Session 1A DPOLY: DPOLY Short Course: Machine Learning for Polymer Physicists I 201

1:00PM 1A.00001: DPOLY Short Course: Machine Learning for Polymer Physicists I — Recent developments in machine learning and related data-driven approaches have created a new paradigm for approaching scientific research. The field of polymer physics has seen important applications in the design of experiments, analysis of scattering data, prediction of molecular properties, and identification of important structural and dynamic patterns. Additionally, the use of high throughput computational and experimental techniques promises to increase the amount of data available to polymer physicists and presents new opportunities for discovery. This day and a half short course will provide an essential introduction to machine learning and data analytics as relevant to polymer physicists, while also showcasing recent advances by leaders in the field. Topics covered will include data capture, design of experiments, varying levels of data quality, model building, optimization and general analysis of both experimental and computational data. Attendees will leave with a sound basis in key algorithmic concepts including when those algorithms are appropriate, an understanding of the state-of-the-art applications, and a foundational understanding of how to incorporate machine learning and data science into their current research.

Session 1B GDS: GDS Short Course: Deep Learning for Image Processing Applications 212
Artificial Intelligence (AI) is a collection of advanced technologies and mathematical methodologies that allows machines to think and act through sensing, comprehending, acting, and learning. This half-century-old field of research has recently garnered renewed attention, partly by several breakthroughs in the design of new AI algorithms, in particular, for image analysis, but also because of the new computing technologies that make the calibration of AI models feasible on personal computers, thus allowing their wide-spread usage by individual researchers in diverse fields of science and engineering. This hands-on workshop will be investigating how deep learning techniques for image analysis can be adapted or developed to address topics and challenges in image analysis and material science. Some of these topics are hyperspectral data analysis in imaging, deep learning applications in active imaging (denoising, drift correction, and deep-learning-based feature extraction), materials discovery, and learning physics from imaging data of mesoscopic and stochastic systems.

Sunday, March 1, 2020 8:00 AM - 4:30 PM

Session 1C GSNP: GSNP Short Course: Machine Learning in Statistical and Nonlinear Physics

Machine learning tools play a growing role in progress in many fields of science. The complex systems addressed by statistical and nonlinear physics are often well suited to exploration with machine learning. In turn, the physics approaches for studying these systems has lead to improvements in machine learning in a new area called the "Physics of Artificial Intelligence." This workshop will include pedagogical talks by experts in our field as well as hands-on computational activities.

Sunday, March 1, 2020 8:15 AM - 4:30 PM

Session 1D DPOLY: DPOLY Short Course: Machine Learning for Polymer Physicists II
Recent developments in machine learning and related data-driven approaches have created a new paradigm for approaching scientific research. The field of polymer physics has seen important applications in the design of experiments, analysis of scattering data, prediction of molecular properties, and identification of important structural and dynamic patterns. Additionally, the use of high throughput computational and experimental techniques promises to increase the amount of data available to polymer physicists and presents new opportunities for discovery. This day and a half short course will provide an essential introduction to machine learning and data analytics as relevant to polymer physicists, while also showcasing recent advances by leaders in the field. Topics covered will include data capture, design of experiments, varying levels of data quality, model building, optimization and general analysis of both experimental and computational data. Attendees will leave with a sound basis in key algorithmic concepts including when those algorithms are appropriate, an understanding of the state-of-the-art applications, and a foundational understanding of how to incorporate machine learning and data science into their current research.

Sunday, March 1, 2020 8:30 AM - 12:30 PM

Session 1E APS: Tutorial 1: Density Functional Theory 607

Density Functional Theory (DFT) provides a practical route for calculating the electronic structure of matter at all levels of aggregation. Five decades after its inception, it is now routinely used in many fields of research, from materials engineering to drug design. Time-dependent Density Functional Theory (TDDFT) has extended the success of DFT to time-dependent phenomena and excitations. Most applications are carried out in the linear-response regime to describe excitation and emission spectra, but the theory is applicable to a much broader class of problems, including strong-field phenomena, attosecond control of electron dynamics, nanoscale transport, and non-adiabatic dynamics of coupled electron-nuclear systems. The tutorial will provide an introduction to the basic formalism of DFT and TDDFT, an overview of state-of-the-art functionals and applications, and a discussion of the most pressing and challenging open questions.

Sunday, March 1, 2020 8:30 AM - 12:30 PM

Session 1F APS: Tutorial 2: Active Learning and AI for Computational and Autonomous Experiments 605
**8:30AM 1F.00001: Tutorial 2: Active Learning and AI for Computational and Autonomous Experiments** — During the course of research, we are often faced with the question of which experimental or computational measurement to perform next. When these measurements are expensive or time-consuming to perform, this question becomes critical. Active learning is a technique in machine learning that provides a framework to systematically answer that question by finding an optimal set of measurements to maximize knowledge gained (given the results already in hand), thus controlling the cost. Machine Learning can then be placed in control of materials synthesis and characterization in a closed-loop system, with active learning providing experiment design on every iteration. Recent examples of autonomous systems include mapping out phase diagrams as well as choosing which computational experiments to perform. In this tutorial, we will introduce the theory of Gaussian processes and active learning using open source python libraries. Here, Gaussian processes are used to learn from prior data and make predictions for the results of future experiments, with associated uncertainty. Active learning then utilizes these predictions to determine the next best experiment to perform. Hands-on exercises will be provided based on actual use cases.

**Sunday, March 1, 2020 8:30 AM - 12:30 PM**

**Session 1G APS: Tutorial 3: Noisy Quantum Devices 601-603**

**8:30AM 1G.00001: Tutorial 3: Noisy Quantum Devices** — The last few years have seen impressive progress in the construction of multi-qubit quantum devices towards the ultimate goal of a fault-tolerant universal quantum computer. However, until we achieve this final goal, we must learn to take advantage of large, but rather noisy devices. Since there are multiple technologies being explored, such as superconducting circuit, ions and spins, we must also learn how to devise tools that are agnostic to the underlying implementation. In this regime there are two main challenges. One challenge is how to characterize and (hopefully) improve errors due to this noise. The other challenge is how to harness the quantum behavior available despite this noisy environment. There are many proposals and some demonstrations for how to obtain a quantum advantage in such systems. These lectures will give an introduction to the types of noise on these devices, typical characterization methods, and applications.

**Sunday, March 1, 2020 9:00 AM - 6:00 PM**

**Session 1H DSOFT: DSOFT Short Course: DNA Nanotechnology Meets Soft Matter 205**
DNA Nanotechnology is a rapidly growing technology impacting many sectors of science and technology, and in particular it is increasingly being harnessed to tackle new and frontier challenges in soft matter science. This course aims to introduce junior researchers in the soft matter field about the elements of DNA Nanotechnology and the state-of-the-art in how it is being applied to address problems in soft matter science and engineering. The course will cover topics outlining the physical chemistry of DNA, the design and assembly of DNA based nanostructures such as DNA tiles and DNA origami, the programming of assembly using DNA, DNA based hydrogels, and DNA-functionalized colloids.

Sunday, March 1, 2020 1:30 PM - 5:30 PM

Session 1J APS: Tutorial 4: Data Analysis and Modern Visualization 607

1:30PM 1J.00001: Tutorial 4: Data Analysis and Modern Visualization — Visualization is an integral part of the scientific process. As an excellent communication tool used by researchers, it is crucial to make complicated scientific data and relations accessible and understandable. This tutorial will train attendees to expand and develop their visualization skills by providing a "from the ground up" understanding of visualization and its utility in error diagnostic and exploration of data for scientific insight. When used effectively, visualization can provide a complementary and effective toolset for data analysis, which is one of the most challenging problems in many scientific domains. We plan to bridge these gaps by providing attendees with fundamental visualization concepts, execution tools, customization, and usage examples. The tutorial will cover different viewpoints, including (1) a rapid introduction to fundamental visualization concepts, (2) an assay of visualization techniques available accompanied by example application scenarios centered around the VisIt software, (3) scientific data visualization using the Blender software, and (4) combination of visualization of data into advanced animations and videos using a full programming language such as Matlab or Python.

Sunday, March 1, 2020 1:30 PM - 5:30 PM

Session 1K APS: Tutorial 5: Medical Metrology 605
1:30PM 1K.00001: Tutorial 5: Medical Metrology — Medicine is becoming increasingly quantitative. Continuing innovation in medical sensors has greatly expanded the range of physical variables that can be accurately measured to probe various aspects of the structure, function, and composition of human body. The analysis of the resulting rich streams of information is enabled by the rapidly developing data science techniques, yielding sophisticated quantitative descriptors of disease and therapeutic response ("quantitative biomarkers"). The trend towards measurement-driven medicine opens exciting opportunities for physicists to contribute their expertise in metrology. This tutorial will cover (i) recent advances in medical sensor technologies (How and what do we measure?), (ii) the discovery and validation of quantitative biomarkers (How do we establish whether a given physical measurement is a biomarker?), and (iii) data analysis techniques that enable clinical decision support based on complex, multi-dimensional biomedical measurements (How do we combine multiple biomarkers into a statistical inference framework?).

**Sunday, March 1, 2020 1:30 PM - 5:30 PM**

**Session 1L APS: Tutorial 6: Quantum Metrology 601-603**

1:30PM 1L.00001: Tutorial 6: Quantum Metrology — Quantum sensing and metrology encompasses a class of techniques and devices that exploit quantum properties such as coherent superposition, wave-particle duality, and entanglement to detect weak or nanoscale signals arising, e.g., from electromagnetic fields, temperature, gravitational gradients, and pressure. As their behavior is tied to physical constants and symmetries, quantum sensors can achieve accuracy, repeatability, and precision approaching fundamental limits. As a result, these devices have shown utility in a wide range of applications spanning across the physical and life sciences —leading to a new generation of real-world technologies with exciting potential. Example quantum sensing platforms to be discussed include atom interferometers; optically-active quantum defects in solids, which have electronic and nuclear spin and can be deployed both for nanoscale sensing with single defects and for bulk sensing with dense ensembles of defects; and atomic vapors constrained in micro-machined ("chip-scale") chambers. (Go to https://march.aps.org/program/tutorial-quantum-metrology/ to view the rest of the tutorial description.)

**Sunday, March 1, 2020 5:00 PM - 6:00 PM**

**Session 1M APS: First-Time Attendee Orientation** Hyatt Mineral B/C - Tag(s): Undergrad Friendly
**5:00PM 1M.00001: First-Time Attendee Orientation** — Join APS staff and leadership to learn how to easily navigate the APS March Meeting. You'll get a crash course on how to use the meeting program to locate sessions you want to see, find out how to use the mobile app to access the meeting program and schedule your events, and find out about interesting and fun events happening throughout the week. You'll also learn about the services APS provides at meetings. Refreshments will be served.

**Sunday, March 1, 2020 6:15 PM - 7:15 PM**

**Session 1Q APS: Future of Physics Days Undergraduate Student Meet-Up** Hyatt Mineral B/C - Tag(s): Undergrad Friendly

**6:15PM 1Q.00001: Future of Physics Days Undergraduate Student Meet Up** — If you would like to informally meet with other undergraduate students from all over to chat about school, professors, science, life, food, ... please check out the undergraduate meet up at the APS March meeting and make some great connections! This is an unstructured meet up with Society of Physics Student leaders and elected leaders of SPS. Once you have assembled we'll grab some snacks and get to know one another.

**Monday, March 2, 2020 8:00 AM - 11:00 AM**

**Session A02 DQI DAMOP: Advances in Atomic Systems** 105 - Daniel Slichter, National Institute of Standards and Technology Boulder - Tag(s): Focus

**8:00AM A02.00001: Trapped Ion Quantum Computing at Honeywell** RUSSELL STUTZ (Presenter), Honeywell Quantum Solutions, Honeywell Intl — Honeywell Quantum Solutions is pursuing a scalable quantum computing architecture based on trapped atomic ions. To this end, Honeywell is developing a broad array of enabling technologies and capabilities, including demonstrations of high-fidelity quantum gate and measurement operations, fast ion transport and re-order, and integration of parallel multi-zone processing of trapped ion qubits to form NISQ devices. We will report recent progress on these and other fronts.
**8:12AM A02.00002: Sandia’s Quantum Scientific Computing Open User Testbed (QSCOUT)**

CHRISTOPHER YALE (Presenter), SUSAN M. CLARK, DANIEL LOBSER, JESSICA M. PEHR, MELISSA C REVELLE, PETER MAUNZ, Sandia National Laboratories — Trapped ions are a leading candidate for quantum computation due to their high-fidelity gate operations, indistinguishability, qubit connectivity, and routes to scalability. Harnessing these advantages, we are developing the Quantum Scientific Computing Open User Testbed (QSCOUT) based on a trapped-ion quantum register at Sandia, using our microfabricated surface electrode traps to host chains of ions with all-to-all connectivity adaptable to diverse algorithms. Here, we present the experimental development of QSCOUT, the current and anticipated capabilities of the testbed, as well as opportunities for use of this platform. As an open testbed, it will feature fully specified operations and hardware allowing users to modify quantum gates and pulse sequences for desired control.

*Sandia National Laboratories is managed and operated by NTESS, LLC, a subsidiary of Honeywell International, Inc., for the US DOE NNSA under contract DE-NA0003525. This work is funded by the US DOE Office of Science ASCR Quantum Testbed Program. The views expressed here do not necessarily represent the views of the DOE or the US Government.

**8:24AM A02.00003: Building a Logical Qubit-sized Ion Trap Quantum Information Processor**

ANDREW RISINGER (Presenter), MICHAEL L GOLDMAN, LAIRD EGAN, CRYSTAL NOEL, DAIWEI ZHU, DEBOPRIYO BISWAS, MARKO CETINA, CHRISTOPHER ROY MONROE, Department of Physics & Joint Quantum Institute, University of Maryland, College Park — We present the system design and architecture of a trapped ion universal quantum processor with high-fidelity quantum gates and addressing of up to 32 qubits. Our approach takes advantage of individual optical addressing to achieve simultaneous high-fidelity operations on a long chain of 171Yb+ ions, resulting in one of the largest academic general-purpose quantum computers. This framework enables long gate-depth, general-purpose algorithms, with the goal of demonstrating an error-corrected logical qubit. We will also cover advances we have made in the control system, specifically in canceling crosstalk and running long experiments.

*This work is supported by the ARO with funding from the IARPA LogiQ program, the NSF Practical Fully-Connected Quantum Computer program, the DOE program on Quantum Computing in Chemical and Material Sciences, the AFOSR MURI on Quantum Measurement and Verification, and the AFOSR MURI on Interactive Quantum Computation and Communication Protocols.

**8:36AM A02.00004: Constructing Trapped Ion Quantum Computers** [Invited]

KENNETH BROWN (Presenter), Duke University — Atomic ion qubits are a promising system for quantum computation with high-fidelity state preparation, measurement, and gates. These systems have already demonstrated complex quantum algorithms from hidden shift problems to quantum simulations. In this talk, I will discuss our experimental work at Duke towards constructing larger ion trap quantum systems. I will also describe the prospects for quantum error correction with trapped atomic ions.

*This work was support by the NSF, IARPA, ARO, and DOE*
A compact room temperature trapped ion system

YUHI AIKYO (Presenter), GEERT VRIJSEN, Department of Electrical and Computer Engineering, Duke University, TOM NOEL, ColdQuanta, JUNGSANG KIM, Department of Electrical and Computer Engineering, Duke University

A trapped ion system is a leading platform for a practical quantum computer. The current gate fidelity is dominated by systematic errors in the control systems delivering the laser beams that drive the gates. The main sources of these errors - mechanical instability and temperature fluctuation - are most effectively addressed by designing compact and robust optical systems. In this work, we present a collaborative work between Duke University and ColdQuanta, where a compact ultra-high vacuum (UHV) chamber operating at room temperature was developed for a trapped ion system. The internal volume of the UHV chamber is only a few cubic centimeters and its vacuum is maintained by a miniaturized ion pump. We demonstrate chain loading of Ytterbium (Yb) ions into a surface trap by ablating a metallic Yb target with a Q-switched Nd:YAG laser. We characterized the vacuum level of this small package by monitoring the hopping rate of an ion in a double well potential, driven by the collision events with background molecules. We also monitored the rate of collision events that cause reordering of the ions in a 6-ion chain containing two isotopes of Yb, one of which appears dark when it is monitored.

*NSF ACQUIRE program, the IARPA LogiQ program and the ARO VISIT STTR program.

A trapped ion system with integrated optics for logical quantum operations

CHRISTOPHER AXLINE (Presenter), KARAN K MEHTA, ROLAND MATT, ROBIN OSWALD, CHIARA DECAROLI, LEON STOLPMANN, JONATHAN P HOME, ETH Zurich

Implementing algorithms using quantum error correction in a quantum computer may require on the order of one million physical qubits. Trapped ion systems have shown long lifetimes and exceptional single- and multi-qubit gate fidelities. It will be critical to preserve these high fidelities while creating a scalable trapping and manipulation scheme. With integrated, independent control of trapped ions within a chain, we can limit noise and simplify the sequence of operations required to realize an error-corrected logical qubit. We are implementing two approaches for individual addressing of $^{40}\text{Ca}^+$ ions in a cryogenic ion trap system; the first involves a fiber array imaged onto an ion string, while the second integrates optical waveguides directly within the ion trap chip. In the same setup, we characterize self-stabilized superconducting magnetic field coils for long-lived coherence. We present designs for operation of multiple trapping zones that could be implemented and interfaced as logical qubits. With such a noise-resilient, configurable system, we aim to demonstrate multi-qubit stabilizer readout towards a powerful ion trap quantum processor.

*We acknowledge support from the Swiss NSF, ETH Zurich Postdoctoral Fellowship, IARPA, and EU Horizon 2020/FET-Open (PIEDMONS).
9:36AM A02.00007: Individual control of an array of neutral atom qubits for quantum computing  
Brian Lester (Presenter), Sabrina Hong, Jonathan King, Stanimir Kondov, Krish Kotru, Mickey McDonald, Remy P.M.J.W. Notermans, Alexander Papageorge, Robin Coxe, Prasahn Sivarajah, Benjamin Bloom, Atom Computing, Inc — Ultracold neutral atoms have emerged as a promising platform for scalable quantum computation. Universal single-qubit control requires high quality state preparation, spatially resolved manipulation, and projective readout of each qubit. For state preparation and readout, neutral atom platforms can apply techniques commonly used in quantum gas microscopes and single atom trapping machines. Furthermore, the ability to isolate the internal spin states of individual neutral atoms from both external fields and neighboring atoms allows for fundamental coherence times exceeding 10 seconds, as demonstrated in recent optical lattice clock experiments. Here, we present initial results on the universal single-qubit control of an array of atomic qubits comprised of neutral strontium atoms. Importantly, the utilized gate scheme enables individual qubit control without relying on global operations that would need to be serialized as the number of qubits is increased.

9:48AM A02.00008: Integrated optical implementation of multi-ion quantum logic*  
Karan Mehta (Presenter), Chi Zhang, Maciej Malinowski, Thanh-Long Nguyen, Martin Stadler, Jonathan P Home, ETH Zurich — Practical and useful quantum information processing will require improvements in operation fidelity and robustness, and simultaneously in scale and integration. Ion qubits’ fundamental qualities are promising for long-term systems, but the optics used to precisely control and measure their quantum states are a challenge to scaling. Previous work with single ions has suggested that trap-integrated optics may make this control more robust, and simultaneously parallelizable [1]. We have designed and implemented planar traps with integrated waveguides and grating couplers, for controlling multiple 40Ca+ ions. We measure 1.5 dB direct fiber-to-chip coupling losses, eliminating the need for beam alignment into vacuum systems/cryostats. Using these photonics, we have realized two-qubit entangling gates with fidelities over 97%, with understood errors suggesting significant possible improvement. The experimental realization of high-fidelity quantum logic in this platform suggests it can enable larger systems in multiple zones connected by transport [2].


*We acknowledge support from the Swiss National Fund, NCCR QSIT, ETH, the EU Flagship, and an ETH postdoctoral fellowship.
10:00AM A02.00009: Efficient Arbitrary Simultaneously Entangling Gates on a trapped-ion quantum computer
NIKODEM GRZESIAK (Presenter), REINHOLD BLUMEL, KRISTIN BECK, KENNETH WRIGHT, VANDIVER CHAPLIN, JASON AMINI, NEAL PISENTI, SHANTANU DEBNATH, JWOSY CHEN, YUNSEONG NAM, IonQ, Inc — Entanglement is a key ingredient in quantum computing. On a trapped ion quantum computer, parallel entangling operations have traditionally been implemented with the help of nonlinear solvers. In this talk, I will present an exact, linear protocol that entangles multiple arbitrary pairs of trapped-ion qubits. The protocol is efficient and can leverage the all-to-all connectivity available on trapped-ion quantum computers to implement up to quadratically many two-qubit gates at the same time. [arXiv:1905.09294]

10:12AM A02.00010: Teleported CNOT Gate in a Mixed-Species Trapped-Ion System
STEPHEN ERICKSON (Presenter), YONG WAN, DANIEL KIENZLER, KARL MAYER, TING REI TAN, JENNY WU, HILMA VASCONCELOS, SCOTT GLANCY, EMANUEL H KNILL, DAVID J WINELAND, ANDREW C WILSON, DIETRICH LEIBFRIED, National Institute of Standards and Technology — Scaling up quantum information processing (QIP) can be aided by distributing qubits across multiple processing zones. Universal quantum computation across such an architecture will require entangling gates between qubits in separate zones. Quantum gate teleportation achieves this, requiring only local operations within each zone, a single entangled ancilla pair split between the two zones, and classical communication. Using this protocol, we demonstrate a teleported CNOT gate between two spatially separated $^9$Be$^+$ ions by means of a split entangled pair of $^{25}$Mg$^+$ ions and measure an entanglement fidelity in the interval $(0.845, 0.872)$ at the 95% confidence level. Our demonstration combines many important tools for scaling trapped-ion QIP, including ion separation and shuttling, individually addressed single qubit rotations and detections, same- and mixed-species entangling gates, and real-time conditional feedforward operations.

*This work was supported by the Office of the Director of National Intelligence (ODNI) Intelligence Advanced Research Projects Activity (IARPA), ONR, the NIST Quantum Information Program, and the National Science Foundation Graduate Research Fellowship Program.
10:24AM A02.00011: Laser-free trapped-ion entangling gates with an oscillating magnetic-field gradient at radio frequency*  
RAGHAVENDRA SRINIVAS (Presenter), SHAUN BURD, University of Colorado, Boulder, ROBERT TYLER SUTHERLAND, Lawrence Livermore National Laboratory, HANNAH M KNAACK, University of Colorado, Boulder, DIETRICH LEIBFRIED, National Institute of Standards and Technology, Boulder, DAVID J WINELAND, University of Oregon, Eugene, ANDREW C WILSON, National Institute of Standards and Technology, Boulder, DAVID THOMAS CHARLES ALLCOCK, University of Oregon, Eugene, DANIEL H SLICHTER, National Institute of Standards and Technology, Boulder — We demonstrate a recently proposed method for trapped-ion entangling gates implemented using an oscillating magnetic-field gradient at radio frequency in addition to two microwave magnetic fields symmetrically detuned about the qubit frequency [1]. This technique enables laser-free entangling gates with reduced sensitivity to qubit frequency errors. The experiment is performed in a surface-electrode trap that incorporates current-carrying electrodes to generate the microwave fields and the oscillating magnetic field gradient. Currently, we achieve a Bell-state fidelity of 0.996(2) with ground-state-cooled ions and 0.991(3) for ions cooled to the Doppler limit (nbar=2). The radio-frequency currents used to generate the gradient also give rise to a tunable differential ac Zeeman shift on the two ions which can be turned on and off. While the gate is insensitive to this shift, it can be used independently to perform single ion addressing. This method of addressing does not require additional control fields or rotation of the ion crystal. We can combine this addressing with an entangling gate to create any Bell state from a given initial state.


*We acknowledge support from the NIST Quantum Information Program.

10:36AM A02.00012: Quantum hopping of frequency-bin entangled photon pairs*  
POOLAD IMANY (Presenter), NAVIN B LINGARAJU, MOHAMMED S ALSHAYKH, DANIEL E LEAIRD, ANDREW M WEINER, Purdue University — Quantum walks of entangled particles have promising applications in simulating many-body physics, as well as in implementing quantum search algorithms. Here, we report continuous quantum walks of a two-photon quantum frequency comb using electro-optic phase modulation to tune the evolution of the state through the quantum circuit. By manipulating the spectral phase of the initial entangled state, we demonstrate either enhanced ballistic energy transport or energy bound states, which are signatures of bosonic and fermionic frequency hopping, respectively. In addition, applying quadratic spectral phase on the initial state creates different subspaces featuring bosonic or fermionic character. We also explore the effect of increasing entanglement dimensionality in frequency domain quantum hopping; our results suggest the potential of our circuit for certifying high-dimensional entanglement.

*National Science Foundation no 1839191-ECCS.
10:48AM A02.00013: Improved Light-Matter Interaction in a Thulium Cavity Memory for Quantum Light Storage  JACOB DAVIDSON (Presenter), Qutech, Delft University of Technology, PASCAL LEFEBVRE, JUN ZHANG, DANIEL OBLAK, Physics, University of Calgary, WOLFGANG TITTEL, Qutech, Delft University of Technology — We design and implement an atomic frequency comb quantum memory using a thulium-doped crystal in an impedance matched optical cavity to create absorption of more than 90% of input signal, resulting in a memory efficiency of 27%. This low finesse optical cavity design enables efficient storage over the conventionally large frequency bandwidths ($\geq$ 500 MHz) present for single photons and high communication rates. We store one member of a photon pair created through spontaneous parametric down-conversion and, by measuring a value of $g(2) = 9.3 \pm 1.2 > 2$ for the cross-correlation function of the photons, verify that the non-classical nature of the light persists after storage in the cavity memory. Using quantum process tomography to measure time-bin qubits after storage in this high-bandwidth memory, we characterize the qubit storage fidelity to be as high as $F = 95.0 \pm 0.1\%$, confirming non-classical qubit storage. These results demonstrate progress toward efficient, faithful, and high bandwidth storage of single photon qubits for quantum networking.

Monday, March 2, 2020 8:00 AM - 10:36 AM


8:00AM A03.00001: Time resolving the loss of crystallinity during detonation in a secondary solid explosive [Invited]  PAMELA BOWLAN (Presenter), LAURA SMILOWITZ, BRYAN HENSON, DENNIS REMELIUS, NATALYA SUVOROVA, DAVID M OSCHWALD, Los Alamos National Laboratory — There are still significant uncertainties in our ability to predict and control detonation in secondary solid explosives which has serious implications for the safety and performance of explosives. One reason is for this uncertainty is that while chemical kinetics are well understood in gases and liquids, much less is known about how chemistry proceeds within a crystalline lattice. Secondly, events like detonation, where a bulk material can go from ambient conditions to pressures of Gigapascals (GPa) and temperatures of about 4000 kelvin (K) within nanoseconds (ns), are extremely difficult to directly observe. To better understand the role of the loss of crystallinity and how this affects temperature and chemical kinetics during a detonation, we developed a technique using visible laser scattering to probe morphology changes on a nanosecond time scale before and during a detonation. We will present our results applying this to several common secondary solid explosives, PETN, HMX and TATB, and considering steady detonation, initiation of detonation, and failure scenarios. These measurements reveal when during a detonation wave, and how fast that the initial crystals change into a less scattering dense product fluid giving new insight into the microscopic mechanism of a detonation in solid explosives.
8:36AM A03.00002: A Hotspot’s Better Half: A Characterization of the Local Potential Energy Rise in Mechanically Induced Hotspots  
BRENDEN HAMILTON (Presenter), Purdue Univ, MATTHEW P KROONBLAWD, Lawrence Livermore National Laboratory, CHUNYU LI, ALEJANDRO H STRACHAN, Purdue Univ — Shock loading of high explosives leads to energy localization into hotspots, which are thought to govern the initiation of detonation. Hotspots are typically characterized in terms of their size and temperature. Criticality of a hotspot depends on a competition between thermal diffusivity and endothermic reactions that tend to quench the hotspot against exothermic reactions that can transform the hotspot into a deflagration wave. However, this view ignores the role of potential energy (PE) as a descriptor of energy localization and criticality. We show through large-scale molecular dynamics simulations of TATB pore collapse that more energy is localized in PE than in kinetic energy (KE). Furthermore, the spatial extent and diffusivity of the PE and KE hotspots are significantly different, and far from expectations based on equipartition. An analysis of the MD trajectories reveals the molecular origin of this puzzling observation. Prepared by LLNL under Contract DE-AC52-07NA27344. Approved for unlimited release, LLNL-ABS-794457.

8:48AM A03.00003: Void collapse in shocked β-HMX single crystals across scales*  
CAMILO DUARTE (Presenter), CHUNYU LI, MARISOL KOSLOWSKI, ALEJANDRO H STRACHAN, Purdue Univ — Heat generation in the vicinity of a void during shock compression plays a critical role on the initiation of detonation in high explosives (HE). Atomistic simulations of under shock compression have shown that the void collapse regime transitions from visco-plastic to hydrodynamic jetting as the shock strength increases in many energetic materials. However, atomistic simulations are limited to nanometer size voids. On the other hand, void collapse experiments have been performed in micron size samples. Here, we present a mesoscale model informed from atomistic simulations to study the anisotropic response of shocked β-HMX single crystals that bridges nanometer to micrometer scales. The shock response of an β-HMX single crystal containing a void is studied with finite element simulations that include plasticity and heat transport. The effect of crystal orientation over a range of impact velocities are discussed. The continuum model is calibrated with non-reactive molecular dynamics simulations of planar socks. The simulations are compared with both atomistic simulations and gas gun experimental results of β-HMX containing a single void.

*US Department of Defense, Office of Naval Research, MURI contract number N00014-16-1-2557, program managers: Chad Stoltz and Kenny Lipkowitz.
9:00AM A03.00004: Mechanisms and Size Effects of Hotspot Formation due to Shock-Induced Collapse of Pores and Cracks  CHUNYU LI (Presenter), BRENDEN HAMILTON, ALEJANDRO H STRACHAN, Purdue Univ — The shock to detonation transition in heterogeneous high energy density materials starts with the spatial localization of mechanical energy into hotspots due to the interaction of the mechanical wave with microstructural features and defects. We present large-scale molecular dynamics simulations of hotspot formation in HMX crystals following the collapse of pores of various shapes and sizes for impact velocities ranging from 0.5 to 2.5 km/s. Hotspots resulting from cracks elongated along the shock direction show significantly higher sensitivity to both shock strength and defect size. Elongated cracks 80 nm in length result in temperatures almost three times higher that voids 80 nm diameter and reach values corresponding to the ideal case of isentropic recompression of a gas. The MD trajectories reveal the atomic origin of this contrasting behavior. While circular voids undergo a transition from viscoelastic pore collapse to a hydrodynamic regime with increasing shock strength, shock focusing in elongated cracks results in jetting and vaporization, which upon recompression leads to increased heating.

9:12AM A03.00005: Time-resolved x-ray imaging of void collapse at micron length scales*  MICHAEL ARMSTRONG (Presenter), RYAN AUSTIN, Lawrence Livermore Natl Lab, PAUL CHOW, YUMING XIAO, Advanced Photon Source, PAULIUS GRIVICKAS, BATIKAN KOROGLU, ERIC V BUKOVSKY, WILLIAM L SHAW, JOSHUA A HAMMONS, TREVOR M WILLEY, ANDREW K ROBINSON, Lawrence Livermore Natl Lab — Pulsed x-ray imaging can provide substantial insight into a wide range of initiation-related phenomena, particularly the in situ imaging of dynamically compressed voids, which are thought to play a fundamental role in explosive initiation. Current models of the dynamic compression behavior of inhomogeneous materials are empirically calibrated to bulk, aggregate experimental data. The development of more fundamental models depends on detailed measurements and corresponding simulations which resolve single void collapse events. Further, since material strength depends on scale, experiments at the scale of actual voids (10 μm) are preferred. Since the field of view for these experiments is relatively small (~100s μm) and void collapse occurs at low pressure, these experiments can be performed with a small scale (100 mJ) laser in a portable experimental setup. Here we present the results of x-ray imaging experiments at the Advanced Photon Source on voids embedded in TNT and silicon using both explosive and laser-driven shocks, which approach the spatial scale of void collapse in actual explosives, 1-10 μm.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
Evaluation of the roles of crystal plasticity and hydrodynamic jetting in hot-spot formation in heterogeneous energetic materials under shocks

OISHIK SEN (Presenter), NIRMAL KUMAR RAI, Univ of Iowa, CAMILO DUARTE, MARISOL KOSLOWSKI, Purdue University, H.S. UDAYKUMAR, Univ of Iowa — Heterogeneous energetic materials are crucial components in munitions and energy-delivery systems. Under shocks, localized hot-spots are formed near voids and microstructural defects in these materials. Hydrodynamic jetting due to void collapse and strain localization due to plastic work are two important mechanisms for hot-spot formation in the material. This work evaluates the relative contribution of these two mechanisms in the formation of hot-spots under shocks in energetic materials. To this end, an Eulerian computational framework is used to study the response of HMXs comprising a single void under shock loading. To study the role of hydrodynamic jetting, the voids are resolved sharply using level-sets and the hot-spot temperatures are tracked at different stages of void collapse. To model heating due to plastic work, an anisotropic crystal plasticity model based on a power-law slip-rate with hardening and thermal softening is used; the localized temperatures in the slip/shear bands formed in the material under shocks are also tracked. Computations are performed for different crystal orientations and shock strength. The presentation will discuss the combined roles of jetting and plastic heating in hot-spot formation in HMXs.

Measurements of State Variables During Exploding Bridgewire Detonator Function

LAURA SMILOWITZ (Presenter), BRYAN HENSON, PAMELA BOWLAN, DENNIS REMELIUS, NATALYA SUVOROVA, Los Alamos Natl Lab — We have studied the behavior of exploding bridgewire detonators using a variety of observables for measuring temperature and density during detonator function. Continuous density movies have been collected using either proton or x-ray radiography and continuous light emission videos simultaneously measured using ultra-high speed video cameras. Spectrally resolved and single broadband pyrometric measures of temperature are also measured. We attempt to provide a description of the mechanism of function for EBW detonators based on the full suite of observations made and comparisons to studies in the literature. In this talk, we will show the results of measurements on PETN and HMX based detonators run in a variety of conditions.

Internal shock structure and thermal response in the function of Exploding Bridgewire Detonators

BRYAN HENSON (Presenter), LAURA SMILOWITZ, PAMELA BOWLAN, NATALYA SUVOROVA, DENNIS REMELIUS, Los Alamos Natl Lab — We have recently shown that the input shock, subsequent initiation and detonation propagation in an Exploding Bridgewire (EBW) detonator exhibits complex internal structure and temporal behavior. Using flash radiography we have observed the prompt emanation of a relatively weak shock wave (3000 m/s) from the region of the bridgewire at the time of vaporization. Abel inversion of the images reveals a highly symmetric, hemispherical structure in the density that propagates through the initial pressing. Visible imaging of the cylindrical surface of the detonator reveals a luminous wavelike structure that appears radially symmetric but lacking the exact symmetry of the density feature. In this talk these structures will be directly compared spatially and temporally for a number of EBW detonators of different sizes and materials. The relationship between shock and detonation like features will be discussed in the context of the mechanism of function of EBW detonators and recent progress in modeling the chemistry of energy release in these applications.
10:00AM A03.00009: Comparing small-scale detonation simulation to experimental data and multi-dimensional initiation sensitivity study  RACHEL MORNEAU (Presenter), MICHAEL J MURPHY, JAMES QUIRK, Los Alamos National Laboratory — We are interested in modeling exploding foil initiator (EFI) detonators to help with design timelines and understanding the fundamental science of detonators. We will discuss efforts to model small-scale detonations in the absence of calibration data that take into account the ignition and growth in PETN sub-centimeter pellets. Several reaction rate models along with parameter studies were performed to show variation in the breakout time and wave shape at the end of the pellet using the hydrocode FLAG. Since 1D initiation does not wholly describe the initiation in these small-scale detonations of interest, we will explore the effect of multi-dimensional ignition on the outcome. We will show several comparisons of simulation data to experimental data and discuss the results.

10:12AM A03.00010: (U) Introducing HEDONIST- A Low Explosive Mass Experiment That Attains Very High Pressures*  CARL JOHNSON (Presenter), JOHN GIBSON, Los Alamos National Laboratory — The proton radiography facility at LANL offers unique experimental capabilities, particularly the planned Pu@pRad line. Pu@pRad limitations however preclude the usage of large quantities of high explosives. We present the hydrocode analysis of a small-scale system (under 30g TNT equivalent) capable of reaching pressures in excess of 2 Mbar. This system utilizes a novel multipoint initiation system to establish converging detonation waves which deliver a strong shock wave onto a sample cell. HEDONIST has been designed to present a low areal density to the pRad beam thereby providing ample signal-to-noise ratio to discern shock waves in sample cell materials from other shocks present. Results from the first two pRad experiments and the comparison to hydrocode simulations will be discussed.

* C. Johnson*, J. Gibson, B. Geesey, A. Fredenburg, S. Ramsey, E. Martinez and A. Llobet Los Alamos National Laboratory, Los Alamos, New Mexico, 87545

10:24AM A03.00011: Modeling and Experimental Analysis of Shaped Charge Jet Characteristics  KEVIN MIERS (Presenter), DANIEL PUDLAK, Detonation Physics and Experimental Research Branch, U.S. Army CCDC Armaments Center — The U.S. Army CCDC Armaments Center at Picatinny Arsenal, NJ uses a variety of computational and analytical tools to predict and validate shaped charge warhead performance. In this work, an 81mm copper lined conical shaped charge loaded with the HMX-based explosive LX-14 is modeled in the hydrocode ALE3D and tested using flash radiography. Jet characterization x-ray films are digitized and analyzed using a series of computer programs developed by Miers and Pham. Experimentally determined jet parameters such as velocity profile and accumulated length/mass/energy are compared with hydrocode predictions. Additionally, the Walsh theory for plastic instability and particulation in stretching metal jets is utilized to predict jet breakup time from hydrocode models, and results are compared with experiment. The resulting effects on armor penetration performance predictions are discussed.

Monday, March 2, 2020 8:00 AM - 10:36 AM
8:00AM A04.00001: Electric Fields, Reorientation, and Water at the Air-water Interface of Iron and other Salt Solutions* [Invited]  HEATHER ALLEN (Presenter), Ohio State Univ - Columbus — Water at the air-water interface organizes and facilitates the accommodation of ion complexes and that of surface active species. The hydration shells of these surface active components are evident by their spectroscopic signatures mostly in the OH stretching regions using both vibrational sum frequency generation and infrared reflection absorption spectroscopies. In addition, surface potential measurements reveal information on the interfacial electric field strength and thus ordering of molecular and ion complexation dipoles in the interfacial region. We report evidence of interfacial iron (III) speciation and other ions and their interfacial hydration effects. We also report on the resistance to dipole reorientation of ion and molecular species at the air-aqueous interface of iron(III) sulfate and nitrate versus iron(III) chloride.

*DOE-BES CPIMS

8:36AM A04.00002: The structure and polarization of the water-graphene interface from molecular dynamics simulations and X-ray reflectivity experiments*  FELIPE JIMENEZ-ANGELES (Presenter), KATHERINE HARMON, TRUNG NGUYEN, Northwestern University, PAUL FENTER, Chemical Sciences and Engineering Division, Argonne National Laboratory, MONICA OLVERA DE LA CRUZ, Northwestern University — Nanconfined water is found in numerous applications across natural and technological systems where water mediates chemical reactions, adsorption, diffusion, ion transport, among other processes. Water affects the interactions among ions, molecules, and surfaces. The electrostatic forces in the systems and processes are modified through polarization which is the collective orientation of the molecules' dipole moment. The polarization of water is different in bulk, in confinement, and at interfaces. Here we study the water structure and polarization next to uncharged graphene surfaces by means of molecular dynamics simulations and X-ray reflectivity experiments. Despite graphene being hydrophobic, our simulations and experiments show an adsorbed water layer on graphene. Even in the absence of an external electric field this adsorbed water layer has a persistent polarization and an induced electrostatic potential. In addition, the adsorbed water molecules form a hydrogen bond network and make the graphene surface repulsive to ions.

*This work was funded by The Sherman Fairchild Foundation; the Center for Hierarchical Materials Design 70NANB19H005; Midwest Integrated Center for Computational Materials 5J-30161-0010A.
8:48AM A04.00003: Polarizable Potentials For Metals: The Density Readjusting Embedded Atom Method (DR-EAM)*  
HEMANTA BHATTARAI (Presenter), Department of Physics, University of Notre Dame, J. DANIEL GEZELTER, Department of Chemistry and Biochemistry, University of Notre Dame, KATHIE ELAINE NEWMAN, Department of Physics, University of Notre Dame — In simulations of metallic interfaces, a critical aspect of metallic behavior is missing from the some of the most widely used classical molecular dynamics force fields. We present a modification of the embedded atom method (EAM) which allows for electronic polarization of the metal by treating the valence density around each atom as a fluctuating dynamical quantity. The densities are represented by a set of additional fluctuating variables (and their conjugate momenta) which are propagated along with the nuclear coordinates. This “density readjusting EAM” (DR-EAM) preserves nearly all of the useful qualities of traditional EAM. We show that DR-EAM can successfully model polarization in response to external charges, capturing the image charge effect in atomistic simulations. DR-EAM also captures behaviors of metals in the presence of uniform electric fields, predicting surface charging and shielding internal to the metal. Our additional studies of DR-EAM used to model a metal-water interface show local surface ordering of water dipoles due to the polarizability of the metal. We also discuss the interfacial thermal conductivity of the metal-water interface calculated using both polarizable and non-polarizable models for the metal and for water.

1. NSF under Grant No. CHE-1663773.

9:00AM A04.00004: Orientational Dynamics of the Hydrogen-bonded OH of Interfacial Water*  
JOHN MCGUIRE (Presenter), School of Physical Science and Technology, ShanghaiTech University, FLORIAN FIGGE, Department of Physics and Astronomy, Michigan State University — We report on the orientational dynamics of the bonded OH (bOH) of interfacial water, i.e., the OH groups in which the H atom participates in a hydrogen bond (HB). A vibrationally resonant infrared-visible sum-frequency signal provides a surface sensitive probe of the dynamics following excitation by a vibrationally resonant infrared pump. Using p-polarized probe beams, we measure the evolution of the pump-induced orientational anisotropy following p- and s-polarized pump excitation. Previous work showed that the dangling OH (dOH) groups (i.e., OH groups in which the H atom does not participate in a HB) reorient much faster than do bulk bOH[1,2]. Measuring the dynamics of interfacial bOH is challenging, though, on account of strong intermolecular resonant vibrational energy transfer (RVET). Using isotopic dilutions down to 1 part H₂O in 19 parts D₂O, we minimize RVET and show that interfacial bOH reorient on the same timescale as do bulk bOH. These dynamics are robust to interfacial ion concentrations and suggest that the interfacial hydrogen bond network becomes bulk-like within a single molecular distance from the surface.

References:

*National Science Foundation (Grant No. CHE-1151590)
Why are Water-Hydrophobe Interfaces Electrically Charged? JAMILYA NAURUZBAYEVA (Presenter), Water Desalination and Reuse Center, King Abdullah University of Science and Technology, ZHONGHAO SUN, Ali i. Al-Naimi Petroleum Engineering Research Center, King Abdullah University of Science and Technology, ADAIR GALLO JUNIOR, MAHMOUD IBRAHIM, Water Desalination and Reuse Center, King Abdullah University of Science and Technology, J. CARLOS SANTAMARINA, Ali i. Al-Naimi Petroleum Engineering Research Center, King Abdullah University of Science and Technology, HIMANSHU MISHRA, Water Desalination and Reuse Center, King Abdullah University of Science and Technology — Mechanisms underlying the electrification of water-hydrophobe interfaces are of much interest in chemical science, but are not entirely clear. In response, a systematic investigation of excess electrical charges carried by water droplets dispensed from capillaries was performed by: (i) studying the deflections of pendant droplets under uniform electric fields, and (ii) the direct measurement of electrical charges of the dispensed droplets using an ultrasensitive electrometer coupled with a Faraday cup. Thus, the effects of the following crucial factors were unraveled: hydrophobicity/hydrophilicity of the capillary, the presence/absence of a water reservoir inside the capillary, water pH, ionic strength, dielectric constant, the dissolved CO₂ content, and the relative humidity. The emerging picture is that the electrification at interfaces of common hydrophobic materials, e.g., polytetrafluoroethylene and polypropylene, is not limited to interfaces with water alone; nor is this phenomenon entirely dependent on the specific adsorption of OH⁻ or H₃O⁺ ions, as commonly believed. Our exhaustive study also draws together an extensive body of literature on this subject.

Free Energy of Water Dissociation at the Water - TiO₂ Interface from Ab Initio Deep Potential Molecular Dynamics* [Invited] ANNABELLA SELLONI (Presenter), Princeton University — TiO₂ is a widely used photocatalyst in science and technology and its interface with water is important in fields ranging from geochemistry to biomedicine. Yet, it is still unclear whether water adsorbs in molecular or dissociated form on TiO₂ even for the case of well-defined crystalline surfaces. To address this issue, we simulated the TiO₂-water interface using molecular dynamics with an ab initio-based deep neural network potential. Our simulations show a 6% equilibrium fraction of water dissociation at room temperature, in agreement with enhanced sampling estimates of the dissociation free energy [1]. Due to the relevance of surface hydroxyl groups to the surface chemistry of TiO₂, our model might be key to understanding phenomena ranging from surface functionalization to photocatalytic mechanisms. Refs: [1] Marcos F. Calegari Andrade, Hsin-Yu Ko, Linfeng Zhang, Roberto Car and Annabella Selloni, submitted.

*This work was conducted within the Computational Chemical Center: Chemistry in Solution and at Interfaces funded by the DoE under Award DE-SC0019394. We also acknowledge the support of DoE-BES, Division of Chemical Sciences, Geosciences and Bio- sciences under Award DE-SC0007347.
10:00AM A04.00007: Laser-Assisted Dissolution of Geological Samples Submerged in Water: Evidence of Hydrothermal Processing*  CHAD DURRANT (Presenter), RAYMOND MARIELLA, JORDAN COMBITSIS, DAVID WEISZ, LLNL — We investigate the use of a 240 ns pulse Nd:YLF (3 kHz, 0.33 mJ/pulse) laser to rapidly break down and dissolve an obsidian sample submerged in water. We propose a mechanism, a hydrothermal surface interaction, by which this laser-assisted dissolution process occurs. The laser fluence is below the ablation thresholds, 0.4-7 J/cm$^2$ vs 10 J/cm$^2$ and is directed onto the submerged sample causing an increase in temperature and pressure at the water-sample interface. Our results indicate that this process is highly efficient at removing, and potentially dissolving, amorphous glassy substrates (i.e. an obsidian sample) at the water-sample interface. This is further shown by the formation of purified SiO$_2$ structures that reform on the surface post-pulse. We additionally show how various parameters (e.g. dwell time, power, repetition rate, and focal length) affect the efficiency of this process.

*Prepared by LLNL under Contract 19-FS-001-LLNL

10:12AM A04.00008: Intrinsic pH of water/vapor interface revealed by ion-induced water alignment*  KUO-YANG CHIANG, LAETITIA DALSTEIN, YU-CHIEH WEN (Presenter), Academia Sinica — Protons at the water/vapor interface are relevant for atmospheric and environmental processes, yet to characterize their surface affinity on the quantitative level is still challenging. Here we utilize phase-sensitive sum-frequency vibrational spectroscopy to quantify the surface density of protons (or their hydronium form) at the intrinsic water/vapor interface, through inspecting the surface-field-induced alignment of water molecules in the electrical double layer of ions. With hydrogen halides in water, the surface adsorption of protons is found to be independent of specific proton-halide anion interactions and to follow a constant adsorption free energy, $\Delta G \sim -3.74 (\pm 0.56) \text{ kJ/mol}$, corresponding to a reduction of the surface pH with respect to the bulk value by 0.66 (±0.10), for bulk ion concentrations up to 0.3 M. Our spectroscopic study is not only of importance in atmospheric chemistry, but also offers a microscopic-level basis to develop advanced quantum-mechanical models for molecular simulations.

*L.D. acknowledges support from Academia Sinica. This work was funded by the Ministry of Science and Technology, Taiwan (grant number 106-2112-M-001-001-MY3; 108-2112-M-001-039-MY3).

10:24AM A04.00009: The behavior of water confined between two hydrophobic surfaces with grafted polymeric segments studied using molecular simulations  RAMIN MEHRANI (Presenter), Mechanical engineering, Ohio University, SUMIT SHARMA, Chemical and Biomolecular engineering, Ohio University — We have performed Indirect Umbrella Sampling (INDUS) molecular simulations to calculate the free energy barrier of evaporation of water confined between two hydrophobic surfaces grafted with polymeric segments. Dependence of the free energy barrier on grafting density and segment flexibility will be discussed. We have calculated the potential of mean force between the two surfaces as a function of the distance between them. The implications of the presence of flexible grafted segments on the hydrophobic collapse of the surfaces will be illustrated.
The control of the photophysical and photochemical properties of molecules through truly quantum mechanisms remains an outstanding goal for the chemical physics community. The strong coupling of spatially confined photons to the electrons of molecules appears among the most promising quantum mechanisms test for molecular control. The formation of cavity polaritons through this strong coupling mechanism has been proposed to amend the excited state structure of molecules embedded in electromagnetic resonantors. Despite these proposals, definite experimental evidence of changes to the dynamics and structure of molecular cavity polaritons remain elusive. In this talk I present experimental results demonstrating the ways in which polariton formation amends the dynamics and structure of strongly cavity-coupled metalloporphyrin molecules. First, I examine how the strong coupling of photons in a nanoscale cavity to the Soret resonance of zinc tetraphenylporphyrin (ZnTPP) affects the competition between excited state absorption and fluorescence processes. I show polariton formation incerases the cross section of excited state absorption relative to stimulated emission. Second, I highlight ultrafast spectroscopic results demonstrating the control of energy gap laws via deterministic polariton formation. In particular, these results show the time scale of populating of an excited singlet state of ZnTPP can be controlled through changes to the Rabi splitting. Third, I propose nonlinear optical spectroscopic methods capable of directly assessing the ways the structure of a molecular excited state change in response to polariton formation. These results demonstrate the power of vibrational light scattering spectroscopies to not only assess structural changes central to the proposed control available through polariton formation, but also novel quantum optical phenomena polaritons may enable.
Optical activity from exciton Aharonov-Bohm effect: a Floquet engineering approach*  
KAI SCHWENNIECKE (Presenter), University of California, San Diego — We theoretically demonstrate that an originally achiral molecular system can exhibit nonzero circular dichroism (CD), through Floquet engineering, when it is driven with elliptically polarized light. More specifically, we consider an isotropic ensemble of small cyclic molecular aggregates in solution whose local low-frequency vibrational modes are driven by a continuous-wave infrared pump. We attribute the origin of the nonzero CD to time-reversal symmetry breaking due to an excitonic Aharonov-Bohm (AB) phase arising from laser-driving and coherent interchromophoric exciton hopping. The obtained Floquet-engineered excitonic AB phases are far more tunable than their analogous electronic AB phases in the nanoscale, highlighting a virtually unexplored potential that excitonic AB phases have in the coherent control of molecular processes and simultaneously introducing new analogues of magneto-optical effects in molecular systems which bypass the use of strong magnetic fields.

*We acknowledge support from the Air Force Office of Scientific Research award FA9550-18-1-0289 for the excitonic design of AB phases and the Defense Advanced Research Projects Agency under Award No. D19AC00011 for the calculation of pseudo-MO effects.

Controlling Coherent Light-Matter Interactions in Semiconductors*  
HUI DENG (Presenter), Univ of Michigan - Ann Arbor — Light-matter interactions are at the heart of quantum electrodynamics and underpin modern photonic technologies. As we develop means to control the properties of light, matter and their interactions, intriguing new phenomena emerge. Using the mature, III-Arsenide semiconductor system, we build a designer cavity platform of polaritons 1. With it, we demonstrate a shot-noise limited polariton lasers with strong nonlinearities 2 and a Bardeen-Cooper-Schrieffer like polariton condensate 3. Coupling two trapped polariton condensates through both coherent tunneling and incoherent dissipation, we form a model system of rich nonlinear dynamics where new, equidistant frequency lines emerge due to limit cycle self-oscillations 4. Extension to larger arrays together with the flexibility to engineer fundamental properties of the polaritons may enable the discovery and understanding of new quantum many-body states. Using two-dimensional van der Waals semiconductors, we establish coherent light-matter coupling in a variety of photonic structures with unprecedented freedom to engineer both the optical modes and excitonic properties 5-7, which may enable new many-body phenomena and novel photonic device concepts.


9:24AM A05.00004: Topological polaritons and magneto-optical materials  SINDHANA SELVI PANNIR SIVA THI (Presenter), JOEL YUEN-ZHOU, University of California, San Diego — In recent years topological polaritons have been theoretically proposed and also observed in experiment. Our work aims to understand the fundamental features for a system to exhibit topological polaritons. We find that topological polaritonic states emerge in magneto-optical materials strongly coupled to surface plasmons in the presence of a magnetic field. In this particular system, we numerically demonstrate unidirectional edge modes.

9:36AM A05.00005: Quantum optics with molecules  CLAUDIU GENES (Presenter), Max Planck Inst for Sci Light —
Recent experimental progress in the collective strong coupling regime of organic molecules with optical cavity or plasmonic modes has shown light-induced modifications of material properties. Experimental and theoretical endeavors go in the direction of charge and energy transport, Förster resonance energy transfer (FRET) enhancement, modified chemical reactivity etc. Oftentimes experiments rely on theoretical models developed for standard cavity quantum electrodynamics with two-level quantum emitters. Molecular systems however have an increased complexity as molecular vibrations and level disorder play a crucial role. We provide a theoretical formalism to tackle the light-electronic-vibrations dynamics modeled via the Holstein-Tavis-Cummings Hamiltonian [1]. We analytically describe aspects such as: polariton asymmetry, molecular branching ratio modification in the Purcell regime and cavity-mediated donor-acceptor FRET processes.


Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A06 GMED FIAP: Physics of Medical Devices 113 - Stephen Russek, National Institute of Standards and Technology Boulder - Tag(s): Focus

8:00AM A06.00001: The Physics of System Integration: Merging Radiotherapy and Magnetic Resonance Imaging to Improve Patient Outcomes* [Invited]  MICHAEL THOMPSON (Presenter), Innovation, ViewRay — The integration of imaging into radiotherapy presents an opportunity to improve the precision and accuracy of radiation delivery to the therapy target. More precise delivery is expected, and has been shown in some cases, to reduce treatment times, radiation toxicity, and improve outcomes. However, to achieve these goals two systems that rely on very accurate electromagnetic fields must be integrated without compromising the performance of either system. In this talk the advantages of integrating low field MRI with radiotherapy will be briefly reviewed. The challenges involved with integrating an MRI system and a linear accelerator to effect superior image guided, and intensity modulated, radiotherapy will be covered in some detail with specific examples.

*The author of this work, and presenter, are employees of ViewRay Inc.
8:36AM A06.00002: Proteomic Assay to Predict Health, Wellness, and Disease [Invited]  JASON CLEVELAND (Presenter), SomaLogic — The ever-changing state of the proteins in your body is arguably one of the most important indicators of health and disease, but, to date, measurements have only been possible on individual proteins or small multiplexes. SomaLogic has commercialized a rapid proteomic scanning platform (SOMAScan) that quantifies over 5000 proteins in blood or urine spanning 7 orders of magnitude in concentration, with sub-pM limits of detection. The assay relies on SOMAmers (Slow-Offrate-Modified AptaMERs), short pieces of DNA with additional chemical diversity that are selected to bind tightly to a specific protein. Rather than directly measure the proteins themselves, the fundamental principle underlying the assay is to turn a protein counting problem into a DNA counting problem. DNA has a few important differences relative to proteins that make the DNA counting problem much more tractable, including that a chemical complement exists, and that DNA can be amplified and sequenced inexpensively. To date, we have measured over 100,000 human samples. Applying machine learning to the large resulting databases has led to a rapidly growing number of health measures, including diabetes and cardiovascular risk, with the ultimate goal of providing hundreds of results from a single liquid sample. I will briefly review the physics underlying the current assay and highlight a few of the health measurements. I will also briefly address some thoughts on future device physics to move the assay from the lab to the home.

9:12AM A06.00003: Light-induced pathogenic bacterial deactivation by using graphene quantum dot and methylene blue*  ERMEK BELEKOV (Presenter), LAUREN COOPER, KHOMIDKHODZA KHOLIKOV, ALI O ER, Western Kentucky Univ — Graphene quantum dots (GQD) is one of the most promising antimicrobial agents with promising potential in photodynamic therapy. GQD was obtained from benzene by focusing high power nanosecond laser pulses. Detailed characterization was performed with transmission electron microscopy (TEM), scanning electron microscopy (SEM), Fourier-transform infrared (FTIR), UV-Visible (UV-Vis), and photoluminescence (PL) spectra. Later, we have attached Methylene Blue (MB), a standard photosensitizer, to graphene quantum dots. The effectiveness of the MB/GQD compound was evaluated on different strains of bacteria such as Escherichia coli and Micrococcus luteus. In addition, MTT assay was used to study human cellular side-effects, cancer and noncancer cellular viability under dark conditions.Combining MB with GQDs caused enhanced singlet oxygen generation and a higher deactivation rate compared to MB and GQD only. These results suggest that the MB/GQD combination is a promising form of photodynamic therapy. Further, ongoing experiments on the germicidal effects of different nanoparticles such as silver (Ag), and aluminum (Al) with MB will be presented.

*Kentucky Biomedical Research Infrastructure Network (KBRIN)
9:24AM A06.00004: Analysis of experimental acoustic waves induced by high energy pulsed X-ray beams*  Farnoush Forghani (Presenter), Adam Mahl, Bernard Jones, University of Colorado, Denver, Mark Borden, University of Colorado, Boulder, Moyed Miften, David Thomas, University of Colorado, Denver — X-ray induced acoustic tomography has recently gained attention for its potential use for 3D dose distribution imaging in radiation therapy and for low dose high resolution 3D imaging in diagnostic therapy. X-ray acoustic waves are produced by the temperature rise following the energy absorption from a pulsed photon beam. While the theory for X-ray acoustics is well established, there is little known about how the X-ray source properties affect the acoustic signal strength and frequency. Here, we present current experimental results of the X-ray acoustic signals obtained by two types of X-ray sources; megavoltage energy with a long pulse width (4 us) and kilovoltage energy with short pulse width (10 ns). The effect of the pulse length and the X-ray source energy on the acoustic signals are investigated. Experimental acoustic signals with high signal to noise ratio are generated when the X-rays strike thin sheets (between 0.1-3 mm) of a high Z material in a water tank. The experimental signals are compared to simulated acoustic waves using Monte Carlo modeling combined with a numerical solver for time domain acoustic wave propagation (kWave).

*This work is supported by American Cancer Society, Colorado Clinical and Translational Sciences Institute, and Cancer League of Colorado.

9:36AM A06.00005: Optimizing coded aperture imaging techniques to allow for online tracking of fiducial markers using high energy scattered radiation from clinical treatment beam.*  Adam Mahl (Presenter), Brian Miller, Moyed Miften, Bernard Jones, University of Colorado, Denver — Real time visualization of fiducial markers and their movement as surrogates for tumor motion during radiotherapy treatment allows for more accurate dose delivery. This project aims to optimize techniques for online tracking by detecting the scattered radiation from clinical treatment beams through a coded aperture (CA).

MCNP6 was used to model radiotherapy beams through phantoms containing gold fiducials. Orthogonal scatter radiographs were collected through a CA geometry. After decoding the simulated radiograph data, the centroid location and FWHM/SNR of the fiducial signals were analyzed. The method was able to accurately localize the markers to within <1mm. The effects of the CA/detector parameters (rank, pattern, and physical dimensions), and the incident beam energy were characterized. Fourier filtering was used to reduce the effects of phantom scatter and decoding artifacts.

Current results will present a proof of concept for a novel real-time imaging method which can be used to further optimize the CA imaging parameter space and guide design and testing of a clinical device.

*Funding comes from the NIH under award number K12CA086913, the University of Colorado Cancer Center/ACS IRG #57-001-53, the American Cancer Society, the Boettcher Foundation, and Varian Medical Systems.
9:48AM A06.00006: Imaging Surgical Devices with Reduced Metal Artifact*  
PENGWEI WU, NIRAL SHETH, ALEJANDRO SISNIEGA, ALI UNERI, RUNZE HAN, ROHAN VIJAYAN, PRASAD VAGDARGI, Johns Hopkins University, BJOERN KREHER, HOLGER KUNZE, GERHARD KLEINSZIG, SEBASTIAN VOGT, Siemens Healthineers, JEFFREY H SIEWERDSEN (Presenter), Johns Hopkins University  
— Imaging in OR is essential to high-precision, minimally invasive spine surgery, but artifacts arising from surgical devices (e.g., implanted screws) present a major challenge to image quality. Such metal objects cause spectral shift (beam-hardening), photon starvation, and scatter, which confound visualization in regions near surgical devices – e.g. to assess the accuracy of screw placement. We present a method to predict patient and device specific orbits of C-arm cone-beam CT system that avoid metal artifacts by acquiring projection data with minimal influence from metal-related polyenergetic bias (spectral shift). The method localizes devices via neural network segmentation in a few low-dose scout views (commonly acquired for patient positioning), and all C-arm rotation and tilt angles are analyzed to identify the orbit with minimal polyenergetic bias. The method was evaluated in simulation, phantoms, and a cadaver with multiple pedicle screws, demonstrating accurate prediction of orbits that optimally avoided metal artifacts. The results yielded ~200-500 HU reduction of shading artifacts, and ~30-45% reduction in blooming artifacts about the screw shaft. Such method can improve the safety and precision of spine surgery.

*Academic-industry partnership with Siemens Healthineers.

10:00AM A06.00007: Personalized radiation attenuating materials for mucosal protection*  
JAMES DONALD BYRNE, Harvard Radiation Oncology Program, JENNIFER PURSLEY (Presenter), KYLA REMILLARD, SAMANTHA EDGINGTON, Department of Radiation Oncology, Massachusetts General Hospital, JONATHAN D SCHOENFELD, Department of Radiation Oncology, Dana-Farber Cancer Institute/Brigham and Women's Hospital, GIOVANNI TRAVERSO, Department of Mechanical Engineering, Massachusetts Institute of Technology — Patients receiving radiation therapy will develop normal tissue injury as a result of treatment. If a radiation attenuating material is placed in normal tissues, it may reduce the radiation received by that tissue. In this study, we measured the radiation attenuating properties of different materials. We investigated the dosimetric impact of three patient-specific radioprotective devices: a 3D-printed intra-oral device for oral cavity cancer patients, and balloon catheters with radioprotective liquids in the esophagus and rectum for lung and prostate cancer patients respectively. The oral cavity and rectum devices demonstrated protective properties in retrospective treatment plans, so in vivo application of these devices was tested in a rat model. Rats treated with the protective devices in place showed decreased ulcerations and erythema of the oral and rectal mucosa compared to control animals. Use of radioprotective devices in patients has the potential to reduce the morbidity of radiation treatments for cancer.

*This work was funded in part by grants from Joint Center for Radiation Therapy Internal Award, NIH Grant No. EB-000244, and Prostate Cancer Foundation Young Investigator Award. G.T. was supported in part by the Department of Mechanical Engineering, MIT.
10:12AM A06.00008: Fast, Small Volume Blood Diagnostics using Homogeneous Thin Solid Films of µL-sized Drops on Super-Hydrophilic Coatings - Impact of Film Properties on Test Accuracy*  
NIKHIL SURESH (Presenter), SHAURYA KHANNA, AMBER A. CHOW, AASHI R GURIJALA, MOHAMMED SAHAL, Department of Physics, Arizona State University, SUKESH RAM, Yale University, SAAKETH R NARAYAN, University of Pennsylvania, NICOLE HERBOTS, THILINA BALASOORIYA, WESLEY PENG, Department of Physics, Arizona State University, ERIC J. CULBERTSON, MicroDrop Diagnostics, LLC, ROBERT J CULBERTSON, Department of Physics, Arizona State University — Blood diagnostic tests require ~7 mL of blood, taking hours for results. Repeated testing can cause Hospital-Acquired Anemia. Accurate blood testing methods with smaller blood volumes and shorter analysis time are needed.

µL-sized blood drops can be rapidly solidified via Super- and Hyper-Hydrophilic HemaDrop™ coatings to yield reproducible Homogeneous Thin Solid Films (HTSFs). HTSFs are investigated for accuracy in measuring electrolytes and heavy metals. Calibration using Balanced Saline Solution allows for conversion of atomic % into concentration in mg/dL, the main metric in blood diagnostics.

Compositions from Ion Beam Analysis, X-ray Photoelectron Spectroscopy, and X-ray Fluorescence are compared at different depths and establish a minimum film homogeneity, volume and surface area to measure blood composition reproducibly and accurately. Relative error analysis shows that reproducibility to <10% can be attained. The damage curve method extracts elemental composition while accounting for possible IBA damage, which is found to be negligible.

Blood HTSFs formed via HemaDrop™ coatings can make accurate solid state analysis of µl blood composition possible.

*We would like to acknowledge SiO2 Innovates and MicroDrop Diagnostics, LLC for providing funding for experimentation.

10:24AM A06.00009: Selection of High Quality Sperm with Lower DNA Fragmentation  
AFROUZ ATAEI (Presenter), ANDY W.C. LAU, THEODORA LEVENTOURI, WASEEM ASGHAR, Florida Atlantic University — The first step of in-vitro fertilization is to sort out the motile sperm from the non-motile. Centrifugation based sperm swim-up and density gradient separation are common methods to sort sperm. However, these methods reduce sperm quality during the repetitive centrifugation steps and isolate sperm with high DNA fragmentation. In this work, we construct a microfluidic device based on the observation that motile sperm can swim against the flow within a specific range of flow rates. This sperm-sorting device consists of two chambers, top and bottom separated by a filter. After 45 minutes the sorted motile sperm is collected from the top retrieval chamber and placed on a glass slide for visual inspection with a light microscopy and data collection. The process is repeated for various flow rates. We find that 1) the most motile and functional sperm pass selectively through the micropores against the flow; 2) the optimum flow rate is the one that gives the highest concentration of motile sperm, the lowest DNA fragmentation and higher percentage of morphologically normal sperm. Our device provides an efficient, inexpensive way to sort sperm-out without the disadvantages of centrifugation.
10:36AM A06.00010: Characterization of neuroblastoma SH-SY5Y cell lines using dielectrophoresis  
SAMANEH RIKHTEHGARAN (Presenter), LUC T WILLE, THEODORA LEVENTOURI, JIANNING WEI, E DU, Florida Atlantic University — Dielectrophoresis (DEP) is a frequency-selective translation of polarized particles under the spatially nonuniform electric field. Particles can move toward the high-field region by positive DEP (pDEP) or away from high-field region by negative DEP (nDEP). This method is label-free, fast and noninvasive characterizing the electrical properties of neuroblastoma SH-SY5Y cell lines. This cell line has been used as an in vitro cell model for the study of Parkinson’s disease or neuronal function and differentiation. We constructed a microdevice that consists of two parts: the interdigitated ITO electrodes to generate AC electric field and a Polydimethylsiloxane (PDMS) with two wells to inject the cells and the media. Then the measured DEP frequency spectra fitted using the spherical shell model to compute electrical properties of the cells.

10:48AM A06.00011: Optimize The Blood Flow In Blood Vessels By Magnet Field To Cure Hypertension*  
RONGJIA TAO (Presenter), Physics, Temple Univ — Sever hypertension comes with headaches, chest pain, shortness of breath, flushing, and visual changes etc. Without timely medical treatment, sever hypertension will lead to heart attack and strokes. Here we report our discovery: the blood flow in blood vessels can be optimized by application of a strong magnetic field along its flow direction. The red blood cells are polarized and aggregated into short chains. The blood viscosity along the flow direction is significantly reduced, turbulence is suppressed, and the flow becomes stable laminar. Hence the blood pressure is lowered down to the normal range. Our clinical trials have more than 250 people tested. The technology is effective for everyone. On average, in 15 minutes the magnetic treatment lowers the blood pressure by 21.4%. The effect lasts more than 24 hours and can be kept continuously if the magnetic treatment is repeated everyday. Our placebo tests have also confirmed that without application of magnetic field, the blood pressure cannot be lowered. The effect is truly produced by improvement of blood flow with magnetic field. We expect that this technology will help people to cure hypertension, preventing cardiovascular diseases.

*American Heart Association

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A07 DQI: Topological Quantum Computing 102 - Tag(s): Focus
**8:00AM A07.00001: Bifurcating entanglement-renormalization group flows of fracton stabilizer models**  
ARPIT DUA (Presenter), PRATYUSH SARKAR, DOMINIC WILLIAMSON, MENG CHENG, Yale University — We investigate the entanglement-renormalization group flows of translation-invariant topological stabilizer models in three dimensions. Fracton models are observed to bifurcate under entanglement renormalization, generically returning at least one copy of the original model. Based on this behavior we formulate the notion of bifurcated equivalence for fracton phases, generalizing foliated fracton equivalence. The notion of quotient superselection sectors is also generalized accordingly. We calculate bifurcating entanglement-renormalization group flows for a wide range of examples and, based on those results, propose conjectures regarding the classification of translation-invariant topological stabilizer models in three dimensions.

*This work is supported by the start-up funds at Yale University (DW and MC), NSF under award number DMR-1846109 and the Alfred P. Sloan foundation (MC)*

**8:12AM A07.00002: Quantum electrodynamics in a topological metamaterial: Part 1**  
EUN JONG KIM (Presenter), XUEYUE ZHANG, ALP SIPAHIGIL, VINICIUS S FERREIRA, JASH BANKER, MOHAMMAD MIRHOSSEINI, OSKAR PAINTER, Caltech — The rich quantum electrodynamical properties arising from topological photonics open new possibilities for studying novel many-body states and implementing topologically protected quantum information processing protocols. It has been recently suggested that a topological waveguide, which realizes a photonic analog of the Su-Schrieffer-Heeger (SSH) model, can host unconventional quantum optical phenomena [Sci. Adv. 5, eaaw0297 (2019)]. We discuss the implementation of the topological waveguide with superconducting metamaterials. We explore the exotic properties of qubit-photon bound states and topological edge states emergent in this system.

**8:24AM A07.00003: Quantum electrodynamics in a topological metamaterial: Part 2**  
XUEYUE ZHANG (Presenter), EUN JONG KIM, ALP SIPAHIGIL, VINICIUS S FERREIRA, JASH BANKER, MOHAMMAD MIRHOSSEINI, OSKAR PAINTER, Caltech — Topological concepts in photonics give rise to novel ways of controlling light or microwaves. By coupling quantum emitters to topological photonic structures, photon-mediated interaction between the emitters inherits the topological properties, which can lead to novel radiative phenomena. Here, we study superconducting qubits coupled to a microwave metamaterial waveguide which is a photonic analog of the Su-Schrieffer-Heeger (SSH) model [Sci. Adv. 5, eaaw0297 (2019)]. We report the observation of novel interaction profiles and scattering properties of the qubits induced by the topological photonic bath.
8:36AM A07.00004: Transition from 2D to 1D topological superconductivity in a triangular island of p-wave superconductor  
AIDAN WINBLAD (Presenter), HUA CHEN, Colorado State University —

We study the connection between 0D and 1D Majorana modes in a triangular island of a model topological superconductor, with the motivation of designing a flexible platform for performing braiding operations on Majorana zero modes for topological quantum computation. Using the mean-field Bogoliubov-de Gennes theory, we solve a tight-binding model with Rashba spin-orbit coupling, out-of-plane Zeeman field, and s-wave pairing on an equilateral triangle, which hosts chiral Majorana edge modes. Using an eigen-value solver we were able to show breaking of the three-fold rotation symmetry of the model by applying an additional in-plane Zeeman field, which is expected to result in an effectively 1D topological superconductor. To further understand the evolution of the pseudo-Majorana states at the corners we treat the corner as a wedge with open boundary conditions and solve the BdG equation analytically.

8:48AM A07.00005: Time-resolved electrical detection of chiral edge vortex braiding*  
INANC ADAGIDELI (Presenter), Sabanci University, FABIAN HASSLER, JARA-Institute for Quantum Information, RWTH Aachen University, AURELIEN GRABSCH, MICHAL PACHOLSKI, CARLO W J BEENAKKER, Physics, Leiden University —  

$2\pi$ phase shift across a Josephson junction in a topological superconductor injects vortices into the chiral edge modes at opposite ends of the junction. When two vortices are fused they transfer charge into a metal contact. We calculate the time dependent current profile for the fusion process, which consists of $\pm e/2$ charge pulses that flip sign if the world lines of the vortices are braided prior to the fusion. This is an electrical signature of the non-Abelian exchange of Majorana zero-modes.

*This research was supported by the Netherlands Organization for Scientific Research (NWO/OCW) and by the European Research Council (ERC).
9:00AM A07.00006: Braiding of Majorana Fermions in a Cavity  MIRCEA TRIF (Presenter), Institute of Physics, Polish Academy of Sciences, PASCAL SIMON, LPS Orsay, University of Paris-Saclay — We study the dynamical process of braiding Majorana bound states (MBS) in the presence of the coupling to photons in a microwave cavity. We show theoretically that the $\pi/4$ phase associated with the braiding of MBS, as well as the parity of the ground state are imprinted into the photonic field of the cavity, which can be detected by dispersive readout techniques [1]. We use a density matrix description for the dynamics of the low energy states in order to account for various relaxation channels both in the adiabatic regime, as well as within the Floquet formalism in the case of periodic driving. We evaluate the average photon number and the second order photon coherence function $g^{(2)}(0)$, and show they are affected by the non Abelian Berry phase accumulated during the braiding process [2]. These manifestations are purely dynamical, they occur in the absence of any splitting of the MBS that are exchanged, and they disappear in the static setups studied previously. Conversely, the cavity can affect the braiding phase, which in turn should allow for cavity controlled braiding.


9:12AM A07.00007: Braiding Majorana Fermions and Creating Quantum Logic Gates with Vortices on a Periodic Pinning Structure*  XIAOYU MA (Presenter), University of Notre Dame, CYNTHIA REICHHARDT, CHARLES REICHHARDT, Los Alamos National Laboratory — We show how vortices that support Majorana fermions when placed on a periodic pinning array can be used for vortex exchange and independent braiding by performing a series of specific moves with a probe tip. Using these braiding operations, we demonstrate realizations of a Hadamard and a CNOT gate. We specifically consider the first matching field at which there is one vortex per pinning site, and we show that there are two basic dynamic operations, move and exchange, from which basic braiding operations can be constructed in order to create specific logic gates. The periodic pinning array permits both control of the world lines of the vortices and freedom for vortex manipulation using a set of specific moves of the probe during which the probe tip strength and height remain unchanged. We measure the robustness of the different moves against thermal effects and show that the three different operations produce distinct force signatures on the moving tip.

*This work was supported by the US Department of Energy through the Los Alamos National Laboratory.
Towards practical self-correction with augmented Majorana stabilizer codes

STEPHAN PLUGGE (Presenter), MARCEL FRANZ, ROBERT RAUSSENDORF, IAN AFFLECK, University of British Columbia — We present design ideas for an augmented Majorana surface code (MSC) that allows improved error-correcting behavior on practically relevant time-scales. The underlying mechanism resembles that of interacting anyon models, and facilitates the protected Hamiltonian-level generation of stabilizer operators in MSCs together with coupling to auxiliary bosonic degrees of freedom. In this talk, I will discuss MSCs and their extensions affording improved error-correction, towards the goal of thermally stable quantum memories in 2D.

We acknowledge funding by NSERC, CIFAR, and the Stewart Blusson Quantum Matter Institute at UBC Vancouver. Further we acknowledge computational resources provided by UBC ARC Sockeye and the Compute Canada network.

Optimizing Clifford gate generation for measurement-only topological quantum computation with Majorana zero modes

ALAN TRAN (Presenter), Physics, University of California, Santa Barbara, ALEX BOCHAROV, BELA BAUER, PARSA BONDESON, Microsoft — One of the main challenges for quantum computation is that while the number of gates required to perform a non-trivial computation may be very large, decoherence and errors in realistic architectures limits the number of physical gate operations that can be performed coherently. Therefore, an optimal mapping of the quantum algorithm into the physically available set of operations is of crucial importance. We examine this problem for a measurement-only topological quantum computer based on Majorana zero modes (MZMs), where gates are performed through sequences of measurements. Such a scheme has been proposed as a practical, scalable approach to process quantum information in an array of topological MZM qubits. Building on previous work that has shown that multi-qubit Clifford gates can be enacted in a topologically protected fashion in such qubit networks, we discuss methods to obtain the optimal measurement sequence for a given Clifford gate under the constraints imposed by the physical architecture, such as layout and the relative difficulty of implementing different measurements. Our methods also provide tools for comparative analysis of different architectures and strategies, given experimental characterizations of particular aspects of the systems under consideration.
9:48AM A07.00010: Computational universality of symmetry-protected topologically ordered cluster phases on 2D Archimedean lattices*  AUSTIN DANIEL (Presenter), RAFAEL ALEXANDER, AKIMASA MIYAKE, University of New Mexico — Which symmetry-protected topologically ordered (SPTO) ground states can be used for universal measurement-based quantum computation in a similar fashion to the 2D cluster state? 2D SPTO states are classified not only by global on-site symmetries but also by subsystem symmetries, which are fine-grained symmetries dependent on the lattice geometry. Recently, all states within so-called SPTO cluster phases on the square and hexagonal lattices have been shown to be universal, based on the presence of subsystem symmetry and associated structures of quantum cellular automata. Motivated by this, we analyze the computational capability of SPTO cluster phases on all vertex-translative 2D Archimedean lattices. There are four subsystem symmetries here called ribbon, cone, fractal, and 1-form symmetries, and the former three are fundamentally in one-to-one correspondence with three classes of Clifford quantum cellular automata. We conclude that nine out of the eleven Archimedean lattices support universal cluster phases protected by one of the former three symmetries, while the remaining lattices possess 1-form symmetry and have a different capability related to error correction.

*This work is supported by NSF grants PHY-1620651 and PHY-1915011. R. N. A. is supported by NSF grant PHY-1630114.

10:00AM A07.00011: Parafermions and $Z_3$ Charge-Flux attachment  PENG RAO (Presenter), Max Planck Institute for the Physics of Complex Systems, VIJAY SHENOY, Indian Institute of Science, INTI SODEMANN, Max Planck Institute for the Physics of Complex Systems — A recent construction (Ann. Phys. 393, 234 (2018)) has introduced an interesting route to bosonization of fermions in two spatial dimensions by implementing a precise lattice version of flux-charge binding. The idea is to modify Kitaev’s Toric code so that the electric charge ($e$) and magnetic flux ($m$) are always created in a tight "dipolar" pair $\varepsilon (=e \times m)$ which is a fermion, providing a way to represent any local fermionic Hamiltonian as a local Hamiltonian of spins. We discuss an extension of these ideas to the case of a $Z_N$ toric which allows a bosonization of anyons with more general statistitical angles. We have focused particularly in the case of $N=3$. We will prove that ground states in the torus in this case are at least three-fold degenerate, and, discuss a model featuring a topological phase transition between a 3-fold degenerate state and a 9-fold degenerate ground state featuring parafermionic excitations.

10:12AM A07.00012: Fun with fractons [Invited]  DOMINIC WILLIAMSON (Presenter), Stanford Univ — Interest in fracton topological order has grown explosively over the past several years, leading to a plethora of models that exhibit exotic topological physics tied to mobility constrained superselection sectors. At the same time a classification of even the simplest class of stabilizer fracton Hamiltonians remains elusive. I will describe some recent efforts to tame the vast array of models with the goal of a systematic construction and classification of all topological phases of matter in three spatial dimensions.

Monday, March 2, 2020 8:00 AM - 11:00 AM
8:00AM A09.00001: Finding Navier-Stokes fluid flows through quantum computing  FRANK GAITAN (Presenter), Laboratory for Physical Sciences; College Park, MD — We present a quantum algorithm that solves an arbitrary set of coupled non-linear partial differential equations and show how it can be used to solve the governing equations for a Navier-Stokes fluid. To test the algorithm we examine the problem of inviscid, compressible flow through a convergent-divergent nozzle. We numerically simulate application of the algorithm to find the steady-state flow when a shockwave is and is not present in the divergent part of the nozzle. In each case excellent agreement is found between the output of the quantum simulation and the exact analytical solution, with the simulation successfully capturing the shockwave when present. We compare the computational cost of the quantum algorithm to that of deterministic and random classical algorithms; discuss future applications as well as the potential long-term significance of quantum computing for the fluid dynamics community.

8:12AM A09.00002: Quantum eigenvalue estimation via time series analysis*  ROLANDO SOMMA (Presenter), Los Alamos National Laboratory — We present an efficient method for estimating the eigenvalues of a Hamiltonian $H$ from the expectation values of the evolution operator for various times. For a given quantum state $\rho$, our method outputs a list of eigenvalue estimates and approximate probabilities. Each probability depends on the support of $\rho$ in those eigenstates of $H$ associated with eigenvalues within an arbitrarily small range. The complexity of our method is polynomial in the inverse of a given precision parameter. Unlike the well-known quantum phase estimation algorithm that uses the quantum Fourier transform, our method does not require large ancillary systems, large sequences of controlled operations, or preserving coherence between experiments, and is therefore more attractive for near-term applications. The output of our method can be used to compute spectral properties of $H$ and other expectation values efficiently.

*This work was supported in part by the Laboratory Directed Research and Development program of Los Alamos National Laboratory and by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Quantum Algorithms Teams program.
**8:24AM A09.00003: A robust algorithm for finding phase factors in quantum signal processing**

YULONG DONG (Presenter), LIN LIN, University of California, Berkeley, XIANG MENG, Peking University, BIRGITTA K WHALEY, University of California, Berkeley — Quantum Signal Processing (QSP) provides a general way to implement matrix functions on quantum computers. The algorithm can be efficiently used to solve quantum linear systems, to perform Hamiltonian simulation, and to prepare Gibbs ensembles, among other applications. QSP can exactly encode a degree-d polynomial transformation of a matrix using d+1 phase factors. However, the current strategies for solving for the phase factors of a given function can be numerically unstable. We present an efficient method to find the phase factors for a general real function, and demonstrate the performance for solving linear systems and eigenvalue problems.

*This work was supported by a Quantum Research Award from Google LLC and also by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Quantum Algorithm Teams Program, under contract number DE-AC02-05CH11231.

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**8:36AM A09.00004: Finding symmetry-broken ground states with variational quantum algorithms**

NICOLAS VOGT (Presenter), SEBASTIAN ZANKER, JAN-MICHAEL REINER, HQS Quantum Simulations GmbH, THOMAS ECKL, ANIKA MARUSCZYK, Robert Bosch GmbH, MICHAEL MARTHALER, HQS Quantum Simulations GmbH — One of the most promising applications for near-term intermediate scale quantum computers (NISQ) is the preparation of the true ground state of strongly correlated electron systems. Besides the ground-state energy the properties of interest of the ground state are its broken symmetries and the corresponding phases of the system.

We study the preparation of broken symmetry ground states on a gate based quantum computer with different variational algorithms, including the variational Hamiltonian ansatz (VHA) with initial state preparation and extensions to the standard VHA. The two-dimensional Hubbard model is used as a toy model, to compare the variational algorithms to each other and to exact diagonalisation. To this end, we simulate the full algorithm including initialization and read-out running on a gate-based quantum computer. We use a hardware model based on the gates available in currently available quantum computers.

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**8:48AM A09.00005: Strategies for digital quantum simulation of bosons**

NICOLAS SAWAYA (Presenter), Intel Labs, TIM MENKE, Physics, MIT, THI HA KYAW, Computer Science, U Toronto, SONIKA JOHRI, Intel Labs, ALAN ASPURU-GUZIK, Computer Science, U Toronto, GIAN GIACOMO GUERRESCHI, Intel Labs — Many prominent bosonic simulation problems are thought to be intractable on a classical computer, including the Bose-Hubbard model, quantum photonics, and molecular vibronics. The behavior of such systems would be efficiently studied on a quantum computer. Before such a simulation is performed, one must choose how to encode the bosonic degrees of freedom into a set of qubits. We present a general methodology for encoding truncated bosons into arrays of qubits, and consider several encoding types. We study the quantum operations and qubit counts for local and composite operators. Importantly, we also consider the utility of interconverting between mappings in the middle of a simulation. These methods lower the quantum resource requirements compared to previous encoding strategies, which may allow for larger problems to be simulated on near-term quantum devices.
**9:00AM A09.00006: A Method of Determining Excited-States for Quantum Computation**

PEJMAN JOUZDANI (Presenter), STEFAN A BRINGUIER, MARK KOSTUK, General Atomics - San Diego — The calculation of molecular ground-state and excited-state energies, or more generally the energy spectra of chemical and material systems, is an application of great interest in a gate-based quantum computational model. In this contribution, we propose a phenomenological approach to the calculation of low-lying excited-states of a given problem Hamiltonian. Specifically, a method is presented in which the ground-state subspace is projected out of a Hamiltonian representation. As a result of this projection, an effective Hamiltonian is constructed where its ground-state coincides with an excited-state of the original problem. Thus, low-lying excited-state energies can be calculated using existing hybrid quantum-classical techniques and variational algorithm(s) for determining ground-state. The method is shown to be fully valid for the H2 molecule. In addition, conditions for the method’s success are discussed in terms of classes of Hamiltonians. A discussion on the broad impact of this method in the era of NISQ devices will also be presented.

*This material is based upon work supported by General Atomics internal R&D funding.

**9:12AM A09.00007: Quantum simulation by qubitization without Toffoli gates**

MARK STEUDTNER (Presenter), Lorentz Institute, STEPHANIE WEHNER, Delft University of Technology — Qubitization is a modern approach to estimate Hamiltonian eigenvalues without simulating its time evolution. While in this way approximation errors are avoided, its resource and gate requirements are more extensive: qubitization requires additional qubits to store information about the Hamiltonian, and Toffoli gates to probe them throughout the routine. Recently, it was shown that storing the Hamiltonian in a unary representation can alleviate the need for such gates in one of the qubitization subroutines. Building on that principle, we develop an entirely new decomposition of the entire algorithm: without Toffoli gates, we can encode the Hamiltonian into qubits within logarithmic depth.

*MS was supported by the Netherlands Organization for Scientific Research (NWO/OCW) and an ERC Synergy Grant. SW was supported by STW Netherlands, an NWO VIDI Grant and an ERC Starting Grant.

**9:24AM A09.00008: Emulation of fractional quantum Hall states with existing quantum hardware**

ARMIN RAHMANI (Presenter), Western Washington University, POUYAN GHAEMI, City College of the City University of New York, ZHANG JIANG, Google Research, Venice, CA, PEDRAM ROUSHAN, Google Inc., Santa Barbara, CA, KEVIN J SUNG, Google Research and the University of Michigan — Emulating strongly correlated phases of matter with existing or near-term quantum hardware is of considerable interest. Here we present quantum circuits to generate both the ground and quasiparticle states corresponding to the Laughlin’s \( \nu = 1/3 \) fractional quantum Hall state in the second-quantized representation. Our circuit depth is linear in the number of qubits. We identify experimentally accessible correlation functions as signatures of this state and discuss the quantum hardware implementation.

*Google Quantum Innovation Award
9:36AM A09.00009: Computing partition functions in the one clean qubit model*  ANIRBAN NARAYAN CHOWDHURY, Physique, Universite de Sherbrooke, ROLANDO SOMMA, YIGIT SUBASI (Presenter), Los Alamos National Laboratory — In this talk we will present a method to approximate partition functions of quantum systems using mixed-state quantum computation. For non-negative Hamiltonians, our method runs on average in time almost linear in \((M/(\varepsilon_{\text{rel}} Z))^2\), where \(M\) is the dimension of the quantum system, \(Z\) is the partition function, and \(\varepsilon_{\text{rel}}\) is the relative precision. It is based on approximations of the exponential operator as linear combinations of certain operations related to block-encoding of Hamiltonians or Hamiltonian evolutions. The trace of each operation is estimated using a standard algorithm in the one clean qubit model. For large values of \(Z\), our method may run faster than exact classical methods, whose complexities are polynomial in \(M\). Using this method we will demonstrate that a version of the partition function estimation problem within additive error is complete for the so-called DQC1 complexity class, suggesting that our method provides an exponential speedup.


9:48AM A09.00010: Reaction dynamics on a quantum computer*  ANDREW TRANTER (Presenter), PETER LOVE, Tufts Univ — The study of quantum chemistry is expected to be a principal use of emergent quantum computing devices. The ability of quantum computers to efficiently provide highly accurate electronic structure data could have major consequences where such accuracy is required, such as in the prediction of the kinetics and dynamics of chemical reactions. However, such simulations often require vast numbers of electronic structure calculations, potentially exacerbating resource limitations of small-scale quantum devices.

In this talk, we present theoretical results characterising the quantum resources required for the simulation of reactions involving small numbers of light atoms through semi-classical trajectory simulation. We consider how this process can be aided by recent optimisations to variational quantum algorithms. Finally, we report simulation results and discuss experimental progress to this end.

*The authors acknowledge Lincoln Labs for financial support.
10:00AM A09.00011: A size-extensive scheme for variational quantum ansatzes without Trotter approximation*  
YAROSLAV HERASYMENKO (Presenter), THOMAS O'BRIEN, Leiden University — One of the most promising applications for quantum computers is simulating the low-energy states of complex quantum systems. In the near-term, this can be done with variational ansatzes. Such ansatzes should follow physical principles to ensure high performance, one of the key principles being size-extensivity. Unfortunately, digitizing such ansatzes into standard operations generally requires the use of the inexact Trotter expansion, which constrains the expected accuracy of the ansatz.

In this work, we resolve this conflict by developing a framework for physically motivated ansatzes, which is fundamentally digital and thereby involves no Trotter errors. Using the stabilizer formalism, we construct a family of digital ansatzes that provably cover the entire Hilbert space with a minimal number of parameters. We show how to compress such parent ansatzes into practical child ansatzes that target specific systems, following the principle of size-extensivity. For this purpose, we develop a convenient diagrammatic approach. We apply our method numerically to the quantum Ising chain, with good convergence outside the critical regime.

*This work was funded by the Netherlands Organization for Scientific Research (NWO/OCW), an ERC Synergy Grant, and Shell Global Solutions BV.

10:12AM A09.00012: Finding the ground state of the Hubbard model by variational methods on a quantum computer with gate errors  
JAN-MICHAEL REINER (Presenter), HQS Quantum Simulations, FRANK WILHELMI, Theoretical Physics, Saarland University, GERD SCHÖN, Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology (KIT), MICHAEL MARTHALER, HQS Quantum Simulations — A key goal of digital quantum computing is the simulation of fermionic systems such as molecules or the Hubbard model. Unfortunately, for present and near-future quantum computers the use of quantum error correction schemes is still out of reach. Hence, the finite error rate limits the use of quantum computers to algorithms with a low number of gates.

The variational Hamiltonian ansatz (VHA) has been shown to produce the ground state in good approximation in a manageable number of steps. Here we study explicitly the effect of gate errors on its performance. The VHA is inspired by the adiabatic quantum evolution under the influence of a time-dependent Hamiltonian, where the -- ideally short -- fixed Trotter time steps are replaced by variational parameters. The method profits substantially from quantum variational error suppression, e.g., unitary quasi-static errors are mitigated within the algorithm. We test the performance of the VHA when applied to the Hubbard model in the presence of unitary control errors on quantum computers with realistic gate fidelities.
10:24AM A09.00013: Quantum algorithm for spectral projection by measuring an ancilla iteratively*

TZU-CHIEH WEI (Presenter), YANZHU CHEN, State Univ of NY - Stony Brook — We propose a quantum algorithm for projecting a quantum system to eigenstates of any Hermitian operator, provided one can access the associated control-unitary evolution for the ancilla and the system. The procedure is iterative by preparing a fresh ancilla state, applying the controlled unitary, and then measuring the ancilla. There are some freedoms in the ancilla state parameter and the control unitary. We give examples to illustrate that the algorithm works. Simulations of the procedure also show that the distribution of the projected eigenstates obeys the Born rule. This algorithm can be used as a subroutine in the quantum annealing procedure by measurement to drive the system to the ground state, and we also simulate this for a quantum spin chain.

*This work was supported by National Science Foundation under grants No. PHY 1620252 and No. PHY 1915165.

10:36AM A09.00014: Quantum Simulation of Quantum Z2 Gauge Theory demonstrated in a GPU Simulator*

YU SHI (Presenter), Fudan Univ — We outline a quantum simulation scheme of quantum Z2 gauge theory using quantum adiabatic algorithm implemented in terms of quantum circuit, and then demonstrate it in the classical simulator QuEST using a CUDA enabled GPU server. In particular, we obtained useful results in (3+1)-dimensional and (2+1)-dimensional theories. It is identified that the quantum phase transition is topological in both dimensions, and is first-order in (3+1) dimensions but second-order in (2+1) dimensions. High-performance classical simulation of quantum simulation, which may be dubbed pseudoquantum simulation, is not only a platform of developing quantum software, but also represents a new practical mode of computation.

*National Science Foundation of China (Grant No. 11574054).

10:48AM A09.00015: Term Grouping Techniques for VQE and Quantum Dynamics Circuits

KAIWEN GUI (Presenter), PRANAV GOKHALE, University of Chicago, TEAGUE TOMESH, Princeton University, YONGSHAN DING, University of Chicago, OLIVIA ANGIULI, University of California, Berkeley, MARTIN SUCHARA, Argonne National Laboratory, MARGARET MARTONOSI, Princeton University, FRED CHONG, University of Chicago — Digital quantum simulations are among the most promising near-term applications of quantum computation. Variational Quantum Eigensolver and time evolution of quantum dynamics are two examples of such algorithms. However, the amount of required quantum resources typically do not scale favorably as the desired accuracy of the calculations increases. Both VQE and quantum dynamics circuits are represented by tensor products of Pauli matrices that are obtained from the second quantization form using transformation methods such as Jordan-Wigner or Bravyi-Kitaev. We demonstrate various grouping techniques that optimize the order of these tensor products, with the goal of optimizing the total quantum resource cost. For VQE circuits, we minimize the number of required measurement operations. For quantum dynamics circuits, we minimize the circuit depth and maximize its fidelity.

Monday, March 2, 2020 8:00 AM - 10:12 AM
8:00AM A10.00001: Scanning Probe Microscope in an Ultra-High Vacuum Cryogen-free Environment*  
ANGELA COE (Presenter), GUOHONG LI, EVA ANDREI, Rutgers University, New Brunswick — Our new design concepts expand the use of scanning probe microscopy (SPM) into an ultra-high vacuum cryogen-free system. Typical cryogen-free systems are too noisy to effectively operate SPM, which require a low noise environment. We have created an internal vibration isolation unit that is able to connect to existing cryogen-free cryostats making their noise level low enough to operate SPMs. Our SPM is a modular design that can accommodate interchangeable probes, including STM, AFM, and MFM. The instrument is equipped with stages for sputtering, e-beam film deposition, and exfoliation for in-situ sample preparation and tip conditioning. The SPM is assembled at room temperature in ultra-high vacuum and a novel low-profile vertical transfer mechanism makes it possible to transfer the SPM, without breaking vacuum, to a variable temperature cryogen-free cryostat and magnet. The integration of all these capabilities into one instrument enables in-situ nano-scale characterization of low dimensional systems.

*Work supported by NSF-DGE 1842213 (A.M.C.), DOE-FG02-99ER45742 (E.Y.A.), NSF-MRI 1337871 (G.L.), and NSF-DMR 1708158 (G.L.).

8:12AM A10.00002: Graphene-based Hall probe magnetic imaging*  
DAVID COLLOMB (Presenter), PENGLEI LI, SIMON J BENDING, Univ of Bath — Hall probe microscopy is a powerful tool for mapping magnetic fields across a sample surface, and can be used to investigate key properties of magnetic and superconducting materials. However, to date the technique has not been widely used under ambient conditions because the figures-of-merit of available GaAs-based Hall probes degrade substantially at room temperature. To address this we have recently demonstrated sub-100nm CVD graphene Hall devices with room temperature field resolutions in the μT/√Hz range, greatly exceeding the performance of GaAs-based Hall probes.¹ Additionally, we have demonstrated improved stability and increased mobility in graphene devices encapsulated in HSQ.² We build upon these developments to optimise CVD graphene Hall probes for high resolution ambient magnetic imaging. We also report progress made in extending the technique to include local susceptometry mapping for, e.g., characterisation of ferromagnetic data storage media.


*Funding was provided by the Lloyds Register Foundation (G0086) and the UK EPSRC (EP/R007160/1).
Absorption of ground-borne vibrations by aggregate of particulate is investigated to determine attenuation versus frequency and material properties. The goal is to mitigate transmission of vibrations from the ground into the building structures. Attenuation depends on mechanical properties of the particulates medium, such as; elastic moduli, contact areas, aggregate size-distribution, and degree of compactness. Experimental findings show that aggregate material behaves as a band-pass filter for vibrations transmitted through them. Some aggregate materials have a frequency band-gap where frequencies in a certain range are strongly attenuated. Media of uniform size particulates are subjected to mechanical vibrations at different frequencies and amplitudes. Vibration attenuation versus frequency is measured as a function of material thickness, aggregate size, and compactness. The results can provide the characteristics of optimal dampers for external vibrations transmitted into the building structures.

The ability to measure and manipulate electrons at the nanoscale gives insight into nanoscale physics and paves way for its applications in electronics and photonics. We present a design and implementation of a scanning probe microscope that is cooled to liquid nitrogen temperature, to image electrons at the nanoscale. The imaging technique relies on a conductive scanning tip that acts as a local, movable electrostatic gate. The tip creates a local change in density of electrons in the material directly underneath it deflecting the electrons away from their original path. This changes the conductance of the device. The conductance is measured as a function of tip position while the tip moves across the material. The conductance change vs. tip position gives the map of the electron flow in the material. To align the tip within a micron of the sample at liquid nitrogen temperature, we use a home-built coarse positioning system. By applying high voltages to a piezo tube, the tip is raster scanned over the sample. With this method, we plan to image the viscous flow of electrons in graphene at liquid nitrogen temperature. Our design also allows us to image electronic flow in other nanoscale materials such as 2D semiconductors and topological insulators.
8:48AM A10.00005: Our software eliminates up to 80% of vibrational noise in a scanning tunneling microscope*  JONATHAN GOETTSCH (Presenter), School of Engineering and Applied Sciences, Harvard University, HARRIS PIRIE, BRYCE PRIMAVERA, Department of Physics, Harvard University, ALBERT CHIEN, School of Engineering and Applied Sciences, Harvard University, JENNIFER E. HOFFMAN, Department of Physics, Harvard University — Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) are globally employed techniques to measure the electronic structure of condensed matter systems with atomic precision. They require extremely stable environments to operate: modern microscopes typically use a combination of pneumatic isolators and massive inertial blocks to reduce ambient vibrations to the picometer scale. However, improvements beyond this benchmark are challenging and even the best microscopes are still limited by residual vibrations. Here we demonstrate a software algorithm that cancels up to 80% of vibrational noise over a 300 Hz bandwidth, even in modern ultra-low-vibration laboratories. Our scheme relies on a precisely calibrated transfer function to accurately propagate geophone-recorded vibrations to the STM tip. These vibrations are then subtracted from spectroscopic and topographic measurements by post processing. Our algorithm mitigates STM vibrational noise in a wide range of experimental environments, including those with high-amplitude noise.

*This work was supported by the Gordon and Betty Moore Foundation under grant number 4536.

9:00AM A10.00006: Progress on the Scanning Majorana Microscope*  ERIC GOODWIN (Presenter), MICHAEL GOTTSCHALK, Michigan State University, ALEX LEVCHENKO, University of Wisconsin - Madison, STUART TESSMER, Michigan State University — Quantum dots have proven to be powerful probes for studying a variety of mesoscopic effects. In general, lithographically-defined surface quantum dots and scanning single-electron-transistor (SET) quantum dot microscopes fulfill different niches, in part due to the inability to bring the scanning SET close enough to the surface to provide strong coupling. We show significant progress on a new type of scanning quantum dot microscope which we call the Scanning Majorana Microscope (SMM). This novel probe is capable of resolving single electrons entering a quantum dot situated at the tip’s apex; and importantly, we are able to position the quantum dot within tunneling range (~1nm) of the surface of a sample. With the ability to strongly couple surface states to the quantum dot and study how the single-electron signal evolves as a function of coupling strength, this probe represents a new tool to study mesoscopic systems, including candidate Majorana states.

*This work is supported by the U.S. Department of Energy, Basic Energy Sciences under Award DE-SC0017888.
CHRISTOPHER LUTZ (Presenter), IBM Research – Almaden — We use a low-temperature scanning tunneling microscope (STM) to perform electron spin resonance (ESR) of individual magnetic atoms on a surface, and employ these atoms as atomic-scale magnetic sensors. This technique combines the single-atom control of STM with the high energy resolution of ESR. We drive spin resonance by using the large electric field available in the tunnel junction, and sense the spin by means of magnetoresistance, using a spin-polarized STM tip. Magnetic coupling between two iron atoms placed a few nanometers apart on an MgO film shows inverse-cube distance dependence, indicating magnetic dipolar interaction. This yields a precise measure of the magnetic moment of the iron atom, which is then used to probe other atoms, such as the bistable magnetic bits formed by individual holmium atoms. We also use STM to drive ESR of titanium and copper atoms, which show free spin-1/2 behavior, in contrast to the high spin and large magnetic anisotropy of iron. Assembled arrays of low-spin atoms show exchange coupling that results in highly entangled magnetic states for quantum simulation of many-body states. ESR also reveals hyperfine coupling between the nucleus and the electrons of each atom. Furthermore, pulsed ESR allows us to perform coherent manipulation of atomic spins in order to observe Rabi oscillation, Ramsey fringes, and spin echoes. The combination of STM with ESR thus provides a versatile tool for exploring nano-scale quantum magnetism.


*We acknowledge funding from the Office of Naval Research.
9:48AM A10.00008: Sputtered Mo-Re SQUID-on-Tip for High-Field Magnetic and Thermal Nanoimaging  KOUSIK BAGANI (Presenter), JAYANTA SARKAR, AVIRAM URI, Department of Condensed Matter Physics, Weizmann Institute of Science, MICHAEL RAPPAPORT, Physics Core Facilities, Weizmann Institute of Science, MARTIN E HUBER, Departments of Physics and Electrical Engineering, University of Colorado Denver, ELI ZELDOV, YURI MYASOEDOV, Department of Condensed Matter Physics, Weizmann Institute of Science — Scanning nanoscale superconducting quantum interference devices (SQUIDs) have attracted attention as highly sensitive microscopic magnetic and thermal characterization tools of quantum and topological states of matter and devices. We present here a technique of collimated differential-pressure magnetron sputtering for the versatile self-aligned fabrication of SQUID-on-tip (SOT), which cannot be produced by conventional sputtering methods due to their diffusive, rather than the required directional point source, deposition. The technique provides access to a broad range of high $H_{c2}$ superconducting materials, alloys and possibly even high-Tc superconductors. This advancement is crucial for expanding the ranges of operating temperatures and magnetic fields essential of SOTs for the study of magnetic phenomena and dissipation mechanisms in a wide variety of quantum systems, unconventional superconductors, and topological materials. As a first example, we have fabricated Mo-Re SOTs with sub-50-nm diameter, that operates up to an unprecedentedly high magnetic field of 5 T with spin sensitivity better than 1.2 $\mu_0$/Hz$^{1/2}$ up to 3 T at 4.2 K, and thermal sensitivity better than 4 $\mu$K/Hz$^{1/2}$ up to 5 T—about five times higher than any previous report [1].


10:00AM A10.00009: Spin-polarized Seebeck effect at the nanoscale measured with scanning tunneling thermovoltage microscopy*  JEWOOK PARK (Presenter), Institute for Basic Science, Pohang, Republic of Korea, FELIX LUEPKE, Oak Ridge National Lab, JUN JIANG, XIAOGUANG ZHANG, University of Florida, AN-PING LI, Oak Ridge National Lab — Spin caloritronic effects have gained recent interest due to, e.g., potential low-power applications of magnetic tunnel junctions in which a temperature gradient-driven tunneling of electrons gives rise to a spin-dependent thermovoltage due to the Seebeck effect. Here, we report spatial mapping of the spin-resolved thermovoltage in a tunneling junction formed by ferromagnetic Co islands on a Cu(111) substrate and the magnetic tip of a scanning tunneling microscope. Our measurements reveal variations of the thermovoltage as function of spin polarization, island size, and stacking orientation of the islands with respect to the substrate. This method allows to reveal nanoscopic heterogeneities of both, the magnetic structures and the spin-dependent thermoelectric power.

*This research was performed at the Center for Nanophase Materials Sciences which is a DOE Office of Science User Facility.

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A11 APS/SPS: Undergraduate Research I 110 - Crystal Bailey, American Physical Society - Tag(s): Undergrad Friendly
Computational and experimental study of the doping of Bi$_2$Fe$_{4-x}$M$_x$O$_9$ (M=Ga, Al, or Ge)*

JOSEPH LANIER (Presenter), DAVID JONATHAN PRYCE MORRIS, Physics, Xavier University, Cincinnati, OH — Transition metal oxides have attracted interest due to the range of physical properties which are of scientific interest and of interest due to their potential applications. Here we report a study into the doping of Bi$_2$Fe$_{4-x}$M$_x$O$_9$. Doping the system with M=Ga, Al, or Ge, allows us to modified the magnetic moment on the iron site and alter the ionic and magnetic order of the material. The structure itself consists of metal oxide polyhedron that are seen throughout the entire crystal. Two edge sharing octahedron are connected to a tetrahedron in all locations, where the bismuth sits outside of these polyhedrons. Monte-Carlo simulations have been performed using the Metropolis algorithm to reduce the Coulomb energy - taking into account ionic radii and charge - to determine whether the M sit on the tetrahedron sites, or the octahedron. As well as using the Heisenberg Model to model the overall magnetic moment of the crystal. Crystals of the material with the three options for M have been grown, and we also report results from magnetization and x-ray measurements that test the simulations.

*John Hauck Foundation Summer Research Program

Surface Plasmon Resonance Dispersion Relation of Gold-Aluminum Thin Films Using the Kretschmann Configuration*

ROBERT KENT (Presenter), ABDUL QADEER REHAN, MARIAMA REBELLO SOUSA DIAS, Physics, University of Richmond — The prevalence of gold (Au) in the excitation of surface plasmon resonance (SPR) has been widely explored, due to these elements' pronounced dip in reflected intensity in the visible and near-IR spectrum, and their integrity in sensors owing to their resistance to oxidization. Other metals such as aluminum also exhibit SPR, but it remains a challenge to work with because of its propensity to form a surface oxide layer which can inhibit the response. Our research explores SPR in gold-aluminum (AuAl) alloyed thin films. We fabricate the thin films using the co-sputtering technique, with some concentrations (Au$_{0.85}$Al$_{0.15}$) showing a higher SPR quality factor than pure gold. The mixture of these elements should reduce the possibility of oxidization of Al, and therefore exhibit a better response. Numerous works have explored SPR using AuAl thin films, but few have done so with such high angular and spectral resolution, over such a wide range, using this many alloys. This is a result of the precision, equipment, and time necessary to take such measurements. We were able to produce high-resolution, homogenous images of SPR for various concentrations of AuAl alloys, that strongly agree with calculations.

*University of Richmond Summer Research Fellowship 2019
8:24AM A11.00003: Simulating Spin Relaxation in Organic Semiconductors*  RICHARD GERST (Presenter), NICHOLAS HARMON, Univ of Evansville — Understanding spin lifetimes in organic semiconductors is important for spin-based applications as well as for devices like organic solar cells and OLEDs. Spin relaxation and diffusion in disordered organic semiconductors is explored with numerical simulations. Previous theories and simulations examined the role of nuclear and spin-orbit interactions in relaxing spin [1, 2]. This work extends and explores in more detail the influence of spin-orbit interactions. Spin relaxation is studied in two regimes: one in which hops are uncorrelated with each other (multiple trapping) and the other where hops are correlated (multiple hopping). For multiple trapping we find agreement with analytic solutions [1]. For multiple hopping we find the simulation gives a smaller spin relaxation rate (a factor of 2/3). Both models are studied in either the semi-classical approximation where the carrier spin is a classical vector or in a quantum model where the carrier spin is a quantum object. We find interesting differences emerge between the two approaches when the hopping rates depends on orbital alignment.


*This work was funded by a UExplore grant from the University of Evansville.

8:36AM A11.00004: Electrically conductive gels of single wall carbon nanotubes and PEDOT:PSS*  ANGELO PORCU (Presenter), LUIS D. RIVAS BAGUER, ANAMARIS MELENDEZ, IDALIA RAMOS, Physics and Electronics, University of Puerto Rico at Humacao, ARJUN G YODH, Physics, University of Pennsylvania, MOHAMMAD F ISLAM, Materials Science and Engineering, Carnegie Mellon University — The development of lightweight, flexible, and electrically conductive carbon aerogels has important technological applications. Their high surface area to volume ratio and electrical conductivity make them suitable for energy storage and chemical sensing. Here, we report on preparation and characterization of highly porous (void volume ~0.9) gels with a range of shapes and sizes and composed of co-networks of single wall carbon nanotubes (SWCNTs) and the conducting polymer poly(3,4-ethylenedioxythiophene)-poly(styrene sulfonate) (PEDOT:PSS), at ratios ranging from 1:5 to 1:9 using concentration dependent sol-gel method. We validated the porous, filamentous microstructure of these gels by imaging their cross-sections using scanning electron microscopy. The aerogels exhibited good electrical conductivity of ~100 S/cm, determined from four-point I-V measurements. We will also present how to enhance the electrical conductivity of the co-gels by the addition of dopants and to fabricate mechanically robust, highly electrically conducting fibers.

*This work was supported by the National Science Foundation (NSF) under grant DMR-PREM 1523463.
Applying uniaxial strain to graphene devices fabricated on flexible substrates*

JUSTIN OH (Presenter), BRIAN T SCHAEFER, Cornell University, VERONIKA SUNKO, Max Planck Institute for Chemical Physics of Solids, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, CLIFFORD W. HICKS, ANDREW P. MACKENZIE, Max Planck Institute for Chemical Physics of Solids, KATJA NOWACK, Cornell University — Strain engineering is a promising avenue for tuning the band structure and electronic properties of two-dimensional materials. We report progress toward applying uniaxial strain to bilayer graphene devices with the ultimate goal of studying their magnetic properties using scanning superconducting quantum interference device (SQUID) microscopy. We fabricate graphene devices on flexible polyimide substrates and use a spring-based strain apparatus [1] to apply uniaxial strain by compressing or stretching the substrate, achieving a planar geometry compatible with scanning probe microscopy. We use Raman microscopy to monitor changes in the Raman peaks of graphene in response to uniaxial strain. Finally, we discuss the effects of strain on the band structure of bilayer graphene and outline our plans for studying this system using scanning SQUID microscopy.


*This work was primarily supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875) and performed in part at the Cornell NanoScale Facility, (NSF NNCI, Grant ECCS-1542081).

Novel Technique for Inducing Large Area Uniaxial Strain in Graphene*

LUCAS HANSON (Presenter), ANGELA COE, GUOHONG LI, EVA ANDREI, Rutgers University, New Brunswick — The effect of uniaxial strain on the electronic band structure of graphene is an exciting topic of inquiry, for both studies into the fundamental physics of 2D electron systems as well as applicative investigations in the design of “straintronics”. Tight binding calculations of the effect of strain in graphene have shown that strain on the order of 20 percent causes the Dirac points to merge, resulting in the formation of a band gap. However, experimental realization of this prediction has yet to be achieved, as current techniques for inducing strain in graphene cannot generate strain exceeding a few percent. We have devised a novel technique for inducing large uniaxial strain in graphene using a piezoelectric mechanism. The mechanism allows for controllable and continuously variable strain, with an expected upper limit on the inducible strain set only by the tearing of graphene at 26 percent. Device functionality and performance are discussed, and strained graphene samples are characterized by Raman spectroscopy. Results are compared with existing Raman spectra of strained graphene.

* Funding Acknowledgements:
Work supported by Richard J. Plano Fellowship (L.C.H), NSF-DGE 1842213 (A.M.C.), DOE-FG02-99ER45742 (E.Y.A.), NSF-MRI 1337871 (G.L.), and NSF-DMR 1708158 (G.L.).
9:12AM A11.00007: Quantum Transport in a Graphene-Superconductor Hybrid Device*
ELIZABETH ZHOU (Presenter), University of Southern California, VIVEK MANU KAKANI, JIAN LIAO, XURUI ZHANG, XIAOYAN SHI, University of Texas at Dallas — The interplay of superconductivity and the two-dimensional (2D) quantum Hall edge states is of great current interest for both fundamental science and applications. It could be an ideal platform to realize the non-Abelian zero modes, which is crucial for topological quantum computation. Here we fabricated an encapsulated few-layer graphene flake, which is in proximity to s-wave superconducting leads to form a Josephson-junction-like structure. At temperatures down to 20 mK, we have studied the magnetotransport properties of the device in a wide range of magnetic fields (both parallel and perpendicular orientations). In addition, the differential resistance has been measured as well. Experiments show multiple peaks at low fields, which may indicate the existence of Andreev reflections.

*This work was supported by the Research Experience for Undergraduates program funded by the National Science Foundation and hosted by the University of Texas at Dallas.

9:24AM A11.00008: Growth of ZnO on Nanosphere templates by Glancing Angle Vapor Deposition and Growth Modeling  DERICK DETELLEM (Presenter), PRITISH MUKHERJEE, SARATH WITANACHCHI, Univ of South Florida — Growth of coatings on a curved surface at steep angles enables the formation of pillar structures. In this research glancing angle laser deposition method was used to deposit Zinc Oxide (ZnO) nanostructures on silica nanoparticle templates in the size range of 3.5um to 250 nm. Self-assembled silica nanosphere templates were prepared by the Langmuir-Blodgett technique. It was observed that the diameter of the pillars and the number of pillars on each nano sphere decreased with decreasing sphere size. A simple model based on the nucleation theory that is adopted for nucleation and growth on a curved surface was developed to predict the evolution of the nanopillar structures. Results pertaining to the morphology, structure, and composition investigated for varying template sphere sizes by SEM, EDS, AFM, and XRD will also be presented.

9:36AM A11.00009: First order reversal curves simulation for core-shell nanoparticles via 3D-Ising model*  NICOLÁS VERGARA (Presenter), EDWIN ER RAMOS, JUAN RAMIREZ, University of the Andes — We studied the magnetic properties of the 3D-Ising model employing Montecarlo simulations. The system is built with a cubic unit cell compound of spherical nanoparticles with a core-shell structure. We have recovered the dynamical magnetic properties such as the susceptibility, energy, heat capacity and equilibrium magnetization for Ferro and Anti-Ferro magnetic couplings. All these properties were studied as a function of nanoparticle size. We found a nanoparticle critical-size limit below which the magnetic properties depart from those of the bulk. In addition, in simulating first order reversal curves (FORC) of the core-shell structures, we found that we were able to identify features on the FORC diagram that allowed us to decouple individual magnetic reversal mechanisms of the core, shell and the interface. Our results suggest that nano-confinement modify bulk properties and that FORC is able to separate individual magnetic contributions to the magnetism that are otherwise hidden in the isothermal hysteresis loops.

*Authors acknowledge support form Colciencias grant 120471250659
9:48AM A11.00010: Plasmonic interactions of gold nanoparticles with MoS$_2$-WS$_2$ Heterostructures

MUMTAZ HASSAN (Presenter), Mechanical Engineering, University of South Florida, HANA HRIM, SHARAD AMBARDAR, DMITRI V VORONINE, Physics, University of South Florida — Scanning probe force microscopic techniques and optical spectroscopy have been widely used for sensing applications. Raman scattering and photoluminescence (PL) signals provide vital spectroscopic information about low vibrational modes and electronic properties of two-dimensional transition metal dichalcogenides (2D TMD). Since Raman signals are generally weak, chemical and electromagnetic mechanisms can enhance these signals using plasmonic materials such as gold nanoparticles (NPs) leading to surface-enhanced Raman scattering (SERS). The effects of the gold NPs deposited on lateral MoS$_2$-WS$_2$ heterostructures has been investigated using a combination of optical spectroscopic techniques. Changes in surface topography have been observed using atomic force microscopy (AFM), Kelvin probe force microscopy (KPFM), Tip-enhanced PL (TEPL) and Raman (TERS) spectroscopy. Contact potential difference obtained through KPFM has decreased as a result of high accumulation of gold NPs. Raman spectroscopy peak intensities have decreased, and PL peaks have been observed to become sharper and narrower which could be a result of the formation of surface cavities on TMD's after the deposition of gold nanoparticles. This information can be applied to nano-optoelectronics and biosensing.

10:00AM A11.00011: Atomistic and Coarse-Grained MD Simulation Studies of the Energetics and Interactions of Regulatory Dib1 Protein Inside a Highly Dynamic Pre-Catalytic Spliceosomal Macromolecular Complex Preceding Pre-Messenger RNA Splicing in Eukaryotic Cells*

RACHEL GOLDSTEIN (Presenter), Trinity University, SARA CHENG, University of Texas at Austin, GABRIELLE ORR, CHRISTIAN SCHREIB, CORINA MAEDER, KWAN CHENG, Trinity University — The spliceosome is a complex RNA/protein macromolecular machine responsible for catalyzing the removal of introns from pre-messenger RNA in eukaryotic cells. As part of the highly dynamic spliceosome assembly pathway, the key protein Dib1 must depart the pre-catalytic B complex prior to pre-mRNA splicing. Experimentally, we have identified several Dib1 temperature-sensitive mutants that disrupt splicing activity and spliceosome assembly. However, the molecular mechanisms underlying how these mutations perturb protein-protein and protein-RNA interactions in the B complex are not known. Using 200ns of atomistic and 2µs of coarse-grained MD simulations, the interactions between Dib1 and its neighboring molecules were determined for spliceosomal B complexes containing wild-type and mutant Dib1 at conditions similar to biochemical experiments. We observed specific changes in the interaction energy, residue-contact, and hydrogen-bonding propensity at the interfacial region between Dib1 and neighboring RNAs and proteins. Our results offer an explanation for the experimental finding that the Dib1 mutations disrupt the transition from B to B$^{act}$ complexes in the splicing pathway.

*Supported by NSF OAC-153159; NIGMS R15GM120720
Electrodepositing switchable photovoltaic window electron and hole transport layers*  
RACHEL THAM (Presenter), University of Illinois at Urbana-Champaign, KEVIN PRINCE, ANICA NEUMANN, Colorado School of Mines, CALEB BOYD, Stanford University, LANCE WHEELER, National Renewable Energy Laboratory — Vertical glass facade buildings, such as skyscrapers, have significant potential for generating electricity using solar window technologies, such as SwitchGlaze, a switchable photovoltaic window, containing a perovskite layer that absorbs visible and UV light. To commercialize these perovksite solar cells, it is essential to optimize electrodeposition, a scalably and controllably fabricate stable transport layers. This technique can then be used to fabricate back contact solar devices to decrease delamination occurrence and allow for more sunlight to directly interact with the perovskite and increase device efficiency. Nickel oxide and tin oxide, are promising transport layers due to higher stability and electron mobility, respectively. A three-electrode system was used to determine, in a range of 0.03 M to 0.1 M electrolyte concentrations, the electrodeposition times, current densities, and annealing times would electrodeposit that produced most uniform, least surface roughness, and thinnest transport layers. Initial results have produced solar cell devices up to about 12% efficiency.

*This work was supported by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS), under SULI.

Manipulating Generation and Spatial Distribution of Plasmon-Generated Hot Electrons via Oxygen Vacancies on Au/TiO$_2$ Heterostructures for Photochemistry*  
GRACE ROHALEY (Presenter), Allegheny College, JIAWEI HUANG, APRIL LO, W. DAVID WEI, Chemistry, University of Florida — Utilizing hot electrons on plasmonic metal/oxide heterostructures offers unique opportunities for solar photocatalysis. However, the role that surface oxygen vacancies (OVs) play in governing plasmon-driven photochemical reactions is poorly understood. Here, we demonstrate that surface OVs on Au/TiO$_2$ heterostructures manipulate plasmon-generated hot electrons in the generation process and spatial distribution for visible-light methylene blue (MB) degradation. Hot electrons originating from the plasmon-mediated electron transfer (PMET) pathway (i.e. the electron transfer from Au to TiO$_2$) and the plasmon-induced energy transfer (PIRET) pathway (i.e. the generation of electrons in TiO$_2$) accumulate under $\lambda > 435$ nm excitations, occupying surface OVs. Together, they result in ca. 5x enhancement in MB degradation than that under $\lambda > 495$ nm excitations, in which hot electrons only originate from the PMET pathway. Taken together, our study demonstrates an essential role played by surface OVs in plasmon-driven photochemistry and reveals two distinct mechanisms clarifying visible-light photocatalytic activity under different excitation conditions.

*The University of Florida Departments of Physics and Chemistry  
NSF REU site: Condensed Matter Physics and Applied Materials (DMR-1852138)
Molecular Dynamics Simulations of the Anorthite-Water System Under Extreme Conditions  
DEVEN ROMINE (Presenter), ROBERT MAYANOVIC, Missouri State Univ — Incorporation of water plays an important role in modifying the physical and chemical properties of silicate melts. Water reacts with the melt constituents causing depolymerization and reduces the viscosity of the melt which directly impacts the eruptive power of magmas and the transfer of mass in magmatic processes. Anorthite is a Ca-bearing aluminosilicate having the chemical formula CaAl$_2$Si$_2$O$_8$. It is an end member of the feldspar series and an important constituent of the rocks comprising the Earth's crust. We have made large simulation-cell molecular dynamics calculations in order to develop a detailed quantitative structural analysis of an hydrous anorthite melt system. ReaxFF reactive force fields are utilized to simulate the reaction between an anorthite melt and water at extreme temperatures. An analysis of bond lengths, pair correlations and bond angles within the hydrous melt is being made in order to determine how the structural properties of the system change under the extremes of pressure and temperature. The extent of depolymerization of the hydrous aluminosilicate melt, as determined from the transformation of Si – O – Si, Si – O – Al, and Al – O – Al bonds into terminating, non-bridging Si – OH and Al – OH bonds, will be discussed.

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A12 APS/SPS: Undergraduate Research II  
Phys AIP - Tag(s): Undergrad Friendly

Simulating Noise in Superconducting Qubits Using Qiskit* 
EVA GURRA (Presenter), ERIC BERG, ELIZABETH DOSS, MATTHIEU DARTIAILH, KASRA SARDASHTI, JAVAD SHABANI, Center for Quantum Phenomena, NYU — Qubits are quantum systems analogous to classical bits. Classically, errors in bits arise from environmental factors like external magnetic fields, and intrinsic factors like dissipation in resistors. To correct for these errors, bits are copied for detection and corrected. In qubits, errors can result from internal factors such as improper state preparation from inaccurate gates, or coupling with the environment, which leads to energy relaxation and decoherence. Error correction in qubits requires a new approach as qubits cannot be copied, and because they exist in superposition, phase information must also be preserved. Through IBM Qiskit, we simulated different noise models such as bit and phase flips, energy relaxation, and decoherence errors to analyze their effect on a singlet state. We generated $T_1$ and $T_2$ times, which denote when the system exponentially decays to 63% of its initial state through energy relaxation. Then, we compared the impact of these models on the singlet state and the preparation process. Lastly, we analyzed the extent to which these models cause a complete loss of information in the qubit state and whether this can be detected and partially reversed.

*US Army URAP/HSAP
Noise Temperature Measurements of Josephson Parametric Amplifiers for the Axion Search at IBS/CAPP

ALLISON SCHROEDER (Presenter), Regis University, ÇAĞLAR KUTLU, Center for Axion and Precision Physics — Josephson parametric amplifiers (JPAs) are promising devices for amplifying the weak signal of the axion in haloscopes due to their low noise amplification and tunable resonant frequency. For the axion experiment, the noise temperature of the JPA needs to be determined at various frequencies, which requires altering the noise source temperature. Optimizing the time required to collect this data is crucial for this experiment. Two methods were used to estimate the noise temperature of the JPA and calculate the standard deviation of the fitted data. First, a modified Y-factor method was developed to calculate the noise temperature using only two noise source temperatures. Then, a method using curve fitting to estimate the noise temperature was applied, utilizing all fifty-three noise source temperature spectra, and the standard deviation was calculated. The fitting method provided much more accurate results, but the measurement time was significantly longer than what would be required for the Y-factor method.

*This work was supported by the Korea Undergraduate Science Program and the Center for Axion and Precision Physics.

Integrating Molecular Rectifiers in AC Circuits

ROBERT BRADFORD (Presenter), ZACHARY LAMPORT, RYAN SULLIVAN, Physics, Wake Forest University, SURYA BANKS, MARK WELKER, Chemistry, Wake Forest University, OANA D. JURCHESCU, Physics, Wake Forest University — The field of molecular electronics exploits single molecules as basic components. Envisioned to provide a route to the continued satisfaction of Moore's Law, these nano-scale components exploit quantum effects to provide functionality at a length scale impossible with current technologies. This presentation focuses on molecular rectifiers based on single molecular layers sandwiched between two electrodes, operating similarly to solid-state diodes. We have developed a new molecule, (E)-1-(4-cyanophenyl)-N-(3-(triethoxysilyl)propyl)methanimine, that allows current rectification with rectification ratios greater than 2500. We further tested the functionality of molecular rectifiers made from this molecule in a standard AC circuit to create a DC rectifier. A test circuit was built where molecular diodes were connected in series with a 1 MΩ resistor and 100 nF smoothing capacitor, using a specially designed 3D-printed low-noise integration system. The rectification ratio of each diode was tested before circuit integration to associate this value with circuit performance. DC voltages measured for a variety of input frequencies show low ripple voltage, the mark of a quality DC rectifier, indicating that the experimental molecular layer acts as a stable diode in AC circuitry.
8:36AM A12.00004: Gating dynamics in ionic-liquid-gated FeS$_2$ single crystals* KEI HELTEMES (Presenter), Department of Physics, Augsburg University, BRYAN VOIGT, Department of Chemical Engineering and Materials Science, University of Minnesota, JEFF WALTER, Department of Physics, Augsburg University, CHRIS LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota — Ionic liquid (IL) gating has proven remarkably effective in voltage control of superconductivity, insulator-metal transitions, and magnetism. This is in large part due to its high electric fields, and thus large accumulated surface charge densities (> $10^{14}$ cm$^{-2}$). Recent studies, however, emphasize the importance of distinguishing electrostatic from electrochemical gating mechanisms in such devices. Here, we present a detailed study of the transport dynamics of IL-gated FeS$_2$ single crystals, where a positive gate voltage is observed to induce a remarkable insulator-metal and diamagnetic-ferromagnetic transition. This transition is found to be highly reversible in transport, which, given the delicate nature of surface conduction in FeS$_2$ [1], strongly evidences an electrostatic gating mechanism. Hysteretic gate voltage sweeps suggest the electrostatic electron accumulation and depletion to be spatially non-uniform, with a sweep-direction-dependent percolation transition. The observation of reversible electrostatic response is discussed in terms of the formation enthalpy and diffusivity of S vacancies in FeS$_2$.


*Work supported by the NSF MRSEC under DMR-1420013 (UMN) and by a Margaret A. Cargill Philanthropies grant (Augsburg).

8:48AM A12.00005: Electrical characterization of a tungsten diselenide/silicon heterostructure* AHMAD MATAR ABED (Presenter), ANAMARIS MELENDEZ, NICHOLAS PINTO, Department of Physics and Electronics, University of Puerto Rico - Humacao, JOSÉ O. SOTERO-ESTEVA, Department of Mathematics, University of Puerto Rico - Humacao, IDALIA RAMOS, Department of Physics and Electronics, University of Puerto Rico - Humacao — A pn diode was fabricated by using a simple method of transferring a p-type two-dimensional WSe$_2$ film onto a cleaved n-Si/SiO$_2$ wafer. The current-voltage characteristics of the device were measured, and the conduction mechanisms analyzed over a temperature range of 80 K–300 K. At high temperatures, the current-voltage characteristics of the diode show that thermionic emission transport dominates. However, tunneling also contributes at low temperatures. To explain the transport behavior of the heterojunction, a model that takes into consideration both thermionic emission and tunneling will be presented. Furthermore, the device was tested as a half-wave rectifier at room temperature at low frequencies. The rectification ratio and low turn-on voltages of the diode make it suitable for optoelectronic applications.

*The WSe$_2$ films were provided by the PSU 2DCC-MIP, which is supported by NSF cooperative agreement DMR-1539916. Research at UPRH was supported by NSF under grant NSF-DMR-1523463 (PENN-UPRH Partnership for Research and Education in Materials).
9:00AM A12.00006: Measuring the Dielectric Constants of Perovskite Nanoparticles in a Polymer Matrix  JOSHUA MORGAN (Presenter), JACKSON BAKER, DANIEL BRITO, GUADALUPE QUIRARTE, ELEANOR RACKOFF, ALBERT DATO, Harvey Mudd College, TODD MONSON, Sandia National Laboratories — Barium titanate (BTO) is a perovskite material used in energy storage applications due to its high dielectric constant [1, 2]. Interestingly, Wada et al. found that BTO nanoparticles ranging from 17 to 500nm exhibited a dependence of their dielectric constant on particle size [2]. Particles with sizes over 300 nm exhibited a dielectric constant of 4000, but a sharp increase in dielectric constant to over 15,000 was observed at a BTO size of 70 nm [2]. To investigate the relationship between the particle size and dielectric constant of BTO, we developed an injection molding process to fabricate polymer-matrix nanocomposites containing BTO powders. Here we present our novel fabrication method and the results of our investigation, which was focused on determining the dielectric constants of nanocomposites containing BTO nanoparticles with sizes ranging from 50 to 500 nm. We will discuss our methods of (1) measuring the dielectric constants of nanocomposites and (2) extracting the dielectric constants of the BTO nanoparticles from those measurements and relating them to particle size and volume loading.


9:12AM A12.00007: Electronic Properties in Strained and Suspended Sheet of MoS\textsubscript{2} on Anodized Aluminum Oxide.*  TAN DAO (Presenter), SHAWNA HOLLEN, Univ of New Hampshire — Two-dimensional materials are as thin as physically possible and have tunable electronic properties that can be useful for the development of faster and smaller electronic devices. One way to tune the electronic properties of 2-D materials is to induce strain by deforming the lattice. In addition to strain impact on the electronic properties, a suspended sheet of 2-D material exhibits higher electrical conductivity. In this project, I induce strain by deforming a semiconductor, MoS\textsubscript{2}, lattice with a nanopatterned substrate, and characterize the strain by atomic force microscopy (AFM) and Raman spectroscopy. Here I present the results of patterning strain and suspension into MoS\textsubscript{2}, and their impact on the electronic properties of MoS\textsubscript{2}. Single layer MoS\textsubscript{2} is isolated via mechanical exfoliation and transferred onto anodized aluminum oxide (AAO) - a substrate with nanoscale valleys and hills. The average strain in the MoS\textsubscript{2} sheet is 0.23% and 0.29%, which obtained from the Raman spectroscopy and AFM data, respectively. AFM techniques such as KPFM, C-AFM, and TERS are used in this project to characterize the electronic properties in the strain-textured MoS\textsubscript{2}.

*This project was supported by the Hamel Undergraduate Reseaarch Center and the McNair Scholars Program.
Understanding the Effects of Controlled Strain on Low Dimensional Material Properties

MICHAEL O'CONNOR (Presenter), MANOJ K SINGH, MICHAEL BOYER, Clark University — A material is typically considered low dimensional if electron movement within the material is limited, for example, to within a particular ionic plane or along an axis. When strain is introduced to an ideal material, lattice deformations may cause substantial changes in structural and electronic properties. Studying the effects strain have on a material can lead to basic insights into the physics governing the material as well as an understanding of how a material's properties can be manipulated for use in applications. Strain can be introduced to a low dimensional material through processes such as sample cleaving, elemental doping, chemical pressure, and external mechanical application. First, we detail our efforts in characterizing the expected strain delivered to the sample from our external application as a function of temperature. We then present resistivity measurements showing the effects strain has on the bulk phase transition temperature of a charge density wave compound. We will discuss how this system can be used in further studies that characterize strain on the nanoscale.

Studying the Crystallization of ALD-Deposited Doped Nb$_2$O$_5$ into NbO$_2$ for Next Generation Electronics Applications

NICOLE ZHE (Presenter), ANDREW H ROWLEY, NICHOLAS MORABITO, ZACHARY ROBINSON, SUNY Brockport, ALEXANDER KOZEN, University at Maryland, LAURA RUPPALT, Naval Research Laboratory — Phase change materials have a variety of applications across many disciplines. They can be used in homes to produce more energy-efficient refrigerators and freezers, or in clothes to help regulate body temperature in varying climates. NbO$_2$ is one such material, and can be used in a variety of electronic applications. In this project, we studied the conversion of amorphous Nb$_2$O$_5$ thin-films doped with either Al$_2$O$_3$ or ZnO (supplied by our collaborators at the Naval Research Laboratory) to crystalline NbO$_2$. Previous studies show Nb$_2$O$_5$ can be converted into NbO$_2$ by annealing to temperatures around 800 C. Systematic anneals in a tube furnace showed how the dopants affect the conversion of Nb$_2$O$_5$ into NbO$_2$. Our results indicate that samples of Nb$_2$O$_5$ doped with Al$_2$O$_3$ convert much slower than pure Nb$_2$O$_5$, and those with ZnO appear to convert faster.
9:48AM A12.00010: A Graphene Encapsulated Growth Method to form Ultra-thin Magnesium Diboride (MgB₂)*

PATRICK RONDONANSKI (Presenter), Department of Physics, Pennsylvania State University, JOAN M REDWING, Department of Materials Science and Engineering and 2D Crystal Consortium - Materials Innovation Platform, Pennsylvania State University, ANUSHKA BANSAL, AZIMKHAN KOZHAKHMETOV, JOSHUA ROBINSON, Department of Materials Science and Engineering, Pennsylvania State University, KE WANG, Materials Research Institute, Pennsylvania State University, ZAKARIA AL BALUSHI, Department of Materials Science and Engineering, University of California - Berkeley — There is interest in coupling 3D topological insulators (TI) with s-wave superconductors (SC) for realizing topological superconductivity (TSC) for quantum computing applications. MgB₂ is an intriguing superconductor for this application as it has $T_c = 39K$ and a hexagonal crystal structure, compatible with common Bi-based TIs. However, MgB₂ oxidizes in air making it difficult to form high quality TI/SC interfaces. Here, we propose a novel approach to synthesize ultra-thin MgB₂ via intercalation between epitaxial graphene (EG) and SiC. EG is used to protect the MgB₂ surface while enabling epitaxial growth of the TI on top. Initial studies investigated Mg intercalation between EG and SiC using a tube furnace. X-ray photoelectron spectroscopy (XPS) and cross section transmission electron microscopy-energy dispersive spectroscopy (TEM-EDS) confirmed Mg intercalation between EG and SiC. Current studies are being performed to optimize process conditions to intercalate Mg. The results of planned investigations to convert Mg to MgB₂ via annealing in B₂H₆ will also be discussed.

*Intel Corporation

Financial support was provided by NSF via an EFRI REM supplement (EFRI-1433378), Grant No. DMR-1410765 and the Penn State 2D Crystal Consortium (DMR-1539916).

10:00AM A12.00011: Temperature Dependent Switching Dynamics in BaTiO₃ at ns Speeds*

ALEXANDER QUALLS (Presenter), ERIC PARSONNET, YIZHE JIANG, WENBO ZHAO, University of California, Berkeley, CHIA-CHING LIN, TANAY GOSAVI, Intel Corp, LANE WYATT MARTIN, RAMAMOORTHY RAMESH, University of California, Berkeley — BaTiO₃ (BTO) is a model ferroelectric, which has been studied extensively, both in bulk crystals and thin films. We have made significant progress, achieving ultra-low coercive fields in thin film BTO samples that hold promise for low-power microelectronics. While there has been extensive work studying switching kinetics in BTO, relatively few studies have performed time-domain experiments on timescales in the low ns regime, since they are typically limited with instrumental constraints (e.g., rise time of oscilloscope or the voltage source). We are able to access this regime by using ultra-low coercive field BTO as a model system and measuring the response to voltage pulses with ~100ps rise time. We present data revealing switching speeds faster than previous reports for BTO, on the order of 1ns. Further, with this setup we study switching dynamics as a function of temperature as we approach the ferroelectric phase transition. The data reveals a decrease in switching time with increasing temperature, which we analyze in the context of classical ferroelectric switching theory.

*Intel Corporation
10:12AM A12.00012: Detection of Phase Transitions in Phase Separated \((La_{1-y}Pr_y)_{1-x}Ca_xMnO_3\) Thin Films*  JONATHAN DESTEFANO (Presenter), A. BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — Phase separated manganites have competing phases that each have unique electronic, magnetic, and structural properties. The similar free energies these phases possess allow for the manipulation of phase transitions with the application of external stimuli. Here we report the role of an external magnetic field and a change in chemical doping ratios on the phase transitions in \((La_{1-y}Pr_y)_{1-x}Ca_xMnO_3\) thin films grown on NdGaO_3. These thin films showed that the nucleation and growth of ferromagnetic metallic regions in an anti-ferromagnetic charge ordered insulating background occurs at a higher temperature when an external magnetic field is applied. At a high enough field strength, these ferromagnetic metallic regions hinder the phase transition from paramagnetic insulating to anti-ferromagnetic charge ordered insulating phase which occurs at a relatively high temperature (close to 200 K). The value of the activation energy for the anti-ferromagnetic charge ordered insulating phase calculated by fitting the resistance vs. temperature data to the Arrhenius equation agrees with direct measurements taken using scanning tunneling spectroscopy.

*NSF DMR-1410237, NSF DMR-1852138

10:24AM A12.00013: Doublons Instability in the Presence of Impurities*  MIRIAM BAITNER (Presenter), LEA SANTOS, Yeshiva Univ — In the presence of strong interactions, particles can bind in pairs forming what became known as doublons. A doublon moves together as a single particle, but contrary to it, doublons move slowly. They emerge in common models of condensed matter physics, such as the anisotropic Heisenberg model and the Bose-Hubbard model. We show that doublons are very stable and do not split up even when this would not violate energy conservation. We illustrate our results using one- and two-dimensional spin models in the presence of impurities.

*We are supported by the NSF Grant No. DMR-1603418

10:36AM A12.00014: Localization in two-dimensional trivial and Chern insulators  SPENSER TALKINGTON (Presenter), RAHUL ROY, University of California, Los Angeles — We investigate the localization properties of two-dimensional tight-binding models using transfer matrix methods. In particular, we numerically determine the localization length for cylindrical lattices with single-particle hamiltonians that have nearest-neighbor and next-nearest-neighbor hopping terms, both in the trivial and Chern insulator phases. We consider the role of disorder strength and particle energy on localization, and construct phase diagrams of conductivity properties. In addition, we use these results to guide an exploration of the critical behavior of localization-delocalization transitions in these models.

Monday, March 2, 2020 8:00 AM - 10:12 AM

Session A15 DFD DSOFT: Flow of Complex Fluids: Rheology, Structure, and Instabilities I 210/212 - Larry Galloway, University of Pennsylvania
8:00AM A15.00001: Bistability in the Flow of Polymer Solutions in Porous Media
CHRISTOPHER BROWNE, AUDREY SHIH, SUJIT DATTA (Presenter), Princeton University — Polymer solutions are often injected in porous media to improve oil recovery or groundwater remediation, but applications are limited by an incomplete understanding of the underlying physics. In a tortuous pore space, the flow becomes unstable at sufficiently large injection rates. However, how the spatio-temporal characteristics of this flow state depend on pore geometry is poorly understood. We shed light on this question by systematically varying the spacing between pores. We find that when the pore spacing is large, unstable eddies form upstream of each pore, similar to the case of an isolated pore. By contrast, when the pore spacing is sufficiently small, the flow exhibits a surprising bistability, stochastically switching between two distinct flow states. We hypothesize that this unusual behavior arises from the interplay between the retention of polymer strain between pores, hysteresis in polymer conformations, and fluctuations in the flow. Moreover, we find that while flow state is correlated between neighboring pores, these correlations do not persist long-range. Our results thus help to elucidate the rich array of flow behaviors that can arise in polymer solution flow through porous media.

8:36AM A15.00002: Shear melting and recovery of cellulose nanocrystal-polymer gels*
ABHINAV RAO, Mechanical Engineering, Massachusetts Institute of Technology, THIBAUT DIVOUX (Presenter), Civil and Environmental Engineering, CNRS / Massachusetts Institute of Technology, GARETH H MCKINLEY, JOHN HART, Mechanical Engineering, Massachusetts Institute of Technology — Cellulose nanocrystals (CNC) are naturally-derived nanostructures of growing importance for the production of composites of attractive mechanical properties. Their fabrication involves extrusion of CNC suspensions and gels in organic solvents, in the presence of additives such as polymers and curing agents. Here, we study the rheological behavior of composite polymer-CNC gels in dimethylformamide, which include additives for both UV and thermal crosslinking. Using rheometry coupled with in-situ infrared spectroscopy, we show that under external shear, CNC-polymer gels display progressive and irreversible failure of the hydrogen bond network that is responsible for their pronounced elastic properties. In the absence of cross-linking additives, polymer-CNC gels show an instantaneous but partial recovery of their viscoelasticity upon cessation of flow, whereas, the presence of additives allows the gels to recover over much longer timescale via van der Waals interactions. By exploring a broad range of shear history and CNC concentrations, we construct master curves for the temporal evolution of the viscoelastic properties of the polymer–CNC gels, illustrating the universality of the observed dynamics with respect to gel composition and flow conditions.

*Procter & Gamble Company
8:48AM A15.00003: Observing phase separation in colloid-polymer mixtures with a custom light-sheet rheoscope*  JING WANG (Presenter), RYAN J. MCGORTY, Univ of San Diego — We study liquid-liquid phase separation (LLPS) with a colloid-polymer system subjected to shear. Our colloid-polymer mixture consists of temperature-responsive PNIPAM microgel particles and polymers acting as a depletant. This mixture separates into two phases: a colloid-poor, or “gas” phase, and a colloid-rich, or “liquid” phase. We observe the process of phase separation using a custom-built light-sheet microscope, which allows for simultaneously acquiring optically-sectioned images of our sample and shearing the sample in a Couette geometry. We measure the size and shape of elongated liquid domains that have been deformed due to flow as a function of shear rate. The temperature-responsive feature of our colloidal particles allows us to further explore the kinetics of phase separation under shear flow. We hope our study of phase separation under shear can provide fundamental insights into hydrodynamics and thermodynamics and provide novel strategies for structuring soft materials.

*American Chemical Society Petroleum Research Fund (#57326-UNI10) and a Research Corporation Cottrell Scholar award

9:00AM A15.00004: Understanding and predicting flow instabilities in self-assembled polymers  PATRICK J MCCAULEY, SATISH KUMAR, MICHELLE CALABRESE (Presenter), University of Minnesota — Shear banding flow instabilities are common in wormlike micelles (WLMs). Despite reported shear banding in polymer WLMs (pWLMs), current research has focused on surfactant WLMs (sWLMs) or linear polymers. Shear banding in linear polymers is typically transient, unstable, or an artifact of slip, fracture, or geometry; conversely, sWLMs dynamically rearrange and break, enabling steady state shear banding. As breakage in pWLMs is limited, the shear banding characteristics likely fall between these limiting cases, though this behavior remains largely unexplored. Here, we use nonlinear rheology and small angle neutron scattering (SANS) to systematically evaluate pWLM shear banding in commercial triblock poloxamers, where the molecular weight, block length, and block ratios are well-controlled. Poloxamer characteristics and micelle features identified via linear rheology and SANS are then used to develop guidelines to predict shear banding a priori, where important parameters include micelle dimensions, solvent penetration, and entanglement degree, among others. Understanding the fundamental role of poloxamer subunit and self-assembled structure provides insight into shear banding mechanisms absent significant breakage, which can be widely used to predict instability formation.
9:12AM A15.00005: Depletion Layer Dynamics of Polyelectrolyte Solutions under Poiseuille Flow*  
JOHN KING (Presenter), SEONG JUN PARK, ANISHA SHAKYA, Center for Soft and Living Matter, 
Institute for Basic Science — The flow of complex fluids over solid surfaces remains an outstanding 
problem in fluid mechanics that is relevant for fields ranging from lubrication to nanofluidics. 
Direct experimental access to depletion layer dimension and composition has been prohibited 
due to the inherently short length scales associated with depletion layers. Here, we develop 
a novel adaptation of super-resolution microscopy based on stimulated emission depletion (STED) 
to directly measure depletion layer composition in real-space with 10s of nanometer resolution. 
The composition and dimension of depletion layers formed in solutions of high molecular weight 
poly(styrene sulfonate) at solid, non-adsorbing walls is measured at equilibrium and under 
Poiseuille flow. Using this novel approach, we 1) confirm concentration profile consistent with 
entropically driven depletion at the interface, 2) observe depletion layer narrowing at low to 
intermediate shear rates, and 3) observe depletion layer composition that approaches pure 
solvent at unexpectedly low shear rates.

*Korean Institute for Basic Science, Project Code IBS-R020-D1

9:24AM A15.00006: Honey bees transport pollen particles of varying shape and size by 
forming them into a permanent granule*  
MARGUERITE MATHERNE (Presenter), SUARJ 
PUVVADA, Georgia Institute of Technology, BEN GUY, Corning, Inc., WILSON POON, The University of 
Edinburgh, DAVID HU, Georgia Institute of Technology — Honey bees (Apis mellifera) carry pollen back 
to their hive by mixing it with nectar and forming it into a pellet, which they carry in the corbcula, 
or pollen basket, on their hind legs. We show that most pellets do not fluidize when subjected to 
vibrations or when brought into contact with a similar suspension of lower volume fraction, 
suggesting that it is a permanent granule. We also explore the behavior of pellets made from 
different size and shaped pollen particles. The bees form the pellet by squeezing small amounts 
of pollen and nectar through the joint of their hind leg, called the pollen press, into the pollen 
basket. Through many repetitions, they form a pellet of up to 2 mm$^3$. This method allows honey 
bees to collect pollen of various sizes and shapes.

*This material is based upon work supported by the National Science Foundation Graduate 
Research Fellowship under Grant No. DGE-1650044.

9:36AM A15.00007: Shear thickening of dense suspensions in the limit of jamming*  
YASAMAN MADRAKI (Presenter), Department of Mechanical Engineering, Ohio University, GUILLAUME 
OVARLEZ, University of Bordeaux, SARAH HORMOZI, Department of Mechanical Engineering, Ohio 
University — In shear thickening suspensions, viscosity appears to increase when the shear rate 
increases. In this work, we focus on the shear thickening phenomenon that occurs in the limit of 
jamming. We have designed a model non-Brownian suspension to experimentally study this 
phenomenon. We have developed a series of comprehensive rheometry tests to provide a 
physical understanding of the problem. We provide a closure for shear stresses in the limit of 
jamming and we test this closure by studying boundary driven flows of dense suspensions.

*NSF Grant No. CBET-1554044-CAREER
9:48AM A15.00008: A new dimensionless number governing dethickening in orthogonally perturbed shear thickened suspensions*  MEERA RAMASWAMY (Presenter), ITAY GRINIASTY, ABHISHEK SHETTY, JAMES PATARASP SETHNA, ITAI COHEN, Cornell University — When concentrated colloidal suspensions are under stress, their viscosity can increase by over an order of magnitude. Previous work has shown that this shear thickened viscosity can be tuned by applying fast oscillatory perturbations orthogonal to the primary shear flows in the system. In this talk, I show that dethickening in the regime where the primary shear flow has fully thickened the suspension, is governed by a single dimensionless parameter – the ratio of the orthogonal shear rate amplitude to that of the primary shear rate. In contrast, a second parameter is required to describe the data in the primary shear flow regime where the suspension is thickening. Understanding these parameters will enable better strategies to tune the properties of shear thickening suspensions for applications ranging from 3D printing to the processing of cement.

*This work is supported by NSF CBET award numbers 1804963 and 1509308.

10:00AM A15.00009: Connecting microscale stresses to macromolecular motion in entangled ring-linear DNA blends*  KARTHIK REDDY PEDDIREDDY (Presenter), MEGAN C LEE, JONATHAN GARAMELLA, RYAN J. MCGORTY, RAE M ROBERTSON-ANDERSON, Univ of San Diego — Ring polymers, as well as mixtures of ring and linear polymers, are ubiquitous in nature yet still poorly understood. Due to the lack of free ends in ring polymers, the motion and dynamics of entangled rings is complex and distinctly different than their linear chain counterparts. As such, the dynamics of entangled blends of ring and linear polymers remain a topic of fervent debate. Here, we use DNA - which occurs naturally in rings and linear forms - as a model system to investigate highly entangled ring-linear blends. To elucidate the dynamics of these blends, we demonstrate a novel technique that combines optical tweezers microrheology with fluorescence imaging and differential dynamic microscopy. This technique enables us to directly image single polymers while performing active microrheology. As a result, we show that it is possible to unambiguously connect the stresses induced by both linear and nonlinear strains to the corresponding macromolecular deformations and network rearrangement in ring-linear polymer blends.

*Air Force Office of Scientific Research (AFOSR- FA9550-17-1-0249) and National Science Foundation (NSF-CBET-1603925)
8:00AM A16.00001: Coherent control of a hybrid superconducting circuit made with van der Waals heterostructures* [Invited] WILLIAM OLIVER (Presenter), Massachusetts Institute of Technology MIT —
In this talk, we present the demonstration of a superconducting transmon qubit realized using a graphene-based weak-link junction. The graphene is encapsulated by hexagonal Boron Nitride (hBN), forming a van der Waals heterostructure. Applying a voltage to a backgate in proximity to the weak-link junction enables voltage tunability of the qubit frequency. We present the coherent control of this qubit, and discuss the promise and the challenges if building superconducting qubits with such van der Waals heterostructures.

*ARO grant no. W911NF-17-S-0001, NSF QII-TAQS, ASDR&E via Lincoln Laboratory under AF contract FA8721-05-C-0002.

8:36AM A16.00002: On-chip microwave spectroscopy of Andreev and Majorana bound states in semiconductor nanowires* [Invited] ATTILA GERESDI (Presenter), Department of Microtechnology and Nanoscience, Chalmers University of Technology — The microscopic picture of the Josephson effect, describing the flow of supercurrent through a weak link, is based on the formation of Andreev bound states, localized at the weak link. In narrow gap semiconductors, such as InAs and InSb, the interplay of induced superconductivity with spin-orbit coupling and magnetic field can give rise to 4π-periodic Andreev levels, signifying the presence of topological superconductivity and Majorana end modes.

In this talk, I will summarize our efforts to understand the Andreev level spectra in proximitized semiconductor nanowires by exploiting the AC Josephson effect and using on-chip microwave detection techniques based on superconducting tunnel junctions. With this technique, we investigate gate-tunable Andreev bound states in ballistic semiconductor nanowire channels [1] and the microwave spectrum of nanowire-based Cooper-pair transistors [2]. I will also showcase our measurements of the 4π-periodic Josephson effect above a threshold magnetic field [3], which is consistent with the topological phase transition and the emergence of Majorana bound states.


*We acknowledge the Netherlands Organization for Scientific Research (NWO) and the European Union’s Horizon 2020 research and innovation programme.
9:12AM A16.00003: Magnetic-field-compatible hybrid superconducting circuits* [Invited]
ANGELA KOU (Presenter), Microsoft Corp, MARTA PITA-VIDAL, ARNO BARGEBOS, Delft University of Technology, CHUNG-KAI YANG, DAVID J. VAN WOERKOM, WOLFGANG PFAFF, Microsoft Corp, NADIA HAIDER, Netherlands Organization for Applied Scientific Research, PETER KROGSTRUP, LEO P KOUWENHOVEN, GIJS DE LANGE, Microsoft Corp — Hybrid circuits that incorporate semiconducting elements into superconducting circuits have recently provided new insights into mesoscopic superconductivity. Extending the capabilities of hybrid circuits to work in large magnetic fields would enable the investigation and control of spin-polarized and topological phenomena. In this talk, I will discuss our work building a magnetic-field-compatible nanowire-based fluxonium. We in-situ tune the Josephson energy of the fluxonium with an electrostatic gate and demonstrate operation of the fluxonium in magnetic fields up to 1T. We use the fluxonium spectrum to map out the dependence of the Josephson energy of the junction on magnetic field and also use it to observe the $\phi_0$-junction effect. Our work demonstrates the utility of hybrid superconducting circuits for exploring mesoscopic physics and paves the way for manipulating Majorana zero modes in these circuits.

*This research was co-funded by the allowance for Topconsortia for Knowledge and Innovation (TKI's) from the Dutch Ministry of Economic Affairs and the Microsoft Quantum initiative.

9:48AM A16.00004: A ballistic graphene superconducting microwave circuit* [Invited] GARY STEELE (Presenter), FELIX SCHMIDT, MARK JENKINS, Quantum Nanoscience, Delft University of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Tsukuba — Josephson junctions are a fundamental component of microwave quantum circuits, such as tunable cavities, qubits and parametric amplifiers. Recently developed encapsulated graphene JJs, with supercurrents extending over micron distance scales, have exciting potential applications as a new building block for quantum circuits. In this talk, I will present our demonstration of a superconducting microwave circuit based on a ballistic graphene Josephson junction. We directly observe a gate-tunable Josephson inductance through the resonance frequency of the device and, using a detailed RF model, we extract this inductance quantitatively. We also observe the microwave losses of the device, and translate this into sub-gap resistances of the junction at $\mu$eV energy scales, not accessible in DC measurements. The microwave performance we observe here suggests that graphene Josephson junctions are a feasible platform for implementing coherent quantum circuits.

*This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement nr. 785219 – GrapheneCore2
10:24AM A16.00005: Coherent Semiconductor-Based Superconducting Quantum Circuits*

[Invited] KARL PETERSSON (Presenter), Microsoft Quantum Lab Copenhagen and Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — The recent development of semiconductors with epitaxial superconducting Al contacts offers new approaches to realizing coherent superconducting quantum devices. In particular, we have demonstrated superconducting transmon qubits with Josephson junctions based on hybrid superconductor-semiconductor nanowire materials [1-2]. These gate tunable transmons (gatemons) have the potential advantage that they can be readily controlled through local electrostatic gating of the junction element. I will discuss progress in improving coherence times and scalability of gatemon qubits. I will also discuss how these hybrid circuits might be used to realize novel qubits that are intrinsically protected against sources of decoherence.


*Research is supported by Microsoft and the Danish National Research Foundation.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A17 DQI: Quantum Machine Learning I

8:00AM A17.00001: Challenges and opportunities for hybrid quantum-classical machine learning and optimization

[Invited] MASOUD MOHSENI (Presenter), Google Inc. — We present an overview of our progress on quantum-inspired and quantum-assisted algorithms for optimization and machine learning at Quantum AI Lab at Google. We develop an end-to-end quantum-inspired discrete optimization platform that uses an interplay of local and non-local thermal updates to sample from inaccessible low-energy states of spin-glass systems that encode high-quality solutions of certain hard combinatorial optimization. We introduce several new techniques for quantum circuit learning on Noisy Intermediate-Scale Quantum (NISQ) processors. We show how we can learn to learn on parameterized quantum circuits via classical recurrent neural networks. We apply this metalearning approach for efficient initialization of Quantum Approximate Optimization Algorithm for Sherrington-Kirkpatrick model and variational Quantum Eigensolver for the Hubbard model. Moreover, we introduce two different layerwise learning for quantum neural networks. In the first method we train layer-wise POVMs to perform variational quantum unsampling of unknown noisy quantum operations. In the second method, we are training varying subsets of the quantum circuit's parameters iteratively while increasing the circuit depth to have sufficient representation of classical or quantum data. In our approach the problem of vanishing gradients or barren plateaus of training landscape can be avoided to a large extent. We provide several applications of such quantum models for characterization of NISQ devices and classification of quantum data.
**8:36AM A17.00002: Variational Quantum Unsampling on an Photonic Quantum Processor**

JACQUES CAROLAN (Presenter), Massachusetts Institute of Technology MIT, MASoud MOHSEni, Google Quantum AI Laboratory, JONATHAN P OLSON, Zapata Computing Inc., MIHIKA PRABHU, CHANGCHEN CHEN, DARIUS BUNANDAR, Massachusetts Institute of Technology MIT, MURPHY YUEZHEN NIu, Google Quantum AI Laboratory, NICHOLAS C HARRIS, Lightmatter, FRANCO N. C. WONG, Massachusetts Institute of Technology MIT, MICHAEL HOCHBERG, Elenion Technologies, SETH LLOYD, DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — Quantum algorithms for Noisy Intermediate-Scale Quantum (NISQ) processors have emerged as promising routes towards demonstrating practical advantage over classical machines. In these systems samples are typically drawn from probability distributions which — under plausible complexity-theoretic conjectures — cannot be efficiently generated classically. Rather than first define a physical system and then determine computational features of the output state, we ask the converse question: given direct access to the quantum state, what features of the generating system can we efficiently learn? Here, we introduce the Variational Quantum Unsampling (VQU) protocol, a nonlinear quantum neural network approach for verification and inference of near-term quantum circuits outputs. We experimentally demonstrate this protocol on a quantum photonic processor. Alongside quantum verification, our protocol has broad applications; including optimal quantum measurement and tomography, quantum sensing and imaging, and ansatz validation.

*This work was supported by the AFOSR MURI for Optimal Measurements for Scalable Quantum Technologies (FA9550-14-1-0052) and by the AFOSR program FA9550-16-1-0391, supervised by Gernot Pomrenke. J.C. is supported by EU H2020 Marie Sklodowska-Curie grant number 751016.

**8:48AM A17.00003: Quantum Hamiltonian-Based Models and the Variational Quantum Thermalizer Algorithm**

GUILLAUME VERDON (Presenter), JACOB MARKS, SASHA NANDA, STEFAN LEICHENAUER, JACK HIDARY, Quantum, X - The Moonshot Factory — We introduce a new class of generative quantum-neural-network-based models called Quantum Hamiltonian-Based Models (QHBMs). In doing so, we establish a paradigmatic approach for quantum-probabilistic hybrid variational learning, where we efficiently decompose the tasks of learning classical and quantum correlations in a way which maximizes the utility of both classical and quantum processors. In addition, we introduce the Variational Quantum Thermalizer (VQT) for generating the thermal state of a given Hamiltonian and target temperature, a task for which QHBMs are naturally well-suited. The VQT can be seen as a generalization of the Variational Quantum Eigensolver (VQE) to thermal states: we show that the VQT converges to the VQE in the zero temperature limit. We provide numerical results demonstrating the efficacy of these techniques in illustrative examples. We use QHBMs and the VQT on Heisenberg spin systems, we apply QHBMs to learn entanglement Hamiltonians and compression codes in simulated free Bosonic systems, and finally we use the VQT to prepare thermal Fermionic Gaussian states for quantum simulation.
9:00AM A17.00004: Variational Fast Forwarding for Quantum Simulation Beyond the Coherence Time*  
ANDREW SORNBORGER (Presenter), Los Alamos National Laboratory, CRISTINA CIRSTOIU, Computer Science, Oxford University, ZOE HOLMES, Controlled Quantum Dynamics Theory Group, Imperial College, JOSEPH IOSUE, QC Ware, LUKASZ CINCIO, PATRICK COLES, Los Alamos National Laboratory — Trotterization-based, iterative approaches to quantum simulation are restricted to simulation times less than the coherence time of the quantum computer, which limits their utility in the near term. Here, we present a hybrid quantum-classical algorithm, called Variational Fast Forwarding (VFF), for decreasing the quantum circuit depth of quantum simulations. VFF seeks an approximate diagonalization of a short-time simulation to enable longer-time simulations using a constant number of gates. Our error analysis provides two results: (1) the simulation error of VFF scales at worst linearly in the fast-forwarded simulation time, and (2) our cost function's operational meaning as an upper bound on average-case simulation error provides a natural termination condition for VFF. We implement VFF for the Hubbard, Ising, and Heisenberg models on a simulator. Finally, we implement VFF on Rigetti's quantum computer to show simulation beyond the coherence time. See full paper at: https://arxiv.org/abs/1910.04292


9:12AM A17.00005: Stochastic Gradient Descent for Hybrid Quantum-Classical Optimization*  
FREDERIK WILDE (Presenter), RYAN SWEKE, JOHANNES JAKOB MEYER, Freie Universität Berlin, MARIA SCHULD, University of KwaZulu-Natal, PAUL K. FÄHRMANN, Freie Universität Berlin, BARTHÉLÉMY MEYNARD-PIGANEAU, Ecole Polytechnique, JENS EISERT, Freie Universität Berlin — Gradient-based methods for hybrid quantum-classical optimization typically rely on expectation values with respect to the outcome of parameterized quantum circuits. In this work, we investigate the fact that the estimation of these quantities on quantum hardware leads to a form of stochastic gradient descent. In many relevant cases estimating expectation values with \( k \) measurements results in optimization algorithms whose convergence properties can be rigorously understood, for any value of \( k \geq 1 \). Moreover, in many settings the required gradients can be expressed as linear combinations of expectation values and we show that in these cases \( k \)-shot expectation value estimation can be combined with sampling over terms of the linear combination, to obtain doubly stochastic gradient descent. For all algorithms we prove convergence guarantees. Additionally, we explore numerically these methods on benchmark VQE, QAOA and quantum-enhanced machine learning tasks and show that treating the stochastic settings as hyper-parameters allows for significantly fewer circuit executions.

*Frederik Wilde acknowledges funding from the DFG under Germany’s Excellence Strategy MATH+: The Berlin Mathematics Research Center, EXC-2046/1 project ID: 390685689.
9:24 AM A17.00006: Robust and efficient algorithms for high-dimensional black-box quantum optimization* ZHAOQI LENG (Presenter), Physics, Princeton University, PRANAV MUNDADA, Electrical Engineering, Princeton University, SAEED GHADIMI, Operations Research and Financial Engineering, Princeton University, ANDREW HOUCK, Electrical Engineering, Princeton University — Hybrid quantum-classical optimization using near-term quantum technology is an emerging direction for exploring quantum advantage in high-dimensional systems. However, precise characterization of all experimental parameters is often impractical and challenging. A viable approach is to use algorithms that rely only on black-box inference rather than analytical gradients. Here, we combine randomized perturbation gradient estimation with adaptive momentum gradient updates to create the AdamSPSA and AdamRSGF algorithms. We prove the asymptotic convergence of our algorithms in a convex setting, and we benchmark them against other gradient-based optimization algorithms on non-convex optimal control tasks. Our results show that these new algorithms accelerate the convergence rate, decrease the variance of loss trajectories, and efficiently tune up high-fidelity (above 99.9%) Hann-window single-qubit gates from trivial initial conditions with twenty variables.

Leng et al. arXiv:1910.03591

*This work was supported by IARPA

9:36 AM A17.00007: A Hybrid Quantum-Classical Algorithm for Training Quantum Boltzmann Machines CHRISTA ZOUFAL (Presenter), IBM Research - Zurich, AURÉLIEN LUCCHI, ETH Zurich, STEFAN WOERNER, IBM Research - Zurich — A Boltzmann Machine is a Machine Learning algorithm based on a measure from statistical mechanics, i.e. the Boltzmann distribution. The respective concepts can also be used with quantum computers which leads to Quantum Boltzmann Machines. These have the potential to outperform classical algorithms in a variety of learning problems and to enable classically intractable tasks, such as discriminative learning with quantum data and generative modeling of classically inaccessible structures. Several implementations have been suggested, but they all face practical difficulties. Firstly, it is often challenging to generate the quantum Gibbs state representing the Boltzmann distribution. Secondly, the training performance is usually impaired as the problem formulation requires that the system must be trained with an upper bound instead of the actual loss function. In this work, we use variational quantum Gibbs state preparation to enable gate-based Quantum Boltzmann Machines which can be trained with the true loss function. Moreover, the algorithm relies on a hybrid quantum-classical optimization algorithm and is, thus, compatible with near-term quantum computers. The applicability of this approach is demonstrated on illustrative examples.
9:48AM A17.00008: Quantum classifier with tailored quantum kernel*  KYUNGDEOCK PARK
(Presenter), KAIST, CARSTEN BLANK, Data Cybernetics, JUNE-KOO(KEVIN) RHEE, KAIST, FRANCESCO PETRUCCIONE, University of KwaZulu-Natal — Kernel methods have broad applications in machine learning. Recently, a link between quantum computing and kernel theory has been formally established, opening up opportunities for quantum enhancements in various machine learning methods. We present a distance-based quantum binary classifier whose kernel is based on the quantum state fidelity between training and test data. The quantum kernel can be tailored systematically with a quantum circuit to assign an exponent to the kernel and assign weights to training data. Our classifier calculates the weighted power sum of fidelities of quantum data in parallel via a swap-test circuit and two single-qubit measurements, requiring only a constant number of repetitions regardless of the number of data. Furthermore, our classifier is equivalent to measuring the expectation value of a Helstrom operator, from which the optimal quantum state discrimination can be derived. We demonstrate the proof-of-principle via classical simulations with a realistic noise model and experiments using an IBM quantum computer.

*This research is funded by the NRF of Korea (2019R1I1A1A01050161 and 2018K1A3A1A09078001), Ministry of Science and ICT, Korea (IITP-2019-2018-0-01402), and South African Research Chair Initiative of the Dept. of Sci. & Tech. and NRF.

10:00AM A17.00009: Machine learning with solid-state NMR using quantum kernel*  TAKERU KUSUMOTO (Presenter), KOSUKE MITARAI, MAKOTO NEGORO, KEISUKE FUJII, MASAHIRO KITAGAWA, Osaka Univ — We employ so-called quantum kernel estimation to exploit complex quantum dynamics of solid-state NMR for machine learning. Kernel method is a popular branch in machine learning algorithms where only the inner products among feature vectors each representing an input datum are required to construct a prediction model. We propose to map an input to a feature space by input-dependent Hamiltonian evolution, and the kernel is estimated by the interference of the evolution. Simple machine learning tasks, namely one-dimensional fitting tasks and two-dimensional classification tasks, are performed as demonstrations. The performance of the trained model tends to increase with the longer evolution time, or equivalently, with a larger number of spins involved in the dynamics. This work can be regarded as one of the baselines for this emerging field.

*TK, KM, MN, and MK are supported by JST CREST JPMJCR1672. KM thanks the METI and IPA for their support through the MITOU Target program. KM is also supported by JSPS KAKENHI No. 19J10978. KF is supported by KAKENHI No.16H02211, JST PRESTO JPMJPR1668, JST ERATO JPMJER1601, and JST CREST JPMJCR1673. MN is supported by JST PRESTO JPMJPR1666. This work is supported by MEXT Quantum Leap Flagship Program (MEXT Q-LEAP) Grant Number JPMXS0118067394.
**10:12AM A17.00010: Hybrid quantum-classical algorithms for generative models**

TENG BIAN (Presenter), SABRE KAIS, Department of Physics, Department of Chemistry, and the Birck Nanotechnology Center, Purdue Univ — Quantum machine learning is a field that combines machine learning techniques and quantum computation together. It has the potential of enjoying impressive data analysis power while improving the time efficiency greatly. We propose a new hybrid quantum-classical circuit design for one major problem from machine learning aspect: generative models. We will discuss different ways to construct generative models using quantum algorithms. We will also apply this new design in example datasets and compare the complexity and the results. This work might help to find hidden patterns behind data and offer applications for near-term quantum devices.

*This material is based upon work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Award Number DE-SC0019215.*

**10:24AM A17.00011: Quantum-tailored machine-learning architectures**

ELIE GENOIS (Presenter), AGUSTIN DI PAOLO, ALEXANDRE BLAIS, JONATHAN GROSS, Institut quantique and Département de Physique, Université de Sherbrooke — Future quantum technologies are expected to be fundamentally challenging to characterize and calibrate. For this reason, a heuristic will most likely be required for this task, and machine learning provides an attractive framework for developing such a heuristic. To this end, we introduce a machine-learning architecture for inferring the dynamics of a quantum device from time-series measurement data. Our architecture is recurrent in nature and leverages quantum-mechanical structure in its design to interpret measurement data from complex quantum devices more efficiently. We investigate how the architectural structure influences the way we learn from data generated by quantum experiments and address applications of our techniques to the calibration and characterization of superconducting quantum devices.

*This work was undertaken thanks in part to funding from NSERC and the Canada First Research Excellence Fund.*
10:36AM A17.00012: Scalable Quantum State Tomography with Attention Network*  
PETER CHA (Presenter), Cornell University, JUAN CARRASQUILLA, Vector Institute for Artificial Intelligence, PAUL GINSPARG, EUN-AH KIM, Cornell University — The problem of many-body wavefunction reconstruction, which suffers from exponential scaling in system size as well as noisy state preparation and measurement, remains a major obstacle to the study of intermediate-scale quantum systems. Recent works found success by recasting the problem of reconstruction to learning the probability distribution of quantum state measurement vectors, a natural task for generative neural network models. Networks based on the attention mechanism, designed to learn long-range correlations in natural language sentences, appear especially well-suited to the task of learning highly entangled wavefunctions. In this work, we demonstrate that an attention mechanism-based generative network, based on the model proposed in "Attention is all you need" by Vishwani et al (2017), can outperform previous neural network based approaches to quantum state tomography. Specifically, in addition to working with state-of-the-art system sizes, the attention mechanism is able to accommodate noise by directly reconstructing the density matrix of mixed states. This work represents an important step forward in the applicability of machine learning to the study of noisy intermediate-scale quantum systems.

*This work was supported by NSF grant 1934714

10:48AM A17.00013: Implementing perceptron models with qubits*  
ROELAND WIERSEMA (Presenter), HILBERT JOHAN KAPPEN, Radboud Univ Nijmegen — We propose a method for learning a quantum probabilistic model of a perceptron. By considering a cross entropy between two density matrices we can learn a model that takes noisy output labels into account while learning. Although some work has been done that aims to utilize the curious properties of quantum systems to build a quantum perceptron, these proposals rely on the ad hoc introduction of a classical cost function for the optimization procedure. We demonstrate the usage of a quantum probabilistic model by considering a quantum equivalent of the classical log-likelihood, which allows for both a quantum model and training procedure. We show that this allows us to better capture noisyness in data compared to a classical perceptron. By considering entangled qubits we can learn nonlinear separation boundaries, such as XOR.

*This research was funded in part by ONR Grant N00014-17-1-256

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A18 FED: Challenges and Best Practices for Preparing Future Physics Teachers  
205 - Monica Plisch, American Physical Society - Tag(s): Careers, Education, Invited, Undergrad Friendly
8:00AM A18.00001: Addressing the Critical Physics Teacher Shortage Through Advocacy
[Invited]  BRIAN PYPER (Presenter), Brigham Young University - Idaho — There is a documented critical shortage of qualified physics teachers in the US today. Data from several sources are confirming this need. Some well-intentioned regulatory demands are exacerbating the problem, but have solutions that you can help with by knowing what they are and wisely advocating for improved policies and processes.

8:36AM A18.00002: Preparing Physics Teachers by Building Bridges Between High Schools and Colleges* [Invited]  THOMAS NOVIELLO (Presenter), Worcester Polytechnic Institute — Physics Education Research has made substantial advancements towards understanding how to offer best practices to ensure equity amongst all learners. However, this has not translated into an increased graduation rate of physics teachers within the United States. PhysTEC aims to address this crisis through granting the funds for universities to hire a Teacher-in-Residence. In this position, the Teacher-in-Residence has a goal of promoting the field of teaching and preparing prospective teachers through direct experience and fieldwork. At Worcester Polytechnic Institute (WPI), a bridge is being built between the university and local high schools through various pathways. One of these pathways is the creation of a science fair course, which is structured project-based learning. A partnership between WPI and Leominster High School affords WPI students the opportunity to engage in curriculum development, and for the high school students to become familiar with research-based approaches to problem solving. Aspirant teachers will not only become familiar with how to engage students throughout a lesson, but will also understand how to apply the elements of backward design to create effective curriculum. It is believed that this will create thoughtful and engaged physics teachers.

*PhysTEC

9:12AM A18.00003: Getting the Facts Out About the STEM Teaching Profession* [Invited]  WENDY ADAMS (Presenter), Physics, Colorado School of Mines — The Get the Facts Out (GFO) project is a joint effort between four national societies and the Colorado School of Mines to change the conversation around grade 7-12 physics, chemistry, and math teaching careers. We have developed a toolkit of recruitment materials which are designed to be customizable and adaptable to the local situation. To develop these materials and better understand best practices around recruiting math and science teachers, GFO has a rigorous research arm. Our research includes the study of both student, faculty, and the general public’s perceptions of the teaching profession including development of instruments to measure these. We also have embarked on a study to identify emotionally engaging ways to share facts about the profession. Finally, to measure the effectiveness of the project, we have an aggressive research design that includes annual collection of qualitative data from eighteen departments and quantitative data from another ~50 departments.

*This work is supported by NSF Grant No's 1821710 & 1821462.
9:48AM A18.00004: Departmental support for future physics teachers: Creating community, nurturing identity* [Invited] ELEANOR W CLOSE (Presenter), HUNTER G CLOSE, JESSICA CONN, DAVID DONNELLY, Texas State University — The physics department at Texas State University has recently experienced a dramatic increase in pre-service physics teachers. We attribute this primarily to students’ experiences in our Physics Learning Assistant (LA) program and to the financial and mentoring support available through our NSF Noyce teacher scholarship program. Our LA program serves all sections of the calculus-based introductory physics sequence, and has a particular focus on supporting LAs’ sense of belonging. LA Program structures are informed by the theory of Communities of Practice. The majority of our majors now serve as LAs for at least one semester. Those who pursue K-12 teacher certification are eligible for Noyce scholarships of $10-15K. Noyce Scholars receive mentoring and professional development through monthly Saturday STEM Seminars, which also serve as a catalyst for community among the Scholars. Together, these programs positively impact students’ identity as physics learners and teachers, and their recruitment into teaching careers.

*This work has been supported in part by NSF grants DUE-1557405, DUE-1557276, DUE-1431578, and PHY-0808790 (PhysTEC).

10:24AM A18.00005: A Research-Based Rubric for Driving Improvement in Physics Teacher Preparation.* [Invited] STEPHANIE CHASTEEN (Presenter), University of Colorado, Boulder, RACHEL E SCHERR, University of Washington Bothell, MONICA J PLISCH, American Physical Society — Given the insufficient number of well-qualified future physics teachers, physics programs often seek guidance for how to address this national need. But, as the saying goes, “if you can’t measure it, you can’t improve it.” Measurement tools can provide useful guidance, both by defining excellence and providing a means to measure progress towards excellence. This talk describes the development of such a measurement tool – the Physics Teacher Education Program Analysis (PTEPA) Rubric. The rubric defines levels of success in several areas that are important for physics teacher education, such as strength of program leadership, or the content of licensure courses, based on observed practices at 8 “thriving” U.S. physics teacher education programs. Initial findings suggest that thriving programs are strong in multiple areas (especially institutional commitment, leadership, and collaboration among partners in education and physics), and that several areas of strength align with those indicated by the existing physics teacher education literature. However, thriving programs are not necessarily strong in all areas, instead reflecting local conditions at the institutional and state level. The rubric and its’ associated supporting materials are intended to shed light on critical practices in physics teacher education, supporting research and hypothesis testing. The rubric is also intended to help program leaders in using a process of continuous improvement to strengthen local programs. We will briefly describe development of the rubric, insights gained from it, and how physics programs can use it to drive improvements.

*We acknowledge funding from NSF-0808790, NSF-1707990 and APS’s 21st Century Campaign for this work.

Monday, March 2, 2020 8:00 AM - 11:00 AM
8:00AM A19.00001: Kang-Kuen Ni Invited Talk [Invited] —

8:36AM A19.00002: Atom arrays of ultracold strontium: new tools for many-body physics and metrology* [Invited] ADAM KAUFMAN (Presenter), Physics, JILA/CU/NIST — The development of microscopic detection of ensembles of neutral atoms has transformed our ability to study complex many-body systems. Techniques like quantum gas microscopy and optical tweezer arrays grant a unique single-particle-resolved perspective on solid-state analogs and idealized quantum spin models, as well as detection capabilities of quantities like entanglement. In this talk, I will describe our group’s progress towards developing these tools for a new atomic species, strontium. In doing so, we establish new prospects enabled by the rich internal degrees-of-freedom associated with alkaline-earth atoms. I will report on our recent results in which we apply our platform to optical atomic clocks, a new application of optical tweezer arrays which indicates a number of strengths for metrology. I will then describe our progress towards engineering entanglement on an optical clock transition, as well as new strategies to coherently control samples with 100s of atoms.

*ARO, AFOSR, NSF-PFC, NIST

9:12AM A19.00003: Rydberg mediated entanglement in a two-dimensional neutral atom qubit array* [Invited] MARK SAFFMAN (Presenter), Physics, University of Wisconsin - Madison — We demonstrate high fidelity two-qubit Rydberg blockade and entanglement in a two-dimensional qubit array. The qubit array is defined by a grid of blue detuned lines of light with 121 sites for trapping atomic qubits. Improved experimental methods have increased the observed Bell state fidelity to FBell = 0.86(2). Accounting for errors in state preparation and measurement (SPAM) and single qubit operations we infer that a Bell state created with the Rydberg mediated CZ gate has a fidelity of 0.89. Comparison with a detailed error model based on quantum process matrices indicates that finite atom temperature and laser noise are the dominant error sources contributing to the observed gate infidelity.

*We acknowledge support from NSF PHY-1720220, the ARL-CDQI, DOE award DE-SC0019465, and ColdQuanta, Inc. .
9:48AM A19.00004: Quantum Science with Ytterbium Rydberg Atoms in Optical Tweezer Arrays* [Invited]  ALEX BURGERS (Presenter), Princeton University — Engineering Rydberg-mediated interactions in arrays of neutral atom qubits is a leading platform for quantum computing and quantum simulation architectures. The advantages of this experimental platform are derived from the strong nature of Rydberg interactions coupled with highly controllable optical tweezer arrays. To date, most neutral atom array experiments utilize alkali atoms, however alkaline-earth-like atoms offer many advantages including extremely long coherence times for nuclear spins in the \( j = 0 \) electronic ground state and narrow optical transitions for use in efficient laser-cooling, metrology and precision measurement. Our experimental approach is to utilize laser-cooled neutral ytterbium (Yb) atoms trapped in optical tweezer arrays. We use the narrow intercombination line, \( ^1S_0 - ^3P_1 \), for cooling and imaging atoms in magic-wavelength (532 nm) optical tweezers and achieve very high atom detection fidelity [1]. An additional advantage of Yb is the ability to stably trap Rydberg states of the atom by leveraging the Yb\(^+\) ion core polarizability for trapping in the optical tweezer. Here we maintain trapping of the Rydberg atom at high \( n \) states thus extending the lifetime for interactions. The expanded interaction time has important implications for quantum computing and simulation with strongly interacting Rydberg atoms. These attributes make Yb atoms in optical tweezers an attractive platform for a wide variety of applications in quantum information science.


*ARO contract W911NF-18-1-0215 and the Sloan Foundation.

10:24AM A19.00005: Quantum Science with Tweezer Arrays [Invited] MANUEL ENDRES (Presenter), Caltech — Recently cold atoms in optical tweezer arrays have emerged as a versatile platform for quantum science experiments. I will review some of these developments, specifically, atom-by-atom assembly [1] as a fast and simple method to generate defect-free atomic arrays and Rydberg-based quantum simulation of spin models. While already reaching competitive results, these systems are still in their infancy and limitations in coherence, detection fidelity, and scalability remain. I will outline how we can improve on these issues and at the same time open new avenues in quantum metrology by using alkaline earth atoms, followed by an overview of recent results: 1) A record in imaging-fidelity for neutral atoms and demonstration of narrow-line cooling in tweezers [2,3]. 2) High-fidelity Rydberg excitation from a clock state, including a record in entanglement-fidelity for two neutral atoms [4]. 3) Demonstration of an optical clock with single-atom detection in tweezer arrays [5].

8:00AM A20.00001: Lessons from Designing Optogenetic Tools* [Invited] ANDREW WOOLLEY (Presenter), Chemistry, University of Toronto — In the course of trying to engineer proteins to have a particular function, unexpected behaviours sometimes arise. I will describe how following up on some odd behaviour observed while trying to engineer photoactive yellow protein as a light-controlled switch, led to interesting, perhaps, general new insights into the behavior of these remarkable molecules

*NSERC (Canada)

8:36AM A20.00002: Engineering and application of a biosensor with focused ligand specificity* DENNIS DELLA CORTE (Presenter), Brigham Young Univ - Provo — Microbial cell factories efficiently converting bio-based precursors to chemicals represent an attractive avenue to a more sustainable economy. Yet screening of genetically diverse strain libraries to identify the best-performing whole-cell biocatalysts is a low throughput endeavor. For this reason, transcriptional biosensors attracted attention as they allow screening of vast libraries in combination with fluorescence-activated cell sorting. However, a broad ligand specificity of many transcriptional regulators often prohibits the development of such ultra-high-throughput screens. We here solved the structure of the transcriptional regulator LysG of Corynebacterium glutamicum detecting all three basic amino acids. Semi-rational engineering of LysG using a FACS-based screening/counterscreening approach yielded a new biosensor bearing a regulator insensitive to l-lysine. Molecular dynamics simulations uncovered the underlying structure-function relationships of a crucial amino acid substitution. As proof of principle, we applied the new biosensor and isolated several l-histidine producing strains by FACS.

*This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program (grant agreement No 638718).
8:48AM A20.00003: Spontaneous Rupture and Entanglement of Human Neuronal Tau Protein Induced by Piconewton Compressive Force* SUSOVAN ROY CHOWDHURY (Presenter), H PETER LU, Bowling Green State University —
Mechanical force vector fluctuations in the living cells can have a significant impact on protein behavior and functions. We have observed abrupt and spontaneous tau protein ruptures under a compressive force ranging from \( \sim 5 \) to \( \sim 125 \) pN, at a biologically available force amplitude range in living cells, using a home-modified atomic force microscopy single-molecule manipulation. The rupture behavior is dependent on the physiological level of the presence of ions, such as K\(^+\) and Mg\(^{2+}\). We observed rupture events in the presence of K\(^+\) but not in the presence of Mg\(^{2+}\) ions. We have also explored the entangled protein state formed following the events of the multiple and simultaneous protein ruptures under crowding. Crowded proteins simultaneously rupture and then spontaneously refold to an entangled folding state, different from either folded or unfolded states of the tau protein, which can be a plausible pathway for the tau protein aggregation that is related to several neurodegenerative diseases, such as the Alzheimer's and Parkinson's Diseases.

*We acknowledge the support of this work from the Ohio Eminent Scholar Endowment fund.

9:00AM A20.00004: Allosteric communications via substrate and linker between domains modulate protein function SUSANTA SARKAR (Presenter), Colorado School of Mines — The relation between structure and dynamics of biomolecules is important for their functions. Intra-domain dynamics occurring at pico- to milli-second timescales have been shown to correlate with activity. However, the correlation of allosteric communications between domains with biomolecular function is poorly understood. Here we show that inter-domain dynamics of matrix metalloprotease-1 (MMP1) on collagen fibrils are correlated with activity. Using single-molecule FRET, we identified the functionally relevant conformations where the two MMP1 domains are far apart, which were significantly absent for inactive MMP1 and could be modulated by inhibitor and enhancer of activity. All-atom and coarse-grained simulations reproduced the experimental features and revealed that dynamics are similar at pico- and milli-second timescales and substrate-dependent. Functional conformations are accompanied by larger catalytic pocket openings, which are increased by the communications mediated by collagen even if the domain linker is absent. Inter-domain communications are likely important for multidomain proteins in general.
9:12AM A20.00005: Disordered Protein Folding and Solubility as a Determinant of Human Disease* [Invited] ZACHARY LEVINE (Presenter), Department of Pathology, Yale University — A longstanding principle in protein biophysics is that a protein’s sequence dictates its threedimensional fold, and that structure is inherently linked to function. However, nearly a third of the human proteome contains intrinsically disordered regions that lack a discernible tertiary structure. Many of these proteins, referred to as intrinsically disordered proteins (IDPs), adopt transient conformations in order to carry out a wide-variety of functions, challenging the classical structure-function paradigm. Dysregulation of IDPs can also lead to the pathological accumulation of proteinaceous plaques and fibrils, which are observed in over 22 degenerative diseases and even in many types of cancers. In this talk, I will summarize our efforts to leverage molecular models of IDPs that populate vast free energy landscapes, reconciling how disordered and often soluble protein intermediates contribute to human disease. I will also discuss how these observations can supplement experiments, where transient protein conformations are often extraordinarily difficult to extract.

*We acknowledge funding from the National Institutes of Health (R01AG057912-01) and XSEDE (MCB170142, MCB180088, MCB190047).

9:48AM A20.00006: Is the Protein Dynamical Transition Useful?* AKANSHA SHARMA (Presenter), DEEPU K GEORGE, ANDREA G MARKELZ, State Univ of NY - Buffalo — Terahertz Time Domain spectroscopy (THz TDS) has been used to characterize the protein dynamical transition [1, 2]. Typically the THz measurements are performed using solutions, however there is some question as to whether the freezing of the solution effects protein structure or dynamics. To address these questions we performed terahertz dynamical transition measurements in the 100-270 K range and between 0.15 – 2.00 THz on buffered solutions, dry glycerol solutions and minimally hydrated glycerol solutions. Buffer solution measurements using chicken egg white lysozyme and myoglobin protein with concentrations between 2 – 30 mM follow Beer’s law concentration dependence below 15 mM from which terahertz molar absorptivity of the hydrated protein can be extracted. For dry glycerol-protein solutions, the dynamical transition is absent, although it is present for 0.5 g water/g protein indicating that freezing of bulk water does not effect the measurements.


*This work is supported by NSF grants DBI 1556359 and MCB 1616529, DOE grant DE-SC0016317 and NIH STTR R41 GM125486.
10:00AM A20.00007: Anti-cancer drug containing apolipoprotein B refolding through first-order-like phase transition process*  CHIA HSIN CHENG (Presenter), WEI-PING CHANG, Department of Biological Science and Technology, National Chiao Tung University, Taiwan, PO YEN LIN, Division of Core Facilities Imaging, Institute of Cellular and Organismic Biology, Academia Sinica, Taiwan, YU CHUAN LIANG, Agricultural Biotechnology Research Center, Academia Sinica, Taiwan, CALEB G. CHEN, Department of Hematology-Oncology, Mackay Memorial Hospital, Taiwan 5Institute of Physics, Academia Sinica, Taiwan, CHIA-CHING CHANG, Department of Biological Science and Technology, National Chiao Tung University, Taiwan — First-order-like phase transition process is a promising approach for protein refolding into functional state. However, lipid binding protein, apolipoprotein B (apoB), reconstitution is challenging until our previous study. At the same time, the reconstituted apoB lipoparticle (rABL) may be an idea vehicle for drug delivery. In this study, we refolded apoB with anti-cancer drug from denatured state to functional state follow a first-order-like state transition model. By characterizing the reconstituted drug loaded rABL (drug@rABL) with circular dichroism (CD), dynamic light scattering (DLS), zeta potential and transmission electron microscope(TEM), we found drug@rABL is similar to rABL and native LDL. Moreover, cell viability assay indicated drug@rABL demonstrated highly anti-cancer efficacy in low concentration. Futhermore, the anti-cancer mechanism of the drug can be revealed, too.

*This study is supported in part by the Ministry of Science and Technology (MOST), Taiwan (ROC) MOST 107-2112-M-009-016-MY3

10:12AM A20.00008: Integrative structural biology: insights from photoactive yellow protein  YICHAO WU, Nanjing University, MASATO KUMAUCHI, Oklahoma State University-Stillwater, WENFEI LI, Nanjing University, AIHUA XIE, WOUTER HOFF (Presenter), Oklahoma State University-Stillwater — The integration of computational approaches with multiple different experimental techniques offers an exciting avenue to address open questions in protein science. We report such an integrative structural biology approach using a bacterial photoreceptor (photoactive yellow protein) as an accessible model system. A coarse-grained model of PYP in its initial pG state and its light-activate pB intermediate was calibrated based on a range of experimental techniques and was used to obtain mechanistic and molecular insights into the structure and energetics of the pB intermediate. Engineered disulfide bonds were used to limit specific molecular motions in PYP. This approach revealed that the pB state is highly glassy, with multiple substates in which the N-terminal region of PYP adopts quite distinct conformations, which in turn greatly alter the lifetime of the pB intermediate. These results reconcile apparent contradictions in published literature regarding the structure of pB, demonstrate that the N-terminal region undergoes Functionally Important Motions (FIMs) during the PYP photocycle, and explains the classic observation that the N-terminal region of PYP modulates pB lifetime.
10:24AM A20.00009: Decoupling between translation al and rotation al motions of water in the proximity of a protein molecule*  PAN TAN (Presenter), LIANG HONG, Shanghai Jiao Tong Univ — The interaction between water and bio macromolecules is of fundamental interest in biophysics and biochemistry. By performing neutron scattering on a perdeuterated protein at various hydration levels, we characterized the dynamics of water in each molecular layer surrounding the biomolecule. We found that the translation al motion of the interfacial water is slowed down more significantly by protein than its rotation, and the retardation effect extends to the second hydration layer for translation while being limited in the first layer for rotation. Molecular dynamics simulation revealed that the observed translation rotation decoupling in hydration water results from that the translation of water is more correlated over space and highly restrained by the spatial confinement on protein. More importantly, water molecules around the structurally most stable protein residues exhibit the most retarded translation while maintaining their rotational freedom. Restraining translation of water around these residues protect the protein stability while maintaining the rotational mobility renders local flexibility to the biomolecule.

*The authors acknowledge NSF China 11974239, 31630002

10:36AM A20.00010: Probing Temperature-Dependent Dynamics of Hemoglobin and Water Molecules in the Hydration Shells Using High Sensitivity Dielectric Spectroscopy*  LUAN C. DOAN (Presenter), ABHISHEK SINGH, CHENGYUAN WEN, SHENGFENG CHENG, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — Hemoglobin, an iron-containing protein in red blood cells, has diverse biological functions including oxygen/carbon-dioxide transport and storage. The functions and behaviors of hemoglobin proteins strongly depend on environmental conditions and temperatures. The complicated quaternary structure of hemoglobin and the hydrogen-bond network in aqueous environments make it a challenge of identifying the conformational dynamics. Employing high-sensitivity dielectric megahertz-to-terahertz frequency-domain spectroscopy, we have systematically examined the dynamics of hemoglobin and the water molecules in their hydration shells as a function of temperature at the molecular level. Combining experiments with molecular dynamics simulations, we have determined the conformational dynamics of hemoglobin and water in aqueous solutions. The results help us identify hemoglobin dynamics and hemoglobin-water interactions that determine the biochemical functions and reactivity of hemoglobin proteins.

*Supported by AFOSR (FA9550-18-1-0263) and National Science Foundation (CHE-1665157)
10:48AM A20.00011: Single Molecule Studies of DNA-Histone Interactions  SANTOSH GAIRE (Presenter), Physics, The Catholic University of America — Mechanically-induced unfolding of protein-compactified-DNA molecules is a powerful tool for studying protein-DNA interactions at the single-molecule level. We perform single molecule experiments using horizontal magnetic tweezers on histones complexed with tethered DNA under tension. Native or hyperacetylated histones purified from cultured cells were used. Our experiments allowed us to characterize the step-length distribution for nucleosomes reconstituted from native histones allowing for a comparison to data from hyperacetylated histones. Here we present preliminary data characterizing the mechanical properties of DNA molecules bound to native and post-translationally modified histones.

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A21 GERA: Energy Storage - Electrode Physics 302

8:00AM A21.00001: Anion charge dependent lithium ion diffusion in solids  ZHENMING XU (Presenter), HONG ZHU, Shanghai Jiao Tong Univ — Our recent studies of the chalcopyrite-structured sulfides and non-spinel-structured halides show that the lithium-ion migration energy barrier can be effectively reduced by comprehensively regulating the anion charge and lithium-ion coordination environments. For example, for lithium ion diffusion between two adjacent lithium-anion octahedrons through a tetrahedral transition state, the greater the anionic charge is, the lower the lithium ion diffusion energy barrier will be. While for lithium ion diffusion between two adjacent lithium-anion tetrahedrons through an octahedral transition state, the smaller the anion charge is, the lower the lithium ion diffusion barrier will be. This new understanding of comprehensively regulating the anion charge and lithium-ion coordination environments to enhance lithium ion transport can be applied for the design and optimization of new superionic conductors.
8:12AM A21.00002: Stable Ionic Conductive Layer on Si Nanoparticles inside Si/C Composite for High-Performance Lithium-Ion Battery Anode  YONG SU KIM (Presenter), Analytical Engineering Group, Samsung Advanced Institute of Technology, HEECHUL JUNG, Energy Laboratory, Samsung Advanced Institute of Technology, JUCHEOL PARK, Business Support Department, Gumi Electronics & Information Technology Research Institute, SEONG HEON KIM, Department of Physics, Myongji University — In this study, we developed a simple and effectual method to form the stable Li ionic conductive layers for Si-based LIB anode materials. (1) For the purpose of maintaining a Li ionic conductive solid electrolyte interphase (SEI) during operation, the protective oxide coating for Si/C composite is practical, which can be simply applied by mixing a poly(vinyl alcohol)-PO₄ with the Si/C composite. The in-depth analysis revealed that the oxide coating reduces the loss of high ionic conductive SEI (Li₂O), resulting in the formation of a stable SEI [1-2]. (2) In the manufacturing step, stable Li ionic conductive layer (Li₂SiO₃) can be successfully fabricated on the Si nanoparticles inside Si/C composite by simply mixing the Li₂O nanoparticles with coal tar pitch. From the electrochemical measurements applied to various cells, it was demonstrated that the Si/C composite with stable Li₂SiO₃ layers show a considerably high performance in stability [3]. The design of this study and analysis provides the direction to enhance the stability of Si-based anode materials at low cost for developing high performance LIB.


8:24AM A21.00003: Creating a Chevrel Hybrid Mo6S₈₋ₓSeₓ to Improve the Performance of Beyond Li-Ion Batteries  TAYLOR JURAN (Presenter), MANUEL SMEU, Binghamton University — Attempting to solve the energy crisis, we consider the use of beyond Li-ion batteries. We are especially interested in the use of Ca and Al metals, due to their abundance within Earth’s crust. Ca and Al are more cost-effective, and environmentally friendly than Li. Additionally, the increased valency increases the energy density. We consider the Chevrel phase (CP), Mo₆X₈ where X= S, Se, Te, as a cathode for Ca-ion batteries. The CP cathode has widely been studied as a cathode for multivalent ion batteries. Several studies have shown that changing the chalcogen X, impacts the potential and diffusion kinetics. Literature shows that the S-rich CP yields a high voltage, with sluggish ion mobility; compared to the Se-rich CP which exhibits a lower voltage and improved ion mobility. We evaluate several S/Se chalcogen concentrations, testing 256 unique configurations, to tune both the potential and diffusion kinetics. Density functional theory is used to investigate the electronic properties, stability, diffusion kinetics, and voltage properties of CaMo6S₈₋ₓSeₓ, where y = 0-8. We implement the SCAN functional, a meta-GGA for an improved level of theory.
**8:36AM A21.00004: An in situ Study of Solid Electrolyte Interface (SEI) Formation on Tungsten Thin Film Electrodes by Neutron Reflectometry with Contrast Variation**  
JOSEPH DURA (Presenter), ERIC D. RUS, National Institute of Standards and Technology — Solid-electrolyte interphase (SEI) formation in LiPF$_6$ in mixed DEC/EC electrolytes was studied in situ by neutron reflectometry (NR) with scattering length density (SLD) contrast variation of the solvent. Tungsten, a non-Li-intercalating material, was used as the working electrode to greatly improve sensitivity to the SEI vs earlier studies.\(^1\) A two-layer SEI was formed upon polarization to +0.25 V vs. Li/Li$^+$. Insensitivity of the inner SEI layer to solvent deuteration at this potential suggested limited incorporation of hydrogen atoms from the solvent molecules. Its low SLD indicated Li$_2$O could be a major constituent. The outer SEI layer SLD scaled with that of the solution, indicating it either had solution filled-porosity or incorporated hydrogen from the solvent, or both. Returning the electrode to +2.65 V removed lithium from both SEI layers, though the effect was more pronounced for the inner SEI layer. Potential cycling increased the solution-derived species content in the inner SEI and decreased the contrast between the outer and inner layers, possibly indicating intermixing of the layers.


*EDR thanks the National Research Council Postdoctoral Fellowship for support*

**8:48AM A21.00005: Aqueous Solutions at Graphitic Interfaces: Effects of Charge Transfer, Ion Hydration, and Confinement on Interfacial Structure and Capacitance**  
CHENG ZHAN (Presenter), MAIRA R CERON, STEVEN A HAWKS, Lawrence Livermore National Laboratory, MINORU OTANI, National Institute of Advanced Industrial Science and Technology (AIST), Japan, BRANDON WOOD, MICHAEL STADERMANN, PATRICK G CAMPBELL, TUAN ANH PHAM, Lawrence Livermore National Laboratory — Improved understanding of aqueous solutions at charged graphitic interfaces is critical for designing new carbon-based materials for energy storage. However, many mechanistic details remain unclear, including how interfacial structure and response are dictated by intrinsic properties of solvated ions under applied voltage. Here, we combine first-principles simulations with electrochemical measurements to investigate adsorption of several alkali-metal cations at the interface with charged graphene and within graphene slit-pores. We confirm that adsorption energy increases with ionic radius, while being highly dependent on pore size under confinement conditions. In addition, in contrast with conventional electrochemical models, we find that interfacial charge transfer contributes non-negligibly to this interaction and can be further enhanced by confinement. Overall, the measured interfacial capacitance trends result from a complex interplay between voltage, confinement, and specific ion effects—including ion hydration and degree of charge transfer.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
9:00AM A21.00006: Stone-Wales type defect induced performance enhancement in BC$_3$ monolayer for Lithium-ion battery anode applications  SIBY THOMAS (Presenter), MOHSEN ASLE ZAEEM, Department of Mechanical Engineering, Colorado School of Mines, Golden, CO-80401, United States, Colorado School of Mines — Based on first-principles density functional theory (DFT) simulations, we systematically explored the possibility of pristine and defective two-dimensional boron carbide (BC$_3$) monolayer for designing high-performance Li-ion battery (LIB) anodes. Our calculations show that the BC$_3$ monolayer possesses significant structural and electronic stability and also noticed that after adsorbing Li atom, the semiconducting characteristic of both pristine and defective BC$_3$ monolayer is transformed into a metallic state, becoming an electrical conductor, which provided enhanced conductivity for LIB application. Our results reveal the Li adsorption in these structures are exothermic and the Stone-Wales type defect filled BC$_3$ shows a higher theoretical specific capacity of 1287 mAhg$^{-1}$ for Li atoms compared to pristine BC$_3$ (1144 mAhg$^{-1}$) and conventional graphite anode (372 mAhg$^{-1}$). We also found that both the pristine and defect filled BC$_3$ possess fast Li mobility with a low diffusion barrier (~ 0.33 eV) as well as a low average open-circuit voltage (< 0.48 V). Because of these excellent properties, our work predicts that the experimentally synthesized BC$_3$ monolayer, especially the one with Stone-Wales defect can be a promising anode material for the development of future LIBs.

9:12AM A21.00007: Structures Properties of Li-S Redox Solid Products* KAH CHUN LAU (Presenter), Physics and Astronomy, California State University, Northridge, QING GUO, RAVINDRA PANDEY, Physics, Michigan Technological University — Among the candidates for high gravimetric energy storage beyond Li-ion battery technology, Lithium-Sulfur (Li-S) battery is considered one of the promising candidates owing to its high gravimetric capacity, and earth-abundant reactant materials (i.e. sulfur). However, despite these attractive attributes, successful commercialization of Li–S batteries is currently hindered by poor cycling performance and capacity retention that is primarily caused by our limited understanding of the Li-S redox products at the level of the nanoscale and atomistic scale. To help us to understand the related materials properties, the state-of-the-art atomistic simulation can be a timely solution. In this talk, I will share with you some of our recent theoretical studies in Li-S redox solid products (e.g. Li$_2$S$_2$, Li$_2$S$_3$) structures properties using first-principles calculations that focus on the fundamental structure-property (e.g. thermodynamic stability, vibrational, mechanical and electronic properties) prediction of these new Li-S solid compounds. The underlying materials properties related design rules and the implications to Li-S battery cycling performance will be discussed.

*CSUN Faculty start-up Fund
9:24AM A21.00008: Insights into the electrochemical behavior of layered oxides intercalated with Na or K  JONAS KAUFMAN (Presenter), University of California, Santa Barbara, MICHAEL TORIYAMA, Northwestern University, ANTON VAN DER VEN, University of California, Santa Barbara — Layered transition-metal oxides, like those used in Li-ion batteries, remain popular candidate electrode materials for the emerging, low-cost Na- and K-ion battery technologies. However, shuttling the larger Na/K ions into and out of these compounds leads to two effects less commonly seen with Li: phase transitions between different stackings of the oxide layers and strong ion-vacancy orderings. Both phenomena are often detrimental, as they can result in mechanical degradation and sluggish ionic transport. To understand this behavior, we have performed first-principles studies of the layered Na$_x$CoO$_2$ and K$_x$CoO$_2$ cathode materials using configurational cluster expansions trained on density functional theory energies. We obtain excellent agreement with the experimentally observed voltage profiles and phase transitions upon cycling. In both systems, we predict several families of stable hierarchical orderings made up of antiphase boundaries between similar ordered regions. We find that K stabilizes unusual distorted phases at high concentrations due to strong K-K repulsion. Our results have important implications for diffusion and may be extended to other layered intercalation compounds.

9:36AM A21.00009: Computational modelling studies on discharge of nanoporous spinel LiMn2O4*  PHUTI NGOEPE (Presenter), Materials Modelling Centre, University of Limpopo — Porosity plays an important role in the performance of Li-ion batteries. Simulated amorphisation recrystallisation methods [1], based on molecular dynamics methods, were used to generate nanoporous LixMn2O4 spinels of approximately 25000 atoms, with different pore sizes. The resulting structures were discharged by lithiation in the concentration range x=1 to 2, and were characterised from XRDs, microstructures and mechanical properties. Generally a transition from the cubic to tetragonal spinel was observed in the range of x=1.5 to 2. In particular, at x=1.75 a broadening of XRD peaks, multiple grain boundarys and a reduction in the yield stress were noted. A pore size that minimises such effects was identified together with associated heterostructures.


*We acknowledge the support of the South African Research Chair Initiative of the Department of Science and Technology, the National Research Foundation in Pretoria and the Centre for High Performance Computing in Cape Town.
9:48AM A21.00010: Influence of Structural Defects on the Electrochemical Properties of MnO$_2$ in Rechargeable Zn/MnO$_2$ Alkaline Batteries: An Ab Initio Study* NIRAJAN PAUDEL (Presenter), BIRENDRA ALE MAGAR, New Mexico State Univ, TIMOTHY N. LAMBERT, Department of Materials, Devices, and Energy Technologies, Sandia National Laboratories, IGOR VASILIEV, New Mexico State Univ — Electrical energy storage is essential for seamless integration of intermittent renewable energy sources into the power grid. Rechargeable alkaline Zn/MnO$_2$ batteries are attractive for large-scale electrical energy storage due to their high energy density, non-toxicity and low cost. The performance of MnO$_2$ electrodes in Zn/MnO$_2$ batteries can be enhanced by nanostructuring and by introducing defects into the crystal structure of MnO$_2$. However, the mechanism of this enhancement is not fully understood. We apply first-principles computational methods based on density functional theory to study the mechanism of hydrogen ion insertion into the crystal structures of pyrolusite ($\beta$), ramsdellite ($R$), and nsutite ($\gamma$) MnO$_2$ polymorphs containing oxygen and cation vacancies. Our calculations show that the presence of oxygen and cation vacancies significantly changes the binding energies of hydrogen ions inserted into the structures of MnO$_2$ polymorphs. The results of our study could explain the influence of structural defects on the electrochemical properties of MnO$_2$ in rechargeable Zn/MnO$_2$ batteries.

*This work was supported by the U.S. Department of Energy, Office of Electricity.

10:00AM A21.00011: Novel states in transition metal oxides: a view based on high-efficiency RIXS of battery electrodes* WANLI YANG (Presenter), Lawrence Berkeley National Laboratory — To meet today’s energy storage requirements for sustainable energy applications, battery electrodes based on transition-metal oxides have been pushed towards very high voltages to achieve a high-energy and high-capacity battery. Such an approach drives the system into a highly oxidized states, which fundamentally leads to stability issues of the battery device. On the other hand, this unconventional state provides a unique playground for studying atypical states in transition metal oxides.

In this presentation, we will discuss spectroscopic studies of battery electrodes, with the focus on ultra-high efficiency mapping of resonant inelastic X-ray scattering (mRIXS). We show that the high voltage operation could trigger redox activities of oxygen (oxygen redox) that could be detected reliably by mRIXS. The spectroscopic results provide striking evidences that oxygen redox, if constrained in the lattice and under control, is not necessarily a detrimental activity as conventionally believed. Understanding and improving energy storage devices are therefore in keen need of collaborating efforts in both materials and fundamental physics.

*BES of the US DOE contract DE-AC02-05CH11231
Energy Biosciences Institute through EBI-Shell program
10:12AM A21.00012: Computational modeling of two-dimensional materials for sustainable energy storage*  
DIBAKAR DATTA, VIDUSHI SHARMA (Presenter), New Jersey Inst of Tech — Two-dimensional materials (2DM) such as graphene, transition metal dichalcogenides (TMD), MXenes, and their heterostructures are among the most promising electrode candidates for radically advanced batteries. In this talk, two important computational aspects of 2DM-based batteries are addressed – (i) 2DM-based anode materials, and (ii) 2DM as van der Waals (vdW) slippery interface. The conventional anode materials have several problems, such as low gravimetric capacity and high volume expansion. We demonstrate that topologically modified 2DM can be utilized as high-capacity anode materials for Li-, Na-, and Ca-ion batteries with a capacity of 1675, 1450, and 2900 mAh/g. Moreover, by building heterostructures made by the stacking of different 2DMs, it is possible to combine the advantage and eliminate the disadvantages of the individual materials. The second part of the talk discusses the interface of anode and current-collector. To combat the issue of high-stress generations at anode-current collector interface during intercalation and deintercalation, we propose the usage of the graphene layer over the current collector as a vdW slippery interface. The computational results are in good agreement with the experimental findings.

*National Science Foundation, CMMI-1911900

10:24AM A21.00013: Crosslinkable Nitroxide Radical Polymer for Energy Storage Applications  
SHAOYANG WANG (Presenter), ALEXANDRA D EASLEY, FEI LI, JODIE LUTKENHAUS, Texas A&M University — Due to the amount of waste generated by lithium-ion batteries disposal, a more environmentally friendly option such as organic batteries is desired to fulfill the need of this large market. Redox-active radical polymers such as poly(2,2,6,6-tetramethylpiperidinyloxy-4-yl methacrylate) (PTMA) are popularly studied as electrode materials for organic batteries. However, linear PTMA may dissolve in the electrolyte and thus degrade the battery's capacity over time. Therefore, crosslinked PTMA is gaining interest as one solution to this challenge.

Here, we present a simple, post-synthetic route to crosslink PTMA while maintaining a relatively high discharge capacity. PTMA monomer is randomly copolymerized with glycidyl methacrylate (GMA). Upon thermal treatment or UV radiation, PTMA is immobilized in a network. The swelling ratio of the crosslinked electrode is calculated from the dry and swelled thickness measured by electrochemical quartz crystal microbalance with dissipation (EQCM-D). The electrochemical properties of the P(TMA-co-GMA) electrodes are obtained using cyclic voltammetry and galvanostatic cycling to evaluate whether crosslinking improves cell performance. Our general finding is that PTMA dissolution was prevented by this crosslinking approach.
10:36AM A21.00014: Highly Mesoporous Carbon Aerogel as Catalyst Support in Proton Exchange Membrane Fuel Cells  ERIC KIM (Presenter), Stuyvesant High School, KEVIN GU, Deerfield Academy, SUNIL SHARMA, STOYAN BLIZNAKOV, MIRIAM RAFAILOVICH, Stony Brook University — Carbon aerogel possesses unique structural and electrical properties, such as high mesopore volume, large specific surface area, and high electrical conductivity, which make it suitable for use as catalyst support in Proton Exchange Membrane Fuel Cell (PEMFC). In this study, we present a novel synthesis of highly mesoporous carbon aerogel via freeze-drying approach and investigate its application in the fuel cell. The structural effects of activation on carbon aerogel will also be discussed. The TEM and XRF, NLDFT and BJH analysis were carried out to observe the morphology and pore structure. Pt on carbon aerogel and activated carbon aerogel show efficient activity in both ORR and HOR reactions compared to Pt on Vulcan XC-72, with increases up to 721% and 194% in specific power density, respectively. The enhanced performance of carbon aerogel is attributed to its large specific surface area, high mesopore to micropore ratio, and even dispersion of catalyst particles. Accelerated stress tests show that carbon aerogel has comparable durability with Vulcan XC-72, while activated carbon aerogel is less durable than both materials. Thus, this mesoporous carbon aerogel provides an efficient, cost-reduced alternative to existing microporous carbon material as catalyst support in PEMFC.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A22 DBIO: Animal Behavior 303 - Gordon Berman, Emory University

8:00AM A22.00001: Uncovering the dynamical structure of behavioral repertoires*  ITAI PINKOVIEZKY, GORDON BERMAN (Presenter), Emory University — Animal behavior consists of an intricate hierarchy of dynamics, from brief muscle twitches to stereotyped behaviors to longer-lived states like hunger, aggression, and parenting. How does an animal bridge these timescales to create complex sequences of actions? The approach that most researchers take when studying sequences of behaviors tends to be probabilistic, observing how discrete states transition in a largely memoryless fashion. In this talk, we take a different approach, fitting dynamical models to long behavioral sequences from fruit flies and other species. We show that these models replicate many summary statistics of the underlying behavioral sequence data and that their fixed points have a geometry that mirrors the geometry of the animals' behavioral repertoires. In addition, we show that the long timescales generated by this model are best explained by a hierarchy of interacting dynamical subsystems that is comparable to the hierarchical structure of behavior. These results suggest a new framework for uncovering the hidden states that modulate the behaviors that an animal performs and predicting how physiology may be linked to behavior.

*HSFP (RGY0076/2018), NIMH (1R01MH115831-01), RCSA (25999)
8:12AM A22.00002: Collective bumblebee foraging in a controlled stochastic environment
DAVID HOFMANN (Presenter), AHMED HEMDAN ROMAN, Physics, Emory University, DONNA ROSA MCDERMOTT, BERRY J BROSI, Environmental Science, Emory University, ILYA M NEMENMAN, Physics, Emory University — We study bumblebees in a flight chamber with 10 artificial flowers to explore and accurately quantify foraging behavior. An RFID system is employed to identify the individual foragers and detect their presence in flowers as well as entry and exit of the hive. Flowers release rewards upon bee's visit with a predefined probability and are divided into two groups of separate reward probabilities and color. Furthermore, we impose a reward refractory period, that is a time span that a bee needs to stay away from a recently triggered flower before it is able to trigger it again.

In this study, an entire colony of tagged bees is kept in the foraging chamber for 4-6 days. We study 7 colonies with 40-70 bees each. We analyze and quantify the operant learning of the relation between flower color and reward probability: bees are able to identify the more rewarding flower type, effectively matching the reward probability ratios. However, the number of bees who are able to do so strongly depends on the length of the imposed refractory period. We conclude that a combined setting of refractory time and reward probability is too challenging for most bumblebees to learn in the given time span and thus leads to suboptimal foraging choices whereas they quickly learn to adapt to Bernoulli trials alone.

8:24AM A22.00003: A Low-Cost Modular Camera System for 3D Pose Estimation in the Field
SCOTT WOLF (Presenter), JULIEN AYROLES, JOSHUA SHAEVITZ, Princeton University — The individual behavior of animals determines the outcome of ecological interactions and drives group organization and community dynamics. Considerable attention has been given to understanding these types of interactions by way of automated tracking of individuals and bio-logging; however, these methods rarely investigate the behaviors performed by animals. Recent developments in deep learning for pose estimation provide a promising avenue for understanding individual behavior at resolutions previously not possible. However, systems for generating datasets appropriate for these methods in the field are lacking. To fill this gap, we developed a low-cost, modular camera platform to generate 3D imaging data compatible with contemporary pose estimation techniques. We use a connected network of solar-powered cameras that supports synchronous capture, triggering, and the integration of multisensory metadata. We initially generated datasets from three camera modules that allow for 3D pose estimation in a large outdoor area of over 600m² and demonstrate its use in an open field experiment at the Mpala Research Centre and Wildlife Foundation in Nanyuki, Kenya. Our system is designed to be modular and extensible, facilitating the use of many camera modules in very large open areas.
8:36AM A22.00004: Bridging time scales in *C. elegans* behavior through transfer operators*
ANTONIO COSTA (Presenter), Vrije Univ (Free Univ), DAVID JORDAN, Department of Genetics, University of Cambridge, GREG STEPHENS, Vrije Univ (Free Univ) — Animal behavior is modulated over multiple timescales: from fast control by neural activity to slower variation due to starvation or aging. Can we extract these hidden processes from the movement dynamics alone? We introduce a principled method to simultaneously reconstruct and partition the dynamical state-space, which we use to approximate the Perron-Frobenius operator. Our operator approximation is built to be maximally predictive and Markovian and its spectral decomposition provides a hierarchy of modes, which evolve over multiple time-scales. Applied to *C. elegans* locomotion, we find coherent structures which represent behavioral motifs, while the dynamics of the long-lived modes capture slower changes in behavioral “strategies”, e.g. the worm’s exploratory propensity. By subsuming the nonlinear dynamics into the process of partitioning and state space reconstruction, we obtain a model of the dynamics which is simple yet still able to faithfully reproduce the complexity of worm behavior from milliseconds to hours.

*Project funding was provided by OIST Graduate University and VU Amsterdam. AC is supported through a program grant from the Netherlands Organization for Scientific Research and DJ is supported by a Herchel Smith postdoctoral fellowship.

8:48AM A22.00005: Inferring behavioral homologies from dynamical models*
KATHERINE OVERMAN (Presenter), ITAI PINKOVIEZKY, GORDON BERMANN, Emory University — Linking the evolution of animal behavior to the genes underlying it has proven challenging, largely due to our inability to find representations of behavior that allow for inter-species comparisons. Animals exhibit variability in many different traits across species, but certain traits are relatively conserved. These traits are known as homologies or homologous structures, and quantitatively identifying these homologies in behavior could provide a new approach for understanding the evolution of behavior. Here, we measure the behavioral repertoires of six fruit fly species, finding both the frequency of behavioral performance, as well as their temporal dynamics. By fitting dynamical models to these transitions, we can reproduce the summary statistics of our dataset, including long timescale dynamics and hierarchical structure. We show that features of these models can be used to define such homologies, providing future avenues for exploring the genetic basis of behavioral evolution.

*RCSA (25999), HFSP (RGY0076/2018), NSF (1806833)
Long timescale dynamics in freely behaving rats

KANISHK JAIN (Presenter), Department of Physics, Emory University, Atlanta, GA, ELENA MENICHINI, TOMASO MUZZU, Institute of Behavioural Neuroscience, Department of Experimental Psychology, University College London, London, United Kingdom, JAKOB MACKE, Departments of Computational Neuroengineering and Electrical and Computer Engineering, Technical University of Munich, Munich, Germany, AMAN SALEEM, Institute of Behavioural Neuroscience, Department of Experimental Psychology, University College London, London, United Kingdom, GORDON BERMAN, Departments of Physics and Biology, Emory University, Atlanta, GA — Natural behavior is composed of rich postural dynamics that contain stereotyped movements performed by the animal. These behaviors span multiple timescales and are performed in a structured manner during spontaneous behavior. Thus, a quantitative understanding of behavioral dynamics is crucial to help unravel the latent physiological states driving behavior. Here, we extract postural information from videos of freely moving rats in an arena using markerless tracking tools. Using these postural time series’ we create a low-dimensional behavioral state space using unsupervised methods that characterizes stereotypic behavioral bouts. We find long, non-Markovian timescales of predictability across novel and familiar trials of light and dark conditions in the arena. These behavioral sequences are found to be arranged in hierarchical clusters, similar to previous results in fruit flies. These results support hierarchical organization of behavior as a general principle across species for generating long timescale dynamics.

Supported by HSFP RGY0076/2018.

Measuring and modeling the dynamics of the thermal memory of C. elegans

AHMED ROMAN (Presenter), Physics, Emory University, KONSTANTINE PALANSKI, ANTIBODY Healthcare Communications, ILYA M NEMENMAN, Physics, Emory University, WILLIAM RYU, Physics, University of Toronto — The roundworm C. elegans learns from its experiences. When placed on a thermal gradient, worms perform thermotaxis to or away from the conditioned temperature, depending on food abundance during the conditioning phase. To quantify this behavior, we developed a novel assay that tracks single worms—each experiencing a Spatio-temporal thermal gradient with thermal precision ±0.01C—in a small (2.8ul) droplets of buffer, arrayed on hydrophobic-printed microscope slides. CCD cameras monitor many worms simultaneously in many droplets, each droplet at 20C midpoint with a thermal gradient of 0.5C/cm. A worm’s thermal preference is summarized as a thermotaxis index, and the index dynamics are tracked at a high temporal resolution for many hours. Initially, worms reared at 15C and 25C exhibit cryophilic or thermophilic tendencies, respectively, and starvation during conditioning or in the droplet reverses these tendencies. This reversal is non-monotonic indicating multiple dynamic processes for learning that operate on different time scales. We build a predictive model with multiple time scales and utilize mutants to detangle the various learning processes. The model predicts the behavior under various conditions.

This work was supported by NIH grant 1T32HD071845 and NSF grant BCS-1822677.
Multi-animal pose tracking using deep neural networks*  
TALMO PEREIRA (Presenter), SHRUTHI RAVINDRANATH, NATHANIEL TABRIS, JUNYU LI, MALA MURTHY, Princeton Neuroscience Institute, Princeton University, JOSHUA SHAEVITZ, Physics, Princeton University — Dissecting behavior in freely moving animals at the fast timescales requires rich representations of their motor dynamics. Recently, we developed a method to automate the estimation of animal pose from videos using deep neural networks (Pereira et al., 2019). This method, termed LEAP, detects body part positions in single animal videos. Extending these techniques to a multi-animal context presents technical challenges, such as assigning body part positions to the correct animal. Here we present a new framework we term SLEAP (Social LEAP Estimates Animal Poses) that can explicitly model the relationship between body parts, enabling accurate multi-animal pose estimation. The framework implements multiple neural network meta-architectures which we empirically evaluate on tracking sub-tasks. We demonstrate the generalizability of this framework by applying this technique to videos of a variety of animals, including a high-resolution dataset of freely interacting fruit flies to construct a map of postural dynamics during courtship.

*This work was supported by the NSF, through the Center for the Physics of Biological Function (PHY-1734030), the GRFP (DGE-1148900), the NSF-IOS BRAIN Initiative EAGER (1451197); by the NIH, through the Targeted BRAIN Circuits Projects (R01 NS104899).

Phenotype to Function: Predicting drug mode of action from behavioural fingerprints  
ADAM MCDERMOTT-ROUSE, ELENI MINGA, ANDRE BROWN (Presenter), Imperial College London — Pesticides and anthelmintics (nematode-killing drugs) are discovered through phenotypic screens in target species. This means that their efficacy is often known early in the development pipeline, but their mode of action is not. Therefore, an important problem in developing new compounds to combat the rise of anthelmintic resistance is determining their mode of action. We record multiple worms from 96-well plates using a multi-camera imaging system and extract behavioural features from tracked animals to define a quantitative phenotype for each well in response to a library of ~80 drugs from 10 known mode of action classes. Because drug dose can have a strong effect on behavioural response, we record worms' response to a range of doses. We combine information across doses using multiple-instance learning to predict a compound's mode of action on unseen data.
Mammals are generalists, capable of flexibly deploying movements across a range of behavioral contexts. However, existing paradigms for studying the genesis of movement in the brain often probe only a narrow range of highly trained behaviors, leaving the neural mechanisms that support this flexibility unclear. To extend the range of behaviors and contexts that can be studied, we developed a new behavioral monitoring system, CAPTURE, that combines motion capture and deep learning to track the 3D movements of twenty points on a freely behaving rat’s trunk and appendages, continuously over week-long timescales. We combined CAPTURE with continuous neural recordings in the dorsolateral striatum, a brain region with a known, if debated, role in controlling diverse aspects of movement and behavior. Within individual behavioral states, striatal neurons displayed tuning to kinematic and behavioral variables. However across states, these tuning properties changed, in a manner that improved the within-state behavioral decodability. This suggests that context-specific coding may be a means to efficiently represent behavioral variables that are flexibly deployed across states, and that representational findings observed in tasks may fail to generalize.

*Vertex-HHWF, NINDS K99/R00 NIH, Simons

10:00AM A22.00011: Speed selection and sampling strategies for terrestrial trail tracking*
GAUTAM REDDY (Presenter), Harvard University, MASSIMO VERGASSOLA, University of California, San Diego, BORIS I SHRAIMAN, University of California, Santa Barbara — Terrestrial animals such as ants, mice and dogs use surface-borne odor trails to establish navigation routes or to find food and mates by following adsorbed chemical traces. Trail-tracking behavior is commonly observed, yet the strategies animals use to track trails are largely unknown. We examine generic features of trail-tracking by posing the problem as a search task of finding the trail after each loss of contact. We show that trail geometry imposes strong constraints on tracking speed; the maximal speed scales as the square-root of the typical radius of trail curvature with a strategy-dependent prefactor. By posing the problem in the reinforcement learning framework, we obtain optimal sampling strategies under various movement constraints and sensor configurations. An exactly solvable model in the Hamilton-Jacobi-Bellman framework recapitulates features of sampling strategies obtained via learning and quantifies the trade-off between movement cost, speed and sampling efficiency. Our work provides a general framework for trail tracking and testable hypotheses on the algorithms that animals use to follow trails.

*This research was supported in part by NSF Grant No. PHY-1748958, NIH Grant No. R25GM067110, and the Gordon and Betty Moore Foundation Grant No. 2919.01.
10:12AM A22.00012: Specialization of control strategies in terrestrial slithering snakes.*
PERRIN E SCHIEBEL (Presenter), Physics, Georgia Institute of Technology, BO LIN, Mathematics, Georgia Institute of Technology, ALEX M HUBBARD, BioE, Georgia Institute of Technology, LILLIAN CHEN, Biology, Georgia Institute of Technology, GREG BLEKHERMAN, Mathematics, Georgia Institute of Technology, DANIEL I GOLDMAN, Physics, Georgia Institute of Technology — Limbless locomotors like snakes use environmental heterogeneities for propulsion. We tested two snake species adapted to different habitats, the desert specialist *C. occipitalis* and the multi-terrain generalist *P. guttatus*, in a model terrestrial terrain—rigid arrays of posts on a low-friction whiteboard substrate. Principal component analysis (PCA) revealed the specialist maintained its stereotyped sand-swimming wave in the arrays, while results for the generalist were inconclusive, indicating either a periodic gait was higher dimensional, or the motion was aperiodic. Persistent homology, a mathematical technique which can identify cycles without reducing dimension, suggested the generalist used aperiodic kinematics. We hypothesized that the generalists instead controlled reaction forces and tested this using a simplified terrain, a single force-sensitive post on whiteboard. The generalist was more effective at using the post, maintaining longer contacts and more consistent force vectors. Our study suggests control specialization; the specialist targets beneficial sand swimming kinematics while the generalist controls for advantageous force generation in accord with early studies of generalist snakes in lattices [e.g. Gray 1955].

*Simons, NSF, DoD

10:24AM A22.00013: Proceed with caution: dynamics of novelty-directed risk assessment behavior in mice* YORIKO YAMAMURA (Presenter), JEFFERY R WICKENS, Okinawa Inst of Sci & Tech — Mice encountering a novel object initially display a distinctive set of behaviors that have been described as "risk assessment," including slow extensions of their snout toward the object followed by rapid retractions. These behaviors have also been observed in mouse models of anxiety, such as during elevated plus maze tasks, and are proposed to reflect a conflict between exploration and risk avoidance. However, a simple conflict does not explain the asymmetry in the speeds of approach and retreat: why do mice spend more time approaching the object than retreating from it, when spending less time near the object overall could reduce their exposure to risk? Analyzing the snout trajectories of mice exploring a novel object, we test the hypothesis that these behaviors reflect an internal evidence accumulation process, in which mice integrate a subjective "risk" while approaching and retreat when the cumulative "risk" crosses a threshold. We ask whether 1) a feed-forward model can predict retreat timings from preceding trajectories of approach, and 2) including feedback from risk to snout velocity explains the asymmetrical dynamics of "risk assessment".

*This work is supported in part by the Research Fellowship for Young Scientists (DC1) from Japan Society for the Promotion of Science.
10:36AM A22.00014: Transitions between stochastic and oscillatory active sensing in pulse-type electric fish  ALEXANDRE MELANSON (Presenter), Département de physique et d'astronomie, Université de Moncton, ANDRE LONGTIN, Department of Physics, University of Ottawa — Rather than wait passively for signals to be detected by their sensors, animals actively move in order to gather information from their environment. Furthermore, when sensing is performed by means of rhythmic movements, reafferent sensory streams are also rhythmic, which is advantageous for sensory processing. Here, we report on and characterize an hitherto unknown behavioural state of pulse-type weakly electric fish during which electrosensory acquisition becomes rhythmic and is coupled to low-frequency movement. The oscillatory nature of this sensory sampling strategy is in stark contrast to that exhibited during other behavioural states, which we show to be well-modelled by jump-diffusion stochastic processes.

To characterize the oscillatory dynamics of these rhythmic behavioural states, we identify and extract them from long-term observations of freely-moving fish. To achieve this, we apply a wavelet transform to the inter-pulse interval time series and use the resulting spectra as input for t-distributed Stochastic Neighbor Embedding. This creates a 2D clustered representation of the data from which we successfully classify different sensory acquisition strategies. This approach reveals that rhythmic sampling in fact occurs over a range of frequencies between 0.5 and 1 Hz.

10:48AM A22.00015: Steering and turning control of C. elegans  KELIMAR DIAZ (Presenter), BAXI CHONG, Georgia Tech, TIANYU WANG, Carnegie Mellon University, KATHLEEN BATES, JIMMY L DING, Georgia Tech, GUILLAUME SARTORETTI, Carnegie Mellon University, HANG LU, Georgia Tech, HOWIE CHOSET, Carnegie Mellon University, DANIEL I GOLDMAN, Georgia Tech — Elongate animals (e.g., snakes, nematodes) propagate waves of body curvature to generate propulsion in dissipative environments. In particular, the nematode worm C. elegans lives in environments (e.g., rotting fruit) where maneuverability is crucial to overcome heterogeneities and post-interaction deformations. To search for steering control principles in undulatory locomotion, we studied C. elegans traversing both agar and liquid buffer. These worms generate a time-dependent omega-like shape for reorientation to achieve body rotation of 150±26° on agar and 84±39° in liquid buffer. Principal component analysis (PCA) revealed the worms use four principal components during turning, superimposing two body traveling waves with two spatial frequencies. A geometric mechanics framework rationalized the observed turning dynamics by properly coupling the amplitude and the phase of the two body traveling waves. Theory predicted omega turns can achieve rotation of 153° on agar and 89° in liquid buffer, in agreement with worm experiments. These results and robophysical experiments implementing the behavior suggest that omega turns are a robust strategy for turning in diverse environments.

Monday, March 2, 2020 8:00 AM - 10:12 AM

Session A23 DBIO: Non-Linear Deformations in Biology 304 - Eva-Maria Collins, Swarthmore Coll - Tag(s): Focus
Mechanics and Elasticity of dynamic cellular monolayers - How *Volvox* embryos turn inside-out

[Invited] STEPHANIE HOEHN (Presenter), PIERRE A HAAS, RAYMOND E GOLDSTEIN, Applied Mathematics and Theoretical Physics, University of Cambridge — Living tissues are intelligent materials that can change their mechanical properties while they develop. In spite of extensive studies in multiple model organisms we are only just beginning to understand these dynamic properties and their role in tissue development. Although many tissues are known to exhibit visco-elastic properties, it is unclear which properties dominate three-dimensional shape changes of cellular monolayers, such as epithelia.

The embryonic *inversion* process in the micro-algal order Volvocales is uniquely suited for studies on epithelial morphogenesis. Volvocalean embryos consist of cup-shaped or spherical cellular monolayers which invert their curvature in order to expose their flagella. *Volvox globator* exhibits one of the most striking processes of cell sheet folding: Through inwards folding at the equator of the initially spherical cell sheet adopts a mushroom shape and eventually turns itself entirely inside-out through an anterior opening [1]. These global deformations are driven by several waves of active cell shape changes [2, 3]. A combination of advanced imaging and computational analyses is used to explore the role of tissue contractility during invagination. The associated internal stresses as well as the elastic properties of the dynamic cell sheet are determined through laser ablation experiments.


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A bilayer model of the non-linear elastodynamics of Hydra mouth opening*  TAPAN GOEL (Presenter), CASSIDY TRAN, University of California, San Diego, ELLEN ADAMS, Swarthmore College, PATRICK HENRY DIAMOND, University of California, San Diego, EVA-MARIA COLLINS, Swarthmore College — Mouth opening in *Hydra* involves extreme deformations, with radial cell strains of up to 30%. *Hydra* consists of two neuronally excitable, mechanically coupled epithelia-muscular cell layers, an outer ectoderm and an inner endoderm. The layers are coupled basally by a viscoelastic extracellular matrix, into which the cells extend contractile fibers (myonemes). In the head, ectodermal myonemes are arranged radially and endodermal myonemes in concentric rings. Experiments show that mouth opening proceeds through a series of radial ‘tugs’ – local myoneme contractions that must synchronize to produce a symmetric opening. We investigate if a bilayer model of viscoelastic sheets containing networks of radial and circular non-linear springs with Poisson distributed compressive forcing can capture mouth opening. Constraining the model using *in vivo* data, we test its ability to reproduce the time history of the mouth area during opening. We compare the kinematics generated by radially travelling contraction pulses with that for simultaneous contractions at all radii. Further, we explore the conditions required for space-time synchronization of ‘tugs’ into a quasi-symmetric opening and the dependence on the ratio of firing rate and the relaxation timescale of the viscoelastic sheet.

**RCSA**

Investigation of Rice Root Tip Circumnutation Functions in Heterogeneous Environments  ERIN MCCASKEY (Presenter), Georgia Inst of Tech, ISAIAH TAYLOR, KEVIN LEHNER, PHILIP N BENFEY, Duke University, DANIEL I GOLDMAN, Georgia Inst of Tech — Circumnutation is the pattern of oscillatory growth widespread among plants. Little is known about the function of circumnutation, particularly in root-heterogeneity interactions. Traits that allow for exploration may be advantageous, as roots can encounter heterogeneities in their environment that prevent productive growth. In this work we used a clear gel-based media to create a growth environment of two gel layers with varying stiffness, which can model soil horizons with varying compaction. A high-throughput automatic imaging system acquired images to visualize the root growth. Roots were grown in either a soft gel upper layer to a stiffer gel bottom layer, or the opposite. Our results show interesting differences in the ability of wild-type and non-circumnutating roots to penetrate the lower gel layer. These differences provide insights into the function of circumnutation.
Mechanics of behavior: Comprehensive search behavior encoded in cytoskeletal dynamics of single cell *Lacrymaria olor*  

ELIOTT FLAUM (Presenter), Program in Biophysics, Stanford University, DEEPAK KRISHNAMURTHY, Mechanical Engineering, Stanford University, SCOTT COYLE, Biochemistry, University of Wisconsin, MANU PRAKASH, Bioengineering, Stanford University — Complex animal behavior arises from interplay between actuators and sensors. Surprisingly, single eukaryotic cells such as protists are also capable of complex behavior, but how an algorithm such as search might be encoded in intrinsic dynamics of a single cell remains unknown. Here we elucidate the mechanics of search behavior in the predatory ciliate *Lacrymaria olor*, which has the ability to extend and contract its “neck” seven body lengths in a second while efficiently searching the space around it for prey in minutes. Our recent work establishes that *L. olor*’s search strategy is encoded in antagonistic active systems: subcellular structures that use surface cilia and the cortical cytoskeleton (Coyle et al, 2019). Here we reveal the underlying geometrical features of the cytoskeleton, and membrane and volume constraints, that together program extension and contraction dynamics of this active filament. Through force spectroscopy and membrane tension experiments in live cells, we reveal the role of this dynamic force landscape and how it shapes the search phase space. Our work combines theoretical active filament models with experimental data to unravel how active mechanics leads to emergent behavior in single cells.

*Howard Hughes Medical Institute, Chan Zuckerberg BioHub

Functional consequences of microscopic skin features on snake locomotion  

JENNIFER RIESER (Presenter), Georgia Inst of Tech, TAI-DE LI, CUNY, DANIEL I GOLDSMAN, Georgia Inst of Tech, JOSEPH MENDELSON, Zoo Atlanta — Interactions between limbless animals and their natural environments, which are essential for movement, are mediated solely through skin contact. We used atomic force microscopy to investigate how surface textures on shed skins vary across snakes and environments. While most snakes have microfibrils oriented longitudinally, a few distantly-related snake species have convergently lost these features in favor of a more isotropic structure. We hypothesize that these microstructures affect the frictional interaction with the substrate and we use resistive force theory to model the effects of frictional anisotropy on snake locomotion. For lateral undulation, we predict that an anisotropic frictional interaction in movement along the body is favored over transverse movement, improving performance (measured in distance traveled per cycle), and that larger anisotropies produce larger displacements. In sidewinding locomotion, however, we predict the opposite trend: decreased frictional anisotropy improves performance. These predictions are consistent with our AFM measurements of small-scale features on snake skins and suggest a functional benefit for the convergent loss of structure shared by sidewinding vipers.
Bioelectrical signaling via domain wall migration*  HAROLD MCNAMARA
(Presenter), RAJATH SALEGAME, ZIAD AL TANOURY, HAITAN XU, SHAHINOOR BEGUM, Harvard University, GLORIA ORTIZ, Chemistry, University of California Berkeley, OLIVIER POURQUIE, ADAM COHEN, Harvard University — Electrical signaling in biology is typically associated with action potentials, transient spikes in membrane voltage that return to baseline. The Hodgkin-Huxley equations of electrophysiology belong to a more general class of reaction-diffusion equations which could, in principle, support patterns of membrane voltage which are stable in time but structured in space. Here we show theoretically and experimentally that homogeneous or nearly homogeneous tissues can undergo spontaneous spatial symmetry breaking into domains with different resting potentials, separated by stable bioelectrical domain walls. Transitions from one resting potential to another can occur through long-range migration of these domain walls. We map bioelectrical domain wall motion using all-optical electrophysiology in an engineered cell line and in human iPSC-derived myoblasts. Bioelectrical domain wall migration may occur during embryonic development and during physiological signaling processes in polarized tissues. These results demonstrate a novel form of bioelectrical pattern formation and long-range signaling.

*This work was supported by the Allen Discovery Center at Tufts University, the Vannevar Bush Fellowship Foundation, the Howard Hughes Medical Institute, and the DOD NDSEG Fellowship.

Modeling the Mechanosensitivity of Crawling Cells*  JOHN MOLINA
(Presenter), RYOICHI YAMAMOTO, Chemical Engineering, Kyoto University — In this work, we study the ability of cells to probe and dynamically adapt to the mechanical properties of their surroundings, i.e., their mechanosensitivity. Experimentally, this can be studied by observing the reorientation of crawling cells over cyclically stretched substrates. To understand the observed cell-specific reorientation, we have introduced a computational model that couples the cyclically stretched substrate to the sub-cellular elements responsible for cell shape and motility: cell membrane, actin cytoskeleton, and focal adhesions. Depending on which sub-cellular process is being probed, and the type of coupling with the substrate, our simulations predict either no reorientation, a bi-stability in the parallel and perpendicular directions, or a complete reorientation. In particular, we show that an asymmetry in the adhesion dynamics during the loading and unloading phases of the stretching can be used to selectively align the cells. Our results provide further evidence for the importance of focal adhesion dynamics in determining the mechanosensitive response of cells.

*This work was supported by the Japan Society for the Promotion of Science (JSPS) Wakate B (17K17825) and KAKENHI (17H01083) grants, as well as the JSPS bilateral joint research projects.
9:48AM A23.00008: Geometry, Elasticity, Growth: The Connection Between Cowrie Growth Dynamics and Shell Form  
MICHAEL GABRIEL LEVY (Presenter), Biophysics Graduate Group, University of California, Berkeley, MICHAEL ROBERT DEWEESE, Physics and Neuroscience, University of California, Berkeley — Thin elastic sheets are currently a hot topic in soft matter physics. We propose a new model illustrating how the physics of bending and wrinkling sheets could underlie the geometry of Cowrie Seashells, offering both qualitative and quantitative insights. This work suggests generally new approaches to the mechanics underlying biological development. Despite both the cowry's import -- in monetary history and as a collector's item -- and a rich history of seashell modeling, we are the first to mechanistically consider cowrie form at all, let alone couple growth, elasticity, and form to recapitulate the shape of the central spiral, the thickening of the shell base, and the ridge-like teeth which form at the shell opening. By connecting elasticity with the biological processes of shell repair and body growth, we suggest that most aspects of form are emergent from the developmental decision to extend the mantle and extrude it over the shell instead of standard volumetric growth. In addition to our theoretical results, we test our model against both published and reported data, suggest previously unreported scaling relations, and demonstrate methods for extracting geometrical information from both three-dimensional scans and two dimensional images.

10:00AM A23.00009: Theoretical tool bridging cell polarities with development of robust morphologies*  
SILAS BOYE NISSEN (Presenter), STEVEN RØNHILD, ALA TRUSINA, KIM SNEPPEN, Niels Bohr Institute, University of Copenhagen — Despite continual renewal and damages, a multicellular organism is able to maintain its complex morphology. How is this stability compatible with the complexity and diversity of living forms? Looking for answers at protein level may be limiting as diverging protein sequences can result in similar morphologies. Inspired by the progressive role of apical-basal and planar cell polarity in development, we propose that stability, complexity, and diversity are emergent properties in populations of proliferating polarized cells. We support our hypothesis by a theoretical approach, developed to effectively capture both types of polar cell adhesions. When applied to specific cases of development – gastrulation and the origins of folds and tubes – our theoretical tool suggests experimentally testable predictions pointing to the strength of polar adhesion, restricted directions of cell polarities, and the rate of cell proliferation to be major determinants of morphological diversity and stability.

*This research has received funding from the Danish National Research Foundation (grant number: DNRF116) and the European Research Council under the European Union's Seventh Framework Programme (FP/2007 2013)/ERC Grant Agreement number 740704.

Monday, March 2, 2020 8:00 AM - 10:36 AM

Session A24 GSNP: GSNP Dissertation, Graduate Student, and Post-doctoral Speaker Awards  
401 - Daniel Lathrop, University of Maryland, College Park - Tag(s): Prize/Award
8:00AM A24.00001: Geometry and Topology in Motion* [Invited] SURAJ SHANKAR (Presenter), Physics, Harvard University — Topological and geometric ideas are now a mainstay of condensed matter physics, underlying much of our understanding of conventional materials in terms of defects and geometric frustration in ordered media, and protected edge states in topological insulators. In this talk, I will argue that such an approach successfully identifies the relevant physics in metamatials and active matter as well, even when traditional techniques fail. Novel topological phenomena acquire unique realizations in active fluids that pose a particular challenge to conventional statistical mechanics, by virtue of being far from equilibrium. I will present some recent results to illustrate this and show how spontaneous flow on complex substrates can mimic synthetic gauge fields allowing them to be fruitfully viewed using topological ideas and analogies with superconductors.

*This work was supported partly by NSF Grant DMR-1609208.

8:36AM A24.00002: Minimal Model for Intermittent Dynamics and "Turbulence" in Many-Body Systems* GURAM GOGIA (Presenter), Emory University — Complex systems are known to exhibit emergent properties that are missing on the constituent level. One particular property shared by many seemingly unrelated complex systems is intermittent switching between distinct dynamical states. Inspired by our previous experimental findings [1], here we present computational results for a particle-based system that exhibits intermittent switching between two distinct phases. The emergent dynamics are a direct consequence of coupling between structural disorder arising from particle polydispersity, inertial dynamics, and external forcing. Modelling the orthogonal mechanical energies of the system using ODEs with both noise and coupling terms based on kinetic arguments surprisingly results into predator-prey-like interactions. Such equations have recently been employed to describe intermittent turbulence in a pipe flow [2]. The only non-dimensional number derived from our equations resembles the Reynolds number in fluid flow and accurately predicts where intermittent dynamics are manifested.


*NSF, DMR-1455086
8:48AM A24.00003: Vortices, space-time braids and loops in the membrane of a living cell
JINGHUI LIU (Presenter), MIT — Topological defects determine the structure and function of matter over a wide range of scales. Many advances have been made in understanding and controlling the defect dynamics in active and passive non-equilibrium fluids. Yet, it remains unknown whether the statistical laws which govern the dynamics of defects in classical or quantum fluids extend to active living matter. Here, we show a defect-mediated turbulence underlies the complex wave propagation patterns of Rho-GTP signaling proteins on the membrane of starfish oocytes. Our experiments reveal that the phase-velocity field extracted from Rho-GTP concentration patterns exhibits vortical defect motions and annihilation dynamics reminiscent of those seen in quantum systems. Space-time analyses of defect trajectories reveal the existence of two characteristic types of braids: loops braided by multiple pairwise creation and annihilation events, and long-lived defect pairs that wiggle and form braid groups. Several key statistics and scaling laws of the defect dynamics, braids and loops can be captured by a generic complex Landau-Ginzburg continuum theory, suggesting space-time braids and loops are useful topological measures for unraveling information scrambling and transmission in dissipative living systems.

9:00AM A24.00004: A mechanical model for supervised learning* MENACHEM STERN (Presenter), University of Chicago — A broad goal of engineering is to make functional machines with specific, programmed input-output responses. When inputs are specified in advance and few in number, this goal is sought through rational design, changing the system elements to obtain desired responses. In the supervised learning framework of computer science, system parameters (synapses) are modified in response to observed examples of the correct input-output mapping (classification).

In this work, we apply the supervised learning framework to self-folding sheets, using a physically motivated learning rule. The trained sheet classifies labeled forces by folding into discrete folded states. These sheets succeed in classifying real-world data like Iris flowers, and also generalize, similar to other learning algorithms. As learning provides a straightforward framework to programming complex input-output relationships, we hope that implementing these ideas in engineering could usher in new classes of machines, that have so far eluded design.

*We acknowledge NSF-MRSEC 1420709 for funding and the University of Chicago Research Computing Center for computing resources.
9:12AM A24.00005: Ecological mechanisms of direct and indirect bacteriotherapies in generalized Lotka-Volterra systems* ERIC JONES (Presenter), University of California, Santa Barbara — Over the last two decades, an association between microbiome composition and some human diseases has been unambiguously established. The correlation between gut microbe composition and these diseases has prompted medical interest into bacteriotherapies, which seek to modify the gut microbiome composition in the hopes of treating the correlated disease. In this work we use generalized Lotka-Volterra (gLV) models to probe the ecological mechanisms through which these bacteriotherapies function. We first describe direct bacteriotherapies, which drive a microbiome to a target state via an instantaneous influx of foreign microbes (e.g. probiotics or fecal microbiota transplantation). Then, we present a novel control framework for indirect bacteriotherapies, which drive a microbiome to a target state by deliberately modifying its environment (e.g. diet, acidity, or nutrients). These dual control methods for gLV systems, interpreted as bacteriotherapies, could eventually inform personalized medicine for the microbiome.

*his work was supported by the David and Lucile Packard Foundation and the Institute for Collaborative Biotechnologies through contract no. W911NF-09-D-0001 from the U.S. Army Research Office.

9:24AM A24.00006: Noisy driven oscillators: Adaptive drives break the fluctuation-dissipation theorem JANAKI SHETH (Presenter), UCLA — The steady-state dynamics of complex nonlinear systems include limit cycles in which the dynamic variables trace a closed path in phase space. Biological systems are replete with examples of such driven oscillators in a diverse range of systems including circadian rhythms, neuronal central pattern generators, and the active mechanics of hearing. These biological systems are inherently noisy, and they are typically controlled by active feedback. We explore the fluctuations and response functions of intrinsically noisy limit-cycle oscillators starting with models of stereocilium dynamics in the inner ear. We show that one can obtain a generalized fluctuations-dissipation theorem (GFDT) for the system in a reference frame comoving with the mean dynamical state moving about the limit cycle. However, in the presence of adaptive drives where there is feedback so that the energy input driving the oscillator depends on the state of the system, as in the driven stereocilium, even these generalized fluctuation theorems fail. We further explore the essential role of these feedback mechanisms in breaking GFDTs in noisy driven systems using a combination of simple computational models, analytical calculations, and stereocilium dynamics data.

9:36AM A24.00007: Diffusive behavior in walking droplets AMINUR RAHMAN (Presenter), Texas Tech University — Fluid droplets walking on a vibrating fluid bath have been observed to display deterministic diffusion. We present an experimental and theoretical investigation of such droplets. In our experiments a droplet is placed into an annular region on a vibrating fluid bath. The droplet motion becomes increasingly diffusive as the bath vibration is intensified above the Faraday wave threshold. This is also captured in our hydrodynamic – kinematic models, which shows close agreement between theory and experiments. Since the model can be studied at a much higher spatio-temporal resolutions than experiments, we use the model to numerically investigate bifurcations and chaotic dynamics suggested by experiments. Finally, we briefly discuss the possibility of model reduction to mitigate computational costs.
9:48AM A24.00008: Exotic Soft Modes in 2D Mechanical Metamaterials Yield Powerful New Analytic Prediction Methods  MICHAEL CZAJKOWSKI (Presenter), Georgia Inst of Tech — Maximally Auxetic behavior, where Poisson’s ratio is the most negative, has been explored and identified in 2D perforated elastic sheets in which rigid square elements are connected at the corners by comparatively flexible elastic “hinges”. While these metamaterials are designed to emulate a uniform zero-energy motion of the free hinge material (mechanism), experiments have revealed qualitatively different non-uniform mechanical response. To understand this, we utilize a coarse graining approach, combined with highly detailed finite element simulations and experiments, to reveal that the perforated elastic sheet mechanics is controlled by a novel set of soft modes that correspond precisely to the well-studied planar Conformal Maps. We exploit this very convenient result to demonstrate new and highly accurate methods of analytically solving for linear and non-linear deformations of real materials. This includes a powerful holographic approach, in which large non-linear deformations may be predictably controlled by simple actuation at the boundary. Finally, we introduce a more general methodology for identifying and controlling the soft modes associated with a broad class of 2D mechanisms including the Miura and Eggbox origami patterns.

10:00AM A24.00009: Low frequency vibrations of deformable particles  DONG WANG (Presenter), Yale University — Disk packings at jamming onset exhibit an excess of low-frequency vibrational modes compared to the number predicted by Debye scaling. The excess number of modes, which controls the mechanical response of packings, decreases as the packings are compressed above jamming onset. In this work, we calculate the spectrum of vibrational modes from the eigenvalues of the dynamical matrix for truly deformable particles at jamming onset as a function of the shape parameter $A = \frac{p^2}{4\pi a}$, where $p$ is the perimeter and $a$ is the area of the particle. We show that there is an excess number of low frequency, collective modes in the density of vibrational modes for jammed packings of deformable particles over a wide range of particle shape both above and below the characteristic value $A \approx 1.15$ at which the system is confluent.
10:12AM A24.00010: Hydrodynamic memory and driven microparticle transport: hedging against fluctuating sources of energy*  
SEAN SEYLER (Presenter), Arizona State University — In a viscous fluid, the motion of an accelerating particle is retained as an imprint on the vorticity field, giving rise to the famous $t^{-3/2}$ decay of the velocity autocorrelation. For nonuniform particle motion at low Reynolds number, this hydrodynamic memory effect is captured by the Basset-Boussinesq-Oseen (BBO) equation, which can be derived from various physical perspectives, including (fluctuating) hydrodynamics and kinetic theory. Moreover, finite-temperature dynamics can be modeled by using fluctuation-dissipation to reincorporate (correlated) thermal noise, turning BBO into a generalized Langevin equation. In this work, we numerically solve the BBO equation to simulate driven microparticles and show that hydrodynamic memory generally reduces transport friction, particularly when driving forces do not vary smoothly. Remarkably, this enables coasting over uneven potentials that otherwise trap particles modeled by pure Stokes drag. Our results are germane to questions surrounding intracellular transport efficiency and, more generally, provide direct physical insight into the role of particle-fluid coupling in microparticle transport.

*Supported by ARO Grant No. W911NF-17-1-0162.

10:24AM A24.00011: Landscapes, nonlinearity, and optimality of ion transport in sub-nanoscale pores*  
SUBIN SAHU (Presenter), University of Maryland, College Park — Biological ion channels evolved to have high transport rates and high selectivity, among other functional characteristics. Synthetic nanoscale pores aim to mimic these properties for applications such as desalination and osmotic power generation.¹ In these systems, ion-ion and ion-channel interactions occur at sub-nanometer distances which entails large electrostatic and dehydration energies.² The balance of these energies determines selectivity and permeation rates. Importantly, the susceptibility of transport and selectivity to minute changes in distances—changes on the order of picometers—is enormous resulting in highly-nonlinear behavior. Biological systems can exploit this susceptibility via variations in protein structure that steer the local electrostatic and structural conditions. We demonstrate how this works in a synthetic selectivity filter and discuss how to probe this system, which will help to experimentally quantify optimal transport conditions and will give the foundation for a robust understanding of more complex biological pores.


*S.S. is supported by the Cooperative Research Agreement between UMD & NIST, Award# 70NANB14H209.
8:00AM A25.00001: Thermodynamics of Open Chemical Reaction Networks: Theory and Applications* [Invited] MASSIMILIANO ESPOSITO (Presenter), University of Luxembourg — After formulating a nonequilibrium thermodynamics for open chemical reaction networks, the theory will be applied to assess the thermodynamics performance of a dissipative self-assembly scheme. Power-efficiency and noise-dissipation trade-offs will be discussed.

References:

*Project NanoThermo ERC-2015-COG agreement no. 681456

8:36AM A25.00002: Universal thermodynamic bounds on nonequilibrium response with biochemical applications JEREMY OWEN (Presenter), Massachusetts Institute of Technology, TODD R GINGRICH, Northwestern University, JORDAN HOROWITZ, University of Michigan — Diverse physical systems are characterized by their response to small perturbations. Near thermodynamic equilibrium, the fluctuation-dissipation theorem provides a powerful theoretical and experimental tool to determine the nature of response by observing spontaneous equilibrium fluctuations. In this spirit, we derive a collection of equalities and inequalities valid arbitrarily far from equilibrium that constrain the response of nonequilibrium steady states in terms of the strength of nonequilibrium driving. Our work opens new avenues for characterizing nonequilibrium response. As illustrations, we show how our results rationalize the energetic requirements of common motifs in biochemical networks, with implications for the thermodynamics of information processing in biological systems.
8:48AM A25.00003: Trade-Offs between Error, Speed, Noise and Energy Dissipation in Biological Processes with Proofreading* JOEL MALLORY (Presenter), ANATOLY BORIS KOLOMEISKY, OLEG A IGOSHIN, Rice Univ —
Fundamental biological processes are highly accurate because the enzymes select the correct substrate out of a pool of chemically similar substrates by activating the so-called proofreading mechanisms. Enzymes with such proofreading ability have remarkably low error rates, e.g., on the order of ~10^{-8}-10^{-10}. While the importance of such proofreading mechanisms is widely accepted, it is still not well understood if enzymes are optimized with respect to certain characteristic properties. We theoretically investigate the trade-offs between four characteristic properties for optimization, i.e., error, speed, noise and energy dissipation, using a discrete-state stochastic framework with a first-passage analysis. Two crucial biological processes are analyzed: DNA replication by T7 DNA polymerase and tRNA selection during protein translation by *Escherichia Coli* ribosome. We developed a quantitative method to rank the importance of the properties. It was determined that the overall reaction speed is the main optimization criterion in both systems, and the energy dissipation comes in second. I will also discuss features of the free energy landscapes that affect the characteristic properties, e.g., error rate and energy dissipation.

*NSF PHY-1427654, Welch Grant C-1559, Welch Grant C-1995

9:00AM A25.00004: Observation of Stochastic Resonance in Transport of the DNA between Entropic Traps* SHAYAN LAME (Presenter), Brown University — We describe a nanofluidic system in which stochastic resonance (SR) could be observed in the motion of single DNA molecules. SR is a nonlinear dynamical phenomenon occurring in bistable systems where a weak signal that is below a sensor’s threshold for detection can be boosted and made detectable with addition of white noise. We fabricated nanofluidic devices with embedded pits that give rise to a bistable landscape for confined DNA molecules. An applied periodic pressure generates a weak periodic force on the DNA that represents a sub-threshold signal. We also developed a technique to control the noise inside a nano-fluidic device using electrokinetic forces. By computing the correlation between the periodic driving signal and the measured hoping of molecules between adjacent wells, the occurrence of SR can be revealed by a peak in that quantity as a function of noise level.

*NSF 1904511
9:12AM A25.00005: Over-damped Brownian dynamics in piecewise-defined energy landscapes*  
EE HOU YONG (Presenter), Nanyang Technological University, THOMAS GRAY, University of Cambridge — We study the over-damped Brownian dynamics of particles moving in piecewise-defined potential energy landscapes $U(x)$, where the height $Q$ of each section is obtained from the exponential distribution $p(Q) = a \beta \exp(-a \beta Q)$, where $\beta$ is the reciprocal thermal energy, and $a > 0$. The averaged effective diffusion coefficient $D_{\text{eff}}$ is introduced to characterise the diffusive motion: $\langle x^2 \rangle = 2 D_{\text{eff}} t$. A general expression for $D_{\text{eff}}$ in terms of $U(x)$ and $p(Q)$ is derived, and then applied to three types of energy landscape: flat sections, smooth maxima, and sharp maxima. All three cases display a transition between sub-diffusive and diffusive behaviour at $a = 1$, and a reduction to free diffusion as $a \to \infty$. The behaviour of $D_{\text{eff}}$ around the transition is investigated and found to depend heavily upon the shape of the maxima: energy landscapes made up of flat sections or smooth maxima display power-law behaviour, whilst for landscapes with sharp maxima, strongly divergent behaviour is observed. Two aspects of the sub-diffusive regime are studied: the growth of the mean squared displacement with time, and the distribution of mean first-passage times.

*Research for this project was made possible by a Start-Up Grant No. M4081583 from Nanyang Technological University, Singapore.

9:24AM A25.00006: An Energy-Accuracy Tradeoff for Nonequilibrium Receptors*  
SARAH HARVEY (Presenter), SUBHANEIL LAHIRI, SURYA GANGULI, Applied Physics, Stanford University — Living systems constantly collect and process information about their surroundings in order to respond to changes in the environment. In particular, single cells are capable of remarkably sensitive chemical concentration sensing using membrane-bound receptors. The physical limit of this sensing capability has been studied since the Berg-Purcell limit in 1977; however, thermodynamic constraints on the design of these sensors have remained theoretically elusive. Here we discuss two novel analytical bounds on signal estimation uncertainty in different limits of the observability of the sensing system. First, we consider estimating a signal based on a fully observable system trajectory, and second we study estimation based only on the coarse-grained occupation time of a subset of states. In the second, more biophysically plausible limit, we derive an energy-accuracy tradeoff for nonequilibrium processes using stochastic thermodynamics and large deviation theory. These lower bounds, supported by numerical simulations, reveal a theoretical limit on the estimation accuracy in terms of the energy consumption of the system and the observation time.

*We acknowledge support from the Stanford Graduate Fellowship, the NDSEG Fellowship, and the Simons Foundation.
9:36AM A25.00007: Functional Thermodynamics for Arbitrary Maxwellian Ratchets
ALEXANDRA JURGENS (Presenter), JAMES P CRUTCHFIELD, University of California, Davis —
Autonomous Maxwellian demons use structured environments as a resource to generate work
by randomizing ordered inputs and leveraging the increased Shannon entropy to transfer energy
from a thermal reservoir to a work reservoir. To date, determining their functional
thermodynamic operating regimes was restricted to information engines for which correlations
among information-bearing degrees of freedom can be calculated exactly via compact analytical
forms - a highly restricted set of engines. Although information engines may be represented as
finite hidden Markov chains, (i) no finite expression for their Shannon entropy rate exists, (ii) the
set of their predictive features is generically uncountably infinite, and (iii) their statistical
complexity diverges. To solve the problems these pose, we adapt recent results from dynamical
systems theory to efficiently and accurately calculate the entropy rates and the rate of statistical
complexity divergence of general hidden Markov chains. The results allow for precise
determination of the thermodynamic functionality of previously-studied Maxwellian demons, as
well as greatly expand the class of analyzable information engines.

9:48AM A25.00008: Trajectory-Class Fluctuation Theorems: Work Decomposition in
Metastable Information Processing  GREG WIMSATT (Presenter), University of California, Davis,
OLLI SAIRA, California Institute of Technology, ALEC BOYD, University of California, Davis, MATTHEW
MATHENY, California Institute of Technology, SIYUAN HAN, University of Kansas, MICHAEL ROUKES,
California Institute of Technology, JAMES P CRUTCHFIELD, University of California, Davis — Information
processing is physical. It requires particular and precise control of the underlying thermodynamic
system. While system parameters in a cyclic control protocol begin and end in the same
configuration, their intermediate paths determine the evolution of the system's informational
states.
The full work distribution generated during thermodynamic computing is surprisingly complex.
Even if simple, efficient, and accurate, the effective information processing may exhibit
thermodynamically-distinct temporal substages. For example, a bit erasure protocol similar to
that of Jun et. al. (2014 PRL 113.190601) consists of four substages, each linearly changing a
single protocol parameter. Combining substage decomposition with partitioning the microscopic
state-space into thermodynamically-metastable regions, a symbolic dynamics emerges that
naturally decomposes the work distribution into canonical components, with each substage
obeying its own fluctuation theorems. Practically, through describing macroscopic observables,
such as net work, these components can be used to diagnose the predominance of specific
microscopic informational failure and success modes. In this way, the trajectory-class fluctuation
theorems can be used to guide optimal protocol design.
10:00AM A25.00009: Quantifying scale-dependent irreversibility using persistent homology
LERON PEREZ (Presenter), KABIR HUSAIN, University of Chicago, SAMIR CHOWDHURY, Stanford University, BENJAMIN SCHWEINHART, Mathematics, Ohio State University, VAHE GALSTYAN, California Institute of Technology, PANKAJ MEHTA, Stanford University, SAMIR CHOWDHURY, Stanford University, BENJAMIN SCHWEINHART, Mathematics, Ohio State University, VAHE GALSTYAN, California Institute of Technology, PANKAJ MEHTA, Stanford University, SAMIR CHOWDHURY, Stanford University, BENJAMIN SCHWEINHART, Mathematics, Ohio State University, VAHE GALSTYAN, California Institute of Technology, PANKAJ MEHTA, Stanford University — Irreversibility is a measure of whether an observer can distinguish a process from its time reversed version. For physical systems, irreversibility is a fundamental property related to dissipation, breaking of detailed balance and non-equilibrium phenomena. But in any real non-equilibrium system, such as in vivo studies of oocytes or in vitro reconstituted actomyosin, irreversibility is associated with the specific timescales of the system's non-equilibrium dynamics: an observer can be fooled into believing a process is reversible if they watch on the wrong timescales. Here, we generalize persistence homology, a scale-dependent topological characterization method, to quantify irreversibility on different scales. While persistence homology is usually used to detect undirected loops, we define a similarity score inspired by statistical physics that captures information about directed circular fluxes. The resulting persistence barcode quantifies irreversibility on different timescales without any prior knowledge of what the relevant variables are.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A26 DBIO GSNP DSOFT DPOLY: Mechanics of Cells and Tissues Across Scales I 403 - Kandice Tanner, National Institutes of Health - NIH - Tag(s): Focus

8:00AM A26.00001: The nematic feedback between cancer cells and the extracellular matrix* [Invited] BO SUN (Presenter), Oregon State Univ — The reciprocal mechanical interaction between cancer cells and their extracellular matrix (ECM) has been shown to play important roles in tumor growth, survival and metastasis. Previous studies have primarily focused on the cell-induced stiffness change of the ECM, which is often characterized using bulk measurement. On the cellular scale, however, ECM produce anisotropic mechanical microenvironment to the cells. Cell generated forces align ECM fibers, and the aligned fiber direct cell polarization and migration through contact guidance. These interactions create a nematic feedback between cancer cells and their local ECM. In this talk I will first discuss quantitative measurements of cellular response to 3D contact guidance cues, which are inevitably noisy and spatially heterogeneous. I will then discuss how cell-induced ECM alignment can be controlled by tumor geometry, and regulate the long-term invasive potential of tumor cells. Together, these results highlight the rich biomechanical functions and powerful control mechanisms of the nematic feedback between cancer cells and extracellular matrix.

*The work is partially supported by the National Science Foundation grant PHY-1844627, as well as SciRIS-II grant from Oregon State University.
8:36AM A26.00002: Mechanical regulation of shape deformation by matrix viscoelasticity in breast tissues  
ALBERTO ELOSEGUI-ARTOLA, ANUPAM GUPTA (Presenter), L MAHADEVAN, DAVID MOONEY, Harvard University — The shape change is one of the phenomena seen in cancerous tissue and the physical mechanism that allows this process to take place has not been clear. The synthetic extracellular matrix (ECM) are typically almost purely elastic. In contrast, the physiological ECM in various tissues, such as brain, liver, adipose tissue, and coagulated bone marrow, etc. are all viscoelastic. Most of the studies to date have focussed largely on elastic properties of ECM. Recently synthetic ECMs have been developed which closely mimic the natural viscoelastic ECMs. In this study, we are further looking into the role of such mechanical properties in inducing the malignant phenotype in normal mammary epithelium MCF10A cell line. Based on these experimental findings we have proposed a mathematical model to capture the qualitative results. This is the first mechanical model to capture this epithelial to mesenchymal transition by changing the viscoelastic properties of ECM. We observe that as you increase the fluidic nature of the ECM, the cell proliferation rate increases, loses its spherical shape, the interface becomes rough and for small viscosities leads to the formation of fingers. We show it in the model that this finger formation can be arrested either by increasing the viscosity or elasticity.

8:48AM A26.00003: Why do rigid tumors contain soft cancer cells?*  
THOMAS FUHS (Presenter), FRANZISKA WETZEL, ANATOL W FRITSCH, Soft Matter Physics Division, University of Leipzig, DAPENG BI, Department of Physics, Northeastern University, ROLAND STANG, STEVE PAWLIZAK, TOBIAS KIESSLING, ERIK MORAWETZ, STEFFEN GROSSER, FRANK SAUER, JÜRGEN LIPPOLDT, FRED RENNER, SABRINA FRIEBE, MAREIKE ZINK, Soft Matter Physics Division, University of Leipzig, LARS-CHRISTIAN HORN, Division of Gynecologic, Breast and Perinatal Pathology, University Hospital Leipzig, BAHRIYE AKTAS, Department of Gynecology, University Hospital Leipzig, KLAUS BENDRAT, Pathology Hamburg-West, MAJA OKTAY, Montefiore Medical Center, AXEL NIENDORF, Pathology Hamburg-West, JOHN S CONDEELIS, Albert Einstein College of Medicine, MICHAEL HÖCKEL, Department of Gynecology, University Hospital Leipzig, M CRISTINA MARCHETTI, M. LISA MANNING, Department of Physics, Syracuse University, JOSEF ALFONS KAES, Soft Matter Physics Division, University of Leipzig — As early as 50 AD, the Roman medical encyclopaedist Celsus recognized that solid tumors are stiffer than surrounding tissue. However, cancer cell lines are softer, which facilitates invasion. This paradox raises several questions: Does softness emerge from adaptation to mechanical and chemical cues in the external microenvironment? Or are soft cells already present inside a rigid primary tumor? We investigate primary samples from patients with mammary and cervical carcinomas on multiple length scales from tissue level down to single cells. We show that primary tumors a highly heterogeneous in their mechanical properties on the tissue level as well as cells do exhibit a broad distribution of rigidities, with a higher fraction of softer and more elongated cells compared to normal tissue. Mechanical modelling based on patient data reveals that tumors remain solid containing a significant fraction of very soft cells. Moreover, it predicts that in such tissues, softer cells spontaneously self-organize into multicellular streams, which we observe experimentally.

*DFG: KA1116/9-1, KA1116/17-1; EU Horizon 2020: "FORCE"; BMBF 13N9366; NSF award ACI-1341006
9:00AM A26.00004: A tug of war between cell-cell and cell-ECM interaction during tumor invasion* YU LING HUANG (Presenter), SUMIT K DEY, CARINA SHIAU, CINDY WU, YUJIE MA, Cornell University, JEFFREY SEGALL, Albert Einstein College of Medicine, MINGMING WU, Cornell University — Tumor invasion within the interstitial space is critically regulated by the force balance between the cell-cell and cell-ECM adhesion. In this talk, we will present a newly developed 3D tumor model in which tumor spheroids were embedded within collagen matrix, and tumor cell dynamics are subsequently imaged and analyzed. We varied cell-cell and cell-ECM adhesion by using three epithelial cell lines with increasing expression levels of E-cadherin (responsible for cell-cell adhesion) and decreasing expression of integrin (responsible for cell-ECM adhesion). Interestingly, our results demonstrated that the tumor cells at the peripheral of the tumor spheroid underwent a tug of war between the cell-ECM and the cell-cell adhesion. Integrin dependent cell-ECM adhesion promoted tumor invasion, while E-cadhesion mediated cell-cell adhesion inhibited tumor invasion.

*NIH National Cancer Institute (Grant no. R01CA221346, GM103388-03, R21CA138366), National Center for Research Resources (5R21RR025801-03), and Cornell Center on the Microenvironment & Metastasis (Award No U54CA143876 from the National Cancer Institute)

9:12AM A26.00005: Understanding the crosstalk between mechanical and chemical guidance in 3D cell migration* PEDRAM ESFAHANI (Presenter), CHRISTOPHER EDDY, JIHAN KIM, RYAN WONG, BO SUN, Physics, Oregon State University — Critical to many physiological and pathological processes, human cells exhibit motility responses to a variety of chemical and mechanical environmental factors. This includes both contact guidance, where cells migrate along the ECM fibers axes; and chemotaxis, in which cells move against the gradient of a chemoattractant. Both cases had been studied extensively. However, there are some synergistic effects that are not fully characterized in 3D cell migration. To reveal the combined effects of mechanical and chemical guidance, and their possible crosstalk, we develop a magneto-microfluidics device to individually control the chemoattractant gradient as well as contact guidance cues. To objectively characterize the cell migration and morphologies, we developed a deep learning based cell tracking method. This novel experimental platform enables us to observe how cells respond to chemotaxis and contact guidance cues in both parallel and perpendicular orientations with respect to each other, as well as in varying strengths. In our continuing work, we will develop a mathematical model to recapitulate our experimental observations and fully characterize the cell response to coupled chemical and mechanical cues.

*National Science Foundation, PHY-1844627
**9:24AM A26.00006: The role of tissue biophysics in organ selectivity in metastasis** [Invited]
KANDICE TANNER (Presenter), National Institutes of Health - NIH — In the event of metastatic disease, emergence of a lesion can occur at varying intervals from diagnosis and in some cases following successful treatment of the primary tumor. Is there a difference in strategy to facilitate outgrowth? Why is there a difference in latency? Genetic factors that drive metastatic progression have been identified, such as those involved in cell adhesion, signaling, extravasation and metabolism. However, organ specific biophysical cues may be a potent contributor to the establishment of these secondary lesions. Here I discuss using optical tweezer based active microrheology to measure the mechanical cues that may influence disseminated tumor cells in different organ microenvironments. I further discuss in vitro and in vivo preclinical models such as 3D culture systems and zebrafish in efforts of understanding the role of the biophysical properties of the stromal architecture on the earliest stage of organ colonization.

**10:00AM A26.00007: Distinct Roles of Tumor-Associated Mutations in Collective Cell Migration**
RACHEL M. LEE (Presenter), MICHELE I. VITOLO, University of Maryland School of Medicine, WOLFGANG LOSERT, University of Maryland, College Park, STUART S. MARTIN, University of Maryland School of Medicine — Recent evidence suggests that groups of cells are more likely to form clinically dangerous metastatic tumors, emphasizing the importance of understanding mechanisms underlying collective behavior. The emergent collective behavior of migrating cell sheets *in vitro* has been shown to be disrupted in tumorigenic cells but the connection between this behavior and *in vivo* tumorigenicity is unclear. Here we use particle image velocimetry to measure a multi-dimensional collective migration phenotype for genetically defined cell types that range in their *in vivo* behavior from non-tumorigenic to aggressively malignant. By using cells with controlled mutations, we show that Ras activation and PTEN deletion lead to opposing effects on collective migration, despite both mutations being frequently found in patient tumors.

*This research was supported by NIH grants T32-CA154274 and R01-CA154624 as well as AFOSR grant number FA9550-16-1-0052 and the American Cancer Society Research Scholar Grant RSG-18-028-01-CSM.

**10:12AM A26.00008: Precision of flow sensing by self-communicating cells**
MICHAEL VENNETTIILLI (Presenter), Physics and Astronomy, Purdue University, SEAN FANCHER, Physics and Astronomy, University of Pennsylvania, NICHOLAS HILGERT, ANDREW MUGLER, Physics and Astronomy, Purdue University — Metastatic cancer cells have been observed to detect the direction of lymphatic flow by “self-communication”: they secrete a chemical which, due to the flow, does not return to the cell surface isotropically. The secretion rate is low, meaning detection noise may play an important role, but the sensory precision of this mechanism has not been explored. Here we derive the precision of flow sensing for two ubiquitous mechanisms: absorption of the chemical and binding/unbinding to surface receptors. We find that the latter mechanism is significantly more precise due to the fact that absorption distorts the signal that the cell aims to detect. Comparing to experiments, our results suggest that the cancer cells operate remarkably close to the physical detection limit. Furthermore, we predict that they should bind the chemical reversibly, not absorb it, a prediction that is supported by endocytosis data for these cells.

*This work was supported by the Simons Foundation.
10:24AM A26.00009: Classification of healthy and cancerous cells using optical rheology and machine learning*  ERIK MORAWETZ (Presenter), DIMITRIJ TSCHODU, JOSEF ALFONS KAES, Univ Leipzig — The optical stretcher (OS) probes single suspended cells with forces around 100 pN. It has been shown, that in the physiological regime of the OS carcinoma cells tend to be softer than their healthy counterparts. Yet, a clear characterization based on rheological data could not be achieved, even though its correlation with cancerous traits is strongly suggested. We use the high throughput of the OS to perform machine learning based discrimination of individual cells with a breast cancer model. We performed around 30,000 single cell stretching experiments on epithelial cells (MCF-10A), carcinoma cells (MDA-MB 436) and fibroblasts (NIH 3T3), and extracted 33 morphological and rheological parameters to use them for classification with random forest and support vector machine algorithms. Our approach allows us to distinguish among the three cell types with an average sensitivity of 71%. These intial results do not only elevate the importance of the mechanics of cells during tumor progression, but also promise live cell sorting for scientific and medical applications.

*European Research Council (ERC-741350/HoldCancerBack), European Union and the European Social Fond in Saxony (ESF-100234741).

10:36AM A26.00010: Modeling biophysical tumor-stroma interactions in 3D co-cultures of pancreatic cancer cells and pancreatic stellate cells  ERIC STRUTH (Presenter), JONATHAN P CELLI, Univ of Mass - Boston — Mechanical interactions between tumor cells and stromal components impact cancer progression and therapeutic response. Tumors of the pancreas in particular are associated with stiff fibrous stroma impacting growth and drug delivery. Here we use time lapse imaging to study contractile force mediated by adhesions between pancreatic ductal adenocarcinoma (PDAC) cells and pancreatic stellate cells (PSCs), a fibroblastic stromal signaling partner, in 3D culture on laminin rich extracellular matrix (ECM). PDAC cells overlaid on ECM form compact multicellular 3D nodules. When PSCs are introduced there is a profound change in growth behavior culminating in the formation of large connected structures mediated by contractile force of activated PSCs. We analyze this behavior using particle image velocimetry, as well as analysis of nodule size distribution. We use immunofluorescence to characterize the E-cadherin/N-cadherin adhesion in these co-cultures and show that E-cadherin deficient PDAC cells are unable to form adhesions with stromal cells and exhibit decreased contractility as a result. Going forward, we are leveraging this system to model and study drug delivery through fibrotic PDAC stroma and evaluate stromal depletion therapies.
AUSTIN NAYLOR (Presenter), DAVID H MCINTYRE, BO SUN, Oregon State Univ — Tumors are known to remodel the local extracellular matrix (ECM) in which they live. This remodeling causes the stiffness of the ECM to change, and is a major footprint in diagnosing tumors, specifically metastatic solid tumors such as breast or brain tumors. However, most studies up to date conduct bulk rheology or macroscopic rigidity experiments on the remodeled ECM. By using optical tweezers based assays, we are able to probe the local remodeling of the ECM and measure the local micromechanics as the tumor continuously expands and invades into the surrounding ECM. We find that the tumor can introduce strong mechanical anisotropy as well as stiffen the ECM. We find that these remodelings are spatially and temporally dependent on the tumor invasion dynamics. We hypothesize that the found remodelings are dominated by two factors, the volume preservation of cells and the traction force generated by cells. We also test our results by using different geometries of tumors.

*National Science Foundation, PHY-1844627

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A27 FIAP: Atomic Structure, Lattice Properties, and Phase Transitions 404 - Nihar Pradhan
8:00AM A27.00001: Electric Field-Induced Metal-to-Insulator Phase Transition in Few-Layered MoSe$_2$* NIHAR PRADHAN (Presenter), Department of Chemistry, Physics and Atmospheric Science, Jackson State University, Jackson, MS-39217, USA, CARLOS GARCIA, Florida State University, Tallahassee, FL 32310, USA, National High Magnetic Field Lab, BHASWAR CHAKRABARTI, Center for Nanoscale Materials, 9700 S-Cass Avenue, Lemont, IL-60439, USA, Argonne National Lab, JAWNAYE NASH, Department of Chemistry, Physics and Atmospheric Science, Jackson State University, Jackson, MS-39217, USA, CHRISTINA S MILLER, Center for Nanoscale Materials, 9700 S-Cass Avenue, Lemont, IL-60439, USA, Argonne National Lab, DHARMARAJ RAGHAVAN, 6525 College Street, NW, Department of Chemistry, Washington DC 20059, Howard University, ALAMGIR KARIM, Department of Chemical & Biomolecular Engineering, S333 Engineering Bldg 1, 4726 Calhoun Rd, Houston, TX 77204, University of Houston, LILIANA STAN, RALU DIVAN, DANIEL ROSENMANN, ANIRUDHA SUMANT, Center for Nanoscale Materials, 9700 S-Cass Avenue, Lemont, IL-60439, USA, Argonne National Lab, STEPHEN A MCGILL, Florida State University, Tallahassee, FL 32310, USA, National High Magnetic Field Lab — The Metal-Insulator phase transition (MIT) is one of the most interesting phenomena to study particularly in two-dimensional transition-metal dichalcogenides (TMDCs). A few recent studies$^{1,2}$ have indicated a possible MIT on MoS$_2$ and ReS$_2$, but the nature of the MIT is still enigmatic due to the interplay between charge carriers and disorder in 2D systems. We will present a potential MIT in few-layered MoSe$_2$ FETs based on four-terminal conductivity measurements. Conductivities measured in multiple samples strongly demonstrate the insulating-to-metallic-like phase transition when the charge carrier density increased above a critical threshold. The nature of the phase transition will be discussed with an existing theoretical model.


*This work was performed, in part, at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, and supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357. This work is also supported by NSF-DMR #1826886 and # 1900692. A portion of this work was performed at the NHMFL, which is supported by the NSF Cooperative Agreement No. DMR-1644779 and the State of Florida

8:12AM A27.00002: Partial Switching in Phase Change Material Sb$_2$Te$_3$ Nanowires to an Intermediate Resistance State by Microwave injection POK LAM TSE (Presenter), Univ of Southern California — Microwave (MW) induced resistance responses on Sb$_2$Te$_3$ nanowire (NW) samples were observed at about 3GHz in the MW frequency sweeps from 0 to 4GHz. The step-wise shifts in resistance occurred for varies samples with Ti/Au or Nb electrodes. The magnitude of electrical resistance change depended on the initial resistance of the NW samples and it appeared to be a crystalline transition into an intermediate state before changed to amorphous. Temperature dependences of NW samples at saturated resistance state of $10^8\Omega$ - $10^9\Omega$ exhibited semiconductor property while pristine NW sample at 500 Ω range had metallic property.
Understanding the Phase Behaviour of Pyrochlore Bi$_2$Sn$_2$O$_7$  

WARDA RAHIM (Presenter), University College London, JONATHAN M. SKELTON, University of Manchester, ARON WALSH, Imperial College London, DAVID SCANLON, University College London — Bi$_2$Sn$_2$O$_7$ exists in a number of polymorphic forms, with an α to β transition occurring at ≈400 K and β to γ transition occurring above 900 K.$^1$ The structural model for γ is undisputed (Fd-3m) but there has been a controversy over the structural models of α and β, with two models existing for α, one with 352 atoms per cell (P1C1)$^2$ and other with 88 atoms per cell (C1c1),$^3$ and recently β belonging to space group Aba2 has been reported.$^3$ We perform DFT lattice dynamics calculations using Phonopy$^4$ starting from γ, and map out the potential energy surfaces$^5$ spanned by imaginary mode eigenvectors, with the aim of elucidating the lowest energy structure. This approach successfully takes us from γ to the new structural model suggested for α, and also shows that β is a thermal average of a lower symmetry structure. The success of the method highlights the strength of ab-intio lattice dynamics in predicting the dynamically stable structural model of a compound and can speed up the exploration of different structures for solid-state applications.

$^2$Evans et al., J. Mater. Chem., 2003, 13, 2098

Electron Transfer in Contact Electrification*  

BENJAMIN J KULBAGO (Presenter), JAMES CHEN, JUN LIU, THOMAS G THUNDAT, State Univ of NY - Buffalo — Contact causes a weak interaction at the interface of two materials. This interaction transforms the surface of the lattice into a perturbed state. This perturbed surface is modeled as a series of dipoles. These dipoles change the surface state of both materials and contribute to a modified work function. The surface dipoles also induce a potential field at the interface, which drives electron transfer across the gap between the materials. A tribopair of Si and SiO2 is used to demonstrate how the modified work function and potential field drive electron transfer, as described by Schrodinger’s equation. The results will also be compared to experimental data.

*This study is supported by U.S. National Science Foundation (grant number 1662879).
8:48AM A27.00005: Density Functional Investigation of Phase Transition in Silicon Nanomembranes  JOEL AMBRIZ PONCE (Presenter), University of Wisconsin - Parkside, EVAN M MACINTOSH, University of Wisconsin - Milwaukee, WILLIAM D PARKER, University of Wisconsin - Parkside — Silicon is an important material at the center of the microelectronic systems industry, and nanomembranes of silicon have a wide range of material, mechanical, optical, and device applications. Recent experimental advances have achieved nanometer-scale flatness, and membrane properties have been found to depend directly on thickness. Using an atomistic slab model, we simulate the electrons with density functional theory in order to investigate the pressure phase transition of silicon in the membrane from semiconducting diamond phase to metallic beta-tin phase. We vary exchange-correlation approximation, comparing to bulk values in each approximation, and we calculate the electronic and vibrational properties of the membranes.

9:00AM A27.00006: Ultra-High Mechanical Flexibility of 2D Silicon Telluride*  ROMAKANTA BHATTARAI (Presenter), XIAO SHEN, Univ of Memphis — Silicon telluride (Si$_2$Te$_3$) is a two-dimensional material with a unique variable structure where the silicon atoms form Si-Si dimers to fill the “metal” sites between the Te layers. The Si-Si dimers have four possible orientations: three in-plane and one out-of-the plane directions. The structural variability of Si$_2$Te$_3$ allows unusual properties, especially mechanical properties. First-principles density functional theory calculations are performed to determine the critical strain of monolayer Si$_2$Te$_3$. The results show that Si$_2$Te$_3$ can sustain a critical uniaxial tensile strain up to 38% with a breaking stress of 8.63 N/m along the direction of Si dimer, making Si$_2$Te$_3$ the most flexible 2D material reported. Because of the high flexibility, a large strain can be used to tune the band structure, and the bandgap can be reduced by up to 1.5 eV. With increasing strain, the bandgap undergoes an unusual indirect-direct-indirect-direct transition. We also find that the uniaxial strain can effectively control the orientation of Si dimers, which may be beneficial for certain applications.

*This work was supported by the National Science Foundation grant # DMR 1709528 and by Ralph E. Powe Jr. Faculty Enhancement Awards from Oak Ridge Associated Universities (ORAU).

9:12AM A27.00007: Entanglement entropy of skeletal regions  ALEX VIGEANT (Presenter), Universite de Montreal — Entanglement entropy (EE) provides deep insights about quantum matter. For most groundstates and spatial regions, the EE is dominated by the celebrated area law. However, much less is known about the EE of skeletal regions, i.e. regions without volume such as a line embedded in 2D. When the boundary and volume coincide, there is little understanding about what is encoded in the EE. Here, we study this question using a 2D harmonic lattice model that leads to a relativistic massless scalar (conformal field theory) at low energy. We find new universal contributions to the EE as a function of the geometry of the skeletal region. We also discuss the field theory interpretation, and outline general open questions.
9:24AM A27.00008: Origin of unexpectedly low thermal conductivity in AMg$_2$X$_2$ ($A = \text{Mg, Ca, Yb}, \ X = \text{Sb, Bi}$) * JINGXUAN DING (Presenter), TYSON LANIGAN-ATKINS, Mechanical Engineering and Materials Science, Duke University, MARIO CALDERON CUEVA, ALEXANDRA ZEVALKINK, Chemical Engineering and Materials Science, Michigan State University, ARNAB BANERJEE, Neutron Scattering Division, Oak Ridge National Laboratory, OLIVIER DELAIRE, Mechanical Engineering and Materials Science, Physics, Duke University — Thermoelectric (TE) materials enable direct conversion of heat into electrical energy. The conversion efficiency is inversely proportional to the thermal conductivity, which is dominated by phonons in semiconductors. Zintl compounds AMg$_2$X$_2$ constitute a class of new TE with excellent performance in n-type Mg$_3$(Sb,Bi)$_2$ alloys, with $zT$ up to 1.6 reported so far. Mg$_3$X$_2$ exhibits very low lattice thermal conductivity (~1 W/m/K at 300K), comparable with PbTe and Bi$_2$Te$_3$, despite a much lighter average ionic mass. We report on inelastic neutron scattering (INS) and first-principles studies of the lattice dynamics of AMg$_2$X$_2$. INS provided the temperature dependent phonon density of states. Extra peaks were found at low frequency in Mg$_3$X$_2$ compared to CaMg$_2$X$_2$ or YbMg$_2$X$_2$, possibly originating from softer low-frequency TA phonons. Considerably stronger softening with temperature is also observed in Mg$_3$X$_2$. The anharmonic effects were examined with first-principles simulations, including ab initio molecular dynamics. We present our analysis of the thermal conductivity based on INS and simulations.

*Neutron scattering and first-principles simulation were supported by the US DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Award No. DE-SC0019299.

9:36AM A27.00009: Anharmonic Effects on Phonon Eigenvectors and $S(Q,E)$ in Quantum Paraelectric SrTiO$_3$ * XING HE (Presenter), Duke University, DIPANSHU BANSAL, Indian Institute of Technology Bombay, BARRY WINN, SONGXUE CHI, LYNN A BOATNER, Oak Ridge National Laboratory, OLIVIER DELAIRE, Duke University — The quantum paraelectric behavior and strongly anharmonic lattice dynamics of SrTiO$_3$ have attracted interest for decades. Inelastic neutron scattering (INS) measurements of SrTiO$_3$ reveal an anomalous evolution of transverse acoustic (TA) phonon intensity with temperature as the transverse optic (TO) mode softens. This reflects the incipient ferroelectric (FE) instability near the quantum critical point and couplings between TA and TO phonons. The experimental trends are confirmed and rationalized using DFT simulations including anharmonic renormalization. By analyzing the temperature-dependent force constants (FC) and eigenvectors, it is found that the structure factors of phonon modes change dramatically with temperature, as a direct consequence of the anharmonicity in this system. We identify that changing Ti and O eigenvectors, originating from FC changes in the Ti-O bonds, are responsible for these striking observations. These results establish how temperature-dependent phonon intensities from INS can provide direct insights into the behavior of phonon eigenvectors, and show how first-principles simulations can rationalize such anharmonic effects.

*This work was supported by the U.S. DOE, Early Career Award No. DE-SC0016166. Calculations were performed using NERSC.
9:48AM A27.00010: Covalency-driven Structural Evolution in the Polar Pyrochlore Series
\( \text{Cd}_2\text{Nb}_2\text{O}_{7-x}\text{S}_x \) *  
DANIEL HICKOX-YOUNG (Presenter), Northwestern University, GENEVA LAURITA, SAMRA HUSREMOVIC, Bates College, JAMES RONDINELLI, Northwestern University — Pyrochlores have attracted considerable interest lately due to their ability to host a variety of interesting phenomena, often derived from their geometrically frustrated interpenetrating sublattices. The triangular arrangement of cations tends to disfavor the coordinated displacements necessary to realize polar structures, but there are a few materials which overcome this frustration and exhibit ferroelectricity. Here we examine the origin and nature of the distortion mechanisms in the oxysulfide series \( \text{Cd}_2\text{Nb}_2\text{O}_{7-x}\text{S}_x \). Using density functional theory, group theoretical methods, and diffraction techniques, we characterize changes in the phase transition under sulfur substitution. We ultimately identify the role of covalent bonding on the Cd-X’ sublattice in shifting the ferroelectric phase transition from proper (x=0) to improper (x=0.25) and eventual elimination (x=0.7). This work sheds light on the origin of polar distortion mechanisms in the pyrochlore structure family, in addition to providing insight into the off-centering mechanisms of complex oxides in general.

*This work is supported by the Army Research Office through Grant No. W911NF-15-1-0017. We would also like to acknowledge the work of our collaborators Jun Li, Arthur W. Sleight, Robin Macaluso, and Mas A. Subramanian.

10:00AM A27.00011: Relationship between multiple degrees of freedom and oxygen interstitial ordering in rare earth ferrites*  
YANG ZHANG (Presenter), Tsinghua University, WENBING WANG, Fudan University, WANDONG XING, RONG YU, JING ZHU, Tsinghua University — Oxygen interstitials and vacancies, as two kinds of common defects in oxide system, usually play an important role in tuning the microstructure and properties of materials. To understand the tuning mechanism resulting from oxygen doping, the precise positions of these point defects and interaction between them and with other degrees of freedom need to be solved. Here, we report how such information can, for the first time, be obtained from the rare earth ferrite \( \text{LuFe}_2\text{O}_{4+x} \) by high-resolution electron microscopy, atomic-resolution spectroscopy and DFT calculations. The oxygen interstitial ordering and related lattice, charge, spin ordering form a new modulation structure, described by the same modulation vector. Meanwhile, we prove the modulation structure can be affected by changing the oxygen interstitial ordering. The interaction between oxygen interstitials and multiple degrees of freedom presented here provide a direct insight into tuning mechanism of oxygen doping in non-stoichiometric oxide systems.

*Chinese National Natural Science Foundation (51788104, 51390471, 51527803, 51525102, 51371102, 51390475, 51761135131, 11834009, 11504053), the National 973 Project of China (2015CB654902), the National Key Research and Development Program (2016YFB0700402, 2016YFA0300702)
First Principle Study of Phase Change Properties of Ag- and In-doped Sb-Te compound as Phase Change Material  

HANJIN PARK (Presenter), YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee Univ - Seoul, DASOL KIM, MANN-HO CHO, Department of Physics and Applied Physics, Yonsei University — Ag- and In- doped Sb-Te binary compounds (AIST) are widely attracted as base material of phase change random access memory (PCRAM) with its fast recrystallization time (ps scale) and less energy consumption in the phase transition than GeTe-Sb$_2$Te$_3$ pseudo-binary compounds (group 1) which are most famous as phase change material (PCM). Although AIST has better phase change behavior than group 1, it has much less investigated such as local structural environments or roles of Ag and In atoms. To reveal phase change properties and local atomic behavior in AIST, we performed molecular dynamics (MD) simulations using \textit{ab initio} density functional theory. AgInSb$_{18}$Te$_4$ is selected as an exemplary model configuration. We identify its crystalline phase with various atomic configurations and evaluating their total energy. Amorphous phase, a representative expanded structure to be a 2×2×2 supercell, is constructed with MD simulation which mimics the melt-quenching experiment process. We explore the phase change mechanism by evaluating the radial distribution function, angle distribution function, solid angle distribution, and order parameter, and find that the In atom plays an important role not only in the phase transition process but also in retaining or stabilizing amorphous phase.

Structural order-by-disorder in framework materials*  

GIAN GUZMAN-VERRI (Presenter), Univ de Costa Rica, PETER B LITTLEWOOD, Materials Science Division, Argonne National Laboratory — Systems which do not order at absolute zero due to a large ground state degeneracy can generate new correlations through thermal or quantum fluctuations and attain long-range order. Here, the internal energy of different ground states is the same, but their free energy can differ because the fluctuations around them give a different entropic weighting to each ground state. This is known as order-by-disorder (ObD) and has proven useful in understanding a wide variety of observed ordering phenomena in magnetic systems such as spin ices and frustrated anti-ferromagnets. Outside magnetism, however, the ramifications of ObD physics remain largely unexplored. In this talk, we propose an ObD mechanism is at play in the observed structural transitions in a class of framework materials (MF$_3$ metal triflourides), which display soft manifold lattice dynamics with an inability to go through a symmetry breaking distortion, providing the required ground state degeneracy analogous to that of frustrated magnetism.

*Work supported by the Vice-rectory for Research at the University of Costa Rica and the DOE Office of Basic Energy Sciences, (Materials Science and Engineering Division).
Electrical properties of ferroelectric 1,4-diaminobutane zinc formate crystals under high hydrostatic pressure.*

ANNA SZEREMETA (Presenter), ANDRZEJ NOWOK, Institute of Physics, University of Silesia in Katowice, ADAM SIERADZKI, Department of Experimental Physics, Wroclaw University of Technology, MIROSLAW MACZKA, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, SEBASTIAN PAWLUS, Institute of Physics, University of Silesia in Katowice — 1,4-diaminobutane zinc formate is an example of metal organic frameworks, MOF, which possesses a nicolite-type structure. This compound is characterized by ordered pore structure, formed by a specific arrangement of atoms formed by coordinating bonds between zinc atoms and formate ligands. Due to its multiferroic properties this compound as well as other MOFs can be applied in memory components.

The electric impedance was measured by means of broadband dielectric spectroscopy (BDS). In the studied crystal one relaxation process was observed. At ambient pressure the phase transition was registered at T = 243 K. The application of Havriliak-Negami model in the description of the relaxation process allowed us to determine relaxation time and consequently activation energy as E_a = 0.48 eV.

The hydrostatic pressure affected both the temperature of phase transition and the relaxation process times. After the sample being pressurized up to 1.7 GPa the phase transition temperature increased by ~ 12 K. Simultaneously the relaxation times got longer which was accompanied by the increase of energy barrier.

*The authors are grateful for the financial support provided by the National Science Centre within the framework of the Opus13 project (Grant No. DEC-2017/25/B/ST3/02321).

Cubic and Tetragonal Perovskites from the Random Phase Approximation*

FANHAO JIA (Presenter), Shanghai University, GEORG KRESSE, CESARE FRANCHINI, PEITAO LIU, Faculty of Physics and Center for Computational Materials Sciences, Vienna University, JIAN WANG, Department of Physics, University of Hong Kong, ALESSANDRO STROPPA, CNR-SPIN, Università degli Studi dell'Aquila, WEI REN, Shanghai University — Evaluating many body correlation effects beyond the commonly applied local or semi-local density functionals has received tremendous attention over the past few years. Using the random phase approximation (RPA) to describe the correlation energy combined with the exact exchange energy, we have investigated twenty cubic ABO_3-type perovskites and three prototypical ferroelectric (tetragonal) perovskites. A quantitative analysis and comparison of the performance of various local and semi-local exchange-correlation functionals (XCFs) shows that the inclusion of dynamical correlation effects allows for an excellent account of the structure and energetics of complex ABO_3-type oxides.

*This work was supported by the National Natural Science Foundation of China (Grants Nos. 51672171, 51861145315 and 51911530124), the National Key Basic Research Program of China (Grant No. 2015CB921600), the fund of the State Key Laboratory of Solidification Processing in NWPU (SKLSP201703). The supercomputing services from AM-HPC and the Fok Ying Tung Education Foundation are also acknowledged.

Monday, March 2, 2020 8:00 AM - 11:00 AM
8:00AM A28.00001: Electrical actuation of DNA-based nanorobotic structures* [Invited]
FRIEDRICH SIMMEL (Presenter), TU Munich — DNA nanotechnology provides efficient methods for the sequence-programmable construction of mechanical devices with nanoscale dimensions. The resulting nanomachines could serve as tools for the manipulation of macromolecules with similar functionalities as mechanical tools and machinery in the macroscopic world. In order to drive and control these machines and to perform specific tasks, fast, reliable and repeatable actuation are required. In this context, we recently developed an effective method for actuating DNA nanostructures using externally applied electric fields. Electrical control allows us to dynamically drive DNA-based nano-robotic systems, which allows us to move and position molecules on a molecular platform with high speed and accuracy.
In this talk we will focus on the physical characterization of this nanorobotic system using single molecule fluorescence techniques as well as a discussion of the physical mechanisms underlying the motion of the robotic arm. We will also touch upon potential applications of such systems in single molecule biosensing and nanoplasmonics

*DFG SFB 1032 TPA2

8:36AM A28.00002: Real-time magnetic actuation of DNA nanodevices* [Invited]
RATNASINGHAM SOORYAKUMAR (Presenter), Department of Physics, The Ohio State University — Recent advances in biomolecular nanotechnology, in particular DNA nanotechnology, have led to molecular devices with precisely designed motion, mechanical properties, and triggered conformational changes. This talk will report an advancement in this field that opens the door to manipulate molecules and nanomaterials with programmed or user-driven magnetic control in real-time.
The magnetic approach to control DNA nano devices that has been developed allow direct manipulation over the device conformation in real-time up to frequencies of several Hertz with tunable applied forces.[1] The technique relies on coupling the motion of micron-sized magnetic beads, which can be easily manipulated using a low-cost platform, to the nanoscale DNA devices via stiff lever arms. The mechanical lever arm has a high aspect ratio, where its cross-sectional dimensions are on the scale of the nanomachines (~25 nm), but the length is on the scale of the actuator (~ 1 µm). While actuation of nano-hinges and nano-rotors is demonstrated, the robust assembly methods can be translated to a variety of molecular devices.
These results thus establish many key advances over several existing methods to actuate molecular devices including sub-second temporal control, the ability to actuate into many different conformations, and capability to manipulate devices with tunable forces.

*This work was supported by the Army Research Office under contract W911NF-14-1-0289 and the National Science Foundation grant ECCS-1916740.
DNA nanotechnology is one of the most powerful methods for constructing nano-mechanical devices. The ability to actuate these devices on-demand would provide a powerful method for creating dynamic nanomachines that can reconfigure nanostructures, apply precisely defined forces, or spatiotemporally control self-assembly. Typically, DNA nanostructures have been temporally modulated by either 1) introducing external toehold-mediated displacement strands, or 2) incorporating photoswitchable azobenzene nucleotides that can reversibly break hybridization. However, these approaches suffer from drawbacks like 1) the need to introduce an exogenous strand (which is not feasible for many applications, especially in biology), and 2) slow kinetics or undesired reversibility. To circumvent these limitations, we have photo-caged the displacement strands within an existing nanostructure, preventing their action until illuminated. These “spring-loaded” nanostructures are in a metastable state until activated by light, whereupon the high local concentration of the displacement strand will drive irreversible nanostructure reconfiguration. To demonstrate this concept, we designed a nano-mechanical tweezer that switches between the closed and open state with UV light. In effect, this device can apply a nano-mechanical force within a few seconds of illumination, paving the way for dynamic nanomachines that can exert controlled motion. The tweezer was analyzed using AFM, FRET, and computational simulations. Our results demonstrate that the photocaged mechanism is efficient and fast, surpassing externally added strand displacement by almost two orders of magnitude. We envision that this approach will allow for light-activated nanomachines in the future for biophysical studies with cells.

N.S. acknowledges startup funds from Arizona State University. This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0053.
Rapid Reconfiguration and Tunable Control of DNA-based Mechanisms

ALEXANDER E. MARRAS (Presenter), Pritzker School of Molecular Engineering, University of Chicago, LIFENG ZHOU, The RNA Institute, University at Albany, State University of New York, ZE SHI, Department of NanoEngineering, University of California, San Diego, GAURAV ARYA, Department of Mechanical Engineering and Materials Science, Duke University, HAI-JUN SU, CARLOS E CASTRO, Department of Mechanical and Aerospace Engineering, Ohio State University — Precise robotic motion is ever-present within our cells with proteins like ATP synthase and kinesin, functioning much like macroscopic machines using multiple components and defined motion paths. Structural DNA nanotechnology enables researchers to construct mechanisms with similar functionality exhibiting nanoscale spatial and dynamic control by employing its vast physical design space and directed self-assembly methods. Our early work contributed to a library of DNA devices with controllable motion, primarily using strand invasion to bind or displace reconfigurable components with timescales of minutes or longer. Here, we present a strategy for tunable actuation in near real time. We demonstrate an approach using a simple modification to existing devices that adds weak binding sites on complementary components. A network of short DNA handles is activated by increasing cation concentration, raising the avidity of the network to join components. Likewise, reconfiguration is quickly reversible in decreased salt conditions. Actuation kinetics are measured via single molecule FRET using buffer exchange through a simple microfluidic system. This level of temporal control over DNA devices serves as a foundation for real-time manipulation of molecular systems.

This work was supported by NSF award no. 1536862.

Hari Subramanian Invited Talk

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A29 DSOFT DBIO GSNP DFD: Active Matter in Complex Environments I

Clogging and Depinning of Active Matter Systems in Disordered Media

CYNTHIA REICHHARDT (Presenter), Los Alamos Natl Lab — We numerically examine the transport of active run-and-tumble particles with steric particle-particle interactions driven with a drift force over random disordered landscapes comprised of fixed obstacles. For increasing run lengths, the net particle transport initially increases before reaching a maximum and decreasing at larger run lengths. The transport reduction is associated with the formation of cluster states that become locally jammed or clogged by the obstacles. We also find that the system dynamically jams at lower particle densities when the run length is increased. Our results indicate that there is an optimal activity level for transport of run-and-tumble type active matter through quenched disorder, and could be important for understanding biological transport in complex environments or for applications of active matter particles in random media.
8:36AM A29.00002: Flocking through disorder  AMÉLIE CHARDAC (Presenter), Laboratoire de Physique, Ecole Normale Supérieure de Lyon, SURAJ SHANKAR, Physics department, Harvard University, M CRISTINA MARCHETTI, Department of Physics, University of California Santa Barbara, DENIS BARTOLO, Laboratoire de Physique, Ecole Normale Supérieure de Lyon — We address the robustness of flocking motion to challenging environments.

The emergence of collective motion in groups of motile bodies arises from the competition between rotational diffusion and polar interactions in ensemble of active particles. This minimal picture was successfully employed to account for the large scale dynamics of systems as diverse as starling flocks and self-propelled colloids.

Building on model experiments based on Quincke rollers, I will show how colloidal flocks lose their orientational order when cruising through disordered lattices. I will present a series of quantitative experiments that elucidate the existence of a novel state of active matter that supports orientational order (through a sparse rivers network) but no net transport. In particular, I will show that this state can be seen as a glass of topological defects.

8:48AM A29.00003: Enhanced bacterial motility in colloidal media*  SHASHANK KAMDAR (Presenter), LORRAINE F. FRANCIS, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota-twin cities — The study of the locomotion of biological and artificial microswimmers in Newtonian and non-Newtonian fluids is gaining rapid momentum with applications in many areas such as pathogenicity, bioremediation, and drug delivery. Here, we experimentally investigate the motility of Escherichia coli, a flagellated bacterium, in colloidal media. We systematically vary the size of passive colloidal particles in the mixture from 20 nm to 1 μm and the volume fraction up to 20%. Using confocal microscopy, we image the motion of fluorescent-labeled bacteria and implement an in-house tracking algorithm to obtain the speeds of bacteria. We observe a substantial increase in bacterial speeds (up to 74%) as the colloid volume fraction increases to 3%, followed by a decrease at higher volume fractions. Additionally, we find that increasing the size of colloidal particles results in larger speed enhancement. We construct a model that qualitatively explains our experiments. Our study highlights the unusual locomotion of swimming microorganisms in colloidal suspensions and illustrates the rich dynamics that arises from swimmers’ interactions with their environment.

*This research is supported by the UMN IPRIIME program.
9:00AM A29.00004: Theoretical Framework to Describe Traveling Waves of Bacteria in Porous Media  DANIEL AMCHIN (Presenter), TAPOMOY BHATTACHARJEE, FELIX S KRATZ, JENNA A OTT, SUJIT DATTA, Princeton University — How bacteria move in porous media like tissues and soil underlies processes like infection and bioremediation. However, existing models of how bacteria coordinate their motion at the population scale cannot fully explain collective migration inside porous media. To address this gap in knowledge, we use confocal microscopy to directly track bacteria deep inside transparent porous media. Similar to the case of free liquid, we find that the cells move together in directed, traveling waves following self-generated nutrient gradients. However, unlike the case of free liquid, the wave speed and shape are also regulated by the structure of the porous medium itself. By analyzing the single cell tracks, we characterize how biased “hopping and trapping” of the individual cells generates traveling waves; surprisingly, in stark contrast to the case of chemotaxis in free liquid, we find that hop length bias is not the dominant contributor to this mode of collective migration. Further, we show how the statistical features of single cell motion can be used to develop a continuum model that can describe collective migration in a porous medium over large length and time scales. Together, our work provides new principles to predict and possibly control bacterial migration in complex environments.

9:12AM A29.00005: The role of diversity for collective bacterial migration through diverse environments*  HENRY MATTINGLY, THIERRY EMONET (Presenter), MCDB & Physics, Yale University — Chemotactic bacteria form expanding wave fronts that allow populations to achieve directed expansion towards new territory (Adler J. Science 1966), which can enhance total population growth. But even isogenic populations exhibit phenotypic heterogeneity in their chemotactic properties, and it has been unclear how this affects their directed expansion with growth. We recently showed that diverse cells can travel together in the expanding front by sorting themselves by chemotactic ability, which compensates for their differences by matching ability to the local chemotactic signal (Fu, Kato et al. Nature Communications 2018). However, this places the lowest-performing cells at the back of the wave and at highest risk of falling behind. Here, through a combination of simulations and theory, we demonstrate the conditions in which diversity is valuable (or not) for collectively-migrating populations that grow and encounter varying environments during travel.

*HM and TE were funded by NIH R01 GM106189. HM was funded by NIH F32 GM131583.
Light-Sensing Microbes in Complex Geometries: Surface Adhesion, Gliding Motility and Self-Organization

ALEXANDROS FRAGKOPOULOS, SEBASTIAN TILL, SEBASTIAN RAUM, RODRIGO CATALAN, OLIVER BAEUMCHEN (Presenter), Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Göttingen, Germany — Life on Earth has evolved under the exposure of sunlight and many microbes are equipped with photoreceptors enabling them to perceive light. The microhabitats of such light-sensing microbes include liquid-infused soil, porous rocks and microdroplets, featuring complex geometric architectures that induce strong spatial and temporal fluctuations of light exposure. In these confined environments the cells frequently encounter and interact with interfaces. We discovered that Chlamydomonas reinhardtii, a soil-dwelling photoactive microorganism and biological model system, can reversibly switch its adhesion to surfaces on and off by light (Kreis et al., Nature Physics, 2018). The adhesiveness is regulated by a blue-light photoreceptor and mediated by their two flagella. Once they are attached to a surface, gliding motility sets in and enables the microbes to maneuver on the surface. Based on cell tracking and statistical analysis, we study the surface adsorption and gliding motility of light-sensing microbes and demonstrate how surface gliding, in conjunction with cell-cell interactions, may control the emergence of microbial self-organization in confinement.

Active Brownian filaments: deviations from blob scaling theory and dynamics inside cavities

SHIBANANDA DAS (Presenter), ANGELO CACCIUTO, Columbia University — Active filaments have become the subject of intense scrutiny in recent years because of their biological implications, and their role as a minimal model where the competition between thermal, elastic and active forces can be systematically studied.

Scaling arguments used to predict the radius of gyration of passive self-avoiding flexible polymers have been shown to hold even under the influence of active fluctuations. Via a numerical study we establish how the standard blob scaling theory representations of a polymer breaks down when dealing with active polymers under confinement. We find that the predicted exponents hold only whenever the persistence length generated on the polymer by the active forces is much smaller than the size of the characteristic blob in the scaling theory. Further, when the activity is directed along the backbone of a semi-flexible filament, while confined in a spherical cavity, a highly dynamic scenario emerges. The filament is capable of escaping local and global energy minima and sample, in a quasi-periodic fashion, an ensemble of conformations usually associated to higher bending energies, and previously observed for passive filaments only under very different degrees of confinement or identified as glassy metastable states.

*NSF Grant No. DMR-1703873
9:48 AM A29.00008: Fitness of cell colonies to navigate obstacles*  BO LI (Presenter), Center for Soft and Living Matter, Institute for Basic Science, SUN-MIN YU, YOON-KYOUNG CHO, School of Biomedical Engineering, Ulsan National Institute of Science & Technology, STEVE GRANICK, Center for Soft and Living Matter, Institute for Basic Science — We confront confluent epithelial cells with the need to adapt from wide-channel to narrow-channel growth. Upconversion from single cell, the colony self-organizes to facilitate migration with greater efficiency than that would be accomplished by fluid hydrodynamics. This is traced to long-range mechanical signaling. Stretched leader cells trigger acceleration of the whole group; the resulting velocity difference, in turn, reinforces stretching of the leaders and establishes positive feedback between cell morphology and mechanical strength, as we confirm by direct visualization of F-actin expression, cadherin localization, and the shapes of cells and their nuclei. The relevance is to show how mechanical signaling promotes a 'smart' group navigation strategy in which adaptations of individual cells to the local environment propagate over long distances to benefit the whole colony.

*IBS-R020-D1

10:00 AM A29.00009: Anomalous size-dependence of bacterial diffusion in a micropillar array  POOJA CHOPRA (Presenter), DAVID A. QUINT, AJAY GOPINATHAN, BIN LIU, University of California, Merced — Microorganisms are endowed with phenotypic variations, including diversities in sizes within the same species, which are crucial to their adaptation to living habitats. Here, we investigate how such size variations affect the transport of bacteria in a structured medium, using an array of microscale pillars and a smooth-swimming mutant of Escherichia coli. In contrast to the common belief that a smaller object can navigate solid obstacles more efficiently, we find that the long-time diffusion of individual E. coli actually decreases with decreasing cell size. By varying the pillar geometries, we determine that such anomalous diffusion is governed by the cell size relative to the pillar curvature: cells with smaller sizes relative to the pillar radius are more easily attracted to the pillar surface and are thus effectively “trapped.” We show that such an attractiveness can be well characterized by a size-dependent residency time that the bacterium spends near the pillar surfaces. We develop an agent-based model that purely relies on the geometry of the micropillars, bacteria and residency time. The numerical model agrees reasonably well with our experimental observations, suggesting that solid structures can affect bacterial transport by purely geometric mechanisms.
HAMID REZA KARANI (Presenter), GAŠPER KOKOT, PETIA M. VLAHOVSKA, Northwestern University — The natural habitat of many microorganisms is not a simple homogeneous environment. A ubiquitous observation is that diffusion becomes anomalous with nonlinear scaling between mean-squared displacement and time. A major challenge in biological sciences and condensed matter physics is to uncover these links to gain insight paramount for design of efficient filter membranes, medical diagnostics and drug delivery, and micro-robots operated in heterogeneous environments.

Building on our recently developed tunable colloidal random walker, we combine microfluidics experiments with theory to characterize and quantify the degree of anomalous diffusion. We define high-order measurable microstructural descriptors which carry information on connectivity and clustering of the designed obstacles that offer a convenient platform to test the theoretical predictions. Results reveal a complex nature of interactions between the colloidal random walker and obstacles which goes beyond a simple correlation between the diffusive behavior and obstacle volume fraction. Using scaling analysis, we provide new quantitative measures for predicting how anomalous diffusion emerges in a heterogeneous micro-environment with known morphological information.

OLEKSANDR CHEPIZHKO (Presenter), THOMAS FRANOSCH, Institute for Theoretical Physics, University of Innsbruck — Microswimmers are exposed in nature to crowded media and their transport properties depend in a subtle way on the interaction with obstacles. Here, we investigate a model for a single circle swimmer exploring a two-dimensional disordered array of impenetrable obstacles. The microswimmer follows the surface of an obstacle for a certain time upon collision. An ideal microswimmer [1] can display long-range transport or be localized in a finite region depending on the obstacle density and the radius of circular orbits. Close to the transition lines from two localized states to a diffusive state the transport becomes subdiffusive, which is rationalized as a dynamic critical phenomenon. We determine the non-equilibrium state diagram and evaluate the diffusivities. For the microswimmer subjected to angular noise [2] increasing the noise tends to amplify diffusion, yet large randomness leads to a strong suppression of transport. We rationalize the suppression and amplification of transport by comparing the relevant time scales of the free motion to the mean-free path time between collisions with obstacles.

1. O. Chepizhko, T. Franosch, Soft Matter, 2019, 15, 452
2. O. Chepizhko, T. Franosch, submitted

*Funding provided by the Austrian Science Fund via grants M 2450-NBL and P 28687-N27.
10:36AM A29.00012: Escape of a Nanoparticle from Cavities in a Porous Matrix  HAICHAO WU (Presenter), BENJAMIN GREYDANUS, DANIEL K SCHWARTZ, University of Colorado, Boulder — Translocation from one cavity to another through a narrow constriction (i.e. a “hole”) represents the fundamental elementary process underlying hindered mass transport of nanoparticles and macromolecules within many natural and synthetic porous materials, including intracellular environments. This process is complex, and may be influenced by long-range (e.g. electrostatic) particle-wall interactions, transient adsorption/desorption, surface diffusion, and hydrodynamic effects. Here, we used a three-dimensional (3D) tracking method to explicitly visualize the process of passive Brownian nanoparticle and self-propelled Janus particle diffusion within periodic porous nanostructures. Specifically, we quantified the spatial dependence of particle motion and the residence times of individual particles in the interconnected confined cavities, allowing us to test hypotheses regarding the effects of self-propulsion on mass transport in confined porous environments.

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A30 DSOFT GSNP: Morphing Matter: From Soft Robotics to 4D Printing I 502 - Pierre-Thomas Brun, Princeton University - Tag(s): Focus

8:00AM A30.00001: Robotic Morphing Matter as Materialized AI [Invited]  LINING YAO (Presenter), Carnegie Mellon Univ — Morphing Matter are physical materials that are transformable, adaptive and autonomous. They are programmable or pre-programmable with inherent sensing, actuating and computational behaviors across scales from the nano to macro. Situating Morphing Matter in the present, it is materialized AI that makes conventional computers disappear and computation weaves itself into the fabric of everyday life - the ultimate dream of ubiquitous computing envisioned by Mark Weiser. These material systems can be leveraged to design soft robots, self-assembling furniture, adaptive fabrics, and self-folding foods. In this talk, Lining presents the recent works in the Morphing Matter Lab, Human-Computer Interaction Institute of School of Computer Science at Carnegie Mellon University and highlights several robotic morphing materials that weave advanced manufacturing, computational tools, and design thinking. Her team believes that the term “robotics” does not only refer to conventional robotic forms and controls but also connects to the artifacts’ abilities to make decisions, adapt, move, and respond to different stimuli. More information from the lab site:
https://morphingmatter.cs.cmu.edu/
8:36AM A30.00002: Spider-morphs: Designing 3D shapes from multiple tapered \textit{elasticae}.
MINGCHAO LIU (Presenter), LUCIE DOMINO, DOMINIC VELLA, Mathematical Institute, University of Oxford — Foldable three-dimensional (3D) structures are important in a wide range of engineering applications. Transforming flat two-dimensional sheets with cuts into 3D structures, or kirigami, has emerged as an exciting manufacturing paradigm. However, achieving a particular 3D shape usually requires multiple materials and/or the application of external stimuli. Here we introduce a design framework for forming approximately axisymmetric 3D structures by harnessing the buckling of multiple tapered elastic sheets (the legs) connected in a central portion (the body). Together this creates a spider-like structure that morphs in 3D: a spider-morph. We design spider-morphs that deform into axisymmetric 3D structures with positive, negative, and variable Gaussian curvature. We conduct both numerical simulations and physical experiments to verify our theoretical approach.

8:48AM A30.00003: Reshapable groovy sheets  ANNE MEEUSSEN (Presenter), Designer Matter, AMOLF, MARTIN VAN HECKE, Leiden University — Most mechanical metamaterials are designed for a single function. But multifunctional metamaterials need to respond distinctly to different kinds of mechanical input. We show that groovy sheets---thin sheets with parallel corrugations---form patterns of snap-through defects and shift into different shapes, depending on how they are actuated. We show that geometric nonlinearities and frustration lie at the heart of the reversible yet multistable behaviour of groovy sheets.

9:00AM A30.00004: Under pressure: Mechanics of swelling hydrogels under confinement
JEAN-FRANCOIS LOUF (Presenter), NANCY LU, MARGARET O'CONNELL, Princeton University, H. JEREMY CHO, Mechanical Engineering, University of Nevada Las Vegas, SUJIT DATTA, Princeton University — Hydrogels are polymer networks that can absorb considerable amounts of water. They are thus promising additives to soil in arid conditions, increasing water retention and decreasing the need for plant irrigation. However, field measurements indicate that confinement in soil alters both the ability of hydrogels to hold water, as well as the properties of the soil itself—and the underlying physical reasons remain unknown. We have developed the ability to directly visualize hydrogel swelling within a three-dimensional porous medium that mimics soil. Using this platform, we quantify how the presence of the solid grains around a hydrogel hinders its ability to swell. By testing different applied loads and sizes of porous media, we show that the deformations of the hydrogel and the medium can be described by a balance between the osmotic swelling pressure of the hydrogel, the local elastic strain energy needed for the hydrogel to swell into the pores, and the frictional interactions holding grains together. Our results thereby provide a general framework by which hydrogel swelling can be understood, potentially improving their ability to help plants survive drought, and informing applications in new settings like oil fields and lab-on-a-chip devices.
9:12AM A30.00005: Delicate and Precise Grasping using Kirigami*  DOUGLAS HOLMES
(Presenter), YI YANG, KATHERINE VELLA, Boston Univ — The ability to precisely and delicately handle deformable, fragile, slippery, or microscale objects remains a significant challenge for robotic grippers. In this work, through a combination of experiments and modeling, we demonstrate how the mechanical actuation of kirigami shells enables both delicate and precise grasping of a wide variety of objects. The design is geometric, so it can be adapted to many material systems, and the geometry was optimized to produce a structure with a high carrying capacity and a low actuation force. We combined individual kirigami grippers in series and in parallel to form gripper arrays capable of grasping slender rods, and simultaneously grasping multiple objects and moving them without changing their relative orientation and position. The kirigami gripper is scalable, lightweight, and can be incorporated with commercially available robotic system to perform delicate and high precision grasping.

*We gratefully acknowledge the financial support from NSF through CMMI-1824882.

9:24AM A30.00006: Design and mechanics of complex inflatable networks  TREVOR J JONES, ETIENNE JAMBON-PUILLET, PIERRE-THOMAS BRUN (Presenter), Princeton University — The use of compliant materials to accomplish complex movements, made difficult or impossible by rigid materials, has inspired a wide array of soft robots. We have recently introduced “bubble casting”, a novel assembly method that leverages the fluidity of curing silicone elastomers to easily fabricate soft actuators with complex shapes. While liquid, an elastomer is first injected in a tube or tubular mold. An inner void is subsequently sculpted by injecting an elongated bubble into the channels, leaving elastomer only on the channels walls. As the elastomer cures into an elastic solid, gravity passively drains the top part of the channel and lifts the bubble to form the final actuator whose cross-section consists of a thin upper membrane attached to a thick lower beam. Here we explore the mechanical response of our soft actuators: while linear actuators are found to curl when inflated owing the asymmetry of their cross section, the deformation of closed shapes, such as loops, or that of connected networks is more intricate. We will discuss the experimental results we obtained with these programmable robots, and the models we have derived to rationalize our observations.

9:36AM A30.00007: Buckling and Metastability in 2D Impurity Arrays  ABIGAIL PLUMMER (Presenter), DAVID R. NELSON, Harvard University — We study a periodic array of impurities that produce local dilations, embedded in a two-dimensional crystalline solid that can buckle out of the plane. These arrays provide a simple elastic model of shape memory. As the size of each impurity increases (or the relative cost of bending to stretching decreases), it becomes energetically favorable for the impurities to buckle either up or down, allowing for a vast number of metastable states. Using discrete simulations and continuum theory, we consider the buckling of isolated impurities as well as impurity arrays, guided by an analogy to the Ising antiferromagnet. We characterize the buckling transition and conjecture ground states for systems with triangular and square lattice microstructures.
4D printing of mechanically programmable shape-shifting liquid crystal elastomers  

MORGAN BARNES (Presenter), RAFAEL VERDUZCO, Rice Univ — 4D printing is a promising method to develop actuators for applications in soft-robotics and biomedical devices where complex structures are required that might be difficult to create using traditional fabrication methods. However, most 4D printing relies on shear alignment upon printing to align liquid crystal or composite fibers that undergo anisotropic expansions/contraction when actuated. This limits the types of shape changes available to researchers as determining the print path required to induce a desired shape change is not trivial. Here, we use a new reactive printing method that enables the printing of a dual network liquid crystal elastomer (LCE) which can be mechanically programmed into the desired shape change. First, a thiol-acrylate Michael addition is completed upon printing an LCE oligomer solution into a catalyst bath. Next, the printed structure is dried, deformed to a desired shape change, and UV cured to crosslink excess acrylates in the network. The resulting LCE transforms between the printed and mechanically deformed shape when heated and cooled, respectively, and is capable reversible strains up to 100%. We demonstrate the versatility of this method by printing a variety of LCE actuators which could not be printed using conventional 4D printing methods.

Versatile and controllable shape morphing using twisted-and-coiled actuators  

JIEFENG SUN (Presenter), JIANGUO ZHAO, Colorado State University — Various shape morphing strategies have been investigated in recent years. Even though existing work has demonstrated complicated shape morphing (e.g., a human face), they can only deform along with a predefined pattern. We propose a different strategy: strategically embedding soft actuators into a soft body to enable versatile shape morphing by actively controlling the deformation of each soft actuator. We utilize a soft actuator, twisted-and-coiled actuators (TCAs), which can be easily fabricated from low-cost sewing threads to generate large force and displacement. We also leverage a jamming-based method to change the stiffness of soft bodies. With these two elements, we realize a shape morphing module that can quickly transform to and hold versatile shapes to adapt to various environments. Different modules can also be combined to generate more complicated shapes. We demonstrate a fast grasping and holding process, which consumes no energy, with a gripper with two shape morphing fingers. We also demonstrate a morphing surface that can hold different 3D configurations. We envision that the concept can be applied to soft robots, medical robots, morphing structures, etc.

*This work is partially supported by the National Science Foundation under Grant CNS-1755766
10:12AM A30.00010: Controlled Shape-morphing of Elastic Sheets by Chemically-driven Fluid Flow*  RAJ KUMAR MANNA (Presenter), OLEG SHKLYAEV, 1Department of Chemical Engineering, University of Pittsburgh, HOWARD A STONE, Department of Mechanical and Aerospace Engineering, Princeton University, ANNA BALAZS, 1Department of Chemical Engineering, University of Pittsburgh — Shape-morphing of two-dimensional (2D) materials into complex three-dimensional (3D) structures provides a wide range of applications from wearable electronics to soft robotics. Convective flows generated by the appropriate chemical reactions provide a mechanism for shape transformation of elastic 2D materials submerged in a flow environment. Here, using a computational model that incorporates interrelated chemical, hydrodynamic and mechanical interactions, we demonstrate how a (2D) enzyme-coated elastic sheet can spontaneously morph into 3D structures in response to specific chemical stimuli introduced in the fluid-filled microchamber. We outline design principles for creating a multi-responsive elastic sheet that self-morphs into different 3D structures. We further develop a theoretical model based on lubrication theory for thin liquid films coupled to the deformations of an elastic sheet that rationalizes our simulation observations and provides insights into the initial dynamics of the transformation of elastic sheets within the microfluidic system.

*The work was supported by NSF Grant 1740630, Centers for Chemical Innovation Phase I, Center for Chemo-mechanical Assembly and computational facilities at the Center for Research Computing at the University of Pittsburgh.

10:24AM A30.00011: Morphing Surfaces formed by Liquid Crystal Elastomer Coatings: Design and Modeling*  ROBIN SELINGER (Presenter), YOUSSEF MOSADDEGHIAN GOLESTANI, JONATHAN SELINGER, SAJEDEH AFGHAH, MICHAEL P VARGA, Kent State Univ - Kent — The suction cups on the arms of an octopus are morphing structures that can actuate to adhere to a non-porous surface, and then release on command. To mimic this functionality in an engineered material, we design and model dynamically morphing surface coatings composed of stimuli-responsive liquid crystal elastomers (LCE). In these programmable materials, patterned molecular orientation gives rise to complex shape transformations, driven by change of temperature. Using a combination of Finite Element Modeling (FEM) and analytical calculations, we design and characterize director patterns that create a variety of surface topographies: a lattice of spikes and/or indentations, an array of parallel microchannels or ridges, and patterned zones of positive and negative Gaussian curvature. To drive a thin film coating to morph into a lattice of suction cup-like indentations, we design an LCE with an array of topological defects, where the orientation of the director near each defect core follows a sigmoid function. By tuning adjustable parameters that define the structure of the defect core, we control the resulting surface topography.

*Supported by NSF CMMI-1663041, DMR-1409658, CMMI-1436565, and by the Ohio Supercomputer Center.
10:36AM A30.0001: Active rapid morphing mechanism of the Venus flytrap  JEONGEUN RYU (Presenter), YOËL FORTERRE, IUSTI, CNRS, Aix-Marseille University, Marseille, France — The Venus flytrap (*Dionaea muscipula*) exhibits rapid snapping in about 100 ms, which has long fascinated scientists as one of the fastest botanical movements. Its motion is mechanically initiated by stimulating the trigger hairs, and accelerated by using the snap buckling instability of the poroelastic curved shell geometry of the leaves. At a macroscopic level, its kinematics and dynamics are well understood. However, the mechanism to actively change its natural curvature remains unknown. Here we first characterise the ‘active’ dynamics of the Venus flytrap by removing the buckling instability. We probe the change of its mechanical properties before and after triggering the closure and investigate the key components driving this rapid motion at a microscopic level. Then we elucidate the physical mechanisms underlying the rapid morphing of the Venus flytrap. A better understanding of active movements in plants could allow us to design new rapid and programmable morphing structures.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A31 DSOFT DFD GSNP: Microflows Meet Soft Matter I: Crystals, Colloids, & Particles 503 - Ivan Christov, Purdue Univ - Tag(s): Focus

8:00AM A31.00001: Wetting and dewetting of nanoscale films of nematic liquid crystal*

[Invited]  LINDA CUMMINGS (Presenter), LOU KONDIC, New Jersey Inst of Tech, MICHAEL LAM, Coastal Hydraulics Laboratory, ENSELA MEMA, Mathematics, West Point Military Academy — The evolution of ultra-thin films (tens of nm) of nematic liquid crystals (NLCs) is considered. Such free-surface films can undergo complex dewetting behavior, as observed in experiments. We present a simplified thin-film model for the free surface evolution that includes strong spatially-varying planar anchoring at the substrate, and weak antagonistic anchoring at the free surface. A number of large-scale simulations are presented, showing good qualitative agreement with experiments. Ongoing work including the effect of spatially-varying electric fields on film evolution is briefly highlighted.

*NSF DMS 1815613
8:36AM A31.00002: A phase-field model for a modulated-disordered interface with varying density* EDUARDO VITRAL (Presenter), PERRY H. LEO, JORGE VINALS, University of Minnesota — Soft modulated phases have been shown to undergo complex morphological transitions at high temperatures, in which the orientation of their layers and the Gaussian curvature play a major role. This is the case of smectic films under thermal treatment, where focal conics can be reshaped into conical pyramids and concentric ring structures. While evaporation-condensation mechanisms have been theoretically and numerically studied for a smectic-isotropic interface, hydrodynamic stresses at the interface and their resulting flows are yet to be analyzed. This is particularly challenging in the case of a smectic-air boundary, due to the large density ratio between the phases. We derive a phase-field model that accounts for a varying density field and represents the smectic layering by an order parameter. The resulting equations govern the evolution of an interface between a modulated and a disordered phase with distinct densities, being able to account for compressibility effects at the interface and accommodate topological transitions. By integrating the equations in time, we investigate the interfacial flow on a disturbed smectic, and verify the implementation based on the derived dispersion relation.

*We thank the support from UMN MSI and XSEDE. EV has been supported by UMN DDF.

8:48AM A31.00003: Non-reciprocal motion in superparamagnetic magnetoelastic membrane patches* CHASE BRISBOIS (Presenter), Northwestern University, MYKOLA TASINKEVYCH, Department of Physics, University of Lisbon, MONICA OLVERA DE LA CRUZ, Northwestern University — Magnetic fields allow for the remote manipulation of bio-orthogonal microscale robots that have applications in drug delivery or microsurgery. We develop a theoretical approach for autonomous locomotion of superparamagnetic membranes through viscous media. Oscillations in triaxial magnetic fields induce non-reciprocal, wave-like motions on circular membrane patches. We show how the strength, angle and frequency of rotating magnetic fields affects circumferential and radial membrane wave propagation. Using the lattice Boltzmann method, we implement hydrodynamic interactions that reveal the flow field of the surrounding fluid and show how truncated circular patches swim at low Reynolds numbers.

*This work is funded by the Center for Bio-Inspired Energy Science (CBES), and Energy Frontier Research Center funded by the Department of energy. DE-SC0000989.

9:00AM A31.00004: Particle motion nearby rough surfaces CHRISTINA KURZTHALER (Presenter), AMIR PAHLAVAN, LAILAI ZHU, HOWARD A STONE, Department of Mechanical and Aerospace Engineering, Princeton University — Interactions between particles and boundaries are ubiquitous in nature and play a pivotal role in microfluidic applications. Here, we study the hydrodynamic couplings between particles and solid, rough boundaries that are characterized by periodic and random surface shapes. Using the Lorentz reciprocal theorem, we derive analytical expressions for the mobility tensor of a spherical particle and investigate its gravity driven sedimentation near a random rough wall. Our theory and experiments show that the particle exhibits translation perpendicular to the gravitation force, in striking contrast to its motion near a planar wall, and follows the surface shape in close proximity to the boundary. Overall, our results should lay the foundation to study microswimmer motion close to random, heterogeneous boundaries.
Growth of clogs in parallel microchannels

EMILIE DRESSAIRE (Presenter), Department of Mechanical Engineering, UCSB, EMMANUEL VILLERMAUX, Universite Aix Marseille, ALBAN SAURET, Department of Mechanical Engineering, UCSB — During the transport of colloidal suspensions in microchannels, the deposition of particles can lead to the formation of clogs. Once a clog is formed in a microchannel, advected particles form an aggregate upstream from the site of the blockage. This aggregate called filter cake grows over time, which leads to a dramatic reduction of the flow rate. We present an analytical description that captures the time evolution of the volume of the aggregates. The results are compared with experiments performed using a pressure-driven suspension flow in an array of parallel microchannels. The coupled dynamics of the aggregates is key to bridge clogging at the pore scale with macroscopic observations of the flow rate evolution at the filter scale.

Flow and Fouling in Elastic Membrane Filters with Complex Pore Morphology

PEJMAN SANAEI (Presenter), Mathematics, New York Institute of Technology, SHI YUE LIU, ZHENGYI CHEN, Mathematics, New York University, Shanghai — Filtration technology has been increasingly used for industrial purposes and the study of membrane science is beneficial for filtration efficacy prediction and performance analysis. Real membranes have complex geometry, with pores inside the membrane branch and interconnected with each other. Membrane fouling, as an indispensable consequence for removing particles, occurs in course of filtration process and deteriorates the membrane permeability. In this work, we consider standard blocking as a fouling mechanism, which decreases membrane porosity. However, for membranes with elastic materials, the pressure within the membrane results in membrane pore radius expansion and further influences the filtration performance. We present a mathematical model with multi-layer bifurcating interior morphology, where two pervasive filtration forcing mechanisms are considered: (i) constant pressure drop; and (2) constant flux through membrane.

*P.S. acknowledges financial support form the NYIT Dean's Faculty Development Fund and the NSF ResearchTraining Group in Modeling and Simulation Grant No. RTG/DMS-1646339. Z.C. and S.Y.L. acknowledge financial support in part by the Summer Undergraduate Research Experience offered by the Courant Institute, New York University.
9:36AM A31.00007: Hydrodynamic shock and instability in sedimenting colloidal suspensions along a surface*

SHAKE KARAPETYAN (Presenter), SAM WILKEN, MICHIO TANAKA, BRENNA SPRINKLE, ALEKSANDAR DONEV, PAUL M CHAIKIN, New York Univ NYU — We combine experiments, large-scale simulations, and a continuum model to study the emergence of a coherent density profile in a suspension of passive particles sedimenting near an inclined plane. Sedimenting colloids form a shock when there are sharp density gradients in the suspension and agree well with a solution to a modified Burger's equation. We also observe the formation of an instability at the front of the shock that is different from the case of driven microrollers¹ and other fluid-like instabilities in that the amplitude does not grow exponentially. The instability is characterized by a wavelength controlled by the gravitational height, the typical height of the particles above the inclined plane.


*This work was supported primarily by the MRSEC Program of the National Science Foundation under Award Number DMR-1420073.

9:48AM A31.00008: Unsteady Sedimentation of a Colloidal Sphere in a Horizontal Channel*

LAUREN ALTMAN (Presenter), DAVID G GRIER, New York Univ NYU — The elementary system of a sphere sedimenting through a viscous fluid under gravity becomes remarkably difficult to treat analytically when the host fluid is bounded by parallel horizontal walls. The simplest treatment, due to Oseen, involves linear superposition of Faxén's classic single-wall correction to the mobility. We investigate the limits of the Oseen superposition approximation in this canonical system by measuring the trajectories of colloidal spheres sedimenting through water in slit pores. Measurements are performed by lifting solid or liquid droplets to the top glass-water interface with holographic optical tweezers and tracking their descent with nanometer precision by interpreting holographic video microscopy data with the Lorenz-Mie theory of light scattering. This analysis also yields precise measurements of the particles' refractive indexes that can be interpreted with Maxwell Garnett effective medium theory to estimate the particles' buoyant masses. Agreement between the hydrodynamic theory and these measurements establishes the limits of validity of the measurement technique and the hydrodynamic model.

*This work was supported by the MRSEC program of the NSF under Award Number DMR-1420073, as well as by the SBIR program of the NIH under Award Number R44TR001590.
Stresslet of colloidal suspensions in a spherical cavity

EMMA DEL CARMEN GONZALEZ GONZALEZ (Presenter), ROSEANNA ZIA, Chemical Engineering, Stanford University — Early studies of force and torque hydrodynamic functions for a colloid in a spherical cavity\(^1\text{-}^3\) paved the way to more sophisticated computational methods, such as the Confined Stokesian dynamics algorithm\(^4\text{-}^5\). However, these studies are restricted to equilibrium situations owing to the lack of stresslet coupling. Currently, the study of confined colloids is gaining traction given its direct application to intracellular transport. In cells, the dynamics are driven out-of-equilibrium by active transport, concentration gradients, and metabolic responses. Furthermore, a predictive model for intracellular transport needs to characterize rheological parameters (\(\eta, OP, \ldots\)), this is only possible by accurately incorporating the stresslet coupling. Here we present the exact solution for stresslet hydrodynamic functions of a colloid in a spherical cavity, and its application to more concentrated suspensions via the Confined Stokesian dynamics algorithm. With this algorithm, we predict high-frequency dynamic viscosities that show non-monotonic behavior throughout the confined domain.


Shape induced segregation and anomalous diffusion of particles under confinement

JIYUAN LI (Presenter), ABHINENDRA SINGH, XIKAI JIANG, University of Chicago, JUAN P. HERNANDEZ-ORTIZ, Colombia/Wisconsin One-Health Consortium, Universidad Nacional de Colombia-Medellin, JUAN DE PABLO, HEINRICH M. JAEGGER, University of Chicago — Diffusive behaviors in a confined environment is a fundamental problem that finds applications in various areas of science and engineering, including cells, supercooled liquids, and mesoporous materials, etc. These behaviors should intuitively be affected by particle shapes and concentrations. However, these effects remain poorly understood due to the computational difficulties in solving hydrodynamic interactions (HIs) between arbitrarily shaped particles in confined space. Here, an immersed boundary–General geometry Ewald-like method (IB-GgEm) is adopted to simulate the dynamics of a mixture of particles of different shapes and relative concentrations with the consideration of both short- and long-range fluctuating HIs. We find that increasing the fraction of cylinders induces particle segregation, where the spherical particles are pushed towards the wall, while the cylinders prefer to be near the center of the cavity. In addition, increasing the fraction of cylinders also affects the diffusive-to-anomalous transition and the degree of anomaly. We believe that our results offer a pathway to understanding fundamental questions in biology, e.g., anomalous macromolecular diffusion in cells, and serve as a route to design and optimize drug-delivering platforms.
10:24AM A31.00011: Equilibrium diffusion, thermodynamics, and rheology of confined Brownian suspensions*  ALP SUNOL (Presenter), ROSEANNA ZIA, Department of Chemical Engineering, Stanford University — Computational modeling of spherically confined, hydrodynamically interacting colloids has led to a new framework for modeling biological cells. While modeling of cellular behavior is robust in atomistic-scale structural biology, with little time evolution, and kinetics-based systems-biology, which abstracts away space, many cellular processes operate over colloidal length scales, where interparticle interactions and particle motion play central and nontrivial roles in whole-cell behavior. Here, we present the results of our dynamic simulation studies using both Confined Stokesian Dynamics and Confined Brownian Dynamics algorithms. We compare the role of thermodynamic structure induced by confinement on the short- and long-time transport properties with and without hydrodynamic interactions. Additionally, we find relations between the variables of particle size and volume fraction within the confinement to rheological properties, such as osmotic pressure and viscosity, and highlight how these findings can play an important role in understanding how prokaryotic cells regulate their function.

*This work was supported in part by a National Science Foundation DGE grant No. 1656518 as well as a J. Hewes Crispin and Marjorie Holmes Crispin Stanford Graduate Fellowship.

10:36AM A31.00012: Auto-phoretic nanorods driven up the wall by gravity  QUENTIN BROSSEAU (Presenter), University of Pennsylvania, FLORENCIO BALBOA USABIAGA, Simons Foundation, ENKELEIDA LUSHI, Applied Mathematics, New Jersey Institute of Technology, YANG WU, Department of Chemistry, New York University, LEIF RISTROPH, CIMS, New York University, MICHAEL WARD, Department of Chemistry, New York University, MICHAEL JOHN SHELLEY, JUN ZHANG, CIMS, New York University — Gravitaxis is the directed upward motion of micro-organisms against gravity, and is observed for a few ciliated organisms like Chlamydomonas, Euglenas or Paramecium. Lacking a dedicated sensor, their gravitactic response relies on bottom-heaviness or shape anisotropy to induce a bias in their swimming direction.

Here we study the gravitaxis of heavy self-electrophoretic Janus nanorods that move upwards on a steeply inclined substrate. Comparisons in experiments and simulations between homogeneous and bottom-heavy nanorods reveals two mechanisms contributing to the gravitactic response of the latter: a buoyancy torque and hydrodynamic interactions with the wall. We show that lubrication forces induce an effective fore-aft asymmetry on nanorods that reinforces the orientation bias to move up the steep wall against gravity.
When microrollers meet anisotropy

ERNEST VAN DER WEE (Presenter), Northwestern University, RAMAKRISHNA KOTNI, ALFONS VAN BLAADEREN, Utrecht University, MICHELLE R DRISCOLL, Northwestern University — Driven colloidal particles can display an array of collective effects. Here we study a system in which these collective interactions are largely driven by hydrodynamics: microrollers. Microrollers can be experimentally realized by driving (weakly) magnetic colloidal particles suspended in a liquid above a wall with a rotating magnetic field. Using fluorescence microscopy and particle tracking we can study their response to the field, as well as their collective interactions. Here, we study how anisotropy in the shape of the rollers alters their dynamics. We explore the collective response of rod-shaped hematite-silica microrollers and how this response is modified by adjusting their concentration and shape. Additionally, we study the role of the alignment of the magnetic moment of the rollers with respect to the anisotropic axis of the rollers themselves. Finally, we will show how these microrollers interact with passive obstacles.

This work is funded by NSF PMP-1706562.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A32 DPOLY: Polymer Networks, Gel, and Elastomers: Fabrication and Architecture 504 - Frederick Phelan, National Institute of Standards and Technology
- Tag(s): Focus

Mechanophore with analogue force readout in a polymer network

KAIKAI ZHENG (Presenter), YIFAN ZHANG, Institute for Basic Science, LINGXIANG JIANG, Jinan University, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences, STEVE GRANICK, Institute for Basic Science — Polymer networks are fundamental from materials science to cellular biology, however their intrinsic properties are normally characterized using common ensemble-averaged methods. In this work, we introduce a synthetic mechanophore to read out the local force, and to show the proof of concept we covalently link it into a PMA (polymethylacrylate) network as crosslink. We observe differing local intensities of different mechanophores as well as their differing evolution during stretch, and from this quantify locally non-affine responses. Interestingly, it seems to be the single-molecule response yet with analogue force readout inaccessible using conventional mechanophores based on irreversible bond scission mechanisms.

This work was supported by the taxpayers of South Korea through the Institute for Basic Science.
Extending the Real Elastic Network Theory to Account for Cooperative Effect of Cyclic Defects

TZYY-SHYANG LIN (Presenter), Massachusetts Institute of Technology MIT, RUI WANG, University of California, Berkeley, JEREMIAH JOHNSON, BRADLEY OLSEN, Massachusetts Institute of Technology MIT — The real elastic network theory, or RENT, has provided insights into how cyclic defects within a phantom network lead to significant lowering of the modulus of polymer networks. However, RENT is a linear theory derived under the ideal loop gas assumption, which is strictly true only in the limit of infinite dilution of defects, rendering RENT inapplicable for networks with nonnegligible loop fraction. To go beyond the linear regime, the cooperative effects of multiple loops are investigated. First, the multi-defect effect is studied through the Virial expansion, in which the behavior of adjacent loops is compared to isolated loops. In most cases, it was found that the Virial coefficients vanish identically except for the first order terms, indicating that the results for the linear approximation are exact. Next, a nonperturbative probability-based theory was developed to capture the nonlinear behaviors. As expected, the nonlinear theory gave predictions almost identical to that of the linear theory in the small loop fraction regime. However, as loop fraction is increased, the nonlinear theory predicts a significant negative deviation from the linear theory, qualitatively matching the behavior observed in experiments.

*This work was supported by the Dow Chemical Company.

WITHDRAWN ABSTRACT

Reactivity-property relationships in photocontrolled polymer networks

JULIA KALOW (Presenter), Chemistry, Northwestern University — In polymer networks based on dynamic covalent bonds, changes in reactivity can be translated into macroscopic responses. Light offers precise, tunable, and noninvasive spatiotemporal control over molecular reactivity. In polymer networks based on dynamic covalent bonds, these changes in reactivity can be translated into macroscopic responses. The Kalow lab has designed crosslinks that allow us to tune the thermodynamics and kinetics of dynamic covalent bonds with light, including visible light, based on the conformation of an adjacent photoswitch. When incorporated into polymer networks, the stability or lifetime of these dynamic covalent bonds can be tuned with light. I will discuss our efforts to elucidate the molecular mechanism underlying these macroscopic changes, as well as rational optimization of the photoswitch to enable applications in 3D cell cultures and recyclable elastomers.

*This material is based upon work supported by the National Science Foundation under grant no. CHE-1847948.
Belousov Zhabotinsky reaction systems: How “far” is far from equilibrium?

VANDANA RAJPUT (Presenter), PRATYUSH DAYAL, Indian Inst of Tech Gandhinagar — Understanding the behaviour of dynamical systems that are far from equilibrium has been a challenge for science and engineering. Belousov Zhabotinsky (BZ) reaction is a system that exhibits chemical oscillations due to periodic oxidation/reduction of the metal ion catalyst. In essence, the oxidized catalyst concentration varies with time crossing its steady state (SS) concentration with each oscillation. Mathematically, the Limit Cycles (LC), which represent self-sustained oscillations occur when the equilibrium (or SS) loses its stability via Hopf bifurcation. The LC resulting from HB, typically, surrounds the equilibrium, which is analogous to variation of oxidized catalyst concentration around SS. Using the Oregonator model, however, we demonstrate that the equilibrium point can be outside the LC under special conditions. Further, we use the nonlinear stability analyses and calculate Lyapunov coefficients to quantify how “far” the LCs are from the corresponding “equilibrium”. In addition, we predict the amplitude and frequency of oscillations, which are in good agreement with our simulation results. These findings can not only be used to characterise behaviours of nonlinear dynamical systems but can also be used to design smart functional materials.

DST-SERB (EMR/2016/007778)

General Approach to Photo-Crosslink Bottlebrush Polymers

RENXUAN XIE (Presenter), SANJOY MUKHERJEE, VERONICA REYNOLDS, CHRISTOPHER BATES, MICHAEL L. CHABINYC, University of California, Santa Barbara — Entanglement-free bottlebrush polymers can form exceptionally soft networks that are compelling in applications ranging from mimics of biological tissue to sensor skins. Controlled polymerizations provide a route to synthesize precisely defined bottlebrush polymers, but require crosslinking to form networks. We have developed a general strategy to photo-crosslink bottlebrush precursors with miscible bis-benzophenone-based additives in ambient conditions without solvent. We demonstrate that this approach is effective with a wide variety of different side-chain chemistries including acrylates, esters, and siloxanes. Current bottlebrush network models assume all crosslinks are elastically effective, which is inadequate for our randomly crosslinked networks formed with benzophenone-based additives. We present a modified Phantom network model that is capable of distinguishing elastically effective crosslinks from the ineffective ones. This model is validated by examining the moduli of networks formed from bottlebrush polymers with different molar masses and side-chain chemistries. We also experimentally verified the minimal amount of crosslinkers predicted to achieve the lowest network modulus and high gel fraction.

Mitsubishi Chemical Center for Advanced Materials
9:36AM A32.00007: Gel Formation in Urethane Liquid Oligomers  PRAVEEN AGARWAL
(Presenter), BOB SAMMLER, LUIGI PELLACANI, ASJAD SHAFI, PRAVEENKUMAR
BOOPALACHANDRAN, DAVID REUSCHLE, Dow — The phenomenon of gel formation is ubiquitous for various materials including polymer solutions, ionomers, biomaterials, and consumer household products. Developing a physical understanding of the interactions that lead to gel formation is essential for rational material design, and controlling the gel formation characteristics is a topic of significant interest. We have investigated a physical gel formed in a urethane oligomer system dispersed in an organic solvent. The mechanism of gel formation was investigated by rheology, polarized optical microscopy and FTIR. We find evidence of hydrogen bonding and ordered structure formation in the gel. Additionally, a rheology-based technique was developed to predict the gel formation characteristics.

9:48AM A32.00008: Modelling Intermolecular Cross-Linking in Collagen Fibrils  MATTHEW LEIGHTON (Presenter), LAURENT KREPLAK, ANDREW RUTENBERG, Dalhousie Univ — Collagen fibrils are microscopic molecular ropes that are structural components in many animal tissues. We present an equilibrium coarse-grained model for the structural and mechanical properties of these cross-linked fibrils. We model enzymatic cross-links as anisotropic Gaussian chains, which allows us to approximate their free-energy contributions. We add additional terms in the free energy for the Frank elastic energy due to the orientation of collagen molecules within the fibril, for the surface tension, and phase-field crystal terms which account for the D-band density modulations observed along the length of collagen fibrils. We computationally minimize the sum of these free-energy terms with respect to imposed strain fields acting on the fibril to obtain equilibrium structures. Using this framework we investigate the effect of strain on various important structural and mechanical properties of the fibril, such as the molecular director field and the stress-strain curve.

10:00AM A32.00009: From Gels to 3-D Networks: Creating Multifunctional Polymer-silica Nanofiber based Aerogels  TAHIRA PIRZADA (Presenter), ZAHRA ASHRAFI, WENYI XIE, SAAD KHAN, North Carolina State University — Gels containing water or solvents abound in applications with considerable efforts being made to fabricate new ones with enhanced functionalities. An area that remains less explored is the creation of aerogels by replacing the liquid matrix of gels with air. Can we preserve the structure of these systems on liquid removal and can we create materials that are just as versatile by doing so? We present a facile and sustainable solid templating approach to fabricate highly porous, flexible aerogels of hybride nanofibers of cellulose acetate and silica which are produced via sol gel electrospinning. SEM micrographs demonstrate a hierarchical architecture consisting of large secondary pores (30-50 μm) interconnected by a network of entangled nanofibers with 2-5 μm primary pores. XPS and in-situ FTIR studies provide evidence that thermal treatment of as-prepared aerogels results in crosslinking the silica-CDA network therefore enhancing their mechanical stability and hydrophobicity without compromising their low bulk density (~10 mg.cm⁻³) and porosity (>98%). Thermal studies demonstrate highly enhanced thermal stability and flame retardancy. These functional features together with ease of processing make these aerogels just as promising, if not more, than their liquid-based analogs!
10:12AM A32.00010: Probing the distribution of localization lengths in amorphous solids via wavelength-dependent elasticity  BOLI ZHOU (Presenter), RAFAEL HIPOLITO, PAUL GOLDBART, University of Texas at Austin — The amorphous solid state exhibited, for example, by randomly crosslinked macromolecular systems has two distinguishing features: (i) it arises via a continuous transition controlled by the crosslink density; and (ii) as a result of the intrinsic randomness, the state is described by a distribution of single-particle localization lengths. Owing to the continuity of the transition, in its vicinity the localization-length distribution is concentrated predominantly at intermediate lengthscales, i.e., lengthscales larger than microscopic but not truly macroscopic. We report on the development of an elasticity theory for the amorphous solid state that is valid not only in the limit of long-wavelength strains but also for strains at wavelengths corresponding to intermediate lengthscales. The corresponding wavelength-dependent shear modulus is sensitive to the distribution of localization lengths, diminishing monotonically with decreasing lengthscale -- a physical reflection of the idea that elasticity at a given lengthscale is primarily supported by particles localized on that or shorter lengthscales. The dependence of the shear modulus on wavelength therefore provides an experimental pathway to probing the distribution of localization lengths.

10:24AM A32.00011: Asynchronous Dynamics in Crosslinked Polymer Networks*  KETAN S KHARE, FREDERICK PHELAN (Presenter), National Institute of Standards and Technology — Recently, we successfully applied time-temperature superposition to obtain master curves of the mean squared displacement (MSD) of atoms in a cross-linked epoxy using atomistic simulations. The resulting curves extend to a macroscopic time-scale \(10^9\) s and can be quantitatively compared with creep compliance obtained from experiments. Here, we show that the MSD trends of the center of mass of molecular units can also be superposed using identical shift factors. Comparison of the master curves and time-scaling exponents of different molecular moieties shows that units which differ in their topological constraints exhibit asynchronous dynamics. We call this feature topology-induced asynchronous (TIA) dynamics and define it as the temporal difference in the dynamics of atoms in a network that vary in their topological constraints. TIA dynamics arise due to the interplay between the chemistry of the epoxy monomer and the crosslinker. We discuss the role of asynchronous dynamics in the thermomechanical behavior of polymer networks composed of non-Gaussian monomers, and how chemistry-specific topological details are important for controlling the polymer dynamics.

*NIST MML-PREP grant 70NANB16H005 to Georgetown University.
XSEDE resources via NSF grant ACI-1053575.
**10:36AM A32.00012: Probing rheology and mechanics of compressed microgel suspensions**

SVETOSLAV NIKOLOV (Presenter), ALBERTO FERNANDEZ-NIEVES, ALEXANDER ALEXEEV, Georgia Inst of Tech —

The unusual and adjustable mechanical properties of compressed microgel suspensions arise from the high deformability and responsiveness to external stimuli, such as temperature and pH, of the constituent microgel particles. Compressed microgel suspensions exhibit a three order of magnitude difference between the bulk and shear moduli that can be further altered by applying an external stimulus which drives the swelling transition in microgels. These properties make compressed microgel suspensions ideal for the development of new materials able to autonomously recover their internal structure after mechanical damage. We use mesoscale simulations to understand the mechanical and rheological response of compressed microgel suspensions and to establish how this response depends on the properties of individual microgels. Our findings show that at high packing fractions deformation occurs mainly as a result of particles shrinking, indicating particle interpenetration is relatively small. We further show that rheological and mechanical responses of the suspensions are directly related to the single particle modulus that sets the scale for particle shrinking.

*This work is supported by NSF DMR-1255288 and DMR-1609841. Simulations used XSEDE resources, supported by NSF ACI-1548562.

**10:48AM A32.00013: Energy Renormalization Approach to Coarse-Grained Epoxy Resins**

ANDREA GIUNTOLI (Presenter), Northwestern University, ZHAOXU MENG, Clemson University, NITIN HANSOGE, SINAN KETEN, Northwestern University —

Cross-linked networks of epoxy resins are ubiquitous materials with a broad range of applications, thanks to the flexibility in their chemical composition that can be fine tuned to obtain the desired properties. The huge parameter space makes it challenging to optimize the material, and modeling efforts can greatly contribute to their development. In particular, many properties of epoxy resins stem from fundamental features like cross-linking density, dynamical heterogeneity and relaxation phenomena that do not depend on the fine atomistic structure of the system.

We developed a new coarse-grained molecular dynamics model for epoxy resins. Thanks to a novel energy renormalization technique, the model parameters can be tuned to match the dynamics and mechanical properties of atomistic simulations over a wide range of temperatures. The coarse-grained nature of the model allows for increased computational efficiency and focus on fundamental physical properties of the resin. We show how tuning these properties affects the dynamical and mechanical behavior of the network.

By highlighting the role of relevant features, the results obtained with this model can guide and accelerate the molecular design and optimization of epoxy resins.

*CHiMaD, award #70NANB14H012 founded through NIST
8:00AM A33.00001: Nanoparticle Structure and Dynamics in Polymer Nanocomposites*  
[Invited]  MICHAEL HORE (Presenter), Case Western Reserve University — The physical properties of polymers can be significantly altered both by embedding nanoparticles within them and by grafting them to nanoparticle surfaces. The ability to predict and measure the structure, dynamics, and thermodynamics of grafted polymers is central to purposefully creating new nanocomposite materials. In particular, one powerful technique for studying these aspects of nanocomposites is neutron scattering. This talk will review recent work we have performed to study the behavior of nanoparticles in nanocomposite materials, with a focus on nanorods and nanospheres. Small-angle neutron scattering measurements of poly(ethylene oxide)-grafted Au nanorods, poly(methyl acrylate)-grafted SiO$_2$ nanospheres, and poly(methyl methacrylate)-grafted Fe$_3$O$_4$ nanospheres will be discussed, along with approaches to interpret the scattering results. The conformation of the grafted polymers will be compared between solution and nanocomposite states. Neutron spin echo measurements of the relaxation dynamics of grafted chain will be discussed, along with opportunities for future research and measurements.

*A portion of this research was funded by the NSF Polymers program (DMR-1651002).

8:36AM A33.00002: Hybrid nanoparticles with continuously tunable scattering length density for the analysis of phase separation in mixed colloidal systems*  
YUE ZHAI, JIN HAN, Carnegie Mellon Univ, WENJIE WU, Chemical and Biomolecular Engineering, University of Houston, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon Univ, ALAMGIR KARIM, Chemical and Biomolecular Engineering, University of Houston, MICHAEL BOCKSTALLER (Presenter), Carnegie Mellon Univ — The modification of nanoparticle surfaces with polymeric chains has emerged as an effective tool to control the interactions and assembly behavior of colloidal systems. Recent results have shown that interactions between chemically distinct polymeric ligands can drive the phase separation of mixed particle systems. This provides opportunities for the fabrication of microstructured hybrid materials that derive functionality from the organization of nanoparticle constituents into microscopic domains.
We will present recent results on the phase separation behavior of polymer tethered particles in thin films. In the thin film state, phase separation resembles the corresponding linear polymer blends provided the length of polymer ligands exceeds a threshold value. However, domain growth kinetics differs from the prediction for diffusion-controlled systems. To elucidate the origin of this deviatory behavior, small angle neutron scattering is performed in the bulk state. A method enabling the continuous variation of the scattering length density of nanoparticles will be presented and its application to the SANS analysis of phase separation in mixed brush particle systems will be demonstrated.

*The authors acknowledge financial support by the Department of Energy via award DE-SC0018784.
**8:48AM A33.00003: Fast solvent induced switchable phase-states of binary polymer-grafted nanoparticle blends**

WENJIE WU (Presenter), MANINDERJEET SINGH, Department of Chemical and Biomolecular Engineering, University of Houston, XIAOTENG WANG, Department of Polymer Engineering, University of Akron, YUE ZHAL, Department of Materials Science and Engineering, Carnegie Mellon University, ZONGYU WANG, Department of Chemistry, Carnegie Mellon University, TANGUY TERLIER, Shared Equipment Authority, SIMS laboratory, Rice University, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, MICHAEL BOCKSTALLER, Department of Materials Science and Engineering, Carnegie Mellon University, ALAMGIR KARIM, Department of Chemical and Biomolecular Engineering, University of Houston — Polymer-grafted nanoparticles (PGNPs) have potential applications in nanoelectronics, photonic devices, and as tough materials with tunable enhanced mechanical properties. However, these applications require the particles to form well-controlled structures. We hypothesize that these can be achieved through liquid-enabled phase-separation as a facile approach. To this end, we developed a method to switch the state of phase-separated structures in a binary blend film of PGNPs, poly (methyl methacrylate) silica (PMMA-SiO\(_2\)) and poly(styrene) silica (PS-SiO\(_2\)), by using a direct solvent immersion annealing (DIA) method. Our results show that by varying the solvents in the DIA solution, interchangeable phase-separated and homogeneous morphologies are formed in the PMMA-SiO\(_2\)/PS-SiO\(_2\) blends within 1 minute. Such homopolymer matrix free PGNP only blend systems are novel, and these switchable transitions are not readily obtainable by thermal annealing due to the large masses and the athermal property of PGNPs involved.

*DOE GRANT #: DE-SC0018854*

**9:00AM A33.00004: PEO / SiO\(_2\) nanocomposites: Correlating Polymer Morphology to Rheological Properties**

KIRIAKI CHRISSOPOULOU (Presenter), SOKRATIS KOGCHYLAKIS, SPIROS H. ANASTASIADIS, FORTH-IESL and Univ. of Crete — Polymer nanocomposites, comprised of a polymer matrix and inorganic additives, possess improved and often innovative physicochemical properties compared to conventionally filled systems. In this work we report on the rheological behavior of a series of poly(ethylene oxide) / silica, PEO/SiO\(_2\), nanocomposites through oscillatory shear rheology measurements. The nanohybrids were synthesized by dispersing spherical SiO\(_2\) nanoparticles of two different radii within high molecular weight (Mw) PEO at different compositions in order to investigate the effect of the additive on the material rheological properties. PEO crystallinity was found to depend on the degree of spatial confinement that the nanoparticles impose as well as their adsorption capacity. Dynamic time and strain sweep tests verify the material thermal stability and linear viscoelastic behavior whereas dynamic frequency sweeps probe its dynamic response. The effect of nanoparticle size and concentration on the behavior is examined to correlate the morphological changes to the rheological response of the materials in an attempt to better understand the structure-properties relationship.

Acknowledgements: This research has been co-financed by EU and Greek national funds (Action RESEARCH – CREATE - INNOVATE, MIS: 5030174).
**9:12AM A33.00005: Decoupling the polymer dynamics and the nanoparticle network dynamics of polymer nanocomposites through dielectric spectroscopy and rheology**

SHIWANG CHENG (Presenter), JIE YANG, Michigan State Univ, WEI YANG, Sichuan University — The dynamics of polymer nanocomposites (PNCs) are dictated by two intertwining components, the polymer matrix and the nanoparticle network, whose characteristics have not been clearly elucidated. Here, we unravel the salient features of the polymer matrix dynamics and the nanoparticle network dynamics through dielectric spectroscopy and rheology. Dielectric measurements show that the dynamics of the polymer matrix of PNCs are almost identical to the neat polymer. In contrast, rheological measurements exhibit a strong deviation in the dynamics of PNCs from that of the neat polymer. Detailed analyses show that the rheology captures both the contributions of the polymer matrix and the nanoparticle network while dielectric measurements are only sensitive to polymer matrix dynamics. Moreover, the dynamics of the polymer matrix and the nanoparticle network have very different temperature dependences, leading to a dynamic decoupling phenomenon and the breakdown of the time-temperature superposition principle in PNCs.

*This research has been founded by Michigan State University. J. Yang (201706240218) acknowledges the financial support from the China Scholarship Council during his visit to Michigan State University.

**9:24AM A33.00006: Segmental dynamics in matrix-free polymer grafted nanoparticles**

MAYANK JHALARIA (Presenter), Columbia Univ, ERIC RUZICKA, University of South Carolina, MADHUSUDAN TYAGI, NIST Center for Neutron Research, VICTORIA GARCIA-SAKAI, Rutherford Appleton Laboratories, BRIAN C BENICEWICZ, University of South Carolina, SANAT KUMAR, Columbia Univ — Polymer grafted nanoparticle based composite materials display a rich spectrum of complex chain and nanoparticle dynamics. Specifically, composite materials constructed using only polymer grafted nanoparticles display several dynamic anomalies—spanning a large range of time and length scales. We focus on the segmental and local dynamics of polymer chains using spatial and temporally sensitive probes with the view of identifying the primary dynamic driving force for penetrant transport in polymers. The composite materials used in the study exhibit enhanced light gas diffusivities highly dependent on the graft chain length and the grafting density, providing a chemically homogenous platform for identification of the relevant dynamics. We find that the segmental motions are highly accelerated in the composites; these speeded up dynamics appear to correlate with the diffusivities observed for these materials, in contrast to localized side group dynamics which are less affected by grafting and do not seem to affect transport. In fact, side group motion is invariant in the presence of high pressures of CO$_2$ further supporting this assertion.

*National Science Foundation (CBET-1629502)*
**9:36AM A33.00007: Modeling the Entanglement Distribution in Polymer-grafted Nanoparticle Systems**

ROBERT J TANNENBAUM (Presenter), Columbia University, TAIJI MIKAMI, GAETAN MAUREL, MARC COUTY, Michelin, SANAT KUMAR, Columbia University — Polymer nanocomposites have become increasingly useful materials due in part to their ability to provide improved strength and mechanical reinforcement over pure polymer systems. Difficulty controlling nanoparticle dispersion in these nanocomposites has lead researchers to use polymer grafted nanoparticles embedded in matrices of free polymer chains. We believe the nature of the improved mechanical properties in grafted systems is the result of graft chains on different filler particles forming an entanglement network. A computational modeling technique was developed that utilizes slipsprings to model the mobility constraints that physical entanglements impose on individual polymer chains. Focusing on the distribution of entanglements, we found that graft chains appear to be more highly entangled than free chains, irrespective of filler particle loading. The amount of inter-particle graft interactions is also always higher than we would expect if the entanglement pairs were randomly distributed based solely on their probability of occurrence.

*Internership funded by the Investissements d'Avenirprogram “Developpement de l'Economie Numerique” through the SMICE project.

**9:48AM A33.00008: Disentangling the role of chain conformation on the mechanics of polymer grafted nanoparticle materials**

JIARUL MIDYA (Presenter), Institute of Physics, Johannes Gutenberg University Mainz, YU CANG, Max Planck Institute for Polymer Research, SERGEI A. EGOROV, Department of Chemistry, University of Virginia, KRZYSZTOF MATYJASZEWSKI, MICHAEL R. BOCKSTALLER, Department of Materials Science and Engineering, Carnegie Mellon University, ARASH NIKOUBASHMAN, Institute of Physics, Johannes Gutenberg University Mainz, GEORGE FYTAS, Max Planck Institute for Polymer Research — The linear elastic properties of isotropic materials of polymer tethered nanoparticles (NPs) are evaluated using noncontact Brillouin light spectroscopy. While the mechanical properties of dense brush materials follow predicted trends with NP composition, a surprising increase in elastic moduli is observed in the case of sparsely grafted particle systems at approximately equal NP filling ratio. Complementary molecular dynamics simulations reveal that the stiffening is caused by the coil-like conformations of the grafted chains, which lead to stronger polymer–polymer interactions compared to densely grafted NPs with short chains. Our results point to novel opportunities to enhance the physical properties of composite materials by the strategic design of the “molecular architecture” of constituents to benefit from synergistic effects relating to the organization of the polymer component.

*German Research Foundation (DFG) through project NI 1487/2. Further, J. Midya received funding by the Impulsfund of Rhineland Palatinate (Germany).
10:00AM A33.00009: Suppression of Creep in Model Polymer Nanocomposites  ENTAO YANG (Presenter), JAMES PRESSLY, ERIC BAILEY, University of Pennsylvania, BHARATH NATARAJAN, ARUNA MOHAN, ExxonMobil Chemical, KAREN WINEY, ROBERT RIGGLEMAN, University of Pennsylvania — While the elastic properties of polymer nanocomposites (PNCs) have been widely studied, the ability of nanoparticles (NPs) to suppress creep in a polymer matrix has received comparatively less attention, and creep suppression is essential for the use of composites in structural applications. It is believed that the primary mechanism of reinforcement in PNCs is the presence of a layer near the NPs' surfaces where the polymer monomers have modified mobility. Thus, understanding how the dynamics in this layer changes as a function of stress, NP size, and polymer-nanoparticle interaction is critical. In this work, we use molecular dynamics simulation to investigate the PNC's creep response with different NP sizes and polymer-nanoparticle interactions. Our results indicate that the small NPs with strong polymer-nanoparticle interaction can best suppress materials' creep response and stiffen the material. A recently developed, machine-learning field called softness is applied to describe the local structures in our composites. We find that the softness is modified near the NP surfaces and largely reduced for attractive polymer-particle interactions, though the range over which softness is modified differs from the range over which the relaxation time is different from the bulk.

10:12AM A33.00010: Nanoparticles with controllable dispersion and localization in immiscible polymer blends  HUSAM ALKHODAIRI (Presenter), SEBASTIAN T RUSSELL, Columbia University, JULIA PRIBYL, BRIAN C BENICEWICZ, University of South Carolina, SANAT KUMAR, Columbia University — Polymer blending is a versatile route to the development of new polymeric materials with enhanced properties and hence applications. However, the unfavorable interaction between most polymer pairs leads to phase-separated systems with unstable morphologies, weak interfaces and poor properties. The use of nanoparticles (NPs) as interfacial stabilizers has gained momentum recently due to their high surface area and strong adsorption at interfaces, but controlling their dispersion and localization in immiscible polymer blends is a major challenge. Recent work has demonstrated that polymer-grafted NPs, which exhibit surfactant-like properties, can self-assemble into a variety of superstructures that depend on the polymer grafting density (σ) and the graft chain length (N). Here, we will show that the location of polystyrene-grafted NPs within an immiscible blend of polymethyl methacrylate (PMMA)/polystyrene (PS) can be determined using $\sigma N^{0.5}$, the brush crowding parameter, and, $1/\alpha$, which describes the entropic effects associated with a mismatch in brush/matrix polymer chain lengths. Using these parameters, the spatial control over NP segregation in immiscible polymer blends is probed and understood.
10:24AM A33.00011: Polymer/Star-Polymer composites: structure and dynamics of bulk and confined materials*  
JINPENG FAN (Presenter), Department of Physics, Wesleyan University, JACK DOUGLAS, Materials Science and Engineering Division, National Institute of Standards and Technology, FRANCIS STARR, Department of Physics, Wesleyan University — Polymer-grafted nanoparticles (NP) are versatile building blocks to create tunable particle superstructures and polymer nanocomposites with customizable properties. Polymer grafted NP are topologically very similar to star polymers. While nanocomposites with polymer-grafted NP have been explored recently, comparatively little is known about composites consisting of star polymers and chain polymers, or star polymers in polymer thin films. We investigate how both the number of arms and molecular weight affect the morphology of self-assembled structures in both a bulk polymer material and an ultra-thin polymer film. Additionally, we study how star polymers affect the glass transition of these composites and films. In doing so, we also examine how star polymers affect the nature of cooperative molecular motions in the matrix and film, and how this potentially relates to changes in the mechanical and rheological properties of the material.

*This work was supported in part by National Institute of Standards and Technology (NIST) Award 70NANB15H282.

10:36AM A33.00012: Tuning structure and dynamics of segmented ionenes with added spherical nanoparticles  
NICHOLAS LIESEN (Presenter), LISA HALL, Ohio State Univ - Columbus — Segmented ionenes can be synthesized such that short ion-containing segments alternate with uncharged segments. By changing the ratio of relatively soft and hard uncharged segment types, material properties can be easily tuned. Incorporating nanoparticles may allow for further manipulation of structure and mechanical behavior. However, the multiple length/time scales involved, the large parameter space, and the nanoparticles’ tendency to aggregate complicates material design. Using efficient coarse-grained molecular dynamics simulations, we aim to establish architecture-structure-property relationships to guide synthetic efforts. Inspired by experimental ammonium ionenes with short polyethylene segments and long, soft segments (such as polyethylene oxide), we study segmented ionenes and spherical nanoparticles using a simple bead-spring model. Soft segment length, the ratio of the two polymer types, and nanoparticle surface chemistry is tuned and structure and dynamics analyzed. We find weight fraction dependent local microphase segregation of soft and hard polymer segments. We also determine the nanoparticle’s impact on the local structure as a function of weight fraction and chemistry.
Polyelectrolyte-Grafted Nanoparticles in Solution

KOTESWARARAO MEDIDHI (Presenter),
Tennessee Tech Univ, PINAR AKCORA, Stevens Institute of Technology, VENKAT PADMANABHAN,
Tennessee Tech Univ — Polyelectrolytes have found applications in fuel cells, solar cells,
membranes, etc. Here, we investigate the structural and flow properties of polyelectrolyte grafted
nanoparticles (PENP) in a solution using coarse-grained molecular dynamics simulations. The
degree of ionization (pH) and the concentration of PENP in solution are systematically varied. For
low pH, the flow properties are dominated by grafted chain entanglements, while at high pH, the
strong electrostatic repulsions between the ionized groups are the major factor. At intermediate
pH, the hydrogen bonding between the ionized and non-ionized groups along with the
concentration of PENP plays a significant role in dictating the solution viscosity. At low PENP
concentrations, intra-particle hydrogen bonds are formed that lowers the viscosity, while at
higher concentrations, inter-particle hydrogen bonds are formed enhancing the viscosity of the
solution.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A34 DPOLY DSOFT: Confinement, Dynamics, and Ion
Interactions in Ion-Containing Polymers I

8:00AM A34.00001: Ion Transport Mechanisms in Ionomers* AMALIE FRISCHKNECHT
(Presenter), BRYCE THURSTON, JONATHAN BOLLINGER, MARK STEVENS, Sandia National
Laboratories, BENJAMIN PAREN, KAREN WINEY, University of Pennsylvania — An understanding of
dynamics in single-ion conducting polymers, such as ionomers with ionic groups covalently
bonded to the polymer backbone, is needed to design these polymers for use as electrolytes. In
melt ionomers, the ions tend to self-assemble into nanoscale ionic aggregates, and the
morphology of these aggregates affects both the ion and chain dynamics. I will describe the ionic
aggregate and ion dynamics in atomistic molecular dynamics (MD) simulations of precise
polyethylene-based ionomers. In particular, the mechanisms for ion transport are the same as
those found in previous coarse-grained MD simulations. In systems with isolated ionic
aggregates, ions move through a process of aggregates merging, rearranging, and breaking up. In
systems with percolated ionic aggregates, ions "shuttle" along the ionic aggregate. From new CG
simulations, we find that the diffusion constant for ions in systems with percolated ionic
aggregates is inversely proportional to an ion "stepping" time scale, which quantifies the cation-
anion association lifetime.

*This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of
8:12AM A34.00002: Confined polyelectrolyte solution driven by an external electric field
DEBARSHEE BAGCHI (Presenter), MONICA OLVERA DE LA CRUZ, Northwestern University — The transport properties of a dilute polyelectrolyte solution, confined inside a charged cylinder and driven by a constant external electric field, are studied using coarse-grained molecular dynamics simulations. The polyelectrolyte is negatively charged and modeled as linear bead-spring chains with explicit monovalent counterions and implicit solvent. We find that, when the confinement walls are negatively charged, the polyelectrolyte mobility is independent of the confinement charge density, whereas, when they are positively charged, the counterion mobility exhibits an intriguing non-monotonic dependence on the surface charge density. We study the dependence of the transport features on the diameter of the confinement, the presence of polarization effects, and on multivalent salts. We also study the mobility of the polyelectrolyte solution when the counterions of the charged surface are placed outside the confinement. In this case, the mobilities remain practically unaffected by the surface charge density, unless excluded volume effects become important.

*This work has been funded by NSF DMR Award No.1611076.

8:24AM A34.00003: Ion Correlations and Transference Number in Model Polymer Electrolytes: Effects of Ion Size and Dielectric Strength
KUAN-HSUAN SHEN (Presenter), LISA HALL, Ohio State Univ - Columbus — Salt-doped polymers have potential as safe electrolytes for batteries but suffer from low ion conductivity. Using bulky anions with delocalized charge may reduce ion agglomeration and increase conduction. However, size asymmetry between ions may increase preferential solvation of cations versus the larger anions, lowering the transference number $t^+$ (fraction of conductivity contributed by the cation). Here, we use coarse-grained molecular dynamics simulations, including a $1/r^4$ potential to capture size-dependent solvation effects, to relate polymer and ion chemistry to $t^+$ and overall conductivity. We calculate conductivity from ion mobilities in an external electric field, which improves accuracy versus the typical use of fluctuation dissipation relationships. We find that there is a discrepancy in $t^+$ estimated from ion diffusion constants and $t^+$ calculated from ion mobilities, especially at large ion size asymmetry or when ion-polymer interactions are strong. By understanding the impact of ion size, polarizability, and polymer dielectric strength on ion correlations, diffusion, and transference number, we aim to help guide design of future materials with improved conduction.

*This work is supported by the National Science Foundation under Grant 1454343.
**8:36AM A34.00004: Influence of Water Content and Morphology on Proton Transport in Biocompatible Conductive Polymer Membranes**

GLORIA BAZARGAN (Presenter), SEAN A FISCHER, DANIEL GUNLYCKE, United States Naval Research Laboratory — Proton transport plays a critical role in many biological processes, including chemical signaling to cells within the human body. Devices that control the flow of protons to biological systems for medicinal and therapeutic purposes are known as bioprotonic devices, and they depend on conductive polymer membranes to facilitate proton transport. The development of bioprotonic devices demands proton-conducting polymers with suitable transport properties and biocompatibility. Herein, the results of theoretical investigations on the transport properties of candidate polymer membranes for bioprotonic devices are described. The effects of water content and morphology on proton transport in these candidate polymer systems are established. This provides a theoretical basis for the design optimization of bioprotonic devices that incorporate biocompatible proton-conducting polymer membranes.

*This work was supported by the Office of Naval Research through the U.S. Naval Research Laboratory.

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**8:48AM A34.00005: Effects of Homopolymer Additives on Conductivity of Salt-Doped Block Copolymers from Molecular Dynamics Simulations**

MENGDI FAN (Presenter), LISA HALL, Ohio State Univ - Columbus — As promising solid electrolyte materials for batteries, salt-doped block copolymers (BCP) simultaneously have ionic conductivity and mechanical robustness, due to the combination of two distinct polymer types. Recent experiments revealed that homopolymer additives, at high enough molecular weight (MW), can increase ionic conductivity in such systems. To understand this effect and guide further study, we employ coarse-grained molecular dynamics (MD) simulations. We analyze the microphase distribution of added homopolymers in salt-doped BCPs and relate this to the overall dynamics and ion conductivity. In particular, we find that longer homopolymers form an interlayer in the middle of the conducting microphase, while shorter chains are more fully integrated across the conducting microphase. This leads to a greater degree of overlap of the ion and homopolymer density profiles with increasing homopolymer MW, which may explain the increased conduction with MW. Ion concentration, segregation strength, and ion solvation energy also affect the ion distribution and can potentially be adjusted to enhance ionic conductivity.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award DE-SC0014209*
9:00AM A34.00006: Can solvation free energy rationalize the phase behavior of ion-doped copolymers?  JIAN QIN (Presenter), KEVIN J HOU, Stanford Univ, WHITNEY LOO, NITASH BALSARA, Chemical Engineering, University of California Berkeley — Previous experimental studies have established the pronounced effects of salt-doping on the morphological behavior of copolymers. The ionic solvation free energy has been recognized as an important factor for this doping effects, which has been encapsulated into an effective $\chi$ parameter that scales linearly with salt concentration. However, no general agreement between experimental and theoretical phase diagrams has been reached. By employing a recently developed ‘free’ ion model for salt-doped copolymers and cultivating the rich experimental data in literature, we show that, for two different molecular weights and over a range of compositions, the morphological variations can be captured by the solvation free energy alone, if the solvation radius is treated as an adjustable parameters.

9:12AM A34.00007: Densely Grafted Polyelectrolyte Brushes Trigger “Water-in-Salt” like Scenarios and Ultraconfinement Effect*  HARNOOR SINGH SACHAR (Presenter), TURASH HAQUE PIAL, PARTH RAKESH DESAI, SAI ANKIT ETHA, YANBIN WANG, PETER W. CHUNG, SIDDHARTH DA, Mechanical Engineering, University of Maryland, College Park — Polyelectrolyte (PE) brushes find use in a plethora of applications like current rectification, ion sensing, biosensing, nanoscale energy conversion etc. We carry out all-atom Molecular Dynamics (MD) simulations of fully ionized PE brushes for various degrees of polymerization and grafting densities. Our brush height results show an excellent match with the existing scaling laws of the non-linear osmotic brush regime. We observe a most remarkable ultraconfinement effect created by the brushes, quantified by orders of magnitude reduction in the mean squared displacement (MSD) of counterions and water molecules. Moreover, we observe that within the PE brushes, the counterion – PE brush complex supersedes the water molecules by both mass and volume above a critical grafting density. This gives rise to a hitherto unknown “water-in-salt” like behavior inside the brushes, with the counterions acting as the cations and the PE brush repeating units acting as the anions. Our calculations reveal a significant lowering of the dielectric constant of water within the brushes due to strong electrostatic binding with the negatively charged PE’s.

*This work has been supported by the Department of Energy Office of Science grant DE-SC0017741.
9:24AM A34.00008: Ion Transport in Pendant and Backbone Polymerized Ionic Liquids

ATSUSHI MATSUMOTO (Presenter), Okinawa Inst of Sci & Tech, PREEYA KURAY, The Pennsylvania State University, TAKERU NODA, Osaka University, CIPRIAN G. IACOB, National Research and Development Institute for Cryogenic and Isotopic Technologies, TADASHI INOUE, Osaka University, MICHAEL A HICKNER, JAMES PATRICK RUNT, The Pennsylvania State University — Polymerized ionic liquids (PILs) are single ion conductors, in which one of the ionic species is incorporated in the polymer chain while the other is nominally free to be transported. PILs are attractive as electrolytes in battery applications and other areas where liquid electrolytes are undesirable. In PILs, the ionic species can either be directly incorporated into the polymeric backbone (backbone PILs (B-PILs)) or placed as pendant groups to the chain (pendant PILs (P-PILs)). Here, we examined the ion transport, morphology, and dynamics of imidazolium-based pendant and backbone PILs with TFSI, CPFSI, and NfO counter-anions. We found that P-PILs yielded higher ionic conductivity when scaled to Tg, but B-PILs exhibited higher ionic conductivity on an absolute temperature scale, likely because of differences in the Tgs of the two systems. We also found that ion transport for B-PILs was coupled to the segmental dynamics below Tg, where the decoupling of ionic conductivity from segmental relaxation was observed for P-PILs. This study gleans insight on relating conductivity of equivalent backbone and pendant PIL structures to morphology, leading to a deeper understanding on the fundamental relationship between conductivity and morphology in PILs.

9:36AM A34.00009: Tailoring Ion Transport Properties of Block Copolymer Electrolytes with End-functionalized Homopolymer Addition

JIHOON KIM (Presenter), MOON JEONG PARK, Pohang Univ of Sci & Tech — Block copolymer electrolytes based on poly(ethylene oxide) (PEO) have been regarded as promising candidates for solid-state lithium batteries, attributed to the good lithium salt-solvating ability of PEO chains and their high ionic conductivity. However, the inherent crystallinity of PEO is tied to a drastic reduction in ionic conductivity at room temperature, limiting its uses in practically viable batteries. In this study, we report a new means of controlling PEO crystallinity of block copolymers by blending end-group functionalized PEO homopolymers. It has been found that the ionic conductivity and morphology of the resultant blends are related to the type and number of terminal moieties in embedded PEO homopolymers. This result suggests that chain folding of PEO is largely modulated by the end-group-driven intermolecular interactions in PEO phases. It has further shown that ion transport properties of blend electrolytes can be improved by this blend approach.
9:48AM A34.00010: Mechanisms of Ion Transport in Polymeric Ionic Liquids* [Invited]
VENKATRAGHAVAN GANESAN (Presenter), University of Texas at Austin — Polymeric ionic liquids (PILs) are an emerging class of materials which combines the attractive properties of ionic liquids with the sequence complexity and mechanical characteristics of macromolecules. While significant advances have occurred in the context of synthesis and characterization of such materials, comparatively less understanding exists on the mechanisms underlying ion transport in such materials. In this talk, I discuss some recent developments in the context of PILs relating to the issue of ion transport in such materials. We focus on the mechanisms of ion transport in such materials, the influence of counterions, and whether such materials do live up to the promise of high transference numbers.

*Robert A. Welch Foundation (Grant F1599) and National Science Foundation (CBET-17069698 and DMR-1721512).

10:24AM A34.00011: Quantifying Intrinsic Interfacial Transport Properties in Block Copolymer Electrolytes
PETER BENNINGTON, DANIEL SHARON, MICHAEL WEBB, JUAN DE PABLO, PAUL F NEALEY, SHRAYESH PATEL (Presenter), University of Chicago — Nanostructure-forming block copolymer electrolytes are of great interest related to their application towards a variety of electrochemical devices. However, questions remain about the nature of ion transport through these nanostructured materials. Specifically, decoupling extrinsic structural effects of tortuosity and grain boundaries from intrinsic phenomena occurring near the block copolymer domain interface has been challenging. This is due to the difficulty in precisely controlling or quantifying the film structure. Here, we present a new platform to probe defect-free single grains of any block copolymer electrolyte. We specifically focus on a model system of polystyrene-block-poly(ethylene oxide) (PS-b-PEO) with LiTFSI to quantitatively demonstrate that interfacial mixing is the predominant factor in reducing ionic mobility near the interface. Using SCFT calculations we directly correlate the interfacial width to reduced ionic conductivity as a function of lithium salt concentration. These findings are supported by atomistic simulations, which give further insight into the exact mechanisms by which this mixing layer restricts ion motion.
Multifunctional polymer electrolyte networks for energy harvesting and storage

HAMAD ALBEHAIJAN, THEIN KYU (Presenter), Polymer Engineering, University of Akron

A novel polymer electrolyte membrane (PEM) was developed based on poly(ethylene imine) (PEI)-co-polyethylene glycol diglycidyl ether (PEGDGE) network, containing lithium tri(fluoromethane sulphonyl) imide (LiTFSI) salt and succinonitrile (SCN) plasticizer. The polymer electrolyte multifunctional-networks have numerous advantages by virtue of the ion-dipole complexation facilitating facile ion conduction, multi-hydrogen bonding for self-healing to prevent electrode cracking, and covalently bonded networks to afford mechanical support. The tensile strength, modulus, and elongation-to-break of the PEI-co-PEGDGE/SCN/LiTFSI PEM films are all high, suggestive of highly flexible and stretchable nature. A wide electrochemical stability window of -0.5 ~ 5.1 V was achieved. In the symmetric Li/PEM/Li cell tests, dendrite formation of lithium crystal was discerned after cycling for 720 h, which motivates us to investigate the mechanism of Li$^+$ dendritic growth through the solid PEM network and develop strategy for preventing such dendritic growth during charge/discharge cycling. The same polymer network showed mechanoelectrical response to bending, exhibiting a flexoelectric coefficient of ~190 μC/m due to polarization/depolarization of oppositely charge dipoles, and dissociated ions.

Low-Voltage Reversible Electro-Adhesion of Ionoelastomer Junctions*

HYEONG JUN KIM (Presenter), LINDSAY PAGUIN, CHRISTOPHER BARNEY, Univ of Mass - Amherst, ZHIGANG SUO, Harvard University, ALFRED J CROSBY, RYAN HAYWARD, Univ of Mass - Amherst — An ionoelastomer is a soft and liquid-free ion conducting network formed by polymerization of an ionic liquid monomer and crosslinker into an elastomer network, such that one ion species is anchored by the network while the other species is mobile. An ‘ionic double layer’ (IDL) is formed at the interface between two oppositely charged ionoelastomers, analogous to the depletion (or space charge) layer formed at a p/n junction of electronic semiconductors. Here, we investigate how the voltage drop across the IDL can be modulated to reversibly control the adhesion between two ionoelastomers. The large electric field developed across the IDL allows for strong adhesion at potentials as low as ~ 1 V, while conventional dielectric electro-adhesives typically require much higher operating voltages (> 1 kV). These ionoelastomer electro-adhesives are also more efficient with regard to force capacity per electrostatic energy, and robust to defects or damage. Our findings provide new fundamental insight into low voltage electro-adhesion and broaden its possible applications.

*This work was supported by the National Science Foundation through grant DMR-1609972
8:00AM A35.00001: Fabrication and characterization of freestanding phononic thermocrystal membranes via block-copolymer directed-self assembly  ELIZABETH ASHLEY (Presenter), Pritzker School of Molecular Engineering, University of Chicago, NAOKI TAMBO, MASAKI FUJIKANE, YASUYUKI NAITO, KOUHEI TAKAHASHI, Technology Innovation Division, Panasonic Corporation, PETER J. DUDA, PAUL F NEALEY, Pritzker School of Molecular Engineering, University of Chicago — Block-copolymer (BCP) directed self-assembly (DSA) is a valuable technique that enables formation of defect-free, single crystal nanostructures over large areas. This is accomplished via a chemical template patterned via ebeam lithography. For perpendicularly oriented cylinder-forming BCPs, which spontaneously form a polycrystalline hexagonally close-packed lattice, controlling the orientation of the DSA pattern enables direct control of the in-plane lattice orientation, total pattern area, and number of periods. For BCPs such as PS-PMMA, the nanostructures can be transferred into an inorganic substrate, such as Si, and integrated into fabrication process flows for complex devices. Here, we present a methodology for integrating cylinder forming PS-PMMA DSA with a novel fabrication process to produce freestanding nanoporous Si membranes that scatter heat-carrying phonons. By controlling the orientation of the hexagonal lattice, a line-of-sight heat transport pathway can be opened or closed, which combined with nanometer scale of the BCP pores, provides the needed device length-scales to probe heat-carrying phonons. In this work, we report fabrication of and measurements on such membranes as a function of porosity, neck size, self-assembled vs DSA pores, and total pattern area.

8:12AM A35.00002: Engineering Block Copolymers To Achieve Equal Surface Free Energy and Tunable $\chi_N$ For Directed Self-Assembly Applications*  HONGBO FENG (Presenter), MOSHE DOLEJSI, University of Chicago, NING ZHU, NanJing Tech University, CHUN ZHOU, STUART J ROWAN, PAUL F NEALEY, University of Chicago — Directed Self-Assembly (DSA) of block copolymers (BCPs) is a promising technique for creating well-defined nanoscale features. The suitable BCPs for this application demand both blocks have equal surface free energies (SFE), a high enough Flory-Huggins parameter ($\chi$) for moderate phase separation but not so high as to prohibit defect annihilation, and high etch contrast. To date, the BCPs that meet these requirements are still very limited. Here we demonstrate a high throughput approach to create a series of BCPs with full pitch sizes from 8-15 nm that meet all these requirements. Furthermore, the capability of incorporation of etch resistant elements is shown to enable potential pattern transfer. We believe the work here will broaden the scope for DSA suitable materials and promote the next generation of nanolithography.

*We gratefully acknowledge the support by National Institute of Standards and Technology through the Center for Hierarchical Materials Design. We acknowledge the MRSEC Shared User Facilities (NSF DMR-1420709) and the Pritzker Nanofabrication Facility of the Pritzker School of Molecular Engineering at the University of Chicago (NSF ECCS-1542205).
8:24AM A35.00003: Enhancing the Scale of Block Copolymer Lamellae Alignment using Ionic Liquid (IL) on a Planar Supporting Substrate*  ALI MASUD (Presenter), University of Houston-Main Campus, JACK DOUGLAS, NIST, SEAN BAILEY, Cornell University, ALAMGIR KARIM, University of Houston-Main Campus — Symmetric Block Copolymers (BCP) such as PS-b-PMMA when cast on Silicon wafer and ordered using thermal annealing assume a parallel lamellar structure in thin films. However, as molecular weight and film thickness increases, attaining complete parallel lamellar structure becomes elusive. Previous study has shown that increasing the thermodynamic driving force for microphase separation, $cN$, where $c$ is the Flory-Huggins interaction parameter between the polymeric blocks and $N$ is the number of segments in the BCP, enhances the degree of BCP ordering and alignment parallel to substrate. In order to control the microstructure of ordering, increasing $N$ or reducing temperature $T$ could be applied at the expense of either slower kinetics, or higher defect formation due to entanglements, higher glass transition temperature ($T_g$) and surface tension. In this work we present a method for parallel alignment of lamellar PS-b-PMMA over notably higher Mw and film thickness regime using IL to enhance $c$, thereby propagating substrate driven parallel layering, while lowering $T_g$ for enhanced molecular mobility for fast kinetics. Such films may be useful in applications barrier materials and batteries, solid state dielectric capacitors.

*NSF-DMR 1905996

8:36AM A35.00004: Combining polymer synthesis with self-assembly of block copolymers  ZHE QIANG (Presenter), School of Polymer Science and Engineering, University of Southern Mississippi, MUZHO WANG, Department of Chemical and Biological Engineering, Northwestern University — Polymer self-assembly is one of the most promising nanopatterning techniques due to its advantages of low cost and high versatility. The key challenge of conventional strategy is its very limited ability to control over chemistry during or after self-assembly in order to alter the nanostructures from its thermodynamic equilibrium state. In this talk, we will demonstrate our recent development of in-film photopolymerization technique for synthesizing polymers within an self-assembled film. The vapor phase monomer is first introduced to swell a photoinitiator-containing block copolymer film, which can be subsequently converted to polymers upon UV irradiation. The synthesized homopolymers blend with BCP films, which alter the thin film nanostructures by changing the underlying polymer composition. As these altered nanostructures are locally near equilibrium, common annealing techniques such as shear aligning can be combined to improve the degree of ordering. With successful integrating polymer chemistry with assembly physics, the in-film polymerization method provides an exciting platform for on-demand manipulation of polymer functionality as well as opening up a new area for radical polymerizations within such geometrically confined, swollen films.
8:48AM A35.00005: Hexagonal pattern coarsening in cylinder-forming PS-b-PMMA block copolymer thin films* GABRIELE SEGUINI (Presenter), MICHELE PEREGO, IMM-CNR — The grain coarsening in thin films (~30 nm) of cylinder forming PS-b-PMMA BCP (N=379-1281) was accomplished by tuning of the annealing temperature and time in a RTP machine. The order of the hexagonal pattern was quantified by measuring the correlation length. The weakly dependence on \( T \) of \( \chi_{S-MMA} \) allows decoupling the control of \( \chi N \) by means of \( N \), and that of the thermally activated kinetic barriers for ordering kinetics modulating \( T \), evidencing the order-disorder transition (ODT) and glass transition (GT) involved in BCP ordering.

Thermodynamically, weak and strong segregation limits are not distinguishable. In weak segregation limit the ordering process switches from a diffusion limited to a curvature driven mechanism. Both single chain and collective motions comply with the extensively evidenced kinetic limited coarsening and the reduced diffusivity, increasing \( N \) and moving away from ODT, and with the thermodynamic limited coarsening and the enhanced diffusivity, decreasing \( N \) and moving towards ODT.

The collective dynamic is further investigated discriminating the behavior of the penta-hepta defects within the hexagonal pattern to give a comprehensive description of thermodynamic, kinetic and topological characteristics of the hexagonal pattern coarsening.

*Project IONS4SET

9:00AM A35.00006: Selective Modification from PS-b-PMMA-b-PtBA Triblock Copolymer for Ultrafiltration Membranes TAESUK JUN (Presenter), Yonsei University, SUNGMIN PARK, Rensselaer Polytechnic Institute, HYE RIN YOON, SEONGJUN JO, CHANG RYU, DU YEOL RYU, Yonsei University — We demonstrate a feasible approach to fabricating nanoporous structures and their functionality using a triblock copolymer of polystyrene-b-poly(methyl methacrylate)-b-poly(tert-butyl acrylate) (PS-b-PMMA-b-PtBA). With casting the samples in the thin films, the continuous-type morphologies were formed as PS matrix consisting cylinders of PMMA and minor PtBA blocks. Perpendicular orientation of cylinder morphologies was exploited near two interfaces of air/polymer and polymer/neutral substrate, sandwiching the random orientation of cylinders in the interior of the film. Nondegradable, selective swelling–deswelling process of cylindrical (PMMA-b-PtBA) blocks generated nanopores with tunable pore sizes. Moreover, a simple hydrolysis of minor tBA blocks functionalized the nanopore surfaces and walls into poly(acrylic acid) layers. The pH-responsive water permeability of nanoporous membranes and their active switching with respect to biomolecules such as bovine serum albumin (BSA) were performed. These results suggest a platform to fabricate a stimuli-responsive ultrafiltration membrane using a tunable multiblock copolymer.
**9:12AM A35.00007: Irreversible Physisorption of PS-b-PMMA for Neutral Layer**

WOOSEOP LEE (Presenter), YEONGSIK KIM, SEUNGYUN JO, Yonsei University, HYUNGJU AHN, Pohang Accelerator Laboratory, DU YEOL RYU, Yonsei University — Polymer chains are irreversibly physisorbed (physically adsorbed) onto impenetrable substrates by intermolecular forces (i.e. H-bonding, vdW force or dipole moment), as the chains favor the conformations which maximizes the segmental contact to compensate the conformational entropy loss. In this study, we succeeded in guiding perpendicular microdomains of polystyrene-b-poly(methyl methacrylate) (PS-b-PMMA) film with the aid of the irreversibly-adsorbed neutral layer made of PS-b-PMMA and evaluated its compositional randomness in terms of the correlation length ($\xi$) between the two phases of PS and PMMA. This method is widely applicable to various substrates without any necessity of random copolymer brushes or mats other than PS-b-PMMA itself.

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**9:24AM A35.00008: Failure and mechanical properties of block copolymer thin films**

TIANREN ZHANG (Presenter), NING WANG, ROBERT RIGGLEMAN, University of Pennsylvania — The physical properties of glassy polymer films can change drastically under nanoscale confinement. These changes are often attributed to increased average molecular mobility and reduction in entanglement density, and both are known to alter mechanical behavior. While most previous work has focused on the properties of homopolymers under confinement, and the mechanical response of block copolymer thin films is still comparatively unexplored. We have used molecular dynamics simulations to investigate the mechanical response of free standing, lamellar-forming block copolymer thin films made from polymer chains that span from slightly entangled to highly entangled at different film thicknesses. We noticed that the failure and mechanical properties become substantially distinct from bulk as the thickness is decreased. The dynamic response of the thinnest films studied show a different local response compared to thicker films. For all the block copolymer films, we find that the plastic rearrangements initially concentrate at the boundary between the two phases of the lamellae until close to failure, when the plasticity moves to the center of a domain.

*NSF*
9:36AM A35.00009: Advanced metrology and molecular dynamics simulations for quantifying counterion condensation in block copolymer electrolyte thin films* QI LEI (Presenter), CHRISTOPHER G ARGES, Louisiana State University, Baton Rouge — Ionic conductivity is an important property of polymer electrolyte membranes and electrode binders. The impact of counterion condensation, a proxy for the extent and strength of ionic group dissociation in polymer electrolytes, on ionic conductivity has received less attention and is not clearly known. This talk highlights our effort to quantify counterion condensation in self-assembled block copolymer electrolyte (BCE) thin films. Advanced metrology (GI-SAXS, QCM, ICP-OES, and LC-MS) were applied to quantify counterion condensation in BCEs. These techniques identified the Donnan concentration during ion-partitioning experiments and determined the activity coefficients of these ions in thin films. Experimental results were compared against the Gibbs-Donnan Model and Manning’s Theory of Counterion Condensation, as well as classical molecular dynamics simulations. The agreements and differences between the experimental and modeling techniques will be presented and discussed.

*The authors acknowledge funding for this work from U. S. Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Subprogram, Award # DE-SC0018989.

9:48AM A35.00010: Modeling Surface Interactions for Block Copolymers and Polymer Brushes under Soft Confinement* JUN-QING SONG, YI-XIN LIU (Presenter), HONG-DONG ZHANG, Fudan Univ — The surface interaction is one of the most important factors that control the nanostructures formed by block copolymers/polymer brushes under soft confinement. In this talk, we introduce a simplified model for surface interactions where the role of soft substrates is decomposed into two independent contributions: the surface preference and the surface softness. Soft substrates are modeled by polymers grated onto hard walls. Their structures on both repulsive and attractive walls are studied by SCFT.[1] Based on this model, we perform a numerical analysis of the stability competition between perpendicular and parallel lamellae of symmetric diblock copolymers on substrates modified by homopolymers.[2] The effects of the surface preference and the surface softness on the alignment of lamellar domains are carefully examined. Applications of this model on understanding the defect removal process in DSA of block copolymer thin films are also demonstrated.[3]


*This work was supported by National Natural Science Foundation of China (21873021, 21004013) and Shanghai Pujiang Program (18PJ1401200).
10:00AM A35.00011: Degradation of Block Copolymer Films*  RYAN SAYKO (Presenter), ZILU WANG, University of Akron, MATTHEW L. BECKER, Duke University, ANDREY DOBRYNIN, University of Akron — We use coarse-grained molecular dynamics simulations to study degradation of films of multiblock copolymers in a solvent. Our simulations were designed to mimic degradation dynamics of glycine, valine, and phenylalanine based poly(ester urea)s in vitro. Simulations show that the rate of copolymer degradation is a result of a fine interplay between chain breaking kinetics, solvent diffusion, and swelling of the domains made of solvophilic blocks. The evolution of the film structure during the degradation process was monitored by calculating the scattering function \( S(q) \) of the copolymer film. The solvent diffusion into the films results in a monotonic shift of the peak position to smaller \( q \). This shift is also accompanied by the increase in scattering intensity at \( q \ll 1 \) in such a way that the peak completely disappears at the later stages of the film degradation. This results in the scattering function \( S(q) \) to have two characteristic power law regimes with \( S(q) \sim 1/q^2 \) and \( S(q) \sim 1/q^4 \), represented by interconnected vesicles with thin shells. The number average degree of polymerization of the copolymer fragments monotonically decreases with time. However, the polydispersity index of the copolymer fragments first increases as a function of time and then decreases.

*ODSA TECG20180022

10:12AM A35.00012: WITHDRAWN ABSTRACT —

10:24AM A35.00013: New insight into self-assembly of block copolymers at the solid-polymer melt interface*  [Invited] TAD KOGA (Presenter), Stony Brook University — I present new pieces of experimental findings on the self-assembling process of block copolymers (BCPs) near nonneutral silicon (Si) substrate surfaces. The key is concurrent physisorption of preferred blocks and non-preferred blocks on the surface. Using an optimized solvent-rinsing approach, we successfully uncovered two different kinds of adsorbed BCP chains: one is the inner strongly adsorbed BCP chains where all constituent blocks lie flat and form a two-dimensional percolating network structure regardless of their chain architectures, microdomain structures, and interfacial energetics. The other is outer "loosely adsorbed chains" which form a poorly packed perpendicularly oriented microdomain structure. I will show that the inner microdomain structures and orientations of BCP thin films are negatively impacted by the loosely adsorbed BCP chains. Interestingly, this undesirable substrate-field effect propagates into the film interior up to the distance of \( \sim 70 \text{ nm} \). Finally, a new surface modification approach to prevent the substrate-field effect is proposed. I will demonstrate that homopolymer chains composed of one of the constituent blocks adsorbed on the Si substrates act as a “structurally neutral” surface coating for directed self-assembly of block copolymer thin films.

*T.K. acknowledges partial financial support from the NSF Grant (CMMI-1332499).
Superconducting quantum processors are controlled and measured in the analog domain and the design of the associated classical-to-quantum interface is critical in optimizing the overall performance of the quantum computer. Control of the processor is achieved using a combination of carefully shaped microwave pulses and high-precision time varying flux biases. Measurement of quantum states is typically achieved using dispersive readout, which requires a low-power pulsed microwave drive and a near quantum-limited readout chain. For control of a single qubit, a typical system employs two high-speed high-resolution (e.g., 1 Gsps/14 bit) digital-to-analog converters (DACs) and a single-sideband modulator to generate microwave control pulses. A third DAC with similar specifications is used for flux-bias control. A typical readout channel may service on the order of five qubits and contains yet another pair of DACs, with a single-sideband modulator employed to generate a stimulus signal. For measurement, the readout chain also employs a series of cryogenic amplifiers followed by further amplification, IQ demodulation, and high-speed digitization at room temperature. For today's prototype systems with on the order of 50-100 qubits, keeping most of the electronics at room temperature makes sense. However, achieving fault tolerance—a long term goal of the community—will require implementing systems with on the order of $10^6$ qubits and today's brute force control and readout approach will not scale to these levels. Instead, a more integrated approach will be required. In this talk, we will present a review of recent work towards implementing a scalable cryogenic quantum control and readout system using silicon integrated circuit technology. After motivating the work, we will describe the design and characterization of a prototype cryogenic XY controller for transmon qubits. Detailed measurement results will be presented. The talk will conclude with a discussion of future work.
Kalman-based IQ Mixer Calibration for Circuit QED

SHAN WILLIAMS (Presenter), RICCARDO BORGANI, MATS OLOV THOLÉN, DAVID HAVILAND, Nanostructure Physics, KTH Royal Inst of Tech — Quantum measurements with superconducting circuits require the generation and detection of signal frequencies in the 2 - 12 GHz range, where frequency conversion is performed by analog devices known as IQ mixers. These mixers generate unwanted image signals upon upconversion, which crowd the already limited frequency spectrum, and become superimposed with the desired signal upon downconversion. Image signals are particularly problematic for frequency-multiplexed qubits [1] as they are a possible source of dephasing when accidentally driving another qubit. These detrimental effects can be minimized by calibrating the IQ mixers.

In this talk we present some simple but elegant methods which do not require a spectrum analyzer, to calibrate both up and downconversion mixers in situ (i.e. without disconnecting the device under test). The downconversion mixer is calibrated with a Kalman filter, providing a minimally distorted estimate of the image-to-signal power ratio. This ratio is then used to calibrate the up-conversion mixer. These techniques, originally developed for wide-band digital communication [2], are well suited for frequency-multiplexed experiments in circuit QED.


Reversible Fluxon Logic with shift registers

WALTRAUT WUSTMANN (Presenter), KEVIN OSBORN, LPS at the University of Maryland, College Park — Reversible digital logic can improve energy efficiency over irreversible logic. Reversible logic gates in superconducting circuits are currently made in the adiabatic type, where drive fields evolve the bit state, but we are developing Reversible Fluxon Logic (RFL) in the ballistic type – key gates are solely powered by bit state inertia. RFL represents the bit states by the two topological charges (flux polarities) of fluxons in a Long Josephson Junction (LJJ). Ballistic gates consist of at least two LJJ connected by a circuit interface and use a resonant conversion of an input fluxon to and from a localized field at the interface. At the end of this process a new fluxon is created in another LJJ and its polarity may deterministically differ from the input bit, thus enabling bit switching. In simulations 1- and 2-bit RFL gates can restore 97% of the input fluxon energy in the output fluxons. While previous RFL 2-bit gates require synchronous input bits, newly developed gates store an internal flux state by which the timing restriction is lifted (asynchronous). This is demonstrated with the shift register – the input state is stored as internal flux while the previously stored flux state transfers to a ballistic output fluxon. We apply a model developed to describe RFL dynamics.
9:00AM A36.00004: Practical Microwave Direct Digital Synthesis for Superconducting Qubit Control*  WILLIAM KALFUS (Presenter), DIANA F. LEE, SPENCER FALLEK, GUILHEM RIBEILL, ANDREW WAGNER, MARTIN V GUSTAFSSON, THOMAS A OHKI, Raytheon BBN Technologies, BRIAN DONOVAN, Systems & Technology Research, DIEGO RIST&Egrave;; Raytheon BBN Technologies — To conduct experiments with higher numbers of superconducting qubits, the availability of scalable control hardware is essential. To address this, we have incorporated custom superconducting qubit control logic into off-the-shelf hardware employing direct RF synthesis at 5 GHz for low-noise and low-latency pulse generation up to 7.5 GHz. Our approach eliminates the need for upconversion (which requires precise calibration to prevent leakage) and highly stable microwave sources (which can be expensive). The wide bandwidth enables efficient experiment configurations, such as control and readout using a single channel. We characterize the performance of the hardware using a five-transmon IBM device and demonstrate no additional decoherence or gate error for one- and two-qubit gates compared to traditional configurations, establishing a foundation for scalable quantum control beyond intermediate-scale systems.

*This document does not contain technology or technical data controlled under either the U.S. ITAR or the U.S. EAR. The project depicted was sponsored by the Dept. of Army, U.S. ARO. The content of the information does not necessarily reflect the position or policy of the federal government, and no official endorsement should be inferred.

9:12AM A36.00005: A scalable FPGA platform for qubit readout and control*  MATS THOLEN (Presenter), RICCARDO BORGANI, SHAN WILLIAMS JOLIN, DAVID HAVILAND, KTH Royal Inst of Tech — Readout and control of superconducting qubits requires high bandwidth signal generation, acquisition and processing, together with the possibility of implementing low latency feedback. These requirements are fulfilled in a new category of Field Programmable Gate Arrays (FPGA) designed for applications in software-defined radio. We adapted the Xilinx Zynq Ultrascale+ RFSoC hardware platform by implementing firmware for pulsed control and readout of qubit circuits. We have also implemented firmware for coherent multifrequency modulation and demodulation of continuous signals. Using the second Nyquist band we perform direct digital synthesis and measurement at microwave frequencies, without analog mixers. With 8 analog input and 8 analog output channels, on-chip integration of DAC, ADC and FPGA, the RFSoC is a promising new platform for experiments with circuit QED.

*WACQT Wallenberg Centre for Quantum Technology
9:24AM A36.00006: High-density cryogenic wiring for superconducting qubits* STEVEN WEBER (Presenter), JOHN CUMMINGS, JOVI MILOSHI, KYLE J THOMPSON, JOHN ROKOSZ, ANDREW JAMES KERMAN, MIT Lincoln Laboratory, WILLIAM OLIVER, Massachusetts Institute of Technology — As superconducting quantum processors continue to scale up in size, it becomes increasingly challenging to route the required number of control lines through a dilution refrigerator to the qubit chip. In this presentation, we will discuss our efforts to develop high-density fridge wiring for use in next-generation quantum annealers. Our wiring solution is based on flexible multi-channel cables with a stripline geometry, designed to achieve low crosstalk and moderate bandwidth. We will describe the electrical performance of these cables, as well as other design considerations such as thermal management.

*This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

9:36AM A36.00007: Single Flux Quantum based electronics for control and readout of superconducting qubits. MANUEL CASTELLANOS-BELTRAN (Presenter), ADAM J. SIROIS, National Institute of Standards and Technology Boulder, JUNLING LONG, Physics, University of Colorado-Boulder, ANNA FOX, DAN SCHMIDT, PAUL DAVID DRESSELHAUS, PETER F. HOPKINS, JOEL N ULLOM, DAVID PAPPAS, SAMUEL P BENZ, National Institute of Standards and Technology Boulder — Superconducting quantum information systems require a mix of continuous-wave AC, pulse-modulated AC, and DC signals for control and readout. There are significant advantages in terms of scaling, physical footprint, latency, signal integrity, and power consumption by moving these sources to 4 K or below, inside the cryostat. In this talk we present an experimental demonstration generating spectroscopy tones at 4 K to measure a transmon qubit’s energy level spacings at 100 mK. The spectroscopy tones are generated by a series of Josephson junctions at 4 K driven by a sigma-delta pulse stream from room temperature. This experiment was our first step in optimizing the Josephson arbitrary waveform synthesizer (JAWS) circuit for controlling quantum systems in a scalable manner. We also discuss further steps needed to generate pulsed signals for qubit preparation, cryogenic readout, and digital superconducting circuits at 4K for signal processing and feedback.
9:48AM A36.00008: Unconditional reset of superconducting qubits and readout resonators using a quantum-circuit refrigerator* VASILII SEVRIUK, JANI TUORILA, JOHANNES HEINSOO (Presenter), CASPAR OCKELOEN-KORPPI, IQM Finland Oy, JONI IKONEN, Department of Applied Physics, Aalto University, KUAN YEN TAN, IQM Finland Oy, ERIC HYYPPÄ, MATTI SILVERI, MATTI PARTANEN, MÁTÉ JENEI, GIACOMO CATTO, TIMM MÖRSTEDT, Department of Applied Physics, Aalto University, LEIF GRÖNBERG, VTT Technical Research Center of Finland Ltd., JAN GOETZ, IQM Finland Oy, MIKKO MOTTONEN, Department of Applied Physics, Aalto University — In quantum information processing with logical qubits, increasing the clock rate of the error correction cycles improves the qubit fidelity. The clock rate is limited by the duration of logical gates, qubit state readout, and initialization of qubits and readout circuits. Linear and non-linear superconducting resonators can be quickly initialized using a quantum-circuit refrigerator based on fast voltage pulsing of an SINIS junction [1,2]. We discuss our latest results to this end.


*IQM Finland OY, European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie Grant No. 795159 and under the European Research Council Consolidator Grant No.681311 (QUESS), from the Academy of Finland Centre of Excellence in Quantum Technology Grant No. 312300, No.316619. and No. 305237, from JST ERATO Grant No. JP-MJER1601, from JSPS KAKENHI Grant No. 18K03486, from the EU Flagship project QMiCS, from the Emil Aaltonen Foundation, from the Alfred Kordelin Foundation, and from the Vilho, Yrjö and Kalle Väisälä Foundation. We acknowledge the provision of facilities and technical support by Aalto University at OtaNano - Micronova Nanofabrication Centre.

10:00AM A36.00009: Simple, smooth 50ns QND circuit-QED measurement pulses FELIX MOTZOI (Presenter), Juelich Forschungszentrum, CHRISTIAN DICKEL, University of Cologne, LUKAS F BUCHMANN, Aarhus University — We demonstrate a technique for greatly reducing the duration and error in circuit QED measurement tasks. We show how to suppress different errors including state discrimination, cavity reset, non-linear cavity effects, bandwidth, filtering, all while retaining QND-ness and staying within a single quadrature. The technique works for a variety of different circuit configurations, including Purcell filters, where two different cavities need to be simultaneously emptied. Moreover, the speed and quantum non-demolition nature is retained as one scales up to more qubits or quantum states, providing a blueprint for scaling up to simultaneously measure leakage state populations, multiple qubits, or multiple network modes. We show for realistic circuit parameters that not only speed can be improved by an order of magnitude but errors as well with 99.9% fidelity well within reach. The technique can be understood in terms of control-theoretic transfer function formalism or shortcuts to adiabaticity, where we can also leverage the adiabatic methodology to cancel unwanted nonlinear effects such as Kerr nonlinearity.
10:12AM A36.00010: Predictive feedback for active noise canceling in superconducting quantum processors* AMIR KARAMLOU (Presenter), ANTTI VEPSALAINEN, RONI WINIK, Research Laboratory of Electronics, Massachusetts Institute of Technology MIT, DAVID K KIM, JONILYN YODER, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, WILLIAM OLIVER, Research Laboratory of Electronics, Massachusetts Institute of Technology MIT — Superconducting qubits are amongst the most promising platforms for building near term practical quantum information processors. However, the coherence time (T2) of these qubits is negatively impacted in the presence of dephasing noise. In this work, we show how to efficiently estimate the noise spectrum experienced by the qubit, employ techniques from machine learning to predict the correlated noise in the future and use fast-feedback with an FPGA to cancel the noise. We propose using this estimate-predict-feedback sequence as a tool to increase gate fidelities while running a quantum circuit.

*This research was funded in part by the ARO MURI W911NF-18-1-0218; and by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. Amir Karamlou is funded by NSF GRFP 2018265551 The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

10:24AM A36.00011: QubiC - An open FPGA based Qubit Control system* GANG HUANG (Presenter), YILUN XU, Lawrence Berkeley National Laboratory, RAVI KAUSHIK NAIK, BRADLEY MITCHELL, Physics, University of California, Berkeley, DAVID SANTIAGO, Lawrence Berkeley National Laboratory, IRFAN SIDDIQI, Physics, University of California, Berkeley — As the number of qubits increases, the flexibility and scalability of the control system become one of the issues limiting the experiments to expand. We developed an FPGA based qubit control system named QubiC. The system generates the physical RF pulses which implemented the quantum algorithm and process the readout and present them to the higher level. Multiple FPGAs can be synchronized via optical fiber, making the system scalable. As a proof of concept, we build a module with the COTS FPGA carrier boards and DAC/ADC boards together with analog frontend boards. We developed the firmware and software to implement the algorithm and demonstrate the basic functionality. In this talk, we describe the system structure, the firmware implementation and the design of the analog front end boards.

*This work was supported by the Department of Energy.
A Scalable Multi-Channel Cryogenic Controller for Spin Qubits/Transmons with Frequency Multiplexing Capability Implemented in Intel 22nm FinFET Technology

BISHNU PATRA, JEROEN P. G. VAN DIJK, Delft University of Technology, Delft, The Netherlands, SUSHIL SUBRAMANIAN (Presenter), Intel, Hillsboro, OR, ANDREA CORNA, XIAO XUE, Delft University of Technology, Delft, The Netherlands, CHARLES JEON, FARHANA SHEIKH, Intel, Hillsboro, OR, ESDRAS JUAREZ HERNANDEZ, BRANDO PEREZ ESPARZA, Intel, Guadalajara, Mexico, HUZAIFA RAMPURAWALA, BRENT CARLTON, Intel, Hillsboro, OR, NODAR SAMKHARADZE, TNO, Delft, The Netherlands, SUREJ RAVIKUMAR, CARLOS NIEVA, SUNGWON KIM, HYUNG-JIN LEE, Intel, Hillsboro, OR, AMIR SAMMAK, TNO, Delft, The Netherlands, GIORDANO SCAPPUCCI, MENNO VELDHORST, LIEVEN M VANDERSYPEN, MASoud BABAIe, FABIO SEBASTIANO, Delft University of Technology, Delft, The Netherlands, EDOARDO CHARBON, EPFL, Neuchatel, Switzerland, STEFANO PELLERANO, Intel, Hillsboro, OR — Scaling a fault-tolerant quantum computer to a very large number of qubits is a daunting challenge. Innovation is required in qubit fabrication, integration and control. Current approaches for controlling qubits operating at cryogenic temperature using room-temperature electronics will not scale to large qubit arrays. We have recently proposed to bring integrated electronics close to the qubits at cryogenic temperatures. Leveraging deeply-scaled CMOS process technologies, complex System-on-Chips (SoCs) with digital, analog and RF capabilities can be integrated with sufficiently low power consumption to be compatible with dilution refrigerators. We demonstrate a cryo-CMOS controller SoC designed to operate at 4K and implemented in Intel 22nm FinFET technology. The SoC is capable of addressing 128 frequency-multiplexed qubits across 4 separate channels over 1GHz RF bandwidth from 2 to 20GHz. The maximum output power is -16dBm at 6GHz with 40dB gain control. Such flexibility enables the control of both spin qubits and transmons with the same chip. By operating our cryo-CMOS controller on the 4K plate in a dilution refrigerator also hosting a Si-based qubit sample at 20mK, we demonstrate Rabi oscillations and coherent x-y rotations of the spin qubit at both 13.7 and 17.5GHz.

Design, Modeling, and Measurement of Through-Silicon Via (TSV) Structures for Superconducting Quantum Computing*

WAYNE WOODS (Presenter), DANNA ROSENBERG, MOLLIE SCHWARTZ, DONNA YOST, JONILYN YODER, WILLIAM OLIVER, MIT Lincoln Lab — We have integrated high-aspect ratio superconducting through silicon vias (TSVs) into routing and control circuitry for superconducting qubits, as well as for dedicated grounding of on-chip ground planes, and for the elimination of chip box modes. We describe our electromagnetic modeling of TSV-embedded routing elements, and we demonstrate their incorporation into design and measurement of superconducting qubits. We also describe the robust modeling and design methodology we use to optimize the combination of compactness, electrical reflections, and dielectric losses.

*This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.
Session A37 FGSA: The Postdoctoral Experience at Universities, Industry Labs, and Military Labs 605 - Tag(s): Careers, Invited, Undergrad Friendly

8:00AM A37.00001: Panel Discussion [Invited] — Invited Panelists are:
Krista Freeman, University of Pittsburgh
Christopher Safranski, IBM TJ Watson Research Center
Ibrahim Boulares, US Army Res Dev & Eng Command

Session A38 FPS: AI and Humanity: Governance, Design, and Ethics 607 -
Savannah Thais, Princeton University - Tag(s): Invited, Undergrad Friendly

8:00AM A38.00001: Theodora Dryer Invited Talk [Invited] —

8:40AM A38.00002: Joaquin Candela Invited Talk [Invited] —

9:20AM A38.00003: An Ecological Approach to Data Governance [Invited] JASMINE MCNEALY (Presenter), University of Florida — Data are currency. They provide the fuel for both decision-making and profit-making. Data offer evidence for enhancing health services, infrastructure, zoning, and for addressing environmental concerns. But data collection and use is spurring conflicts between cities, corporate and civil society organizations, and constituents on the grounds of data ownership, access, privacy, and security, spilling into the courts, the media, and public discourse.
In this talk I trace these conflicts to our perception of data as a singular piece of property. A better metaphor for data would be that of a networked representation or observation in an ecosystem. I argue that we require an ecological approach for understanding this era of emergent technology and data -- both for creating adequate policy, and for protecting the vulnerable.

10:00AM A38.00004: Physicists' Involvement in AI and AI Ethics [Invited] SAVANNAH THAIS (Presenter), Princeton University — Physicists in many subfields are increasingly employing Machine Learning and Artificial Intelligence techniques in their research; furthermore, in some cases physics principles and research are informing the development of new algorithms and learning methods. Physics and AI are now inextricably linked and thus physicists must critically consider the broader impact of AI developments on people and society. This talk will summarize current areas of physics-informed AI research and will provide suggestions and context for how physicists can meaningfully engage in these discussions.

10:15AM A38.00005: Panel Discussion [Invited] —
8:00AM A39.00001: Plasmon-induced excited-state catalysis understood via embedded correlated wavefunction theory [Invited] JOHN MARK P. MARTIREZ, Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, JUNWEI L. BAO, Department of Mechanical and Aerospace Engineering, Princeton University, EMILY CARTER (Presenter), Office of the Chancellor, University of California, Los Angeles — Metallic nanoparticles (MNPs) with nearly-free-electron-like valence electrons have enhanced ability to scatter/absorb light by means of local surface plasmon resonances (LSPRs). Such LSPRs produce amplified electric fields that can excite molecules or other materials coupled to the MNPs. Photocatalysis mediated by MNPs exploits this unique optical phenomenon. First-principles quantum mechanics can aid in understanding such light-driven chemistry but the methods used must properly account for both electronic excitations and surface reactions. Embedded correlated wavefunction (ECW) theory is ideally suited for this purpose, wherein the extended surface is described by an embedding potential derived from density functional embedding theory (DFET). The chemical reaction then is treated with CW theory subject to this DFET-derived potential. ECW calculations of a variety of endoergic reactions on pure and doped surface-plasmon-active metals reveal that enhanced kinetics can occur on excited-state reactive potential energy surfaces accessed via plasmon-enhanced light absorption or resonance energy transfer. Our calculations explain experimentally observed plasmon-driven enhanced rates and suggest candidate MNPs for photocatalytic nanoplasmonics.
8:36AM A39.00002: Ultrafast dynamics of plasmons and strong plasmon-molecule coupling at the nanoscale: Insights from first-principles modeling*  
TUOMAS ROSSI (Presenter), PAUL ERHART, Department of Physics, Chalmers University of Technology — Localized surface plasmons render metal nanoparticles efficient light absorbers at their resonance frequencies. After light absorption by the plasmon mode, the system can display different femtosecond-scale processes: The plasmon can decay into incoherent electrons and holes or a coherent energy exchange can take place between plasmon and other strongly-coupled electronic excitations. In this presentation, we employ time-dependent density-functional theory (TDDFT) for providing first-principles insights on these ultrafast processes at the nanoscale. We analyze the electron-hole transitions involved in photoabsorption and in the subsequent dynamics of the electronic system, which enables us to scrutinize the plasmonic character [1], follow the plasmon decay into hot electrons and holes [2], and dissect the symmetric and antisymmetric hybrid modes caused by strong coupling between plasmon and molecular excitation [3]. Our work paves the way for addressing spatiotemporal dynamics of plasmon-enhanced processes down to the atomic-scale details.


*EU Horizon 2020 research and innovation programme, Marie Sklodowska-Curie grant No 838996

8:48AM A39.00003: Decoherence in First-Principles Simulation of Excited Electron Dynamics in Nanomaterials and at Interfaces*  
JIAN CHENG WONG (Presenter), YOSUKE KANAI, Univ of NC - Chapel Hill — Understanding hot carrier dynamics in nanomaterials and at molecule-material interfaces is central to gain scientific insights into the operation of various future optoelectronic technologies. We investigate the excited electron dynamics at molecule-material interfaces using first-principles simulation based on the fewest switches surface hopping (FSSH) method. Within the FSSH method, identification of trivial crossings poses a major numerical challenge in practice as it can influence simulation results in a few different ways. In particular, calculation of the decoherence rate from the energy autocorrelation function is found to be rather sensitive to the trivial crossings. In addition to discussing how decoherence influences both hot electron relaxation and transfer at interfaces, we propose a numerical method to treat trivial crossings and discuss the extent to which trivial crossings affect the calculated decoherence rate.

*Work primarily supported by the Alliance for Molecular PhotoElectrode Design for Solar Fuels, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001011.
9:00AM A39.00004: First-principles calculations of the ultrafast dynamics of coupled electrons and phonons
XIAO TONG (Presenter), MARCO BERNARDI, Caltech — Progress on experiments probing the ultrafast electron dynamics calls for the development of accurate simulations of materials in the time domain. However, widely employed approaches to model the coupled nonequilibrium dynamics of electrons and atomic vibrations (phonons) employ empirical or approximate interactions, or are limited to femtosecond timescales. Here we show a numerical approach to evolve in time the coupled Boltzmann transport equations (BTEs) of electrons and phonons, using ab initio electron-phonon and phonon-phonon interactions together with a parallel algorithm to explicitly time step the BTEs. Our approach can simulate the dynamics up to hundreds of picoseconds (with a femtosecond time resolution) and provide microscopic insight into the scattering mechanisms. The accuracy of the interactions used in the calculations can be validated by computing transport properties. We show example calculations on graphene and semiconductors, for which we compute carrier cooling rates, mode-resolved phonon dynamics, transient absorption, structural snapshots and diffuse X-ray scattering. Possible extensions to include static electric or electromagnetic fields will also be discussed. Our findings open new avenues for quantitative simulations of ultrafast dynamics in materials.

9:12AM A39.00005: Spin-phonon relaxation in diverse materials from a universal ab initio density matrix approach*
JUNQING XU (Presenter), University of California, Santa Cruz, ADELA HABIB, SUSHANT KUMAR, Rensselaer Polytechnic Institute, FENG WU, University of California, Santa Cruz, RAVISHANKAR SUNDARARAMAN, Rensselaer Polytechnic Institute, YUAN PING, University of California, Santa Cruz — We present a new, universal first-principles methodology based on Lindbladian dynamics of density matrices to calculate the spin-phonon relaxation time of solids with arbitrary spin mixing and crystal symmetry. In particular, this method describes contributions of the Elliott-Yafet and D’yakonov-Perel’ (DP) mechanisms to spin relaxation, corresponding to systems with and without inversion symmetry, on an equal footing. Our \textit{ab initio} predictions are in excellent agreement with experiment data for a broad range of materials, including metals and semiconductors with inversion symmetry (silicon and iron), and materials without inversion symmetry (MoS$_2$ and MoSe$_2$). We find strong magnetic field dependence of electron and hole spin relaxation in MoS$_2$ and MoSe$_2$. As a function of temperature, we find the spin relaxation time to be proportional to carrier/momentum relaxation time in all cases, consistent with experiments but distinct from the commonly-quoted inverse relation for simplified models of the DP mechanism. We emphasize that first-principles spin-orbit coupling and electron-phonon scattering is crucial for general, accurate prediction of spin relaxation in solids.

*We acknowledge financial support from the National Science Foundation under Grant No. DMR-1760260.
9:24AM A39.00006: Predicting weak-to-strong light-matter coupling in cavities from first principles*  
DEREK WANG (Presenter), TOMAS NEUMAN, JOHANNES FLICK, PRINEHA NARANG, Harvard University — Quantum electrodynamical density functional theory (QEDFT) is a first principles, non-perturbative framework for interactions of quantum matter with quantized electromagnetic fields. QEDFT studies have usually considered lossless cavities. Experimentally accessible cavities, however, exhibit finite photon lifetimes leading to incoherences that dominate dynamics of the light-matter excitations. Here we extend QEDFT by considering lossy cavity modes. This allows us to study ab initio correlated optical interactions in matter ranging from the weak-coupling to strong-coupling regime. As an example, we study excited-state dynamics and spectral responses of benzene and chlorobenzene under weak-to-strong light-matter coupling. By tuning the coupling we achieve cavity-mediated energy transfer between electronic excited states. We interpret the first principles results using a Fano-like model parametrized with the (QE)DFT data. This extension to QEDFT moves toward closing the loop between first principles calculations employed in electronic structure theory and parametric models of the quantum optics community.

*This work was supported by the DOE ‘Photonics at Thermodynamic Limits’ Energy Frontier Research Center under grant DE-SC0019140. DW is an NSF Graduate Research Fellow.

9:36AM A39.00007: Local basis formulation for the Floquet theory of electronic stopping of ion projectiles*  
NICOLO' FORCELLINI, MARJAN FAMILI (Presenter), EMILIO ARTACHO, Univ of Cambridge — Ions shooting through solids are slowed down by electronic excitation in the so-called electronic stopping process. This century-old problem is of fundamental and applied interest in various contexts, including nuclear, space and biomedical industries. The electronic stopping problem is approached theoretically from two prevalent paradigms, one based on linear response for weak effective interactions, the other on the homogeneous electron liquid, a successful model for simple metals. A more general theory for crystalline solids has been introduced recently based on exploiting a discrete translational invariance along a space-time diagonal, the Floquet theory of electronic stopping [1]. Here we will present how to formalise this theory using a local basis for the practical solution of the unconventional scattering problem that arises from the theory.


*This work was supported by the EPSRC grant EP/N509620/1 (NF), Leverhulme Trust, UK, RPG-2018-254 (MF, EA)
9:48AM A39.00008: The effect of pressure ($P$) on the intrinsic optical dynamics of nitrogen-vacancy NV$^+$ colored centers in diamond: reexamining the intersystem crossing (ISC) with $\Delta$SCF calculations within density functional theory (DFT) combined to the extended Hubbard model

MARIYA ROMANOVA (Presenter), Ecole Polytechnique, Laboratoire des Solides Irradiés, JELENA SJAKSTE, CNRS, Laboratoire des Solides Irradiés, MICHELE CASULA, CNRS, Sorbonne Université, Institut de Minéralogie, de Physique des Matériaux, et de Cosmochimie, NATHALIE VAST, CEA-Saclay, Laboratoire des Solides Irradiés — The sensitivity of the NV center to its surrounding magnetic field is expected to be a powerful tool to detect the onset of superconductivity at ultrahigh $P$ in diamond anvil cells. In this work, we propose a combined approach to study the many-body excited states of the NV$^+$ center under $P$: the extended Hubbard model with all of the parameters fit on $\Delta$SCF-DFT calculations of the differences of total energies with constrained occupations, thereby including the electron-hole interaction for any $P$.

We study the behavior of all of the many body states under $P$. In particular, we compute for the first time the pressure coefficients of the singlet-singlet emission consecutive to the ISC for the two models reported in the literature [1,2], and show that they are widely different, the application of hydrostatic pressure being an effective tool to discriminate between them.


*Results have been obtained with the Quantum ESPRESSO package and our home-developed code, and computer time granted by PRACE (Project No. 2019204962) and by French GENCI-CINES and GENCI-TGCC (Project 2210). Support from labex PALM and DIM SIRTEQ (région Île-de-France) is acknowledged.

10:00AM A39.00009: Magnetocrystalline Anisotropy and Potential Switching in Antiferromagnetic Fe$_2$As

KISUNG KANG (Presenter), KEXIN YANG, DAVID CAHILL, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Antiferromagnetic Fe$_2$As attracts interest due to its tetragonal chemical structure with easy-plane magnetism and metallic electrical conductivity. To understand the electrically-activated switching process of the Néel vector in this material, anisotropy energy becomes an important parameter as an energy barrier. Anisotropy energy originates from spin-orbit interaction (SOI) and magnetic dipole-dipole interaction (MDD). We use density functional theory and classical modeling to investigate SOI and MDD, and find that in-plane anisotropy is dominated by SOI, which is two times larger than the MDD contribution to out-of-plane anisotropy. The in-plane anisotropy presents four-fold symmetry and is 276.5 J/m$^3$ which is confirmed by torque magnetometry, and total out-of-plane anisotropy energy is 829772 J/m$^3$ with two-folded symmetry. Based on anisotropy energy and magnetic susceptibility, the lowest frequency spin wave is predicted to have a frequency of 0.64 THz and out-of-plane anisotropy dominates. This suggests that easy-plane antiferromagnetic materials might exhibit fast dynamics and high speed of switching similar to uniaxial materials. However, these materials might suffer from low thermal stability, due to the extremely small in-plane anisotropy.

*Illinois MRSEC NSF DMR-1720633
First-principles study of the phonons and crystal-field excitations in the magnetodielectric regime of Ce2O3* YUEQING CHANG (Presenter), ASTHA SETHI, JOHN SLIMAK, LUCAS WAGNER, S. LANCE COOPER, University of Illinois at Urbana-Champaign — The mechanism associated with the giant magnetodielectric effect that was recently reported in A-type Ce2O3 remains an open question [1]. Recent Raman measurements indicate that there are vibronic excitations in its magnetodielectric regime, which in turn suggest a strong coupling between its spin, lattice and electronic degrees of freedom [2]. In this study, we apply density functional theory with LDA+U+SOC functional to disentangle the multiple coupling channels. The results show that strong coupling exists between the phonons and crystal-field excitations. This study helps to elucidate the underlying mechanism of the strong magnetodielectric effect in Ce2O3.


*This work was funded by the grant DOE FG02-12ER46875 (SciDAC).

Matter-Beam Interactions: Photochemistry with Virtual Photons?* DAVID LINGERFELT (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JACEK JAKOWSKI, Center for Nanophase Materials Sciences & Computational Sciences and Engineering Division, Oak Ridge National Laboratory, PANCHAPAKESAN GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, BOBBY SUMPTER, Center for Nanophase Materials Sciences & Computational Sciences and Engineering Division, Oak Ridge National Laboratory — It has recently been appreciated that the convergent electron beams used in scanning transmission electron microscopes (STEMs) can not only be employed for purposes of structural determination, but also for inducing local chemical transformations. STEMs have already been used to build heterostructures from substitutional defects in two-dimensional materials with atomic precision; a feat with transformative technological implications. However, the mechanisms underlying the chemical processes initiated by the matter-beam interaction are not yet well-understood. I will present our recent progress towards first principles methods for describing the electronic response of materials to high energy electron irradiation. I will also discuss the selection rules for electronic excitations that can occur in the materials, which depend explicitly on the incident electron's point of impact. Finally, I will give an overview of a study in which these methods are applied to reveal defect-centered excited states of silicon-doped graphene nanostructures, and the effects of beam-induced population of these exited states on the reactivity of the silicon defect.

*This work was performed at the Center for Nanophase Materials Sciences, a U.S. Department of Energy Office of Science User Facility.
10:36 AM A39.00012: Discretized Diagonalization for Efficient Berry Curvature Integration: Application to Electric Polarization  
JOHN BONINI (Presenter), DAVID VANDERBILT, KARIN M RABE, Rutgers University, New Brunswick — An important property in characterizing the response of a material to an electric field is the induced change in electric polarization. For periodic systems, the modern theory of polarization relates this change to a change in the Berry phase, raising the question of the correct choice of branch. In this talk, I present a new method for predicting the electric-field-induced change in polarization using only the wavefunctions of only the initial and final states, based on finely subdividing the relevant phase change into gauge-invariant pieces. The underlying assumptions are automatically checked within the method and are valid for most known ferroelectrics, allowing the computation of switching polarization without the need to identify an explicit path or to perform calculations for intermediate states. The extension of this approach to the computation of other quantities expressed in terms of Berry curvature, notably topological invariants, will be discussed.

10:48 AM A39.00013: Study of the near-edge optical properties of monoclinic HfO$_2$ from first-principles*  
XIAO ZHANG (Presenter), ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — HfO$_2$ is a wide band gap dielectric material, that has applications in optical coatings, rendering the importance of a precise description of its optical properties. The full understanding, however, has been limited by the lack of a consistent explanation of a shoulder-like feature near the absorption onset, reported in multiple experimental studies. In this work, by solving the Bethe-Salpeter equation (BSE) for the optical polarization function, we compute the optical spectra of monoclinic HfO$_2$ from first-principles. From these results we show that the shoulder-like effect is intrinsic to the crystal and is related to excitonic effects. Further, we show that since HfO$_2$ is a polar material, lattice screening, especially beyond the current static screening approximation, can potentially be important in describing dielectric screening of the electron-hole Coulomb interaction. In this work, we explored the effect of \textit{dynamical} lattice screening in HfO$_2$, and aim at describing the influence of lattice screening on the near-edge optical spectra.

*This work is supported by the National Science Foundation (No. DMR-1555153) and is part of the Blue Waters sustained-petascale computing project, supported by the NSF (No. OCI-0725070 and ACI-1238993) and the state of IL.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A40 DCOMP DCMP DPOLY DBIO: Building the Bridge to Exascale: Applications and Opportunities for Materials, Chemistry, and Biology | 705 - Jack Wells, Oak Ridge National Lab - Tag(s): Focus
8:00AM A40.00001: A Path to the Exascale for Atomistic Simulations with Improved Accuracy, Length and Time Scales* [Invited] MITCHELL WOOD (Presenter), AIDAN THOMPSON, STEVEN JAMES PLIMPTON, Sandia National Laboratories, ANDERS NIKLASSON, DANNY PEREZ, Los Alamos National Lab — With exascale super computers arriving in the near future, it is timely to ask whether our simulation software is capable of matching this unprecedented computing capability. While many research challenges in material physics, chemistry and biology lie just out of reach on peta-scale machines due to length and time restrictions inherent to Molecular Dynamics(MD), questions of the accuracy of our simulations will continue to linger. Simply running the same peta-scale simulations with more atoms on a larger computer (weak scaling) does not advance the accessible timescales, nor does it avoid the pitfalls of empirically developed constitutive models. This talk will overview the U.S. Department of Energy* EXAALT (EXascale Atomistics for Accuracy, Length and Time) project and our efforts to provide software tools for MD that not only scale efficiently to huge atom counts, but also enable efficient MD simulations for smaller systems too. New parallel time-acceleration methods such as sublattice-ParSplice and local hyperdynamics have been developed along with quantum accurate machine learned interatomic potentials to study damage accumulation in plasma facing materials.

*This work is funded through the Exascale Computing Project (No. 17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

8:36AM A40.00002: Accelerating Quantum Molecular Dynamics simulations: Can GPUs really help?* JEAN-LUC FATTEBERT (Presenter), Oak Ridge National Laboratory, CHRISTIAN F. A. NEGRE, JAMAL MOHD-YUSOF, TOKS ADEDOYIN, Los Alamos National Laboratory, DANIEL OSEI-KUFFUOR, Lawrence Livermore National Laboratory, SUSAN MNISZEWSKI, Los Alamos National Laboratory — GPU accelerators on the most powerful supercomputers give us an opportunity to speed up time-to-solution for large-scale Quantum Molecular Dynamics simulations that would otherwise be too slow for practical purposes. But using this type of hardware in an efficient manner presents serious challenges. Besides having to possibly rewrite large amounts of codes, algorithmic changes may be required for optimal efficiency. Even then, using GPUs at full capacity is not straightforward, in particular if there is not enough work for each GPU. In this talk we will present some software library solutions in development to facilitate porting electronic structure codes to new architectures, as well as parallel strategies and algorithms that can help speed up time-to-solution in real applications.

*This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration. This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
8:48AM A40.00003: Multibillion Atom Molecular Dynamics Simulations of Cellular Membranes  
NOAH TREBESCH (Presenter), Center for Biophysics and Quantitative Biology, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, EMAD TAJKHORSHID, Department of Biochemistry, Center for Biophysics and Quantitative Biology, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign — Membranes are the basic organizational and defensive unit of the cell, and they thus play a vital role in biological function. Electron microscopy (EM) can provide 3D structures of these membranes, and, with the advent of exascale computing, there is a new opportunity to use molecular dynamics (MD) simulations to elucidate the intricate biophysical connection between the complex structure and function of these membranes. To take advantage of this opportunity, we have developed xMAS (Experimentally-Derived Membranes of Arbitrary Shape) Builder, software designed to turn low resolution EM-based structures of cellular membranes into atomistic models that are suitable for MD. Using xMAS Builder, we have built the first cell-scale (~4.5 billion atom) model of a representative cellular membrane (a helicoidal system from the endoplasmic reticulum), and we have also built several models of a smaller synthetic system with equivalent complexity. Preliminary simulations of these models have demonstrated their potential to reveal fundamental insights into the general behavior of cellular membranes, supporting the expectation that xMAS Builder will soon enable MD simulations that leverage exascale computing to provide detailed biophysical characterization of these key biological systems.

9:00AM A40.00004: Unveiling the structural properties of HIV-1 vesicle from atomistic molecular dynamics simulations  
FABIO GONZALEZ, Univ of Delaware, TYLER REDDY, Los Alamos National Laboratory, JUAN PERILLA (Presenter), Univ of Delaware — The HIV-1 viral particle contains all the macromolecular components to infect host cells, typically CD4 + T human cells, by fusion of the viral envelope with the cell plasma membrane. Such macromolecular components correspond to phospholipids, membrane glycoproteins, genomic RNA, and gag polyproteins; which are assembled during infection to furthermore undergo maturation and structural re-arrangements to form the virion. Here, exploiting the advances of molecular modeling, we present the first insights towards the construction of an all-atomistic model of the HIV-1 mature and immature virion. The model includes a twenty-four lipids bilayer with membrane glycoproteins, and the capsid protein. We review over the techniques proposed to build and prepare the system, as well as the steps required to simulate, analyze and characterize the HIV-1 virion model, which contains over 800 million atoms.
9:12AM A40.00005: Molecular Understanding of Membranes for the Water-Energy Nexus in the Exascale Realm*  
DVORA PERAHIA (Presenter), Clemson University, GARY GREST, Sandia National Laboratories — Polymeric membranes are used for a large variety of clean energy, medical, and environmental applications. Their use remains limited by tradeoffs of permeability, selectivity and longevity. A fundamental paradigm shift from a descriptive continuum approach to a predictive atomic and molecular level understanding of ion transport is essential for transformative progress to programable smart membranes. The need to control the interrelation of membrane structure, dynamics, transport and stability over a wide range of length and time scales is in the core of design of new membranes. Here we will present molecular dynamics simulation results that depict the structured motion and transport in polymeric membranes that consists of units, or blocks, with different chemical structures, tailored into a macromolecule with targeted roles. The impact of fundamentals that underline the structure/processing/properties relations that will be attained through exascale computing will be discussed.

*DOE SC0019284, NERSC, NSF DMR 1611136; NSF DMR, 1905407.

9:24AM A40.00006: Multi-GPU parallelization of Deep Potential Molecular Dynamics for high-performance computing  
DENGHUI LU (Presenter), College of Engineering, Peking University, Beijing 100871, P. R. China., WEILE JIA, University of California, Berkeley, CA, 94720, USA, MOHAN CHEN, College of Engineering, Peking University, Beijing 100871, P. R. China., HAN WANG, Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Huayuan Road 6, Beijing 100088, People's Republic of China, LINFENG ZHANG, Program in Applied and Computational Mathematics, Princeton University, Princeton, NJ 08544, USA — The recently developed Deep Potential Molecular Dynamics [1,2] (DPMD) builds many-body potentials for atomic systems based on the deep neural network and has been successfully applied to a variety of systems. The DPMD model owns the quantum mechanical accuracy and the linear growth computational complexity. In this work, we develop the multi-GPU parallelization for DeePMD-kit [3], an implementation of DPMD, and optimize the workflows when the package interfaces with LAMMPS and TensorFlow. We demonstrate that the resulting package is well-suited for high-performance computing with the aim of performing large-scale molecular simulations with quantum mechanical accuracy.

9:36AM A40.00007: Scalable Frameworks for Reinforcement Learning for Control of Self-Assembling Materials and for Chemistry Design  PAUL WELCH (Presenter), Theoretical Division, Los Alamos National Laboratory, CHRISTINE SWEENEY, Los Alamos National Laboratory, MALACHI SCHRAM, Pacific Northwest National Laboratory, LOGAN WARD, Argonne National Laboratory — The ExaLearn Exascale Computing Project has developed scalable frameworks for reinforcement learning (RL) to control scientific processes such as the self-assembly of block copolymers and chemical design. These policies could drastically reduce the time required to navigate large parameter spaces, optimizing experimental protocols. This accelerated search methodology may thus guide materials annealing experiments, exploration of candidate structures for battery materials, or evaluation of the configurational space for low-energy water clusters. The frameworks use various RL algorithms, environments and fast-running scientific simulations for the training process. RL training can be thought of as creating a sequence of moves in a game; at each move the player (agent) may decide to exploit previous knowledge (a policy) or explore new parameters (run a simulation). Scalability is achieved by running many RL training episodes on different nodes and aggregating models. Challenges include developing simulations, fully utilizing CPU and GPU resources on each node, and aggregating policies so as not to impede learning. We present results for full single node and preliminary multi-node computing resource utilization performance.

9:48AM A40.00008: Exascale-ready neural network interatomic potentials with CabanaMD*  SAM REEVE (Presenter), Lawrence Livermore Natl Lab, SAKETH DESAI, Purdue University, JAMES BELAK, Lawrence Livermore Natl Lab — Computational predictions for materials require sufficiently accurate physics models which can be simulated in a reasonable amount of time. In the drive towards exascale computing, new hardware and software technologies are enabling more complex, accurate, and expensive models, but only with rethinking of algorithms, communication patterns, and data layouts. We exemplify this trend with a re-implementation of the Behler-style neural network potential (NNP), for classical molecular dynamics (MD) with near-quantum level accuracy. We use the Co-design center for Particle Applications (CoPA) Cabana particle library which, i) is built on Kokkos for on-node parallelism on various hardware, ii) provides performant particle-centric functionality, including MPI communication and neighbor lists, and iii) enables optimization of data structure for a given architecture through arrays-of-structs-of-arrays (AoSoA), intermediate between AoS and SoA. The NNP is added to the CabanaMD proxy app, where we show performance portability, including many-core CPU and GPU.

*Work performed under the auspices of the U.S. DOE by LLNL under contracts DE-AC52-07NA27344 and supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. DOE Office of Science and the NNSA.
10:00AM A40.00009: DOE Software Center for Non-perturbative Studies of Functional Materials Under Non-equilibrium Conditions (NPNEQ)*  

TADASHI OGITSU (Presenter), XAVIER ANDRADE, ALFREDO A. CORREA, Lawrence Livermore Natl Lab, LIANG TAN, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, SRI CHAITANYA DAS PEMMARAJU, SLAC, AARON LINDENBERG, SLAC/Stanford — Fundamental processes that underlie transformations of energy and information in material systems are intrinsically non-equilibrium in character as they involve additional coupling of electronic and ionic degrees of freedom to external time-dependent perturbations such as light or electrical voltages. Understanding and controlling the quantum non-equilibrium nature of functional materials on the characteristic Angstrom (Å, 10^{-10} m) length scales and femtosecond (fs, 10^{-15} s) time scales of electronic motion is a crucial component in the rational design of energy-relevant materials and devices. In this presentation, we will introduce the software center, NPNEQ, where the open-source real-time time-dependent density-functional-theory (RT-TDDFT) code is being developed. We will also discuss about joint theory-experiment scientific research plan that will fully take advantage of the RT-TDDFT code that exploits the full potential of the GPU-CPU architectures as well as the ultrafast experimental capability at SLAC.

*The work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344 and was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division.

10:12AM A40.00010: Towards fast and accurate exascale density functional theory calculations using DFT-FE -- a massively parallel real-space code using adaptive finite-element discretization*  

SAMBIT DAS (Presenter), PHANI MOTAMARRI, VIKRAM GAVINI, Univ of Michigan - Ann Arbor — Kohn-Sham density functional theory (DFT) calculations have been instrumental in providing many crucial insights into materials behavior and occupy a sizable fraction of world’s computational resources today. However, the stringent accuracy requirements in DFT needed to compute meaningful material properties, in conjunction with the asymptotic cubic-scaling computational complexity with number of electrons, demand huge computational resources. Thus, these calculations are routinely limited to material systems with at most few thousands of electrons. In this talk, we present a significant advance in the state-of-the-art for accurate DFT calculations -via- the development of DFT-FE, that has enabled fast, scalable and accurate large-scale DFT calculations on material systems with tens of thousands of electrons. This has been facilitated by (i) the development of efficient and accurate spatially adaptive discretization strategies using higher-order finite-element discretization; (ii) developing efficient and scalable algorithms in conjunction with mixed-precision strategies; (iii) implementation innovations, both on many core and hybrid architectures, that significantly improve performance.

*DoE-BES Award Number DE-SC0008637 and Toyota Research Institute
10:24AM A40.00011: Massively-Parallel Real-Time TDDFT Simulations of Electronic Stopping in Solvated DNA under Proton Irradiation* DILLON C YOST (Presenter), YI YAO, CHRIS SHEPARD, YOSUKE KANAI, Univ of NC - Chapel Hill — We discuss massively-parallel real-time, time-dependent density functional theory (RT-TDDFT) simulations for investigating electronic stopping in DNA solvated in water. We have developed RT-TDDFT capabilities within the Qbox/Qb@ll code, based on a planewave-pseudopotential formalism [1], which is applied to study the electronic excitation dynamics of solvated DNA under proton irradiation. In electronic stopping processes, massive electronic excitations are produced by fast energetic charged particles like protons. Electronic stopping is central to DNA damage by ion irradiation, which is central to ion beam cancer therapy. We discuss the scalable implementation and performance of the RT-TDDFT simulations and recent results for solvated DNA, a system which includes more than 13,000 electrons.


*This work was financially supported by the NSF under Awards No. CHE-1565714/OAC-1740204. Computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program This research used resources of the Argonne Leadership Computing Facility (ALCF), which is a DOE Office of Science User Facility supported under Contract No. DE-AC02-06CH11357.

10:36AM A40.00012: Spatiotemporal Mapping of Polymer Dynamics* JIHONG MA (Presenter), JAN-MICHAEL CARRILLO, BOBBY SUMPTER, YANGYANG WANG, Oak Ridge National Laboratory — Polymers present unique challenges to computational science, as their structures and dynamics are characterized by a remarkably wide range of length scales and timescales. The recent advances in high performance computing systems have afforded new opportunities to investigate the slow dynamics in polymeric liquids. In this talk, we demonstrate a novel approach to resolve the fine spatiotemporal features of entangled polymer dynamics, by leveraging the computational resources at the Oak Ridge Leadership Computing Facility. Potential applications of this new method will also be discussed.

*The research is supported by the Laboratory Directed Research and Development Program (LDRD) of the Oak Ridge National Laboratory.
Towards adaptive exascale workflows for simulating long timescales

JOHN OSSYRA (Presenter), University of Tennessee, Knoxville, ADA SEDOVA, JEREMY SMITH, Oak Ridge National Laboratory — Molecular dynamics simulations integrate trillions of short simulation steps and are reaching hardware-bound performance limits for clock time per step. Despite this, most biologically relevant processes occur over seconds to hours, orders of magnitude slower than feasible simulation timescales. Workflow-based methods harnessing complex statistical mechanics analyses are increasingly used with the hope of achieving kinetic estimates on experimentally relevant timescales from swarms of short parallel simulations. We present a highly scalable workflow software, AdaptiveMD, that implements a massively parallel adaptive-sampling algorithm to build a Markov-state model of long-timescale biomolecular kinetics. The software was ported to the Summit pre-exascale machine at the Oak Ridge Leadership Computing Facility (OLCF), after initial development on OLCF Titan, and demonstrated excellent scalability and fault tolerance. Summits software and hardware features allow for an unprecedented ability to simulate large biomolecular systems within this framework. These results suggest that this method at exascale may allow us to tackle grand challenges in biomolecular simulations.

*This work was supported from a Laboratory Directed Research and Development award from the US Department of Energy.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A41 GMAG DMP FIAP DCOMP: 2D Magnetic Materials

8:00AM A41.00001: Discovery of Intrinsic Two-dimensional Ferromagnetism in CrTe$_2$ Thin films

XIAOQIAN ZHANG, JACOB COOK (Presenter), QIANGSHENG LU, GUANG BIAN, Univ of Missouri - Columbia — Two-dimensional (2D) layered ferromagnetic (FM) materials have attracted much interest recently since the discovery of intrinsic 2D ferromagnetism in atomically thin layers. Due to the reduced dimensionality, 2D magnets usually exhibit weak magnetic ordering compared to conventional bulk magnets. In this work, we report robust 2D ferromagnetism in chromium ditelluride (CrTe$_2$) nanofilms whose electronic structure and magnetic properties are clearly resolved by angle-resolved photoemission spectroscopy (ARPES), superconducting quantum interference device (SQUID) and X-ray magnetic circular dichroism (XMCD). The robust ferromagnetism has been experimentally evidenced, and persists up to 250 K. In addition, the electron band structure of the ferromagnetic ground state was clearly resolved by in-situ ARPES. These experimental evidences establish CrTe$_2$ nanofilms as an outstanding 2D vdW magnet for spintronics applications.

*G.B. is supported by the US National Science Foundation (NSF-DMR#1809160)
8:12AM A41.00002: Magnetic field- and temperature-dependent resonant Raman spectroscopy of bulk CrI₃

SIWEN LI (Presenter), Univ of Michigan - Ann Arbor, ZHIPENG YE, Texas Tech University, XIANGPENG LUO, Univ of Michigan - Ann Arbor, GAIHUA YE, Texas Tech University, SHANGJIE TIAN, HECHANG LEI, Renmin University of China, KAI SUN, Univ of Michigan - Ann Arbor, RUI HE, Texas Tech University, LIUYAN ZHAO, Univ of Michigan - Ann Arbor — The van der Waals magnet CrI₃ has been thought to host ferromagnetism in its bulk form and interlayer antiferromagnetism in its few-layer form. The magnetic excitations in bulk CrI₃ have been probed by inelastic neutron scattering, while those in CrI₃ films have been studied with inelastic magneto-tunneling spectroscopy and Raman spectroscopy. Despite such intensive effort, it remains mysterious till now how the interlayer magnetism evolves from the ferromagnetic type in bulk to the antiferromagnetic one in thin films and what the low energy magnetic excitations are in CrI₃. In this talk, we will present our results on temperature- and magnetic field-dependent resonant Raman spectroscopy studies on bulk CrI₃. We will show our experimental evidences on the complex spin wave structures in bulk CrI₃ and their intricate magnetic field dependence. We will further discuss the magnetic field dependence of phonons and explore the interplay between the lattice and the spin degrees of freedom in bulk CrI₃.

*Supported by NSF CAREER Grants No. DMR-1760668 and No. DMR-1749774.

8:24AM A41.00003: Electric-Field Control of 2D Magnetism in Bilayer VI₃

THI PHUONG THAO NGUYEN (Presenter), KUNIHIKO YAMAUCHI, TAMIO OGUCHI, Institute of Scientific and Industrial Research Osaka University — The recent discovery of two-dimensional van-der-Waals (vdW) magnetic materials has received much interest owing to its potentials for future spintronics device applications. There is a large number of recent publications on two-dimensional honeycomb ferromagnet CrI₃, which belong to the family of transition-metal trihalides MX₃ with X = Cl, B, and I, as a promising candidate materials for spintronics and magnetoelectronic applications. VI₃ is a new discovered material that belongs to the transition-metal trihalides. While its structure and bulk properties have been investigated, there is a lack of information about the magnetism in the thin film. In this presentation, we will present our first-principle study on the magnetic properties in bilayer VI₃ and the influence of applied electric-fields on the magnetism. We predict that the magnetic stability of bilayer VI₃ systems can be tuned by external electric fields and the effect is comparable with the case of bilayer CrI₃. To understand the physics behind, the geometry, stability, and electronic and magnetic properties of bilayer VI₃ will be discussed by presenting the projected density of state and the band structure.
Light-controlled magnetism in vanadium-doped tungsten disulfide monolayers

VALERY ORTIZ JIMENEZ (Presenter), YEN THI HAI PHAM, VIJAYSANKAR KALAPPATTIL, Physics, University of South Florida, FU ZHANG, MAURICIO TERRONES, Materials Science and Engineering, Pennsylvania State University, MANH-HUONG PHAN, Physics, University of South Florida — Transition metal dichalcogenides (TMDs) have received growing attention for their outstanding electrical and optical properties. A promising way to induce long-range ferromagnetism (FM) in TMDs is by introducing magnetic dopants to form a dilute magnetic semiconductor. Our recent study shows room temperature (RT) FM in V-doped monolayer WSe$_2$ (V-WSe$_2$), which is an important step for TMDs based spintronics. In this work, we show light-mediated magnetism in V-WS$_2$ at RT. We probe this effect using the magnetic LC-resonance principle which employs a soft FM Co-based microwire coil driven near resonance with an RF signal. Combined with an excellent giant magneto-impedance effect, the coil becomes highly sensitive to changes in magnetic flux through its core. The monolayer, placed at the core of the coil, is excited with a laser as we measure the change in magnetization. Interestingly, the magnetization depends on laser power and doping concentration, demonstrating the light control of 2D magnetism. We attribute this to the generation of electron-hole pairs which mediate the magnetization of the monolayer. These findings provide a promising route to exploit light-controlled FM in 2D spintronic devices.

*Work was supported by U.S. DoE (DE-FG02-07ER46438) and VISCOSTONE (VS-1253113200).

Strain Tuning of Magnetic Order in Two-dimensional Magnets

SHENGWEI JIANG (Presenter), HONGCHAO XIE, Cornell University, DANIEL WEBER, JOSHUA GOLDBERGER, Ohio State University, JIE SHAN, KIN FAI MAK, Cornell University — The recent discovery of two-dimensional (2D) van der Waals magnetic materials has received growing attention. Of particular interest are the thickness-dependent magnetic ground states in atomically thin CrI$_3$. The competing ferromagnetic and anti-ferromagnetic interlayer exchange interactions result in a competing magnetic order that is sensitive to external perturbations including magnetic field, electrostatic gating, and hydrostatic pressure. Here we demonstrate that the magnetic order in 2D CrI$_3$ can also be effectively tuned by applying in-plane strain. Our result demonstrates the potential for the application of 2D magnets in spin-mechanical devices.
9:00AM A41.00006: Tuning Magnetism of Monolayer Tungsten Disulfide by Transition Metal Doping* YEN THI HAI PHAM (Presenter), VALERY ORTIZ JIMENEZ, VIJAYSANKAR S KALAPPATTIL, Univ of South Florida, FU ZHANG, MAURICIO TERRONES, Pennsylvania State University, MANH-HUONG PHAN, Univ of South Florida — The recent discoveries of intrinsic ferromagnetism (FM) in two-dimensional (2D) materials have drawn particular attention on encoding the spin behavior at low dimensions. Theoretical investigations of 2D transition metal dichalcogenides (TMDs) have predicted promising perspectives for inducing intrinsic FM in 2D TMD semiconductors by transition metal doping. This has motivated us to experimentally exploit magnetic functionality in monolayer Fe- and V-doped WS₂ - a semiconducting TMD with outstanding optoelectronic and valleytronic properties. Pristine and Fe/V-doped monolayer tungsten disulfide films were grown on SiO₂ substrates by a single-step solution-based method. We observe that while monolayer WS₂ possesses a weak ferromagnetic ordering on its diamagnetic background, Fe:WS₂ and V:WS₂ monolayers exhibit strong, intrinsic FM at room temperature, which is also tunable by controlling dopant concentration. This, coupled with high-resolution TEM images, has suggested the mechanism of strong ferromagnetism in the films, resulting from the magnetic dopants and spatial-dependent ferromagnetic ordering between them. Our findings offer a prospect of developing novel 2D dilute magnetic semiconductors for future spintronic applications.

*Work was supported by VISCOSTONE (VS-1253113200).

9:12AM A41.00007: Magnetic Correlations in the Quasi-2D Semiconducting Ferromagnet CrGeTe₃ TRAVIS WILLIAMS (Presenter), ADAM ACZEL, Oak Ridge National Laboratory, BRENDEN ORTIZ, PAUL SARTE, STEPHEN WILSON, University of California, Santa Barbara — The quasi-two-dimensional, semiconducting ferromagnets CrSiTe₃ and CrGeTe₃ have been studied as candidates for spintronics applications due to the relatively accessible transition temperatures and large magnetic moments. While CrSiTe₃ has been more studied due to the ease of growing crystals, CrGeTe₃ is more interesting due to the higher transition temperature $T_C = 61$ K. In this study, we use neutron scattering to measure the static and dynamic magnetic properties. Neutron diffraction was used to study the 3D order below $T_C$, as well as two dimensional static correlations above the transition. Preliminary inelastic measurements shed light on the nature of the spin gap and magnetic correlations that drive the magnetism in this material, which can be contrasted to previous work on CrSiTe₃.
First-principles theory of proximity spin-orbit torque on a two-dimensional magnet: Current-driven antiferromagnet-to-ferromagnet reversible transition in bilayer CrI$_3$ KAPILDEB DOLUI (Presenter), MARKO PETROVIC, Department of Physics and Astronomy, University of Delaware, USA, KLAUS ZOLLNER, University of Regensburg, Germany, PETR PLECHAC, Department of Mathematical Science, University of Delaware, USA, JAROSLAV FABIAN, University of Regensburg, Germany, BRANISLAV NIKOLIC, Department of Physics and Astronomy, University of Delaware, USA — The recently discovered two-dimensional (2D) magnetic insulator CrI$_3$ is an intriguing case for basic research and spintronic applications since it is a ferromagnet in the bulk, but an antiferromagnet in bilayer form, with its magnetic ordering amenable to external manipulations. Using first-principles quantum transport approach, we predict that injecting unpolarized charge current parallel to the interface of bilayer-CrI$_3$/monolayer-TaSe$_2$ van der Waals heterostructure will induce spin-orbit torque (SOT) and thereby driven dynamics of magnetization on the first monolayer of CrI$_3$ in direct contact with TaSe$_2$. By combining calculated complex angular dependence of SOT with the Landau-Lifshitz-Gilbert equation for classical dynamics of magnetization, we demonstrate that current pulses can switch the direction of magnetization on the first monolayer to become parallel to that of the second monolayer, thereby converting CrI$_3$ from antiferromagnet to ferromagnet while not requiring any external magnetic field. The transition can be detected by passing vertical read current through the vdW heterostructure, encapsulated by bilayer of hexagonal boron nitride and sandwiched between graphite electrodes, where we find tunneling magnetoresistance of 240% [1].


Large anomalous Nernst effect in a van der Waals ferromagnet Fe$_3$GeTe$_2$ JINSONG XU (Presenter), WILLIAM ADAM PHELAN, CHIA-LING CHIEN, Johns Hopkins University — Anomalous Nernst effect, a result of charge current driven by temperature gradient, provides a probe of the topological nature of materials due to its sensitivity to the Berry curvature near the Fermi level. Fe$_3$GeTe$_2$, one important member of the recently discovered two-dimensional van der Waals magnetic materials, offers a unique platform for anomalous Nernst effect because of its metallic and topological nature. Here, we report the observation of large anomalous Nernst effect in Fe$_3$GeTe$_2$. The anomalous Hall angle and anomalous Nernst angle are about 0.07 and 0.09 respectively, far larger than those in common ferromagnets. By utilizing the Mott relation, these large angles indicate a large Berry curvature near the Fermi level, consistent with the recent proposal for Fe$_3$GeTe$_2$ as a topological nodal line semimetal candidate. Our work provides evidence of Fe$_3$GeTe$_2$ as a topological ferromagnet, and demonstrates the feasibility of using two-dimensional magnetic materials and their band topology for spin caloritronics applications.

*This work was supported by the US Department of Energy, Basic Energy Science Aeard Grant No. DE-SC0009390. The bulk crystals growth was supported by the National Science Foundation under Cooperative Agreement No. DMR-1539918.
Unconventional magnetic behavior in two-dimensional layered CrTe$_2$ films*  

HANG CHI (Presenter), YUNBO OU, Massachusetts Institute of Technology, DON HEIMAN, Northeastern University, JAGADEESH MOODERA, Massachusetts Institute of Technology — Quasi two-dimensional (2D) transition metal dichalcogenides (TMDs) often exhibit nontrivial topological phenomena. Here, we explore the behavior of a new van der Waals (vdW) TMD, CrTe$_2$ epitaxial films with apparent C$_6$ in-plane symmetry. Rich magnetic/transport properties develop upon varying film thickness. In the few monolayer (ML) regime, films display perpendicular magnetic anisotropy with a Curie temperature $T_C \sim 160$ K for 40 ML thickness. Apart from the ordinary Hall effect (OHE) with linear field dependence, the anomalous Hall effect (AHE) manifests a unique temperature-dependent sign reversal. Interestingly, a novel feature arising from the topological Hall effect (THE) is observed as well. These features likely originate from the strained substrate/film interface, which is believed to modify the topology of the electronic band structure and stabilize the formation of magnetic skyrmions in layered TMD. The vdW nature of CrTe$_2$ makes it appealing for interfacial Berry-phase engineering. The ferromagnetic CrTe$_2$ films with novel noncoplanar spin textures and novel electronic properties offer new opportunities for spintronics devices using vdW TMDC architectures.

*Supported by ARO W911NF-19-2-0015 and W911NF-19-2-0041, NSF DMR 1700137, ONR N00014-16-1-2657 and CIQM-NSF 1231319.

Ultimate tunability of ferromagnetic anisotropy in chromium mixed halides*  

FAZEL TAFTI (Presenter), THOMAS TARTAGLIA, FARANAK BAHRAMI, JOSEPH TANG, Boston College — In recent years, chromium iodide, bromide, and chloride have received attention due to exhibiting ferromagnetic ordering in 2D which is ideal for ultrathin magneto-optical devices. Also, it has been demonstrated that by alloying the halides, the magnetic easy axis can be tuned. Here, we show the ultimate case of such alloying, by presenting a new material CrClBrI where all three halides are mixed in one composition. The crystals of CrClBrI are thin and exfoliate. We present a phase diagram of all compositions of mixed halides and demonstrate how the critical temperature, Weiss constant, and magnetic anisotropy are continuously tuned across the series.

*NSF-DMR-1708929
10:12AM A41.00012: Spin-dependent scattering in 2D van der Waals ferromagnet Fe\textsubscript{0.29}TaS\textsubscript{2} and its heterostructure  
RANRAN CAI (Presenter), PENG LV, WENYU XING, YUNYAN YAO, YANG MA, HUIBIN ZHOU, BONING LI, YANGYANG CHEN, SHUANG JIA, Department of physics, ICQM, Peking University, IGOR ZUTIC, Department of physics, University at Buffalo, XINCHENG XIE, QING-FENG SUN, WEI HAN, Department of physics, ICQM, Peking University — The recent emergence of two-dimensional (2D) van der Waals ferromagnets has provided a new platform for exploring magnetism in the flatland and for designing 2D ferromagnet-based spintronics devices. In this talk, we will present the spin-scattering mechanisms in quasi-2D van der Waals ferromagnet. Via systematically measuring Fe\textsubscript{0.29}TaS\textsubscript{2} devices with different thickness, it is found that the dominant AHE mechanism is found to be skew scattering in bulk single crystal, and the contribution from intrinsic mechanism emerges and become more relevant as the Fe\textsubscript{0.29}TaS\textsubscript{2} thickness decrease. At the end, the spin-dependent scattering at the Fe\textsubscript{0.29}TaS\textsubscript{2}/superconductor interface will be discussed.

10:24AM A41.00013: Stacking Dependence of the Chern Number in a Ferromagnetic Topological Magnon Insulator Heterostructure*  
STEPHEN HOFER (Presenter), Physics, Southern Illinois University Carbondale, TRINANJAN DATTA, Chemistry and Physics, Augusta University, DIPANJAN MAZUMDAR, Physics, Southern Illinois University Carbondale — Recent advances in topological materials have shown that 2D magnetic insulators can be promising hosts for topologically non-trivial magnons. In this work we focus on the topological magnetic features of these materials as they might be grown in the few-layer regime. Particularly, we explore the AA and AB stacking dependencies on the Chern numbers of a layered ferromagnetic honeycomb topological magnon insulator heterostructure. Based on our bandstructure and Berry curvature calculations we show that the evolution of the Chern numbers depend non-trivially on the number of layers and the stacking arrangement, AA or AB. Additionally, we also discuss the physical consequences of sandwiching topological and non-topological ferromagnetic layers.

*NSF CAREER grant (ECCS: Award#1846829).

10:36AM A41.00014: Quantum critical point and ferromagnetic semiconducting behavior in p-type FeAs\textsubscript{2}  
BING-HUA LEI (Presenter), YUHAO FU, ZHENZHEN FENG, DAVID SINGH, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211-7010, USA — Ferromagnetic semiconductors are of interest due to the unusual combination of physical properties and because if tunable they may offer opportunities for studying magnetic quantum critical points. Here, we illustrate an approach for studying suitable materials based on itinerant magnetism, different from conventional magnetic semiconductors. We show that p-type FeAs\textsubscript{2} is an example. The complex non-parabolic band structure of this material leads to a ferromagnetic instability when doped, while at the same time allowing for a modest transport effective mass. This leads to an analogy between magnetic semiconductors and thermoelectric materials.

*This work was supported by the Department of Energy, award number DE-SC0019114.
Temperature Dependence of the Anomalous Hall Effect from Electron Interactions

SONGCI LI (Presenter), ALEX LEVCHENKO, University of Wisconsin - Madison — We consider the impact of electron-electron interactions on the temperature dependence of the anomalous Hall effect in disordered conductors. The microscopic analysis is carried out within the diagrammatic approach of the linear response Kubo-Streda formula with an account of both extrinsic skew-scattering and side-jump mechanisms of the anomalous Hall effect arising in the presence of spin-orbit coupling. We demonstrate the importance of electron interactions in the Cooper channel even for nominally non-superconducting materials and find that the corresponding low-temperature dependence of the anomalous Hall conductivity is asymptotically of the form $T^{1/2}/\ln(T_0/T)$ in three dimensions and $\ln[\ln(T_0/T)]$ in two dimensions, where the scale of $T_0$ is parametrically of the order of Fermi energy. These results, in particular, may provide an explanation for the recently observed unconventional temperature dependence of the anomalous Hall effect in HgCr$_2$Se$_4$.

*This work was supported by NSF Grant No. DMR-1653661 and No. DMR-1743986.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A42 GMAG DMP: Chiral and Topological Spin Textures 709/711 -
Lucas Caretta, University of California, Berkeley - Tag(s): Focus
8:00AM A42.00001: Manipulation of topological spin structures at ultrathin magnetic interfaces by oxygen adsorption and interlayer exchange coupling* TZU-HUNG CHUANG (Presenter), Scientific Research Division, National Synchrotron Radiation Research Center, LIANG-WEI LAN, Department of Physics, National Sun Yat-sen University, MING-CHING WU, CHIA-CHI LIU, Scientific Research Division, National Synchrotron Radiation Research Center, YAO-JUI CHAN, Department of Physics, National Sun Yat-sen University, CHIH-HENG HUANG, International PhD Program for Science, National Sun Yat-sen University, DER-HSIN WEI, Scientific Research Division, National Synchrotron Radiation Research Center, CHIEN-CHENG KUO, Department of Physics, National Sun Yat-sen University — Magnetic skyrmions have been investigated from fundamental physics to applications for next generation high-density information encoding. Such non-collinear magnetic structures at interfaces are usually attributed to the Dzyaloshinskii-Moriya interaction (DMI) when the inversion symmetry is broken. Here we report two ultrathin ferromagnetic systems, where the first one demonstrates a microscopic insight on how the oxygen adsorption modulates the spin reorientation transition (SRT) of a Fe/Ni bilayer on Cu(100) and consequently impacts on the DMI of the interface. The second case shows that even in a negligible DMI interface, such as Co/Au(111), magnetic skyrmion bubbles can be stabilized at room temperature in the metastable phase of spin canting configuration within the SRT by interlayer exchange coupling across a non-magnetic spacer layer. The magnetic images are measured by X-ray magnetic circular dichroism (XMCD) based photoemission electron microscopy (PEEM), and the experimental results are discussed with the help of micromagnetic simulations.

*Supported by MOST 105-2112-M-213-012-MY2, MOST 107-2112-M-213-008, and National Synchrotron Radiation Research Center

8:12AM A42.00002: Equilibrium thermodynamic properties of chiral skyrmions in ferromagnetic materials* ROBERTO ZIVIERI (Presenter), Univ of Messina — The equilibrium statistical thermodynamics of chiral magnetic skyrmions developing in a ferromagnetic material having the shape of an ultrathin cylindrical dot is investigated. This is accomplished by determining via analytical calculations for both hedgehog and vortex-like skyrmions: 1) the internal energy of a single chiral skyrmion; 2) the skyrmion radius depending on magnetic and geometric parameters; 3) the skyrmion configurational entropy; 4) the partition function; 5) the free energy; 6) the pressure and 7) the equation of state of a skyrmion diameters population. For the calculation of the thermodynamic functions we make the analogy between the skyrmion diameters population and the three-dimensional Maxwell-Boltzmann distribution of particles of an ideal gas [1]. It is shown that, in correspondence of the average skyrmion volumes, the pressure curves of the skyrmion diameters population intersect the pressure curves of the ideal gas at different temperatures. These results could advance the field of materials science with special regard to skyrmionics.


*The author acknowledges support by Gruppo Nazionale per la Fisica Matematica (GNFM) and Istituto Nazionale di Alta Matematica (INdAM) “F. Severi.”
8:24AM A42.00003: Theory of the Lifetime of Metastable Skyrmions in Chiral Magnets*  
PO-KUAN WU (Presenter), JAMES R ROWLAND, MOHIT RANDERIA, Department of Physics, Ohio State University — Understanding the lifetime of metastable skyrmions in chiral magnetic materials is both of fundamental interest and of practical importance. We use the Landau-Lifshitz-Gilbert equation with thermal noise to derive the activated rate for an isolated metastable skyrmion to decay into the stable ferromagnetic state. Our formalism includes damping as well as the effects of entropic corrections to the energy barrier within a Gaussian approximation. We show that the nature of the saddle point that needs to be crossed for the decay of a skyrmion changes from a Bloch point singularity in 2D systems to a chiral bobber in films with thickness \( L > L_D = 2\pi J/D \). We will present numerical and variational results as a function of ferromagnetic exchange \( J \), Dzyaloshinskii-Moriya interaction \( D \), effective anisotropy \( K \), and the external field \( B \), and discuss the relation between the size and lifetime of metastable skyrmions.

*Research supported by DARPA Grant No. D18AP00008

8:36AM A42.00004: Melting the skyrmion lattice - from solid to liquid via a hexatic phase*  
[Invited]  PING HUANG, State Key Laboratory for Mechanical Behaviour of Materials, Xi'an Jiaotong University, THOMAS SCHOENENBERGER (Presenter), MARCO CANTONI, Ecole Polytechnique Federale de Lausanne, LUKAS HEINEN, Institut fuer Theoretische Physik, Universitaet zu Koeln, ARNAUD MAGREZ, Ecole Polytechnique Federale de Lausanne, ACHIM ROSCH, Institut fuer Theoretische Physik, Universitaet zu Koeln, FABRIZIO CARBONE, HENRIK RONNOW, Ecole Polytechnique Federale de Lausanne — The most commonly seen phase transition is possibly "melting", a transition from ordered crystalline solids to disordered isotropic liquids. While melting in three-dimensions is always a single, first-order phase transition, in two-dimensional systems a scenario of two continuous phase transitions separated by an intermediate "oriented liquid" state, the so-called hexatic phase, has been proposed theoretically and evidenced experimentally in colloidal systems, Wigner solids and liquid crystals. Fundamentally different from these real-matter particles, skyrmions are countable soliton configurations localized in continuous fields with non-trivial topology, and these emergent quasi-particles can form two-dimensional lattices, whose melting dynamics remains unexplored. Here we show, by direct imaging with cryo-Lorentz transmission electron microscopy, that the phase of the skyrmion ensembles in the material Cu2OSeO3 can be tuned by magnetic field from two-dimensional skyrmion solids, through the long-speculated skyrmion hexatic phase, to skyrmion liquids, with the local spin order preserved throughout the whole process. Remarkably, our quantitative analysis demonstrates that this mesoscopic phase transition can be well described as topological-defect-induced crystal melting in two dimensions. By uncovering the novel phase behaviors of skyrmionic quasi-particles, we demonstrate skyrmion ensembles as an ideal platform for exploring novel properties in two-dimensions.

*This work was supported by the Swiss National Science Foundation (SNSF) through project 166298, the Sinergia network 171003 for Nanoskyrmionics, and the National Center for Competence in Research 157956 on Molecular Ultrafast Science and Technology (NCCR MUST), as well as the ERC project HERO. P. Huang also acknowledges the financial support from the Young Talent Support Plan of Xi'an Jiaotong University and the National Natural Science Foundation of China (No. 11904277).
9:12AM A42.00005: Quantifying Order in Magnetic Systems with Convolutional Neural Networks*  
GARY DOWNING (Presenter), MARIJAN BEG, HANS FANGOH, SRINANDAN DASMAHAPATRA, ONDREJ HOVORKA, University of Southampton — Quantifying the order parameters in simulations of disordered magnetic systems to reliably represent magnetic states requires efficient interpretation of the often irregular magnetic patterns contained in large data sets. In helimagnetic materials with impurities, or at non-zero temperatures, the helical and skyrmion textures become distorted and embedded in noisy backgrounds with varying topological properties. Standard approaches based on quantifying the order parameters by averaging the spin states over a lattice, or computing pair correlation functions often become inconclusive. In this presentation, we discuss an approach based on applying convolutional neural networks (CNNs) to extract representative features of skyrmionic textures from simulated snapshots of complex magnetic backgrounds. Using large-scale micromagnetic simulations of a broad class of helimagnetic materials we show that CNNs are capable of not only accurately resolving the underlying magnetic textures, but also allow for regression to accurately predict classes of micromagnetic models representative of the observable magnetic textures. We then draw general conclusions about the uniqueness and invertibility of micromagnetic models of helimagnetic materials.

*This work was supported by EPSRC grant EP/L015382/1

9:24AM A42.00006: Creation of magnetic skyrmions by surface acoustic waves in Pt/Co/Ir trilayer films  
TOMOYUKI YOKOUCHI (Presenter), Center for Emergent Matter Science (CEMS), RIKEN, SATOSHI SUGIMOTO, National Institute for Materials Science (NIMS), BIVAS RANA, Center for Emergent Matter Science (CEMS), RIKEN, SHINICHIRO SEKI, Department of Applied Physics and Institute of Engineering Innovation, The University of Tokyo, NAOKI OGAWA, Center for Emergent Matter Science (CEMS), RIKEN, SHINYA KASAI, National Institute for Materials Science (NIMS), YOSHICHIKA OTANI, Institute for Solid State Physics (ISSP), The University of Tokyo — A magnetic skyrmion, a particle-like noncoplanar topological spin structure characterized by a nonzero topological integer called the skyrmion number, has great potential for various spintronic applications. In particular, efficient and practical means to create skyrmions is an important technological issue. However, creation of skyrmions has been achieved by only using currents so far, and moreover, in these methods, the skyrmions are only created at a specific position in the films.

In this presentation, we demonstrate a novel approach for skyrmion creation by employing surface acoustic waves (SAWs); in asymmetric multilayers of Pt/Co/Ir, we experimentally observed at room temperature that skyrmions can be created by propagating SAWs in a wide area of the magnetic film due to the long propagation length of SAWs. Micromagnetic simulation reveals inhomogeneous torque arising from both SAWs and thermal fluctuations creates a pair of Néel and antiskyrmion-like structure, which subsequently transforms to Néel skyrmion due to the instability of antiskyrmion-like structure in systems with interfacial Dzyaloshinskii-Moriya interaction. Our finding provides a novel guiding principle for efficient manipulation of topological spin objects without Joule heating dissipation.
9:36AM A42.00007: Thermal Collapse of a Skyrmion* AMEL DERRAS-CHOUK (Presenter),
Physics, The Graduate Center, City University of New York, EUGENE M CHUDNOVSKY, DMITRY
GARANIN, Physics, Herbert H. Lehman College — Thermal collapse of an isolated skyrmion on a two-
dimensional spin lattice has been investigated. The method is based upon solution of the system
of stochastic Landau-Lifshitz equations for up to 104 spins. The recently developed pulse- noise
algorithm has been used for the stochastic component of the equations. The collapse rate
follows the Arrhenius law. Analytical formulas derived within a continuous spin-field model
support numerically-obtained values of the energy barrier. The pre-exponential factor is
independent of the phenomenological damping constant that implies that the skyrmion is
overcoming the energy barrier due to the energy exchange with the rest of the spin system. Our
findings agree with experiments, as well as with recent numerical results obtained by other
methods.

*Grant No. DEFG02- 93ER45487 funded by the U.S. Department of Energy, Office of Science.

9:48AM A42.00008: Operando study of chiral magnetic textures under electrical bias using
Lorentz scanning transmission electron microscopy* ALBERT PARK (Presenter), ZHEN CHEN,
LIJUN ZHU, ROBERT BUHRMAN, DAVID MULLER, GREGORY FUCHS, School of Applied and Engineering
Physics, Cornell University — We develop a device fabrication process that is compatible with
operando Lorentz Scanning Transmission Electron Microscopy (LSTEM) for studying chiral
magnetic textures and their electric current dependent behavior with nanometer-scale spatial
resolution. Chiral magnetic spin textures appear in our samples as a result of the interplay
between magnetic energy terms including interfacial Dzyaloshinskii-Moriya Interaction and
perpendicular magnetic anisotropy (PMA) at heavy metal/ferromagnet interfaces. High-resolution
LSTEM can resolve the internal structure of spin textures including details as small as a few nm.
As a first step, we examine stripe domain and field nucleated Néel Skyrmions in devices as we
vary the stack repetition and ferromagnet thicknesses. We find rich magnetic textures with a
strong history dependence as the magnitude of PMA approaches zero.

*We acknowledge support from the DARPA TEE program (D18AC00009).
10:00AM A42.00009: Robust magnetization dynamics and magnetocaloric anomalies across the phase diagrams of noncollinear magnets  ELEANOR CLEMENTS (Presenter), Univ of South Florida, RAJA DAS, Phenikaa University, GANESH POKHAREL, LING LI, DAVID MANDRUS, University of Tennessee, Knoxville, MICHAEL OSOFSKY, Naval Research Lab, HARIHARAN SRIKANTH, MANH-HUONG PHAN, Univ of South Florida — Incommensurate magnetic structures stabilized by the Dzyaloshinskii-Moriya interaction exhibit long-range phase coherence over macroscopic length scales. Depending on the crystal symmetry, the magnetocrystalline anisotropy controls the orientation of the propagation vector and may also enhance the robustness of the magnetic texture. We present recent studies on the magnetic phase evolution of noncollinear spin textures analyzing the nonlinear ac magnetic response and magnetocaloric effect for selected crystalline magnetic materials with broken inversion symmetry: Cr$_{1/3}$NbS$_2$, GaV$_4$S$_8$, and MnSi. Each realize solitonic spin textures of varying dimension and helicity due to distinct differences in magnetocrystalline anisotropy. By analyzing the anomalous nonlinear response and dynamic magnetic loss, we characterize the rigidity of the various spin textures against an ac magnetic field. Additionally, our magnetocaloric measurements uncover phase regimes characterized by field-induced spin fluctuations, where entropy increases across the metamagnetic transition. The combined analysis reveals details about the complex ordering and magnetization processes that may be useful for identifying new magnetic phases emerging from long-period spin textures.

10:12AM A42.00010: Surface acoustic waves (SAW) and pinning of magnetic domain walls in a ferromagnetic multilayer.*  ANIL ADHIKARI (Presenter), SHIREEN ADENWALLA, Physics and Astronomy, University of Nebraska - Lincoln — The pinning of magnetic domain walls (DW) results in reduced velocities and non-deterministic motion of domain walls. Perpendicular anisotropy (PMA) materials display narrow, stable DWs but the pinning barriers have a significant effect due to the small width. We investigate the effects of SAW on pinning and motion of domain walls in films of Cr(2nm)/Pt(2nm)/[Co(0.3nm)/Pt(0.6nm)]$_5$ that are patterned into micron wide stripes between a pair of inter-digital transducers (IDTs), all on a 128 -Y cut LiNbO$_3$ substrate. Measurements were made using a magneto-optical Kerr effect microscope. Preliminary measurements of DW motion using magnetic field pulses, varying both the width and the height of the pulse identified the location, pinning potential and critical field of highly reproducible strong pinning sites. The effect of SAW on these well characterized pinning sites indicate that SAW are able to depin DW even from deep pinning potentials. The standing wave generated by the IDT pair allows for measurements at both the and antinodes of the SAW. Between these deep pinning sites, DW motion is consistent with creep behavior, with increasing SAW amplitude increasing the DW velocity.

*NSF (DMR-1409622) and NSF Nebraska MRSEC (DMR-1420645).
Skyrmions and antiskyrmions from current-induced boundary instabilities

SHANE SANDHOEFNER (Presenter), ALDO RAELIARJAONA, RABINDRA NEPAL, University of Nebraska - Lincoln, DALTON SNYDER-TINOCO, California State University at San Bernardino, ALEXEY KOVALEV, University of Nebraska - Lincoln — We study generation and dynamics of skyrmions and antiskyrmions using current-induced torques at interfaces between adjacent regions with differing properties such as DMI (Dzyaloshinskii-Moriya interaction), anisotropy, exchange, etc.. The generation of skyrmions and antiskyrmions can be interpreted as a current-induced Doppler shift acting on the magnons localized at the interface. These localized modes are analyzed by using the Bogoliubov-de-Gennes Hamiltonian written for magnons. We confirm our theoretical predictions using micromagnetics simulations, where we observe that a current pulse closes the magnon band gap, leading to instabilities in the magnetic texture at the interface between different regions. From micromagnetic simulations, we observe that the closure of the magnon band gap effectively causes the system to form skyrmions and/or antiskyrmions, depending on the type of DMI present.

Stability of biskyrmions in centrosymmetric magnetic films

DANIEL CAPIC (Presenter), DMITRY GARANIN, EUGENE M CHUDNOVSKY, CUNY-Lehman Coll — In [1], we investigate analytically and numerically the stability of biskyrmions in films of finite thickness, taking into account the nearest-neighbor exchange interaction, perpendicular magnetic anisotropy (PMA), dipole-dipole interaction (DDI), and the discreteness of the atomic lattice. The biskyrmion is characterized by the topological charge Q=2, the spatial scale λ, and another independent length d that can be interpreted as a separation of two Q=1 skyrmions inside a Q=2 topological defect in the background of uniform magnetization. We find that biskyrmions with d of order λ can be stabilized by the magnetic field within a certain range of the ratio of PMA to DDI in a film having a sufficient number of atomic layers Nz. The shape of biskyrmions has been obtained by the numerical minimization of the energy of interacting spins in a 1000×1000×Nz atomic lattice. It is close to the exact solution of the Belavin-Polyakov model when d is below the width of the ferromagnetic domain wall. We compute the magnetic moment of a biskyrmion and discuss ways of creating biskyrmions in experiment.


*Grant No. OSR2016-CRG5-2977 from KAUST
10:48AM A42.00013: Magnetic domain dynamics in an insulating quantum ferromagnet
CHRISTOPHER TANG (Presenter), DANIEL SILEVITCH, Caltech, JIAN XU, James Franck Institute,
University of Chicago, KARIN ANDREA DAHMEN, Department of Physics, University of Illinois at Urbana-
Champaign, THOMAS F ROSENBAUM, Caltech — The structure of free-energy manifolds with many
local minima are of great interest in the context of quantum computation and optimization. In
the disordered ferromagnet, LiHo_xY_1-xF_4, quenched disorder and frustration, driven by the
combination of chemical substitution and the anisotropic magnetic dipolar coupling, give rise to
one such example of a complex, traversable free-energy landscape. We probe the structure of
this landscape and the dynamics of the driven system by measuring the statistics and form of
magnetic avalanches due to domain-wall motion. For large avalanches at temperatures
approaching the Curie point, we find a response free of the signatures of drag effects. By
contrast, in the low temperature limit, drag effects contribute to the dynamics, which we attribute
to enhanced pinning from local random fields due to the disorder. Furthermore, as an applied
transverse magnetic field is increased, the dynamics of the system can be tuned by progressively
strengthening the random-field pinning and then increasing the quantum tunneling rate. Tuning
from a classical regime to a quantum regime dominated by tunneling reveals the structure of the
free-energy surface and barriers to domain reorientation, with applications to quantum
annealing.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A43 DCOMP DAMOP DCMP: Precision Many-Body Physics I: Ab
Initio Methods 702 - Moritz Binder, Duke University - Tag(s): Focus
**8:00AM A43.00001: Ab initio finite-temperature and excited state computations by auxiliary-field quantum Monte Carlo** [Invited] SHIWEI ZHANG (Presenter), Center for Computational Quantum Physics (CCQ), Flatiron Institute — Development in the ground-state auxiliary-field quantum Monte Carlo (AFQMC) approach over the past decade has allowed accurate computations in a broad array of systems ranging from Hubbard-like models, ultracold Fermi gases, to solids and quantum chemistry. I will discuss recent progress in generalizing the approach to non-zero temperatures. Two bottlenecks had to be removed. The first is the sign or phase problem which appears in most cases, similar to ground-state calculations. The second is the unfavorable scaling of finite-temperature, grand-canonical computations as \( N^3 \) (\( N \) is the size of the lattice or basis set) in contrast with \( N*M^2 \) in ground-state computations (\( M \) is the number of fermions), a major obstacle in any realistic calculations aiming to describe the continuum limit, where \( N/M \) needs to be extrapolated to infinity for convergence. We remove the sign or phase problem by constraining the path-integrals in field space with a gauge condition; a self-consistent procedure is formulated to improve the accuracy of the constraint iteratively [1]. We then introduce a systematically controllable low rank factorization which changes the scaling of the computations to \( N*M^2 \) [2]. The method is applicable to both models and real materials. Results will be presented on magnetic and stripe orders in the repulsive Hubbard model, as well as pairing and other properties in the strongly interacting two-dimensional Fermi gas as a function of temperature.


*Flatiron Institute is a division of the Simons Foundation. Partial support from NSF.

**8:36AM A43.00002: Effects of charge self-consistency in DFT+DMFT calculations for complex transition metal oxides** ALEXANDER HAMPEL (Presenter), Center for Computational Quantum Physics, Flatiron Institute, SOPHIE BECK, CLAUDE EDERER, ETH Zurich — During recent years, the combination of density functional theory (DFT) and dynamical mean-field theory (DMFT) has become a widespread tool to calculate properties in correlated materials. The basic idea of the method is that the electronic degrees of freedom can be separated into a weakly interacting part, for which a standard DFT treatment is adequate, and a correlated subspace, which requires a more elaborate treatment of the electron-electron interaction. The latter leads, in general, to a redistribution of electrons within the correlated subspace compared to the DFT result. This change should then enter, in a self-consistent way, the effective potential felt by the weakly interacting electrons, which is achieved by iterating between DFT and DMFT steps. However, such a charge self-consistent (CSC) DFT+DMFT calculation leads to a higher computational cost compared to simpler one-shot calculations, where this charge rearrangement is neglected. Here, we examine the effect of CSC in DFT+DMFT calculations compared to simpler one-shot calculations for two instructive example materials, CaVO\(_3\) and LuNiO\(_3\), to clarify in which cases the more complex CSC treatment is necessary and in which cases the simpler one-shot calculation is sufficient.
DFT+eDMFT Study of Finite-temperature Properties of Filled Skutterudite CeGe_{4}Pt_{12}∗

KHANDKER QUADER (Presenter), Physics, Kent State University, Kent, OH 44242, USA, GHEORGHE PASCUT, MANSiD Research Center and Faculty of Forestry, Stefan Cel Mare University (USV), Suceava 720229, Romania, KRISTJAN HAULE, Physics & Astronomy, Rutgers University, New Brunswick, NJ, USA 08854, MICHAEL WIDOM, Physics, Carnegie-Mellon University, Pittsburgh, PA 15213, USA — Current interest in the filled skutterudites stem from a range of observed physical phenomena, such as superconductivity, Kondo-lattice, heavy fermion, Fermi liquid behavior, etc, and due to thermoelectric properties at room temperature. Following up on our comprehensive density functional theory (DFT) study (PRB 100, 125114 (2019)) of the RPt_{4}Ge_{12} (R=La, Ce, Pr) compounds, we have been performing temperature dependent calculations on these systems using first-principles self-consistent density functional theory with embedded-dynamical mean field theory (DFT+eDMFT). Here we present results for CeGe_{4}Pt_{12}, namely the temperature dependence of spectral function, density of states, hybridization, effective mass, susceptibility, and resistivity, and compare with experiments. Based on our calculations, we suggest that CeGe_{4}Pt_{12} exhibits Curie-Weiss behavior at high temperature (indicating presence of local moments), a Kondo-lattice like behavior at intermediate temperatures (~80-50K), and a Fermi liquid state of screened local moments at low temperature (~10-5K).

∗Work supported in part by the Department of Energy Grant No. DE-SC0014506 (Widom)

Efficient implementation of ab initio dynamical mean-field theory for periodic systems

TIANYU ZHU (Presenter), ZHI-HAO CUI, GARNET CHAN, Division of Chemistry and Chemical Engineering, California Institute of Technology — We present an ab initio quantum chemical framework for dynamical mean-field theory (DMFT) in periodic systems. Our DMFT scheme employs ab initio Hamiltonians defined for impurities comprising the full unit cell or a supercell of atoms and for realistic quantum chemical basis sets. We avoid double counting errors by using Hartree-Fock as the low-level theory. Intrinsic and projected atomic orbitals (IAO+PAO) are chosen as the local embedding basis, facilitating numerical bath truncation. Using an efficient integral transformation and coupled-cluster Green's function (CCGF) impurity solvers, we are able to handle large embedded impurity problems with several hundred orbitals. We apply our ab initio DMFT approach to study a hexagonal boron nitride monolayer, crystalline silicon, and nickel oxide in the antiferromagnetic phase, with up to 104 and 78 impurity orbitals in spin-restricted and unrestricted cluster DMFT calculations and over 100 bath orbitals. We show that our scheme produces accurate spectral functions compared to both benchmark periodic coupled-cluster computations and experimental spectra.
9:12AM A43.00005: Efficient Hybridization Fitting for Dynamical Mean-Field Theory via Semi-Definite Relaxation* CARLOS MEJUTO ZAERA (Presenter), University of California, Berkeley, LEONARDO ZEPEDA-NÚÑEZ, Mathematics, University of Wisconsin-Madison, MICHAEL LINDSEY, Courant Institute of Mathematical Sciences, NORM TUBMAN, Quantum Artificial Intelligence Lab., NASA Ames Research Center, BIRGITTA K WHALEY, LIN LIN, University of California, Berkeley — Hamiltonian-based solvers for dynamical mean-field theory (DMFT) can compute spectral properties directly in the real axis and are applicable to impurity Hamiltonians presenting general interactions. This flexibility comes at the prize of having to truncate the formally infinite bath, transforming the DMFT self-consistent condition into a non-linear optimization problem. Fulfilling the self-consistency condition exactly with a finite bath is impossible. Furthermore, the large number of degrees of freedom in the optimization problem makes it likely to fall into local minima, which may result in the DMFT calculation converging to the wrong physical solution. As a consequence, the optimization step in Hamiltonian-based DMFT can become the most difficult part of the calculation. In this work¹, we propose a nested optimization procedure using semi-definite relaxation which addresses and improves many of the issues that plague the optimization step in Hamiltonian-based DMFT.

¹: arXiv:1907.07191

*Funded by DOE, Grant No. DE-AC02-05CH11231, AFOSR, Award Number FA9550-18-1-0095, NSF Graduate Research Fellowship Program, Grant DGE-1106400, and Obra Social “La Caixa”. Computational resources provided by XSEDE, which is supported by the NSF Grant No. OCI-1053575.

9:24AM A43.00006: Electronic Structure of Strongly Correlated f-electron System: DFT+DMFT Approach VIJAY SINGH (Presenter), Department of Physics, University of Illinois at Chicago Chicago, Illinois, 60607, USA, UTHPALA HERATH, Department of Physics, West Virginia University, Morgantown, WV 26506, USA, BENNY WAH, Department of Physics, University of Illinois at Chicago Chicago, Illinois, 60607, USA, ALDO H ROMERO, Department of Physics, West Virginia University, Morgantown, WV 26506, USA, HYOWON PARK, Department of Physics, University of Illinois at Chicago Chicago, Illinois, 60607, USA — Computational materials design of strongly correlated materials (SCM) has been challenging in modern condensed matter physics since it requires the development of more accurate methodologies beyond density functional theory (DFT). In the present talk, I will discuss our recent development of an efficient computational method so called DMFTwDFT to treat dynamical correlations in SCM accurately. I use dynamical mean-field theory (DMFT) in combination with DFT to compute the electronic structure of strongly correlated f-electron systems, specifically, rare-earth metals. The main point of the debate in f-electron system is related to the understanding of the role played by f electrons — they are localized or itinerant, or more exactly how many f electrons are localized or itinerant. For this reason, the theoretical and experimental investigations of the electronic structure of rare-earth metals have always occupied an important position in rare-earth research. Here, I use the DMFT+DFT method implemented using the maximally localized Wannier function as the local basis set and combining various DFT codes to study electronic properties of these materials. Our results will be also compared to other DMFT+DFT codes employing different local basis sets and DFT implementations.
**9:36AM A43.00007: Kondo route to quantum interference in prototypical single molecule transistors**

SUDESHNA SEN (Presenter), ANDREW MITCHELL, Univ Coll Dublin — Single molecule transistors offer a fascinatingly diverse range of physics due to their ultrasmall size, chemical complexity, and strong electronic interactions. They constitute a playground for exploring the fundamental physics of correlations on the nanoscale, and their signatures in transport. Understanding these systems is also an essential prerequisite for possible advanced technological applications utilizing their quantum characteristics. In this talk I examine prototypical molecular junctions π-conjugated hydrocarbon molecular junctions using a combination of perturbative scaling, numerical renormalization group, and machine learning methods [1] after reducing them to effective multi-orbital impurity systems. The interplay of Kondo effect and emergent many body quantum interference effects are explored in the context of quantum boosted functionalities.

Reference:

*We acknowledge funding from the Irish Research Council Laureate Awards 2017/2018 through grant IRCLA/2017/169.

**9:48AM A43.00008: Density Matrix Embedding Theory: From Lattice Models to Realistic Materials**

ZHI-HAO CUI (Presenter), TIANYU ZHU, GARNET CHAN, Caltech — In the past few years, density matrix embedding theory (DMET) [Phys. Rev. Lett. 109, 186404] has emerged as a successful wavefunction-based embedding scheme for both lattice models and molecules, but with few applications to ab initio periodic Hamiltonians. In this work, we will discuss a unified formalism for both lattice models and realistic solids. We will highlight some practical considerations in the simulation of realistic materials with DMET, including the choice of orbitals and mapping to a lattice, treatment of the virtual space and bath truncation, and the lattice-to-embedded integral transformation. We apply our DMET framework to both Hubbard-like lattice models and several realitic materials, e.g. hexagonal boron nitride monolayer, crystalline silicon, and nickel monoxide in the antiferromagnetic phase, using large embedded clusters with up to 300 embedding orbitals.

*This work is partially supported by US Department of Energy via award no. DE-SC19390. Additional support was provided by the Simons Foundation via an Investigatorship and through the Simons Collaboration on the Many-Electron Problem.
10:00AM A43.00009: Out of equilibrium thermometry with pump-probe x-ray photoemission spectroscopy  
OLEH MATVYEYEV (Presenter), Department of Physics, Georgetown University, ANDRIJ SHVAIKA, Department of Quantum Statistics, Institute for Condensed Matter Physics, JAMES FREERICKS, Department of Physics, Georgetown University — We calculate the spectral function of a deep core-level hole in a pump-probe x-ray photoemission spectroscopy experiment. Here, an intense light pulse pumps electrons to higher energies, and a second high-energy x-ray probe pulse is used to knock out an electron from a deep core-level. Electrons from the conduction band feel the effects of the core-hole potential and react by screening it. This creates particle-hole excitations within the conduction band until the core-hole has been filled. We examine the spinless Falicov-Kimball model, which possesses a metal-Mott-insulator transition, and has an exact solution within dynamical mean-field theory. In linear response, it is well known that the shape of the core-hole spectra depends strongly on temperature in the high-temperature regime. We employ this effect in nonequilibrium, and describe an ultrafast "thermometer," which can determine the energy content of the conduction electrons with a nondestructive in situ measurement on an ultrafast time scale.

10:12AM A43.00010: Electronic structure of bulk manganese oxide and nickel oxide from coupled cluster theory*  
YANG GAO (Presenter), Caltech, QIMING SUN, Tencent America LLC, JASON YU, UC Irvine, MARIO MOTTA, IBM Almaden Research Center, JAMES MCCLAIN, ALEC F WHITE, AUSTIN MINNICH, GARNET CHAN, Caltech — We describe the ground- and excited-state electronic structure of bulk MnO and NiO using coupled cluster theory with single and double excitations (CCSD). Starting from a Hartree-Fock reference, we find fundamental gaps of 3.46 eV and 4.83 eV for MnO and NiO respectively for the 16 unit supercell, slightly overestimated compared to experiment, although finite-size scaling suggests that the gap is more severely overestimated in the thermodynamic limit. From the character of the correlated electronic bands we find both MnO and NiO to lie in the intermediate Mott/charge-transfer insulator regime, although NiO appears as a charge transfer insulator when only the fundamental gap is considered. While the lowest quasiparticle excitations are of metal 3d and O 2p character in most of the Brillouin zone, near the Γ point, the lowest conduction band quasiparticles are of s character. Our study supports the potential of coupled cluster theory to provide high level many-body insights into correlated solids.

*G. K. C. acknowledges support from de-sc0018140. Partial support for Y. G. was from de-sc0019330. A. F. White was supported by MURI FA9550-18-1-0095. J.M.Y. acknowledges support from NSF Grant DGE-1745301. Y. G. and A. J. M. acknowledge the support of ONR under Grant No. N00014-18-1-2101.
10:24AM A43.00011: The electronic structure of \( n \)-doped ABO\(_3\) perovskite metals from quantum Monte Carlo.*  

MICHAEL BENNETT (Presenter), GUOXIANG HU, PANCHAPAKESAN GANESH, JARON KROGEL, Oak Ridge National Laboratory — Some perovskites (PVs) are known to undergo metal-to-insulator transitions (MITs) when \( n \)-doped. In particular, the PV ferromagnet strontium cobaltite (SrCoO\(_3\)), undergoes an MIT when a critical level of ordered oxygen vacancies are present in the system. Concomitant topotactic and magnetic transitions can also occur, e.g., the oxygen-deficient SrCoO\(_{2.5}\) phase is an anti-ferromagnet with a brownmillerite crystal structure. The cause of this nonintuitive MIT in these oxygen-deficient systems is not well understood. Density functional theory (DFT) calculations suggest that charge disproportionation is often associated with the transition, but these systems have strong correlations that are beyond DFT. Furthermore, counting formal oxidation states in the oxygen-rich systems hints at the presence of ligand holes which would conceivably lead to passivation after \( n \)-doping. Here, we hypothesize that these systems are indeed self-hole doped and use diffusion Monte Carlo methods that include electron correlations exactly to gain clarity on the electronic/magnetic/structural transitions.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, as part of the Computational Materials Sciences Program.

10:36AM A43.00012: ThetaPhi - a new program for calculation of Bardeen-Cooper-Schrieffer and Magnetic Superstructure Electronic States  

EVGENY PLEKHANOV (Presenter), Physics, Kings College London, ANDREI TCHOUGREEFF, A.N. Frumkin Institute of Physical Chemistry and Electrochemistry of RAS, Moscow, Russia — We propose the Theta-Phi package [1] which addresses two of the most important extensions of the essentially single-particle mean-field paradigm of the computational solid state physics: the admission of the Bardeen-Cooper-Schrieffer electronic ground state and allowance of the magnetically ordered states with an arbitrary superstructure (pitch) wave vector. Both features are implemented in the context of multi-band systems which paves the way to an interplay with the solid state quantum physics packages eventually providing access to the first-principles estimates of the relevant matrix elements of the model Hamiltonians derived from the standard DFT calculations. Several examples showing the workability of the proposed code are given.

We present a numerically exact Inchworm Monte Carlo method for equilibrium multi-orbital quantum impurity problems with general interactions and hybridizations. We show that the method, originally developed to overcome the dynamical sign problem in certain real-time propagation problems, can also overcome the sign problem as a function of temperature for equilibrium quantum impurity models. This is shown in several cases where the current method of choice, the continuous-time hybridization expansion, fails due to the sign problem. Our method therefore enables simulations of impurity problems as they appear in embedding theories without further approximations, such as the truncation of the hybridization or interaction structure or a discretization of the impurity bath with a set of discrete energy levels, and eliminates a crucial bottleneck in the simulation of ab initio embedding problems.

G.C. acknowledges support by the Israel Science Foundation (Grant No. 1604/16). E.E. and G.C. acknowledge support by the PAZY foundation (Grant No. 308/19), and E.G. was supported by DOE ER 46932. Computational support was provided by the NegevHPC project. International exchange and collaboration was supported by Grant No. 2016087 from the United States-Israel Binational Science Foundation (BSF).
8:00AM A44.00001: Exploiting Orbital Locality in Real Space to Enable Large-Scale Condensed-Phase Ab Initio Molecular Dynamics with Hybrid Density Functional Theory
[Invited] ROBERT DISTASIO (Presenter), Cornell University — By including a fraction of exact exchange (EXX), hybrid functionals reduce the self-interaction error in semi-local density functional theory (DFT), and thereby furnish a more accurate and reliable description of the underlying electronic structure in systems throughout chemistry, physics, and materials science. However, the high computational cost associated with hybrid DFT has limited its applicability when treating large-scale condensed-phase systems. To overcome this limitation, we have devised a linear-scaling yet formally exact approach that utilizes a local representation of the occupied orbitals to exploit the sparsity in the real-space evaluation of the quantum mechanical exchange interaction in finite-gap systems. Here, we present a detailed description of the theoretical and algorithmic advances required to perform ab initio molecular dynamics (AIMD) simulations of large-scale condensed-phase systems with hybrid DFT. We focus our theoretical discussion on integrating this approach into the framework of Car-Parrinello AIMD, and provide a comprehensive description of our algorithm, which is implemented in the open-source Quantum ESPRESSO program and employs a hybrid MPI/OpenMP parallelization scheme to efficiently utilize the high-performance computing (HPC) resources available on supercomputer architectures. This is followed by a critical assessment of the accuracy and parallel performance (e.g., strong and weak scaling) of this approach when performing AIMD simulations of liquid water in the canonical (NVT) and isobaric-isothermal (NpT) ensembles. With access to HPC resources, we demonstrate that our algorithm enables hybrid DFT based AIMD simulations of condensed-phase systems containing ~1000 atoms with a wall-time cost that is comparable to semi-local DFT. In doing so, this work takes us one step closer to routinely performing AIMD simulations of large-scale condensed-phase systems for sufficiently long timescales at the hybrid DFT level of theory.

8:36AM A44.00002: Improving the Scalability of Condensed-Phase Hybrid Density Functional Theory: Computation, Communication, and Load Balancing
HSIN-YU KO (Presenter), JUNTEENG JIA, Cornell University, MARCOS ANDRADE, Princeton University, ZACHARY SPARROW, ROBERT DISTASIO, Cornell University — Ab initio molecular dynamics (AIMD) simulations at the hybrid density functional theory (DFT) level provide a semi-quantitative description of complex condensed-phase systems such as molecular liquids and crystals. For finite-gap systems, we have developed a linear-scaling and formally exact algorithm for computing the exact exchange interaction in real space based on a localized representation of the occupied orbitals (e.g., maximally localized Wannier functions). Although a massively parallel implementation of this algorithm in Quantum ESPRESSO already enables hybrid DFT based AIMD simulations of condensed-phase systems containing 500-1000 atoms, we have identified three nearly equal contributions to the walltime cost of this approach: computation events, communication overhead, and processor idling due to workload imbalance. In this work, we present a three-pronged strategy that we have employed to attack these contributions and reduce the overall walltime cost by approximately an order of magnitude.

*DOE EFRC (Grant No. DE-SC0019445)
8:48AM A44.00003: SPARC-X: Real-space Density Functional Theory for large length and time scales*  PHANISH SURYANARAYANA (Presenter), Georgia Inst of Tech — In this talk, previous and current efforts of the speaker to develop efficient real-space formulations and massively parallel implementations for Density Functional Theory (DFT) will be discussed. These include (i) SPARC: A general purpose framework for performing large-scale electronic structure calculations based on DFT; (ii) Cyclic DFT: A framework for studying systems possessing cyclic symmetry, with application to the bending deformations in nanostructures; (iii) Helical DFT: A framework for studying systems possessing helical symmetry, with application to the torsional deformations in nanostructures; and (iv) SQDFT: A linear-scaling framework for studying materials under extreme conditions. Overall, the speaker will discuss how the above developments enable electronic structure simulations at large length and time scales.

*NSF, DOE, and LLNL

9:00AM A44.00004: A Scalable Eigensolver for Real-space Pseudopotential Density Functional Theory: A Polynomial-filtered Spectrum Slicing Method*  KAI-HSIN LIOU (Presenter), University of Texas at Austin, CHAO YANG, Lawrence Berkeley National Laboratory, JAMES CHELIKOWSKY, University of Texas at Austin — First-principles electronic structure calculations are a popular avenue for understanding and predicting properties of materials. However, solving the electronic structures of the materials of interest, such as complex biomolecules, nanostructures, and interfacial systems can require descriptions of systems with many atoms, e.g., systems with over 10,000 atoms. Systems of this size pose a challenge to current electronic structure computation software. We will present recent work using a spectrum-slicing algorithm, which is implemented in a real-space pseudopotential density functional theory code, PARSEC. The spectrum slicing method builds an additional layer of parallelization on top of the Chebyshev-filtered subspace iteration. Our approach provides more flexibility to fully utilize the computing power of modern distributed parallel computers. We will demonstrate the scalability of the algorithm and discuss outstanding challenges.

*Work at Texas is supported by a subaward from the Center for Computational Study of Excited-State Phenomena in Energy Materials at LBNL, which is funded by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231, as part of the Computational Materials Sciences Program.
9:12AM A44.00005: Treecode-Accelerated Green's Iteration for Kohn-Sham DFT* NATHAN VAUGHN (Presenter), ROBERT KRASNY, VIKRAM GAVINI, Univ of Michigan - Ann Arbor — We present a real-space method for Kohn-Sham Density Functional Theory based on an integral equation formulation of the Kohn-Sham equations, called Treecode-Accelerated Green's Iteration (TAGI). In this approach, the eigenvalue problem for the Kohn-Sham differential operator is converted to a fixed point problem for an integral operator by convolution with a Green's function, then the fixed points are computed using Green's iteration. Essential to this method is the accurate and efficient evaluation of the convolution integrals arising in the iteration. TAGI achieves accuracy and efficiency through the use of adaptive mesh refinement to represent the fields, singularity subtraction schemes to reduce the quadrature error due to the singular Green's functions, and a GPU-accelerated treecode to reduce the computational complexity of the convolution integrals. We have performed all-electron calculations on non-periodic systems and demonstrated systematic convergence to chemical accuracy with respect to tightly converged reference values.

*This work was supported by National Science Foundation grant DMS-1819094, and the Mcubed program and Michigan Institute for Computational Discovery and Engineering (MICDE) at the University of Michigan.

9:24AM A44.00006: Accelerating real-space methods by discontinuous projection* JOHN PASK (Presenter), Lawrence Livermore Natl Lab, QIMEN XU, PHANISH SURYANARAYANA, Georgia Institute of Technology — By virtue of multiple advances in the past two decades, real-space electronic structure methods have surpassed planewave methods in large-scale calculations of isolated and extended systems alike. Combining advances in both finite-difference and finite-element methods over the decades, we discuss a new approach to accelerate real-space methods further still, while retaining the simplicity, systematic convergence, and parallelizability inherent in the methodology. The key idea is to compress the large, sparse real-space Hamiltonian by projection in a strictly local, systematically improvable, discontinuous basis spanning the occupied subspace. We show how this basis can be constructed and employed to reduce the dimension of the real-space Hamiltonian by up to three orders of magnitude. Molecular dynamics step times of a few minutes for systems containing thousands of atoms demonstrate the scalability of the methodology in a discontinuous Galerkin formulation [1]. Results for 1D, 2D, and 3D systems demonstrate the additional advantages afforded by the new projection formulation [2].


*This work was performed, in part, under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.
A Space-filling Curve Based Grid Partition to Accelerate Real-space Pseudopotential Density Functional Theory Calculations

ARIEL BILLER (Presenter), Weizmann Institute of Science, KAI-HSIN LIOU, University of Texas at Austin, DEENA ROLLER, LEEOR KRONIK, Weizmann Institute of Science, JAMES CHELIKOWSKY, University of Texas at Austin — Density functional theory (DFT) has become a popular tool to verify, explain, and predict experimental discoveries in materials. In conjunction with pseudopotentials, we can now achieve simulations of systems with tens of thousands of atoms as “routine work.” Real-space DFT has advantages when simulating confined or semi-periodic systems, such as defects, charged systems, and interfaces. Within a finite-difference method, the Hamiltonian matrix is often large and sparse, and requires an efficient implementation of matrix-vector multiplication. We will show through space-filling curves that we can construct a real-space grid whose grid points have excellent locality. Consequently, the communication between compute nodes is reduced. We will also demonstrate that this space-filling curve based grid partition improves the scalability of the matrix-vector multiplications, which is beneficial to polynomial filtering based eigensolvers.

Work at Texas is supported by a subaward from the Center for Computational Study of Excited-State Phenomena in Energy Materials at LBNL, which is funded by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231, as part of the Computational Materials Sciences Program.

Reduce Noise in Stochastic Density Functional Theory

MING CHEN (Presenter), Department of Chemistry, University of California, Berkeley, DANIEL NEUHAUSER, Department of Chemistry and Biochemistry, University of California, Los Angeles, ROI BAER, Institute of Chemistry, The Hebrew University of Jerusalem, ERAN RABANI, Department of Chemistry, University of California, Berkeley — Large scale density functional theory (DFT) calculations are necessary for understanding the physics of complex materials. Steep numerical scaling of conventional DFT methods prohibits the routine application to large systems containing tens of thousands of electrons. An alternative to conventional DFT is based on representing the density and density matrix using stochastic sampling of the occupied subspace, allowing for linear or even sub-linear scaling DFT method at the cost of introducing a well-controlled statistical error. It becomes an important task to develop approaches that reduce the stochastic noise in order to improve accuracy and reliability of stochastic DFT. Two different noise reduction techniques have been introduced in stochastic DFT. One is based on decomposing the system into overlapped fragments and the other approach divides the occupied subspace into subspaces according to energy windows. Both noise reduction techniques can significantly reduce the noise level in electronic structures, which leads to orders of magnitude reduction in computational costs. This talk will provide a look into both methods including analysis of noise reduction, scaling, and performance. Illustrations will be given for semiconductor materials with nearly 16,000 electrons.
10:00AM A44.00009: A general approach towards continuous translational symmetry in finite difference real-space calculations  TIAN QIU (Presenter), University of Pennsylvania, LEO OR KRONIK, Weizmann Institute of Science, ANDREW MARSHALL RAPPE, University of Pennsylvania — We have developed a new scheme to install pseudopotentials on a finite real-space grid that significantly reduces unphysical fluctuations of quantities for fractional grid-point shifts in real space. Instead of interpolating the potential on the grid, this scheme chooses a reference position and use a translation method to represent positions of atoms in real space. This translation is exact for integer grid-point shifts and is designed to minimize the "egg box" effect for fractional grid-point shifts. It provides nonlocal but banded representations for local potentials and is compatible with nonlocal pseudopotential operators. As a demonstration, this scheme is tested in one dimension for three types of potentials: a local ionic potential, a local ionic potential plus a nonlocal operator, and a local ionic potential plus the Hartree and exchange-correlation potential. Fluctuations of examined quantities are reduced by four orders, four orders, and three orders, respectively. This scheme does not require the manipulation of grids and can be easily extended to the three-dimensional case.

10:12AM A44.00010: Discrete discontinuous basis projection (DDBP) method for large-scale electronic structure calculations.  QIMEN XU (Presenter), PHANISH SURYANARAYANA, Georgia Inst of Tech — The large number of grid points per atom required for accurate real-space Kohn-Sham Density Functional Theory (DFT) calculations restricts their efficiency. In this work, we present an approach to accelerate such calculations several fold, without loss of accuracy, by systematically reducing the cost of the key computational step: the determination of the Kohn-Sham orbitals spanning the occupied subspace. This is achieved by systematically reducing the dimension of the discrete eigenproblem that must be solved, through projection into a highly efficient discrete discontinuous basis. In calculations of quasi-1D, quasi-2D, and bulk metallic systems, we find that accurate energies and forces are obtained with 8–25 basis functions per atom, reducing the dimension of full-matrix eigenproblems by 1-3 orders of magnitude.
Fast all-electron density functional theory calculations in solids using orthogonalized enriched finite elements*  
NELSON DAVID RUFUS (Presenter), BIKASH KANUNGO, VIKRAM GAVINI, Univ of Michigan - Ann Arbor — We present a computationally efficient approach to perform real-space all-electron Kohn-Sham DFT calculations for bulk solids using an enriched finite element (FE) basis, wherein the classical FE basis are augmented with atom-centered numerical basis functions constructed from atomic solutions to the Kohn-Sham problem. We term these atom-centered numerical basis functions as enrichment functions. Notably, to improve the conditioning we orthogonalize the enrichment function with respect to the classical FE basis, without compromising on the locality of the resultant basis. In addition to improved conditioning, this orthogonalization procedure also renders the overlap matrix block-diagonal, greatly simplifying its inversion. Subsequently, we use a Chebyshev polynomial based acceleration technique to efficiently compute the occupied eigenspace in each self-consistent iteration. We demonstrate the accuracy and efficiency for periodic unit-cells and supercells, ranging up to 5000 electrons (containing as many as 500 atoms). We observe a staggering 50-100x speedup over the classical FE basis. We also benchmark with (L)APW(\(+lo\)) basis for accuracy and performance. Finally, we demonstrate parallel scalability for a system with ~216 Si and C atoms.

*DoE BES, Award Number DE-SC0017380
Under applied shear, amorphous solids flow via a succession of plastic rearrangements of localized particles. Numerous numerical and experimental studies have shown that plastic instabilities in glasses are triggered by spatially localized soft spots in direct analogy with dislocations present in crystalline solids, although the population and microscopic structure of the former are significantly different from the latter. In addition, many research groups have developed methods for identifying such defects, although these methods have not been systematically compared. Here we use a swap Monte Carlo algorithm to prepare equilibrium amorphous configurations with very different stabilities that exhibit a range of behaviors under shear, from ductile flow to brittle failure. We compute various structural indicators ranging from purely structural to highly non-linear metrics that require the knowledge of the interactions between constituents. We compare these metrics on the same data sets, quantifying how well these metrics perform in predicting plastic deformation across this range of glass stabilities. Moreover, we use these structural metrics to quantify the spatial distribution of plastic defects for different preparation protocols, as well as the evolution of these defects across the yielding transition, allowing us to precisely characterize how the microscopic structure encodes the differences between ductile and brittle materials.

*This work was supported by the Simons Foundation Grant No. 454947.
8:36AM A45.00002: Yielding of Ultrastable Computer Glasses  MISAKI OZAWA (Presenter), Ecole Normale Superieure, LUDOVIC BERTHIER, Universite Montpellier, GIULIO BIROLI, Ecole Normale Superieure, ALBERTO ROSSO, Universite Paris-Sud, GILLES TARJUS, Sorbonne Universite, MURARI SINGH, Universite Montpellier, WEI-TING YEH, KUNIMASA MIYAZAKI, TAKESHI KAWASAKI, Nagoya University —

We study mechanical yielding of ultrastable computer glasses generated by optimized swap Monte-Carlo simulations for polydisperse particles [1,2] as well as more realistic multi-component metallic glass models [3]. We observe brittle yielding associated with a sharp system-spanning shearband in various rheological settings, such as uniform shear and oscillatory deformation in two and three dimensions [4,5,6]. The observed behaviors are qualitatively different from the standard computer glasses that have been studied previously. Thus, our computational scheme opens up new opportunities to investigate the mechanical behaviors of metallic glasses in experimentally relevant conditions. As an application, we numerically test the scenario of shearband nucleation by artificially inserting a soft spot into a stable glass sample. We argue that brittle yielding in macroscopic samples is triggered by rare droplets of the soft spot [4].

[3] Parmar, Ozawa, and Berthier
[4] Ozawa, Berthier, Biroli, and Tarjus
[5] Singh, Ozawa, and Berthier
[6] Yeh, Ozawa, Miyazaki, Kawasaki, and Berthier

8:48AM A45.00003: When does local structure play a role in sheared jammed packings?*
SEAN RIDOUT (Presenter), University of Pennsylvania, JASON ROCKS, Boston University, ANDREA JO-WEI LIU, University of Pennsylvania — In jammed packings, it is usually assumed that local structure only plays a significant role in specific regimes. For instance, it is known that in jammed packings the variance of the relative excess coordination, $\delta Z/Z_c$, decays like $1/d$, so that local structure should play no role at high spatial dimensions. Furthermore, in any fixed dimension $d \geq 2$, lowering the pressure results in a diverging length scale, again suggesting that local structure should not be sufficient to describe response. Here we address the validity of the assumption that local structure does not matter in these cases. Focusing on jammed packings under athermal, quasistatic shear, we utilize machine learning to identify a local structural variable, softness, that has been shown to be strongly predictive of rearrangements in many disordered systems. We apply the softness analysis to plastic events in jammed packings across many dimensions and pressures, and find that local structure is perhaps more predictive than one might have guessed.

*This work was funded by the Simons Foundation through the collaboration “Cracking the glass problem” (454945) (for AJL and SAR), by the US Department of Energy under award DE-FG02-05ER46199 (JWR). the an NSERC PGS-D fellowship to SAR, and an NSF graduate fellowship to JWR.
Connecting thermal relaxation to local yield stress in glassy systems
MATTHIAS LERBINGER (Presenter), ARMAND BARBOT, SYLVAIN PATINET, DAMIEN VANDEMBROUCQ, PMMH, ESPCI Paris — We study a binary Lennard-Jones mixture in the supercooled regime using molecular dynamic simulations. At low temperatures, thermal relaxation proceeds in a series of activated jumps between inherent structures, i.e. local minima of the potential energy landscape. From these inherent dynamics we recover information about the location of thermally activated rearrangements. We observe a strong connection between the thermal relaxation and areas where the structure has been previously identified as being soft using a local, direct probing of shear stress thresholds. Using the probability distribution of local shear stresses we are able to capture features of the system’s dynamical relaxation processes. We thus can establish a link between structural and dynamical properties of the supercooled liquid. Furthermore, we extend our analysis to out of equilibrium dynamics by studying the effects of rejuvenation and aging on the local yield stress distribution in both glasses and liquids at different temperatures.

Correlation between local structural order and ductility of glasses
AYA NAWANO (Presenter), Department of Mechanical Engineering and Materials Science, Yale University, YUAN-CHAO HU, Institute of Industrial Science, University of Tokyo, JAN SCHROERS, Department of Mechanical Engineering and Materials Science, Yale University, MARK SHATTUCK, Department of Physics and Benjamin Levich Institute, City College of New York, COREY SHANE O’HERN, Department of Mechanical Engineering and Materials Science, Yale University — Bulk metallic glasses (BMGs) are amorphous metallic alloys with desirable material properties such as high yield strength and superior corrosion resistance compared to conventional crystalline alloys. However, their use as structural materials has been limited because of their brittle behavior, especially in tension. In this work, we identify atomic-scale structural signatures in undeformed metallic glasses that are able to predict their mechanical response to tension or pure shear tests. In particular, we employ molecular dynamics simulations to prepare different types of glasses using a range of cooling rates and interaction potentials, including highly polydisperse soft-repulsive spheres, binary Lennard-Jones spheres, atomic systems that interact via the Stillinger-Weber potential, and binary and ternary alloys described by the embedded atom method. We then perform quasi-static tension or pure shear tests on the glassy samples, and measure the shear stress and local structural order as a function of strain. For each model system, we find a strong correlation between the measure of local structural order in the undeformed sample and the mechanical response at finite strain.

*A. N. and C.S.O acknowledge support from NSF Grant No. CMMI-1901959.
9:24AM A45.00006: Understanding shear bands characteristics and formation in model glasses through the measure of the local yield stress. ARMAND BARBOT (Presenter), MATTHIAS LERBINGER, PMMH, CNRS UMR 7636, ESPCI Paris, PSL University, Sorbonne Université, Université de Paris, F-75005 Paris, France, ANAËL LEMAÎTRE, Université Paris-Est, Laboratoire Navier (UMR 8205), CNRS, ENPC, IFSTTAR, 2 allée Képler, F-77420 Marne-la-Vallée, France, DAMIEN VANDEMBROUCQ, SYLVAIN PATINET, PMMH, CNRS UMR 7636, ESPCI Paris, PSL University, Sorbonne Université, Université de Paris, F-75005 Paris, France — Many phenomena remain poorly understood in amorphous materials such as plasticity and shear banding, their brittleness and disordered structure making it difficult to study them experimentally. As a consequence, we employ a two-dimensional Lennard-Jones numerical model of glasses and measure their local yield stress, a measure of the local softness presented in [1]. This method is nonperturbative and gives access to a quantitative property on a well-controlled length scale. Applying it on deeply quench glasses under simple shear loading, we show that the plastic events create a local yield stress [2] decrease in the material which cause the emergence of a shear band [3]. We finally focus on the shear bands formation by looking for a relevant localization criterion to understand the influence of the system size and quench protocol.


9:36AM A45.00007: Atomic nonaffinity as structural indicator of protocol-dependent plasticity in amorphous solids* BIN XU (Presenter), Beijing Computational Science Research Center, MICHAEL FALK, Johns hopkins university, SYLVAIN PATINET, Physique de Mécanique des Milieux Hétérogènes laboratory, PENGFEI GUAN, Beijing Computational Science Research Center — Structural heterogeneity of amorphous solids challenges the prediction of plastic events which is intimately connected to their mechanical behaviors. Here we report the atomic nonaffinity, as a structural indicator with intrinsic orientation, which is derived from the total nonaffine modulus based on a perturbation analysis of the potential energy landscape. We find that the atomic nonaffinity can efficiently characterize the locations of plastic events, which is comparable to other indicators. More importantly, it can accurately predict the protocol-dependent response of plastic events by quantitatively analyzing the relation between its softest direction and shear loading direction. These results shed light on the characterization and prediction of the mechanical response of amorphous solids.

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**9:48AM A45.00008: Unveiling the predictive power of static structure in glassy systems**

VICTOR BAPST (Presenter), THOMAS KECK, AGNIESZKA GRABSKA-BARWINSKA, CRAIG DONNER, DeepMind, EKIN DOGUS CUBUK, SAM SCHOENHOLZ, Google Brain, ANNETTE OBIKA, ALEXANDER NELSON, TREVOR BACK, DEMIS HASSABIS, PUSHMEET KOHLI, DeepMind — Despite decades of theoretical studies, the nature of the glass transition remains elusive and debated, while the existence of structural predictors of the dynamics is a major open question. Recent approaches propose inferring predictors from a variety of human-defined features using machine learning. We learn the long time evolution of a glassy system solely from the initial particle positions and without any hand-crafted features, using a powerful model: graph neural networks. We show that this method strongly outperforms state-of-the-art methods, generalizing over a wide range of temperatures, pressures, and densities. In shear experiments, it predicts the location of rearranging particles. The structural predictors learned by our network exhibit a correlation length which increases with larger timescales to reach the size of our system. Beyond glasses, our method could apply to many other physical systems that map to a graph of local interactions.

**10:00AM A45.00009: Identifying flow units by machine learning in a model metallic glass**

YICHENG WU (Presenter), Beijing Computational Science Research Center, HAIYANG BAI, Institutes of Physics, Chinese Academy of Sciences, PENGFEI GUAN, Beijing Computational Science Research Center — Characterizing and predicting the flow units directly from the atomic structure are longstanding challenges in metallic glasses. We report the successful identification of flow units in the model Zr<sub>50</sub>Cu<sub>50</sub> metallic glass above and below its glass transition temperature by machine learning methods. We find that the differences of the structural characteristics between flow units and the rest of the system are beyond short-range order, and further confirmed by the local structural entropy. Our study demonstrates that machine learning provides an unconventional tool to understand the intrinsic heterogeneities in metallic glasses, and sheds light on the structural indicator of heterogeneous dynamic behaviors in amorphous solids.

**10:12AM A45.00010: Residual stress distributions and mechanical noise in athermally deformed amorphous solids from atomistic simulations**

*CÉLINE RUSCHER, Quantum Matter Institute, University of British Columbia, JOERG ROTTLER (Presenter), Dept. of Physics and Astronomy and Quantum Matter Institute, University of British Columbia — The distribution P(x) of local residual stresses in amorphous packings governs the statistical properties of global collective failure events at the yielding transition. We reveal the evolution of P(x) upon deformation by combining atomistic simulations with the frozen matrix approach. A pseudogap form P(x) ~ x<sup>Θ</sup> is observed in the freshly quenched state and in the early stages of deformation. After a few percent strain, however, P(x) starts to develop a plateau p<sub>0</sub> in the small x-limit, where p<sub>0</sub> ~ L<sup>-p</sup> with L the system size. A direct comparison with the system size scaling of the stress drops shows that the distribution of avalanche sizes are controlled by Θ in the transient regime and the plateau exponent p in the steady state flow. The broad distribution of mechanical noise P(|Δx|) ~ |Δx|<sup>-1-µ</sup> is characterized by a Levy-exponent µ and can be related to the behavior of P(x) via a mean-field description.

*JR thanks the Alexander von Humboldt foundation for financial support. Computing resources were provided by Compute Canada.
10:24AM A45.00011: Interplay between rearrangements, strain, and softness and during avalanche propagation*  
GE ZHANG (Presenter), SEAN RIDOUT, ANDREA JO-WEI LIU, University of Pennsylvania — Disordered solids yield at a common shear strain of about 3%, but the behavior beyond yield is different for different systems and for systems with different histories. Foams can deform indefinitely without fracturing, many systems exhibit crackling noise or avalanche behavior, and still others exhibit shear banding and brittle fracture. Here we study an athermal, jammed packing of Hertzian particles that is sheared quasistatically. We identify the stress drops associated with rearrangements and then use steepest descent dynamics to study the evolution of the avalanches. We find that the avalanches consist of localized events that appear sequentially in well-separated locations of the sample. To understand this behavior, we study the interplay between rearrangements, strain, and softness, a machine-learned structural descriptor that predicts the propensity of a particle to rearrange. We find that each rearrangement gives rise to a shear strain field that can immediately trigger other rearrangements, while also causing an isotropic strain field that changes the softness of other particles; this may affect subsequent rearrangements over a much longer time scale. We compare our results to elasto-plastic and mean-field models of avalanches.

*We thank U.S. DOE award DE-FG02-05ER46199.

10:36AM A45.00012: Structural evolution of amorphous systems during avalanches*  
ETHAN STANIFER (Presenter), M. LISA MANNING, Syracuse University — Under applied shear strain, granular and amorphous materials deform. At zero temperature, the deformation can be separated into elastic branches where the particles do not change neighbors and rearrangements where they do. Some rearrangement events are small and localized, while others involve large or system-spanning avalanches. Using numerical simulations of soft spheres, we find that avalanches can be decomposed into a series of localized excitations, and we develop an extension of persistent homology to isolate these excitations. Next, we develop a method to study the linear response of unstable systems during an avalanche, by extending existing tools for identifying structural defects using the Hessian and study how the population of structural defects evolves during an avalanche. We find that localized excitations in the avalanche correlate strongly with localized excitations in the linear spectrum, and investigate how these excitations are created and coupled during the avalanche. These data should help to constrain elastoplastic models for glasses and granular matter.

*Simons Foundation MMLS grant #446222
10:48AM A45.00013: The behavior of jammed packings under correlated random forces*
SUDESHNA ROY (Presenter), ETHAN STANIFER, M. LISA MANNING, Syracuse University — Mean-field calculations suggest that the response of a system to global shear and random forces are essentially equivalent in infinite dimensions. However, it remains an open question whether this is true for systems in lower dimensions. To address this, Morse and collaborators have recently developed a method for driving 2D jammed packings of disks quasi-statically, with random, infinitely-persistent, active forces, and found striking similarities and differences between sheared and actively forced systems. Here, we extend that previous work by studying how changing correlation length of the random forcing affects the mechanical response. We find that both the effective modulus with respect to the random forcing direction, as well as the average effective strain between rearrangements or saddle points, does change systematically with correlation length. This paves the way for a deeper understanding of the connection between shear and active driving in lower dimensions.

*This work was supported by a grant from the Simons Foundation (#454947, Lisa Manning).”

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A46 GMAG DMP: Magnon and Spin Dynamics 708 - Eric Montoya, University of California, Irvine

8:00AM A46.00001: Theoretical model for direct evidence of spatial stability of Bose-Einstein condensate of magnons*  
IGOR BORISENKO, BORIS DIVINSKIY, VLADISLAV DEMIDOV, Institute for Applied Physics and Center for Nanotechnology, University of Muenster, GANG LI (Presenter), Texas A&M Univ, THOMAS NATTERMANN, Institute of Theoretical Physics, University of Cologne, VALERY L POKROVSKY, Texas A&M Univ, SERGEJ DEMOKRITOV, Institute of Applied Physics and Center for Nanotechnology, University of Muenster — Bose-Einstein condensation of quasi-equilibrium magnons is one of few macroscopic quantum phenomena observed at room temperature. However, for a long time it remained unclear, what physical mechanisms can be responsible for the spatial stability of the magnon condensate. Indeed, since magnons are believed to exhibit attractive interaction, it is generally expected that the magnon condensate should be unstable with respect to the real-space collapse, which contradicts all the experimental findings. Here, we provide direct experimental evidence that magnons in a condensate exhibit repulsive interaction resulting in the condensate stabilization and propose a mechanism, which is responsible for the interaction inversion. Our experimental conclusions are additionally supported by the theoretical model based on the Gross-Pitaevskii equation. Our findings solve a long-standing problem and provide a new insight into the physics of magnon Bose-Einstein condensates.

*This work was supported in part by the Deutsche Forschungsgemeinschaft (Project No. 416727653). The theoretical work was supported by the University of Cologne Center of Excellence QM2 and by William R. Thurman’58 Chair in Physics, Texas A&M University.
8:12AM A46.00002: Thermal Hall Effect in Collinear Antiferromagnets on a Square Lattice*
NISHCHAY SURI (Presenter), YINHAN ZHANG, Carnegie Mellon Univ, SATOSHI OKAMOTO, Oak Ridge National Laboratory, DI XIAO, Carnegie Mellon Univ — We show that the thermal Hall effect is possible in collinear antiferromagnets on a square lattice once the magnon-phonon interaction due to the Dzyaloshinskii-Moriya interaction (DMI) is taken into account. We discuss the field- and DMI-dependence of the thermal Hall coefficient. We show that the thermal Hall conductivity is controlled by the resonant contribution from the anticrossing points between the magnon and phonon branches, and estimate its size in real materials.

*Work at CMU is supported by DE-SC0019443 and DE-SC0012509.
The research by S.O. is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

8:24AM A46.00003: Magnon contributions to dielectric constant in spiral magnets
FRANCESCO FOGGETTI (Presenter), Quantum Materials Theory, Italian Institute of Technology; University of Genova, SERGEY ARTYUKHIN, Quantum Materials Theory, Italian Institute of Technology — Magnetic frustration often results in interesting magnetic and dielectric properties. Spiral spin structures are common in magnetic perovskites due to competing exchange interactions and may give rise to ferroelectric polarization via inverse Dzyaloshinskii-Moriya mechanism. Here we model chiral domain walls in the spiral magnetic order and characterize the excitation spectrum using a model Hamiltonian describing spins interacting with polar ionic displacements. We explore the contributions of domain wall localized excitations to the low-frequency dielectric constant in spiral multiferroics (i.e. TbMnO$_3$, MnWO$_4$).

8:36AM A46.00004: Goos-Hänchen effect of spin waves at heterochiral interfaces
ZHENYU WANG (Presenter), YUNSHAN CAO, PENG YAN, University of Electronic Science and Technology of China — One of the most robust methods for measuring the Dzyaloshinskii-Moriya interaction (DMI) is the Brillouin light scattering spectroscopy (BLS) at present. But measuring the DMI parameter in a narrow magnetic strip is always a difficult problem because of the big laser spot size subjected to the diffraction limit of lights. In previous work, we proposed a nonlocal scheme to measure the DMI in a narrow magnetic strip by three-magnon processes, but it is only feasible for the magnetic strip with the width in the range of 50–100 nm. In this work, we observe a Goos-Hänchen shift of spin waves at the heterochiral interface when the spin-wave beam is totally reflected. We further explore the GH shift of spin waves by narrow DMI strips of different widths. It is found that the induced shift is independent of the strip width down to 10 nm, offering an approach to measure the DMI strength of ultranarrow magnetic strips of sub-50-nm scales. Our findings are helpful to understand the GH effect in chiral magnets and enable us to measure the DMI for ultranarrow magnetic strips via the magnonic GH shift, which fills in the gap of current technology.
8:48AM A46.00005: Magnon spectrum in Ferromagnet-Superconductor heterostructure
BISHAL PARAJULI (Presenter), University of California, Merced, SHIZENG LIN, Los Alamos National Lab, CHIH-CHUN CHIEN, University of California, Merced — Research on ferromagnet-superconductor heterostructures gives rise to novel quantum phases and excitations. Spin-waves (Magnons) can propagate in a ferromagnetic thin film while magnetic fields penetrate through a type-II superconducting thin film forming a vortex lattice. Here, we study the magnon spectrum in ferromagnetic thin films in the presence of a vortex lattice in a superconducting thin film separated by an insulating film. It was revealed that the spin-waves interact with the vortex lattice and the magnon spectrum is modified. Because of the periodic modulation of the magnetic field from the vortex lattice, the ferromagnetic film influenced by the vortex lattice acts as a magnonic crystal and results in the formation of bandgaps in the spin wave spectrum. The vortex lattice depends on the magnitude of the applied magnetic field, which can then be used to tune the spin wave band gaps for possible magnonic applications.

9:00AM A46.00006: Imaging spin-wave propagation and interference with electron spins in diamond
IACOPO BERTELLI (Presenter), JORIS JIP CARMIGGELT, BRECHT SIMON, COOSJE POTHOVEN, Delft University of Technology, JAN AARTS, Leiden University, TOENO VAN DER SAR, TAO YU, Delft University of Technology, GERRIT BAUER, Institute for Materials Research and WPI-AIMR and CSRN, Tohoku University, YAROSLAV M. BLANTER, Delft University of Technology — The coherent transport of spin information in magnetic insulators is not associated with the heat dissipation of electronic currents. Therefore, it is envisioned that the next generation of information-processing devices could be based on spin waves, the elementary excitations of magnets that can reach nanometer wavelengths and terahertz frequencies. Here we use electron spins in diamond to probe coherent spin-wave transport in the magnetic insulator yttrium-iron-garnet (YIG). We image propagating spin-waves and their interference, we extract the dispersion relation, demonstrate time-domain control and quantify the magnetization oscillations carried by these excitations. These results pave the way for fundamental studies of spin-wave transport and to harness spin-wave interference in magnonic devices.
**9:12AM A46.00007: Experimental observation of exceptional surface in synthetic dimensions with magnon polaritons**

XUFENG ZHANG (Presenter), Argonne Natl Lab, KUN DING, Imperial College London, XIANJING ZHOU, JING XU, DAFEI JIN, Argonne Natl Lab — Exceptional points (EPs) are singularities of eigen-energies in non-Hermitian systems. Intriguing phenomena have been previously observed around EPs. However, previous demonstrations are limited to 0-dimensional points and 1-dimensional lines. Here we report, to the best of our knowledge, the first experimental observation of an exceptional surface (ES) in a magnon polariton system. Magnon polaritons are hybrid excitations of electromagnetic waves and spin waves, which have recently emerged as a promising candidate for coherent information processing. We took advantage of the excellent tunability in magnon polaritons and introduced a 4-dimensional synthetic space, which enabled the observation of ES. In addition, we also observed an exceptional saddle point in the ES, which exhibits unique anisotropic behaviors in both the real and imaginary part of the eigenfrequencies. Our findings open up new opportunities for high-dimensional control of non-Hermitian systems and novel sensing applications.

*This work was performed, in part, at the Center for Nanoscale Materials, a U.S. DOE Office of Science User Facility, and supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357. K.D. acknowledges funding from the Gordon and Betty Moore Foundation.

**9:24AM A46.00008: Magnon spectrum of the chiral ferrimagnet Cu$_2$OSeO$_3$: a coarse-grained approach**

YI LUO (Presenter), GUY G MARCUS, Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University, BENJAMIN TRUMP, NIST Center for Neutron Research, National Institute of Standards and Technology, JONAS KINDERVATER, Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University, MATTHEW STONE, Neutron Scattering Division, Oak Ridge National Laboratory, TYREL MCQUEEN, OLEG TCHERNYSHYOV, COLLIN LESLIE BROHOLM, Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University — We report a comprehensive neutron scattering study of low energy magnetic excitations in the breathing pyrochlore helimagnetic Cu$_2$OSeO$_3$. Fully documenting the four lowest energy modes that leave the ferrimagnetic configuration of the "strong tetrahedra" intact (ℏω<13 meV), we find quadratic dispersion at the Γ point for energies above 0.2 meV with any gap less than 0.19 meV, two doublets separated by 1.6(2) meV at the R point, and a bounded continuum at the X point. Our constrained rigid spin cluster model relates these features to Dzyaloshinskii-Moriya(DM) interactions and the incommensurate helical ground state. Combining conventional spin wave theory with a spin cluster form-factor accurately reproduces the measured equal time structure factor through multiple Brillouin zones. An effective spin Hamiltonian describing the complex anisotropic inter-cluster interactions is obtained.

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DESC0019331. Collin Broholm and Jonas Kindervater were supported by the Gordon and Betty Moore Foundation under the EPQS program grant number GBMF-4532.
9:36AM A46.00009: Modeling Hall viscosity in magnetic Skyrmions  BOM KIM (Presenter), Loyola University Maryland — Magnetic Skyrmions are topologically stable objects that are made with a bunch of spins tightly arranged in a smooth fashion. Their topological nature provides unusual and complex transport properties, such as Skyrmion Hall effect. Extensive Hall data have further revealed asymmetry between Skyrmion and Anti-Skyrmion Hall angles, which cannot be accounted by known mechanisms. Here, we explain this asymmetry by utilizing another universal transport coefficient called ‘Hall viscosity,’ extensively studied in quantum Hall systems. Hall viscosity is modeled in steady-state Skyrmions motion by generalizing the Thiele equation with a transverse velocity component and is independent of the Skyrmion charge. Our analyses, based on available asymmetric Hall angle data, reveal this transverse force amounts 3% - 5.4% of the force due to Skyrmion Hall effect. Further clarification of Hall viscosity will be essential for designing next generation storage devices properly, not to mention for our deeper understanding of fundamental properties of nature.

9:48AM A46.00010: Spin dynamics in the skyrmion host lacunar spinel GaV₄S₈  GANESH POKHAREL (Presenter), HASITHA SURIYA ARACHCHIGE, Department of Physics and Astronomy, The University of Tennessee, GEORG EHLERS, Neutron Technologies Division, OakRidge National Laboratory, SEUNGHWAN DO, Materials Science and Technology Division, OakRidge National Laboratory, MATTHEW STONE, MARK D LUMSDEN, Neutron Scattering Division, OakRidge National Laboratory, HAO ZHANG, CRISTIAN BATISTA, Department of Physics and Astronomy, The University of Tennessee, YIMING QIU, NIST Center for Neutron Research, National Institute of Standards and Technology, RANDY FISHMAN, Materials Science and Technology Division, OakRidge National Laboratory, DAVID MANDRUS, Materials Science and Engineering, The University of Tennessee, ANDREW D CHRISTIANSON, Materials Science and Technology Division, OakRidge National Laboratory — In the lacunar spinel GaV₄S₈, the interplay of spin, charge, and orbital degrees of freedom results in a complex phase diagram that includes ferroelectric, orbitally ordered and Néel type skyrmion phases. Below 12.7 K, GaV₄S₈ exhibits a cycloidal state at zero field and a Néel type skyrmion spin structure with the application of field. To understand the physics driving the formation of these novel phases, we have carried out inelastic neutron scattering measurements on GaV₄S₈ above and below the ordering temperature of 12.7 K. Dispersive spin excitations with a zone boundary energy 5.65 meV are observed along the [100], and [110] directions within the magnetically ordered phase. The excitation spectrum softens along the third high symmetry direction, [111]. Using a Heisenberg model with near-neighbor exchange couplings and Dzyaloshinskii-Moria (DM) interactions, the excitation spectra are simulated. Simulation shows ferromagnetic inter-tetrahedral couplings with J= -0.69(3) meV. It is also observed that the DM interactions are around an order of magnitude weaker than the near-neighbor exchange interactions. A small and finite value of the DM interaction at 2 K provides evidence that the ground state of GaV₄S₈ is a cycloid below the ordering temperature in zero applied field.
**10:00AM A46.00011: Dynamics of a vortex near the edge of a thin-film ferromagnet**

MICHAEL BJERNGAARD (Presenter), Johns Hopkins University, DEREK REITZ, UCLA, OLEG TCHERNYSHYOV, Johns Hopkins University — The low-frequency dynamics of magnetization in a thin-film ferromagnet with an easy-plane anisotropy can be efficiently described by a mapping to electrodynamics in 2+1 dimensions. Magnons turn into photons, whereas vortices become massless particles with an electric charge equal to the vortex number. In a previous work [1], we showed that a vortex-antivortex pair with equal skyrmion numbers revolve around the geometrical center and gradually spiral down towards annihilation. Their motion was accurately modeled by considering the balance of forces acting on these topological defects: the Coulomb attraction, the gyroscopic forces, and the viscous force from Gilbert damping. A vortex-antivortex pair with opposite skyrmion numbers will move mostly in the same direction, gradually approaching each other. A similar motion is expected of a vortex near a straight edge, which creates the image of an antivortex attracting the vortex toward the edge. We study this motion numerically and model it analytically.


*Supported as part of the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331

**10:12AM A46.00012: Soliton Bound States in Large-Spin Anisotropic Antiferromagnets**

HARRY LANE (Presenter), University of Edinburgh, FRANK KRÜGER, ELLIOT CHRISTOU, London Centre for Nanotechnology, University College London, CHRIS STOCK, University of Edinburgh, RUSSELL EWINGS, ISIS Facility, Rutherford Appleton Laboratory — It has long been known that the low-energy dynamics of spin systems are well-described by classical linear spin-wave theory. This is particularly true in the case of systems with a large spin moment, where one can expand in powers of $1/S$. For large-spin antiferromagnets, linear spin wave theory predicts dispersive magnon modes which are gapped in the presence of anisotropy. Such spectra are found time and again in the literature, but can the quantum nature of spin give rise to exotic excitations that are not well described by linear spin-wave theory?

Using a path integral approach [1], we show that the movement of domain walls in an anisotropic large-spin antiferromagnetic chain can be described by solitons. In the presence of coupling to other chains, the frustration induced by this soliton propagation leads to a nonlinear confinement potential that can support bound states. We will then show experimental evidence for these soliton bound states [2], demonstrate strong agreement with our theoretical model and offer insights into where one might expect to find such a phenomenon.

10:24AM A46.00013: Tuning high-Q nonlinear dynamics in a disordered quantum magnet*

DANIEL SILEVITCH (Presenter), CHRISTOPHER TANG, Caltech, GABRIEL AEPPLI, ETH Zurich, THOMAS F ROSENBAUM, Caltech — Quantum states cohere and interfere. Atoms arranged imperfectly in a solid rarely display these properties. Here we demonstrate an exception in a disordered quantum magnet that divides itself into nearly isolated subsystems. We probe these coherent spin clusters by driving the system nonlinearly and measuring the resulting hole in the linear spectral response. The Fano shape of the hole encodes the incoherent lifetime as well as coherent mixing of the localized excitations. For the Ising magnet LiHo$_{0.045}$Y$_{0.955}$F$_4$, the quality factor $Q$ for spectral holes can be as high as 100,000. We tune the dynamics by sweeping the Fano mixing parameter $q$ through zero via the ac pump amplitude as well as a dc transverse field. The zero crossing of $q$ is associated with a dissipationless response at the drive frequency. We then explore the dynamics of this dissipationless state, focusing on the decoherence of the extended spin clusters. Identifying localized two-level systems in a dense and disordered magnet advances the search for qubit platforms emerging from strongly interacting, many-body systems.

*The work at Caltech was supported by US Department of Energy Basic Energy Sciences Award DE-SC0014866.

10:36AM A46.00014: Enhanced self-focusing effect of spin-wave by a pulsed flat-top excitation field in a multi-domain state

KIM HYO SEOK (Presenter), JONGSEOK LEE, IN HYEOK CHOI, Gwangju Institute of Science and Technology — Spin-wave (SW) or its quantum, magnon, is studied with renewed interest as a basis for wave-based classic information processing. Along with other physical waves, SWs also have wave-like properties, such as radiation, propagation, reflection, and refraction, which have been extensively investigated in order to manipulate SWs. Especially, there have been many methods reported to focus the SW via a nonlinearity, a graded refractive index, and a phase-controlled SW sources. In this work, we explore another efficient way of the SW focusing by using the spatially and temporally tailored magnetic field excitations. Using a micro-magnetic simulation, we explain how the SW propagates and is focused in a ferromagnetic thin film with a perpendicularly magnetized anisotropy after its excitation by a pulsed magnetic field having a flat-top amplitude distribution. In particular, we observe that the focusing appears more efficiently in the multi-domain state divided by Bloch walls compared to that in the single-domain state. Based on these results, we suggest the flat-top excitation of the magneto-static wave as an efficient way to create magnetic droplets in a multi-domain state of a perpendicularly magnetized system.
We study in detail the structural and magnetic excitations of CrI$_3$ in single crystalline thin flakes using inelastic light scattering in a magnetic field. We find that for fields above 6 T we observe the scattering from the zone center magnon, the ferromagnetic resonance, with a linear dependence on the magnetic field in this range. This behavior is well explained by the classical Kittel formula that predicts a value of the zero-field resonance at approximately 45 GHz with an effective g-factor of ~ 2. We also find that as a function of the scattered polarization angle with respect to the incoming polarization, the intensity has a two-fold symmetric pattern without nodes (i.e. the signal does not vanish). We will discuss the possible reasons for this behavior and compare it to that expected for the lattice excitations for the expected magnetic point group symmetry.

*Work at OSU was supported by the Center for Emergent Materials, an NSF MRSEC under grant DMR-1420451. Work at NIST was supported by the NIST/NRC Postdoctoral Research Associateship Program and NIST-STRS.
8:00AM A47.00001: Low-temperature magnetic proximity effects in Mg(Al,Fe)₂O₄/Bi₂Se₃ bilayers* LAUREN RIDDIFORD (Presenter), Applied Physics, Stanford University, PENG LI, Electrical and Computer Engineering, Auburn University, ALEXANDER GRUTTER, National Institute of Standards and Technology, YURI SUZUKI, Applied Physics, Stanford University — Topological insulators (TIs) are of significant interest in spin current-based electronics due to their strong spin-orbit coupling from spin-momentum locking of surface states. Bi₂Se₃ is a 3D topological insulator with a semiconductor gap in the bulk and gapless surface states. However, conduction near room temperature is typically bulk-dominated due to Se vacancies. Bilayers of Mg(Al,Fe)₂O₄ (MAFO), a magnetic insulator, and Bi₂Se₃ show highly efficient spin pumping in the bulk-dominated regime at room temperature. At low temperature, below 45 K, we have found evidence of proximity-induced magnetism in the TI. To understand the underlying mechanism of this proximity-induced magnetism, we performed polarized neutron reflectometry which indicates a sharp interface and a magnetic moment in the TI up to at least 45 K. In transport measurements, we observed both the anomalous Hall effect (AHE) and a large unidirectional magnetoresistance in the TI. The AHE, around 1 Ω at 2 K, was observed up to ~40 K and was amplified by electrically gating Bi₂Se₃. These results suggest that the induced magnetism in Bi₂Se₃ is primarily due to the coupling between MAFO and the surface states of Bi₂Se₃.

*Funded by the Vannevar Bush Faculty Fellowship of the DoD under Grant #N00014-15-1-0045 and NSF GRFP.

8:12AM A47.00002: Exotic coupling in garnet-ferromagnet heterostructures* PATRICK QUARTERMAN, National Institute of Standards and Technology, YABIN FAN, LUQIAO LIU, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, ALEXANDER GRUTTER (Presenter), National Institute of Standards and Technology — Metallic and insulating ferromagnets (FM) have been extensively studied for use in spintronic like structures—the former for spin transfer and spin orbit torques and the latter for generation of magnon spin currents [1,2]. Recently, we have shown that in yttrium iron garnet (YIG)/permalloy (Py) bilayers, grown on Si, the YIG preferentially aligns antiparallel to the Py at low field and can be used to form a magnon spin valve [3]. However, the observed coupling in YIG/FM is quite complex and is heavily dependent on the sample geometry—for example when the same bilayers are grown on Gd₃Ga₅O₁₂ (GGG) substrates, no antiparallel coupling has been observed. In this work, we discuss the coupling of YIG to Py and Co when grown on Si and GGG substrates by measuring the magnetic depth profile using polarized neutron reflectometry. The effect of texture and choice of FM on coupling to the underlying YIG layer will be presented in detail.


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8:24AM A47.00003: Angle-dependent magnetoresistance of Pt/EuO\(_{1-x}\) thin films

NARENDRA SHRESTHA (Presenter), JOSEPH R MURPHY, SUBASH KATTEL, WILLIAM RICE, JINKE TANG, Uni of Wyoming — Europium monoxide (EuO) has attracted a great deal of attention in spintronic research due to its unique ferromagnetic and semiconducting properties. Here, we have prepared Pt/EuO thin films by pulsed laser deposition. We study the magnetic and transport properties as a function of temperature and field. The magnetic data shows enhanced Curie temperature to 140 K, which is a signature of oxygen deficiency. Transport measurements reveal a metal-insulator transition below 70 K associated with the ferromagnetic ordering of EuO. Angle-dependent magnetoresistance exhibits behavior that cannot be explained solely on the basis of anisotropic magnetoresistance of EuO: rather, the MR shows a strong angular dependence as the magnetic field, \(H\), is rotated from in-plane to perpendicular-to-plane, while keeping \(H\) perpendicular to the current – a feature consistent with spin Hall magnetoresistance. We discuss the possible origins of the angular dependence by considering the strong spin-orbit coupling present in the system, magnetic proximity effect, interface properties, and the hetero-structure nature of the films.

*This work was supported by NSF (DMR-1710512) and the USDOE (DE-SC0020074).

8:36AM A47.00004: Magnetoresistance and second harmonic Hall measurement of Pt/CoFe\(_2\)O\(_4\) bilayers

ZEXUAN ZHANG (Presenter), PHILLIP DANG, JOSEPH CASAMENTO, XIANG LI, YONGJIAN TANG, TIANXIANG NAN, DANIEL C. RALPH, HUILI XING, DEBDEEP JENA, Cornell University — CoFe\(_2\)O\(_4\) (CFO), a room temperature ferrimagnetic insulating spinel ferrite, is a promising candidate for energy efficient spintronics. Magnetic proximity effect was believed to be absent in Pt/CFO bilayers grown by sputtering or pulsed laser deposition (PLD), but was recently observed in Pt/CFO (001) bilayers grown entirely by molecular beam epitaxy (MBE) [Amamou, Walid et al. Physical Review Materials 2, 011401 (2018)]. Here, we report the observation of magnetic proximity effect in \textit{ex situ} sputtered Pt on MBE grown CFO (001) at room temperature. Angle dependent magnetoresistance measurements in the direction insensitive to spin Hall magnetoresistance (SMR) indicates that magnetic proximity effect is a relatively robust phenomenon. We also studied high quality CFO (111) on multiferroic LuFeO\(_3\) (111) using MBE, since the impact of crystal orientation of CFO on magnetic interaction has been reported to be significant between Pt and CFO. In the same Pt/CFO (001) and Pt/CFO (001) stacks we also carried out the second harmonic Hall measurement and found Nernst effect dominating the signal.

*This work was supported by the Semiconductor Research Corporation (SRC) as nCORE task 2758.001 and NSF under the E2CDA program (ECCS 1740286) and NewLAW EFRI 1741694.
8:48AM A47.00005: Hydroxide-based Magneto-ionics

ALBERTO QUINTANA-PUEBLA
(Presenter), Physics Department, Georgetown University, ABIGAIL A. FIRME, Physics Department, University of Wyoming, CHRISTOPHER J JENSEN, KAI LIU, Physics Department, Georgetown University —

Recently, magneto-ionics has attracted a lot of interests where controlled motion of ions, e.g., under an electric field, is employed to modify metal/oxide interfaces and their magnetic responses in a reversible and non-volatile fashion. Despite the promising initial oxygen-based magneto-ionic systems, it has been demonstrated that hydrogen-based system showed better performance.

In this work, we aim to study the magneto-ionic effects in cobalt hydroxide (Co(OH)₂) / gadolinium (Gd) heterostructures. In contrast to other works, in our system both O²⁻ and H⁺ are contained in the initial sample. Cobalt hydroxide films are grown by electrochemical methods from a cobalt nitrate electrolyte and confirmed by x-ray diffraction. Magnetometry results showed the paramagnetic character of the sample in the as-grown state. However, after the cobalt hydroxide film is sputter-coated with a Gd layer, a clear magnetic hysteresis loop arises. Since the Tc of Gd is 292 K, the observed magnetism arises solely from the spontaneous reduction of Co(OH)₂ to Co and the formation of Gd(OH)ₓ. Finally, we have also demonstrated that the magnetic moment can be tailored with electric fields.

*This work has been supported in part by the SRC/NIST SMART Center and the NSF (DMR-1659532, ECCS-1933527, DMR-1828420).

9:00AM A47.00006: Current-induced magnetization switching in all-oxide heterostructures

LIANG LIU (Presenter), QING QIN, WEINAN LIN, CHANGJIAN LI, QIDONG XIE, SHIKUN HE, XINYU SHU, CHENGHANG ZHOU, ZHISHIUH LIM, JIHANG YU, National University of Singapore, WENLAI LU, Shanghai University, MENGSHA LI, National University of Singapore, XIAOBING YAN, Hebei University, STEPHEN J PENNYCOOK, JINGSHENG CHEN, National University of Singapore —

The electrical switching of magnetization through spin-orbit torque (SOT) holds promise for application in information technologies. Materials with strong spin-orbit coupling, such as heavy metals can convert a charge current into a spin current. The spin current can then execute a transfer torque on the magnetization of a neighboring magnetic layer, usually a ferromagnetic metal like CoFeB, and reverse its magnetization. Here, we combine a ferromagnetic transition metal oxide with an oxide with strong spin-orbit coupling to demonstrate all-oxide SOT devices. We show current-induced magnetization switching in SrIrO₃/SrRuO₃ bilayer structures. By controlling the magnetocrystalline anisotropy of SrRuO₃ on (001)- and (110)-oriented SrTiO₃ (STO) substrates, we designed two types of SOT switching schemes. For the bilayer on the STO(001) substrate, a magnetic-field-free switching was achieved, which remained undisturbed even when the external magnetic field reached 100 mT. The charge-to-spin conversion efficiency for the bilayer on the STO(110) substrate ranged from 0.58 to 0.86, depending on the directionality of the current flow with respect to the crystalline symmetry.

Spin-charge interconversion in complex oxide SrIrO₃ has been studied extensively. Spin Hall angle of SrIrO₃ thin film has been reported, varying from 0.5⁴ to 1⁵. Given the large resistivity mismatch between semimetal SrIrO₃ thin films and typical metal ferromagnets such as CoFeB, CoFe and NiFe, spurious effects and current shunting would be unavoidable in transport measurements. The oxide ferromagnet La₀.₃Sr₀.₇MnO₃ (LSMO) exhibits high Curie temperature, small coercive field and resistance comparable to SrIrO₃ thin films, making it a more suitable candidate for the study of intrinsic spin Hall effects in SrIrO₃ thin films. Also, in situ epitaxial growth of LSMO/SrIrO₃ bilayer system by PLD provides us a platform for engineering the bilayer interface, realizing a fine control of spin dependent interface properties such as effective spin mixing conductance (g↑↓). g↑↓ that is one orders higher than NiFe/2DES, two orders higher than YIG/Heavy metals has been measured.


The relationship between spin-orbit coupling (SOC), emergent topological states, and spin Hall effects, which are highly relevant for spintronics, has driven the recent interest in materials with strong SOC. To probe the influence of SOC at 3d-5d complex oxide interfaces, we have investigated ferromagnetic La₀.₇Sr₀.₃MnO₃/SrIrO₃ bilayers deposited on SrTiO₃. We find that depending on the growth order, the coercive field of the magnetization loop differs significantly at low temperatures. Similar to previous reports, a net moment on Ir has been recorded with element specific XMCD experiments, which is aligned antiparallel to the Mn moments within the manganite. We find that the Ir moment does not follow the same temperature dependence as the magnetization of the manganite, and is limited to the interface. The origins and implications of this result will be discussed.

*Work at Argonne National Laboratory was supported by the U.S. DOE, Office of Science, BES, MSED. This research used resources of the Advanced Photon Source, a U.S. DOE, Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Neutron scattering at the Spallation Neutron Source at ORNL was supported by the DOE, Office of Science, BES.
9:36AM A47.00009: Current-manipulated propagation of spin waves in antiparallel coupled stripe domains of La 0.67 Sr 0.33 MnO 3 thin films [Invited] HAIMING YU (Presenter), BeiHang University — Spin waves may enable low-power devices based on spin information transmission that is free of Joule heating. Antiferromagnetic-type spin waves have intrinsic advantages, such as high speed, dual-polarized and robust against external field perturbation. To date, antiferromagnetic-type propagating spin waves excitation and manipulation have remained challenging. Here, we demonstrate current-controlled stripe domains with alternating upward and downward magnetization in La 0.67 Sr 0.33 MnO 3 thin films, which host spin-wave propagation. A frequency mode around 10 GHz higher than the ordinary low-frequency modes is observed and the dispersion of this mode is different from the low-frequency ones. We developed a theoretical model based on two oppositely oriented coupled domains, which accounts the high-frequency mode an effective antiferromagnetic spin-wave mode. The spin waves can even propagate at zero magnetic field, with group velocities of 2.6 km s$^{-1}$. The orientation of the stripe domains can be controllably modified by an electric current pulse with a density of only 10 5 A cm$^{-2}$, which opens up perspectives for reconfigurable magnonic devices[1].


10:12AM A47.00010: Anisotropic magnon spin diffusion length in ultra-thin spinel ferrite thin films RUOFAN LI (Presenter), TIANXiang NAN, Cornell University, PENG LI, YURI SUZUKI, Stanford University, DANIEL RALPH, Cornell University — Magnon-mediated spin transport in magnetically ordered insulators is of interest in the field of spintronics as it enables transport of spin information with ultra-low-dissipation. Long-distance spin transport has been demonstrated previously in low-damping iron garnets with the film thickness typically above 100 nm. For this large thickness, strain relaxation in the film impedes the study of strain control of magnons. Here we demonstrate anisotropic magnon spin transport in coherently-strained ultra-thin epitaxial films of magnesium aluminum ferrite (MgAl$_{0.5}$Fe$_{1.5}$O$_4$, MAFO) with low Gilbert damping and thickness of 6 nm. Using nonlocal measurements with the spin polarization injected from Pt bars, we found a $\sim$50 % enhancement of the magnon spin diffusion length for propagation in the [110] direction compared to [100], for both electrically and thermally excited magnons. We correlate this anisotropy to the biaxial magnetic anisotropy in MAFO induced by tetragonal distortion. Our finding suggests that epitaxial strain can be used to further engineer magnon spin transport.
**10:24AM A47.00011: Low Magnetic Damping in Epitaxial Li$_{0.5}$Fe$_{2.5}$O$_4$ Thin Films**  
XIN YU ZHENG (Presenter), LAUREN RIDDIFORD, JACOB WISSE, YURI SUZUKI, Stanford Univ — One of the major challenges in the field of spin-current based electronics is the development of low-loss ferromagnetic insulators capable of generating spin currents without an accompanying charge current. Bulk phase Li$_{0.5}$Fe$_{2.5}$O$_4$ (LFO) is known to have the lowest Gilbert damping parameter ($\alpha \approx 0.002$) among the spinel ferrites, but the growth of LFO thin films with desirable microwave properties has remained elusive due to the volatility of lithium. In this talk, we demonstrate the realization of epitaxial LFO ultra-thin films (~3nm) on MgAl$_2$O$_4$ substrates with an ultra-low damping of $\alpha \approx 0.0005$ and an FMR linewidth of 7.5 Oe at 15GHz. These values rival those of yttrium iron garnet (YIG), the gold standard of low-loss magnetic insulators. LFO also offers distinct advantages over YIG such as smaller external field requirements and thinner interfacial layers crucial for magnetic switching. Our results place LFO as an attractive new candidate for low-loss microwave materials in the field of spintronics.

*This work was supported by the U.S. Department of Energy, Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Contract No. DESC0008505.

**10:36AM A47.00012: Interface ferromagnetism and anomalous Hall effect of CdO/ferromagnetic-insulator heterostructures**  
YANG MA (Presenter), Peking Univ — The experimental observation of quantum anomalous Hall effect (QAHE) in magnetic topological insulators has stimulated enormous interest in condensed-matter physics and materials science. For the purpose of realizing high-temperature QAHE, several material candidates have been proposed, among which the interface states in the CdO/ferromagnetic insulator heterostructures are particularly interesting and favorable for technological applications. Here, we report the experimental observation of the interfacial ferromagnetism and anomalous Hall effect in the Fe$_3$O$_4$/CdO/Fe$_3$O$_4$ heterostructures grown via oxide molecular-beam epitaxy. Systematical variation of the CdO thickness reveals the interface ferromagnetism as the major cause for the observed planar magnetoresistance and anomalous Hall effect. Our results might pave the way to engineer oxide interface states for the exploration of QAHE towards exotic quantum-physical phenomena and potential applications.
10:48AM A47.00013: Structural, Magnetic and Electrical Transport Properties of YIG Thin Films with Heavily Reduced Oxygen Content  SHU MI (Presenter), VENKATA SWAMY GOLLAPOTHU, Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, HAOLIANG HUANG, YALIN LU, CAS Key Laboratory of Materials for Energy Conversion, Hefei National Laboratory for Physical Sciences at the Microscale & National Synchrotron Radiation Laboratory, Universi, YONGGANG ZHAO, Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University — Yttrium iron garnet (YIG) is very promising for spintronic devices due to its insulating nature, low damping and large magnon decay length. Moreover, YIG films have greatly facilitated the research on spin pumping, spin Seebeck effect and topological spintronics [1]. So far, many studies have shown that oxygen content is essential for tuning the structural and magnetic properties of YIG films [2]. But the effect was not so remarkable because only a small amount of oxygen content has been reduced. We have investigated the effect of oxygen content on structural, magnetic and electrical transport properties of YIG films with heavily reduced oxygen contents, obtained via annealing with the presence of carbon. Both the saturation magnetic moment and lattice parameter of YIG decrease with reduced oxygen content, and the electrical resistivity of YIG decreases several orders of magnitude with the lowest value of 0.23 Ωcm at 300 K. The electronic transport behaviors are analyzed in detail by variable-range hopping (VRH) and trap-controlled space charge limited (SCL) conduction. This work is helpful for understanding the effect of oxygen content on the properties of YIG.

References

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A48 DCMP: Superconductivity: Critical Current and Vortex Dynamics  Mile High Ballroom 1A - Morten Eskildsen, University of Notre Dame

8:00AM A48.00001: Confined Vortex Matter with Anisotropic Interaction  LIHAO YAN (Presenter), BOLDIZSAR JANKO, XIAOYU MA, WENZHAO LI, University of Notre Dame — In this project, we study confined superconducting vortex matter, when Abrikosov vortices are confined into a mesoscopic container. When the container is large, the vortices are arranged in a triangular Abrikosov vortex lattice. In contrast, in a mesoscopic container, vortices are arranged in other geometries strongly influenced by the container symmetry. In order to systematically study the system of confined vortices, we use the Molecular Dynamics (MD) simulation. In this work, we investigate the stability and melting of mesoscopic vortex matter as a function of vortex number, container size, and container geometry. We identify the so-called “magic number” states which correspond to very stable vortex configurations. We investigate the effect of container symmetry and size on these magic number states and differentiate between the so-called angular melting and general melting transitions. Finally, we explore the influence of anisotropic vortex interactions on the structure of mesoscopic vortex matter.
8:12AM A48.00002: Solid and liquid vortex phases in superconducting Nb/V hybrids* JOSE VICENT (Presenter), Univ Complutense, VICTOR ROLLANO, IMDEA-Nanociencia, ALICIA GOMEZ, Centro de Astrobiología (CSIC-INTA), ALVARO MUNOZ-NOVAL, Univ Complutense, JAVIER DEL VALLE, UCSD, MARIELA MENGHINI, MARINA CALERO DE ORY, IMDEA-Nanociencia, JOSE LUIS PRIETO, ISOM-UPM, ELENA NAVARRO, ELVIRA MARIA GONZALEZ, Univ Complutense — We have studied the vortex dynamics in a periodic potential created by local enhancement of superconductivity. This has been achieved by an array of Nb nanodots embedded in a V film of slightly lower critical temperature. A sample of Cu nanodots embedded in a V film is used as witness sample. In the former hybrid (Nb/V) the array of superconducting Nb dots induces: i) vanishing of commensurability effect between the vortex lattice and the Nb array; ii) hysteresis effects of the vortex dynamics in the solid phase; iii) softening of the vortex lattice, and iv) broadening of the liquid vortex phase. These outcomes can be controlled varying the temperature and/or the in-plane applied magnetic field.

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8:24AM A48.00003: Nonlinear Dynamics and Dissipation of a Curvilinear Vortex Driven by a Strong Surface Current* MANULA RANDHIKA PATHIRANA WALIVE PATHIRANAGE (Presenter), ALEXANDER V GUREVICH, Old Dominion University — We report extensive numerical simulations of large-amplitude oscillations of a trapped vortex line subject to a strong ac magnetic field $H(t) = H_0 \sin(\omega t)$ parallel to the surface. The power dissipated by an oscillating vortex segment driven by the Meissner current was calculated by taking into account the nonlinear vortex line tension, vortex mass and a nonlinear Larkin-Ovchinnikov (LO) viscous drag force. It is shown that oscillations of trapped vortices perpendicular to the surface can radically change the field dependence of a residual surface resistance $R_i(H_0)$ due to the LO decrease of the viscous drag coefficient with the vortex velocity. As the frequency increases, the conventional increase of $R_i(H_0)$ with $H_0$ at low $\omega$ evolves into a non-monotonic dependence of $R_i(H_0)$ at larger $\omega$, so that $R_i(H_0)$ decreases with $H_0$ at higher fields. As the electron mean free path on nonmagnetic impurities gets shorter, the field onset of the anomalous decrease of $R_i(H_0)$ shifts to smaller field, and the drop of $R_i(H_0)$ with $H_0$ becomes more pronounced.

*This work was supported by NSF under Grants PHY-100614-010 and PHY-1734075 and by DOE under Grant and by DOE under grant No. DE-SC0010081.
8:36AM A48.00004: Melting of the 2D vortex lattice in thin α-MoGe films

BAL POKHAREL (Presenter), JASMINKA TERZIC, DRAGANA POPOVIC, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State University, SURAJIT DUTTA, JOHN JESUDASAN, PRATAP RAYCHAUDHURI, Tata Institute of Fundamental Research, ILLARIA MACCARI, KTH-Royal Institute of Technology, LARA BENFATTO, Dept. of Phys., Sapienza Univ. of Rome — The vortex lattice in a 2D type II superconductor is expected to melt via a BKT transition that involves an intermediate liquid phase ("hexatic fluid"), which preserves orientational order. Recent experiments combining transport and STM imaging made it possible to identify the hexatic state in α-MoGe thin films, showing that vortex diffusivity in the hexatic fluid state is strongly reduced with respect to the isotropic vortex liquid. To fully characterize the melting transition, we performed systematic transport measurements on weakly disordered, 22 nm-thick α-MoGe films down to 0.020 K and in magnetic fields up to 18 T. Our results unambiguously show that the persistence of orientational correlations in the hexatic phase significantly slows down the vortex motion, leading to vanishingly small flux-flow resistance. This effect is consistent with numerical simulations.

* Supported by NSF DMR-1707785 and NHMFL via NSF DMR-1644779 and the State of Florida.

8:48AM A48.00005: Strong irradiation-induced vortex pinning in (Cu,C)Ba$_2$Ca$_3$Cu$_4$O$_{11+d}$

WAI-KWONG KWOK (Presenter), ULRICH WELP, ALEXEI KOSHELEV, Argonne Natl Lab, ASGHAR KAYANI, PRASHANTA NIRAULA, Dept. of Physics, Western Michigan University, YUE ZHANG, CHENGPING HE, HAI-HU WEN, Dept. of Physics, Nanjing University — We report on the strong enhancement of vortex pinning in the 115K-superconductor (Cu,C)Ba$_2$Ca$_3$Cu$_4$O$_{11+d}$ following irradiation with 6 MeV protons. While $T_c$ decreases by only ~2K after doses of up to $10^{17}$ p/cm$^2$, the critical current density $J_c$ is enhanced by a factor of 40 in fields above 2 Tesla and at temperatures above 60 K, matching well the range of intended applications. We estimate $J_c$ from magnetization hysteresis measurements on polycrystalline samples using the Bean model. The whole-sample $J_c$ values, deduced by using the sample size as dimension in Bean's model, approach 5000 A/cm$^2$ at 77 K and 1 T. These values are comparable to those of grain-aligned YBa$_2$Cu$_3$O$_x$ intended for trapped-field magnets, underlining the application potential of this material if produced for instance in film form. The evolution of the field dependence of $J_c$ with irradiation dose is consistent with a model of strong pinning by large-size inclusions.

* Materials characterization at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division. Sample synthesis at Nanjing University was supported by National Key R&D Program of China and National Natural Science Foundation of China.
The superconducting vortex lattice (VL) of MgB$_2$ hosts three structural phases associated with distinct rotations of the VL with respect to the crystal lattice. One of these phases, the L phase, contains two degenerate orientations with respect to the $a$ axis, causing the VL to fracture into domains. Domain boundaries inhibit structural transitions to and from the L phase, giving rise to robust metastability and an activation barrier which grows rapidly as the VL approaches equilibrium [1]. These domain-dominated kinetics are ubiquitous in material science, from martensitic phase transitions to ferroelectric domain switching, however, unique to the VL of MgB$_2$ is the ability to externally tune this behavior. By rotating the crystal with respect to the applied field, we can suppress the geometric degeneracy between the two domain orientations and inhibit domain wall formation. In this talk, we will discuss the effect of this broken symmetry on both the VL phase diagram and the kinetic behavior of the structural phase transitions.


*This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Award No. DE-SC0005051.
9:24AM A48.00008: Peak effects in NbSe$_2$ with artificial pinning centers*  
TSUYOSHI TAMEGAI (Presenter), WENJIE LI, SUNSENG PYON, Department of Applied Physics, The University of Tokyo, SATORU OKAYASU, Advanced Science Research Center, Japan Atomic Energy Agency, ATARU ICHINOSE, Central Research Institute of Electric Power Industry, Electric Power Engineering Research Laboratory — Irradiations of swift particles into superconductors modify their vortex states and lead to the enhancement of critical current density, $J_C$, via creation of point defects (PDs) or columnar defects (CDs). Such an enhancement of $J_C$ was demonstrated in cuprate superconductors [1] as well as in conventional [2] and iron-based superconductors [3]. However, how the $J_C$ is enhanced depends strongly on the target material and ion species, energy, and density of swift particles. In some cases, $J_C$ is monotonically enhanced, while in other cases, non-monotonic magnetic field dependence of $J_C$, peak effect, is observed after the irradiation. In the present study, we compare the effect of PDs and CDs on the $J_C$ - $H$ behavior of NbSe$_2$. With increasing the density of PDs by proton irradiation, the field range for the peak effect close to $H_{c2}$ broadens significantly. In the case of CDs, the $J_C$ - $H$ behavior changes sensitively as a function of the direction of CDs and magnetic field with respect to the c-axis.


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9:36AM A48.00009: Large and uniform critical currents in finite magnetic fields  
IVAN SADOVSKYY (Presenter), Microsoft Corp, ANDREAS GLATZ, ALEXEI KOSHELEV, ULRICH WELP, WAI-KWONG KWOK, Argonne National Lab — Loss-free superconducting transport is tremendously important for technological and energy applications. Heat dissipation from drifting magnetic vortices is one of the main limiting factors for superconductors usage. Here we discuss defect configurations that trap vortices almost independently of their direction. As a result, such pinning configurations produce near uniform critical current as a function of applied magnetic field angle. To cover the broadest class of pinning landscapes we employ a genetic algorithm varying the size, position, and orientation of each defect individually. We report several notable results and analyse them in details. The highest uniform critical current is 22% of the depairing current at the magnetic field 10% of the second critical field.
9:48AM A48.00010: New paradigm for a disordered superconductor in orbital magnetic field  AMIT GHOSAL (Presenter), ANUSHREE DATTA, ANURAG BANERJEE, IISER Kolkata, NANDINI TRIVEDI, Physics, Ohio State University — Orbital magnetic field, as well as disorder, weaken superconductivity when acting individually on a s-wave superconductor. The Abrikosov vortex lattice in a clean type-II superconductor, resulting from an orbital magnetic field, transforms into a metal beyond a critical magnetic field $H_c$ once vortices start overlapping. Similarly, disorder drives a transition from a superconductor to an insulator past a critical disorder strength. Here we show that acting simultaneously on a two-dimensional superconductor, disorder and magnetic field lead to an intriguing evolution of the superconducting state. While for weak disorder, the critical field $H_c$ for the suppression of superconducting energy gap matches the critical field at which the superfluid density collapses, the two diverge from each other with increasing disorder creating a pseudogap phase. Our results provide a natural explanation of the long standing puzzle of a strong magnetoresistance peak observed as a function of orbital magnetic field in thin disordered superconducting films. Our results also explain why the characteristic Caroli-de Gennes-Matricon zero bias peak in the local density of states in the vortex core of a clean superconductor might be absent in the presence of disorder, as observed in some recent experiments.

10:00AM A48.00011: Microwave flux-flow Hall effect of superconductors: (1) Method RYO OGAWA, FUYUKI NABESHIMA, ATSUTAKA MAEDA (Presenter), Dept. of Basic Sci., Univ. Tokyo — The bound states in the vortex core of superconductors can be classified in terms of the cleanliness of the vortex core. High $T_c$ cuprate superconductors are expected to be in the clean limit because of the large superconducting gap. However, previous measurements of the effective viscous drag coefficient, $\eta^*$, for wide range of cleaness found that the vortex cores of high $T_c$ cuprates were in the moderately clean limit, as a universal trend [1]. These results may suggest that there exists an extra dissipation mechanism due to the vortex motion which have not been considered so far. However, $\eta^*$ is the mixture of the longitudinal viscous drag coefficient and the Hall coefficient [2]. Thus, $\eta^*$ measurement may not reflect the true electronic states in the vortex core. Therefore, it is necessary to directly measure the flux flow Hall effect and to evaluate the true core states. In order to neglect pinning, we need high frequencies. Thus, we developed a new method for microwave Hall effect measurement using a cross shaped bimodal cavity. In this talk, we will show the detail of the measurement and the analysis. We applied our system to Bi, and obtained a good result.
10:12AM A48.00012: Microwave flux-flow Hall effect of superconductors: (2) Experiments in Bi$_2$Sr$_2$CaCu$_2$O$_y$  
RYO OGAWA (Presenter), FUYUKI NABESHIMA, ATSUTAKA MAEDA, Dept. of Basic Sci., Univ. Tokyo — We have developed a new system to measure the microwave flux-flow Hall effect [1]. The new method enables us to measure microwave Hall effect of materials with high conductivity at low temperatures. Using the system, we investigate the flux flow Hall effect of high T$_c$ cuprate superconductor, Bi$_2$Sr$_2$CaCu$_2$O$_y$. In the vortex state, with increasing magnetic field, Hall angle, tanq, approaches to a constant value at each temperature. We obtained $\omega_0\tau \approx 2-3$ in the low temperature limit ($\omega_0$ and $\tau$ are the level spacing of quasiparticle in the vortex core and the quasiparticle scattering time in the vortex core, respectively), which is larger than the estimated value by the effective viscous drag coefficient $\eta^*$. In this talk, we will discuss the implication of the results.


10:24AM A48.00013: Dynamic Penetration Field of Vortices in a Superconductor in a Time-Dependent Magnetic Field*  
AHMAD SHEIKHZADA, ALEXANDER V GUREVICH (Presenter), Old Dominion University — We address the nonlinear dynamics of penetration of vortices in a superconductor subject to a periodic magnetic field $H(t) = H_0 \sin \omega t$ parallel to the surface. The time-dependent Ginzburg-Landau equations for a gapped superconductor were simulated numerically to calculate the frequency and temperature dependencies of the field onset $H_p(T, \omega)$ of vortex penetration at $T \approx T_c$. It is shown that $H_p(T, \omega)$ can exceed the dc superheating field $H_s$ at which the Meissner state becomes unstable. Here $H_p(T, \omega)$ increases with $\omega$ and approaches $\sqrt{2}H_s(T)$ at $\omega \tau \geq 1$, where $\tau(T)$ is the energy relaxation time of quasiparticles on phonons. We also investigated the effect of surface topographic defects on $H_p(T, \omega)$ and showed that they can substantially reduce $H_p(T, \omega)$ and cause additional power dissipation.

*This work was supported by DOE under grant No. DE-SC0010081.
Glassy and plastic vortex creep regimes in superconducting (Y,Gd)Ba$_2$Cu$_3$O$_y$ films and coated conductors$^*$ LEONARDO CIVALE (Presenter), BORIS MAIOROV, IVAN NEKRASHEVICH, Los Alamos Natl Lab, MASASHI MIURA, Graduate School of Science and technology, Seikei University — Large thermal fluctuations in high $T_c$ superconductors give rise to fast vortex dynamics that promotes the time relaxation of the metastable supercurrents, which is detrimental for applications. We are pursuing a general understanding of the lowest achievable flux creep rate ($S$) for a superconductor at any temperature ($T$) and magnetic field ($H$). Initially, we found that there is a universal lower limit for $S$ in the Anderson-Kim (A-K) regime at $T<<T_c$ (Eley et al., Nat. Mat. 2017). Later, we expanded our quest to higher $T$ and $H$ outside the A-K limit, where the universality is lost and different regimes occur. We will present results on (Y,Gd)Ba$_2$Cu$_3$O$_y$ coated conductors with randomly distributed BaHfO$_3$ nanoparticles. These samples exhibit extremely strong vortex pinning, with critical current densities among the highest in any known superconductor. We identify several glassy and plastic dynamics regimes, the boundaries among which are determined either by intrinsic vortex properties or by thickness effects. In particular, we find a thickness-controlled “second A-K regime” at high $T$, which sets the lowest $S(T,H)$ limit in thin samples in technologically relevant $T$-$H$ conditions.

$^*$Work funded by US DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A49 DCMP: Superconducting Proximity Effect and Josephson Junctions Mile High Ballroom 1B - Dmitry Smirnov, National High Magnetic Field Laboratory
8:00AM A49.00001: Gate-Dependent Transport in Multi-Terminal Josephson Junctions*
GINO GRAZIANO (Presenter), University of Minnesota, JOON SUE LEE, SEAN HARRINGTON, MIHIR PENDHARKAR, CHRIS J PALMSTROM, University of California, Santa Barbara, VLAD PRIBIAG, University of Minnesota — Josephson coupling of three or more superconducting leads through a material with few conducting modes has been predicted to give rise to topological effects. Such behavior, of relevance for topologically-protected quantum bits, would lead to specific transport features measured between terminals, with topological phase transitions occurring as a function of relative phase and voltage biases. Here we study the effects on transport of several top-gating arrangements on multi-terminal Josephson junctions with many conducting modes based on an InAs 2DEG proximitized with an epitaxial aluminum layer and many conducting modes. The superconducting features can be accurately simulated by a network of RCSJ junctions. [1]


*This work was supported primarily by the National Science Foundation under Award No. DMR-1554609. The work at UCSB was supported by the Department of Energy under Award No. DESC0019274. The development of the epitaxial growth process was supported by Microsoft Research.

8:12AM A49.00002: Gate tunable multi-terminal Josephson effect
NATALIA PANKRATOVA (Presenter), HANHO LEE, ROMAN KUZMIN, KAUSHINI S WICKRAMASINGHE, University of Maryland, College Park, MAXIM G VAVILOV, University of Wisconsin - Madison, JAVAD SHABANI, New York University, VLADIMIR MANUCHARYAN, University of Maryland, College Park — Junctions of more than two superconducting terminals are required for implementing braiding operations on Majorana fermions. Moreover, such multi-terminal Josephson Junctions (JJ) were predicted to support topological state and host zero-energy quasiparticles. Unlike conventional two-terminal JJs where the value of critical current is a number, the multi-terminal JJs exhibit a novel feature – the critical current contour (CCC) [1]. We report the measurement of non-trivial CCC shapes as a function of gate voltage and magnetic field in hybrid semiconductor/superconductor (InAs/Al) multi-terminal JJs. Multi-terminal junctions can host two different regimes: a strong neighbor-coupling regime and a multi-terminal regime, depending on the gate voltage. The geometry of a junction is also an important factor defining the operating regime. The effect of an out-of-plane magnetic field indicates an observation of the Fraunhofer interference pattern in multi-terminal JJs.

8:24AM A49.00003: Unconventional Superconductivity in monolayer Transition Metal Dichalcogenides via proximity  VIVEK AJI (Presenter), ROBERT DAWSON, University of California, Riverside — Single layer Transition Metal Dichalcogenides (TMDCs) provide a unique platform to study the interplay of spin-orbit coupling, topology and electron-electron interactions. In addition, the ultrathin 2D geometry allows for proximal coupling to other materials particularly magnets and superconductors. In this talk we report on the nature of the induced superconducting state when coupled to a conventional superconductor. Going beyond the tunneling model we solve a self-consistent Bogoliubov-De Gennes equations for the heterostructure to establish the nature of the paired state. Introducing a third device component, a ferromagnet such as Chromium tri-iodide, breaks time reversal allowing access to the topologically nontrivial electronic states of the TMDC. Modifications of the induced phase and conditions for realizing topological superconductivity will be discussed.

8:36AM A49.00004: Induced superconductivity and multiple Andreev reflections in multilayer WTe$_2$ Josephson junctions*  XURUI ZHANG (Presenter), XIAOYAN SHI, University of Texas at Dallas — Introducing superconductivity into topological materials has become a focus of attention in condensed matter physics as an effective way to realize Majorana modes. It has been predicted that Majorana bound states could arise from the proximity effect between an s-wave superconductor and the surface states of a strong topological insulator (TI). As one of the transition metal dichalcogenides, the topological properties of WTe$_2$ have been verified in both bulk (type-II Weyl semi-metal) and monolayer materials (topological insulator). Here we fabricated SNS junctions based on multilayer WTe$_2$ flakes. We report the observations of the proximity effect induced superconductivity revealed by magnetoresistance (MR) and I-V measurements. Distinct zero-bias conductance peaks in differential conductance measurements, might be as a sign of Majorana state, were also observed. In addition, the multi-dips of differential resistance at low temperature and magnetic field marks multiple Andreev reflections which might result from the intrinsic multi-gap superconducting states of WTe$_2$.

*This work was supported by UT Dallas research enhancement fund.
8:48AM A49.00005: Proximity induced Superconductivity in low carrier density Bi$_x$Sb$_{2-x}$Te$_3$*

YANG BAI (Presenter), XIANGYU SONG, GUANG YUE, ALEXEY BEZRYADIN, DALE J VAN HARLINGEN, JAMES ECKSTEIN, University of Illinois at Urbana-Champaign — To investigate superconductivity in topological insulators, we have fabricated and measured arrays of islands of diameter about 160nm on topological insulators grown by molecular beam epitaxy. Typical island spacing is about 40 nm. The superconductivity is induced via the proximity effect which is strongly dependent on the electronic properties of the underlying TI film. Earlier work with n-type Bi$_2$Se$_3$ where the carrier density was 3E13 carriers per square cm showed the emergence of superconductivity with a 2D critical current density of more than 1A/m at 0.7 mK. In these samples, both bulk and 2D topological surface states were made superconducting. To study proximity effect coupling into only the topological surface states we used thin films of the alloy Bi$_x$Sb$_{2-x}$Te$_3$. In these materials, the total carrier density can be tuned such that the Fermi surface is completely topological and no bulk states are occupied. In samples with carrier density of 7E12 carriers per square cm, we observed the superconducting proximity effect coupling through the surface states above 0.8 K. Nonlinear transport and magnetoresistance results will be presented and discussed. This study reveals how surface and bulk carriers participate in superconductivity in TIs.

*Air Force Office, NSF and DOE
9:00AM A49.00006: Superconducting Proximity Effect in Magnetically-Doped Topological Insulators using Bulk Single Crystals*  
RIKIZO YANO (Presenter), KOHEI TSUMURA, Applied Physics, Nagoya University, HISHIRO T. HIROSE, Laboratory for Materials and Structures, Tokyo Institute of Technology, MASAHIRO YAMAMOTO, Applied Physics, Nagoya University, ANDREI KUDRIASHOV, TQPSS, Moscow Institute of Physics and Technology, MASAO KOYANAGI, HIROMI KASHIWAYA, National Institute of Advanced Industrial Science and Technology, YASUHIRO ASANO, Center of Topological Science and Technology, Hokkaido University, VASILY STOLYAROV, TQPSS, Moscow Institute of Physics and Technology, TAKAO SASAGAWA, Laboratory for Materials and Structures, Tokyo Institute of Technology, SATOSHI KASHIWAYA, Applied Physics, Nagoya University — Superconducting proximity effect on magnetic topological insulators (TIs) is expected to induce unconventional superconductivity, some of which can host the Majorana fermion. Recently, we observed some unusual behaviors on Nb/Fe-doped TI/ Nb Josephson junctions: e.g., a unique three-peak structure and a $4\pi$-periodic Josephson current. However, those origins are still under debate due to possible contributions from the bulk and the edge modes to the proximity effect.

In this study, we prepared another magnetic TI with a high bulk resistivity and fabricated its Josephson junctions without edge contacts. As a result, a similar three-peak structure was also observed, suggesting that the observed unique behaviors found in the former junction also came from the surface contribution. Furthermore, we observed a unique magnetic response possibly related to bulk magnetic properties. We believe that those results promote our understanding of the proximity effect on topological materials.

*This study was supported by JST CREST (Grant No. JPMJCR16F2) and KAKENHI (Grant Nos. JP15H05851, 15H05853, 16H03847, and 18H01243). Crystal growth was supported by the CRP of MSL-Tokyo Tech. The fabrication process was performed at the AIST-NPF, supported by NTPJ of the MEXT, Japan.

9:12AM A49.00007: Compensated CoGd Ferrimagnets in Magnetic Josephson Junctions*  
ALEXANDER MADDEN (Presenter), JOSHUA WILLARD, REZA LOLOEE, NORMAN BIRGE, Michigan State Univ — The rare earth-transition metal ferrimagnet Co$_{1-x}$Gd$_x$ has been studied for application in superconducting electronics. At a carefully chosen Gd concentration, the Co and Gd moments perfectly cancel leading to a zero-moment compensation point. Point-contact Andreev reflection measurements [1] have shown that at the compensation point there is still a net spin polarization of the transport current. This raises the possibility of application in electronics requiring a magnetic material with little stray field, such as cryogenic magnetic memory. As the compensation point can vary significantly as a function of temperature and thickness, we present SQUID VSM data on thin films taken at cryogenic temperatures. We also present the results of transport measurements on superconductor-ferrimagnet-superconductor Josephson junctions over a range of thicknesses for CoGd alloys near their compensation point.


*This research is based upon work supported by the ODNI, IARPA, via ARO contract number W911NF-14-C-0115. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the ODNI, IARPA, or the U.S. Government.
Superconducting pairing symmetry and spin-orbit coupling in proximitized graphene

ABDULRHMAN ALSHARARI (Presenter), University of Tabuk, SERGIO E ULLOA, Ohio University — Graphene has been shown to exhibit unusual topological phases upon proximity to different dichalcogenide substrates [1]. However, the effect of these perturbations in the presence of superconducting correlations has not been explored. We study the effect of different superconducting symmetry pairings over a range of chemical potential. We analyze the symmetry and identify the topological characteristics of the resulting quasiparticle spectrum at the mean field level.

Interestingly, the system with nearest neighbor spin-singlet superconductivity order parameter may exhibit inverted bands in the quasiparticle band structure, reminiscent of the electronic bands [1]. As the system parameters change, the corresponding edge states in such phase appear after a transition to a regime that closes the bulk bandgap. As we will show, however, both gapped phases belong to a topologically trivial regime, as the results of their invariant number Z2 indicate.

Our results also show that the phases in a time-reversal-invariant 2D-superconductor are not dependent on the magnitude of the singlet and triplet order parameter, and/or the chemical potential, as the topological invariant number remains unchanged.


Chaos and Chimera in Hysteretic RF SQUID Metamaterials*

JINGNAN CAI (Presenter), STEVEN ANLAGE, University of Maryland, College Park — RF SQUIDs have been established as viable building blocks for microwave frequency metamaterials [1,2]. The RF SQUID resonance is tunable under applied DC flux, with upper-frequency range scaling as $\sqrt{1+\beta_{rf}}$. Our previous design restricted the parameter $\beta_{rf}$ below unity to avoid hysteresis, thus limited the resonance range. We have built new arrays of RF SQUID meta-atoms in the hysteretic regime to explore their interesting properties with the ultimate goal of extending the resonance frequency tunability. In particular, a strong and positive out-of-plane coupling among the SQUIDs is achieved through an alternating-overlapping-loop geometry, potentially mitigating the hysteresis from high-$\beta_{rf}$ SQUID meta-atoms. Much theoretical work has predicted chaotic dynamics and chimera states in such systems. Observations of the above nonlinear phenomena in microwave transmission measurements and laser scanning microscopy [3] will be reported.


*This work is supported by DOE through grant # DESC0018788.
**9:48AM A49.00010: Josephson current mediated by odd-frequency equal-spin triplet pairing on the surface of Weyl nodal loop semimetals**  PARAMITA DUTTA (Presenter), ANNICA M BLACK-SCHAFFER, Department of Physics and Astronomy, Uppsala University — We explore proximity-induced pairing on the surface of a Weyl nodal loop semimetal (WNLS) sandwiched between two conventional spin-singlet s-wave superconductors in a Josephson junction set-up. The fully spin-polarized drumheadlike surface states (DSSs) and the intrinsic spin-orbit interation of the WNLS cause odd-frequency (odd-ω) equal-spin triplet pairing to be induced on the surface of the WNLS, whereas, the spin-singlet pairing decays inside the WNLS very fast. We show finite Josephson current in the junction contributed by the equal-spin triplet odd-ω pairing. Odd-ω mixed-spin triplet pairing can be generated by placing an additional ferromagnet in the junction if the direction of the magnetization of the ferromagnet opposes the spin-polarization direction of the DSSs. The pairing and the current are not affected if the magnetization direction is orthogonal to the DSS spin polarization, which further confirms the equal-spin structure of the odd-ω pairing.

*We acknowledge financial support from the Swedish Research Council (Vetenskapsradet, Grant No. 621-2014-3721), the Knut and Alice Wallenberg Foundation, and the European Research Council (ERC) under the European Union’s Hori- zon 2020 research and innovation program (ERC- 2017-StG- 757553).

**10:00AM A49.00011: Critical Current Decay in Josephson Junctions Containing Antiferromagnetic Ni$_{41}$Mn$_{59}$**  ROBERT M KLAES (Presenter), REZA LOLOEE, NORMAN BIRGE, Michigan State University — We report on the fabrication and measurement of antiferromagnetic (AF) S/N/AF/N/S Josephson junctions where Ni$_{41}$Mn$_{59}$ is used as the AF layer, Nb as the S layer, and Cu as the N layer. From measurement of critical current in samples with NiMn thicknesses in the range from 1.2 nm to 6.0 nm, we measure the characteristic decay length within NiMn to be 2.1 nm. One potential application of AF layers inside Josephson junctions is to pin the magnetization of an adjacent ferromagnetic (F) layer by exchange bias. We have characterized NiMn/NiFe and NiMn/Ni bilayer sheet films magnetically to confirm the pinning behavior of NiMn. Such a bilayer AF/F system could potentially be used as a pinned hard layer in a proposed cryogenic memory cell whose design takes the form of an S/F/F'/S spin valve where the two ferromagnetic layers [F, F'] have different switching fields [1]. This design requires a robust magnetization of the hard layer which would be strengthened by the exchange bias effect.


*This research is based on work supported by Northrop Grumman Corporation.*
Magneto-transport of electrons in near surface InAs quantum wells in contact with NbTiN* Mehdi Haftepour (Presenter), William Mayer, Noah Gooss, William Makoto Strikland, Joseph Yuan, Kaushini S Wickramasinghe, Kasra Sardashti, New York University, Tzu-Ming Lu, Sandia National Laboratories, Javad Shabani, New York University — Indium Arsenide (InAs) near surface quantum wells have become the focus of recent interest for their use in heterostructures with superconductors. An interface between a superconductor and quantum Hall edges is predicted to exhibit excitations with non-abelian statistics. NbTiN-InAs is a promising candidate as NbTiN can sustain strong magnetic fields where InAs can host integer quantum Hall states. In this work, we study the proximity effect by monitoring the current flow along the superconductor-semiconductor interface. The data suggest the enhanced conductance is due to Andreev reflection when edge states are formed in the presence of a strong magnetic field.

This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. DOE's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. This work was supported partially by NSF EAGER under award number DMR-1836687.

Superconductor-Semiconductor Devices with 2D Holes in Germanium* Kushagra Aggarwal (Presenter), Andrea Hofmann, Daniel Jirovec, Ivan Prieto Gonzalez, Institute of Science and Technology Austria, Amir Sammak, Menno Veldhorst, Giordano Scappucci, QuTech, Delft University of Technology, Georgios Katsaros, Institute of Science and Technology Austria — The coupling of superconductors to semiconductors receives widespread interest due to their potential for realizing topological superconductivity, interferometers and Andreev Bound State devices [1, 2]. The quality of the induced gap, heavily influenced by the transparency of the superconductor-semiconductor interface, presents a crucial challenge for realizing such devices. Here, we study proximity induced superconductivity in germanium quantum wells coupled to aluminium. The presence of strong spin-orbit interaction, tunable g-factor and high mobility make germanium an attractive semiconducting platform. Combined with the ease of ohmic contact formation due to Fermi level pinning, Ge-Al is a promising material system for hybrid semiconductor-superconductor devices. We achieved transparencies of 65% and $I_C R_N$ products of up to 50μV, about three times higher than previously reported [3, 4].


*The project received financial support from NOMIS foundation.
Transport properties of ultra-scaled Ge/Si core/shell nanowires with highly transparent Al contacts. *JOVIAN DELAFORCE (Presenter), Université Grenoble Alpes, CNRS, Institut NEEL UPR2940, Grenoble, France, MASIAR SISTANI, Institute of Solid State Electronics, TU Wien, Gußhausstraße 25-25a, 1040 Vienna, Austria, ROMAN KRAMER, NICOLAS ROCH, Université Grenoble Alpes, CNRS, Institut NEEL UPR2940, Grenoble, France, MINH-ANH LUONG, Université Grenoble Alpes, CEA, IRIG-DEPHY, F-38054 Grenoble, France, MARTIEN DEN-HERTOG, Université Grenoble Alpes, CNRS, Institut NEEL UPR2940, Grenoble, France, ERIC ROBIN, Université Grenoble Alpes, CEA, IRIG-DEPHY, F-38054 Grenoble, France, JUERGEN SMOLINER, Institute of Solid State Electronics, TU Wien, Gußhausstraße 25-25a, 1040 Vienna, Austria, JUN YAO, Department of Electrical and Computer Engineering, Institute for Applied Life Sciences, University of Massachusetts, Amherst, Massachusetts, 01003, USA, CHARLES M LIEBER, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, 02138, USA, CÉCILE NAUD, Université Grenoble Alpes, CNRS, Institut NEEL UPR2940, Grenoble, France, ALOIS LUGSTEIN, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, 02138, USA, OLIVIER BUISSON, Université Grenoble Alpes, CNRS, Institut NEEL UPR2940, Grenoble, France — Superconducting-semiconducting hybrid systems provide a rich domain for the investigation of electronic and quantum transport. Further, promising developments in their application in high performance nanoelectronics and quantum devices has motivated significant research and development. Nanowire heterostructures are of particular interest due to their quantum confinement properties allowing one to investigate transport in quasi one-dimensional systems. However, critical to their success is the fabrication of high quality and reproducible semiconductor-superconductor interfaces. Using a novel annealing technique, we have realised nanowire heterostructures consisting of crystalline-Al/Si core/shell leads contacting tuneable Ge/Si core/shell segments with atomically precise interfaces. We will present results of temperature dependent DC transport measurements on ultra-scaled devices. Reporting on the gate tuneable transport properties of these highly transparent devices including quantized conductance, tuneable Josephson current and multiple Andreev reflections and their applications as quantum devices.

*J. Delaforce acknowledges the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 754303.
10:48AM A49.00015: Gate-tunable proximity effect in epitaxial Al-InAs Josephson junctions using hBN gate dielectric*  JOSHUA THOMPSON (Presenter), Physics, University of Arkansas, WILLIAM MAYER, FATEMEH BARATI, JOSEPH YUAN, KAUSHINI S WICKRAMASINGHE, KASRA SARDASHTI, Physics, New York University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, JAVAD SHABANI, Physics, New York University, HUGH CHURCHILL, Physics, University of Arkansas — The transparent interface of epitaxial Al-InAs heterostructures provides an excellent platform for potential advances in topological superconductivity and superconducting quantum computation. Josephson junctions built on these heterostructures can be gated, allowing for tuning of the supercurrent. We report the fabrication and measurement of gate-tunable Al-InAs Josephson junctions in which the gate dielectric in contact with the InAs was mechanically exfoliated hexagonal boron nitride (hBN). We discuss fabrication processes that enable compatibility between layered material transfer and Al-InAs heterostructures. By comparing these devices with others using a conventional AlOx gate dielectric, we show that hBN is a suitable gate dielectric for the Al-InAs material platform. Specifically, the product of normal resistance and critical current, is comparable for both types of devices, but higher $R_N$ for the hBN-based devices suggests the possibility of less unintentional doping of the InAs by the gate dielectric.

*We acknowledge support from NSF DMR-1610126 and NSF DMR 1836687.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A50 DCMP: Antiferromagnetic Order and Instabilities Mile High
Ballroom 1C - Md Mofazzel Hosen
8:00AM A50.00001: First single crystals of a new itinerant antiferromagnet without magnetic elements

JAIME MOYA (Presenter), Rice University, ALANNAH HALLAS, Physics and Astronomy, University of Bristish Columbia, EMILIA MOROSAN, VAIDEESH LOGANATHAN, ANDRIY NEVIDOMSKY, Rice University, FRANZISKA WEICKERT, Los Alamos National Laboratory, JAMES W BEARE, YIPENG CAI, GRAEME LUKE, McMaster University, CHIEN-LUNG HUANG, Rice University — Magnetism exists on a spectrum spanning the local to itinerant limit. Theory in the local moment extreme is experimentally confirmed in many magnetic insulators where the magnetism originates from unfilled electronic shells. However, in the itinerant limit, where magnetism stems from band effects, experiment lags theory as there are only three known purely itinerant magnets: ZrZn$_2$ and Sc$_{3.1}$In, both FM, and TiAu an AFM. While ZrZn$_2$ has been made in single crystal form, no single crystals have been made of a purely itinerant AFM, until now. We present the results on single crystals of a new itinerant AFM with no magnetic constituent elements which orders at $T_N = 11$ K. The paramagnetic moment is large, 1.0 $\mu_B$/FU, compared to the saturated moment of 0.25 $\mu_B$/FU, leading to a Rhodes-Wohlfarth ratio of 4. The entropy release is small, just 0.7%$R\ln 2$, yet muon spin relaxation measurements confirm the order is intrinsic. DFT calculations confirm the small moment and conclude a Fermi surface nesting mechanism is responsible for the magnetic order. Having the first purely itinerant AFM crystal paves the way for advance experiments that will allow a fundamental understanding of this class of materials for the first time.

*This work supported by NSF DMR 1903741.

8:12AM A50.00002: Magnetochiral dichroism in a collinear antiferromagnet MnTiO$_3$ with zero magnetization

TATSUKI SATO (Presenter), NOBUYUKI ABE, Univ of Tokyo-Kashiwanoha, SHOJIRO KIMURA, Tohoku University, YUSUKE TOKUNAGA, TAKA-HISA ARIMA, Univ of Tokyo-Kashiwanoha — Symmetry breaking induces specific optical effects. Magnetochiral dichroism (MChD) - nonreciprocal directional asymmetry in the propagation of unpolarized light - has been found to be induced by simultaneous breaking of the space-inversion and time reversal symmetries. After the first discovery [1], it has been established that net magnetization along with the light path causes MChD in various chiral magnets. In contrast, MChD in antiferromagnets without magnetization is less explored. Here we report the MChD in a collinear antiferromagnet MnTiO$_3$ in the absence of magnetization. We observed some asymmetry in the absorption coefficient between the light beams propagating parallel and antiparallel to the net staggered magnetization. Exploiting the linear magnetoelectric coupling [2], we also demonstrate the electric-field and magnetic-field induced switching of absorbance in MnTiO$_3$. In our presentation, we will propose the microscopic description of the origin of the MChD in MnTiO$_3$ from the viewpoint of local symmetry on each Mn site.


*This work was partly supported by JSPS KAKENHI Grants No. 16K13828, 16H01065, 18H04309, 19H01835, and JP19H05826.
Highly nonlinear magnetoelectric effect in antiferromagnetic $\text{Co}_4\text{Ta}_2\text{O}_9$ single crystals

DONGGUN OH (Presenter), NARA LEE, Yonsei University, SUNGKYUN CHOI, Rutgers University, JAE YOUNG MOON, JONG HYUK KIM, HYUN JUN SHIN, HWAN YOUNG CHOI, Yonsei University, SON KWANGHYO, Max Planck Institute for Intelligent Systems, MATTHIAS J GUTMANN, Rutherford Appleton Laboratory, GIDEOK KIM, Max Planck Institute for Solid State Research, VALERY KIRYUKHIN, Rutgers University, JURGEN NUSS, Max Planck Institute for Solid State Research, YOUNG JAI CHOI, Yonsei University — A class of antiferromagnetic honeycomb lattices compounds, $\text{A}_4\text{B}_2\text{O}_9$ ($\text{A} = \text{Co, Fe, Mn}; \text{B} = \text{Nb, Ta}$), have been explored owing to the occurrence of linear magnetoelectricity. We observe a highly nonlinear magnetoelectric effect on single crystals of $\text{Co}_4\text{Ta}_2\text{O}_9$ (CTO), distinctive from the linear behavior in the isostructural $\text{Co}_4\text{Nb}_2\text{O}_9$.

Ferroelectricity emerges primarily along the [110] direction under magnetic fields, with the onset of antiferromagnetic order at $T_N = 20.5$ K. For in-plane magnetic field, a spin-flop occurs at $H_C \approx 0.3$ T, above which the ferroelectric polarization gradually becomes negative and reaches a broad minimum. Upon increasing magnetic field further, the polarization crosses zero and increases continuously to $\sim 60 \mu\text{C/m}^2$ at 9 T. In contrast, the polarization for a magnetic field perpendicular to the hexagonal plane increases monotonously and reaches $\sim 80 \mu\text{C/m}^2$ at 9 T. This observation of a strongly nonlinear magnetoelectricity suggests that two types of inequivalent $\text{Co}^{2+}$ sublattices generate magnetic field-dependent ferroelectric polarization with opposite signs. These results motivate fundamental and applied research on the intriguing magnetoelectric characteristics of these honeycomb lattice materials.

Gapless antiferromagnetic behavior in newly synthesized marcasite-phase $\text{CoAsSe}$

YIYAO CHEN (Presenter), GEORGE YUMNAM, ASHUTOSH DAHAL, Univ of Missouri - Columbia, JOSE RODRIGUEZ-RIVERA, GUANGYONG XU, National Institute of Standards and Technology, THOMAS HEITMANN, DEEPAK K SINGH, Univ of Missouri - Columbia — $\text{CoAsSe}$ belongs to the CoXY chalcogenide family and is reported to crystalize in different phases depending on the synthesizing temperature and pressure, including a half metallic phase according to DFT calculations. For the first time, we have synthesized marcasite-phase $\text{CoAsSe}$ in large amount to perform neutron scattering measurements. Elastic neutron scattering measurements revealed weak magnetic peaks below $T \sim 38$ K at momentum transfer positions of $(0, 0.5, 0)$ and $(1, 0, 0)$ in reciprocal lattice units. Detailed inelastic measurements in low temperature revealed a broad excitation spectrum in the energy transfer-momentum transfer map. We will present the magnetic structures of the newly synthesized marcasite phase $\text{CoAsSe}$ and discuss its relationship to electrical measurement results.

*The research at MU is supported by DOE, Office of Basic Energy Sciences under grant no. DE-SC0014461.
8:48AM A50.00005: Microscopic insights to ARPES spectra of doped quantum anti-ferromagnets  FABIAN GRUSDT (Presenter), Department of Physics and Arnold Sommerfeld Center for Theoretical Physics (ASC), Ludwig-Maximilians-Universität München, Theresienstr. 37, München D-80333, Germany, ANNABELLE BOHRDT, Department of Physics and Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany, FRANK POLLMANN, Department of Physics, T42, Technical University of Munich, D-85748 Garching, Germany, MICHAEL KNAP, Department of Physics and Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany — The phase diagram of cuprates, often modeled by the 2D Fermi Hubbard or $t-J$ model, remains poorly understood at low doping. Here we present new theoretical insights to the ARPES spectrum of quantum anti-ferromagnets at low doping: We argue that, at strong coupling $t \gg J$, the spectrum directly reflects the spectral function of a spinon which forms a universal bound state with the chargon created in the measurement. Our result is relevant to cuprates in the pseudogap regime: we interpret the observed Fermi-arcs in a fractionalized Fermi liquid (FL*) picture and argue that the strongly suppressed spectral weight on the back-side of the hole pocket is a signature for the Dirac-fermion nature of the underlying spinons. We present DMRG calculations of the one-hole spectrum, which support the existence of the universal spinon-chargon bound state we assume at strong couplings. Our results are also relevant for the search of Dirac spinons in a larger class of frustrated quantum magnets.

9:00AM A50.00006: Optical conductivity of CrAs across the paramagnetic to antiferromagnetic transition  ALEXANDRE ZIMMERS (Presenter), RICARDO LOBO, ESPCI, CNRS, Sorbonne University, Paris-France, AMIR-ABBAS HAGHIGHIRAD, MATTHIEU LE TACON, Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany — We report the optical spectroscopy of monopnictide crystal CrAs. This system exhibits a PM to AF transition at $T_N \approx 265K$. This AF phase gradually disappears under pressure with the emergence of 2.2K superconductivity at 0.7GPa. To understand this rich phase diagram, various technics have investigated similarities of this material with the parent iron-pnictide superconductors. Here we studied the PM to AF transition by measuring the reflectivity from 300K to 5K at ambient pressure from 17meV to 3eV. As a function of incident photon energy, the reflectivity shows a gradual decay for all temperatures. The optical conductivity was extracted using Kramers–Kronig. Below 50meV, a Drude peak is clearly found only for temperatures below $T_N$. Extrapolation to zero frequencies of the conductivity is in agreement with previous reported DC transport measurements. In the mid-infrared range, the optical response of the AF order ($T=250K$) shows a rounded gap features with respect to the PM phase ($T=300K$): suppression in the low frequency optical conductivity, alongside a spectral weight transfer from low to high frequencies. The spectral weight transfer dip-hump structure will be compared to previous SDW gaps found in iron-based superconductors and electron doped cuprates.
9:12AM A50.00007: Gapless spin liquid state of the spin-1/2 honeycomb antiferromagnetic Gamma model*  XIAOQUN WANG (Presenter), School of Physics and Astronomy, Shanghai Jiao Tong University, QIANG LUO, Department of Physics, Renmin University of China, JIZE ZHAO, School of Physical Science and Technology & Key Laboratory for Magnetism and Magnetic Materials of the MoE, Lanzhou University — We propose a choreographed model by introducing a bond-modulated Heisenberg interaction J in addition to the Gamma term. With varying an angular parameter of vartheta=atan(Gamma/J)in[0,pi], the ground state is shown to change from a zigzag magnetic order to a stripy magnetic order through a mixed phase as well as a noncoplanar phase based on a parallel tempering Monte Carlo simulation. In the quantum case where we resort to large scale density matrix renormalization group calculations, two classical intermediate phases merge into one which is gapless and nonmagnetic, signaling a quantum spin liquid (QSL), in a wide range of 0.50\leq vartheta/pi\leq 0.66(1) for the thermodynamic limit. It turns out that the ground state of HCGammaA is affirmed to be the gapless QSL since it corresponds to vartheta=\pi/2 in the phase diagram. Our findings are further verified with scanning the variable parameter vartheta on a long cylinder.

*Natural Science Foundation of China (Grant No. 11874188, No. 11574200 and No. 11974244) and the Fundamental Research Funds for the Central Universities and Key Research Project (Grant No. 2016YFA0300501)

9:24AM A50.00008: Evidence for a Field-Induced Quantum Phase Transition in Ising-like D-Er$_2$Si$_2$O$_7$*  GAVIN HESTER (Presenter), TIM DELAZZER, DANIELLE YAHNE, COLIN SARKIS, KATE ROSS, Colorado State University — Exploring the magnetic properties of the rare-earth pyrosilicate (RE$_2$Si$_2$O$_7$) family of compounds is of interest due to their variety of crystal structures and anisotropic pseudo-spin ½ moments. D-Er$_2$Si$_2$O$_7$ (space group P2$_1$/b) was previously found to have a large g-tensor anisotropy (g$_{xx}$ = 2.6, g$_{yy}$ = 3.4, g$_{zz}$ = 13.4) and magnetization consistent with Ising exchange [1]. In this work we have performed specific heat, magnetometry, and inelastic neutron scattering (INS) on a polycrystalline sample to further characterize the magnetism of D-Er$_2$Si$_2$O$_7$. The zero-field specific heat and magnetometry data corroborate previous measurements indicating antiferromagnetic ordering at 1.9 K. The INS data shows a gapped excitation at 0.6 meV in zero field, consistent with Ising exchange. This gap closes with the application of a magnetic field of ~1 T, consistent with a quantum critical point. Magnetization measurements on single crystal samples suggest that the mode softening is due to the field acting on the direction perpendicular to the Ising moments. Our data suggests that D-Er$_2$Si$_2$O$_7$ could be a new experimental system in which to study the quantum Ising model.


*NSF: DMR-1611217
Nonthermal interacting-magnon dynamics in an optically driven 2D Heisenberg antiferromagnet

MONA KALTHOFF (Presenter), Max Planck Institute for the Structure and Dynamics of Matter, DANTE KENNES, Institut für Theorie der Statistischen Physik, RWTH Aachen University, ANDREW MILLIS, Center for Computational Quantum Physics, Flatiron Institute, MICHAEL SENTEF, Max Planck Institute for the Structure and Dynamics of Matter — Recent theory results demonstrate a dynamical phase transition involving nonthermal magnon populations in the antiferromagnetic phase of the 2D Hubbard model upon laser driving [Walldorf et al., Phys. Rev. B 100, 121110(R) (2019)]. These results were obtained in a one loop non-interacting magnon theory. Here we present first steps towards a full interacting theory of this dynamical phase transition using a Dyson Maleev large Spin expansion and a Boltzmann formalism to investigate the effects of magnon-magnon interactions on the dynamical phase transition. The dynamical phase transition will be more completely characterized and implications for pump-probe experiments and ultrafast materials design of strongly correlated magnetism will be discussed.

*DFG Emmy Noether program SE 2558/2-1, US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering Grant No. DE SC0012375, the Flatiron Institute is a Division of the Simons Foundation, the Max Planck-New York Center for Nonequilibrium Quantum Phenomena

Coherently driven phonons coupled to antiferromagnetic order

VALENTIN KASPER, SERGI JULIA (Presenter), RAVINDRA CHHAJLANY, MACIEJ A LEWENSTEIN, ICFO — The possibility to coherently drive single phonon modes in strongly correlated materials opens the possibility to analyze and manipulate quantum matter via the electron-phonon coupling. In this work we study the effect of a single coherent phonon mode coupled to antiferromagnetic order. In particular, we calculate the dynamic spin structure factor and discuss the possibility of an emergent quasiparticle due to the coupling between phonons and magnons. Further, we explore the possibility to observe self-similar behavior in the occupation number of magnons.
10:00AM A50.00011: Refinement of exchange parameters and magnetic form factor of Mn$_3$Ir from neutron spectroscopy measurements.* MARTIN D LEBLANC, Physics and Astronomy, Memorial University of Newfoundland, ADAM ACZEL, GARRETT E GRANROTH (Presenter), Neutron Scattering Division, Oak Ridge National Laboratory, BYRON W SOUTHERN, Physics and Astronomy, University of Manitoba, STEPHEN E NAGLER, Neutron Scattering Division, Oak Ridge National Laboratory, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, JOHN P. WHITEHEAD, MARTIN PLUMER, Physics and Astronomy, Memorial University of Newfoundland — Inelastic neutron scattering measurements of the fcc kagome antiferromagnet Mn$_3$Ir were performed using the SEQUOIA spectrometer at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL). Comparison of the observed magnetic excitations to calculated spin waves, using exchange parameters derived from Density Functional Theory (DFT) calculations\(^1\), confirms that 4 exchange parameters are needed to describe the spectra. However the values from DFT underestimate the bandwidth of the excitations. Using these values as initial parameters, fits to the model modified the 2 largest exchange parameters to match the bandwidth. A spin orbit correction to the the magnetic form factor was also provided by the fit. These results are consistent with effective spin orbit coupling mentioned in\(^2\). Physically this means the magnetic moment is more extended than the free ion value.


*This work was supported by the Natural Sciences and Engineering Council of Canada, the Canada Foundation for Innovation, and Compute Canada. A portion of this research used resources at the SNS a DOE Office of Science User Facility, and the CADES cloud computing resource at ORNL.

10:12AM A50.00012: Orbital magnetization in magnetic neutron scattering HUA CHEN (Presenter), Colorado State University — Magnetic neutron scattering has been a powerful tool to reveal the microscopic magnetic structures of ordered and disordered magnetic systems. For magnetically ordered crystalline systems it has been a common practice to fit the elastic neutron cross-section to models of periodically arranged localized magnetic moments. However, it is unclear how the orbital magnetization which has an itinerant nature manifests in neutron scattering. The question is relevant to, e.g., metallic antiferromagnets and 4d/5d transition metal materials. We show that magnetic neutron scattering in general maps out the equilibrium electric current distribution inside the material but leaves the magnetization density unfixed because of a gauge freedom. We discuss the connection between the equilibrium current density and the modern theory of orbital magnetization, and provide examples on calculating the orbital contribution to elastic neutron cross-section using models and first-principles methods.
10:24AM A50.00013: Numerical evidence for a continuous phase transition between Neel and valence bond solid phases on a spin-ladder system  TAKUHIRO OGINO (Presenter), RYUI KANEKO, SATOSHI MORITA, NAOKI KAWASHIMA, Univ of Tokyo-Kashiwanoha — We investigate the possibility of deconfined quantum criticality in the J-Q-like model in one spatial dimension. As the simplest example, we study a spin-1/2 two-leg XXZ ladder with a four-spin interaction by using the Variational Uniform Matrix Product State (VUMPS), which can directly calculate physical quantities in the thermodynamic limit. We focus on the quantum phase transition between Neel and valence bond solid phases, which are characterized by breaking of SU(2) and space inversion symmetry, respectively. We find evidence for a continuous phase transition between the two phases, which is unconventional according to the Landau-Ginzburg-Wilson paradigm.

10:36AM A50.00014: Monte Carlo study of microscopic models for Néel-to-plaquette VBS transition on 2D square lattice*  JUN TAKAHASHI (Presenter), Institute of Physics, Chinese Academy of Sciences, ANDERS W SANDVIK, Boston Univ — The theory of deconfined quantum criticality (DQC) predicts an interesting connection between the Néel and the valence-bond solid (VBS) states, resulting in critical quantum phase transitions beyond the Ginzburg-Landau paradigm with emergent higher symmetry [1]. DQC with columnar VBS (CVBS) phase has been numerically confirmed in microscopic models [2]. Although there are interesting recent proposals on the possibility of the plaquette VBS (PVBS) phase behaving differently from CVBS due to the immobility of the spinons [3], there were no sign-problem free microscopic models that exhibits the Néel-PVBS transition that could be studied in detail. Here, we construct such a model, and probe the nature of the transition with quantum Monte Carlo simulations. Our results show that the transition is weakly first-order with enhanced SO(5) symmetry, similar to previous results of a system with different symmetry [4].


*A. W. S. was funded by the NSF under Grant No. DMR-1710170 and by the Simons Foundation.
10:48AM A50.00015: Terahertz 2D coherent spectroscopy of transverse field quantum Ising model with further neighbor interactions  YIHUA QIANG (Presenter), YURIY SIZYUK, Department of Physics and Astronomy, Iowa State University, THAIS VICTA TREVISAN, Ames Laboratory, PETER ORTH, Department of Physics and Astronomy, Iowa State University — Recent advances in optical experimental methods in the terahertz range made terahertz 2D coherent spectroscopy (2DCS) possible. It has been a successful tool to probe interactions in various systems ranging from biexcitons in semiconductors to magnons in magnetic insulators. Here, we report results for the nonlinear 2DCS susceptibilities in the transverse field quantum Ising model including further neighbor interactions. Using a Jordan-Wigner transformation the model can be mapped to interacting fermions, for which we compute the 2DCS spectrum in a field-theoretical Keldysh approach. Information contained in the 2DCS can be used to identify interactions among the fermions, corresponding to next-nearest neighbor spin exchange couplings in the magnetic system.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A51 DCMP: Electronic Properties of Graphene Based Twisted Heterostructures: Transport Studies

8:00AM A51.00001: Dynamic rotation of monolayer van der Walls heterostructures  JOSH SWANN (Presenter), SHAOWEN CHEN, NATHAN FINNEY, DERICK GONZALEZ-ACEVEDO, MATTHEW A YANKOWITZ, CORY DEAN, Columbia University — Emerging at a twist angle of around 1.1 degrees, the flat band dispersion of twisted bilayer graphene (tBLG) provides an exciting means of studying the physics of strongly correlated states. These strong correlations have recently been shown in a number of studies to give rise to superconducting and correlated insulating states as well as anomalous Hall effects. However, the physics of these states is highly sensitive to slight changes in the twist angle away from the so called ‘magic angle’. We report on a new technique for fabricating twisted bilayer graphene devices using an Atomic Force Microscope to control this angle with a high degree of precision. Techniques that enable monolayers to be rotated to arbitrary angles while also preventing the twist angle from relaxing to the Bernal stacking phase will be discussed.

8:12AM A51.00002: Shear phonon modes in twisted bilayer 2D crystals  SEOUNG-HUN KANG (Presenter), KISUNG CHAE, Korea Inst for Advanced Study, MIKITO KOSHINO, Department of Physics, Osaka University, YOUNG-WOO SON, Korea Inst for Advanced Study — Based on large scale first-principles computations and molecular dynamics simulations, we present variation of low energy in-plane phonon modes in twisted bilayer 2D crystals such as graphene and transition metal dichalcogenides. It is shown that the shear phonon modes soften as the twisted angle increases to 30 degrees while layer breathing modes does not. Discussions regarding on relation between the shear phonon softening, stability of quasicrystalline ordering and interlayer friction will be present.
Correlated insulating and superconducting states in twisted bilayer graphene below the magic angle

EMILIO CODECIDO (Presenter), Ohio State Univ - Columbus, QIYUE WANG, The University of Texas at Dallas, RYAN KOESTER, SHI CHE, HAIDONG TIAN, RUI LV, SON TRAN, Ohio State Univ - Columbus, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, FAN ZHANG, The University of Texas at Dallas, MARC BOCKRATH, CHUN NING LAU, Ohio State Univ - Columbus — The emergence of flat bands and correlated behaviors in “magic angle” twisted bilayer graphene (tBLG) has sparked tremendous interest, though its many aspects are under intense debate. Here we report observation of both superconductivity and the Mott-like insulating state in a tBLG device with a twist angle of ~0.93°, which is smaller than the magic angle by 15%. At an electron concentration of ±5 electrons/moiré unit cell, we observe a narrow resistance peak with an activation energy gap ~0.1 meV. This indicates additional correlated insulating state, and is consistent with theory predicting a high-energy flat band. At doping of ±12 electrons/moiré unit cell we observe resistance peaks arising from the Dirac points in the spectrum. Our results reveal that the “magic” range of tBLG is in fact larger than what is previously expected, and provide a wealth of new information to help decipher the strongly correlated phenomena observed in tBLG.

Interaction effects in ultra-clean ABC trilayer/hexagonal boron nitride moire heterostructures

TIAN XIE (Presenter), HAOXIN ZHOU, University of California, Santa Barbara, JAMES R. EHRETS II, Department of Physics, Harvard University, ERIC SPANTON, California NanoSystems Institute, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, ANDREA YOUNG, University of California, Santa Barbara — ABC-stacked trilayer graphene aligned to hexagonal boron nitride hosts narrow, isolated low energy bands which have been shown to ferromagnetism and superconductivity. In addition, these bands can be tuned with an out-of-plane electric field. The main challenge of fabricating this type of samples is the metastability of the ABC-stacking order, which tends to relax to the lower-energy ABA-stacking during the fabrication process. Here we will describe techniques to identify and isolate ABC domains in trilayer graphene and incorporate them into dual-graphite gated heterostructures while preserving the stacking order. Preliminary transport data reveals electric field tunable transitions between resistive states at partial band filling.
8:48AM A51.00005: Characterization of correlated insulating states and superconductivity in twisted bilayer graphene: Part 1*  Harpreet Arora (Presenter), Robert Polski, Watson Laboratory of Applied Physics, California Institute of Technology, Yiran Zhang, Youngjoon Choi, Department of Physics, California Institute of Technology, Hechen Ren, Watson Laboratory of Applied Physics, California Institute of Technology, Kenji Watanabe, Takashi Taniguchi, National Institute for Materials Science, Stevan Nadj-Perge, Watson Laboratory of Applied Physics, California Institute of Technology — Magic Angle Twisted Bilayer Graphene (MATBG) has emerged as an exciting platform to explore correlated insulating states and unconventional superconductivity due to its gate tunable nature. Even though several theoretical models have been proposed, the nature of the many body physics leading to these exotic states is not fully understood. Here we study correlated insulating and superconducting states for a range of angles around the magic angle value. Transport measurements as a function of carrier density, temperature and magnetic field reveal new insights in this correlated system.

*This work has been supported by the GIST-Caltech memorandum of understanding and partly by NSF CAREER program (DMR-1753306). S. N-P also acknowledges support from the IQIM (NSF funded physics frontiers center).

9:00AM A51.00006: Characterization of correlated insulating states and superconductivity in twisted bilayer graphene: Part 2*  Robert Polski (Presenter), Harpreet Arora, Watson Laboratory of Applied Physics, Caltech, Yiran Zhang, Youngjoon Choi, Physics, Caltech, Hechen Ren, Watson Laboratory of Applied Physics, Caltech, Kenji Watanabe, Takashi Taniguchi, National Institute for Materials Science, Stevan Nadj-Perge, Watson Laboratory of Applied Physics, Caltech — Near magic-angle (~1.1°) twisted bilayer graphene (TBG) has emerged as a promising system for studying electron correlations due to the wide tunability of its band structure—using twist angle—and electron/hole density through gating. However, many details on the nature of correlations and their evolution with twist angle have yet to be resolved. We report sub-Kelvin magnetotransport measurements on TBG for several angles near the magic angle, including measurements of correlated insulators and superconductivity on both hole and electron sides.

*This work has been partly supported by the NSF CAREER program (DMR-1753306) and Gist-Caltech memorandum of understanding. S. N-P also acknowledges support from the IQIM (NSF funded physics frontiers center). R. P and S. N-P also acknowledge the support of the DARPA Topological Excitations in Electronics (TEE) program.
9:12AM A51.00007: Engineering Low-Disorder Superlattice Potentials in Graphene-Based Van der Waals Heterostructures  LIAM COHEN (Presenter), ERIC SPANTON, ANDREA YOUNG, University of California, Santa Barbara, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science — Long wavelength periodic potentials have led to the observation of a variety of electronic phenomena in graphene, including the Hofstadter butterfly, fractional Chern insulators, and flat band physics at zero magnetic field. Typically, such potentials arise due to Moiré patterns generated through lattice or rotationally mismatched layers. While Moiré patterns produce high quality, low-pitch potentials, they do not allow tuning of lattice strength, symmetry, or pitch. Here we present the fabrication of sub 40nm pitch, ultra-clean, lithographically defined metal superlattices. Using bulk capacitance measurements, we show that integrating the superlattices into a multilayer heterostructures allows controllable screening of the disorder potential while preserving a finite strength superlattice potential. I will present our progress towards engineering correlated states in artificial superlattices.

9:24AM A51.00008: Transport study of transition metal dichalcogenide morié superlattices  TINGXIN LI (Presenter), LIZHONG LI, YANHAO TANG, JIACHENG ZHU, Cornell University, SONG LIU, KATAYUN BARMAK, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, JIE SHAN, KIN FAI MAK, Cornell University — Morié superlattices formed in van der Waals materials have emerged as a new platform to explore strongly correlated physics and other emergent phenomena in two-dimensional electronic systems. Superconductivity, correlated insulating states, and ferromagnetism have recently been discovered in the twisted bilayer graphene and ABC trilayer graphene/boron nitride systems. In contrast to the graphene systems, in which spin, valley, and layer degeneracies are all present, the spin and layer degeneracies are lifted in semiconducting transition metal dichalcogenide (TMD) heterobilayers by strong spin-orbital interactions and layer asymmetry. The large band mass and band gap of the TMDs also allow the flat bands to be present for a large range of twist angle. In this talk, we will present a transport study of angle aligned WSe$_2$/WS$_2$ bilayers and discuss properties of the observed correlated insulating states at half filling (i.e. one particle per morié site).

9:36AM A51.00009: High sensitivity thermodynamic measurements of fractional quantum Hall states in graphene  FANGYUAN YANG (Presenter), ALEXANDER A ZIBROV, RUIHENG BAI, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, ANDREA YOUNG, University of California, Santa Barbara — Thermodynamic quantities such as chemical potential and entropy provide information about many-body ground states that cannot be directly revealed by conventional transport measurements. In this talk, I will present a technique for high sensitivity measurement of the chemical potential in ultra-clean graphene heterostructures, based on a multilayer heterostructure with an embedded graphene layer that functions as an electrometer. An integrated on-chip heater further allows rapid modulation of the temperature, from which we extract the entropy per particle, $\Delta S/\Delta N = -\Delta \mu/\Delta T$. We apply this technique to a high mobility monolayer graphene 2D electron gas at high magnetic fields, measuring the chemical potential and entropy of fractional quantum Hall states in $N = 0$ and $N = 1$ Landau levels (LLs) and electron solid states in the $N = 2$ and N=3 Landau levels. We compare our experimental sensitivity with that required to detect the ground state entropy associated with non-Abelian anyons, as are thought to appear at several filling factors in bilayer graphene.
**9:48AM A51.00010: Van der Waals Force Driven Ultrahigh-Density Piezoelectric Nano-Generators Arrays**  
YUHANG JIANG (Presenter), JINHAI MAO, University of Chinese Academy of Sciences, COLIN ROBERT WOODS, School of Physics & Astronomy, University of Manchester, SLAVISA MILOVANOVIC, FRANCOIS M PEETERS, Departement Fysica, University of Antwerp, KONSTANTIN S NOVOSELOV, School of Physics & Astronomy, University of Manchester, EVA ANDREI, Department of Physics and Astronomy, Rutgers University — The elegance of Van der Waals heterostructure emerges as the possibilities to design its function on-demand when choosing different functional materials. When two layers materials are taken to form moire lattice, the Van der Waals force between the two layers could stimulate even more fascinating features forming spontaneously. Here we show, when graphene and single layer BN (SLBN) are minimally twisted superposed, the interlayer interactions propel the two lattices rearrangement and induces a spatial modulated strain configuration. The moire pattern reconciled strain superlattice in single layer BN, companied by its inversion symmetry broken, induces an oscillating charge polarization as revealed by the scanning tunneling microscope. This moire pattern driven charge polarization in SLBN allows us to get a highly ordered nano-generators array with a giant density.

*DOE-FG02-99ER45742 , NSF-DMR 1708158

**10:00AM A51.00011: Tunable extra Dirac points in one-dimensional graphene superlattice induced by periodic ferroelectric domains**  
TIANLIN LI (Presenter), HANYING CHEN, KUN WANG, YIFEI HAO, LE ZHANG, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln — In this work, we investigate the transport signature of one-dimensional superlattice (SL) in monolayer graphene induced by pre-patterned periodic domains in an interfacial ferroelectric bottom layer. We work with 50 nm single crystalline ferroelectric Pb(Zr,Ti)O$_3$ (PZT) films deposited on (La,Sr)MnO$_3$ buffered SrTiO$_3$ substrates, and create periodic polarization up (P$_{up}$) and down (P$_{down}$) stripe domains on PZT using conductive atomic force microscopy. The domain periodicity varies from 200 nm to 300 nm, and the number of periods changes from 60 to 100. We then transfer hBN-graphene stacks onto the pre-patterned domains and fabricate them into top-gated field-effect devices. The difference in carrier density between the two polarization regions reaches around 3$\times$10$^{13}$ cm$^{-2}$ at 2 K due to the pyroelectric effect. We observe extra Dirac points in R(V$_g$) by applying voltage to the hBN top gate, which is attributed to the SL modification of the band structure. We discuss the effects of the SL period and the width ratio between the P$_{up}$ and P$_{down}$ domains on the position of the extra Dirac points, and the magnetotransport properties of these SLs.

*This work was primarily supported by the U.S. Department of Energy, BES, under Award No. DE-SC0016153.
Contact electrodes with high workfunctions can enable significant enhancement in optoelectronic device performance due to their important role in efficient extracting/injecting carriers especially from optically active materials. With such materials becoming increasingly important in emerging solar cell technologies, the need for high workfunction electrodes has become of timely importance. In this work, p-doped graphene is investigated using first principles calculations, as a potential high workfunction contact electrode material for device applications. We found that chemical doping based on the adsorption of different non-metallic adatoms on graphene allows tuning the workfunction which can reach as high as 5.76 eV due to charge transfer from the graphene to the p-dopants. Therefore, our results are necessary to bring out the capabilities graphene-based electrodes.

*Thanks, Qatar National Research Foundation for the support Grant No.NPRP X-107-1-027.
Heat transfer in nanostructures is of fundamental and practical interest. Sufficient cooling is critical for the operation of superconducting nanowire single-photon detectors (SNSPDs), which can support large current densities (~5 MA/cm²) just prior to being switched into a high resistivity (~250 μΩ·cm) normal state by an incident photon, leading to substantial local heating. The thermal boundary conductance (TBC) between the nanowire and the substrate determines the cooling rate, and hence the reset time, and potentially impacts the quantum efficiency of SNSPDs. Despite the TBC’s importance, open questions remain about its correct description in few-nm thick films, and little experimental data exists on patterned nanowire devices.

Here, we show that simple DC electrical measurements can be used to estimate the TBC between the nanowire and the substrate. Our results suggest that the heat transfer from these devices is well-described by phonon black-body radiation into the substrate, with a phonon-emissivity that depends on the acoustic properties of the wire and substrate. Calculations using the acoustic mismatch model assuming two semi-infinite elastic media match the phonon-emissivity extracted from measurements. One-dimensional numerical simulations validate our approach.
**10:36AM A51.00014: Conductance quantization in cleaved edge overgrowth GaAs quantum wires**

HENOK WELDEYESUS (Presenter), TARAS PATLATIUK, CHRISTIAN SCHELLER, Department of Physics, University of Basel, CH-4056, Basel, Switzerland, GILAD BARAK, AMIR YACOBY, Department of Physics, Harvard University, Cambridge, MA, 02138, USA, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, Princeton, NJ, 08544, USA, DOMINIK ZUMBUHL, Department of Physics, University of Basel, CH-4056, Basel, Switzerland —

Cleaved Edge Overgrowth (CEO) quantum wires (QW) are among the cleanest 1D systems available, showing conductance quantization and Luttinger liquid effects such as charge fractionalization and spin-charge separation. Previously, we have studied the conductance quantization of CEO QWs as a function of temperature in Scheller et al. PRL112, 066801 (2014), finding that the first wire plateau goes from \(2 \frac{e^2}{h}\) at high \(T > 10K\) to \(1 \frac{e^2}{h}\) at low \(T < 0.1K\). This was interpreted as evidence for a nuclear spin helix, as proposed theoretically by Braunecker, Simon and Loss PRB80, 165119 (2009).

Here, we look at the dependence on wire length, and observe a steeper slope over increasing temperatures in short 2 μm wires compared to 6 μm wires. This is consistent with theory from Aseev et al. PRBB95, 125440 (2017) and may allow an estimate of the Luttinger charge interaction parameter.

Further, we report on the velocities of quantum Hall edge states measured on the same CEO sample using momentum resolved tunneling spectroscopy. Using a multi terminal measurement of the voltage drop, the velocities agree very well with theory. In the future, fractional and topological edge states could be studied with this technique.

*Supported by Swiss NSF, Swiss Nano Institute, and European Microkelvin Platform*

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**10:48AM A51.00015: Emergence of dynamical energy gap in an oscillating graphene membrane**

NANCY SANDLER (Presenter), Ohio University, DAWEI ZHAI, The University of Hong Kong —

One intriguing aspect of graphene is the effect of strain on its electronic properties, which manifests as a pseudo-magnetic field producing peculiar local charge distributions and Landau level-like flat bands. It is challenging however, to generate global energy gaps for semiconductor applications- the strain needed is either too large or requires precise engineering. Irradiation with polarized light has been proposed as a mechanism for gap generation, but the high frequency and intensity needed may induce sample damage. Oscillating mechanical deformations appear like an alternative that is particularly well suited for suspended samples. Besides, spatial strain variation allows more flexibility in gap engineering. We study the effect of a Gaussian-shaped deformation in graphene with a time-periodic amplitude. Using an effective Floquet Hamiltonian, we predict the appearance of anisotropic dynamical gaps with Green's function methods and degenerate perturbation theory. The profile of the gap closely follows the modulations in the local density of states caused by strain. We find that the optimal regime for gap generation occurs when a deformation extends over the whole sample, with a magnitude determined by its geometrical parameters.

*This work is supported by NSF (DMR-1508325).*
Monday, March 2, 2020 8:00 AM - 10:36 AM

Session A52 DCMP: Surface Adsorption, Dynamics, and Defects Mile High Ballroom 1E - Daniel Dougherty, North Carolina State University

8:00AM A52.00001: Quantitative measurements of total yields from electron stimulated desorption of ice  BRIAN FERRARI (Presenter), KATERINA SLAVICINSKA, CHRIS BENNETT, Univ of Central Florida — Sputtering yields from electron stimulated desorption (ESD) are typically neglected by planetary science models, although mid-energy (200-1000eV) electrons can produce significant sputtering yields. Here, we investigated the total and relative yields from ESD on comet ice analogs in an Ultra-High Vacuum (UHV) chamber with base pressure of 3x10^{-11} torr. Gas was introduced to the chamber, then condensed on a sample holder, which was then irradiated with an electron source at various energies. A quartz-crystal microbalance (QCM) was used for precise mass desorption measurements, while a quadrupole mass spectrometer (QMS) was used to measure the positive, negative and neutral species that desorbed off the ice. These processes are relevant for various planetary science environments which are subjected to high intensity of electron bombardment, such as the rings of Saturn, Icy Moons, and interstellar ices. The results of our experiments will provide more accurate yields for modeling sputtering from airless bodies.

8:12AM A52.00002: Investigation of atomic layer deposited amorphous alumina films for the prevention of water-based corrosion of glass  MIRIAM ELISABETH HIEBERT, ETHAN HYDE, MSE, University of Maryland, College Park, EDWARD P VICENZI, Museum Conservation Institute, Smithsonian Institution, JAMIE WEAVER, NCNR, NIST, RAYMOND PHANEUF (Presenter), MSE, University of Maryland, College Park — Water is corrosive to a wide range of materials, including silicate glasses, for which contact results in an exchange of modifier ions for protons, swelling of the altered glass, and eventually crack network evolution leading to mechanical failure; this process is referred to commonly as “glass disease”. Atomic layer deposition (ALD) of metal oxide thin films provides a seemingly near-ideal approach toward the protection of silicate glass from water-based corrosion, combining optical, transparency, and potentially high resistance to permeation by water. In this talk I’ll discuss the results of accelerated aging experiments in which ALD alumina-coated silicate glass is immersed in water at elevated temperatures and the rate of ion leaching into the water is monitored as a function of time. We find the application of such films to be capable of slowing water-mediated corrosion by at least an order of magnitude. Finally, I’ll discuss the role of film defects that limit the effectiveness of ALD alumina in preventer water-based corrosion.

*Work supported by a Big Ten Academic Alliance Smithsonian Fellowship and a UM/SI Seed Grant
8:24AM A52.00003: Tuning single-atom electron spin resonance in a vector-magnetic field*
PHILIP WILLKE, APARAJITA SINGA, XUE ZHANG, TANER ESAT, Center for Quantum Nanoscience, Institute for Basic Science, CHRISTOPHER LUTZ, IBM Almaden Research Center, ANDREAS J HEINRICH, TAEYOUNG CHOI (Presenter), Center for Quantum Nanoscience, Institute for Basic Science — Scanning tunneling microscopy (STM) has been one of highly versatile surface science tools to investigate electronic and magnetic properties of individual atoms and molecules on surfaces. Recently, successful combination of electron spin resonance (ESR) technique and STM has demonstrated electron spin of individual atoms on ultrathin insulating MgO films can be coherently driven. Utilizing a 2D vector magnetic field and the local stray field from the magnetic STM tip, we optimize the ESR signal and characterize the role of the tip field. We demonstrate single atom ESR using the tip-field only, under zero external magnetic field, which promises to make this technique available in many existing STM systems.

*We acknowledge support from the Institute for Basic Science under grant IBS-R027-D1 and Ewha Womans University.

8:36AM A52.00004: Reactive MD simulation on the formation of amorphous sub-nano alumina layer* YUXUAN LU (Presenter), DEVON ROMINE, Missouri State Univ, JAGARAN ACHARYA, JUDY WU, University of Kansas, RIDWAN SAKIDJA, Missouri State Univ — In this study, we systematically performed the large-scale classical reactive molecular dynamics (MD) simulations of Atomic Layer Deposition (ALD) processes to model the formation of amorphous alumina sub-nanolayer water. The ALD process used water and (Trimethyl-Aluminum) TMA precursors deposited onto the surface of an aluminum wetting layer. We varied the sizes of the substrate and the concentrations of water/hydroxide precursors with a range of temperature to design the most favorable configurations for the subsequent TMA precursors to add onto. The role of crystallographic orientation of the Al wetting layer was also investigated and compared with the experimental findings.

*The support from NSF (Grant No. 1809284) “Collaborative Research: Development of Atomically Thin Tunnel Barriers for High-Performance Tunnel Junctions” from the Electronics, Photonics and Magnetic Devices (EPMD) Program is gratefully acknowledged.
8:48AM A52.00005: Quantum-well states and electronic coherence in bimetallic Pb/Ag thin films  
CHI-RUEI PAN, Georgia Institute of Technology, WOOJOO LEE, CHIH-KANG SHIH, University of Texas at Austin, MEI-YIN CHOU (Presenter), Academia Sinica — It has been well established that the presence of quantum-well states in metal thin films plays an essential role in determining the thickness dependence of many physical properties. Here we present first-principles calculations and measurements by angle-resolved photoemission spectroscopy for electronic states in a bimetallic film composed of 10 layers of Pb and 9 layers of Ag in the (111) direction on a Si substrate. It is found that the original quantum-well states in individual Pb and Ag films evolve into new states in the bimetallic film by extending into the additional space, instead of directly coupling with each other as one would have expected. The new set of quantum-well states therefore have modified effective masses and energy values compared with the parent ones. Even though the Pb/Ag interface is incommensurate, the coherence of the electronic states across the whole bimetallic film is verified by supercell configurations with different rotational arrangements in the calculation. The excellent agreement between theory and experiment in the energy dispersion of the quantum-well states confirms the physical picture proposed in this work, which could form the basis in exploring the electronic structure in multiple stacked thin films.

9:00AM A52.00006: Investigation of oxidation mechanisms of Pt nanoparticles in water – a molecular dynamics study  
KARIM GADELRAH (Presenter), NATHAN CRAIG, Research and Technology Center, Robert Bosch LLC — Platinum oxide (PtO) formation has a direct link to nanoparticle passivation as well as Pt dissolution in proton exchange membrane fuel cells (PEMFCs). During potential sweep, place exchange mechanism between Pt and O atoms is first triggered followed by irreversible Pt surface roughening at high potential. In this work, we employ molecular dynamics (MD) to capture atomic level processes of Pt extraction by O atoms from Pt(111) surface. As a benchmarking system, we correlate oxygen coverage with the onset of different Pt surface evolution mechanisms in the presence of water. Local O coordination of Pt atoms, concurrent Pt extraction, and generation of surface vacancies are major factors shaping the final surface structure. In addition, the MD simulation is employed to investigate the oxidation process of Pt nanoparticles. Our results show that in addition to PtO formation on faceted surfaces, Pt atoms desorption into water is a strong function of oxygen coverage. This is particularly true for under-coordinated atoms at edges and corners. The atomistic details described by the MD setup provides valuable insights into Pt-O interaction and stability of Pt nanoparticles in a complex environment.
9:12AM A52.00007: Atomic Defects of the Hydrogen-Terminated Silicon Surface Imaged with nc-AFM  JEREMIAH CROSHAW (Presenter), THOMAS DIENEL, TALEANA R HUFF, ROBERT A WOLKOW, Univ of Alberta — The hydrogen-terminated silicon (H:Si) surface has been shown to be a viable candidate for the development of atom-scale devices\textsuperscript{1,2}; however, the creation of such devices is currently limited by the need for constant user-guided interaction during the fabrication process. Attempts to automate fabrication using deep learning successfully demonstrated the training of a neural network which was able to identify common defects\textsuperscript{3}. Building upon these recent works we present our efforts at creating a comprehensive catalog containing many of the commonly found defects of the H:Si-100(2x1) surface. By imaging the defects using different imaging parameters in STM and two different tip contrasts in non-contact AFM\textsuperscript{4}, we determine the structures of the defects, their likely origins and potential removal, and a path to improved accuracy for their automated detection. A deeper understanding will enable the creation of better defect-free samples for atomic fabrication.


9:24AM A52.00008: A first-principles study of the physical properties and secondary electron emission of 4d and 5d FCC metal surfaces with and without a vacancy defect* LEOPOLDO DIAZ III (Presenter), MAHDI SANATI, Department of Physics and Astronomy, Texas Tech University, RAVINDRA P JOSHI, Department of Electrical and Computer Engineering, Texas Tech University — In this study we have introduced a vacancy defect to the 100, 110, 111 surfaces of the 4d and 5d FCC metals to understand the impact the defect will have on their physical properties and secondary electron emission. We have used density functional theory (DFT) to calculate the formation energy (FE), the work function (WF), and the dielectric constant for each metal surface. To ensure accuracy, the calculations were performed using both the local density approximation (LDA) and the generalized gradient approximation (GGA) exchange correlation functionals. For all the FCC metals we have identified the following trend for the vacancy FE and the WF: $\varphi_{111} > \varphi_{100} > \varphi_{110}$ for surfaces with and without a vacancy. We have also calculated the Q-factor for each of the metals allowing for predictions to be made about the secondary electron yield expected by each metal, including which metal would be best for vacuum or near-vacuum devices.

*This research was supported in part by a Department of Defense MURI. Also supported through grants from the Office of Naval Research (ONR) and the Air Force Office of Scientific Research.
Probing non-equilibrium dynamics of photoexcited polarons on a metal oxide surface with atomic precision

CHAOYU GUO, Xiangzhi Meng, Physics, Peking University, Huixia Fu, Physics, Chinese Academy of Sciences, Qin Wang (Presenter), Physics, Peking University, Sheng Meng, Physics, Chinese Academy of Sciences, Ying Jiang, Physics, Peking University — Understanding the non-equilibrium dynamics of photoexcited polarons at atomic scale is of great importance for improving the performance of photocatalytic and solar-energy materials, but remains a grand challenge in experiment so far. Using a pulsed-laser-combined scanning tunneling microscopy and spectroscopy, we succeeded to resolve the photoexcitation and recovery dynamics of single polarons bound to oxygen vacancies on a prototypical photocatalyst, rutile TiO$_2$(110). The visible-light excitation of the defect-derived polarons leads to depletion of the polaron states and delocalized free electrons in conduction band. We found that the formation time of polarons becomes considerably shorter when the polaron is bound to two surface oxygen vacancies than that to one. In contrast, the lifetime of photogenerated free electrons is insensitive to the atomic-scale distribution of the defects but correlated with the averaged defect density within a nanometer-sized area. The results shed new lights on the photocatalytically active sites at the metal oxides surface.

TDDFT approach on laser field enhancement by carbon nanotube and photo-decomposition of water

Hong Zhang (Presenter), Physics, Sichuan University, China — In this presentation, we discuss field enhancement of femtosecond laser by carbon nanotubes and application to accelerating water photo-decomposition. The real-time time-dependent density functional theory (TDDFT) was employed for simulating water photo-decomposition near (8,0) semiconducting carbon nanotube. A short pulse with full-width of half-maximum 10fs was considered. When optical field is perpendicular to the tube axis, we found significant laser field enhancement corresponding to laser-power enhancement by factor 2 with laser wavelength 800 nm, and by factor around 8 with wavelength 400 nm. The enhancement is due to polarizability and wall-curvature of carbon nanotube that helps to reduce threshold power for photo-decomposition of water.

*H.Z. acknowledges the National Natural Science Foundation of China (Grants No. 11974253). and the financial support from the National Key R&D Program of China (2017YFA0303600)
The dissociative adsorption of O₂ on the bimetallic Pd₃M₂ clusters (M=Ag, Au, Co, Cu, Mn, Ni, Pt, and Ru) by density functional theory

NUSAIBA ZAMAN (Presenter), ABDELKADER KARA, Univ of Central Florida — We use density functional theory to systematically investigate the adsorption and reactivity of oxygen on the bimetallic Pd₃M₂ clusters (M = Ag, Au, Co, Cu, Mn, Ni, Pt, and Ru). This is because small bimetallic clusters with high surface area to volume ratio often offer higher stability, greater selectivity and sometimes superior activity than the pure metal counterparts. We explore different adsorption sites for molecular oxygen, which can be oriented in a vertical or horizontal direction with respect to the cluster, as well as atomic oxygen on these bimetallic Pd₃M₂ clusters. The reaction path for dissociation of oxygen molecule on these bimetallic clusters is studied using the nudge elastic band method. We will present our result for the calculated energy barriers for O₂ dissociation on these bimetallic clusters and how it changes depending on the composition of the bimetallic clusters. Moreover, we will present the effect of O₂ adsorption on the electronic properties of these Pd₃M₂ clusters. Bader charge analysis is performed to probe how the charges are transferred between the molecule and the clusters.

Partial support is provided from the U.S. Department of Energy Basic Energy Science under Award number DE-SC0007045. We used computational resources of NERSC and UCF-Stokes.

Impact of solvation on the structure and reactivity of the Co₃O₄(001)/H₂O interface: a molecular dynamics study.

STEPHANE KENMOE (Presenter), TIM KOX, ECKHARD SPHR, Univ Duisburg — The spinel Co₃O₄ has many beneficial properties of potential use in catalysis. In operando, water is always present and alters the properties of the catalysts. To improve these properties and allow a rational design of catalysts, a fundamental understanding of the active crystal facets and their reactivity upon water adsorption is essential. We use ab initio molecular dynamics to understand the effect of water, aqueous solutions and solvation on the structure and reactivity of the Co₃O₄(001) surface.

Confined Catalysis under 2D silica: A CO Oxidation Study

CALLEY EADS (Presenter), J. ANIBAL BOSCOBOINIK, ASHLEY HEAD, DARIO STACCHIOLA, SAMUEL TENNEY, Brookhaven National Laboratory — Open metal surfaces play an active role in heterogeneous catalysis reactions such as the prolific CO oxidation reaction to produce CO₂. The addition of a nanostructured film on the metal surface changes the reaction kinetics and dynamics due to confinement effects under the cover. We illustrate the role of porous 2D silica grown on Pd(111) in the model reaction of CO oxidation at the interface of palladium and silica using in situ infrared reflection-absorption spectroscopy (IRRAS), mass spectroscopy (MS) and ambient pressure X-ray photoelectron spectroscopy (APXPS). Our findings suggest that 2D silica more effectively converts CO and O₂ to CO₂ under industrially-relevant conditions than the bare Pd(111) alone. 2D confinement effects enhance CO₂ production even with less CO bound species involved in the reaction.
**A52.00014: Probing two-dimensional ices with scanning probe microscopy**

YE TIAN (Presenter), RUNZE MA, DUANYUN CAO, International Center for Quantum Materials, School of Physics, Peking University, CHONGQIN ZHU, Department of Chemistry and Department of Chemical & Biomolecular Engineering and Department of Mechanical & Materials Engineering, University of Nebraska-Lincoln, Lincoln, N, JINBO PENG, JING GUO, International Center for Quantum Materials, School of Physics, Peking University, JI CHEN, XIN-ZHENG LI, School of Physics, Peking University, Beijing 100871, P. R. China, JOSEPH S FRANCISCO, Department of Earth and Environmental Sciences, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA, XIAO CHENG ZENG, Department of Chemistry and Department of Chemical & Biomolecular Engineering and Department of Mechanical & Materials Engineering, University of Nebraska-Lincoln, Lincoln, N, LIMEI XU, International Center for Quantum Materials, School of Physics, Peking University, ENGE WANG, University of Chinese Academy of Sciences, Beijing 100190, P. R. China, CAS Center for Excellence in Topological Quantum Computation, YING JIANG, International Center for Quantum Materials, School of Physics, Peking University — Two-dimensional (2D) water/ices are responsible for a broad spectrum of phenomena in materials science, chemistry, and biology. Particularly, the edges of 2D ice play key roles in the ice growth, melting and catalytic reaction, but atomic-scale structural characterization still remains a big challenge due to the fragileness and high reactivity of the ice edges. Here we report atomic-scale imaging of the edge structures of a 2D bilayer ice grown on Au(111) surface with weakly perturbative non-contact atomic force microscopy (1, 2). We found a new type of edge, aligning along the armchair direction but reconstructed with 5756-member rings, coexisting with the zigzag edge commonly observed in two-dimensional hexagonal crystals. We were further able to deduce different growth behaviors for the zigzag and armchair edges from the frozen metastable structures at the two edges. In addition, we explore the impact of alkali metal ions on the structure of 2D ice. By changing the concentration of alkali metal ions, various new ice phases can be obtained. Those results reveal new understanding of the stability and growth of 2D ices.

*This work was supported by the National Key R&D Program under Grant No. 2017YFA0205003, the National Natural Science Foundation of China under Grant No. 11634001.

**Monday, March 2, 2020 8:00 AM - 11:00 AM**

**Session A53 DMP DCOMP: 2D Semiconductors: Transport and Devices**

Mile High Ballroom 1F - Xia Hong, University of Nebraska-Lincoln - Tag(s): Focus
8:00AM A53.00001: Electron-hole liquid in a van der Waals heterostructure photocell at room temperature [Invited] NATHANIEL GABOR (Presenter), TREVOR ARP, DENNIS PLESKOT, VIVEK AJI, University of California, Riverside — Condensation - the familiar process underlying the formation of clouds and the distillation of ethyl alcohol into whiskey - is the phase transition of gas into liquid droplets. In semiconductors, at sufficiently high electron-hole (e-h) densities or low temperatures, the gas of non-equilibrium electrons and holes may undergo condensation into one of several potential liquid-like phases. In this talk, I present recent results on the gas-to-liquid phase transition of electrons and holes in ultrathin van der Waals heterostructure photocells revealed through multi-parameter dynamic photoresponse microscopy (MPDPM). By combining rich visualization with comprehensive analysis of very large data sets acquired through MPDPM, we find that ultrafast laser excitation at a graphene-molybdenum ditelluride-graphene interface leads to the abrupt formation of ring-like spatial patterns in the photocurrent response as a function of increasing optical power. These patterns, together with extreme sublinear power dependence and picosecond-scale photocurrent dynamics, provide strong evidence for the formation of a two-dimensional e-h liquid. While our imaging experiments mark the first observation (in over 50 years of study) of an e-h liquid at room temperature, I will discuss our results within the greater context of strongly correlated electronic condensates.

8:36AM A53.00002: Intrinsic disorder effects on device performance of few-layer MoS₂ field-effect transistors* HAO-WEI TU, CHE-CHI SHIH, CHIN-LUNG LIN, JIAN-JHONG LAI, WEN-BIN JIAN (Presenter), CHENMING HU, Natl Chiao Tung Univ — Field-effect transistors (FETs) made by two dimensional (2D) materials attract attention because of high on-off ratios and negligible short-channel effects. The 2D material of MoS₂ has been studied for years while problems from contact, interface, and structural disorders have not been solved. There are a lot of reports to give a wide range of electron mobility and the best performance of a single-layer MoS2 FET is still in debate. We present a large variation of disorders in MoS₂ flakes exfoliated from the same bulk. The disorder dominate the low performance of FETs. In particular, for high performance devices, the mobility increases with decreasing temperature and the device reveals metallic behaviors. Setting the FET in an on state, the conductivity of high-performance devices is close to e²/h, giving a standard to check the quality. There are some disorders resulting in a large decrease in conductance as well as in the FET mobility. On the other hand, the subthreshold swings are independent from the mobility. The disorder effects dominate to low performance thus growth of perfect 2D crystals is essential for the application of 2D FETs.

*This work was supported by the Ministry of Science and Technology, Taiwan.
8:48AM A53.00003: Control of valley-polarized exciton currents in 2D heterostructures*

ALBERTO CIARROCCHI (Presenter), DMITRII UNUCHEK, AHMET AVSAR, ZHE SUN, Ecole Polytechnique Federale de Lausanne, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ANDRAS KIS, Ecole Polytechnique Federale de Lausanne — Valleytronics is an alternative to charge-based electronics aiming at encoding data in the valley degree of freedom, which could enable new paradigms for computing devices. Transition metal dichalcogenides (TMDCs) are an ideal platform for this due to the combination of unique spin-valley physics and direct bandgap, allowing optical initialization and readout of the valley state. Recent developments in the control of interlayer excitons in heterostructures of these materials offer an effective way to realize valley-optoelectronic devices [1]. Here, we show the generation and transport over mesoscopic distances of valley-polarized excitons in a device based on a type-II TMDC heterostructure. Engineering of the interlayer coupling results in enhanced diffusion of valley-polarized excitons, which can be controlled and switched electrically [2]. Furthermore, using electrostatic traps we can increase the exciton concentration by an order of magnitude, reaching densities higher than $10^{12} \text{ cm}^{-2}$, a promising approach to obtain coherent quantum states of excitons.


*Swiss National Science Foundation, H2020 European Research Council and Marie Curie-Sklodowska-Curie Action

9:00AM A53.00004: Frequency Stability of MoS$_2$ drum resonators at Room Temperature*

NISHTA ARORA (Presenter), AKSHAY NAIK, Indian Institute of Science — Nanomechanical resonators hold great promise for ultrasensitive mass and force sensing. The discovery of two-dimensional (2D) materials having ultralow mass and exceptional mechanical properties have made them an ideal choice for NEMS. 2D resonators tend to be a great platform for sensing applications since the minimum detectable mass is proportional to mass of the resonator itself. The limit of detection is also, directly dependent on the measurement uncertainty of resonant frequency ($\delta f/f$). Thus, frequency stability is an important performance metric for such resonators. We report frequency stability at room temperature on MoS$_2$ drum resonators. The Allan deviation (AD) was observed to be of the order of $10^{-5}$ at 150ms integration time for 24V VgDC and AC drive of 70mV. This corresponds to a mass sensitivity of few attograms. We observe that increasing VgAC leads to more improvement in AD as compared to that of VgDC drive. This is due to an enhanced signal to noise ratio. We estimate various types of noise associated with MoS$_2$ resonator. This work holds promise for ultrasensitive sensing and realizing ultrastable oscillators from 2D materials.

*We acknowledge NNfC and MNCF at CeNSE, IISc, Bengaluru. N.A. acknowledges fellowship support under Visvesvaraya Ph.D. Scheme, MeitY, India.
9:12AM A53.00005: Probing anisotropic transport in atomically thin ReS$_2$ via ferroelectric domain controlled nanowire patterning*  
DAWEI LI (Presenter), SHUO SUN, ZHIYONG XIAO, JINGFENG SONG, DING-FU SHAO, EVGENY Y TSYMBAL, STEPHEN P DUCHARME, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln — The layered van der Waals material ReS$_2$ exhibits highly anisotropic band structure in the 1T' phase. In this work, we probe the effect of the band anisotropy on the transport properties of single- and few-layer ReS$_2$ via ferroelectric field effect combined with ferroelectric domain patterning. We fabricated mechanically exfoliated ReS$_2$ flakes into two-point transistor devices sandwiched between a SiO$_2$/Si back gate and a ferroelectric polymer PVDF-TrFE thin film top layer. The polarization of PVDF was then controlled at the nanoscale using conductive atomic force microscopy. By uniformly polarizing the ferroelectric top layer into the up ($P_{up}$) and down ($P_{down}$) directions, we induced up to $10^5$ current switching in bilayer ReS$_2$ channel at 300 K. We then polarized the entire channel into the insulating state, and created a nanoscale line-domain across the channel, leading to a conductive nanowire. By creating nanowires at different orientations, we mapped out the angular dependence of ReS$_2$ conductivity, which reveals more than one order of magnitude difference between the directions along and perpendicular to the $b$-axis. We compared the results with DFT calculated band structure of ReS$_2$.

*This work was primarily supported by the DOE, BES, under Award No. DE-SC0016153.

9:24AM A53.00006: Electronic transport in two-dimensional MXenes for energy storage*  
NESRINE BOUSSADOUNE (Presenter), OLIVIER NADEAU, GABRIEL ANTONIUS, Hydrogen Research Institute, Université du Québec à Trois-Rivières — MXenes are a large family of two-dimensional transition metal carbides and carbonitrides, which is attracting great research attention in the energy storage devices, including supercapacitor, due to their excellent electrical conductivity. In order to assist the design of supercapacitor electrodes based on these materials, we study the electronic conductivity of selected MXenes from first principles, and we aim to understand how their conductivity depends on their chemical composition and surface termination. We use the Abinit software to perform first-principles calculations. First, the total energy, the electronic band structure and the density of state (DOS) are investigated using density functional theory (DFT). Second, we employed density functional perturbation theory (DFPT) to obtain the phonon band structure and electron-phonon coupling. Finally, we solve the linearized Boltzmann equation in order to obtain the phonon-limited electronic mobility. We will show preliminary results for Ti$_3$C$_2$F$_2$ and Ti$_3$C$_2$(OH)$_2$.

*We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC), [funding reference numbers RGPIN-2019-07149 and DGECR-2019-00008], and from UQTR. The computational resources were provided by Calcul Québec and Compute Canada.
9:36AM A53.00007: Anisotropic carrier transport of black phosphorus encapsulated by h-BN*  MYEONGJIN LEE (Presenter), WON JONG YOO, Sungkyunkwan Univ — Anisotropic two-dimensional (2D) materials are promising candidates for novel electronics and optoelectronics because in-plane anisotropy in 2D materials can be used for polarization controlled infrared sensors, directionally controlled heat dissipators, and the angle control between adjacent 2D layered materials. Black phosphorus (BP), one of the anisotropic 2D materials, is known to have strong p-type in-plane anisotropic properties [1]. But, researches of anisotropic properties of BP in the tightly controlled fabrication environment and device structure are still elusive. Here, we report the anisotropic electrical properties of the BP field effect transistor (FET) by precisely aligning the FET channel along its pre-determined in-plane directions. Using angle-resolved polarized Raman spectroscopy (ARPR), we were able to identify BP into zigzag (ZZ) and armchair (AC) directions. Field effect mobility and resistances of AC direction was found to be better than that of ZZ direction at room and low temperature respectively.

*This work was supported by the Global Research Laboratory (GRL) Program (2016K1A1A2912707) and Global Frontier R&D Program (2013M3A6B1078873), both funded by the Ministry of Science, ICT & Future Planning via the National Research Foundation of Korea (NRF).

9:48AM A53.00008: Characterization of the metal/MoS₂ top contact based on first-principles quantum transport calculations  TAE HYUNG KIM (Presenter), YONG-HOON KIM, School of electrical engineering, KAIST, MYUNG HO BAE, KRISS — We have recently reported the experimental achievement of Ohmic van der Waals (vdW) contacts at the indium (In)/MoS₂ devices thorough a novel thermal evaporation process, and based on the combined density functional theory and matrix Green's function calculations concluded that the nature of the ideal Ohmic contact is characterized by the abrupt and rigid shift of TMDC bands across the In/MoS₂ interface (i.e. no band bending) together with the formation of metal-induced gap states (MIGS) [1]. In this work, we extend the analysis by considering four other metal species, Ag, Au, Sc, and Pd. Systematically considering how the electrode contact-region MoS₂ electronic structure develops into that of the channel region in different metal cases, we conclude that the identification of MIGS (rather than band bending) as the main determining factor for the clean metal/MoS₂ contacts is generally valid irrespective of the differences in the metal work function and wettability.

**10:00AM A53.00009: Photo-Induced Anomalous Hall Effect in 2D Transition-Metal Dichalcogenide**  
*PHUONG NGUYEN (Presenter), WANG KONG TSE, Department of Physics and Astronomy, University of Alabama, Tuscaloosa — Illumination of a circularly polarized a.c. pump field induces a valley polarization in two-dimensional transition metal dichalcogenides (TMDs), which results in an anomalous Hall voltage in response to a d.c. bias. In this work, we develop a theory for this photovoltaic valley-resolved anomalous Hall effect in undoped TMDs. A quantum kinetic equation is used to study the non-equilibrium carrier populations and time-averaged transport currents under the simultaneous influence of the strong a.c pump field and the weak d.c probe field. Our results for the photo-induced longitudinal and Hall conductivities show strong resonant features when the pump field frequency reaches the spin-split band-to-band transition energies.

*This work was supported by the US Department of Energy, Office of Science, Basic Energy Sciences under Early Career Award No. DE-SC0019326 and by the Research Grants Committee funds from the University of Alabama.

**10:12AM A53.00010: Density-functional prediction of a strong Orbital Hall effect in the monolayer WX2 (X = Te, S)**  
*PRATIK SAHU (Presenter), SAYANTIKA BHOWAL, SASHI SEKHAR SATPATHY, Univ of Missouri - Columbia — The orbital Hall effect (OHE) is the transverse flow of the orbital angular momentum in response to the applied electric field, analogous to the charge current flow in the standard Hall effect. Even though the OHE has been proposed about a decade ago, it has not been directly observed experimentally to our knowledge. We have recently proposed that the 2D transition metal dichalcogenides (TMDC) with non-centrosymmetric crystal structure may be a good candidate for a robust OHE. In this talk, we evaluate the effect for the 2D-TMDC materials WTe2 and WS2 where there is a strong spin-orbit coupling present, both for the non-centrosymmetric (2H) and the centrosymmetry (1T') cases. As anticipated, the OHE in the 2H structure is much stronger, due to the existence of the intrinsic orbital moment in different parts of the Brillouin zone, which flow in different directions, as opposed to the centrosymmetric (1T') structure, where the OHE occurs due to the induced orbital moment in the presence of the Hall electric field. Our results are based on density-functional calculations as well as minimal tight-binding models.

*Work supported by the Department of Energy under Grant No. DEFG02-00ER45818
Heterojunctions from Coulomb-Engineered Transition Metal Dichalcogenides  
MALTE ROESNER (Presenter), Theory of Condensed Matter Department, Radboud University, CHRISTINA STEINKE, TIM WEHLING, Institute for Theoretical Physics, University of Bremen — The band structure and the band gap of semiconducting layered materials are strongly affected by the Coulomb interaction between carriers within the layer. At the same time we can externally modify this interaction by means of dielectric substrates or dielectric coating. This Coulomb-engineering can thus be used to tailor the fundamental electronic properties of layered materials.

Here we use a combination of the GdW [1] and WFCE [2] approaches to systematically study the environmental-screening effects to monolayers of semiconducting transition metal dichalcogenides on a material-realistic level. We compare static and dynamic screening effects of homogeneous substrates and derive an effective modeling scheme for spatially-varying heterogeneous substrates. The latter allows for the external and non-invasive induction of heterojunctions within the otherwise homogeneous monolayer. Our calculations show that spatial band gap modulations on the length scale of a few lattice constants are possible and are just limited by the heterogeneous substrate.


Quasi-1D TiS₃ Nanoribbons: Mechanical Exfoliation, Thickness-Dependent Raman Spectroscopy and Electronic Properties  
ALEXANDER SINITSKII (Presenter), University of Nebraska - Lincoln — Quasi-one-dimensional (quasi-1D) materials enjoy growing interest due to their unusual physical properties and promise for miniature electronic devices. We investigated the micromechanical exfoliation of representative quasi-1D crystals, TiS₃ whiskers, and demonstrate that they typically split into narrow nanoribbons with very smooth edges and clear signatures of 1D TiS₃ chains. Theoretical calculations show that the energies required for breaking weak interactions between the 2D layers and between 1D chains within the layers are comparable, and in turn are considerably lower than those required for breaking the covalent bonds within the chains. We systematically studied the exfoliated TiS₃ crystals by Raman spectroscopy and identified the Raman peaks whose spectral positions were most dependent on the crystals’ thickness. Finally, we fabricated TiS₃-based electronic devices and tested their transport properties. The conclusions established in this study for the exfoliated TiS₃ crystals can be extended to a variety of transition metal trichalcogenide materials as well as other quasi-1D crystals. The possibility of exfoliation of TiS₃ into few-nm wide crystals with smooth edges is important for realization of miniature device channels with reduced edge scattering.
Molybdenum disulfide (MoS$_2$) has emerged as a prototypical material among the 2D transition metal dichalcogenides for its stability, low cost and unique electronic, optical and mechanical properties. Its electronic properties can be tuned using different control parameters. This great sensitivity presents an opportunity to functionalize its properties through defect engineering, strain or by proximity to another material. We use high resolution low temperature STM/STS to study the local electronic properties of monolayer MoS$_2$. We were able to induce strains up to 3% before slipping effects take place and relaxation mechanisms prevail. We found a reduction of the quasiparticle bandgap of about 400 meV per percent local strain with a minimum gap of 1.2 eV. Heterostructures based on MoS$_2$ offer another viable possibility to tune its electronic properties. In this case, interactions between the planes of different materials are expected to modify the electronic properties of the constituent materials and open unprecedented possibilities of combining them for technological use.

*This work was supported by the US DOE, under grant No. DE-SC0004556 and by the Center for Complex Materials from First Principles (CCM), an Energy Frontier Research Center under Award No. DE-SC0012575.
8:00AM A54.00001: Evidence for topological surface states in amorphous Bi$_2$Se$_3$*  PAUL CORBAE (Presenter), SAMUEL CIOCYS, University of California, Berkeley, DANIEL VARJAS, QuTech and Kavli Institute of NanoScience., Delft University of Technology, ADOLFO G GRUSHIN, Néel Institute, ALESSANDRA LANZARA, FRANCES HELLMAN, University of California, Berkeley — Crystalline symmetries and classification schemes have played a central role in the identification of topological materials [1-3]. We address whether amorphous topological materials, which lie beyond this classification, exist in the solid state [4]. Amorphous Bi$_2$Se$_3$ thin films show a metallic behavior and an increased bulk resistance. The low field magnetoresistance due to weak antilocalization reveals a significant number of two-dimensional surface conduction channels. Angle-resolved photoemission spectroscopy data is consistent with a dispersive two-dimensional surface state with a distinct node. Spin resolved photoemission spectroscopy shows this state has an anti-symmetric spin-texture resembling that of the surface state of crystalline Bi$_2$Se$_3$.

Experimental results are consistent with an amorphous tight-binding model that utilizes a realistic amorphous structure. Evidence of amorphous materials with topological properties uncovers topological matter outside the current classification scheme, enabling materials discovery and scalable topological devices.


*PC is funded by the NSF GRFP Grant No. 1752814.

8:12AM A54.00002: Atypical Highly-Dispersive Band Structure in Putative Amorphous Topological Insulator*  SAMUEL CIOCYS (Presenter), PAUL CORBAE, University of California, Berkeley, DANIEL VARJAS, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, ADOLFO G GRUSHIN, Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, FRANCES HELLMAN, ALESSANDRA LANZARA, University of California, Berkeley — In typical amorphous and highly disordered materials, Anderson Localization guarantees flat valence bands. This effect is so dramatic and pervasive in the amorphous field of study that the density of states is assumed to be momentum-independent, serving as the full characterization of an amorphous system's electronic structure. In this work, we discover an exception to this rule in amorphous Bi$_2$Se$_3$ films. Angle-resolved photoemission spectroscopy uncovers an amorphous surface-state band structure with strong momentum-dependence and spin-momentum locking. We observe a Fermi surface with repeated annuli and reveal a spherically-parameterized momentum-space picture that warrants a re-evaluation of amorphous band structure on the most fundamental level.

*S.C. was supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE1852814 and DGE1106400.

Gordon and Betty Moore Foundation's EPiQS grant GBMF4838
Towards Realistic Amorphous Topological Insulators

MARCIO COSTA, GABRIEL SCHLEDER, Brazilian Nanotechnology National Laboratory (LNNano), CNPEM, Brazil, MARCO BUONGIORNO NARDELLI, Department of Physics, University of North Texas, USA, CAIO LEWENKOPF (Presenter), Physics Institute, Universidade Federal Fluminense, Brazil, ADALBERTO FAZZIO, Brazilian Nanotechnology National Laboratory (LNNano), CNPEM, Brazil — The topological properties of materials are, until now, associated with the features of their crystalline structure, although translational symmetry is not an explicit requirement of the topological phases. Recent studies of hopping models on random lattices have demonstrated that amorphous materials can display a non-trivial topology. Using ab initio calculations we show that amorphous materials can also display topological insulator properties. More specifically, we present a realistic study of the electronic and transport properties of amorphous bismuthene systems, showing that they are topological insulators. These systems are characterized by the topological index \( Z_2 = 1 \) and bulk-edge duality, and their linear conductance is quantized, \( G = \frac{2e^2}{h} \), for Fermi energies within the topological gap. Our study opens the path to the investigation of amorphous topological insulator materials.

This work was partially supported by the Brazilian funding agencies CNPq, FAPESP, and FAPERJ.

Numerical signatures of disordered topological phases

DOMINIC REISS (Presenter), FENNER HARPER, RAHUL ROY, University of California, Los Angeles — We investigate a number of numerical signatures which distinguish the topological and trivial phases of clean and disordered insulators. In particular, we consider two dimensional systems and suggest a procedure for numerically constructing a sequence of maximally localized mutually orthogonal states which span the Hilbert space. The localization lengths of states constructed using our procedure is numerically shown to diverge as a power law for systems with non-zero Chern number, and conversely saturate for systems with zero Chern number. We construct and numerically verify a scaling argument which suggests this exponent is universal. Finally, we discuss extensions of this approach to other spatial dimensions and symmetry classes.

D. R., F. H., and R. R. acknowledge support from the NSF under CAREER DMR-1455368 and the Alfred P. Sloan Foundation.

Topological Phase Transition in a Disordered Inversion-Symmetric Chain

SAAVANTH VELURY (Presenter), BARRY BRADLYN, TAYLOR L HUGHES, University of Illinois at Urbana-Champaign — Topological crystalline phases are states which are protected by crystalline symmetries. When translational invariance is broken by bulk disorder, the topological nature of these states may change depending on the type of disorder that is applied. In this work, we characterize the phases of a one-dimensional (1D) chain with inversion and chiral symmetries where the disorder preserves the inversion symmetry on every configuration. By using a basis-independent formulation for the inversion invariant and chiral winding number, we are able to construct phase diagrams for both quantities when disorder is present. Unlike the chiral winding number, the inversion invariant is prone to fluctuations past the spectral gap closing at strong disorder. Using the real-space renormalization group, we are able to compare how differently the inversion invariant and chiral winding number behave at low energies when disorder is present.
**9:00AM A54.00006: Dislocation defect as a bulk probe of monopole charge of multi-Weyl semimetals**

RODRIGO SOTO GARRIDO (Presenter), ENRIQUE MUNOZ, Pontif Univ Catolica de Chile, VLADIMIR JURICIC, NORDITA — We consider the electronic scattering in multi-Weyls semimetals due to dislocations defects which can be represented as an emergent effective magnetic field. We use partial wave analysis to analytically obtain the transmitted current and the conductance. From the conductance peaks as a function of the bias voltage, we can deduce monopole charge $n$ of the corresponding multi-Weyl semimetal as well as the effective flux of the dislocation defect. We argue that this provides a simple and a robust way to measure the monopole charge of a multi-Weyl semimetal.

*This work was supported by Fondecyt (Chile) Grant No 1190361*

**9:12AM A54.00007: Bound-state spectrum of superconductors with magnetic-texture defects**

 DANIEL STEFFENSEN (Presenter), BRIAN M. ANDERSEN, Niels Bohr Institute, PANAGIOTIS KOTETES, ITP-CAS — Recent experiments [1] provided evidence for zero-energy Majorana bound states (MBSs) when magnetic adatoms are deposited onto a superconductor. Such observations are reconcilable by means of 0D-like defects which trap MBSs. Existing explanations rely on the presence of isolated magnetic skyrmions or vortices in the spin-orbit coupling field. These need to be contrasted to the standard mechanism, in which MBSs are trapped in vortices of the superconducting order parameter. Inspired from the above, we explore a novel promising path towards realizing MBSs, which relies on 0D defects in the order parameter describing a textured magnetic order that coexists with spin-singlet superconductivity. This scenario appears relevant for iron-pnictides, where a theoretical study [2] has revealed that textured magnetism is accessible in doped BaFe$_2$As$_2$ and LaFeAsO. Here, we perform a thorough numerical investigation of the bound-state energy spectrum arising when vortices are introduced in the order parameter of spin-spiral and -whirl magnetic orders. Our preliminary results indicate that the defect-induced MBSs are accessible in superconductors which yield a nodal spectrum in the absence of the magnetic order.

In-gap excitations due to defects in topological superconductor with spin-orbit coupling

*ANDREJ MESAROSH (Presenter), Laboratoire de Physique des Solides, CNRS, GERBOLD MÉNARD, Niels Bohr Institute, Copenhagen, Denmark, CHRISTOPHE BRUN, FRANÇOIS DEBONTRIDDER, DIMITRI RODITCHEV, Institut des NanoSciences de Paris, Sorbonne Université, PASCAL SIMON, Laboratoire de Physique des Solides, Université Paris-Sud, TRISTAN CREN, Institut des NanoSciences de Paris, Sorbonne Université — Recent microscopy experiments on superconducting monolayer of lead(Pb) grown over clusters of cobalt atoms have raised urgent questions about in-gap electronic states in presence of strong spin-orbit coupling and magnetism.

Using analytics and numerics we find that a topological defect in Rashba spin-orbit coupling (in contrast to a vortex in superconducting pairing) fully explains puzzling features of this experiment: 1) Two different zero-modes, one point-like at center of cluster and the other ring-shaped around it; 2) The zero mode pair is protected by a large energy gap; 3) The localization lengthscale inside the cluster is far smaller than superconducting coherence length, but comparable to it outside. The theory predicts that this is a Majorana pair, with remarkable isolation in energy thanks to the defect in strong spin-orbit coupling. We discuss the role of magnetic textures in our theoretical scenario.

*Supported by the French Agence Nationale de la Recherche through the contract ANR Mistral, and by the Region Ile de France through the DIM Nano-K project ETERNAL.

CT-symmetric Non-linear Topological Defect Modes

*DO HYEOK JEON (Presenter), Wesleyan University, MATTIS REISNER, FABRICE MORTESSAGNE, ULRICH KUHL, Institut de Physique de Nice (INPHYNI), TSAMPIKOS KOTTOS, Wesleyan University — Topologically protected states have recently been a subject of increasing interest due to their unique robustness against disorder. Such property is beneficial for a variety of photonics applications ranging from lasers to optical isolators and receiver protectors. On the other hand, an essential piece of information associated with the interplay between optical nonlinearity and topological protection is still missing. Such a question cannot be ignored, since nonlinearity is prevalent in realistic circumstances. Using a non-linear SSH model we have theoretically analyzed the topological nature of an emerging nonlinear defect mode associated with a non-linear defect. To this end, we have devised a theoretical formalism which is based on Green’s functions and prove that for certain type of nonlinearities the nonlinear defect mode is spectrally protected by a charge-conjugation (CT) symmetry. We demonstrate the validity of our study via direct measurements using a CROW SSH array in the microwave domain.

*Partial support under NSF Grant EFMA1641109 and ONR Grant N00014-19-1-2480.
9:48AM A54.00010: Aperiodic Topological Boundary Modes: Revisiting Quasi-Periodic Localization  
DAN BORGNIA (Presenter), ROBERT-JAN SLAGER, ASHVIN VISHWANATH, Harvard University — Although physical systems are generically aperiodic, most work on non-interacting topological materials focuses on translation-invariant cases. These systems are well described by band theory and perturbatively resistant to the disorder of real world conditions, however, the regime of strong aperiodicity is not frequently discussed in the context of topological materials. Aiming to better understand such systems, this work generalizes key results in translation-invariant systems to their aperiodic counterparts. We then apply these techniques to the canonical Andre-Aubrey-Harper (AAH) Model and its 1D Metal-Insulator Transition (MIT). We uncover a deep connection between the known non-commutative topological properties of the model and the MIT. This not only highlights the power of this non-commutative technology, but also separates the AAH model from its disordered counterparts. The 1D MIT in the AAH model and its peculiar properties are indeed topological in nature. This suggests quasiperiodic systems form their own special class of topological materials distinct from their translation-invariant counterparts.

10:00AM A54.00011: The existence of robust edge currents in Sierpinsky Fractals* 
MIKAEL FREMLING (Presenter), MICHAL VAN HOOFT, CRISTIANE MORAIS SMITH, LARS FRITZ, Univ of Utrecht — We investigate the Hall conductivity in a Sierpinski carpet, a fractal of Hausdor dimension \( d_f = \ln(8) / \ln(3) \approx 1.893 \), subject to a perpendicular magnetic field. We compute the Hall conductivity using linear response and the recursive Green function method. Our main finding is that edge modes, corresponding to a maximum Hall conductivity of at least \( \sigma_{xy} = \pm e^2/h \), seems to be generically present for arbitrary finite field strength, no matter how one approaches the thermodynamic limit of the fractal. We discuss a simple counting rule to determine the maximal number of edge modes in terms of paths through the system with a fixed width. This quantized edge conductance, as in the case of the conventional Hofstadter problem, is stable with respect to disorder and thus a robust feature of the system.

*We acknowledge the SFI/HEA Irish Centre for High-End Computing (ICHEC) for the provision of computational facilities and support through project nmphy013b. This work is part of the D-ITP consortium, a program of the Netherlands Organisation for Scientific Research (NWO) that is funded by the Dutch Ministry of Education, Culture and Science (OCW).
10:12AM A54.00012: Tracking the mechanism behind graphene ripple inversion with LAMMPS  JAMES MANGUM (Presenter), PAUL M THIBADO, Univ of Arkansas-Fayetteville — Freestanding graphene spontaneously forms ripples. If a sheet is under sufficient compressive strain, the ripples form a bi-stable system (concave or convex). The rate at which a ripple inverts is lower than the small thermal oscillation frequency. This rate decreases with increased compressive strain, and increases with increased temperature. We ran ten simulations, using LAMMPS molecular dynamics simulation software, for a single ripple of graphene, with different compressive strains at 3000 K. The z-component (out of plane) average and center values were tracked to identify when inversion occurs. Atoms that make up a cross-section of the ripple were also tracked. Changes in the cross-section profile that occur during inversion show that the mechanism behind inversion is the formation of smaller sub-ripples.

10:24AM A54.00013: Anomalous Hall effect in chiral superconductors from impurity superlattices* ZHIQIANG WANG (Presenter), James Franck Institute, University of Chicago, YU LI, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, WEN HUANG, Shenzhen Institute for Quantum Science and Engineering and Department of Physics, Southern University of Science and Technology — Unlike anomalous quantum Hall insulators, clean single-band chiral superconductors do not exhibit intrinsic Hall effect at the one-loop approximation. Finite ac Hall conductance was found to emerge beyond one-loop, such as with vertex corrections associated with extrinsic random impurity scatterings. In this work, we consider the effect of impurities embedded in chiral superconductors in a superlattice pattern, instead of in random distributions. The impurity-induced Bogoliubov quasiparticle bound states hybridize to form subgap bands, constituting an emergent low-energy effective theory whose anomalous Hall effect can be studied with ease. We demonstrate that the occurrence of the Hall effect depends on the superlattice geometry and the parity of the chiral pairing. In particular, due to the composite particle-hole character of the subgap states, the Hall conductance arises at the one-loop level of the current-current correlator in our effective model. Generalized to random impurities, our theory sheds new light on the physics of impurity-induced anomalous Hall conductivity in chiral superconductors.

*This work is supported in part by a startup grant at the Southern University of Science and Technology.
We consider the interplay between topology and disorder on the surface fluids of topological superconductors (TSCs). In the case of a single 2D Majorana cone, only “quenched gravitational disorder (QGD)” is allowed, i.e. a static modulation of the effective speed of light. Although disorder effects near zero energy have been understood for a long time, recent numerical results uncovered an unexpected result: finite energy TSC surface states form “stacks” of quantum critical wave functions, with universal, energy-independent statistics [1,2,3]. In classes CI and AIII, one finds stacks of quantum Hall plateau transition states [1,2]. For the single Majorana cone with QGD in class DIII, the stacked critical states appear to belong to a new class [3]. In order to shed light on the DIII results, we consider a semiclassical approach. We find that kinetic theory predicts a divergent conductivity at all temperatures. We further study the statistical properties of the null geodesics in the 2+1-D quenched random spacetime metric that can be associated to QGD.

[2] B. Sbierski, J. Karcher, M. S. Foster, unpublished

*Welch Foundation, Grant No. C-1809
10:48AM A54.00015: Antisite defect enhanced thermoelectric performance of topological crystalline insulators*  
MUHAMMAD USMAN MUZAFFAR, SHUNHONG ZHANG, PING CUI (Presenter), University of Science and Technology of China, Hefei 230026, China, JIAQING HE, Southern University of Science and Technology, Shenzhen 518055, China, ZHENYU ZHANG, University of Science and Technology of China, Hefei 230026, China — As the first experimentally established topological crystalline insulator (TCI), SnTe also exhibits superior thermoelectricity upon proper doping; yet to date, whether such doping will preserve or destroy the salient topological properties in achieving outstanding thermoelectric performance remains elusive. Using first-principles calculations combined with Boltzmann transport theory, we uncover the elegant role of antisite defect in optimally enhancing the thermopower of SnTe while simultaneously preserving its topological nature. We first show that Sn\textsubscript{Te} antisite defect effectively induces pronounced variations in the low-energy density of states rather than rigidly shifting the chemical potential, resulting in higher Seebeck coefficient and power factor. Next, we demonstrate that in a wide temperature range the Seebeck coefficient of antisite doped SnTe distinctly outperforms previously identified systems invoking extrinsic dopants. We further confirm that such intrinsic antisite doping preserves the nontrivial topology, which in turn favors high electrical conductivity and thermoelectricity. These findings render antisite doping as a natural and powerful avenue to optimize the overall thermoelectric performance of TCIs and related systems.

*Supported by NNSF of China and MOST.

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A55 DCMP: Dirac and Weyl Semimetals: Theory I  
Mile High Ballroom 2B - Herbert Fertig, Indiana Univ - Bloomington

8:00AM A55.00001: Chiral Qubit: Implementing a Qubit Using Chiral Charge and Chiral Anomaly*  
EVAN PHILIP (Presenter), SAHAL KAUSHIK, DMITRI E KHRZEEV, State Univ of NY - Stony Brook — Dirac and Weyl semimetals are capable, due to chiral anomaly, of a nearly dissipationless current in the presence of a chirality imbalance and magnetic field (Chiral Magnetic Effect). We propose an implementation of the qubit based on this. Superconducting qubits require low operating temperatures and are limited in operating frequency by the superconducting gap—two limitations that the "chiral qubit" could potentially overcome. I will present our theoretical model and estimates regarding the chiral qubit.

*U.S. Department of Energy Awards DE-FG-88ER40388 (E. P. and D. K.), DE-SC-0017662 (S. K. and D. K.), and DE-AC02-98CH10886 (D. K.)
8:12AM A55.00002: Two-body interaction induces axion/phason field in Weyl semimetals
DAVID SCHMELTZER (Presenter), The City College of New York, AVADH SAXENA, Los Alamos National Lab — Following our results that the two-body interaction can induce a space and time dependent topological axion term $\theta(z,t)\left[\frac{e^2}{2\pi \hbar}\right](E,B)$, we show that by applying this theory to a Weyl semimetal with two nodes in a magnetic field a one-dimensional sliding charge density wave (CDW) emerges which replaces the asymptotic effective topological representation, in agreement with the recent experimental finding of J. Gooth et al. [Nature, https://doi.org/10.1038/s41586-019-1630-4 (2019)].

8:24AM A55.00003: Chiral vector field-induced collective fermionic excitations in Weyl semimetals
ALBERTO CORTIJO (Presenter), CSIC - Madrid, ERIK VAN DER WURFF, Institute for theoretical physics, Utrecht University — We study the single-particle fermionic spectrum of Weyl semimetals in three dimensions taking into account the axial vector character of the electron-phonon interaction. We find that, together the expected standard quasi-particle peak, a second peak appears in the spectral function. The main features of this new fermionic excitation are to be intrinsically anisotropic and gapped. We will discuss also the potential impact of these collective fermionic modes on the transport phenomena in Weyl semimetals.

*E.C.I. van der Wurf acknowledges financial support from the Stichting voor Fundamenteel Onderzoek der Materie (FOM), part of the D-ITP consortium, a program of the Netherlands Organisation for Scientific Research (NWO) that is funded by the Dutch Ministry of Education. A. C. acknowledges financial support through MINECO/AEI/FEDER, UE Grant No. FIS2015-73454-JIN and European Union structural funds and the Comunidad Autonoma de Madrid (CAM) NMAT2D-CM Program (S2018-NMT-4511).

8:36AM A55.00004: Theoretical Study of Resonant Inelastic X-ray Scattering for Monopole Density-wave Order and Superconductivity in Weyl Semimetals
ERIC BOBROW (Presenter), Johns Hopkins University, PETER ABBAMONTE, University of Illinois at Urbana-Champaign, YI LI, Johns Hopkins University — Resonant Inelastic X-ray Scattering (RIXS) spectra can provide useful information for phase-sensitive bulk detection. A difference of RIXS spectra for cross-polarized X-rays has been previously proposed to detect the topological windings of single-particle Weyl nodes in, for example, TaAs. We generalize this idea to investigate various topological excitations near the emergent Weyl nodes in exotic nodal superconducting and density-wave ordered Weyl semimetal systems characterized by monopole harmonic symmetry.

*This work is supported by NSF CAREER DMR-1848349 and in part by the Alfred P. Sloan Research Fellowships and the Gordon and Betty Moore Foundations EPiQS Initiative through Grant No. GBMF4305.
8:48AM A55.00005: Nonlinear Planar Hall as Another Signature of Chiral Anomaly in Weyl Semimetals*  RUIHAO LI (Presenter), SHULEI ZHANG, Department of Physics, Case Western Reserve University, ANTON BURKOV, Department of Physics and Astronomy, University of Waterloo, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory — Weyl semimetals (WSMs) are a newly discovered class of quantum materials which can host a number of exotic quasiparticles called Weyl fermions. One of the defining properties of WSMs is chiral anomaly – a pair of Weyl nodes with opposite chirality act as source and drain of electrons in the presence of electric and magnetic fields that are not perpendicular to each other. To date, the most remarkable phenomenon induced by chiral anomaly is the longitudinal negative magnetoresistance, which is a linear response effect. In this work, we theoretically investigate the transport properties of WSMs in the nonlinear regime, and predict a nonlinear planar Hall effect as another manifestation of chiral anomaly in transport. Intuitively, a steady-state density difference between a pair of Weyl nodes may be established when the chiral pumping and internode relaxation reach a balance, which conspires with anomalous velocity to give rise to the nonlinear Hall effect. In contrast to the intrinsic quantum nonlinear Hall effect, this effect does not rely on a finite Berry curvature dipole.

* R. L. and S. Z. were supported by College of Arts and Sciences Case Western Reserve University. A. B. and O. H. were supported by CATS, an Energy Frontier Research Center funded by the U.S. DOE, Office of BES.

9:00AM A55.00006: Viscosity as a probe of nodal topology  MARIANNE MOORE (Presenter), University of British Columbia, PIOTR SUROWKA, Max Planck Inst, VLADIMIR JURICIC, NORDITA, BITAN ROY, Lehigh University — Electronic materials can sustain a variety of unusual, but symmetry protected touchdowns of valence and conduction bands, each of which is identified by a distinct topological invariant. Well known examples include linearly dispersing pseudo-relativistic fermions in monolayer graphene, Weyl and nodal-loop semimetals, bi-quadratic (-cubic) band touching in bilayer (trilayer) graphene, as well as mixed dispersions in multi-Weyl systems. We here show that depending on the underlying band curvature, the shear viscosity in the collisionless regime displays unique power-law scaling with frequency at low temperatures, bearing the signatures of the band topology, which are distinct from the ones when the system resides at the brink of a topological phase transition into a band insulator. Therefore, besides density of states (governing specific heat, compressibility) and dynamic conductivity, shear viscosity can be instrumental to pin nodal topology in electronic materials.

9:12AM A55.00007: Large enhancement of thermopower at low magnetic field in compensated Dirac/Weyl semimetals  XIAOZHOU FENG (Presenter), BRIAN SKINNER, Ohio State Univ - Columbus — We theoretically study the thermoelectric properties of compensated Dirac/Weyl semimetals subjected to a magnetic field. Previous work has shown that Dirac/Weyl semimetals without compensation can exhibit a large enhancement of thermopower in the extreme quantum limit of magnetic field. Here we show that in compensated systems a huge enhancement of thermopower can be obtained even at much smaller magnetic field, provided that $\omega_c \tau \gg 1$. We discuss our results in light of recent measurements on the compensated Weyl semimetal tantalum phosphide, in which an enormous magnetothermoelectric effect was observed.
A55.00008: Charged Domain Wall of Electric Polarizations in Topological Nodal-Line Semimetals  AKIHIKO SEKINE (Presenter), RIKEN, NAOTO NAGAOSA, RIKEN & University of Tokyo — We study theoretically the electronic structure of three-dimensional topological nodal-line semimetals. We show that, in the presence of a gap-opening spatially dependent mass term that forms a domain wall, an in-gap charged localized mode emerges at the domain wall. It turns out that such a domain wall is realized by head-to-head (or tail-to-tail) bulk electric polarizations. The localized mode has a topological origin, i.e., a topological confinement is realized, which is understood by a semiclassical topological number defined in the semiclassical momentum-real space. Namely, a stable charged domain wall of electric polarizations is realized in nodal-line semimetals. In sharp contrast to the well-known band bending mechanism, the origin of the charged domain wall in this study is purely electronic, i.e., due to the band topology. Moreover, in contrast to previous studies, our study demonstrates a topological confinement at the interface between two insulators without bulk topological numbers. The dispersion of the localized mode evolves from gapless to gapped as the bulk bandgap increases, which means that its conductivity is externally tunable. We discuss a possible experimental realization of the stable, electrically-tunable charged domain wall.

A55.00009: Spin and Pseudo-Spin Collective Modes in Doped Graphene  ABHISHEK KUMAR (Presenter), DMITRII MASLOV, University of Florida — Collective modes in graphene has been an active area of research during the last decade. As any two-dimensional electron system, graphene harbors a gapless plasmon mode which disperses as $q^{1/2}$. Gapped collective modes in graphene are, however, less explored. The goal of this work is two-fold: a comprehensive study of collective modes in graphene (a) without spin-orbit coupling (SOC) and (b) in the presence of Rashba and valley-Zeeman SOC. For a short-range electron-electron interaction, we find that in case (a) there exists a collective mode below the continuum, corresponding to oscillations of pseudospin. In case (b), we show that, in graphene with Rashba SOC, there exists a collective spin mode consisting of three branches: a double-degenerate branch, corresponding to oscillations of in-plane magnetization, and a non-degenerate branch corresponding to oscillations of out of plane magnetization. For graphene with valley-Zeeman SOC, there exists only a single branch of the collective mode corresponding to out of plane oscillation of the magnetization. We also study the case of an unscreened Coulomb interaction, solved by reducing the sum of ladder diagrams for a vertex function to a Dirac equation with non-local interaction.

A55.00010: Quantum oscillations in Dirac magnetoplasmons  JOHANNES HOFMANN (Presenter), Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Centre for Mathematical Sciences, University of Cambridge — The plasmon frequency in standard electron gases with a parabolic single-particle dispersion is a purely classical quantity that is not sensitive to electron interactions or the equation of state. We demonstrate that this canonical result no longer holds for plasmons in three-dimensional semimetals, which can thus be used to probe many-body effects. In particular, we show that the plasmon frequency in an external magnetic field displays quantum oscillations, which is not the case for the electron gas. Using the random phase approximation, results are presented for the magnetoplasmon dispersion and the loss function in Dirac semimetals. We include a full discussion of the loss function in a magnetic field as a function of the direction of propagation with respect to the magnetic field direction and discuss the transition from large magnetic fields to the low-field limit.
10:00AM A55.00011: Fermi-arcs and non-local collective modes in thin-film Weyl systems
SONU VERMA, DEBASMITA GIRI, Physics, Indian Institute of Technology Kanpur, HERBERT FERTIG, Physics, Indiana university Bloomington, ARIJIT KUNDU (Presenter), Physics, Indian Institute of Technology Kanpur — Fermi-arcs in Weyl semimetals carry signatures of their topological origin. In a thin-film geometry, in the presence of Coulomb interactions, particle-hole excitations can take place either on the same surface, or between the two surfaces, giving rise to the possibility of unique non-local collective modes. We study, in particular, plasmonic modes that are non-locally bound in a thin-film Weyl semimetal carrying the signature of bulk and surface mixing and analyze the possibility of their application.

* DST/SERB (India), CSIR (India), MHRD (India)

10:12AM A55.00012: Effect of charge renormalization on electric and thermo-electric transport along the vortex lattice of a Weyl superconductor
GAL LEMUT (Presenter), MICHAL PACHOLSKI, Leiden University, INANC ADAGIDEI, Sabanci University, CARLO W J BEENAKKER, Leiden University — Building on the discovery that a Weyl superconductor in a magnetic field supports chiral Landau level motion along the vortex lines, we investigate its transport properties out of equilibrium. We show that the vortex lattice carries an electric current $I=1/2(Q_{\text{eff}}^2/h)(\Phi/\Phi_0)V$ between two normal metal contacts at voltage difference $V$, with $\Phi$ the magnetic flux through the system, $\Phi_0$ the superconducting flux quantum, and $Q_{\text{eff}}<e$ the renormalized charge of the Weyl fermions in the superconducting Landau level. Because the charge renormalization is energy dependent, a nonzero thermo-electric coefficient appears even in the absence of energy-dependent scattering processes.

* This project has received funding from the Netherlands Organization for Scientific Research (NWO/OCW), from the TUBITAK grant No. 114F163, and from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program.

10:24AM A55.00013: Effect of Disorder on Edge States in Nodal Topological Materials
SAUMITRAN KASTURIRANGAN (Presenter), XUZHE YING, FIONA BURNELL, ALEX KAMENEV, University of Minnesota — Many nodal topological materials exhibit gapless flat-band boundary modes which are protected by non-trivial topology in momentum space. Here we ask the question of whether, as is the case for weak topological insulators [1], these boundary flat-bands maintain their integrity in the presence of disorder – and whether this leads to observable signatures in transport. To do this, we study the effects of various types of quenched short-range disorder on the energy spectrum, localization, and transport properties of the boundary states of a 2D topological semi-metal in symmetry class BDI. Our primary example is graphene with time-reversal and particle-hole symmetry. We discuss the implications of our results for experimentally detecting the boundary modes of nodal topological superconductors in 2D.


* This work was partially supported by NSF: DMR-1352271 and NSF: DMR-1928166
10:36AM A55.00014: Topologically protected Landau level in the vortex lattice of a Weyl superconductor*  
MICHAL PACHOLSKI (Presenter), CARLO W J BEENAKKER, Leiden University, INANC ADAGIDELI, Faculty of Engineering and Natural Sciences, Sabanci University — The question whether the mixed phase of a gapless superconductor can support a Landau level is a celebrated problem in the context of $d$-wave superconductivity, with a negative answer: The scattering of the subgap excitations (massless Dirac fermions) by the vortex lattice obscures the Landau level quantization. Here we show that the same question has a positive answer for a Weyl superconductor: The chirality of the Weyl fermions protects the zeroth Landau level by means of a topological index theorem. As a result, the heat conductance parallel to the magnetic field has the universal value $G = \frac{1}{2} g_0 \Phi / \Phi_0$, with $\Phi$ the magnetic flux through the system, $\Phi_0$ the superconducting flux quantum, and $g_0$ the thermal conductance quantum.

*This research was supported by the Netherlands Organization for Scientific Research (NWO/OCW), an ERC Synergy Grant, and by the TUB ITAK grant No. 114F163.

A55.00015: Nonlocal Response Mediated by Weyl Orbits*  
ZHE HOU (Presenter), QING-FENG SUN, Peking Univ — Nonlocality is always an interesting topic in quantum physics and is usually mediated by some unique quantum states. Nonlocal phenomena in three dimensional systems mediated by trivial bulk states are rarely reported however. Here we investigate a Weyl semimetal slab and find an exotic nonlocal correlation effect when placing two potential wells merely on the top and bottom surfaces. This nonlocal response is totally carried by the bulk states inside the Weyl orbit, which is a result of the peculiar band structure of Weyl semimetals. A giant nonlocal transport signal and a body breakdown by the Weyl fermions are further uncovered, which can serve as signatures for verifying this nonlocal phenomenon experimentally. Our results extend a new member in the nonlocality family and have potential applications for designing new electric devices with fancy functions.

*This work was financially supported by National Key R and D Program of China (Grant No. 2017YFA0303301), NSF-China (Grant No. 11921005), the Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. DB28000000), and Beijing Municipal Science & Technology Commission (Grant No.Z181100004218001).

**Monday, March 2, 2020 8:00 AM - 11:00 AM**

**Session A56 DCMP GMAG: Kitaev Model Theory and Experiment**  
Mile High Ballroom 2C - Joseph Paddison, Oak Ridge National Lab
8:00AM A56.00001: Pressure Induced Quantum Spin Liquids in Extended Kitaev Model
JIUCAI WANG (Presenter), ZHENG-XIN LIU, Department of Physics, Renmin University of China, Beijing 100872, China — The Kitaev's Honeycomb lattice model has exactly solvable spin liquid ground states and has attracted lots of research interest. However, most Kitaev materials possess both Kitaev and non-Kitaev interactions, resulting in magnetically ordered ground states. A possible way to suppress the magnetic order and to drive the system to quantum spin liquid phases is exerting high pressure, assuming that the bond-dependent interaction strength can be adjusted by the external pressure. We illustrate this possibility by studying a (pressure caused) anisotropic spin model with variational Monte Carlo method. While the anisotropic pure Kitaev model contains only two phases, the presence of non-Kitaev interactions result in a much richer phase diagram and give rise to several gapless spin liquids whose low-energy spinon excitations contain different number of cones. We show that these gapless spin liquids can be distinguished experimentally. Furthermore, a small out-of-plane magnetic field opens a gap to these spin liquids and results in different chiral spin liquids, all of which are belonging to the Kitaev 16-fold classification.

8:12AM A56.00002: Transport and chaos in lattice Sachdev-Ye-Kitaev models* HAOYU GUO (Presenter), YINGFEI GU, SUBIR SACHDEV, Department of Physics, Harvard University — We compute the transport and chaos properties of lattices of quantum Sachdev-Ye-Kitaev islands coupled by single fermion hopping, and with the islands coupled to a large number of local, low energy phonons. We find two distinct regimes of linear-in-temperature (T) resistivity, and describe the crossover between them. When the electron-phonon coupling is weak, we obtain the “incoherent metal” regime, where there is near-maximal chaos with front propagation at a butterfly velocity $v_B$, and the associated diffusivity $D_{\text{chaos}} = (v_B)^2/(2\pi T)$ closely tracks the energy diffusivity. On the other hand, when the electron-phonon coupling is strong, and the linear resistivity is largely due to near-elastic scattering of electrons off nearly free phonons, we find that the chaos is far from maximal and spreads diffusively. We also describe the crossovers to low T regimes where the electronic quasiparticles are well defined.

*This research was supported by the U.S. Department of Energy under Grant No. DESC0019030. Y.G. is also supported by the Gordon and Betty Moore Foundation EPiQS Initiative through Grant (GBMF4306). This work was performed in part at the Aspen Center for Physics, which is supported by National Science Foundation Grant PHY-1607611.
8:24AM A56.00003: Low-rank Sachdev-Ye-Kitaev Models*  JAEWON KIM (Presenter), XIANGYU CAO, EHUD ALTMAN, University of California, Berkeley — Motivated by recent works on atom-cavity realizations of fast scramblers, and on Cooper pairing in non-Fermi liquids, we study a family of solvable variants of the (q=4) Sachdev-Ye-Kitaev model in which the rank and eigenvalue distribution of the coupling matrix J are tuneable. When the rank is proportional to the number of fermions, the low temperature behavior is sensitive to the eigenvalue distribution. We obtain a complete classification of the possible non-Fermi liquid quantum phases. These include two previously studied phases whose fermion scaling dimension depends continuously on the rank; we show that they are maximally chaotic, but necessitate an extensively degenerate or negative semidefinite coupling matrix. More generic distributions give rise to "almost Fermi liquids" with a scaling dimension Delta = 1/2, but which differ from a genuine Fermi-liquid in quasi-particle decay rate, quantum Lyapunov exponent and/or specific heat.

*We acknowledge support from the ERC synergy Grant UQUAM and DOE grant DE-SC0019380.

8:36AM A56.00004: Soft modes in the complex Sachdev-Ye-Kitaev model*  YINGFEI GU, Harvard University, ALEXEI KITAEV, Physics, Caltech, SUBIR SACHDEV, GRIGORY TARNOPOLSKY (Presenter), Harvard University — We discuss soft modes in the Sachdev-Ye-Kitaev model for complex fermions with large N flavors and a global U(1) charge. The conserved charge leads to a compact scalar field in the effective action, from which we derive the many-body density of states and extract the charge compressibility. We compute the latter via three distinct numerical methods and obtain consistent results.

*Y.G. is supported by the Gordon and Betty Moore Foundation EPIQS Initiative through Grant (GBMF-4306) and DOE grant, DE-SC0019030. A.K. is supported by the Simons Foundation under grant 376205 and through the “It from Qubit” program, as well as by the Institute of Quantum Information and Matter, a NSF Frontier center funded in part by the Gordon and Betty Moore Foundation. S.S. and G.T. are supported by DOE grant, DE-SC0019030. G.T. acknowledges support from the MURI grant W911NF-14-1-0003 from ARO and by DOE grant DE-SC0007870
Dynamical and thermal magnetic properties of the Kitaev spin liquid candidate α-RuCl₃*

PONTUS LAURELL (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, SATOSHI OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory — α-RuCl₃ is a promising Kitaev spin liquid candidate, but orders magnetically, the description of which necessitates additional interaction terms. The nature of these interactions, their magnitudes and even signs, remain an open question. In this work we investigate dynamical and thermal magnetic properties of proposed effective Hamiltonians. We calculate $T=0$ inelastic neutron scattering (INS) intensities using exact diagonalization, and magnetic specific heat, $C(T)$, using a thermal pure quantum states method. We find that no single current model satisfactorily explains all observed phenomena of α-RuCl₃. In particular, we find that Hamiltonians derived from first principles can capture the experimentally observed high-temperature peak in $C(T)$, while overestimating the magnon energy at $q=0$. In contrast, other models reproduce important features of the INS data, but do not adequately describe $C(T)$. We propose a modified ab initio model that is consistent with both magnetic specific heat and low-energy features of INS data.

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

Thermal and magnetoelastic properties of a-RuCl₃ in the field-induced low temperature states

RICO SCHOENEMANN (Presenter), Los Alamos National Laboratory, SHUSAKU IMAJO, University of Tokyo, FRANZISKA WEICKERT, Los Alamos National Laboratory, YASUMASA TAKANO, University of Florida, STEPHEN E NAGLER, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee, MARCELO JAIME, Los Alamos National Laboratory — Magnetocaloric effect, thermal expansion, and magnetostriction measurements on single crystal α-RuCl₃ samples in applied magnetic fields are discussed. α-RuCl₃ has been established as a promising candidate for the sought-after physical realization of the Kitaev model, which describes $S=1/2$ spins on a honeycomb lattice with bond dependent Ising interactions, hosting Majorana fermions as well as a topological quantum spin liquid (QSL) ground state. Recent experimental data indicate signs of a QSL state that emerges in applied magnetic fields, once the antiferromagnetic (AFM) transition temperature $T_N$ observed in zero field below 7K is suppressed. In order to identify the nature of the phase transitions below $T_N$ and to map the phase diagram as a function of magnetic field, we conducted measurements of the magnetocaloric effect in pulse magnetic fields as well as thermal expansion and magnetostriction measurements in static fields up to 15 T. The results are discussed in the context of possible quantum critical and QSL behavior in α-RuCl₃.
9:12AM A56.00007: Multipartite Entanglement in the Kitaev Honeycomb Model  JAMES LAMBERT (Presenter), ERIK SORENSEN, McMaster Univ — Quantum spin liquid (QSL) phases of matter have proven extremely elusive from both experimental and theoretical perspectives. In the theoretical domain, examining the topological entanglement entropy has been a primary tool for diagnosing whether or not a model exhibits QSL physics in its groundstate. We study the Kitaev honeycomb model, a prototype of QSL physics in two dimensions, using the quantum Fisher information (QFI), which is both experimentally accessible and well defined at finite temperature. We explore he behaviour of the QFI in both the gapped and gapless phases and in the regions around the transition.

9:24AM A56.00008: Spin-one Kitaev-Heisenberg model on a two-dimensional honeycomb lattice  XIAOYU DONG (Presenter), Ghent University, DONNA SHENG, California State University, Northridge — We study the Kitaev-Heisenberg model with a spin-1 local degree of freedom on a two-dimensional honeycomb lattice numerically by density matrix renormalization group method. We obtain the phase diagram with two spin liquid phases and four symmetry broken phases. We identify that the spin liquid is gapless and has short-ranged spin-spin correlations within the whole phase. Comparing to its spin-1/2 counterpart, the spin-1 spin liquid has more gapless modes.

9:36AM A56.00009: Microscopic route to magnetic anisotropy in higher-spin honeycomb lattice: application to CrI$_3$  PANAGIOTIS PETER STAVROPOULOS (Presenter), HAE-YOUNG KEE, Univ of Toronto — In the past decade transition metal (TM) compounds have generated a wealth of theoretical and experimental research on frustrated magnetism, especially TM compounds that host local 1/2 moments. Spin-orbit coupling (SOC) of the TM cation sites plays a key role for the appearance and dominance of frustrated terms such as the Kitaev spin-1/2 term. Very recently it has been recognized that SOC of the anion sites is a viable route to realizing frustrated higher spin model terms from super-exchange paths [1]. We present the microscopic origin of frustrated S=3/2 model terms in d$^3$ systems. The appearance and competition of the Kitaev term with conventional spin model terms are presented. Applications of the theory to CrI$_3$ and related materials are also discussed.

9:48AM A56.00010: Two-Magnon Bound States in the Kitaev Model in a [111]-Field
SUBHASREE PRADHAN (Presenter), NIRA CVKUMAR PATEL, NANDINI TRIVEDI, Ohio State Univ - Columbus — It is now well established that the Kitaev honeycomb model in a magnetic field along the [111]-direction harbors an intermediate gapless quantum spin liquid (QSL) phase sandwiched between a gapped non-abelian QSL at low fields $H<H_c^1$ and a partially polarized phase at high fields $H>H_c^2$. Here, we analyze the low field and high field phases and phase transitions in terms of single- and two-magnon excitations using exact diagonalization (ED) and density matrix renormalization group (DMRG) methods. We find that the energy to create a bound state of two-magnons $\Delta_p$ becomes lower than the energy to create a single spin flip $\Delta_s$ near $H_c^2$. In the entire Kitaev spin liquid $\Delta_p<\Delta_s$ and both gaps vanish at $H_c^2$. We make testable predictions for magnon pairing that could be observable in Raman scattering measurements on Kitaev QSL candidate materials.

10:00AM A56.00011: Phase diagram of the spin-1/2 Kitaev-Gamma chain and emergent \`\`partial" SU(2) symmetry  WANG YANG (Presenter), ALBERTO NOCERA, TARUN TUMMURU, Physics, University of British Columbia, HAE-YOUNG KEE, Physics, University of Toronto, IAN AFFLECK, Physics, University of British Columbia — We study the phase diagram of a one-dimensional version of the Kitaev spin-1/2 model with an extra \`\` $\Gamma$'-term", using analytical, density matrix renormalization group and exact diagonalization methods. Two intriguing phases are found. In the gapless phase, the low energy theory is described by an emergent SU(2)$_1$ Wess-Zumino-Witten (WZW) model though the exact symmetry group is discrete. On the other hand, the relations between the local spin operators and the WZW currents and primary field contain SU(2) breaking coefficients. A modified nonabelian bosonization formula is proposed to capture such exotic emergent \`\`partial" SU(2) symmetry. In the ordered phase, there is numerical evidence for an $O_h \rightarrow D_8^\infty$ spontaneous symmetry breaking.

10:12AM A56.00012: Ab initio quantum chemical study of magnetic interactions in the honeycomb Kitaev-Heisenberg systems $\text{Cu}_2\text{IrO}_3$ and $\text{H}_3\text{LiIr}_2\text{O}_6$  MOHAMED ELDEEB (Presenter), RAVI YADAV, IFW - Dresden, NIKOLAY BOGDANOV, Max Planck Institute for Solid State Research, RAJYAVARDHAN RAY, SATOSHI NISHIMOTO, JEROEN VAN DEN BRINK, LIVIU HOZOI, IFW - Dresden — The magnetic interactions in honeycomb iridium oxide compounds are studied using quantum chemical wavefunction-based methods. Mapping the results onto the corresponding effective spin model shows the crucial dependence of the anisotropic magnetic couplings, in particular Kitaev exchange, on the precise position of inter-layer species and on additional geometrical factors such as Ir-O-Ir bond angles and Ir-O bond lengths. While the latter define the actual superexchange path between magnetic centers, the former may come into play through strong out-of-plane polarization of ligand 2p orbitals mediating intersite hopping [1,2].

**10:24AM A56.00013: Kitaev material candidates beyond the Iridates**

ARUN RAMANATHAN (Presenter), MARCUS DAUM, MARTIN MOURIGAL, HENRY S LA PIERRE, Georgia Inst of Tech — Na2MO3 (M = a tetravalent metal) based Mott insulators have been studied recently as potential candidates to realize Kitaev spin model. 4d5 or 5d5 systems on a Honeycomb lattice exhibit spinorbit assisted Mott insulating ground states. At the strong SOC regime, the ground state for these ions in an octahedral crystal field is dominated by Jeff=1/2 states resulting in bond-dependent anisotropic magnetic exchange in the plane, essential to realize the Kitaev spin model. However, candidates to realize the Kitaev spin model are not limited to 4d/5d systems. Lanthanide elements with significant SOC and inherent anisotropy can also be considered in this context. In this talk, I will present our work on a new lanthanide-based, Kitaev material candidate with a potential Jeff=1/2 ground state. Synthesis and structure of the material will be discussed. Physical property measurements coupled with inelastic neutron scattering results will be utilized to understand the single-ion characteristics of the lanthanide and to unveil the rich low-temperature physics of the material.

**10:36AM A56.00014: Ferrimagnetism and anisotropic phase tunability by magnetic fields in Na2Co2TeO6**

WEILIANG YAO (Presenter), YUAN LI, Peking Univ — Na2Co2TeO6 is a honeycomb-lattice compound with a zigzag antiferromagnetic order [1,2]. It has recently been proposed to be a Kitaev-like magnet based on high-spin d7 electron configuration [3,4]. To assess how close it is to realizing Kitaev quantum spin liquids, we have measured magnetization and specific heat on high-quality single crystals in magnetic fields applied along high-symmetry directions [5]. With small training fields, we find a canonical ferrimagnetic behavior below 27 K, which reveals additional Neel-type order of canted moments. Moreover, moderate fields in the honeycomb plane can suppress the thermal transition at 27 K, and seem to partly reverse the moment-canting when applied perpendicular to the zigzag chains. In contrast, out-of-plane fields leave the transition largely unaffected, but promotes another transition below 10 K, possibly also related to canting reversal. Our study indicates the magnetism of Na2Co2TeO6 is highly anisotropic and close to tipping points between competing phases.

We study magnetic structures and excitations in the series of A2PrO3 (A: alkali metals) by performing neutron scattering experiments. In these compounds, tetravalent praseodymium ions reside in edge-sharing PrO6 octahedra and the 4 f1 electrons exhibit Jeff=1/2 ground state doublet which result from a strong spin-orbital coupling and a weak octahedral crystal field. Furthermore, it was proposed that for A=Li, Na, the interactions are anti-ferromagnetic and dominantly Kitaev-type and therefore offer a potential playground for quantum spin liquid. We show evidence of anti-ferromagnetic phase transitions in such materials and provide possible effective Hamiltonians that will guide further searches for Kitaev spin liquids in rare earth compounds.

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A57 DMP: Electronic and Optical Properties of 2D Materials I
Mile High Ballroom 3A - Jie Shan, Case Western Reserve University - Tag(s): Focus

8:00AM A57.00001: Substituient Modified Covalent Organic Frameworks for Applications in Size Selective Separations*  VALERIE KUEHL (Presenter), PHUOC H.H. DUONG, JIASHI YIN, KATIE LI-OAKEY, WILLIAM D. RICE, BRUCE PARKINSON, JOHN HOBÉRG, Univ of Wyoming — Despite efforts, controlled placement of atoms, dopants, vacancies, and intercalates into crystalline lattices is only achieved in few systems and limited circumstances. Recent developments using metal or covalent organic frameworks (MOFs/COFs) show promise as synthetically configurable motifs. COFs are frameworks whose crystals are punctuated by a lattice of ordered nanopores where size, spacing, and filling are controlled. These nanopores are populated with substituents creating tailored properties for charge/size selective separations, particular emission properties, and Fermi level control. Here, we present the synthesis, characterization, and functional properties of four different COFs. Characterization includes atomic force microscopy, X-ray diffraction, and electron microscopy to show that the COFs are 2D, crystalline, and uniform, respectively. Finally, we show that COFs can be used to separate ions and proteins by size/charge, demonstrating the technological utility of these materials.

*Funding provided by the Department of Energy Grant #DE-SC0020100, National Institute of General Medical Sciences (P20GM103432) from the National Institutes of Health, Wyoming Water Development Commission (RN 20616), and U.S. Geological Survey/Department of Interior (G11AP20075).
8:12AM A57.00002: Anharmonic renormalization of flexural acoustic modes in graphene and their effect on the mechanical stability of the membrane UNAI ASEGINOLAZA (Presenter), AITOR BERGARA, ION ERREA, Centro de Física de Materiales — The mechanical stability and long-range crystalline order of two dimensional materials has always been under debate [1], however, since the discovery of graphene, the debate is only theoretical. 2D materials are invariant upon any rotation by putting the axis in the plane where the system is. This symmetry obliges the harmonic dispersion of the acoustic out-of-plane modes to be quadratic close to the point gamma in the first Brillouin zone, instead of linear, and this functionality makes the membrane unstable. The instability is translated as diverging atomic displacements as a function of the sample size and finite line width of phonons with very low crystal momentum [2].

These instabilities arise within the harmonic approximation, however, an anharmonic approach may suppress them. In this work we apply an anharmonic method named stochastic self-consistent harmonic approximation [3]. We see that the inclusion of anharmonic effects suppresses the divergence in the atomic displacements and provides a vanishing line width to the phonons with very low crystal momentum.


8:24AM A57.00003: Phonon lifetimes and scattering processes in carbon fiber systems JENNIFER NIEDZIELA (Presenter), ANDREW MISKOWIEC, JOHN J LANGFORD, ZACHARY BRUBAKER, SARA B ISBILL, ASHLEY SHIELDS, ROGER J KAPSIMALIS, Oak Ridge National Lab — Carbon fibers show ultrahigh strength to weight ratio and are sought as a replacement for steel in numerous industries. The basic morphology of carbon fiber is a collection of graphitic regions, with a higher degree of graphitization correlated with a higher stiffness fiber. Currently carbon fiber applications are limited by the inability to obtain high strength and high stiffness in the same fiber, which is presumably due to the effect of defects in the carbon fiber matrix. Here we present an overview of the microstructure and spectral features of carbon fiber obtained from Raman and x-ray scattering spanning a broad range of carbon fiber mechanical properties. The combined results show a direct correlation between estimated interdefect distance and ultimate fiber strength and a reduction in overall phonon lifetime for defect-mediated modes for high strength fibers. Efforts to understand phonon transport across defect boundaries in large scale models of defected graphite analogues are underway and will be briefly discussed.
8:36AM A57.00004: Role of grain orientation mismatch in friction of graphene layers using the Lennard-Jones and DRIP potentials*  HUYAN LI (Presenter), WOO KYUN KIM, Univ of Cincinnati — Graphene, as a one-atom thick 2-D material, is an ideal solid lubricant for small length scale devices such as micro/electro-mechanical systems. Without an accurate interatomic potential, the friction property of graphene is difficult to predict properly. In this study, two interatomic potentials, Lennard-Jones (LJ) and dihedral-angle-corrected registry-dependent interlayer (DRIP), are used to model interlayer interactions in friction simulations of multilayer graphene models. Both potentials have similar attractive interactions, but the DRIP potential considers the dihedral angle as well as the bond distance to model the repulsive interaction. We investigate the friction properties between a pristine layer and a single grain layer with different orientation angles using molecular dynamics (MD) simulations. The simulation results reveal that the LJ potential shows an increase in friction at misorientation angle of about 0.3° compared to a model with an angle of 0°. On the contrary, the DRIP models exhibit a monotonous decrease with increasing misorientation angle, which is attributed by the change in potential energy surface due to the dihedral angle.

*Acknowledgement: This work was in part supported by NSF CMMI 1662666.

8:48AM A57.00005: Particle swarm optimized interatomic potentials for novel 2D materials for temperature dependent vibrational properties  OGUZ GULSEREN (Presenter), ARASH MOBARAKI, Bilkent Univ, CEM SEVIK, Mechanical Engineering, Eskisehir Technical University — Two-dimensional materials are expected to become key components for novel applications because of their exotic properties. Predicting the mechanical and thermal properties of two dimensional materials is an essential task necessary for their implementation in device applications. Fully understanding of most of the material properties needs an atomistic description. Although, rigorous density functional theory based calculations are able to predict mechanical and electronic properties, mostly they are limited to zero temperature. Classical molecular dynamics facilitates the investigation of temperature dependent properties, but its performance highly depends on the potential used for defining interactions between the atoms. In this study, we calculated temperature dependent phonon properties of several single layer 2D systems including graphene, silicene, group III nitrides, i.e GaN, AlN and BN, and TMDs by developing particle swarm optimized Stillinger-Weber type potentials with respect to the first-principles datasets. These potentials validated by comparing the resulted phonon dispersion curves and thermal conductivities with available first-principles and experimental results.
Several layered transition metal dichalcogenides (TMDs) exhibit unusually high transition temperatures to different charge-density-wave (CDW) symmetry-reducing phases, revealing interesting physics, and opening possibility for practical applications of such materials. One of the most promising materials, 1T-TaS2, has the CDW transition between the nearly-commensurate (NC-CDW) and the incommensurate (IC-CDW) phases at 350 K, the transition to the normal metal phase at 550 K – 600 K. In this invited talk, I will review our recent results on controlling the CDW phase transitions in 2D materials with applied electric bias, and monitoring them via low-frequency electronic noise spectroscopy [1-6]. The noise spectroscopy has been particularly effective for monitoring the switching from the IC-CDW phase to the normal metal phase in 1T-TaS2. The noise spectral density exhibits sharp increases at the phase transition points, which correspond to the step-like changes in resistivity. The noise spectroscopy was instrumental in revealing the “hidden phase transitions” in vertical 1T-TaS2 devices. Preliminary data on the “narrow-band noise” in quasi-2D CDW devices will also be presented. We found that the 1T-TaS2 CDW devices reveal exceptional hardness against X-ray and proton radiations. We explained this property of the CDW devices by the high carrier concentration in all their phase states, two-terminal design, and the thin-film channel geometry.


*This work was supported, in part, by NSF through DMREF: Data Driven Discovery of van der Waals Bonded Solids, and by the UC – National Laboratory Collaborative Research and Training Program.
Impact of intrinsic and extrinsic imperfections on the electronic and optical properties of MoS$_2$* [Invited]  

URSULA WURSTBAUER, University of Muenster, JULIAN KLEIN (Presenter), Walter Schottky Institute of Munich Technical University — Substrate, environment and lattice imperfections have strong impact on the local electronic structure and the optical properties of atomically thin transition metal dichalcogenides. Moreover, luminescent centers can be created on demand and with nm lateral precision using a focused helium ion beam [1,2]. We report on a combined optical and scanning tunneling spectroscopy (STS) study of MoS$_2$ on SiO$_2$ and hBN substrate. We demonstrate that apparent band gap for MoS$_2$ on SiO$_2$ is significantly reduced compared to MoS$_2$ what can be explained by a substantial amount of band tail states near the conduction band edge of MoS$_2$. The presence of those states in STS can be linked to a broad red-shifted PL peak that are all strongly diminished or even absent using high quality hBN substrates [3]. Suppression of the L peak by hBN encapsulation enables to spectrally isolate a very narrow emission potentially serving as single photon source that can be precisely engineered by the focused helium ion beam [4].


*Work was done in close collaboration with J. Klein, A. Kerelsky, M. Lorke, M. Florian, F. Sigger, J. Kiemle, M. C. Reuter, T. Taniguchi, K. Watanabe, J. J. Finley, A. Pasupathy, A. W. Holleitner, F. M. Ross. We acknowledge financial support by DFG.

Nanocharacterization of 2D Hybrid Materials by Near-Field Microscopy*  

TETYANA IGNATOVA (Presenter), Nanoscience, Univ of NC - Greensboro, SLAVA V. ROTKIN, Engineering Science and Mechanics, Penn State University — Methods of Near-Field Microscopy are high-throughput non-destructive techniques, which can be used for characterization of 2D Hybrid Materials with sub-micrometer resolution as well as for device inspection. Here we show near field data on 2D samples with various electronic properties, from metals to semiconductors. Simple physical models are proposed for near-field analysis.

*To the Pennsylvania State University 2DCC-MIP supported by NSF cooperative agreement DMR-1539916. To the JSNN, a member of Southeastern Nanotechnology Infrastructure Corridor (SEニック) and National Nanotechnology Coordinated Infrastructure (NNCI), supported by NSF ECCS-1542174. To the UNCG Faculty First Award.
10:24 AM A57.00009: One Dimensional Electronic Structure Studies on Monolayer MoS$_2$ Grain Boundaries  
JUN JUNG (Presenter), YONG-HYUN KIM, Department of Physics, KAIST — On the boundary of the material, low dimensional electronic states, which are localized on the boundary, can be created. In this research, we have investigated grain boundaries of monolayer MoS$_2$ as a platform of one-dimensional (1D) physics. We have studied the electronics structures by density-functional theory calculations. We have designed a specific atomic structure of the boundary so that defect states show significantly low bandwidth, comparing to the bulk band. Due to low bandwidth, electrons can create spin or charge order on the boundary. Magnetism is obtained when electron doped case, which can be realized by MoS$_2$/Graphene heterojunction. Energetically the system favors antiferromagnetism compared to ferromagnetism. These magnetic orders solely derived from electronic structure instabilities. In addition to that, charge density wave can also be formed on the boundary of the grains. Our research suggests possibility of 1D interacting electrons on transition metal dichalcogenide grain boundaries.

10:36 AM A57.00010: Analysis of Raman scattering spectra of single-layer graphene doped with an ionic liquid*  
DAIKI INUKAI (Presenter), TAKESHI KOYAMA, Nagoya Univ, KENJI KAWAHARA, HIROKI AGO, Kyushu Univ, HIDEO KISHIDA, Nagoya Univ — Fundamental understanding of the electronic states of electrochemically doped single-layer graphene is essential for achievement of electric and electronic graphene devices. We fabricated a planar-type electrochemical cell operated with an ionic liquid, which is suitable for spectroscopic measurements. In the cell, the electric double layer induced by application of voltage results in high doping density. We observed Raman active phonon modes of graphene at various doping levels. The spectral shape of the G phonon mode reflects the effect of Fano resonance between the phonon excitation and the electronic excitation and becomes asymmetric depending on the degree of the effect. We performed a fitting analysis using a Breit-Wigner-Fano function to estimate the strength of the Fano coupling. On basis of the analysis, we discuss the electronic states of the single-layer graphene doped with ionic liquid.

*This work was supported by DII Collaborative Graduate Program for Accelerating Innovation in Future Electronics, Nagoya University and JSPS KAKENHI Grant Numbers 17H02764 and 18H03864.

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A58 DCP DCOMP DPOLY DCMP: DFT and Beyond I Mile High Ballroom 3B
- Jianwei Sun, Tulane Univ - Tag(s): Focus
The Predictive Power of Exact Constraints and Appropriate Norms in Density Functional Theory

JOHN P. PERDEW (Presenter), Depts. of Physics and Chemistry, Temple University — Approximations to the density functional for the exchange-correlation energy of Kohn-Sham theory can be constructed by fitting to data sets for bonded systems, or by satisfying exact mathematical constraints on the functional and appropriate norms (such as the uniform electron gas), or both. Fitting is interpolative, and can predict accurately for systems similar to those in the data sets, while satisfying exact constraints makes a functional more widely predictive over the immense space of possible molecules and materials. For example, the SCAN (strongly constrained and appropriately normed) functional [1] satisfies all 17 exact constraints that a computationally-efficient meta-generalized gradient approximation can, and has been remarkably successful for some complex materials (like liquid water [2]) and some strongly-correlated materials (like the cuprate high-temperature superconducting materials [3,4]). Prospects for an improved SCAN and for the correction of its residual self-interaction error will also be discussed.


**8:36AM A58.00002: Assessment of DFAs in predicting the magnetization of transition metal solids**

ALBERTO VELA (Presenter), CINVESTAV-IPN, KARLA A BOTELLO MANCILLA, ESIQIE, IPN, ANGEL M ALBAVERA MATA, CINVESTAV-IPN, SAMUEL TRICKEY, Quantum Theory Project, Department of Physics and Department of Chemistry, University of Florida, JOSE L GAZQUEZ, Chemistry, UAM-Iztapalapa — It has been recently reported that SCAN over stabilizes higher magnetic moments for the itinerant magnets Fe, Co and Ni.[1-4] Here we present and discuss the performance of a variety of generalized and meta-generalized gradient approximations, including our recently proposed locally parameterized GGAs, on the magnetic properties of a set composed of 3d, 4d and 5d metals, a total of 29 solids. Detailed analyses of the itinerant magnets further show different behaviors between the band structures calculated with SCAN versus those with PBE [5] and SCAN-L [6,7] at the magnetization saturation.


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**8:48AM A58.00003: The Importance of Smoothness with Exact Constraints in Functional Design**

JAMES FURNESS (Presenter), Physics and Engineering Physics, Tulane University, AARON KAPLAN, JOHN P. PERDEW, Temple University, JIANWEI SUN, Physics and Engineering Physics, Tulane University — There are two core goals in exchange-correlation functional design: accuracy and efficiency. Whilst modern semi-local functionals have greatly improved accuracy, this has often been at the cost of efficiency. Our previous work [1], and that of others [2], has shown the iso-orbital indicator $\alpha$ as a key component in this sensitivity, compounded by sharply varying interpolation functions. In a recent publication [2] Bartók and Yates propose a regularised SCAN (rSCAN) that resolves these numerical problems for the SCAN functional [3] at the expense of breaking some exact constraints. The uniform electron gas and slowly varying density limits are broken, along with incorrect coordinate scaling of the regularised iso-orbital indicator $\alpha_r$.

We restore these constraints while preserving regularisation to give a new functional, $r^2$SCAN. We explore how constraint restoration affects accuracy and efficiency in simple systems for which exact constraints are important.


*U.S. DOE, Office of Sciences, Basic Energy Sciences Grant No. #DE-SC0019350
Analysis of over-magnetization of elemental transition metal solids from the SCAN and three related density functionals.*

DANIEL MEJIA-RODRIGUEZ (Presenter), SAM TRICKEY, University of Florida — Recent investigations have found that the strongly constrained and appropriately normed (SCAN) meta-generalized gradient approximation exchange-correlation functional significantly over-magnetizes elemental Fe, Co, and Ni solids [1]. The difficulty does not occur in SCAN-L (deorbitalized SCAN) [2]. The problem have been traced to the tendency to favor integer occupations, similar to a DFT+U treatment [3]. We discuss what properties of the SCAN, revSCAN and rSCAN functional forms are responsible for such errors, and why the SCAN-L functional does much better in this respect [2].


*This work was supported by U.S. Department of Energy grant DE-SC0002139.
S.B.T. also was supported by U.S. Department of Energy Energy Frontier Research Center grant DE-SC0019330.

Failure of the SCAN functional for itinerant magnets and the reasons*

DAVID SINGH (Presenter), YUHAO FU, Univ of Missouri - Columbia — The SCAN functional fails dramatically in its description of itinerant magnets including the elements Fe, Ni and Co. We report that SCAN is closer in behavior to functionals that yield localized behavior, such as hybrid functionals, than other semilocal functionals that are tested. The results are understood in terms of a tendency to differentiate orbitals, favoring integer occupation, which is necessary for a correct description of atomic systems, but inappropriate for the open shell metallic ferromagnetic metals. This has to do with the fitted nature of SCAN where it reproduces selected “norms”.

*Work supported by the U.S. Department of Energy, Basic Energy Sciences, Award DE-SC0019114.
9:24AM A58.00006: Assessment of SCAN and regularized SCAN functional with and without self-interaction correction

ALAN SALCEDO (Presenter), YOH YAMAMOTO, TUNNA BARUAH, RAJENDRA ZOPE, University of Texas at El Paso — The Strongly Constrained and Appropriately Normed (SCAN) is a non-empirical meta-GGA functional that satisfies all the known 17 exact constraints that a meta-GGA functional can. Its numerical implementation is challenging and its use requires extremely fine numerical grids. The numerical issues become even more pronounced for the Perdew-Zunger (PZ) self-interaction correction (SIC) method as it requires evaluating the functional and its derivatives with orbital density that varies rapidly compared to total density. Bartok and Yates recently proposed a modification to SCAN, called regularized SCAN (rSCAN) to remove some of the numerical instabilities of SCAN. We have implemented rSCAN functional in our Fermi-Lowdin Self-Interaction Correction code and performed assessment of rSCAN for various molecular properties using standard datasets. We find rSCAN gives similar results to SCAN despite violation of some of the constraints and requires comparatively coarser grids than SCAN. However, like SCAN, rSCAN also shows numerical instabilities in PZ-SIC calculations where orbital densities are used. This problem is due to the use of variable $\alpha$ in these functionals. A solution to this numerical instability is suggested and implemented.

*U.S. DOE under grants DE-SC0018331 and DE-SC0006818.

9:36AM A58.00007: Systematizing Approximate Density Functional Design

AARON KAPLAN (Presenter), Temple University, JAMES FURNESS, JIANWEI SUN, Tulane University, JOHN P. PERDEW, Temple University — A meta-GGA with well-rounded accuracy and efficient numerical performance for all many-electron systems has proved to be elusive. TPSS, while accurate for many systems, never reaches predictive accuracy. SCAN [1], motivated by a need to systematize development of approximate density functionals, is often predictive, but falters for metallic systems [2]. In this talk, I'll discuss the need to further systematize the construction of approximate density functionals. The design of possible successors to SCAN, with results for transition metals and weakly-bonded systems, as well as improvements in meta-GGA numeric efficiency from new iso-orbital indicators [3] will also be discussed.


*This work was supported by DOE, BES, grant No. DE-SC001255.
Evaluating exchange correlation performance on structural prediction from GGA to metaGGA*  
PEDRAM TAVADZE (Presenter), Department of Physics, West Virginia University, MATTHIEU J VERSTRAETE, Department of Physics, Université de Liège, ALDO H ROMERO, Department of Physics, West Virginia University — The use of density functional theory in materials prediction and structural characterization is a very well-established field. We use this methodology in a high throughput framework, where thousands of materials are analyzed and classified in databases. This step has become quite standard and many databases do not discuss their most basic approximation: which exchange correlation functional has been used. While much work has been done on the functional dependency of the cell parameters and ground state space group, little is known for the internal degrees of freedom. A crystal structure can be reduced to the cell parameters and the Wyckoff positions (WPs), some of which can add additional degrees of freedom to the crystal structure. In this work we analyze the effect on the internal degrees of freedom of more than 1500 structures, both metallic and semiconductor materials from completely local functionals as LDA up to meta-GGAs using the recently introduced SCAN.

*WVU Thorny Flat supercomputer, DMREF-NSF 1434897, NSF OAC-1740111 and DOE DE-SC0016176 projects

Single Hamiltonian for self-interaction corrected DFT with Fermi-Lowdin orbitals  
TUNNA BARUAH (Presenter), MARK PEDERSON, University of Texas, El Paso — The self-interaction error in density functional approximation arises from the incomplete cancellation of self-Coulomb by self-exchange. The self-interaction correction proposed by Perdew and Zunger corrects for this error through an orbital by orbital scheme. The resulting SI corrected potential for the electrons becomes orbital dependent. The original SI corrected energy was not unitarily invariant with respect to orbital transformations. The energy minimization requires finding the set of orbitals that minimizes the total energy. Recent development of Fermi-Lowdin orbital based self-interaction correction scheme is a step forward in that energy is unitarily invariant under orbital transformation to localized Fermi Lowdin orbitals. We show that within the Fermi-Lowdin orbital based self-interaction correction scheme it is also possible to derive a single Kohn-Sham multiplicative Hamiltonian for all orbitals which decreases the computational complexity. Implementation of this method is discussed and the results show that the energy is slightly lower and required time is significantly less than other approximate methods for obtaining the canonical orbitals.
10:12AM A58.00010: Self-interaction correction and dielectric properties of molecules
KUSHANTHA WITHANAGE (Presenter), ALEXANDER I JOHNSON, JUAN PERALTA, Central Michigan Univ, YOH YAMAMOTO, RAJENDRA ZOPE, TUNNA BARUAH, Physics, University of Texas, El Paso, KOBLAR ALAN JACKSON, Central Michigan Univ — We recently used the Fermi-Löwdin orbital implementation of the Perdew-Zunger self-interaction correction (FLO-SIC) to study the impact of self-interaction error on the prediction of dipole moments of molecules and polarizabilities for atoms (DOI: 10.1103/PhysRevA.100.012505). Using FLO-SIC in conjunction with the local spin density approximation (LSDA), the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation, and the strongly-constrained and appropriately normed (SCAN) meta-GGA, we have found that application of SIC generally improves predictions, but typically results in overshooting reference values. In this talk, we examine this overcorrection and discuss simple approaches to overcome it.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0018331.

10:24AM A58.00011: Fermi-Löwdin self-interaction correction for ground and excited states
SANTOSH ADHIKARI (Presenter), Department of Physics, Temple University, RAJENDRA RZOPE, CARLOS DIAZ, Department of Physics, The University of Texas at El Paso, ADRIENN RUZSINSZKY, Department of Physics, Temple University — Self-interaction error (SIE) is strongly present in ground-state density functional theory (DFT) and propagates into time-dependent DFT as well. A significant requirement of the self-interaction correction (SIC) is the localization of the orbitals, as required by size-consistency. In 2014, Pederson and collaborators recommended a computationally much more attractive version of the earlier Perdew-Zunger (PZ) SIC [1]. This SIC utilizes Fermi orbitals, greatly restricting the number of possible unitary transformations of the occupied Kohn-Sham orbitals. This work is a straightforward continuation of the Fermi orbital PZ-SIC to test crucial physical properties relevant for both ground, and excited states, with the potential to eliminate SIE for excitation energies.


*This work was supported by the Department of Energy under Grant No. DE-SC0018331.
Assisting the performance of self-interaction-corrected SCAN meta-GGA functional using an orbital scaling approach

YOH YAMAMOTO (Presenter), RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — Semilocal density functional approximations (DFAs) suffer from self-interaction (SI) error which limits their applicability. The Perdew-Zunger SI correction (PZSIC) improves the description of properties such as barrier heights or dissociation energies where SI error is dominant but it degrades already good performance of DFAs when applied to GGA and meta-GGA functionals. We implemented the orbital scaling approach of Vydrov et al.[1] that scales down orbital wise PZSIC in the FLOSIC code and use it with SCAN functional to assess its performance for a wide range of properties such as total energies, ionization potentials, and electron affinities for atoms, and atomization energies, dissociation and reaction energies, and reaction barrier heights of molecules. Our results show that orbital scaling recovers the performance of SCAN that is lost with SIC. We suggest a modification to recover \(-1/r\) asymptotic behavior of the potential lost by the scaling scheme of Vydrov et al. We also discuss the cases where the orbital scaling is not successful. General strategies of applying the scaling and how to improve its performance will be discussed in this talk.


*U.S. DOE under grants DE-SC0018331 and DE-SC0006818.

Monday, March 2, 2020 8:00 AM - 10:48 AM

Session A59 DMP: Magnetic Weyl Semimetals: Materials Discovery

High Ballroom 3C - Tag(s): Focus
Stabilizing ferromagnetism in the Weyl semimetal candidate EuCd$_2$As$_2$*

BRINDA KUTHANAZHI (Presenter), NA HYUN JO, YUN WU, Iowa State University/Ames Laboratory, TAE-HOON KIM, LIN ZHOU, Ames Laboratory, ERIK I TIMMONS, Iowa State University/Ames Laboratory, LIN-LIN WANG, ANDRIY PALASYUK, Ames Laboratory, KYUNGCHAN LEE, BENJAMIN SCHRUNK, Iowa State University/Ames Laboratory, BENJAMIN UELAND, Ames Laboratory, ANTON BURKOV, University of Waterloo, RUSLAN PROZOROV, SERGEY L. BUD’KO, ADAM KAMINSKI, PAUL C CANFIELD, Iowa State University/Ames Laboratory — EuCd$_2$As$_2$ is predicted to host a variety of topological features in its band structure depending on its magnetic ground state. A ferromagnetic state with spins oriented along the crystallographic c axis is expected to have a single pair of Weyl points near the Fermi energy. [1] Previously published work on EuCd$_2$As$_2$ report it to have an antiferromagnetic ground state. [2,3] Here, we present the synthesis and characterization of single crystals of EuCd$_2$As$_2$ that, with varying initial stoichiometries, can be tuned from an antiferromagnetic ground state (T$_N$ ~ 9.5 K) to a ground state with a clear ferromagnetic component (T$_C$ ~ 30 K). Measurements of magnetization, magneto-optical Kerr rotation, specific heat and resistivity will be presented and discussed.


*This work was carried out at Iowa State University and supported by Ames Laboratory, US DOE, under Contract No. DEAC0207CH11358 and the Center for Advancement of Topological Semimetals, an Energy Frontier Research Center funded by the U.S. DOE, Office of Basic Energy Sciences and by the Gordon and Betty Moore Foundation (NHJ).

A New Magnetic Topological Quantum Material Candidate by Design: EuSn$_2$P$_2$

XIN GUI (Presenter), Louisiana State University, Baton Rouge, IVO PLETIKOSIC, Princeton University, HUIBO CAO, Oak Ridge National Lab, HUNG-JU TIEN, National Cheng Kung University, XITONG XU, Peking University, RUIDAN ZHONG, Princeton University, GUANGQIANG WANG, Peking University, TAY-RONG CHANG, National Cheng Kung University, SHUANG JIA, Peking University, TONICA VALLA, Brookhaven National Lab, WEIWEI XIE, Louisiana State University, Baton Rouge, ROBERT J. CAVA, Princeton University — Magnetism, when combined with an unconventional electronic band structure, can give rise to forefront electronic properties such as the quantum anomalous Hall effect, axion electrodynamics and Majorana fermions. Here we report the characterization of high-quality crystals of EuSn$_2$P$_2$, a new quantum material specifically designed to engender unconventional electronic states plus magnetism. EuSn$_2$P$_2$ has a layered, Bi$_2$Te$_3$-type structure. Ferromagnetic interactions dominate the Curie-Weiss susceptibility, but a transition to antiferromagnetic ordering occurs near 30 K. Neutron diffraction reveals that this is due to two-dimensional ferromagnetic spin alignment within individual Eu layers and antiferromagnetic alignment between layers - this magnetic state surrounds the Sn-P layers at low temperatures. The bulk electrical resistivity is sensitive to the magnetism. Electronic structure calculations reveal that EuSn$_2$P$_2$ might be a strong topological insulator, which can be a new magnetic topological quantum material (MTQM) candidate. The calculations show that surface states should be present, and they are indeed observed by ARPES measurements.
8:24AM A59.00003: Angle resolved photoemission spectroscopy study on EuCd$_2$As$_2$*  

HYUN JO (Presenter), YUN WU, Department of Physics and Astronomy, Ames Laboratory/Iowa State University, LIN-LIN WANG, Ames Laboratory, KYUNGCHAN LEE, BRINDA KUTHANAZHI, BENJAMIN SCHRUNK, SERGEY L. BUD'KO, PAUL C CANFIELD, ADAM KAMINSKI, Department of Physics and Astronomy, Ames Laboratory/Iowa State University — Recently, DFT calculations on EuCd$_2$As$_2$ in a FM ordered state with Eu moments aligned along the c-axis revealed a single pair of Weyl points. However, previous experimental studies on EuCd$_2$As$_2$ show that the magnetism is an A-type AFM with $T_N \approx 9.5$ K. Here, by discovering and taking advantage of EuCd$_2$As$_2$ chemical tunability, we report successful growths of single crystals of EuCd$_2$As$_2$ with two different magnetic ground states: FM-EuCd$_2$As$_2$ and AFM-EuCd$_2$As$_2$. Angle resolved photoemission spectroscopy shows an anomalous suppression of scattering in ferromagnetic Weyl semimetal candidate EuCd$_2$As$_2$. Unexpectedly, scattering rate is suppressed only in one of the bands over limited energy range that is controlled by presence of another, completely filled band. Such selectivity is highly unusual and can have potential impact on spin transport.

*This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering. The research was formed at the Ames Laboratory. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358. NHJ, BK, LLW, were supported by the Center for Advancement of Topological Semimetals, an Energy Frontier Research Center.

8:36AM A59.00004: Ultrafast carrier dynamics in the ferromagnetic semimetal EuCd$_2$As$_2$*  

KENNETH O'NEAL (Presenter), LAMOYNE TYLER MIX, MIN-CHEOL LEE, Los Alamos National Laboratory, BRINDA KUTHANAZHI, NA HYUN JO, SERGEY L. BUD'KO, PAUL C CANFIELD, Ames Laboratory, Iowa State University, ROHIT P PRASANKUMAR, DZMITRY YAROTSKI, Los Alamos National Laboratory — We report the near-infrared pump-probe ultrafast response of the ferromagnetic candidate for Weyl semimetal EuCd$_2$As$_2$. A non-pulsewidth limited rise dynamic is followed by two distinct decay processes – a sub-picosecond decay attributed to electron-phonon relaxation and a several picosecond long process which stems from demagnetization of the in-plane magnetic moment. Exponential fits of the decay processes down to 6 K reveal sensitivity to the long range magnetic ordering. These findings indicate strong coupling between charge and spin degrees of freedom, a step towards magnetic field or light control of topological Weyl states.

*Research presented in this presentation was supported by the Laboratory Directed Research and Development program of Los Alamos National Laboratory under project number E1TT.
8:48AM A59.00005: Single crystal growth of Weyl semimetal candidates  SUDHA KRISHNAN (Presenter), TIGLET BESARA, Missouri State Univ — Following the discovery of topological Weyl semimetals in non-magnetic materials, ferromagnetic Weyl semimetals have now been discovered with materials such as YbMnBi$_2$, Co$_2$MnGa, and Co$_3$Sn$_2$S$_2$. With the different structures of the already discovered ferromagnetic Weyl semimetals, this suggests that more ternary intermetallic compounds can be found displaying the connection between ferromagnetism and topology. Here, we report a systematic growth study and search for other ternary intermetallics displaying magnetism and topology. We utilize metallic self-flux methods to grow single crystals of compounds isostructural to YbMnBi$_2$ and Co$_2$MnGa.

9:00AM A59.00006: Giant room temperature anomalous Hall effect and magnetically tuned topology in the ferromagnetic Weyl semimetal Co$_2$MnAl* PEIGANG LI, Tulane University, JAHYUN KOO (Presenter), Weizmann institute of science, WEI NING, Pennsylvania state University, JINGUO LI, Chinese Academy of Sciences, LEIXIN MIAO, LUJIN MIN, YANGLIN ZHU, YU WANG, NASIM ALEM, CHAO-XING LIU, Pennsylvania state University, ZHIQIANG MAO, Tulane University, BINGHAI YAN, Weizmann institute of science — Weyl semimetals have been extensively studied due to their exotic properties such as topological surface states and anomalous transport phenomena. Their band structure topology is usually predetermined by material parameters and can hardly be manipulated once the material is formed. By calculations and experiments, we reveal a tunable, giant anomalous Hall effect in the ferromagnet Co$_2$MnAl. The transition between Weyl points and nodal rings occurs when rotating the magnetization axis. We propose a material recipe to generate the giant anomalous Hall effect by gaping nodal rings without requiring the existence of Weyl points. In addition, experiments show the strong anomalous Hall effect even at room temperature with a large Hall angle 21%. Our work reveals an ideal intrinsically magnetic platform to explore the interplay between magnetic dynamics and topological physics for the development of a new generation of spintronic devices.

*We acknowledge the Willner Family Leadership Institute for the Weizmann Institute of Science, the Benoziyo Endowment Fund for the Advancement of Science, Ruth and Herman Albert Scholars Program for New Scientists, and the European Research Council (ERC grant No. 815869).
9:12AM A59.00007: Magnetotransport properties and fermiology in a layered rare-earth intermetallics*  TAKASHI KURUMAJI (Presenter), MIN GU KANG, Physics, MIT, SHIANG FANG, Physics, Harvard University, DAVID E GRAF, NHMFL, LINDA YE, Physics, MIT, YANG ZHAO, NIST, MUN K. CHAN, NHMFL, TAKEHITO SUZUKI, RICCARDO COMIN, Physics, MIT, JEFFREY LYNN, NIST, JOSEPH G CHECKELSKY, Physics, MIT — While a growing number of nonmagnetic topological phases are being proposed and discovered, the search for materials that combine nontrivial electronic topology with strong correlations has advanced at a slower pace [1]. Most studies have focused on doping magnetic elements into nonmagnetic topological materials [2] in which random disorder and low magnetic transition temperature are inevitable. Realization of magnetic topological state in stoichiometric compounds has the potential to enable an approach to the intrinsic properties of the system, and provide a chance to design candidates for higher temperature quantized anomalous Hall effect and axion electrodynamics [3]. We will discuss our recent attempts to design, synthesize, and characterize magnetic topological semimetals with a focus on layered materials with non-trivial magnetic order arising from rare-earth ions. We will describe transport, spectroscopic, and neutron scattering measurements as well as ab-initio calculations to develop an understanding of their underlying electronic/magnetic structure.

References

*This research was supported in part by a JSPS overseas research fellowship.

9:24AM A59.00008: Layered Rare-Earth Intergrowth Compounds: A Platform for Correlated and Topological Properties*  [Invited] JULIA CHAN (Presenter), ASHLEY WEILAND, GREGORY MCCANDLESS, Chemistry, University of Texas at Dallas — The single crystalline growth of lanthanide based intermetallics has garnered much interest in the last two decades, primarily due to their unusual magnetic and electrical properties. To study the intrinsic and physical properties of highly correlated quantum systems, the growth of single crystalline intermetallics is critical. With our ongoing efforts to grow single crystals of rare earth materials, the opportunity exists to discover new compositions or robust structure types enabling subsequent substitution for correlation studies for compounds with competing magnetic behavior. In this talk, examples of the strategic selection of rare earth layered intergrowth compounds will be presented. In particular, we will present a new class of Ce-based intermetallics for fundamental correlation between the subunits and structural motifs common in highly correlated materials. To advance the field, discovering new families of highly correlated material is vital to the advancement of correlated and topological materials.

*NSF-DMR: 1700030
10:00AM A59.00009: Synthesis and characterization of a new topological semimetal enabled by a charge density wave*  SHIMING LEI (Presenter), JINGJING LIN, Princeton University, ANDREAS TOPP, CHRISTIAN R AST, Max Planck Institute for Solid State Research, N. PHUAN ONG, LESLIE SCHOOP, Princeton University — Formation of charge density waves (CDWs) is a known mechanism to induce an energy gap or partial energy gap at the Fermi surface. Therefore, introducing a CDW can be a way to modify the band structure. In this work, we discuss the potential of a CDW being the key to realize materials with clean topological semimetal band structures, by gapping out unwanted trivial states at the Fermi level. We will introduce a class of materials that exhibits CDWs and discuss the effect of the structural distortion on the electronic structure. Finally, we will present electrical transport and angle resolved photoemission spectroscopy (ARPES) data on one magnetic topological semimetal candidate, which was identified through this method.

*This research was supported by NSF through the Princeton Center for Complex Materials, a Materials Research Science and Engineering Center DMR-1420541 and by the Arnold and Mable Beckman foundation.

10:12AM A59.00010: Quantum Anomalous Hall Effect in Intrinsic Magnetic Topological Insulator MnBi₂Te₄  YUJUN DENG (Presenter), YIJUN YU, Fudan University, MENG ZHU SHI, University of Science and Technology of China, ZHONGXUN GUO, Fudan University, ZIHAN XU, SixCarbon Technology, JING WANG, Fudan University, XIANHUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Fudan University — In a magnetic topological insulator, nontrivial band topology conspires with magnetic order to produce exotic states of matter that are best exemplified by quantum anomalous Hall (QAH) insulators and axion insulators. Here, we probe quantum transport in MnBi₂Te₄ thin flake—a topological insulator with intrinsic magnetic order. In this layered van der Waals crystal, the ferromagnetic layers couple anti-parallel to each other, so bulk MnBi₂Te₄ is an antiferromagnet. Atomically thin MnBi₂Te₄, however, becomes ferromagnetic when the sample has odd number of septuple layers. Signatures of QAH effect are observed in few-layer MnBi₂Te₄ samples. Our results establish MnBi₂Te₄ as an ideal arena for further exploring various topological phenomena.
10:24AM A59.00011: Routes to quantum anomalous Hall effect from superlattice-like magnetic topological insulators* QIHANG LIU (Presenter), HONGYI SUN, PENGFEI LIU, Department of Physics, Southern University of Science and Technology, NI NI, CHAOWEI HU, Department of Physics and Astronomy, University of California, Los Angeles, KYLE GORDON, DANIEL DESSAU, University of Colorado, Boulder — Recently, MnBi$_2$Te$_4$ thin films were observed to manifest the quantum anomalous Hall effect (QAHE) at a temperature of 4.5 K under magnetic field. By realizing a bulk MnBi$_4$Te$_7$ with alternating [MnBi$_2$Te$_4$] and [Bi$_2$Te$_3$] layers, we suggest that MnBi$_4$Te$_7$ is a Z$_2$ antiferromagnetic topological insulator with a small out-of-plane saturation field of ~ 0.2 Tesla [1]. Using model Hamiltonian analysis and first-principle calculations, we then establish a topological phase diagram and map on it with different two-dimensional configurations, which is taken from the recently-grown magnetic topological insulators MnBi$_4$Te$_7$ and MnBi$_6$Te$_{10}$. These configurations manifest various topological phases, including quantum spin Hall effect with and without time-reversal symmetry, as well as QAHE. We then provide design principles to trigger QAHE by tuning experimentally accessible knobs, such as slab thickness and magnetization [2]. Our work reveals that superlattice-like magnetic topological insulators with tunable exchange interaction serve as an ideal platform to realize the long-sought QAHE in pristine compounds.


*This work was supported by the National Natural Science Foundation of China under Grant No. 11874195

10:36AM A59.00012: A new method for tuning topological insulators with large carrier densities (~10$^{20}$/cc) to CNP and beyond* HAIMING DENG (Presenter), LUKAS ZHAO, The City College of New York, KYUNGWHA PARK, Physics, Virginia Tech, LIA KRUSIN-ELBAUM, The City College of New York — We report a new powerful method for tuning chemical potential in topological materials, capable of changing carrier densities by more than 10$^{20}$/cc. It involves the incorporation of H$^+$ into the device structure. The process is reversible by low-temperature annealing (< 100°C), and a finetuning of the chemical potential is easily achieved. We demonstrate this method to be effective in a variety of 3D bulk topological insulators (TIs) (e.g. Bi$_2$Te$_3$ and Sb$_2$Te$_3$), as well as in intrinsic magnetic TIs, such as Mn(Bi, Sb)$_2$Te$_4$. For example, Bi$_2$Te$_3$ which is initially p-type with hole carrier densities of >10$^{19}$/cc is converted to n-type with n >10$^{19}$/cc. This electron doping method should apply to other materials as well. Using a proper annealing protocol, the chemical potential is finetuned across the charge-neutral point (CNP), where the Hall resistance exhibits the ambipolar behavior and $R_{xx}$ has a maximum at the type conversion. This method does not create additional defects that reduce carrier mobility, nor induce any significant top-bottom surface asymmetries typical of electrostatic gating. The mechanism responsible for the H$^+$ doping will be discussed.

*NSF-DMR-1420634, NSF HRD-1547830
Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A60 DMP: Topological Materials: Thin Films and Hybrid Structures Mile High Ballroom 4A - Seongshik Oh, Rutgers University, New Brunswick - Tag(s): Focus

8:00AM A60.00001: Exploring topological superconductivity in topological insulator – superconductor hybrid devices* [Invited] MORTEZA KAYYALHA (Presenter), Pennsylvania State University — Topological insulators (TIs) coupled to s-wave superconductors (SC) are predicted to harbor a topological superconducting phase. In this talk, I will first talk about the SC-TI-SC junctions, where an anomalous enhancement of the critical current at low temperatures and a highly non-sinusoidal current-phase relation were observed. These results suggest superconductivity is induced in the spin-helical topological surface states and point toward nearly ballistic nature of superconducting transport. I will then introduce our recent work about the induced SC in a quantum anomalous Hall (QAH) insulator, as a potential platform for the realization of “chiral Majorana modes”. A recent transport experiment claimed the half-quantized two-terminal conductance plateau in a millimeter-size QAH – Nb hybrid structure as evidence for the chiral Majorana modes. However, there are serious concerns about this interpretation because non-Majorana mechanisms can also generate similar signatures, especially in a disordered QAH system. I will present a systematic study of the superconducting contact transparency and its influence on the two-terminal conductance measurements and provide a non-Majorana explanation for the appearance of the half-quantized plateau in the QAH – Nb hybrid devices.

*This work is supported by the NSF-CAREER award (DMR-1847811) and the ARO grant (W911NF1810198).

8:36AM A60.00002: Majorana π-junctions in full-shell nanowire SQUIDs* DAVYDAS RAZMADZE (Presenter), EOIN C O’FARRELL, PETER KROGSTRUP, CHARLES MARCUS, Niels Bohr Institute, University of Copenhagen — Recent studies of InAs nanowires covered by full-shell Al superconductor showed signatures of Majorana zero modes (MZMs) around one applied axial-flux quantum [1]. Here, we study such wires in dc-SQUID geometry with a naturally-formed normal quantum dots in the Josephson junctions. In the trivial regime around zero axial-flux we find 0-π transition as the occupancy of a quantum dot is changed; the transition vanishes at one axial-flux quantum. In addition, we find that the critical currents of the Josephson junctions increase in the topological regime. Tunneling spectroscopy of a junction in the π-state reveals a discrete zero-energy state at one applied axial-flux quantum. Our observations are consistent with the theoretical models of MZMs coupling through a normal quantum dot [2,3].


*Research is supported by Microsoft Project Q and the Danish National Research Foundation. CMM acknowledges support from the Villum Foundation.
8:48AM A60.00003: Quantum anomalous Hall effect using interfacial Green’s function method for an accurate mass gap  JINWOONG KIM (Presenter), DAVID VANDERBILT, Rutgers University, New Brunswick — By using a Green’s function method with DFT-based tight-binding parameters, we investigate the quantum anomalous Hall (QAH) effect at the interface between topological insulators (SnTe, SnSe) and magnetic insulators (EuS, EuSe, EuTe). QAH or axionic states, a subject of recent broad interest, are achieved by introducing an effective Zeeman field to a topological insulator whose surface Dirac cone then acquires a mass gap, resulting in exotic electromagnetic responses within the mass gap. A number of studies have demonstrated the appearance of such states by using diverse interfacial, magnetic-element-doped, and magnetic-topological systems in agreement with predictions. Although achieving a large mass gap is critical for further investigations and room temperature devices, the microscopic mechanisms determining the size of the mass gap have not been clearly addressed. In this study, we enumerate several combinations of topological crystalline insulators and magnetic insulators in a search for an optimal electronic structure, where a large mass gap is isolated inside a bulk insulating gap. The underlying mechanisms and their dependence on factors such as an external field will be discussed.

9:00AM A60.00004: Topological phase transition in epitaxial single layer FeTe$_{1-x}$Se$_x$/SrTiO$_3$(001)*  QIANG ZOU (Presenter), ZHUOZHI GE, CHENHUI YAN, HUIMIN ZHANG, LIAN LI, West Virginia University — Recent work shows evidence of topological superconductivity on the (001) surface of FeTeSe bulk crystals. In this work, we demonstrate both superconducting and topological phase transitions at higher temperature in FeTe$_{1-x}$Se$_x$ thin films, by reducing its thickness down to one atomic layer. High quality single layer FeTe$_{1-x}$Se$_x$ films are grown on SrTiO$_3$(001) substrate by molecular beam epitaxy and characterized by in situ scanning tunneling microscopy/spectroscopy and angle-resolved photoemission spectroscopy. We find the topological and superconducting properties to be strongly dependent on the Te concentration, which controls spin-orbit coupling. With increasing Te, the top of the valence band at the Γ point moves towards and then crosses the Fermi level, accompanied by a change of the band profile from parabolic to linear. Above a critical Te concentration of 80%, the linear valence band reverts back to parabolic and shifts back down below the Fermi level, characteristic of a topological phase transition. These findings and their implications for the emergence of topological phases in Fe-based superconductors at reduced dimensions will be presented at the meeting.

*This research is supported by DOE (DE-SC0017632).
Tuning the electrical properties of GdSb thin films by epitaxial strain

HADASS INBAR (Presenter), Materials, University of California, Santa Barbara, SHOUVIK CHATTERJEE, MIHIR PENDHARKAR, Electrical & Computer Engineering, University of California, Santa Barbara, YU HAO CHANG, MAXWELL MILES BOCHEFF, TAOZHI GUO, TOBIAS L BROWN-HEFT, Materials, University of California, Santa Barbara, ALEXEI V FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, DAN READ, School of Physics and Astronomy, Cardiff University, CHRIS J PALMSTROM, Materials and Electrical & Comp. Eng, University of California, Santa Barbara — Early studies of rare-earth monopnictide (RE-V) thin films have focused mainly on their applications as buried ohmic contacts for III-V semiconductors, THz emitters and detectors, thermoelectrics, diffusion barriers, and plasmonic heterostructures. Recent predictions of topological semimetallic states and observations of extremely large magnetoresistance (XMR) in RE-Vs, and specifically GdSb, have opened up a new research front aimed at studying the interplay between magnetic ordering and XMR. Here we demonstrate the epitaxial growth and characterization of GdSb thin films with thickness varied from 3-60 nm and biaxial strains ranging from -2% to +2% lattice-mismatch. Utilizing x-ray diffraction, in-vacuo angle-resolved photoemission spectroscopy, SQUID magnetometry and magnetotransport measurements we map out shifts in energy bands and trends in exchange interaction parameters due to dimensional confinement and biaxial strain.

*Synthesis and ARPES experiments are supported by the US DOE (Contract No. DE-SC0014388). Development of the growth facilities and low temp. magnetotransport measurements are supported by the ONR VBFF Award No. N00014-15-1-2845. This research used resources of the ALS, which is a DOE Office of Science User Facility under contract No. DEAC02- 05CH11231.
Quantum transport in in-plane selective area InSb-Al nanowire quantum networks

DI XU (Presenter), QuTech and Kavli Institute of Nanoscience, Delft University of Technology, ROY OP HET VELD, Department of Applied Physics, Eindhoven University of Technology, VANESSA SCHALLER, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, JASON JUNG, Department of Applied Physics, Eindhoven University of Technology, QINGZHEN WANG, MICHIEL DE MOOR, BART HESSELMANN, KIEFER VERMEULEN, JOURI BOMMER, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, JOON SUE LEE, California Nanosystems Institute, University of California Santa Barbara, MIHIR PENDHARKAR, CHRIS J PALMSTROM, Electrical and Computer Engineering, University of California Santa Barbara, ERIK BAKKERS, Department of Applied Physics, Eindhoven University of Technology, LEO P KOUWENHOVEN, HAO ZHANG, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Strong spin-orbit semiconductor nanowires coupled to a superconductor are predicted to host Majorana zero modes. Exchange (braiding) operations of the Majorana modes form the logical gates of a topological quantum computer and require a network of nanowires. Here, we implement an in-plane selective-area growth technique for InSb-Al allowing complex semiconductor-superconductor nanowire networks with excellent quantum transport properties. Essential quantum transport phenomena for topological quantum computing are demonstrated in these structures including phase-coherent transport up to 5 harmonics of Aharonov-Bohm oscillations with a phase coherence length of ~10 μm. Tunneling spectroscopy on hybrid InSb-Al nanowires demonstrates a hard superconducting gap, accompanied by 2e-periodic Coulomb oscillations with an Al-based Cooper pair island integrated in the nanowire network. The results, together with possible Majorana signatures, confirm the high quality of the InSb nanowire networks, holding great promise for this platform for scalable topological networks.
Microwave spectroscopy reveals the quantum geometric tensor of topological Josephson matter*  
RAFFAEL KLEES (Presenter), GIANLUCA RASTELLI, Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany, JUAN CARLOS CUEVAS, Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain, WOLFGANG BELZIG, Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — Quantization effects due to topological invariants such as Chern numbers have become very relevant in many systems, yet, key quantities as the quantum geometric tensor [1] providing local information about quantum states remain experimentally difficult to access. Recently, it has been shown that multiterminal Josephson junctions constitute an ideal platform to synthesize topological systems in a controlled manner [2]. We theoretically study properties of Andreev states in topological Josephson matter and demonstrate that the quantum geometric tensor of Andreev states can be extracted by synthetically polarized microwaves [3]. The oscillator strength of the absorption rates provides direct evidence of topological quantum properties of the Andreev states.


*This work was supported by the DFG through SFB 767 and Grant No. RA 2810/1. J.C.C. acknowledges the support via the Mercator Program of the DFG in the frame of the SFB 767.

Observation of the non-Hermitian Skin effect in topoelectric circuits*  
TOBIAS HELBIG (Presenter), TOBIAS HOFMANN, University of Wurzburg, CHING HUA LEE, National University of Singapore, MARTIN GREITER, RONNY THOMALE, University of Wurzburg — A contemporary frontier of metamaterial research is the challenge non-Hermitian systems pose to the established characterization of topological matter. There, one of the most relied upon principles is the bulk-boundary correspondence (BBC): energy eigenvalues and eigenstates exhibit a perturbatively small change as the boundary conditions are modified from periodic to open by changing a single bond. The framework of BBC captures the emergence of protected surface states at the boundary of a system with non-trivial bulk topology. In this talk, we present a periodic circuit network, where gain and loss conspire with the violation of reciprocity to affect this principle dramatically. Switching from periodic to open boundary conditions results in a non-perturbative change of all eigenmodes in this system. We experimentally observe the non-Hermitian Skin effect with extensive mode localization at open boundaries for the first time.


10:00AM A60.00009: Reciprocal skin effect and its realization in a topolectrical circuit*

TOBIAS HOFMANN (Presenter), TOBIAS HELBIG, Institute for Theoretical Physics and Astrophysics, University of Wurzburg, FRANK SCHINDLER, Department of Physics, University of Zurich, CHING HUA LEE, Department of Physics, National University of Singapore, MARTIN GREITER, Institute for Theoretical Physics and Astrophysics, University of Wurzburg, TITUS NEUPERT, Department of Physics, University of Zurich, RONNY THOMALE, Institute for Theoretical Physics and Astrophysics, University of Wurzburg —

The non-Hermitian Skin effect constitutes a new paradigm in synthetic metamaterial research. The established notion of the Skin effect requires specifically tailored gain and loss conspiring with the breaking of reciprocity. In this talk we present a model which shows extensive eigenmode localization at its boundaries while preserving reciprocity. In contrast to non-reciprocal implementations of the Skin effect requiring external energy supply, this model can be realized with exclusively passive components. We demonstrate this novel phenomenon in a passive RLC circuit network. The reciprocal Skin effect suggests itself for realizations in further metamaterial platforms with limited availability of active components.


*Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through Project-ID 258499086 - SFB 1170 and through the Wuerzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter - ct.qmat Project-ID 39085490 - EXC 2147
10:12AM A60.00010: Tuning Electronic Band Properties in Binary Chalcogenides with Extrinsic and Intrinsic Strain: A First-Principles Study  THOMAS REID (Presenter), Institute of Materials Science, University of Connecticut, SANJEEV K NAYAK, Materials Science and Engineering, University of Connecticut, R.M. GEILHUF, NORDITA, KTH Royal Institute of Technology; Department of Physics, University of Connecticut, PAMIR ALPAY, Materials Science and Engineering, University of Connecticut, ALEXANDER BALATSKY, NORDITA, KTH Royal Institute of Technology; Department of Physics, University of Connecticut — We assess the relationship of the electronic band structure and atomic relaxation in Bi$_2$Se$_3$ and Bi$_2$Te$_3$. We use first-principles Density Functional theory (DFT) method to control for the influence of the exchange-correlation functional (XCF) and slab thickness. After a thorough analysis, in which we modulate the input parameters over a broad swathe of the computational space, we conclude that the GGA+vdW functional reproduces experimental results with best relative computational efficiency. In addition, we conclude that the use of experimental lattice parameters (ELP)—instead of ab initio ones—is sufficient to generate accurate descriptions of the electronic properties. After making this determination, we study the effect of doping on the electronic structure of As$_2$Te$_3$ and Bi$_2$Se$_3$, in the context of another study on the effect of biaxial strain on the same. In accordance with the first set of results, we use GGA+vdW as the XCF, and we use the ELP as the basis of both materials’ unrelaxed structure. Our results are valuable for the development of mechanisms for tuning the electronic properties of topological and trivial insulators.

10:24AM A60.00011: Predicting two-dimensional topological phases in Janus materials by substitutional doping in transition metal dichalcogenide monolayers*  ANICETO B. MAGHIRANG III, ZHI-QUAN HUANG, ROVI ANGELO B. VILLAOS, CHIA-HSIU HSU, LIANG-YING FENG, Physics, National Sun Yat-sen University, EMMANUEL FLORIDO, Institute of Mathematical Sciences and Physics, University of the Philippines Los Baños, HSIN LIN, Institute of Physics, Academia Sinica, ARUN BANSIL, Physics, Northeastern University, FENG-CHUAN CHUANG (Presenter), Physics, National Sun Yat-sen University — Ultrathin Janus two-dimensional (2D) materials are attracting intense interest currently. Substitutional doping of 2D transition metal dichalcogenides (TMDs) is of importance for tuning and possible enhancement of their electronic, physical and chemical properties toward industrial applications. Using systematic first-principles computations, we propose a class of Janus 2D materials based on the monolayers MX$_2$ (M=V, Nb, Ta, Tc, or Re; X=S, Se, or Te) with halogen (F, Cl, Br, or I) or pnictogen (N, P, As, Sb, or Bi) substitution. Nontrivial phases are obtained on pnictogen substitution of group VB (V, Nb, or Ta), whereas for group VIIB (Tc or Re), the nontrivial phases are obtained for halogen substitution. Orbital analysis shows that the non-trivial phase is driven by the splitting of M-d$_{yz}$ and M-d$_{xz}$ orbitals. Our study demonstrates that the Janus 2D materials have the tunability and suitability for synthesis under various conditions.

*Ministry of Science and Technology of Taiwan under Grants No. MOST-107-2628-M-110-001-MY3; US Department of Energy (DOE), Office of Science, Basic Energy Sciences grant number DE-FG02-07ER46352, DOE grant number DE-AC02-05CH11231, and DE-SC0012575.
Controlling in-gap states in graphene nanoribbons via tunable topological phases  
FANGZHOU ZHAO (Presenter), STEVEN LOUIE, University of California, Berkeley — Graphene nanoribbons (GNRs) possess distinct symmetry-protected electron topological phases that depend on structure and termination. We show, through first-principles calculations, that by applying an experimentally accessible transverse electric field, certain designer GNRs may be tuned from a topologically trivial to a nontrivial phase or vice versa. With a spatially varying field, junctions of GNRs with distinct topological phases can be created, with localized topological in-gap interface states emerging at these junctions. We further study the formation of in-gap end states inside different energy gaps around the Fermi level for a finite GNR segment, including the conditions for end state to emerge in energy gaps other than the charge-neutrality gap. This work is supported by the National Science Foundation and the Office of Naval Research under the Muri Program. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

Dynamic nuclear spin polarization induced by Edelstein effect at Bi(111) surfaces*  
ZIJIAN JIANG (Presenter), VICTORIA SOGHOMONIAN, JEAN J HEREMANS, Virginia Tech — Nuclear spin polarization and its Overhauser field, induced by hyperfine interaction and the Edelstein effect, were investigated by quantum transport in individual micrometer-sized Bi(111) thin film samples. A high current density was applied at low temperatures to generate a non-equilibrium carrier spin polarization in the Bi(111) surface states by the Edelstein effect and strong spin-orbit interaction, which then induced dynamic nuclear polarization by hyperfine interaction. The antilocalization magnetotransport measurements showed that as the polarization duration or the polarization current increased, the carrier quantum phase decoherence times decreased while the spin-orbit decoherence times increased, which allowed a quantification of the Overhauser field from the nuclear polarization. By using delay times between polarization and measurement, an exponential decay of the Overhauser field was observed, driven by a nuclear spin relaxation time. Application of an external magnetic field during polarization showed that the carrier spin polarization itself was sufficient to overcome dipolar interactions between nuclear spins. Comparative studies of the transport properties of Bi(111)-on-mica and Bi(111)-on-Si(111) will also be discussed.

*DOE DE-FG02-08ER46532

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A61 DMP DCMP DCOMP: Fe-Based Superconductors - Nematicity I  
Mile High Ballroom 4B - Ulrich Welp, Argonne Natl Lab - Tag(s): Focus
8:00AM A61.00001: Specific Heat and Critical Behavior in BaFe$_2$(As$_{1-x}$P$_x$)$_2$* [Invited] CAMILLA MOIR (Presenter), CRIEPI, SCOTT C. RIGGS, JOSE A GALVIS, PAULA GIRALDO-GALLO, NHMFL, JIUN-HAW CHU, Physics, University of Washington, PHILIP WALMSLEY, IAN FISHER, Stanford University, ARKADY SHEKHTER, GREGORY SCOTT BOEBINGER, NHMFL — With $T_c$'s below 40 K and evidence of a quantum critical point [1], the iron-based high-temperature superconductor BaFe$_2$(As$_{1-x}$P$_x$)$_2$ is an appealing system for investigating the behavior underlying superconductivity in high-$T_c$ superconductors. By applying magnetic fields up to 35 T, we are able to suppress superconductivity and reveal the normal state of overdoped BaFe$_2$(As$_{1-x}$P$_x$)$_2$. We observe $\sqrt{H}$ behavior indicating a nodal superconducting gap, saturation of the heat capacity at a magnetic field corresponding to the onset of the normal state, and enhancement of the quasiparticle mass sum as calculated from electronic specific heat coefficient as optimal doping is approached [1]. Our comparison of specific heat as a function of magnetic field to specific heat as a function of temperature, as well as other measurements, forms a consistent treatment of specific heat measurements in high-temperature superconductors.


*BaFe$_2$(As$_{1-x}$P$_x$)$_2$ samples were grown at The Geballe Laboratory for Advanced Materials at Stanford University supported by the Department of Energy, Office of Basic Energy Sciences under contract DE-AC02-76SF00515 and the Gordon and Betty Moore Foundation. DC-field measurements were performed at the DC Magnet Facility of the National High Magnetic Field Laboratory (NHMFL) in Tallahassee, FL. Thermometer calibrations were performed in the Pulsed Field Facility of the NHMFL in Los Alamos, NM. The work at the NHMFL was supported through the National Science Foundation Cooperative Agreements DMR-1157490 and DMR-1644779, the United States Department of Energy, and the State of Florida.
Quantum critical nematic fluctuations and spin excitation anisotropy in the iron pnictides*  

CHIA-CHUAN LIU (Presenter), Rice Univ, ELIHU ABRAHAMS, University of California, Los Angeles, QIMIAO SI, Rice Univ — Quantum criticality in iron pnictides involves nematic and antiferromagnetic degrees of freedom in a concurrent way [1,2], but the relationship between the two types of fluctuations has yet to be clarified. To elucidate the nematic correlations, we study the spin excitation anisotropy defined by the difference between the dynamical spin susceptibilities at (π,0) and (0,π) [3]. We start from an effective Ginzburg-Landau theory for both the Ising-nematic and antiferromagnetic fluctuations in the presence of a small external uniaxial potential, which breaks the C4-symmetry in B1g channel, and establish an identity that connects the spin excitation anisotropy with the dynamical magnetic susceptibility and static nematic susceptibility. Using this identity, we show that the dynamical nematic susceptibility in the quantum critical regime can be determined, and we illustrate it by considering the case of the optimally Ni-doped BaFe2As2 [3].

References:

*DOE BES Award # DE-SC0018197 and Welch Foundation Grant No. C-1411
Quantum phase transition of correlated iron-based superconductivity in LiFe$_{1-x}$Co$_x$As*

NANA SHUMIYA (Presenter), JIAJIN YIN, SONGTIAN SONIA ZHANG, Princeton University, GUANGYANG DAI, Institute of Physics, Chinese Academy of Sciences, YUANYUAN ZHAO, School of Physics and Optoelectronic Engineering, Nanjing University of Information Science and Technology, ANDREAS KREISEL, Institut für Theoretische Physik, Universität, GENNEVIEVE MACAM, National Sun Yat-Sen University, BRIAN M. ANDERSEN, University of Copenhagen, FENG-CHUAN CHUANG, National Sun Yat-Sen University, HSIN LIN, Institute of Physics, Academia Sinica, ZIQIANG WANG, Boston College, CHANGQING JIN, Institute of Physics, Chinese Academy of Sciences, YUNKYU BANG, Asia Pacific Center for Theoretical Physics and Department of Physics, POSTECH, ZAHID HASAN, Princeton University — We use scanning tunneling microscopy (STM) to image the electronic impact of Co atoms on the ground state of the LiFe$_{1-x}$Co$_x$As system. We observe that impurities progressively suppress the global superconducting gap and introduce low energy states near the gap edge, with the superconductivity remaining in the strong-coupling limit. Unexpectedly, the fully opened gap evolves into a nodal state before the Cooper pair coherence is fully destroyed. Our systematic theoretical analysis shows that these new observations can be quantitatively understood by the nonmagnetic Born-limit scattering effect in a $s\pm$-wave superconductor, unveiling the driving force of the superconductor to metal quantum phase transition.

*Experimental and theoretical work at Princeton University was supported by the Gordon and Betty Moore Foundation (GBMF4547/ Hasan) and the United States Department of energy (US DOE) under the Basic Energy Sciences programme (grant number DOE/BES DE-FG-02-05ER46200).

Nematic and Antiferromagnetic Quantum Criticality in a Multi-Orbital Hubbard Model for Iron Pnictides*

LEI CHEN (Presenter), Rice University, WENJUN HU, University of Tennessee, HAOYU HU, Rice University, RONG YU, Renmin University, HSIN-HUA LAI, Rice University, LUCA FAUSTO TOCCHIO, DISAT, Politecnico di Torino, FEDERICO BECCA, University of Trieste, QIMIAO SI, Rice University — The extent to which quantum criticality drives the physics of iron pnictides is a central question in the field. While the issue had been addressed by effective field theories [1,2], how to approach it in the multi-orbital Hubbard model has been a long-standing challenge due to the limitation in methods for intermediate correlations. Here [3] we study this problem within a multi-orbital Hubbard model containing both the Hubbard and Hund's interactions, by a variational Monte Carlo method based on Jastrow-Slater wave functions that allow for a non-perturbative treatment of the electron correlations. We find strong evidence for the existence of a unique quantum critical point, where both nematic and ($\pi$, 0) antiferromagnetic orders develop, in the bad-metal regime of the phase diagram. A robust signal for unconventional superconducting pairing is also found as the system approaches the quantum critical point from the paramagnetic side.


*DOE BES Award # DE-SC0018197 and Welch Foundation Grant No. C-1411
9:12AM A61.00005: Fluctuating orders induced non-Fermi-liquid behavior near quantum critical point in iron-based superconductors  RONG LI (Presenter), ZHEN-SU SHE, Peking Univ — The non-Fermi-liquid behavior near quantum critical point (QCP) in iron-based superconductors (IBSCs) is a matter of considerable debate. Recently, we have proposed a novel transport theory quantifying scattering by multi-order fluctuations, yielding a new resistivity model, i.e., $\rho = \rho_a + (\rho_b + \alpha^2 T^2 + \beta^2 B^2)^{1/2}$ (see also another contributed talk, She and Li, "A symmetry-breaking analysis for non-Fermi-liquids induced by order fluctuations in correlated electron systems"). For IBSCs near QCP, the theory quantitatively explains the widely observed low-$T$ plateau as a result of scattering by antiferromagnetic (AFM) fluctuations, and the unusual linear $T$ and $B$ scaling at high $T$ and $B$ induced by thermal- and magnetic-vortex fluctuations. Furthermore, the scaling transition from $T^2$ to $T$ under increasing $T$ and doping is explained by the increase of vortex fluctuations relative to AFM fluctuations. We present supporting evidence by comparing the predictions with data of dozens of samples. It thus forms a novel framework to clarify the difference between IBSCs and cuprates, successfully quantifying the feature of weaker AFM fluctuations in LiFe$_{1-x}$Co$_x$As, and stronger vortex fluctuations in BaFe$_2$(As$_{1-x}$P$_x$)$_2$ based on the link between macroscopic resistivity and microscopic fluctuating orders.

9:24AM A61.00006: Manifestation of the multiband nature in the BCS-BEC crossover of FeSe$_{1-x}$S$_x$  TAKAHIRO HASHIMOTO (Presenter), YUICHI OTA, AKIHIRO TSUZUKI, TSUBAKI NAGASHIMA, AKIKO FUKUSHIMA, Institute for Solid State Physics, University of Tokyo, SHIGERU KASAHARA, YUJI MATSUDA, Department of Physics, Kyoto University, KOHEI MATSUURA, YUTA MIZUKAMI, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, University of Tokyo, SHIK SHIN, University of Tokyo, KOZO OKAZAKI, Institute for Solid State Physics, University of Tokyo — The crossover from the superconductivity of Bardeen-Cooper-Shrieffer (BCS) regime to Bose-Einstein condensation (BEC) regime holds the key to understanding the nature of pairing and condensation of fermions [1]. In electron systems in solids, however, it is generally difficult to control the pairing strength of the electrons, and complete evidence of the BCS-BEC crossover has been elusive so far. Here, we provide the first example of complete evidence for the BCS-BEC crossover in an iron-based superconductor FeSe$_{1-x}$S$_x$ from laser-excited angle-resolved photoemission spectroscopy, and propose a multiband mechanism for BCS-BEC crossover in this system.


*This research is supported by Photon and Quantum Basic Research Coordinated Development Program of MEXT and partially supported by Grants-in-Aid for Scientific Research (KAKENHI) (Grant Numbers JP25220707, JP16K17741, JP25220710, JP15H02106, JP15H03688), and on Innovative Areas Topological Material Science (Grant Number JP15H05852) from Japan Society for the Promotion of Science (JSPS). T. H. acknowledges the JSPS Research Fellowship for Young Scientists (DC2).
Unusual BCS-BEC crossover in FeSe$_{1-x}$S$_x$ superconductors* YUTA MIZUKAMI (Presenter), Univ of Tokyo-Kashiwanoha, MASAHIRO HAZE, Kyoto University, OHEI TANAKA, KOHEI MATSUURA, Univ of Tokyo-Kashiwanoha, DAIKI SANO, Kyoto University, JAKOB BÖKER, ILYA EREMIN, Ruhr-Universität Bochum, SHIGERU KASAHARA, YUJI MATSUDA, Kyoto University, TAKASADA SHIBAUCHI, Univ of Tokyo-Kashiwanoha — The BCS-BEC crossover from strongly overlapping Cooper pairs to non-overlapping composite bosons in the strong coupling limit has been a long-standing issue of interacting many-body fermion systems. It has been extremely challenging to realize such a crossover state in electronic systems over the past decade. Recently, FeSe semimetal emerged as a high-$T_c$ superconductor located in the BCS-BEC crossover regime, owing to its very small Fermi energies. In FeSe, however, an ordinary BCS-like heat-capacity jump is observed at $T_c$, posing a fundamental question on the characteristics of the BCS-BEC crossover. Here we report on high resolution heat capacity, magnetic torque, and scanning tunneling spectroscopy measurements in FeSe$_{1-x}$S$_x$. When the nematic order is suppressed at $x > 0.17$, an unusual BEC-like transition is found in the thermodynamic quantities with giant superconducting fluctuations extending far above $T_c$. However, no pseudogap formation is observed in the tunneling spectra. These results illuminate highly unusual features of the BCS-BEC crossover in superconductors with multiband electronic structure and competing electronic instabilities.

*This work has been supported by KAKENHI (Nos.19H00649,18H05227) from JSPS.

FeSe as a Polymorphous Network* ZHI WANG (Presenter), XINGANG ZHAO, University of Colorado, Boulder, SIMON J L BILLINGE, Department of Applied Physics and Applied Mathematics, Columbia University, ALEX ZUNGER, University of Colorado, Boulder — The observed electronic structure of FeSe has lower apparent symmetry than the one that would be suggested by its macroscopic crystallographic structure. It has been argued that such nematicity must be electronic symmetry lowering, driven by strong correlations, rather than a local structural symmetry lowering, the latter being judged on the basis of global structural probes to be too small. Standard structure predictions use small unit cells that cannot accommodate structural symmetry lowering. Using a predictive first principles minimization of the internal total energy without restricting it to a small unit cell reveals that the lowest energy configuration whose average macroscopic symmetry is tetragonal consists, in fact, of a distribution of different local low-symmetries. This polymorphous network explains the PDF pattern in both the local and long-range regions without a fit. When used as input to electronic structure calculations, the predicted polymorphous structure reveals electronic symmetry breaking that is unique to this unusual compound.

*supported by NSF-DMREF-1921949.
The recent discovery of superconductivity in the two-leg ladder compounds BaFe$_2$X$_3$ ($X$=S, Se) started the novel field of quasi-one-dimensional iron-based superconductors. Here, we predict that the previously barely explored ladder compound RbFe$_2$Te$_3$ should be magnetic with a CX-type arrangement[1]. Moreover, at $n = 6.0$ our DFT phase diagrams (with/without lattice tetramerization) reveal that the stable magnetic states could be either a 2x2 magnetic Block-type, as for $X$=Se, or a previously never observed before CY-type state. In the Te-based studies, electrons are more localized than in S, implying that the degree of electronic correlation is enhanced for the Te case. This potential relevance of strong correlation in $n$=6 Te-123 ladders could also induce exotic phenomena [2], such as Block-type order, the orbital selective Mott physics, and superconductivity under high pressure. Our overarching conclusion is that experimental studies of iron ladder tellurides are worth pursuing.


*U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, National Natural Science Foundation of China.

For insight into the composition-dependent electronic structure of iron pnictides, we performed a systematic study of spatial structure and electronic states by x-ray diffraction and x-ray absorption. A large number of compositions in the (Ba,Sr)(Fe,$TM$)$_2$(As,P)$_2$ family of compounds was investigated, covering the substitution of Ba by Sr; of Fe by transition metals ($TM$); and of As by P. Our observations on doping effects upon such substitutions include “reluctant” doping (charge carriers are only partially transferred away from the substituent) or “site-decoupled” doping (transferred charge carriers affect either Fe sites or As sites but not both). Here, we focus on isovalent substitutions. Our findings suggest that Indirect, structural effects of substitution appear to be more important for magnetism and superconductivity in iron pnictides than the direct, charge-carrier doping effects.
10:24AM A61.00011: Isovalent S and Te substitution effect on superconductivity in FeSe thin films* FUYUKI NABESHIMA (Presenter), TOMOYA ISHIKAWA, NAOKI SHIKAMA, YUKI SAKISHITA, SOTA NAKAMURA, HODACA KUROKAWA, ATSUTAKA MAEDA, Univ of Tokyo — We investigated chemical pressure effects from positive to negative (S and Te substitution) and in-plane strain effect from tensile to compressive on physical properties in FeSe thin films. Both S and Te substitution suppresses the structural transition temperature. The behavior of superconducting transition temperature, \( T_c \), is completely different between S and Te substitution at the composition when the structural transition disappears. \( T_c \) increases drastically for Te substitution at the ortho.-tetra. boundary, while \( T_c \) shows monotonic decrease in S substituted samples. These results demonstrate that the relationship between the nematicity and the superconductivity is not universal in FeSe[1]. A magneto-transport study revealed a positive correlation between carrier densities and \( T_c \) in our films[2,3]. Our results suggest that the structural transition affects the electronic structure differently between Fe(Se,S) and Fe(Se,Te) and that this is the direct cause of the difference in the \( T_c \) behaviors at the ortho.-tetra. boundary[3].


*This work was supported by JSPS KAKENHI Grant Number 18H04212 and 19K14651 and The Murata Science Foundation.

10:36AM A61.00012: Resistivity and Magnetic Susceptibility Under Pressure (0–2.0 GPa) of \( \text{Fe}_{1+\varepsilon}\text{Te}_{0.5}\text{Se}_{0.5} \) and \( \text{R}_{1-x}\text{Ce}_x\text{NiO}_3 \) \( \text{[R = (La,Y), Pr]} \)** ZACHARY P. KUKLINSKI, GREGORIO PONTI, QUINN D. B. TIMMERS, RABIA HUSAIN (Presenter), JOHN MARKERT, Department of Physics, University of Texas at Austin — We report measurements of the ac magnetic susceptibility of the iron-based mixed-chalcogenide superconductor \( \text{Fe}_{1+\varepsilon}\text{Te}_{0.5}\text{Se}_{0.5} \), and of the electrical resistivity of doped nickel-oxide compounds \( \text{R}_{1-x}\text{Ce}_x\text{NiO}_3 \), with \( \text{R = Pr or (La,Y)} \), over the pressure range 0–20 kbar (0–2.0 GPa). Our iron-based material is optimized \((\varepsilon \approx 0.07)\) for bulk superconductivity, exhibiting an ambient-pressure superconducting transition at \( T_c \approx 14 \text{ K} \), well above the transition of bulk FeSe \((T_c = 9 \text{ K})\). With applied pressure, we observe an immense, nearly linear increase of \( T_c \), with \( dT_c/dP = +7.0\pm0.5 \text{ K/GPa} \). We have prepared bulk “113” doped nickelates using high-oxygen-pressure (150–200 bar), high-temperature \((T \approx 1000^{\circ}\text{C})\) synthesis. For undoped \( \text{PrNiO}_3 \), the metal insulator transition temperature decreases with pressure, with reported \( dT_{\text{MI}}/dP \approx -42 \) to \(-76 \text{ K/GPa} \) [1,2]. For \( \text{Pr}_{1-x}\text{Ce}_x\text{NiO}_3 \) with \( x \approx 0.0–0.2 \), we are exploring variations in \( dT_{\text{MI}}/dP \). We consider both steric (e.g., band-broadening, bond-straightening), electron-doping, and hole-filling contributions to this behavior.


**Support from University of Texas, College of Natural Sciences Freshman Research Initiative.
**10:48AM A61.00013: Unconventional quantum criticality in a two-dimensional fermion-boson coupled system**  
JIANQIAO LIU (Presenter), RYUICHI SHINDOU, Peking Univ — We study a two-dimensional two-band Fermi system with finite Fermi surfaces that couples with a $\phi^4$ action of O(3) vector boson field with dynamical exponent $z = 1$ through Yukawa-type coupling. By using RG analysis, we show that quantum criticality associated with an ordering of the O(3) vector field is controlled by a new saddle-point fixed point instead of the Wilson-Fisher fixed point. The new fixed point has a finite fermion-boson coupling and the boson velocity is strongly renormalized by the Yukawa coupling. We discuss possible superconducting instability near such a quantum critical point.

**Monday, March 2, 2020 8:00 AM - 11:00 AM**

**Session A62 DMP: Nanostructures and Metamaterials I**  
Mile High Ballroom 4C - Natalia Litchinitser, Duke University - Tag(s): Focus

**8:00AM A62.00001: Flying Micro-Lightsails: Optical Levitation and Propulsion of Nanostructured Ultralight Macroscopic Objects**  
HARRY ATWATER (Presenter), Applied Physics and Materials Science, California Institute of Technology — The Breakthrough Starshot Initiative initiated in 2016 defined an audacious goal of sending a spacecraft beyond to a neighboring star, Proxima Centauri within the next half-century. Its vision for an ultralight spacecraft that can be accelerated by laser radiation pressure from an Earth-based source to ~20% of the speed of light demands the use of materials with extreme properties. Here we examine stringent criteria for the lightsail materials design, thermal management and dynamical stability, and discuss lightsail design and first experimental steps by exploration of small (<1 mm$^2$) microscale lightsails. We explore nanophotonic design of materials, thermal management, and self-stabilizing optical manipulation, levitation and propulsion of lightweight macroscopic (i.e., mm, cm, or even meter-scale) micro-lightsails via radiation pressure. We consider the materials characteristics required to realize robust, thermally stable building blocks, and find that stable trajectories for dynamic motion of macro-objects can be achieved by controlling the anisotropy of light scattering along the object surface. With radiative cooling being the sole mechanism for passive thermal management in vacuum or space, we quantify the stringent requirements on material absorptivity that enable these structures to withstand high laser intensities and prevent excessive heating and mechanical failure. Achievement of stable optical manipulation and propulsion of macroscale (i.e., >> wavelength in size) structures, via radiation pressure appears to be possible by the use of structured optical beams and tailored nanophotonic design. Reaching this goal requires the conception and design of new ultralight photonic structures composed of materials with extreme optical, mechanical and thermal properties.

*This work was supported by the Air Force Office of Scientific Research under grant FA9550-19-1-0279.*
8:36AM A62.00002: Fundamental Limits on Electromagnetic Scattering in Nanostructured Materials: Upper Bounds on Extinction, Purcell Enhancement, and Absorption* PENGNING CHAO (Presenter), SEAN MOLESKY, PRASHANTH S VENKATARAM, Princeton University, WEILIANG JIN, Stanford University, ALEJANDRO RODRIGUEZ, Princeton University — Advances in computational optimization (inverse design) and experimental fabrication techniques suggest the possibility of approaching the fundamental limits of optical control, which remain largely unknown. Through algebraic analysis of the scattering properties of Maxwell's equations, we formulate new constraints on various optical scattering processes, such as extinction and absorption, and apply these to establish upper bounds on thermal emission, radiative heat transfer, and Purcell enhancement in nanostructured materials. These bounds are general and useful in that they apply to arbitrary structures while incorporating the most relevant aspects of any photonic design problem: the material a given structure will be made of and the volume it will occupy. In particular, the bounds demonstrate the degree to which large metallic response and nanostructuring can be exploited to enhance light-matter interactions, with applications to single-photon extraction, photovoltaics, LEDs, and Raman scattering. They also reveal a transition from quasistatic (subwavelength) to ray optics behavior, and are shown to be nearly tight by comparison with structures discovered through inverse design.

*The authors would like to acknowledge support from NSF (DMR-1454836) and DARPA (HR0011182004).

8:48AM A62.00003: Hot-Electron Generation and Photothermal Effect in Plasmonic Nanostructures and Metamaterials ALEXANDRE GOVOROV (Presenter), Ohio Univ, LUCAS VAZQUEZ BESTEIRO, UESTC, China and INRS, Canada — Generation of energetic (hot) electrons and photo-heating are intrinsic properties of any plasmonic nanocrystal under illumination [1,2]. While the photo-heating effect is well described classically, the generation of hot electrons (HEs) is a quantum process and its theoretical description requires advanced quantum approaches [2]. The energy efficiency of such hot-electron processes is always limited. However, there are interesting possibilities to achieve the hot-electron enhancement [1]. The generation of high-energy HEs is a key mechanism for several applications such as plasmonic photodetectors, photocatalysis and ultrafast spectroscopy [1,2]. In particular, photochemistry induced by HEs and heating represent a very active area, which also involves chiral metamaterials and chiral photocatalysis [3].

9:00AM A62.00004: Optical and Thermal Metamaterials for Scalable Applications [Invited]
XIAOBO YIN (Presenter), University of Colorado Boulder — Micro/nano-structured materials offer significantly new opportunities for high efficiency devices and systems for energy harvesting, conversion and storage. Fundamental understanding at the small scale enables us to design structures and materials with unprecedented performances. However, there is a tremendous gap between the proof-of-principle demonstration at small scale and the intrinsically large scale real-world thermal and energy systems. In this talk, I will give an overview on our research and, more specifically, present our recent metamaterial development for emerging food, energy and water applications.

9:36AM A62.00005: Self-Cleaning and Tunable Structural Color Generation by TiO$_2$/Ti nanostructures* Gaurav Shukla (Presenter), Angappane Subramanian, Centre for Nano and Soft Matter Sciences — Structural colors are known for its long term sustainability in comparison to dyes, pigments, etc., but generating self-cleaning structural colors by nano/micro structuring is quite challenging. Here, we report self-cleaning structural color generation by TiO$_2$ nanorods and thin films on Ti sputtered glass and polyethylene terephthalate (PET) substrates deploying glancing angle deposition (GLAD) method. Reflected colors are tuned by varying height of TiO$_2$ nanorods or thin film on Ti films. Both the front and back surface of the samples show different colors, called Janus optical effect, due to altered dielectric constant on both sides of Ti film. All as-deposited TiO$_2$ nanorods and thin film samples are hydrophobic and hydrophilic respectively while both is transformed to reversible superhydrophilic state, a self-cleaning state, by UV irradiation. Further, annealing of samples on glass substrates has made the samples semi-transparent or transparent having superhydrophilic surface. Besides, structural colors are demonstrated for information encryption and optical ethanol sensing. Nevertheless, these structural colored specimens are promising for immense applications in the field of color printing, smart windows etc.

*S.A. thanks DST-Nanomission for the funding (SR/NM/TP-25/2016).
Two-dimensional nanostructured materials for catalytic activities: a combined experimental and theoretical study

TEKALIGN TERFA DEBELA (Presenter), Institute for Application of Advanced Materials, Jeonju University, HONG SEOK KANG, Department of Nano and Advanced Materials, College of Engineering, Jeonju University — Two-dimensional (2D) MoS$_2$ nanostructures have attracted much attention in recent years because of their excellent electrocatalytic activity toward the hydrogen evolution reaction (HER). Herein, we report unique 2D hybrid nanostructures of MoS$_2$ and melamine synthesized via a one-step solvothermal process.[1] The hybrid complexes with 7% intercalated melamine exhibited excellent HER Performance, with a current of 10 mA cm$^{-2}$ at 0.136 V (vs. RHE) and a Tafel slope of 37 mV dec$^{-1}$. Our first-principles calculations showed that the intercalation of hydrogen-bonded melamine clusters could stabilize the $1T'$ phase MoS$_2$ via substantial charge transfer. In addition, I will discuss our results on the selective reduction of CO$_2$ to formic acid using indium-zinc bimetallic nanocrystals.[2]


This study was supported by grants 2017H1D3A1A01014082 and 2018R1A2B2006474, which were funded by the Ministry of Science and ICT of Korea. We would also like to thank Jeonju University for providing partial financial support.

Nanostructured gold thermocouple for photodetection

MAHDIYEH ABBASI (Presenter), CHARLOTTE EVANS, LONGJI CUI, XIFAN WANG, DOUGLAS NATELSON, Rice Univ — The Seebeck coefficient of a metal depends on the energy-dependent electrical conductivity, which in turn depends on the energy-dependent electron mean free path and the material band structure. At the nanoscale, when the geometric size is comparable with the mean free path of the electrons, single metal thermocouples can be fabricated by changing the material geometry across the thermocouple. By using plasmonically-resonant structures, different device geometries and sizes can be used for wavelength sensitive light detection. We will present experimental data and simulations of single metal gold nanostructures with different geometries that are plasmonically active with IR laser illumination. We will discuss how these devices can be used for photodetection and discuss future applications for these measurements.

*The authors acknowledge support from NSF ECCS 1704625.
The advances on hybrid metamaterial design using bottom-up fabrication technique bring multiple advantages toward sensing and large-scale nanophotonic device integration. In our work, a two-phase plasmonic framework with Au nanoantenna arrays being embedded inside a titanium nitride (TiN) matrix was demonstrated, with easy access of controlling the packing density or aspect ratio. Advantages include sub-10 nm nanoantenna arrays, high crystalline quality, inch-scale throughput as well as high durability. Such geometrical flexibility brings tunable resonance frequency and anisotropic dielectric dispersion at optical regime. We demonstrate effective molecular sensing affected by the surface-enhanced plasmonic substrate with built-in Au antenna array. Our functional hybrid thin film template, as a first step, can be applied to multiple three-dimensional metamaterial designs. We will show some of our latest research progress on nanostructures and applications using such hybrid template.

*National Science Foundation (DMR-1565822)
10:36AM A62.00010: Three-dimensional printing of piezoelectric materials with designed anisotropy and their applications in underwater transducers  
HUACHEN CUI (Presenter), RYAN HENSLEIGH, DESHENG YAO, University of California, Los Angeles, DOMINIC LOPINTO, Virginia Tech, XIAOYU ZHENG, University of California, Los Angeles — We describe design and manufacturing routes to previously inaccessible classes of piezoelectric materials that have arbitrary piezoelectric coefficient tensors. Our scheme is based on the manipulation of electric displacement maps from families of structural cell patterns. We implement our designs by additively manufacturing free-form, perovskite-based piezoelectric nanocomposites with complex three-dimensional architectures. The resulting voltage response of the activated piezoelectric metamaterials at a given mode can be selectively suppressed, reversed or enhanced with applied stress. To demonstrate our novel design method and fabrication capability, we designed and fabricated underwater transducers consisting of rationally designed metamaterials to accommodate diverse situations, in which the piezoelectric composites convert mechanical vibrations into electrical voltages and vice versa. Through tuning geometry of the micro-architectures, resonance frequencies of these transducers can vary from 100Hz to 10MHz while the impedance is close to water. Moreover, we showed the feasibility and applicability of these transducers for the purpose of source detection, liquid quality monitoring, and directional sensing.

10:48AM A62.00011: 3D printable multi-directional piezoelectric sensor  
DESHENG YAO (Presenter), HUACHEN CUI, RYAN HENSLEIGH, XIAOYU ZHENG, University of California, Los Angeles — The electromechanical coupling behaviors of the piezoelectric materials enable their wide applications in sensing systems. However, the comprehensive measurement of the stress tensor presented significant challenges for current piezoelectric sensing devices. Notably, the evaluation of the surface shear stress requires complicated structural designs along with intricate fabrication processes. Herein, we present the design methodology and manufacturing route to simultaneously extracting all individual components of the stress tensor. Our scheme is based on manipulating the deformation mechanism of each individual ligament within the piezoelectric micro-lattice structures. We implement our design principle via three-dimensional printing of free-form, piezo-active feedstock with high-resolution micro-architectures. The presented piezoelectric multi-mode sensor owns the capability of isolating the target stress components when subjecting to multiple external inputs. Innovated by these findings, the applicability of the multi-mode sensors is demonstrated by embedding them to the gas-solid interface as the conformal, flexible airflow sensor that is able to monitor the status of the airflow, as well as a self-sensing fluid pipe for liquid velocity field mapping.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A63 DMP: Structure and Crystallography of Halide Perovskites

Mile High Ballroom 4D - Luisa Whittaker-Brooks
8:00AM A63.00001: Deciphering the nature of anharmonicity in CH$_3$NH$_3$PbI$_3$ by THz range Raman crystallography  
RITURAJ SHARMA (Presenter), Department of Materials and Interfaces, Weizmann Institute of Science, Israel, ZHENBANG DAI, Department of Chemistry, University of Pennsylvania, Philadelphia, USA, THOMAS M. BRENNER, LENA YADGAROV, Department of Materials and Interfaces, Weizmann Institute of Science, Israel, LINGYUAN GAO, Department of Chemistry, University of Pennsylvania, Philadelphia, USA, YEVGENY RAKITA, ROMAN KOROBKO, Department of Materials and Interfaces, Weizmann Institute of Science, Israel, IDDO PINKAS, Department of Chemical Research Support, Weizmann Institute of Science, Israel, ANDREW MARSHALL RAPPE, Department of Chemistry, University of Pennsylvania, Philadelphia, USA, OMER YAFFE, Department of Materials and Interfaces, Weizmann Institute of Science, Israel — Methylammonium lead iodide (CH$_3$NH$_3$PbI$_3$ or MAPI) shows many seemingly contradictory characteristics, like low diffusion but high carrier lifetime, small Urbach energy but defect tolerance etc., which are intimately connected to its anharmonic structural dynamics. Therefore, the fundamental understanding of the anharmonicity in MAPI is critical for harnessing its full potential in future optoelectronic devices. We combine THz-range Raman crystallography and ab initio computation to elucidate the microscopic mechanisms governing the strongly anharmonic structural dynamics in MAPI. Correlation between observed Raman intensity modulations with PbI$_6$ octahedral tilting patterns provides a direct evidence of highly anharmonic and anisotropic nature of such low-frequency vibrations. The anisotropy and anomalous broadening of the Raman features throughout the tetragonal phase is manifested by athermal anharmonicity. Conversely, thermally induced all-axes relaxational rotation causes anharmonicity and consequently, isotropy in cubic phase. Our study delineates the anharmonic structural dynamics of the technologically relevant tetragonal phase MAPI and offer insights to utilize anharmonicity to engineer favorable optoelectronic properties in materials with long term stability.

8:12AM A63.00002: Local Structure of 3D Halide Perovskites at High Pressure  
SAMUEL GIRDZIS (Presenter), Stanford University, YU LIN, SLAC National Accelerator Laboratory, WENDY MAO, Stanford University — Over the past decade, halide perovskites have emerged as promising materials for solar cells, due to their low-cost synthesis and robust semiconducting properties. Challenges remain in terms of improving the chemical stability of these materials, for instance to air, water, and heat, and in terms of reducing their toxicity, as the best performing halide perovskites still incorporate a lead (Pb) cation. Numerous studies have used compression to investigate structure-property relationships in these materials. However, previous structural investigations have only looked at long-range periodicity changes at high pressure. Here, we have performed in situ synchrotron X-ray total scattering at high pressure on a selection of 3D halide perovskites, including the archetypal composition, methylammonium lead iodide (MAPbI$_3$), to understand the evolution of their short-range, local structure. Preliminary results indicate local disorder due to octahedral tilting which has not been observable through conventional diffraction experiments. Insight into the local structural behavior has the potential to guide future synthetic efforts toward stable, non-toxic perovskite photovoltaics.
8:24AM A63.00003: Bias stress effects in organic-inorganic halide perovskites  LAURA FLANNERY (Presenter), DANIEL POWELL, LUISA WHITTAKER-BROOKS, University of Utah — The power conversion efficiencies of organic-inorganic halide perovskites (OIHP) have been improved over the last decade using a wide variety of methods, such as composition manipulation, dopant introduction, and interfacial buffers. These methods, however, have taken little regard for the electronic and interfacial effects such alterations may cause within devices under voltage bias stress. A condition required for most device operation. Using two efficient and commonly studied OIHP compositions, CH$_3$NH$_3$PbI$_{2.87}$Cl$_{0.13}$ and Cs$_{0.1}$(MA$_{0.17}$FA$_{0.83}$)$_{0.9}$Pb(I$_{0.83}$Br$_{0.17}$)$_3$, we investigate the effect of halide and cation substitution in OIHP structures to understand the unique current behavior while under a range of voltage bias stress in both light and dark conditions. With the use of a second device structure, without transport layers, the same bias stress effects unique for the different OIHP structures are observed. Confirming the difference in the current trends, for the two materials, is due to intrinsic behavior of the perovskite material itself, rather than the interfacial recombination and interactions with the transport layers. In this study, we continue to flush out how the changes in morphological defects and ion migration in the two OIHP materials are influencing charge transport.

8:36AM A63.00004: Structural phase transitions and photoluminescence mechanism in a layer of 3D hybrid perovskite nanocrystals  YURI GLINKA (Presenter), RUI CAI, XIAN GAO, DAN WU, RUI CHEN, XIAO WEI SUN, Electrical and Electronic Engineering, Southern University of Science and Technology — Although the structural phase transitions in the single-crystal hybrid methyl-ammonium (MA) lead halide perovskites (MAPbX$_3$, X = Cl, Br, I) are common phenomena, they have never been observed in the corresponding nanocrystals. Furthermore, although these materials are promising for the future electronics, optoelectronics, and solar energy harvesting applications, the nature of quasiparticles governing their unique photoluminescence (PL) and transport properties is still unclear. Here using two-photon excited PL spectroscopy, we provide evidence that the structural phase transitions in a layer of 3D MAPbBr$_3$ nanocrystals may occur at about the same temperatures as those in the corresponding single crystals. We also show that room-temperature PL originates from the radiative recombination of the optical-phonon vibrationally excited polaronic quasiparticles with energies might exceed the ground-state Fröhlich polaron and Rashba energies due to optical-phonon bottleneck. Because of small masses and large radii of these polaronic quasiparticles, their high mobility and long-range diffusion become possible.
**8:48AM A63.00005: Doping of Halide Perovskites**  
ZHIQIANG ZHANG (Presenter), ANDERSON JANOTTI, Univ of Delaware — Methylammonium lead iodide (MAPbI3) based organic-inorganic hybrid perovskites (OIHP) have emerged as promising solar photovoltaic absorbers, with power conversion efficiency increasing from 3.8% to 23.7% in the last 10 years. Such high efficiency combined with low-temperature solution fabrication process make OIHP promising candidates for the next generation of photovoltaic materials. Current solar cell designs use semi-insulating or low carrier density layers coupled to hole and electron transport contact materials. Controlled doping, both n and p-type, would allow for tuning electrical conductivity and fabrication of p-n homojunctions, opening great opportunities in device applications that go beyond solar cells. In this presentation we discuss possible approaches to doping of MAPbI3, exploring substitutional and interstitial impurities, on both organic and inorganic sites. Using density functional theory and hybrid functional calculations we explore all possible configurations of the various dopants, analysing formation energies, thermodynamic transition levels, and dopant solubilities.

**9:00AM A63.00006: Anharmonic Lattice Dynamics in CsPbBr3**  
TYSON LANIGAN-ATKINS (Presenter), XING HE, Duke University, MATTHEW KROGSTAD, RAYMOND OSBORN, STEPHAN ROSENKRANZ, DUCK YOUNG CHUNG, Argonne National Laboratory, MERCOURI KANATZIDIS, Northwestern University, DANIEL PAJEROWSKI, GUANGYONG XU, Oak Ridge National Laboratory, OLIVIER DELAIRE, Duke University — CsPbBr3 is a promising material for use in solar cells and thermoelectrics. The suitability of halide perovskites as photovoltaics derives from the long lifetimes of photoexcited carriers before recombination and it has been theorized that this is due to local polar fluctuations. Furthermore, CsPbBr3 has been shown to exhibit ultralow thermal conductivity which makes it attractive for use in thermoelectrics. CsPbBr3 has several lattice instabilities undergoing a cubic to tetragonal transition at ~400K before transforming to an orthorhombic phase at ~360K.

We report inelastic neutron scattering (INS) studies, supported by anharmonic first-principles simulations, on CsPbBr3 across its three phases. These momentum-resolved measurements allow us to investigate phonon behavior across the Brillouin zone and hence phonon-phonon scattering rates which directly impact thermal conductivity. We find large overall broadening of phonons, even at low temperature, but also a large temperature-dependent anisotropy in the anharmonicity.

*U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Award No. DE-SC0019299.*
Structural Studies of Halide Perovskite Photovoltaic Systems

SIZHAN LIU, New Jersey Inst of Tech, MAHALINGAM BALASUBRAMANIAN, SUYIN WANG, YU-SHENG CHEN, Argonne National Laboratory, ROGER LALANCETTE (Presenter), Rutgers University, SANJIT GHOSE, Brookhaven National Laboratory, YONG YAN, San Diego State University, TREVOR TYSON, New Jersey Inst of Tech — The lead halide perovskite systems have been studied intensively recently for applications as photovoltaic materials due to their very high conversion efficiency. To develop accurate models of these systems, it is critical to understand their structural phases and atomic level properties. High-resolution single crystal x-ray diffraction, Raman spectroscopy, x-ray absorption spectroscopy, x-ray pair distribution function measurements, and differential scanning calorimetry measurements are being used to determine the long-range and local structures and assess the stable phases. A discussion of the structure on different length scales over a broad temperature range will be given.

This work is supported by NSF Grant No. DMR-1809931.

Particle Ordering and A-site Composition Effects in Hybrid Organic-Inorganic Metal Halide Perovskite Quantum Dot Films

JULIAN VIGIL (Presenter), Stanford Univ, MICHAEL TONEY, SLAC National Accelerator Laboratory, JOSEPH LUTHER, National Renewable Energy Laboratory — The promising optoelectronic properties of bulk metal halide perovskite semiconductors have motivated recent developments in nanoscale and quantum well perovskite congeners, including layered structures and nanocrystalline quantum dots (QDs). In addition to the ability to tune the optical bandgap and improve photoluminescence efficiency, confining the nanocrystalline dimensions has proven valuable in accessing compositions[1] and crystallographic phases[2] that are unstable in the bulk.

Herein, we report on structural studies of FA$_x$Cs$_{1-x}$PbI$_3$ (FA = formamidinium) QD films by synchrotron X-ray scattering techniques. 15-nm FA$_x$Cs$_{1-x}$PbI$_3$ QDs (x = 0, 0.1, 0.25, 0.5, 0.75, 1) were deposited from colloidal solution and investigated by grazing incidence wide-angle X-ray scattering (GIWAXS). GIWAXS patterns indicate coherent particle ordering on the substrate for thin spin-coated films, while the subsequent ligand exchange and particle depositions lead to isotropic ordering of the particles. The patterns also show evidence of crystallographic phase inhomogeneities and a transition from cubic (FAPbI$_3$) to tetragonal (Cs$_{0.5}$FA$_{0.5}$PbI$_3$) to orthorhombic (CsPbI$_3$) character in the composition series.

9:36AM A63.00009: Stress effects on vibrational spectra of orthorhombic and tetragonal hybrid perovskites.* KUNTAL TALIT (Presenter), DAVID STRUBBE, University of California, Merced — Strain plays an important role in semiconductor performance and stability. Strains may develop in organic metal-halide perovskites which affect carrier mobility, non-radiative recombination, degradation and other optoelectronic properties. Measuring spatially varying strains is difficult but imperative for understanding these effects. We have used DFT to investigate effects of applied strain on the vibrations of tetragonal and orthorhombic methylammonium lead iodides (MAPI), building on our previous study of the high-temperature pseudo-cubic phase [arXiv:1907.03673]. Applying small uniaxial strains along three crystal axes, we have analyzed changes in frequency and phonon displacement patterns. We identified favorable modes for experimental measurements of local strain by Raman microscopy, and we calculated mode Grüneisen and Grüneisen parameters in different directions to connect with reports of negative thermal expansion in c-direction. Our study gives insight into the interaction between strain, structural changes and vibrational modes which may help to understand degradation.

*Merced nAnomaterials Center for Energy and Sensing, MERCED cluster at UC Merced and NERSC supercomputer at LBNL.

9:48AM A63.00010: Pressure-induced Phase Changes in Cesium Lead Bromide Perovskite Nanocrystals with Planar Defects* SORB YESUDHAS (Presenter), Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, MARIA V MORRELL, Department of Chemical Engineering, University of Missouri - Columbia, Missouri 65211, USA, MATTHEW J ANDERSON, CARSTEN A. ULLRICH, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, CURTIS KENNEY-BENSON, HPCAT, X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont IL, 60439, USA, YANGCHUAN XING, Department of Chemical Engineering, University of Missouri - Columbia, Missouri 65211, USA, SUCHISMITA GUHA, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA — Lead halide perovskites have a rich landscape of structural and optical properties, which can be explored and possibly controlled by applying high pressure. CsPbBr$_3$ NCs with Ruddlesden-Popper (RP) faults, formed via post-synthetic fusion growth, are significantly larger in size than as-synthesized NCs and display exceptional emission stability. We compare synchrotron-based high pressure X-ray diffraction and photoluminescence (PL) properties of CsPbBr$_3$ (without RP) and RP-CsPbBr$_3$ (with RP), and resolve their crystal structure under pressure for the first time. CsPbBr$_3$ undergoes a phase transition from ambient orthorhombic (S.G: Pnma) to cubic (S.G: Pmm) phase at 1.7 GPa and RP-CsPbBr$_3$ transforms from Pnma to monoclinic (S.G: P2$_1$/m) phase at 0.74 GPa in addition to several isostructural transitions. Density-functional calculations predict a narrowing of the band gap with pressure, concomitant with the PL energies. The RP-CsPbBr$_3$ NCs exhibit enhanced PL intensity at 1 GPa and show band gap opening at high pressures. This study opens new strategies for tuning not just the structural properties but also tuning planar defects in alkali lead halide crystals for improved optical properties.

*This work was supported by National Science Foundation under Grant No. ECCS-1807263
Two-dimensional (2D) Ruddlesden-Popper (RP) perovskites, with high quantum efficiency, good photostability and chemical stability, are promising for optoelectronic devices. Blancon et al. reported firstly the lower photoenergy edge emission at those \((BA)_{2}(MA)_{n-1}Pb_{n}I_{3n+1}\) 2D RP perovskites when \(n\geq3\) in 2017[1]. Then, significant attention was attracted to explore the mechanism of edge emission. A theoretical work following them was published to assert that this edge emitting originates from interface strain[2]. After that, another work declared that the edge emission is induced by water molecules[3]. The discussion of Zhao et al. indicated that the loss of part BA at edges should be responsible for the edge emission[4]. While, a reliable and consistent explanation is still missing till now. In this work, we observe the edge emission in 2D exfoliated perovskites and clarify the mechanism of edge emission. This work reveals the nature of the edge emission and pave a way for developing the new optoelectronic devices based on the 2D RP hybrid perovskites.


The air-stable, optically active CsPbI\(_3\) perovskite phase is one of the promising candidates for applications in solar cells. However, the black CsPbI\(_3\) perovskite is thermodynamically unstable and spontaneously converts to a yellow non-perovskite phase at room temperature. We report that a black perovskite phase can persist at room temperature by tuning the tilt of \([PbI_6]^{4-}\) octahedra of high temperature perovskites with pressure, which shows improved stability and remains unchanged after releasing pressure to ambient conditions. Synchrotron X-ray diffraction, Raman spectroscopy, and photoluminescence measurements indicate that the preserved CsPbI\(_3\) crystallizes into an orthorhombic perovskite structure and has a robust PL signal at ~702 nm. First-principles calculations reveal that the tilt of the \([PbI_6]^{4-}\) octahedra play a significant role on stabilizing CsPbI\(_3\) perovskite to room temperature. Our results present a promising approach to prepare superb stable black CsPbI\(_3\) for perovskite solar cells.

*The authors acknowledge the funding support of DE-AC02-76SF00515, DE-AC02-05CH11231, EAR 1606856, DE-AC02-06CH11357 and ECCS-1542152
Monitoring Electron−Phonon Interactions in Lead Halide Perovskites Using Time-Resolved THz Spectroscopy

DAMING ZHAO (Presenter), HONGWEI HU, REINHARD HASELSBERGER, Nanyang Tech Univ, RUDOLPH A MARCUS, California Institute of Technology, MARIA-ELISABETH MICHEL-BEYERLE, YENG MING LAM, Nanyang Tech Univ, JIAN-XIN ZHU, Los Alamos National Laboratory, CHAN LA-O-VORAKIAT, King Mongkut's University of Technology Thonburi, MATTHEW C BEARD, National Renewable Energy Laboratory, EE MIN CHIA, Nanyang Tech Univ — Lead halide perovskites have low-frequency phonon modes within the lead halide sublattice and thus are considered to be soft. The soft lattice is considered to be important in defining their interesting optoelectronic properties. Electron−phonon coupling governs hot-carrier relaxation, carrier mobilities, carrier lifetimes etc. Directly observing the interplay between free charge carriers and phonons can provide details on how phonons impact these properties. Here, we observe a delicate interplay among carriers, phonons, and excitons in mixed-cation and mixed-halide perovskite films by simultaneously resolving the contribution of free carriers and phonons in time-resolved THz photoconductivity spectra. We observe directly the increase in phonon population during carrier cooling and discuss how thermal equilibrium populations of carriers and phonons modulate the carrier transport properties, as well as reduce the population of carriers within band tails. We are also able to observe directly the formation of free carriers when excitons interact with phonons and dissociate and to describe how free carriers and exciton populations exchange through phonon interactions. Finally, we also time-resolve how the carriers are screened via the Coulomb interaction at low and room temperatures.

Stabilizing Metal-Halide Perovskites via Nanoconfined Crystallization

XIAOQING KONG, STEPHANIE LEE, YI YANG (Presenter), Stevens Inst of Tech — Metal-halide perovskites undergo multiple polymorph transitions, with the smallest bandgap phases thermodynamically favored at elevated temperatures. We explore nanoconfinement as a strategy to shift the thermodynamics of polymorph transitions in order to stabilize high-performance phases against temperature-induced polymorph transitions and humidity-induced degradation. Specifically, when crystal sizes are reduced, the surface free energy contribution to the total Gibbs free energy of the crystals becomes increasingly important. By exploiting the dependence of the surface free energy on the symmetry of the crystal structure, it is possible to shift polymorph transitions to lower temperatures under nanoconfinement compared to the bulk. These nanoconfined crystals also exhibit excellent stability against humidity-induced degradation, with no change in their X-ray diffraction patterns over a period of at least two years of storage in air.


*We acknowledge support from the Public Service Enterprise Group to advance energy innovation at Stevens.
10:48AM A63.00015: Dimensional Confinement-Deconfinement Along the Crystallographic C Axis: A Desorption Mediated Band Engineering of Methylammonium Lead Iodide
SAYANTAN SASMAL (Presenter), Material Science Programme, IIT Kanpur — Strong optical absorption, long diffusion length, benign intrinsic defects established organic-inorganic hybrid perovskites as one of the most important materials in the area of photovoltaics. Unfortunately, the formation of photogenerated halide rich trap centers during conventional halide exchange methods limits the use of hybrids perovskite in multi-junction solar cells.

In this report, we demonstrate band gap engineering of MAPbI$_3$ film due to systematic dimensional deconfinement along the crystallographic c axis during gas induced growth. There are some distinct interrelated events occurring during gas induced reaction, which involves (i) in situ formations of hexylamine from 2D (HA)$_2$PbI$_4$ upon exposure to methylamine, (ii) selective adsorption of hexylamine on the Pb sites of growing MAPbI$_3$ leading to the anisotropic growth, (iii) systematic desorption of hexylamine during exposure of methylamine leading to continuous band gap tuning (2.18 eV to 1.69 eV). Most importantly, this dimensional confinement-deconfinement leads to extremely smooth, homogeneous film without having the halide rich trap centres, thereby establishing the importance of this novel route in the context of hybrid perovskite photovoltaics.

Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A64 DMP: High Mobility, Wide Bandgap Oxides for Electronics
Mile High Ballroom 4E - Turan Birol, University of Minnesota - Tag(s): Focus

8:00AM A64.00001: Complex Oxide Heterointerfaces - New Materials, Terminations, and Orientations [Invited]  MARK RZCHOWSKI (Presenter), University of Wisconsin - Madison — In this talk I discuss our recent research activity in complex oxide heterostructures, addressing effects arising from spin-orbit coupling, novel spin structures, and interface modifications across a range of systems, highlighting similarities and differences. I will discuss two-dimensional charge liquids at heterointerfaces and their dependence on new materials, crystallographic orientation, and termination, magnetoelectric coupling in multiferrioc and composite oxide heterostructures, and materials and heterostructures exhibiting Berry curvature effects and interfacial coupling arising from crystalline and spin structure.
8:36AM A64.00002: Structural, Electronic, and Optical Properties of 2D Titanium Oxide Layers on MgO (001)*  STEPHEN ELTINGE (Presenter), KIDAE SHIN, SANGJAE LEE, JUAN JIANG, CHARLES H AHN, FREDERICK J WALKER, SOHRAB ISMAIL-BEIGI, Yale University — Two-dimensional transition metal oxides (2DTMOs) are a promising addition to the growing array of functional 2D materials, with potential applications related to their long-lived, strongly bound excitons. In addition, 2DTMOs are expected to be more stable than other 2D materials since they do not react with water or oxygen species. However, unlike some other chalcogenides, 2DTMOs do not naturally occur in stackable van der Waals-bonded layers, so they present challenges for structural prediction and characterization. We report on ab initio density functional theory simulations of 2D titanium oxide layers on the (001) surface of MgO. We consider both monolayer TiO$_2$, including various surface reconstructions, and few-layer Mg$_2$TiO$_4$ based on a bulk inverse spinel structure. We examine the feasibility of various interfaces between the Mg$_2$TiO$_4$ overlayer and the MgO(001) substrate. We report on calculations of the optical absorption spectrum of low-energy structures in order to compare to experiment. Finally, we describe the improved treatment of the orbital energies of low-energy structures using a nonlocal hybrid functional.

*This work is supported by the NSF EAGER program, award 1838463. SE is also supported by an NSF Graduate Research Fellowship.

8:48AM A64.00003: Ab initio calculation of ionic oxidation states in metal oxides*  SOHRAB ISMAIL-BEIGI (Presenter), Yale University — The concept of the oxidation state of ions is intuitive and useful for determining or predicting the stability, metallicity, and/or magnetism of metal oxides (as well as other materials). Determining the oxidation state of an ion is almost always a straightforward exercise in the use of the periodic table together with atomic electronegativities. However, calculating the charge state of an atom in a crystal, i.e., assigning electrons to atoms, is a notoriously difficult and ill-defined problem. After a brief discussion of some of the most popular approaches used for assigning electrons to atoms and their relative merits, we discuss the relation of oxidation state to the band structure, band occupancy and band symmetry in metal oxides and what is required and what it means to compute oxidation states from the band structure. Examples of insulating and metallic bulk metal oxides as well as superlattices and interfacial systems will illustrate the ideas.

*This work was supported primarily by the NSF via MRSEC DMR-1119826 (CRISP).
9:00AM A64.00004: Radical-based MBE growth, chemical doping, and electronic transport in SrSnO$_3$ films
TRISTAN TRUTTMANN (Presenter), FENGDENG LIU, ABHINAV PRAKASH, JIN YUE, Chemical Engineering and Materials Science, University of Minnesota - Twin Cities, THOMAS E MATES, Materials Department, University of California, Santa Barbara, BHARAT JALAN, Chemical Engineering and Materials Science, University of Minnesota - Twin Cities — In this talk, we present our recent study of radical-based molecular beam epitaxy (MBE) growth, and controlled doping in coherent, epitaxial $n$-doped SrSnO$_3$/GdScO$_3$ (001) films using La and Nd as dopants. By combining detailed growth, structural characterizations, secondary ion mass spectroscopy (SIMS) and temperature-dependent magnetotransport measurements, we show films with one-to-one correlation between dopant and activated carrier concentration. Carrier density exceeding $1 \times 10^{20}$ cm$^{-3}$ was achieved in doped SrSnO$_3$ films, which is in excellent agreement with the dopant-solubility limit predicted by density functional theory calculations. A record-high room-temperature mobility of 70 cm$^2$ V$^{-1}$ s$^{-1}$ at $1 \times 10^{20}$ cm$^{-3}$ was obtained in a 12 nm La-doped SrSnO$_3$ film, making this the thinnest perovskite oxide semiconductor with electron mobility exceeding 25 cm$^2$ V$^{-1}$s$^{-1}$ at room temperature. We discuss the structure - dopant - scattering mechanisms - transport property relationships, providing essential knowledge for the design of electronic devices using these materials.

9:12AM A64.00005: Electronic and Magnetic Characterization of Doped Perovskite Stannate Epitaxial Thin Films*
EMILY LINDGREN (Presenter), Geballe Laboratory for Advanced Materials, Stanford University, HANJONG PAIK, Platform for the Accelerated Realization, Analysis, & Discovery of Interface Materials (PARADIM), Cornell University, CAROLINA ADAMO, Geballe Laboratory for Advanced Materials, Stanford University, ALPHA T. N’DIAYE, Advanced Light Source, Lawrence Berkeley National Laboratory, DARRELL SCHLOM, Platform for the Accelerated Realization, Analysis, & Discovery of Interface Materials (PARADIM), Cornell University, YURI SUZUKI, Geballe Laboratory for Advanced Materials, Stanford University — La-doped BaSnO$_3$ thin films have been identified as a promising high mobility semiconducting oxide, which could play an important role in the development of an all-oxide power electronics platform. In order to incorporate spin functionality into these materials, we explore magnetic doping of the conducting perovskite stannates. We have fabricated La and Ru doped BaSnO$_3$ and SrSnO$_3$ films on (001) SrTiO$_3$ substrates grown by molecular beam epitaxy (MBE) and pulsed laser deposition (PLD). X-ray diffraction (XRD) was used to verify epitaxial growth and confirm high crystalline quality, with typical omega rocking curve FWHM of 0.05° deg. Films are optically transparent as verified by UV-vis spectrometry. They are also conductive, with room temperature mobilities up to 105 cm$^2$/Vs, and standard carrier electron concentrations of 1-2x10$^{20}$ /cm$^3$. Films show evidence of paramagnetism both in the field and temperature dependence of magnetization.

*We acknowledge support from the National Science Foundation (Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)) under Cooperative Agreement No. DMR-1539918, as well as the National Science Foundation under grant #1762971.
9:24AM A64.00006: Weak Electron-Electron Interaction effects in La-doped SrSnO$_3$ Films
TIANQI WANG (Presenter), JIN YUE, LAXMAN R. THOUTAM, ABHINAV PRAKASH, BHARAT JALAN, Department of Chemical Engineering and Materials Science, University of Minnesota — Alkaline-earth stannates with perovskite structures have attracted significant research interest recently due to their wide bandgap, high optical transparency, and high room temperature mobility. These characteristics make them promising candidates for transparent electronics and power electronics applications. Significant progress has been made in the synthesis, characterization and device demonstration, but there are still many open fundamental questions regarding the electronic transport in stannates.

In this talk, we present the temperature and magnetic field dependent transport study of La-doped SrSnO$_3$ (SSO) films. We demonstrate that the electron-electron interaction effect is primarily responsible for an increase in the Hall coefficient in the La-doped SSO films below 50 K accompanied by an increase in the sheet resistance. Magnetoresistance fitting yielded a large electron phase coherence length exceeding 450 nm at 1.8 K and revealed the electron-electron interaction to be the electron phase-coherence breaking mechanism in La-doped SSO films. These results while providing critical insights into the fundamental transport behavior in doped stannates also indicate the potential applications in quantum coherent electronic devices owing to their large phase coherence length.

9:36AM A64.00007: Large Hysteretic Magnetoresistance in La-doped SrSnO$_3$

**Heterostructures: An Evidence of Magnetism?**
LAXMAN RAJU THOUTAM (Presenter), TRISTAN TRUTTMANN, ANIL K RAJAPITAMAHUNI, BHARAT JALAN, University of Minnesota — In this talk, we present our recent observation of a robust, hysteretic magnetoresistance (MR) in low-doped Sr$_{1-x}$La$_x$SnO$_3$ films grown on GdScO$_3$ (001)$_{pc}$ using radical-based MBE approach. At low temperatures, sample showed a transport behavior consistent with Efros-Shklovskii variable range hopping. The MR shows negative values for 6 K ≤ T ≤ 200 K whereas it crosses over to positive values at lower temperatures, 1.8 K ≤ T ≤ 5 K. A large anisotropy was observed at 1.8 K between the out-of-plane and the in-plane MR values with MR exceeding 100% for magnetic field in the plane of the sample. Significantly, a robust hysteretic behavior was observed at low temperatures, which disappears only at temperature above 5 K. We discuss the physical origin of the hysteresis, and the origin of large in-plane MR in low-doped SrSnO$_3$ providing important and critical insights into the role of defects, strain and the choice of substrates on the electronic and magnetic properties.

*Work supported by UMN NSF MRSEC*
Strain Dependent Characterization of Flexible BaSnO$_3$ Nanomembranes

PRASTUTI SINGH (Presenter), Department of Applied Physics, Stanford University, SEUNG SAE HONG, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory & Stanford University, VARUN HARBOLA, Department of Physics, Stanford University, HAROLD HWANG, Department of Applied Physics, Stanford University — Doped BaSnO$_3$ is a wide band-gap semiconductor that is known to exhibit high electron mobility at room temperature, showing great prospects as an alternative transparent conducting oxide to the industry standard indium-tin-oxide. Flexible transparent conducting oxides are of special interest for future photonics and optoelectronic devices but realizing high-quality films as flexible materials has been a challenge. In this work, we will discuss our efforts to fabricate nanometer thick, freestanding La-doped BaSnO$_3$ film that are highly conducting and transparent using a water-soluble and lattice matched Ba$_3$Al$_2$O$_6$ buffer layer$^1$. Using this technique, we can transfer the nanomembranes onto a flexible device platform and characterize the physical and electronic properties of La-doped BaSnO$_3$ as a function of strain.


Structural characterization and optimization of PAMBE-grown Ga$_2$O$_3$ on STO (001)*

TOBIAS HADAMEK (Presenter), Physics, University of Texas at Austin, ERIC DOMBROWSKI, Staib Instruments, AGHAM POSADAS, Physics, University of Texas at Austin, MARTHA R. MCCARTNEY, DAVID JOHN SMITH, Physics, Arizona State University, ALEXANDER DEMKOV, Physics, University of Texas at Austin — Wide band-gap semiconductor Ga$_2$O$_3$ is in the focus of research as a promising material for high-power device applications. Here, we report on the structural properties of Ga$_2$O$_3$ grown by plasma-assisted MBE on STO as a function of growth temperature. At elevated temperatures above 550 °C we observe two out-of-plane orientations of the beta-polymorph (1-2-2) and (100), each with four in-plane rotational domain orientations by XRD and RHEED. As we lower the temperature the high-energy surface (1-2-2) becomes suppressed and we obtain single-out-of-plane oriented (100) beta-Ga$_2$O$_3$. The possibility of thin interfacial layers of gamma-Ga$_2$O$_3$ is investigated by means of STEM. The relevance of the integration of Ga$_2$O$_3$ on STO is that STO can be epitaxially grown directly on Si (001) and hence, can function as a template layer for the integration of Ga$_2$O$_3$ onto the Si platform. A low temperature growth is therefore preferable.

*The work is supported by the Air Force Office of Scientific Research under grant FA9550-18-1-0053.
Temperature-dependent Magnetotransport Study of Si-doped β-Ga$_2$O$_3$ Films

ANIL RAJAPITAMAHUNI (Presenter), LAXMAN RAJU THOUTAM, Department of Chemical Engineering and Materials Science, University of Minnesota-Minneapolis, PRANEETH RANGA, SRIRAM KRISHNAMOORTHY, Department of Electrical and Computers Engineering, The University of Utah, BHARAT JALAN, Department of Chemical Engineering and Materials Science, University of Minnesota-Minneapolis. — Monoclinic β-Ga$_2$O$_3$ has generated significant excitement due to the wide bandgap, high electrical breakdown and high electron mobility at room temperature. In this work, we will discuss temperature-dependent magnetotransport study of homoepitaxial Si-doped β-Ga$_2$O$_3$ (010) films grown via metal-organic vapor-phase epitaxy (MOVPE). Temperature dependent Hall measurements were carried out using Van der Pauw configuration. Hall measurement at room temperature yielded a linear slope and a carrier density ($n$) of ~ 4 x 10$^{17}$ cm$^{-3}$. A non-linear Hall resistance was however observed at 10 K < T < 150 K indicating the presence of multiple channel conduction. A transport model using two-channel conduction was used to fit the experimental magnetotransport data resulting in carrier densities, $n_1$, $n_2$ and the corresponding mobilities of $\mu_1$, and $\mu_2$ respectively. With decreasing temperature, $n_1$ showed a freeze-out behavior with an activation energy of ~ 15 meV, whereas $n_2$ remained nominally unchanged. By combining electrostatic gating using ion-gel as a gate-dielectric, detailed magnetotransport and transport modeling, we will discuss the origin of multiple carriers, defect-mobility relationship, and the relevant scattering mechanisms in MOVPE grown Si-doped β-Ga$_2$O$_3$.

*Work supported by UMN MRSEC

Stabilizing extraordinary disorder in single crystal high entropy oxides

WENRUI ZHANG (Presenter), ALESSANDRO MAZZA, ELIZABETH SKOROPATA, THOMAS ZAC WARD, Oak Ridge National Lab. — In functional oxides, compositional changes to the cation sublattice(s) enables tunability to electronic and/or magnetic phases. For correlated systems, even low levels of cation substitution can have a dominating influence on behavior due to the near degeneracy of the spin/charge/orbital energy scales. Further, the local distortion fields near doping sites often act as the catalysis for phase transitions. Controlling the type, number, and magnitude of these local distortions is highly desirable but often not experimentally accessible. We demonstrate the creation of exceptionally high disorder fields in single crystal oxides. Examples of epitaxial perovskite, spinel, and layered Ruddlesden-Popper phases possessing 5 or more elements randomly distributed on one or more of their cation sublattices. Synthesis of these materials relies on precise control of configuration entropy to dominate the free energy landscape, thus avoiding phase separation generally inherent in complex multinary systems. The impact of changing spin, charge, and lattice distortion field uniformity in these high entropy oxides will be discussed.

*This work was supported by the DOE Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
10:36AM A64.00012: Epitaxial Oxides on Glass: A Platform for Integrated Oxide Devices*

JOHN E ORTMANN, University of Texas at Austin, MARTHA R. MCCARTNEY, Arizona State University, AGHAM POSADAS (Presenter), University of Texas at Austin, DAVID JOHN SMITH, Arizona State University, ALEXANDER DEMKOV, University of Texas at Austin — The fabrication of epitaxial, ultra-thin SrTiO$_3$ (STO) on thick SiO$_2$ without the need for complicated wafer-bonding processes has been demonstrated. The resulting transition metal oxide (TMO)-on-glass layer stack is analogous to traditional silicon-on-insulator (SOI) wafers, where the crystalline device silicon layer of SOI has been replaced by a crystalline functional TMO layer. Fabrication starts with ultra-thin body SOI on which crystalline STO is grown epitaxially by molecular beam epitaxy. The device silicon layer is subsequently fully oxidized by ex situ high-temperature dry O$_2$ annealing, as confirmed by X-ray photoelectron spectroscopy, X-ray reflectivity, and high-resolution electron microscopy. STO maintains its epitaxial registry to the carrier silicon substrate after annealing and no evidence for degradation of the STO crystalline quality as a result of the TMO-on-glass fabrication process is observed. The ease of fabricating the TMO-on-glass platform without the need for wafer bonding will enable rapid progress in the development of state-of-the-art TMO-based electronic and photonic devices.

*The work at UT Austin was supported by the Air Force Office of Scientific Research under Grant No. FA9550-18-1-0053.

10:48AM A64.00013: Growth and structure of Mg$_2$TiO$_4$ on MgO (001)*

KIDAE SHIN (Presenter), STEPHEN ELTINGE, SANGJAE LEE, Yale University, HYUNGKI SHIN, University of British Columbia, JUAN JIANG, Yale University, HAWOONG HONG, Argonne National Laboratory, BRUCE DAVIDSON, KE ZOU, University of British Columbia, SOHRAB ISMAIL-BEIGI, CHARLES H AHN, FREDERICK J WALKER, Yale University — The unique properties of two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides, have been used for applications such as high mobility channels and as hosts for quantum optical phenomena. In transition metal oxides (TMOs), a similarly broad range of properties and devices may be possible to realize by leveraging the diverse properties and structures found in these materials and synthesizing them as ultrathin 2D films. In order to use 2D TMOs, understanding the limits of 2D oxide heteroepitaxy is crucial. Here, we report that growth of TiO$_2$ on MgO using molecular beam epitaxy (MBE) results in formation of epitaxial Mg$_2$TiO$_4$. Using a combination of in situ crystal truncation rod (CTR) measurements and first-principles density functional theory (DFT) calculations, the layer-resolved structure of Mg$_2$TiO$_4$ that is a few unit cells thick is determined, and the thermodynamic driving force behind Mg$_2$TiO$_4$ formation is calculated. These measurements resolve distinct structural features at the Mg$_2$TiO$_4$ interface with MgO, which is due to the polarity of Mg$_2$TiO$_4$, pointing to new ways to synthesize distinct 2D electronic structures in thin films.

*NSF EAGER- 1838463

Monday, March 2, 2020 8:00 AM - 11:00 AM
It was found recently that 2D electron fluids can support collective excitations that are not subject to Landau's $T^2$ dissipation [1,2,3]. This surprising collective behavior originates from the head-on carrier collisions, a process that dominates angular relaxation at not-too-high temperatures $T<<T_F$ due to the interplay of Pauli blocking and kinematic constraints. As a result, a large family of exceptionally long-lived excitations emerges, associated with the odd-parity harmonics of momentum distribution. This leads to "tomographic" dynamics: fast 1D spatial diffusion along the unchanging velocity direction accompanied by a slow angular dynamics that gradually randomizes velocity orientation. The abnormally slow angular relaxation originates from correlated angular dynamics involving "lock-step" angular displacements along the Fermi surface occurring in collinear two-particle collisions. The slow loss of directional memory is described as non-Brownian angular random walk, "superdiffusion" on the Fermi surface. The collective behavior with directional memory dominates at moderately long times, pushing the onset of conventional hydrodynamics to abnormally large timescales. The tomographic regime features an unusual hierarchy of time scales and scale-dependent transport coefficients manifest in fractional-power current flow profiles and unusual conductance scaling vs. temperature and sample size. This exotic behavior can be directly probed by transport measurement techniques, as well as by momentum-resolved tunneling measurements.

3. P J Ledwith, H Guo, L Levitov, Angular Dynamics and Directional Memory in Two-Dimensional Electron Fluids, 2019
8:36AM A66.00002: Levy flights and non-local transport in Dirac and Weyl systems* [Invited]
JOERG SCHMALIAN (Presenter), Karlsruhe Institute of Technology — We show that hydrodynamic collision processes of Dirac and Weyl systems can be described in terms of a Fokker-Planck equation with fractional derivative, corresponding to a Lévy flight in momentum space. Thus, electron-electron collisions give rise to frequent small-angle scattering processes that are interrupted by rare large-angle events. The latter give rise to superdiffusive dynamics of collective excitations. We argue that such superdiffusive dynamics is of more general importance to the out-of-equilibrium dynamics of quantum-critical systems.

*We acknowledge support by the European Commission's Horizon 2020 RISE program Hydrotronics (Grant Agreement 873028.

9:12AM A66.00003: Mirage and hidden collective modes in two dimensional Fermi liquids* [Invited] AVRAHAM KLEIN (Presenter), University of Minnesota, DMITRII MASLOV, University of Florida, ANDREY CHUBUKOV, University of Minnesota — I will show that two-particle correlation functions in 2D Fermi liquids have a nontrivial topological structure. The structure manifests itself in two exotic types of zero-sound collective modes: sharp propagating “hidden” modes that cannot be detected by spectroscopy and “mirage” modes that appear as sharp peaks in spectroscopy but don’t determine the Fermi liquid’s response. I will discuss how these features are associated with the existence of a two-sheet Riemann surface defined by the dynamical susceptibility $\chi(q,\omega)$. The hidden modes reside below the branch cut gluing the sheets, and the illusory modes reside on an unphysical sheet of the Riemann surface. Although neither the existence of a hidden mode, nor the illusory nature of a mirage mode, appear in spectroscopic probes, both can be readily identified in time-dependent measurements in pump-probe configurations.

*This work was supported by the NSF DMR-1523036 (A.K. and A.V.C.), and NSF-DMR-1720816 (D.L.M.).
Motivated by the recent development of terahertz pump-probe experiments, we investigate the short-time dynamics in superconductors with multiple attractive pairing channels. Studying a single-band and multiband superconductors, we find the signatures of collective excitations of the pairing symmetries (known as Bardasis-Schrieffer modes) as well as the order parameter amplitude (Higgs mode) in the short-time dynamics of the spectral gap and quasiparticle distribution after an excitation by a pump pulse. We show that the polarization and intensity of the pulse can be used to control the symmetry of the non-equilibrium state as well as frequencies and relative intensities of the contributions of different collective modes. We find particularly strong signatures of the Bardasis-Schrieffer mode in the dynamics of the quasiparticle distribution function. In the multiband superconductors we particularly address the collective modes and the short time dynamics of the superconducting state with $s + i s$-wave order parameter using an effective four-band model with two hole and two electron pockets. The amplitude and phase modes are coupled giving rise to a variety of collective modes and we further uncover a new coupled collective soft mode. Our work shows the potential of modern ultrafast experiments to address the collective excitations in unconventional superconductors and highlights the importance of sub-dominant interactions for the non-equilibrium dynamics in these systems.

* work done in collaboration with Marvin A. Müller, Pengtao Shen, Maxim Dzero, Pavel A. Volkov, and Indranil Paul

** the work is supported by the joint DFG-ANR Project (ER 463/8-1)
10:24AM A66.00005: Spectroscopies of superconducting collective modes: new advances and open questions [Invited] LARA BENFATTO (Presenter), Sapienza University of Rome, Italy — In the last few years, a number of experiments carried out with very intense THz fields, either in transmission or in pump-probe configuration, have shown the possibility to excite superconducting collective modes via light pulses. The signatures of the superconducting excitations manifest either in third-harmonic generation, in the case of narrowband pulses, or in well-defined oscillations of the transmitted field as a function of the pump-probe delay, in the case of broadband pulses. In the latter case, the phenomenon is completely analogous to the well-known excitations of Raman-active phonons in insulating and metallic systems. Despite the clear interest in the fundamental and applicative aspects of these techniques, a clear theoretical paradigm for the description of these experiments is still lacking. In this talk I will present a general scheme we recently developed [1,2] to describe step-by-step the processes behind the pump-probe detection of collective excitations, that can be equally well applied to ordinary phonons as well as electronic collective modes. I will then discuss a direct application of our interpretative scheme to the light-induced excitation of the so-called superconducting phase Leggett mode in the multi band MgB2 superconductor[2], and its connection to the phenomenon of the third-harmonic generation in superconductors[3,4]. Finally, I will present some recent results [5] on the role of the superconducting phase mode for the non-linear optical response in unconventional curate superconductors.


Monday, March 2, 2020 8:00 AM - 11:00 AM

Session A67 DCMP: Thermal Hall Effect in Quantum Materials Four Seasons
2-3 - Leon Balents, University of California, Santa Barbara - Tag(s): Invited

8:00AM A67.00001: Thermal Hall conductivity of spin liquids at low temperatures* [Invited] N. PHUAN ONG (Presenter), PETER CZAJKA, TONG GAO, Physics, Princeton University — I will describe results on low-temperature thermal Hall conductivity Kxy of several quantum spin liquids based on honeycomb and triangular lattices, primarilty α-RuCl3, and Na2BaCo(PO4)2. In α-RuCl3, I will describe recent evidence suggesting the existence of a neutral Fermi surface. Results on the thermal Hall conductivity at temperatures performed at temperatures down to 0.4 K will be presented. The difficult challenges facing Kxy measurements will be discussed.

*Supported by Dept of Energy (Contract DE-SC0017863), NSF MRSEC (award DMR 1420541) and the Gordon and Betty Moore Foundation (Grant GBMF4539).
For several years, the compound $\alpha$-RuCl$_3$ is considered as one prime candidate material to host a Kitaev topological quantum spin liquid (TQSL). Such a TQSL has been predicted for the spin-1/2 Kitaev model on a honeycomb lattice in an external magnetic field [1]. The zero field ground state is a quantum spin liquid with itinerant Majorana fermions and immobile gauge fluxes as elementary excitations. An external magnetic field gaps out the Majorana bulk states and topological Majorana edge states emerge. Indeed, for $\alpha$-RuCl$_3$ there is evidence for a significant Kitaev interaction acting between neighboring $j_{\text{eff}}=1/2$ moments. However, the ground state of $\alpha$-RuCl$_3$ shows long-range antiferromagnetic order, indicative of additional Heisenberg-type and anistropy terms in the spin Hamiltonian. An in-plane field of about 8 T suppresses the magnetic order, which opens the question whether the field-induced ground state bears the main signatures of the Kitaev TQSL. In this talk, I will discuss our experimental efforts to probe the elementary magnetic excitations of $\alpha$-RuCl$_3$ by thermal transport. After summarizing the main findings for the longitudinal heat conductivity $\kappa_{xx}$ [2], and briefly discussing new data which extend our findings to very large magnetic fields and lower temperature, I will focus on the surprising and sizeable thermal Hall effect $\kappa_{xy}$ with a field perpendicular to the RuCl$_3$-planes [3] as well as on our attempts to study this quantity for different field orientations.


*We acknowledge financial support from the DFG through SFB 1143 (project-id 247310070) and through projects HE3439/12 and HE3439/13.
The nature of the pseudogap phase of cuprates remains a major puzzle. Although there are indications that this phase breaks various symmetries, there is no consensus on its fundamental nature [1]. Fermi-surface, transport and thermodynamic signatures of the pseudogap phase are reminiscent of a transition into a phase with antiferromagnetic order, but evidence for an associated long-range magnetic order is still lacking. Here we report measurements of the thermal Hall conductivity $\kappa_{xy}$ in the normal state of four different cuprates and show that a large negative $\kappa_{xy}$ signal is a property of the pseudogap phase, appearing with the onset of that phase at the critical doping $p^*$ [2]. It is also a property of the Mott insulator at $p \approx 0$, where $\kappa_{xy}$ has the largest reported magnitude of any insulator. Since this negative $\kappa_{xy}$ signal grows as the system becomes increasingly insulating electrically, it cannot be attributed to conventional mobile charge carriers. Nor is it due to magnons, since it exists in the absence of magnetic order. Our observation is reminiscent of the thermal Hall conductivity of insulators with spin-liquid states [3, 4, 5] pointing to neutral excitations with spin chirality in the pseudogap phase of cuprates.

9:48AM A67.00004: Thermal Hall effect in quantum paramagnets and cuprates [Invited] JUNG HOON HAN (Presenter), Physics, Sungkyunkwan University — Several theoretical aspects of thermal Hall transport in magnetic insulators are discussed in light of recent experimental progress in frustrated magnets and in undoped cuprates. A general formalism for calculating thermal Hall conductivity in magnets is presented[1,2] and used to compute such quantity for kagome ferromagnets[1] and antiferromagnets[3] under the perpendicular magnetic field. Both calculations bear close resemblance to actual experimental data. Furthermore I discuss our recent theoretical effort to understand the remarkable yet puzzling observation of large thermal Hall conductivity in undoped to lightly doped cuprates[4]. A tentative scenario in terms of spinon Fermi surface is presented to work, to a certain extent, in matching the observation, albeit on weak experimental foundation. The talk covers materials learned from collaboration with Hyunyong Lee, Jin-Hong Park, Patrick Lee, and Yamashita group at ISSP.


10:24AM A67.00005: Thermal Hall effect in square-lattice spin liquids: an application to cuprates* [Invited] MATHIAS SCHEURER (Presenter), Harvard University — Recent experiments [1] have revealed an enhanced thermal Hall effect in the pseudogap phase of several different cuprates compounds. The large signal even persists in the undoped system and, thus, challenges our understanding of the antiferromagnetic phase fundamentally. In this talk, I will analyze possible mechanisms that can give rise to a thermal Hall effect in the square-lattice Heisenberg antiferromagnet [2,3]. In particular, I will discuss the possibility [3] that the magnetic field drives the Néel state close to a transition to a phase where Néel order coexists with a chiral spin liquid. A spinon lattice model for this transition is shown to give rise to a large thermal Hall conductivity that also features a similar magnetic field and temperature dependence to experiment. We will derive the low-energy continuum field theory for the transition, which is characterized by an emergent global SO(3) symmetry and has four different formulations that are all related by dualities.


*Research supported by National Science Foundation (Grant No. DMR-1664842). In addition, MS: German National Academy of Sciences Leopoldina, LPDS 2016-12, SC: ERC synergy grant UQUAM.
Session A68 DPOLY: 100 Years of Polymer Science  Four Seasons 4 - Connie Roth, Emory University - Tag(s): Invited, Undergrad Friendly

8:00AM A68.00001: Equilibration and Dynamics in Block Copolymer Micelles  [Invited]
TIMOTHY LODGE (Presenter), University of Minnesota — Block copolymers provide a remarkably versatile platform for achieving desired nanostructures by self-assembly, with length scales ranging from a few nanometers up to several hundred nanometers. In particular, block copolymer micelles in selective solvents are of great interest across a range of technologies, including drug delivery, imaging, catalysis, lubrication, and extraction. While block copolymers generally adopt the morphologies familiar in small molecule surfactants and lipids (i.e., spherical micelles, worm-like micelles, and vesicles), one key difference is that polymeric micelles are typically not at equilibrium. The primary reason is the large number of repeat units in the insoluble block, \( N_{\text{core}} \), which makes the thermodynamic penalty for extracting a single chain (“unimer exchange”) substantial. As a consequence, the critical micelle concentration (CMC) is rarely accessed experimentally; however, in the proximity of a critical micelle temperature (CMT), equilibration is possible. We use time-resolved small angle neutron scattering (TR-SANS) to obtain a detailed picture of the mechanisms and time scales for chain exchange, for systems at or near equilibrium. The dependence of the rate of exchange on the key variables – concentration, temperature, \( N_{\text{core}} \), \( N_{\text{corona}} \), and chain architecture (diblock versus triblock) – will be discussed. We will also address measurements of micelles prepared far from equilibrium, which equilibrate by fragmentation processes, using dynamic light scattering, small-angle X-ray scattering, and liquid-state TEM.
Over the last few decades, there has been rapidly growing interest in soft, stimuli-responsive polymeric materials ("mushy, squishy systems") that exhibit a global response to a local signal. One motivation for creating such polymers arises from a technological need to produce energy efficient devices that can amplify or convert a small-scale input into a large-scale action. Another inspiration for focusing on responsive polymers comes from biology. One of the exquisitely evolved properties of biological systems is the ability to convert local information into a global action. Few synthetic materials can match the ability of biological systems to undergo large-scale, rapid motion in response to local changes. There are a number of design challenges that must be met in order to create such efficient systems. First, the polymeric material must be capable of not only sensing a local signal, but also reacting in a specified manner. Second, the polymers should ideally be capable of transducing one form of energy (e.g., electromagnetic, optical, chemical) into a mechanical action and thus must be "active". Developing such responsive polymeric materials poses significant and intriguing scientific challenges, and necessitates the development of robust theoretical and computational models for the behavior of active materials systems. A few examples of these kinds of modeling approaches will be discussed, highlighting efforts that are valuable for developments in future technologies, such as soft robotics and autonomously operating devices.
The surprising flow behavior of entangled polymer melts and solutions has been a subject of enduring interest. In the last 30 years, substantial progress has been made in mechanistic understanding of entangled polymer rheology, based on the tube ansatz of Edwards and de Gennes. I will summarize the essential physics of the “success stories”: 1) linear dynamic rheology of entangled linear chains, stars, star-linear blends, H-polymers, polydisperse multiply branched chains, and polydisperse linear chains; and 2) nonlinear extensional flow of linear chains and branched polymers.

With that progress, how well do we understand where the tube comes from? Simulations have been helpful: we can observe the “skeleton” of the tube with various chain-shrinking methods, and “see” the tube using isoconfigurational averaging. And, we can relate the tube to a measure of how many knots the melt can tie, the “topological entropy”.

But can we predict the tube diameter from chain architecture? I will describe a new scaling theory that joins previous predictions for flexible chains and stiff chains. Overall, entanglement is governed by close encounters between chains, when they can “zig” one way or “zag” the other as they pass. These encounters are governed by 1) the larger of the packing length $p$ or chain diameter $d$, and 2) whether an entanglement strand is flexible.

Scaling based on packing length and flexible chains (Lin-Noolandi, or LN) describes a wide range of real polymers; but commonly simulated linear bead-spring chains behave as entangled “threads”, with no role for $p$. However, if we “bulk up” linear bead-spring chains with sidegroups, we can observe LN scaling in simulations. This raises the question of how to *measure* the packing length, which we do by asking how far from a given monomer most of the density comes from its own chain. Packing length measured this way is consistent with LN scaling, and differs from simple estimates based on the effective diameter of chains.
From the first numerical simulations of single polymer chains in dilute solution to current exascale simulations of highly entangled polymer melts, computer simulations have played a critical role in polymer physics. Numerical simulations have provided microscopic insight into macroscopic behavior. Here the potential of computations to polymer physics in the realm of new computer architectures will be introduced in view of the fundamental insight connecting theory and experiments attained thus far. Capturing the wide range of coupled length and time scales that govern the unique macroscopic, viscoelastic behavior of polymers has been one of the major challenges to surmount. Starting with the simple bead-spring models, through atomistically inspired coarse-grained approaches, it is now possible to capture not only the mobility of the chain but also the viscoelastic properties of entangled polymers. With current and future computational resources, numerical simulations will provide the understanding of viscoelastic response and shear and extensional viscosity of entangled melts for complex architectures bridging the dynamics on the length scale of the atomic level with the macroscopic response.

*This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under Contract No. DE-NA-0003525.
We first introduce the field of “Entangled Active Matter”. Active systems span an enormous range of length scales, from the cytoskeleton of individual living cells to tissues and animal groups such as fish or insect swarms. We will focus on “entangled active matter”, where the building blocks are transiently bound. We will point out strong similarities of mechanical properties between aggregates of cells, swarm of ants, of cells and inert viscous pastes.

We characterize the tissue mechanical properties (surface tension, elasticity, viscosity) using pipette aspiration technique. Cellular aggregates exhibit a viscoelastic response in analogy to ultra-viscous polymer melts. When we apply oscillating pressures, we observe a reinforcement of the tissue at high frequencies. We developed a model to determine the main mechanical properties of the system as a function of the oscillation frequencies. Unlike inert polymer melts, we observe aggregate's reinforcement with pressure, which gives rise to pulsed contractions or “shivering”, interpreted as a mechano-sensitive active response of the acto-myosin cortex.

We then describe the spreading of aggregates on rigid and soft substrates, varying both intercellular and substrate adhesion. We find both partial and complete wetting, with a precursor film forming a dense cellular monolayer in analogy with the stratified spreading of viscous polymer melts. On soft substrate, the precursor film is unstable, leading to a symmetry breaking of cells polarity causing the aggregate to move spontaneously as a giant keratocytes.

References:
F Brochard-Wyart et al, *Entangled Active Matter: from ants to living cells* EPJE 2015

*The authors greatly acknowledge the Nikon Imaging Center and the PICT-IBiSA Imaging core facility at Institut Curie-CNRS.*
8:00AM A70.00001: Dynamics of nanoparticles in polyelectrolyte solutions* ALI H SLIM, Univ of Houston, RYAN POLING-SKUTVIK, University of Pennsylvania, JACINTA CONRAD (Presenter), Univ of Houston — Recent theories indicate that nanoparticle dynamics in semidilute solutions of neutral, flexible polymers couple to the segmental relaxations of polymer chains. How nanoparticle dynamics couple to relaxations of charged, semiflexible polymers remains incompletely understood. Here, we probe the dynamics of polystyrene nanoparticles in solutions of a polyelectrolyte, sodium polystyrene sulfonate, using fluorescence microscopy. When the ionic strength of the solution is high, such that the polymer adopts a Gaussian conformation, the nanoparticle dynamics are coupled to the bulk solution viscosity across the dilute and semidilute regimes of polymer concentration. In near-salt-free solutions, in which the polymer adopts an extended conformation, the nanoparticle dynamics do not follow the Stokes-Einstein prediction based on the bulk viscosity across all polymer concentrations, and furthermore do not collapse onto a master curve as a function of normalized length scales. This result suggests that the coupling of nanoparticle and polymer segmental dynamics are altered by polymer conformation.

*Welch Foundation (E-1869), NSF (CBET-1705968)

8:12AM A70.00002: Correcting the Generalized Stokes-Einstein Relation to Include Effects of Hydrodynamic Interactions from Periodic Images* JEFFREY ETHIER (Presenter), Illinois Institute of Technology, POURIA NOURIAN, RAJESH KHARE, Texas Tech University, JAY SCHIEBER, Illinois Institute of Technology — In microrheology, the mean squared displacement (MSD) of micron-sized particles is measured to extract linear viscoelastic properties of entangled polymer melts using the generalized Stokes-Einstein (SE) relation. Probe rheology from molecular dynamics (MD) simulations has a significant computational cost due to the large simulation box sizes required to reduce the effect of the probe’s hydrodynamic interactions with its periodic images. Here, we use an analytical solution for Stokes flow around a body-centered cubic array of spheres to introduce a correction factor to the generalized SE relation. We show that this correction factor is a function of the ratio ($R/L$), where $R$ and $L$ are particle radius and simulation box length, and the fluid mass fraction. We then predict the dynamic moduli of an entangled melt of bead-spring polymer chains from the MSD of a probe particle at various $R$ and $L$. Lattice Boltzmann simulations are also performed to calculate the transient drag force and velocity of a particle in a Newtonian fluid to account for effects of inertia at higher frequencies. This added correction factor should allow a reduction of at least one order of magnitude in MD simulation costs.

*This work is supported by the National Science Foundation under DMR Award No. 1610115.
8:24AM A70.00003: Resolving structure-property-dynamics relationships in model polymer nanocomposite systems* BENJAMIN YAVITT (Presenter), DANIEL SALATTO, ZHIXING HUANG, MAYA ENDOH, State Univ of NY - Stony Brook, LUTZ WIEGART, ANDREI FLUERASU, YUGANG ZHANG, MASAFUMI FUKUTO, RUIPENG LI, Brookhaven National Laboratory, VERA BOCHAROVA, Oak Ridge National Laboratory, ALEXEI SOKOLOV, University of Tennessee, Knoxville, TAD KOGA, State Univ of NY - Stony Brook — Understanding the origins of mechanical enhancement in polymer-nanoparticle composites (PNC) is necessary to design materials with optimized mechanical properties. We use a combination of techniques to resolve the dynamics-structure-property relationships governing mechanical enhancement in a model PNC system of attractive SiO2 nanoparticles embedded in a glassy P2VP polymer matrix over a wide range of NP concentrations (1 – 25 vol.%). By tuning the interparticle distance between neighboring NPs, the formation of the proposed “structural bridge” and the resulting contribution to mechanical enhancement are resolved [1]. The nanoscale structure is investigated by SAXS and TEM while the micro/macro dynamics are resolved by x-ray photon correlation spectroscopy (XPCS) and shear rheology respectively. As concentration increases, the characteristic relaxation times increase dramatically. The dynamics transition to collective motion at the gel point, which correlates to the formation of a sample spanning network. Identification of “rubbery” and “glassy” bridges are discussed in the context of the observed dynamics. [1] Chen, Q.; et al. ACS Macro Lett. 2015, 4 (4), 398–402.

*Donors of the American Chemical Society Petroleum Research Fund

8:36AM A70.00004: Role of soft interactions in enhanced diffusivity of polymer-grafted nanoparticles in heterogeneous environments RYAN POLING-SKUTVIK (Presenter), University of Pennsylvania, JACINTA CONRAD, RAMANAN KRISHNAMOORTI, University of Houston — The dynamic behavior of dilute solutions of polymers is well described by the colloidal model or the Zimm model. In denser systems, the colloidal description fails as interactions with the environment become important. Here, we investigate the behavior of polymer-grafted nanoparticles (PGNPs), where the grafting to the nanoparticle surface causes a high self-concentration of the polymer chains. When dispersed in semidilute polymer solutions, the grafted polymer chains compress and their dynamics are confined by neighboring chains. This change in grafted polymer dynamics arises from the soft repulsive interaction between PGNPs and surrounding polymer chains. This soft interaction profile also affects the dynamics on longer length and time scales. Whereas hard sphere diffusivity decouples from bulk predictions in polymer solutions when the particle becomes comparably sized to the polymer, the diffusivity of soft PGNPs decouples from solution viscoelasticity even when they are larger than the surrounding polymer. Furthermore, the PGNP dynamics strongly depend on the ratio of free to grafted polymer molecular weights. These findings indicate that soft interactions allow PGNPs to diffuse faster than hard spheres in heterogeneous materials.
8:48AM A70.00005: Dynamic Behavior of Polystyrene Soft Nanoparticles by Neutron Spin Echo  
JACOB FISCHER (Presenter), MARK DADMUN, University of Tennessee, Knoxville, ANTONIO FARAOONE, NCNR, NIST — The inclusion of soft polystyrene nanoparticles improves the dynamic properties of bulk polystyrene, a behavior that is not yet fully understood. To provide insight into this phenomenon, the dynamics of the nanoparticles are evaluated using neutron spin echo (NSE) spectroscopy. These particles consist of a crosslinked polystyrene core with loosely connected loops and tails, which we term a fuzzy interface. NSE spectroscopy of dilute solutions of the nanoparticles (NPs) show the nanoparticle with the lowest crosslinking density and molecular weight exhibits the most Zimm-like dynamics. Varying the synthetic procedure to create nanoparticles with lower molecular weights and fuzzier surfaces results in more heterogeneous relaxation processes, indicating that the dynamics of the core differs significantly from that of the outer shell. Combined with our previous studies showing the relationship between the fuzziness of the nanoparticle and diffusion of bulk polystyrene, these results exemplify the importance of the NP molecular weight and the interaction of the fuzzy interface with linear chains in determining the dynamics of all polymer nanocomposite system.

9:00AM A70.00006: Universality in Microstructural Evolution of Deformed Polymer Melts as Revealed by Small-Angle Neutron Scattering and Molecular Dynamics Simulation*  
WENSHENG XU, CHRISTOPHER N LAM, JAN-MICHAEL CARRILLO, BOBBY SUMPTER, YANGYANG WANG (Presenter), Oak Ridge National Lab — The viscoelastic properties of polymers are strongly influenced by the entanglement phenomenon. Historically, distinct theoretical models have been developed to understand the rheology of entangled and unentangled polymer melts. Using small-angle neutron scattering and nonequilibrium molecular dynamics simulations, we show that the microstructural evolutions of deformed entangled and unentangled polymer melts share a number of universal traits that cannot be comprehended within the classical theoretical framework. Our analysis suggests that interchain correlations play a fundamental role in nonlinear polymer melt rheology.

*The research is supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Early Career Research Program Award KC0402010, under Contract DE-AC05-00OR22725.
Nanoparticle effect on multiscale polymer dynamics in nanocomposites: insights from neutron and x-ray spectroscopy [Invited]  ERKAN SENSES (Presenter), Koc University — Dynamics of polymers in presence of nanoparticles has attracted much attention due to immediate consequences on the rheological behavior of polymer nanocomposites. Bulk techniques are usually insufficient to study the component dynamics mainly due to lack of space-time resolution required for intrinsically complex relaxation mechanisms. In our studies, we applied extensive neutron and x-ray scattering techniques, specifically backscattering, neutron spin echo, and x-ray photon correlation spectroscopy to gain microscopic insight on the role of nanoparticle size, shape, loading, dispersion state, polymer-particle interfaces and confinement on multiscale polymer dynamics as well as on slow nanoparticle relaxation in attractive nanocomposites [1, 2]. These interconnected and often competing effects result in the unusual rheological behavior, the origin of which has long been debated. By simultaneously accessing time scales from sub-nanosecond to hundreds of nanoseconds, and length scales from monomers to entanglement spacing, we directly measured the key dynamical parameters- Rouse rate and reptation tube size- in nanocomposites, and correlated them with the macroscopic mechanical relaxation and the nanoscale particle motion [3].


Molecular Dynamics Simulations of a Polymer Star under Shear Flow
JAN-MICHAEL CARRILLO (Presenter), YANGYANG WANG, BOBBY SUMPTER, WEI-REN CHEN, Oak Ridge National Lab — We performed large-scale coarse-grained molecular dynamics simulation of a polymer star in a melt of short polymer chains under shear flow in dilute star concentrations. The temperature of the system was maintained using a dissipative particle dynamics (DPD) thermostat to conserve momentum and model hydrodynamic interactions. Simulations at the quiescent state was used to determine the timescale for which the end-to-end vector of the star’s arm as it relaxes. The star has sixteen arms and its motion under shear in high Weissenberg numbers is characterized by a cycle of collapse and extension of the star’s arm, which is in line with expected tank-treading motion. We used the trajectories of these simulations to calculate quantities pertinent to neutron scattering experiments, such as small angle neutron scattering under high shear stress, or SANS in the rheo-SANS environment, and predict the resulting spectra from these experiments. Specifically, we calculate the star’s anisotropic single-molecule structure factor through the spherical harmonic expansion approach.
**10:00AM A70.00009: Dynamics and Rheology of THF Swollen Ionic Polymer Melts: Molecular Dynamics Simulation Study**

SHALIKA D. K. MEEDIN (Presenter), CHATHURIKA KOSGALLANA, MANJULA SENANAYAKE, Department of Chemistry, Clemson University, Clemson, SC, United States, 29634., GARY GREST, Sandia National Laboratories, Albuquerque, NM 87123, DVORA PERAHIA, Department of Chemistry, Clemson University, Clemson, SC, United States, 29634. Department of Physics, Clemson University, Clemson, SC, United States, 29631. — The macroscopic dynamics of ionic polymers are often constrained by the formation of ionic clusters. Traces of solvents however affect the structure, dynamics and viscoelastic response of these melts. Here, we probe the effects of THF on the dynamics of polystyrene sulfonate (PSS) melts by fully atomistic molecular dynamics simulations. We hypothesize that THF penetrates both hydrophilic and hydrophobic domains, affecting their interrelation. Melts swollen with THF as the sulfonation fraction is varied were studied. We find that with the addition of THF the average cluster size decreases. The number of THF molecules associated with ionic groups increases with increasing sulfonation fraction \( f \). Shear measurements show that the addition of small amounts of THF decreases the viscosity dramatically. Correlations of the dynamics of swollen melts on different time and length scales as determined by MSD and \( S(q, t) \) with the rheology studies will be discussed.

*DOE funding DE-SC0019284

**10:12AM A70.00010: Influence of Chain Architecture on the Kinetics of Chain Exchange Between BCC-Ordered Copolymer Micelles: A Dynamical Self-Consistent Mean-Field Theory Study**

MARK HOLDEN (Presenter), ROBERT WICKHAM, Univ of Guelph — Motivated by recent time-resolved small-angle neutron scattering results, we study the kinetics of symmetric ABA and BAB triblock copolymer exchange between BCC-ordered spherical micelles using dynamical self-consistent field theory simulations. We characterize the equilibrium properties of micelles in pure melts of AB, ABA, and BAB copolymers, and systematically examine the decay time of the fraction of core (A) blocks remaining in their original micelle, as well as the chain self-diffusion constant, as a function of segregation. Differences in the equilibrium micelle structure between these cases complicate comparison of the dynamical behaviour for the different chain architectures. This complication is overcome by simulating tracer triblock copolymers in a constant background of BCC-ordered diblock micelles, allowing for direct comparison of the chain diffusion for the different chain architectures, as a function of segregation.
10:24AM A70.00011: Revealing Structures and Dynamics of Bound Chains in Filler-Reinforced Elastomers  
DANIEL SALATTO (Presenter), BENJAMIN YAVITT, MAYA ENDOH, Stony Brook University, TOMOMI MASUI, HIROYUKI KISHIMOTO, Sumitomo Rubber Industries Ltd., JAN-MICHAEL CARRILLO, ORNL, TAKASHI TANIGUCHI, Kyoto University, MICHIIRO NAGAO, NIST, TADANORI KOGA, Stony Brook University — Filler-reinforced elastomers have been of great interest to the broad materials community for at least the last three decades. The addition of nanofillers such as carbon black or silica to elastomers affects the overall rheological and mechanical properties mainly due to the creation of a few nanometer-thick bound polymer layer (BPL) on a filler surface at which the polymer is expected to have different structural and dynamical behavior from the bulk. However, the detailed descriptions of the BPL remain a challenge due to the lack of experimental techniques that directly probe the BPL. In this presentation, using simplified industrial carbon black (CB) filled polybutadiene in conjunction with contrast-matched neutron scattering and spectroscopy techniques, we resolve the buried structure at the nanometer-scale and the dynamics at the picosecond-to-nanosecond time scales in the polymer matrix.

10:36AM A70.00012: The Effect of Rubbery/Glassy Block Copolymer Brushes on the Dynamic Behaviors of Silica Particles in Nanocomposite Elastomer  
CHAO-HUNG CHENG (Presenter), SHIORI MASUDA, NATTANEE DECHNARONG, KENTO FUKADA, KIYU UNO, KAZUTAKA KAMITANI, Kyushu Univ, TAIKI HOSHINO, SPring-8 Center, RIKEN, KEN KOJOI, ATSUSHI TAKAHARA, Kyushu Univ — Matrix-free elastomer nanocomposites with high strength was prepared by rubbery/glassy block copolymer-grafted silica nanoparticles (BCP-g-SiNP). Investigation of dynamic behavior of the nanocomposites can help us to know the dynamic structure and properties. However, the dynamic behavior of SiNP in the BCP-g-SiNP has not been well-studied. In this study, X-ray photon correlation spectroscopy (XPCS) was utilized to analyze the dynamics of BCP-g-SiNP with inner poly(butyl acrylate) and outer poly(methyl methacrylate). The XPCS measurement revealed that the relaxation rates of SiNP were proportional to $q$ value, indicating that the behavior of SiNP in the block copolymer-grafted SiNP was non-Brownian and hyperdiffusion motion. At the same $q$ value, the relaxation rates increased dramatically as the temperature exceeded $T_g$. This is due to the outer PMMA phase changed to the rubbery state, and the restriction of SiNP motion by PMMA decreased. Moreover, during elongation, the relaxation rates of SiNP in the direction perpendicular to elongation was faster than in the direction parallel to elongation. The extended polymer chains might restrict the motion of SiNP, leading the slower relaxation rate of SiNP in the direction parallel to elongation.
The Role of Fast Relaxations in Cross-Linked Polymer Networks for Impact Mitigation

CHRISTOPHER SOLES (Presenter), KANAE ITO, ADAM B BURNS, MADHUSUDAN TYAGI, National Institute of Standards and Technology, DANIEL KNORR, KEVIN A MASSER, JOSEPH L LENHART, Army Research Laboratory — Composites for ballistic impact resistance integrate high strength reinforcements, such as high strength fibers or ceramic, with a polymeric binder that imparts ductility to the system. Together these components provide the strength plus ductility to realize tough ballistic composites. The binder is often a cross-linked polymer networks where the reactive liquid monomers can be impregnated into the composite structure and then be cross-linked into a rigid component. To this end, there is a significant interest in the molecular origins of toughness in cross-linked networks - why some systems lead to tough resins whereas others lead to a brittle response. Here we explore a series of model epoxy networks with moderate toughness to a series dicyclopentadiene networks which display incredible toughness deep into the glassy state. Quasielastic neutron scattering (QENS) is used to quantify molecular motions on the time scale of ps to ns in these networks. This reveals a strong correlation between these fast polymer relaxations and toughness. Collective many atom vibrations are important for toughness, but not enough. The many atom vibrations must lead to dissipative, many atom relaxations in order to dissipate energy and enhance toughness under ballistic impact conditions.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B01 DAMOP DCMP: Disorder and Localization in AMO Systems

Many-body delocalization of ultracold bosons in lattices [Invited]

CHRISTIAN GROSS (Presenter), Max-Planck-Institute of Quantum Optics — Many-body localization describes the phenomenon of localization and vanishing charge transport in closed quantum many-body systems. It is well accepted by now that MBL is stable in one dimension and many of its properties have been revealed. Much less is known in two dimensions. Here we present our recent results on the study of the stability of the localization in 2d bosonic lattice systems. Our observation is consistent with persistent localization if the system is brought in contact with a small quantum bath, but localization is clearly destroyed for larger baths. The dynamics towards the steady state differs strongly in the two cases.
11:51AM B01.00002: Instability of subdiffusive spin dynamics in strongly disordered Hubbard chain

MAKSYMILIAN SRODA (Presenter), Department of Theoretical Physics, Wroclaw University of Science and Technology, PETER PRELOVSEK, J. Stefan Institute, MARCIN MIERZEJEWSKI, Department of Theoretical Physics, Wroclaw University of Science and Technology — We study spin transport in a Hubbard chain with a strong, random, on-site potential and with spin-dependent hopping integrals $t_\sigma$. For the SU(2) symmetric case $t_\uparrow = t_\downarrow$, such a model exhibits only partial many-body localization with localized charge and (delocalized) subdiffusive spin excitations [1,2]. In our work [3], we demonstrate that breaking the SU(2) symmetry by even weak spin asymmetry, $t_\uparrow \neq t_\downarrow$, localizes spins and restores full many-body localization. To this end, we derive an effective spin model where the spin subdiffusion is shown to be destroyed by arbitrarily weak $t_\uparrow \neq t_\downarrow$. Instability of the spin subdiffusion originates from an interplay between random effective fields and singularly distributed random exchange interactions.


* (1) National Science Centre, Poland via Project No. 2016/23/B/ST3/00647
(2) Program No. P1-0044 and Project No. N1-0088 of the Slovenian Research Agency
(3) Polish National Agency of Academic Exchange (NAWA) PPN/PPO/2018/1/00035

12:03PM B01.00003: Many-body localization from a one-particle perspective in the disordered 1D Bose-Hubbard model

MIROSLAV HOPJAN (Presenter), FABIAN HEIDRICH-MEISNER, Institute for Theoretical Physics, University of Göttingen, Germany — We numerically investigate 1D Bose-Hubbard chains with onsite disorder by means of exact diagonalization. Consistent with previous studies, we observe signatures of transition from the ergodic to the many-body localized (MBL) regime when increasing the disorder strength or energy density. Apart from the entanglement entropy as a conventional but indirect measure for the ergodic-MBL transition we utilise the one-particle density matrix (OPDM) to characterize the system [1]. We show that the natural orbitals (the eigenstates of OPDM) are extended in the ergodic phase and real-space localized when one enters into the MBL phase. Furthermore, the distributions of occupancies of the natural orbitals as well as the diagonal part of OPDM (i.e., the site occupancies) can be used as measures of Fock-space localization in the respective basis [2]. Moreover, the full distribution of the densities of the physical particles provides a one-particle measure for the detection of the ergodic-MBL transition which could be directly accessed in experiments with ultra-cold gases.

12:15PM B01.00004: Localization dynamics in a centrally coupled system  NATHAN NG (Presenter), University of California, Berkeley, RAJAGOPALA SEELAM, SEBASTIAN WENDEROTH, University of Freiburg, MICHAEL KOLODRUBETZ, University of Texas at Dallas, ERAN RABANI, University of California, Berkeley, MICHAEL THOSS, University of Freiburg — We investigate a disordered Ising chain in which all spins couple to a central qudit, through which spin flip interactions are mediated. For small but finite coupling, the trivial localization of the non-coupled limit survives as a form of many-body localization (MBL). By using an exact wavefunction propagation method, we are able to observe the dynamics of large system sizes (L~50-100) to intermediate timescales and establish the existence of slow or vanishing relaxation. This allows us to address the question of the proper scaling of the qudit size with L in the thermodynamic limit, the suppression of effective all-to-all coupling to protect MBL, and the dependence of localization on energy density.

12:27PM B01.00005: Strongly resonating clusters around the ergodic-MBL transition* BENA JM VILLALONGA (Presenter), BRYAN CLARK, University of Illinois at Urbana-Champaign — An interacting quantum system can transition from an ergodic to a many body localized (MBL) phase under the presence of sufficiently large disorder. Both phases are radically different in their dynamical properties, which are characterized by highly excited energy eigenstates. One of the differences between both phases is in the statistics of their energy levels: while in an ergodic phase levels experience repulsion and follow GOE statistics, in MBL they largely lack repulsion and follow Poisson statistics. Here, we argue that the transition between both behaviors is accompanied by the formation of resonating clusters in the eigenstates of the Hamiltonian. Using a basis of local integrals of motion (l-bits), we observe that these clusters take the form of cat states over a subset of l-bits on a 1D spin chain. While such resonances are rare in MBL, they proliferate around the transition, and are absent well into the ergodic phase. Finally, the spatial structure of the resonating clusters suggests correlations that are scale invariant in the chain, which we check numerically for finite size systems.

*This research is part of the Blue Waters sustained-petascale computing project, supported by the National Science Foundation (OCI-0725070 and ACI-1238993) and the state of Illinois.

12:39PM B01.00006: Inverted many-body mobility edge in a central qudit problem SAEED RAHMANIAN KOSHAKI (Presenter), MICHAEL KOLODRUBETZ, University of Texas at Dallas — We study the disordered Ising model with transverse and longitudinal fields coupled globally to a d-level system (qudit). In the center of the many-body spectrum, earlier work [PRL 122, 240402 (2019)] found a regime where many-body localization (MBL) survives global coupling to the cavity. In this work, we study the dependence of MBL on energy. Most strikingly, we discover an inverted mobility edge, where high energy states are localized while low energy states are delocalized. Our results are supported by shift-and-invert eigenstate targeting and Krylov time evolution up to L=13 and 18 respectively, with large central spin d=12 that is effectively infinite. We argue for critical energy of the MBL to thermal phase transition which scales as $E_c \sim L^{\frac{1}{2}}$, consistent with finite size numerics. We also show evidence for a reentrant MBL phase at even lower energies despite the presence of strong effects of the central qudit in this regime.
Emergent ergodicity at the transition between many-body localized phases — RAHUL SAHAY (Presenter), BINGTIAN YE, FRANCISCO MACHADO, NORMAN YAO, University of California, Berkeley — Due to their failure to thermalize, systems in the many-body localized (MBL) phase can support non-trivial order (e.g., order characterized by spontaneously broken symmetries or symmetry-protected topological order) even in highly excited, many-body eigenstates. However, the stability of MBL as a system transitions between different ordered phases remains a mystery. In particular, it is unknown whether the competition between two orders near a phase boundary inevitably destabilizes the MBL and restores ergodicity to the system. Here, we present evidence that, indeed, a direct transition between different MBL phases cannot occur, and between any two MBL phases, an intervening finite-width thermalizing phase emerges. We probe the emergence of this thermalizing phase by numerically studying the level statistics of a variety of different models exhibiting either symmetry broken order or symmetry-protected topological order, both in the static and driven case. We complement our numerical analysis by providing an analytic picture for the instability of MBL around the phase transition.

Critical properties of the many-body Aubry-Andre model localization-delocalization transition — TAYLOR COOKMEYER (Presenter), University of California, Berkeley, JOHANNES MOTRUK, Lawrence Berkeley National Lab, JOEL MOORE, University of California, Berkeley — As opposed to random disorder, which localizes single-particle wave-functions in 1D at arbitrarily small disorder strengths, there is a localization-delocalization transition for quasi-periodic disorder in the 1D Aubry-Andre model at a finite disorder strength. On the single-particle level, many properties of the ground-state critical behavior have been revealed by applying a real-space renormalization-group scheme; the critical properties are determined solely by the continued fraction expansion of the incommensurate frequency of the disorder. We investigate the many-particle localization-delocalization transition in the Aubry-Andre model with and without interactions. In contrast to the single-particle case, we find that the critical exponents depend on a Diophantine equation relating the incommensurate frequency of the disorder and the filling fraction which generalizes the dependence, in the single-particle spectrum, on the continued fraction expansion of the incommensurate frequency. Numerical evidence suggests that interactions may be irrelevant at at least some of these critical points, meaning that the critical exponent relations obtained from the Diophantine equation may actually survive in the interacting case.

Single doublons as ergodic bubbles — ULRICH KRAUSE, Frei Universität Berlin, THÉO PELLEGRIN, Univ of Geneva, PIET W BROUWER, Frei Universität Berlin, DMITRY ABANIN, MICHELE FILIPPONE (Presenter), Univ of Geneva — We illustrate a remarkably simple mechanism in which single doublon excitations trigger the generation of ergodic bubbles, which thermalize extensive localized systems. We provide analytical estimates showing how the critical disorder strength for such mechanism depends on singlon densities, which are nicely supported by numerical exact-diagonalization simulations. Our predictions equally apply to fermionic and bosonic systems and are definitively accessible by ongoing experiments simulating synthetic quantum lattices.

*FNS/SNF Ambizione Grant PZ00P2 174038
1:27PM B01.00010: Quasi-1D limit of the integer quantum Hall transition as a disordered Thouless pump* MATTEO IPPOLITI (Presenter), Stanford Univ, RAVINDRA NAUTAM BHATT, Princeton University — We study the quantum Hall plateau transition on rectangular tori. As the torus aspect ratio is increased, the 2D critical behavior (where a subextensive number of topological states exist in a vanishing energy window around a critical energy) changes drastically. In the thin-torus limit, the entire spectrum is Anderson-localized; however, an extensive number of states retain a nonzero Chern number. This apparent paradox is resolved by mapping the thin-torus quantum Hall system onto a disordered Thouless pump. We show that the Chern number maps onto the winding number of an electron’s path in real space during a pump cycle, and that the electrons’ paths become random walks of diverging length, giving rise to the proliferation of large and essentially random Chern numbers across the spectrum. Building on this thin-torus limit result, we characterize quantitatively the crossover between the 1D and 2D regimes for large but finite aspect ratio. Possible realizations of this physics in quantum simulation platforms (e.g. cold atoms, microwave cavity arrays) are discussed.


*This work was supported by DOE BES grant n. DE-SC0002140.

1:39PM B01.00011: Spin transport in disordered long-range interacting spin chain* BENEDIKT KLOSS (Presenter), Chemistry, Columbia Univ, YEVGENY BAR LEV, Physics, Ben-Gurion University of the Negev — We numerically study spin transport and spin-density profiles after a local quench in a disordered one-dimensional spin-chain with long-range interactions, in the regime where delocalization is predicted by all existing theories. We observe a transient super-diffusive transport, followed by asymptotic diffusive behavior. We provide a phenomenological explanation by properly generalized Griffiths picture.

*This research was supported by the Israel Science Foundation (grants No. 527/19 and 218/19). Benedikt Kloss acknowledges funding through the National Science Foundation (Grant No. CHE-1464802).
1:51PM B01.00012: Complex network description of phase transitions in the classical and quantum disordered Ising Model*  MINA FASIHI (Presenter), HALEY COLE, LINCOLN CARR, Colorado School of Mines, GUILLERMO GARCIA PEREZ, SABRINA MANISCALCO, Physics and Astronomy, University of Turku — Complex network analysis is a powerful tool to describe and characterize classical systems such as the Ising model in a transverse magnetic field. Measuring spin-spin correlations gives rise to the adjacency matrix, representing a weighted network. In this study, the spin-spin correlations at different temperatures are analytically calculated, yielding phase-dependent complex networks, from simple networks in the low temperature ferromagnetic limit to random ones at high temperature. The network structure varies as the transverse field and temperature change, recovering the phase diagram and providing initial insight into correlations in the critical region. Analyzing the resulting complex network using a variety of network measures such as the degree histogram, average clustering, betweenness centrality and the graph entropy, the complexity is characterized. This method is applied for both the disordered classical Ising and quantum Ising lattice, demonstrating the role of finite temperature and disorder in generation of complexity.

*Funded by NSF

2:03PM B01.00013: Probing Slow Scrambling in MBL and the Random Singlet Phase  IAN MACCORMACK (Presenter), MAO-TIAN TAN, JONAH L KUDLER-FLAM, SHINSEI RYU, University of Chicago — We characterize the spreading of operators and entanglement in two paradigmatic non-thermalizing phases - the many body localized phase and the random singlet phase - using out-of-time-ordered correlators, the entanglement contour, and operator entanglement. We contrast these phases with strongly thermalizing holographic conformal field theories and fully localized Anderson insulators. We obtain a phenomenological description of the operator and state dynamics of these phases and provide credence to the utility of the entanglement contour and operator entanglement measures as useful probes of slowly scrambling and non-thermalizing dynamics.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B02 DAMOP: Strongly Interacting Bose and Fermi Gases
11:15AM B02.00001: Fermionic superfluidity in confined one-dimensional spin-imbalanced systems: A configuration-space Hartree-Fock-Bogoliubov approach* KELLY PATTON (Presenter), Physics and Astronomy, Georgia Southern University, DANIEL E SHEEHY, Physics and Astronomy, Louisiana State University — We study pairing and density correlations in imbalanced one-dimensional Fermi systems with short-range interactions that are spatially confined by either a harmonic or a hard-wall (or “box”) trapping potential. It has been hoped that such systems, which can be realized using ultracold atomic gases, would exhibit the long-sought-after Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superfluid phase. Our approach applies a general Hartree-Fock-Bogoliubov (HFB) transformation to handle spatially-inhomogeneous pairing and density correlations on an equal footing to yield predictions for the ground state of confined 1D Fermi gases in harmonic and hard-wall traps. We find that while both cases yield a spatially modulated FFLO pairing amplitude in the imbalanced regime, in the case of a harmonic trap the corresponding signature in the local density is rather weak. In contrast, in the hard-wall case, we find a strong reflection of the FFLO pairing in the local in situ densities. In particular, we find that the excess spins are strongly localized near nodes in the pairing amplitude, thus creating an unmistakable signature of the FFLO state in a hard-wall box trap.

*K.P. would like to thank Georgia Southern University for generous startup funding, which contributed to this work.

11:27AM B02.00002: Ferromagnetism in the SU(n) Hubbard model with nearly flat band* KENSUKE TAMURA (Presenter), HOSHO KATSURA, Univ of Tokyo — Recently, the SU(n) (n>2) Hubbard model describing multi-component fermions with SU(n) symmetry has been a focus of interest, as it is expected to exhibit a rich phase diagram. However, very little is known rigorously about the model with n>2. Here we study the model on a one-dimensional Tasaki lattice and derive rigorous results for the ground states. We first study the model with a flat band at the bottom of the single-particle spectrum. We prove that the ground states are SU(n) ferromagnetic when the number of particles is half the number of lattice sites, generalizing the previous result in Ref. [1]. To discuss SU(n) ferromagnetism in a non-singular setting, we perturb the flat-band model and make the bottom band dispersive. Then we find that SU(n) ferromagnetism in the ground states of the perturbed model at the same filling can be proved if each local Hamiltonian (independent of the system size) is positive semi-definite (p.s.d.). Furthermore, we prove that the local Hamiltonian is p.s.d. for sufficiently large interaction and band gap [2].


*JSPS Grant-in-Aid for Scientific Research on Innovative Areas: No. JP18H04478 (H.K.) and JSPS KAKENHI Grant No. JP18K03445 (H.K.)
11:39AM B02.00003: One-dimensional Spin-polarized Fermi Gas near resonances*  YUTA SEKINO (Presenter), RIKEN, YUSUKE NISHIDA, Department of Physics, Tokyo Institute of Technology — We study a quantum field theory for resonantly interacting spinless fermions in one dimension. This fermions are known to correspond to one-dimensional bosons with delta-function interaction [1]. We perform the renormalization group analysis and clarify that three-body coupling, which is zero in the ultraviolet theory, emergently appears in the infrared limit [2]. This running coupling allows us to rederive the energy relation, i.e., the expression of energy in terms of a momentum distribution and contact parameters characterizing local corrections of the system. The obtained energy relation is consistent with that previously derived in the first quantization formalism [3].


*The work is supported by JSPS KAKENHI Grants No. JP15K17727 and No. JP19J01006.

11:51AM B02.00004: Dynamical Fermionization and Scaling Behaviour for a Strongly Repulsive Spinor Gas after Quench*  SHAH SAAD ALAM (Presenter), TIM SKARAS, LI YANG, HAN PU, Rice Univ — Dynamical fermionization has been theoretically demonstrated for trapped 1D bosonic and anyonic gases in the Tonks-Girardeau limit. It refers to the phenomenon where, after the initial harmonic confinement is turned off, the momentum distribution of the system asymptotically approaches that of a trapped Fermi gas. Evidence of dynamical fermionization was experimentally shown for 1D hard core bosonic gases recently. We extend this study to a harmonically confined 1D spinor gas in the hard core and strongly repulsive regimes, and analytically prove the existence of dynamical fermionization. We further discuss numerical investigation of two particle and few particle calculations for specific spinor systems. Finally, we present the Tan contact for a strongly interacting spinor system, as well as its scaling during expansion.

*NSF, Welch Foundation
12:03PM B02.00005: Dynamics of Macroscopic Quantum Tunneling from Superfluid to Mott Insulating Regimes*  
DIEGO ALCALA (Presenter), MARIE MCLAIN, LINCOLN CARR, Colorado School of Mines — In 1928 quantum tunneling was discovered to explain alpha decay, and in 2002 the Mott-Superfluid quantum phase transition was experimentally observed. How would the transition between a Superfluid and Mott insulator alter the tunneling dynamics of a many-body system? Specifically, we study bosons in a quasi one-dimensional meta-stable trap, modeled by the Bose-Hubbard Hamiltonian, using matrix product state methods which grant access to many-body observables, and compare to mean-field, which fails for strong interactions. We quantify how the barrier and interaction energies can amplify or reduce number fluctuations by an order of magnitude. Bond entropy is found to maximize when nearly half of the atoms have escaped in a Superfluid, while Mott-dominated interactions result in a maximum when only one quarter of the atoms have escaped. Mott-dominated dynamics also produce strong, long-range, and off-diagonal correlations. We find significantly different time scales in observables, i.e., when bond entropy and fluctuations maximize. Periodic fluctuations in time derivatives are found for several observables, scaling with the size of the meta-stable trap. Finally, preliminary results suggest that interaction energies can alter the escape velocity of atoms.

*Funded by NSF.

12:15PM B02.00006: On the possible existence of an effective momentum-momentum coupling in a correlated electronic system  
AMIR O. CALDEIRA (Presenter), THAIS VICTA TREVISAN, State University of Campinas, GUSTAVO MONTEIRO, The City College of New York — In this talk, we present a study on how to partly reincorporate the effects of localized binding electrons on the dynamics of their itinerant counterparts in Hubbard-like Hamiltonians. This is done by relaxing the constraint that the former should be entirely frozen in the chemical bonds between the underlying lattice sites through the employment of a Bohr-Oppenheimer ansatz for the wavefunction of the whole electronic system. Accordingly, the latter includes itinerant as well as binding electron coordinates. It is then argued that going beyond the adiabatic approximation, which will be properly justified in due time, we are able to show that the net effect of virtual transitions of binding electrons between their ground and excited states is to furnish the itinerant electrons with an effective inter-electronic momentum-momentum interaction. Once expressed in a localized orbital basis, this term generates new two-body processes which cannot be found even among those neglected in obtaining the Hubbard Hamiltonian. Although we have applied these ideas to the specific case of rings, we are sure they can be easily generalized to higher dimensional systems sharing the required properties of which we have made use herein.
12:27PM B02.00007: Superfluid vs. Mott-Insulator Phase in Imperfect Multi-Rods Lattices*
OMAR ABEL RODRÍGUEZ-LÓPEZ (Presenter), M. A. SOLÍS, Theoretical Physics, Universidad Nacional Autónoma de México — We calculate the ground state (GS) energy and the static structure factor at zero temperature of an interacting Bose gas confined by a one-dimensional, periodic, multi-rods lattice created by an external Kronig-Penney potential. We employ the Diffusion Monte Carlo (DMC) method to estimate the physical properties exactly up to a statistical error. In the limit of zero external potential, we recover the results for the well-known Lieb-Liniger model. Using the Luttinger Liquid formalism for the low-energy properties of 1D systems, we find a phase transition from the superfluid state to the Mott insulator state as the lattice height increases. Also, we report that the introduction of a barrier defect in the lattice favors the superfluid phase with respect to the Mott insulator phase.

*We thank the partial support from grants CONACyT 221030, and PAPIIT 110319.

12:39PM B02.00008: Optimized pairing from repulsive interactions in Fermi-Hubbard ladders and its static and dynamic signatures*
THOMAS KOEHLER (Presenter), ADRIAN KANTIAN, Uppsala Univ — Experiments on Fermi-Hubbard models, implemented via lattice-confined ultra-cold gases, are moving towards temperatures where their charge gap and possibly their spin gap can be resolved. It is thus important to obtain accurate quantitative theory for those systems in order to optimize the chance of observing any possible unconventional pairing from repulsive interactions at the given temperatures of the ongoing experiments. In this talk we will present such results for the Fermi-Hubbard ladder, which is proven to have unconventional pairing, and that allows us to optimize this pairing via changes in ladder structure and interactions based on highly accurate numerical theory such as matrix-product-state-based methods. We further demonstrate quantitatively how the temperature ranges at which repulsively mediated pairing may be experimentally observable is very strongly dependent on these optimizations, and how it may be detected with established techniques in both the static regime as well as via dynamically generated excitations.

*Funding through the ERC Starting Grant from the European Union's Horizon 2020 research and innovation programme under grant agreement No 758935 is greatfully acknowledged.
12:51PM B02.00009: Matrix Product States in the Continuum and Cold Atomic Gases*
JOSEPH PEACOCK (Presenter), ALEKSANDAR LJEPOJA, C. J. BOLECH, University of Cincinnati — Cold atomic gases are an ideal laboratory to explore the physics of interacting degenerate quantum gases due to the high degree of tunability possible in the experiments. In particular, special trapping arrangements allow, among other things, to control the effective dimensionality of the systems. In this talk we present an update on the continuum formulation of Matrix Product States (cMPS) to describe one dimensional dilute quantum gases. The goal is to develop cMPS as an accurate predictive tool to plan and analyse past and future experiments. To that end, we shall present results for the cases of trapped single-species and multi-species bosonic and fermionic atoms, as well as their mixtures. When available, we make quantitative comparisons of cMPS results with the exact results for solvable cases.

*We acknowledge support from NSF (Grant No. PHY-1708049) and the Ohio Supercomputing Center.

1:03PM B02.00010: Spin Imbalance Effect in a Mixture of Spinor Fermions and Hard-Core Bosons
RAMÓN GUERRERO SUÁREZ (Presenter), Universidad Nacional de Colombia, Bogota, JUAN MENDOZA ARENAS, Universidad de los Andes, ROBERTO FRANCO PÉALOZA, JERESON SILVA VALENCIA, Universidad Nacional de Colombia, Bogota — Mixtures of bosons and fermions have been the subject of research since the first studies of $^3$He-$^4$He system. With the current cold atoms setups, these types of mixtures can be realized and the inter- and intraspecies interactions can be readily tuned. By means of a Bose-Fermi Hubbard Hamiltonian, mixtures of bosons and fermions can be studied theoretically. Different superfluids, Mott Insulators, phase separation, spin and charge density waves, together with Wigner crystals have been reported for these systems. We study numerically the effect that spin imbalance can have in these mixtures, specifically for a system of spinor fermions and in the hard-core bosonic limit. Using DMRG we explore the phase diagram of the ground state, finding new insulator states that appear only when there is imbalance in the system. This happens for both attractive and repulsive intraspecies interactions and for both attractive and repulsive fermionic interactions, implying that the new insulator states are due to the coupling between bosons and fermions.
1:15PM B02.00011: *Ab initio* auxiliary-field quantum Monte Carlo study of finite-temperature properties of the two-dimensional Fermi gas*  
YUAN-YAO HE (Presenter), HAO SHI, SHIWEI ZHANG, Center for Computational Quantum Physics, Flatiron Institute  
Finite-temperature properties of the two-dimensional unpolarized Fermi gas with a zero-range attractive interaction are studied by a numerically exact auxiliary-field quantum Monte Carlo method [1]. This system has generated strong experimental and theoretical interest as a clean and well-controlled testground for a rich set of physics combining strong interaction and superfluidity in two dimensions. To reliably reach the continuum limit, we adopt a new finite-temperature algorithm [1], which has computational scaling as linear in lattice size instead of cubic as in the standard algorithm. Numerically exact results for the equation of state, contact parameter, momentum distributions as well as pairing properties are obtained across the BCS-BEC crossover, spanning the entire temperature range and connecting with exact zero-temperature results [2]. We also investigate the Berezinskii-Kosterlitz-Thouless transition and possible pseudogap physics in this system.

References:

*The Flatiron Institute is a division of the Simons Foundation.

1:27PM B02.00012: Universal intrinsic high-rank spin Hall effects*  
JUNPENG HOU (Presenter), CHUANWEI ZHANG, University of Texas at Dallas  
Spin Hall effect (SHE) is one of the key concepts in modern condensed-matter physics since its first discovery more than two decades ago. In this work, we introduce the concept dubbed high-rank spin Hall effect, in which the usual (charge) Hall effects and SHEs are incorporated as rank-0 and rank-1 SHEs. The first non-trivial example is then rank-2 SHE and we showcase a minimal intrinsic model in a spin-1 Fermionic system (a three-component Fermion or triply-degenerate point), which exhibits an universal rank-2 spin Hall conductivity $e/4\pi$. As a generalization to larger spin, we further provide another model in a spin-3/2 system. A simple experimental setup is proposed based on recently experimentally realized 2-dimensional spin-orbit coupling in cold atoms and the effects of Zeeman fields are investigated. Our work reveals interesting spin transport phenomena in large-spin systems and may lead to novel applications in spintronic and quantum-mechanical devices.

*This work is supported by AFOSR (FA9550-16-1-0387), NSF (PHY-1806227) and ARO (W911NF-17-1-0128).
Beyond mean-field corrections to the quasiparticle spectrum of superfluid Fermi gases

SENNE VAN LOON (Presenter), JACQUES TEMPERE, HADRIEN KURKJIAN, Univ of Antwerp — The notion of quasiparticles is an essential tool for the study of interacting many-body systems. In superfluid Fermi gases, two types of elementary excitations can be identified: the fermionic branch of broken pairs, and the bosonic collective mode describing the collective motion of the pairs. These can be observed in systems of ultracold fermionic atoms, where, due to Fesbach resonances, a whole range of superfluids can be studied. Measurements of the quasiparticle spectrum are already available [1], though the theoretical study of corrections to the fermionic branch remains limited [2]. Here, we investigate this quasiparticle branch in the BCS-BEC crossover and calculate the quasiparticle lifetime and energy shift due to its coupling with the collective mode. Close to the minimum of the branch the quasiparticles are undamped, allowing us to find the energy correction in a self-consistent way, that we express in experimentally relevant quantities.


Prediction of Exotic Electron Transport Properties using the Shape Effect of the Fermi Surface

ELENA DERUNOVA (Presenter), Max Planck Institute of Microstructure Physics, YAN SUN, Max Planck Institute for Chemical Physics of Solids, MAZHAR ALI, Max Planck Institute of Microstructure Physics — The intrinsic anomalous Hall and spin Hall effects (AHE/SHE) provided evidence of exotic electronic transport phenomena relating to a topological connection between bands around the Fermi energy. Currently, the calculation of Berry curvature and the Kubo formalism based on Green functions is used to quantify bands’ topological connection and predict the AHE, SHE and other effects. Here we show that the topological connection of the bands also leads to particular shapes of the corresponding Fermi surfaces (FS) and that geometric analysis of these shapes can be used to predict transport properties. For the AHE/SHE we developed a qualitative indicator, $H_F$, based on Gaussian curvature of the FS and found that $H_F$ is linearly correlated with the experimentally measured AHE (R-square 0.97) in a variety of famous AHE compounds as well correlated with the Kubo calculated SHE. We show that consideration of the geodesic flow on the FS gives rise to FS based equations in a semiclassical style, which contain information about the electron transport properties aside from longitudinal conduction. Going beyond just AHE/SHE, a full understanding of the Shape Effect of the FS (SEFS) opens the door to simple prediction of exotic electron transport property in materials in a novel and facile way.
B02.00015: Superfluidity of interacting fermions in optical lattices: Interplay of population imbalance, dimensionality, and lattice-continuum mixing*  QIJIN CHEN (Presenter), University of Science and Technology of China, JIBIAO WANG, LIN SUN, Department of Physics, Zhejiang University — In this talk, I will discuss the superfluid behavior of ultracold atomic Fermi gases in 1D and 2D optical lattices (OL), subject to a short range pairing interaction, and show the highly unusual behavior as a consequence of the interplay between population imbalance, dimensionality and more importantly lattice-continuum mixing. These systems are different from pure 3D continuum or 3D lattices, in that each lattice "site" now contains many fermions. Using a pairing fluctuation theory, we demonstrate that this feature leads to unexpected enhancement of pair hopping in the presence of population imbalance and thus possible enhancement of Tc on the BEC side of the unitary limit. For 1DOL, the superfluid phase exists only for a very limited range of parameters, and the truncated momentum space in the lattice dimension in combination with the enhanced pair hopping may give rise to enhance Tc in the BEC regime, with an constant BEC asymptote. For 2DOL, the further truncated momentum space helps to strongly suppress pairing fluctuation contributions to the pseudogap, so that Tc gradually approaches its high mean-field value in the deep BEC regime.


*Supported by NSF of China, grant No. 11774309.

Monday, March 2, 2020 11:15 AM - 1:51 PM

Session B03 GSCCM: Materials in Extremes: Energetic and Reactive Materials: Novel Approaches 107 - Pamela Bowlan, Los Alamos National Laboratory - Tag(s): Focus

11:15AM B03.00001: Safety and performance characteristics of thermite systems: from powders to 3D printed lattices [Invited]  KYLE SULLIVAN (Presenter), Lawrence Livermore Natl Lab — The reaction in thermite powders is a highly complex process. Developing a true understanding of this process involves an understanding of the various length and time scales, as well as the non-equilibrium and equilibrium processes as fuel and oxide particles react to form mixed-phase products on a rapid time scale. In this work, we present an overview of our work, which ranges from loose-powder combustion testing to 3D printed lattices of thermite. Specifically, we explored the dynamic formation of mesoparticles and the resultant multi-phase expansion of these particles as they are entrained in a gas stream. Additive manufacturing (AM) was then used to probe how the printed architecture can be used to manipulate the reactivity, by affecting the forward energy transport through design of the structure. A materials design plot (i.e., an "Ashby Diagram") was constructed to quantify the control AM offers for these materials.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
11:51AM B03.00002: High Velocity Impact Testing of Structural Reactive Projectiles*  ALAN WILLIAMS (Presenter), COLT CAGLE, MICHELLE PANTOYA, Texas Tech Univ — This study examined the dynamic response of structural reactive projectiles penetrating through an aluminum target then impacting an inert steel anvil at speeds up to 1500 m/s. The impact testing is performed using a High-velocity Impact-ignition Testing System (HITS). The projectiles consist of a thermite with a high loading ductile metallic binder, consolidated into a cylindrical pellet contained in a .410 caliber shot gun case. The thermite includes aluminum fuel particles that were stress altered prior to their consolidation. This study considers the effect of stress altering aluminum particles on the overall penetration dynamics and reactivity of the projectile. Results demonstrate the range of plate deformation mechanics and overall transient pressure data that can be used to interpret reactivity. A threshold impact velocity was observed that corresponds with fragmentation of the projectile and is a function of stress-altered particles. The differences in reactivity between stress altered and untreated aluminum powder likely stem from the fragmentation field created upon penetration of the plate. Results provide a fundamental understanding of penetration and impact events with structural reactive formulations.

*Office of Naval Research

12:03PM B03.00003: Modeling PBX 9501 High Explosive Cylinder Experiments and an Evaluation of WSD and AWSD Parameter Sets  MARVIN ZOCHER (Presenter), TARIQ D ASLAM, Los Alamos Natl Lab — Cylindrical assemblies are often used in experiments aimed at calibrating and validating continuum level models of reactive burn, and of the so-called equation of state model (constitutive model for the spherical part of the Cauchy tensor). Such is the case in work to be discussed here. In particular, work will be described involving the modeling of a series of experiments involving PBX 9501 encased in a copper cylinder. The objective of the work is to test and perhaps refine a set of phenomenological parameters for the Wescott-Stewart-Davis (WSD) and Arrhenius-WSD (AWSD) reactive burn models. The focus of this talk will be on modeling the experiments, which turned out to be non-trivial. Always difficult to handle due to the extremely short reaction zone of PBX 9501, scaling is employed to address issues related to detonation velocity. The modeling is conducted using ALE methodology.
12:15PM B03.00004: High Explosive Shock Initiation Model Based on Hot Spot Temperature

LAURENCE FRIED (Presenter), MATTHEW P KROONBLAWD, Lawrence Livermore Natl Lab — We describe a new shock initiation model based on the Cheetah thermochemical code. The model is based on a multiple stage picture of the shock initiation process and uses hot spot temperature as an auxiliary variable to control the initial stages of reaction. Unlike using rates controlled by other thermodynamic variables, this approach captures physical sub-zonal differences between the bulk temperature and the substantially higher local hot spot temperature that actually governs ignition chemistry. In the model, a single representative hot spot diameter is chosen and the hot spot temperature is controlled by shock pressure and thermal conductivity. The practical utility of a sub-zonal hot spot temperature model will be discussed, as well as evidence for co-existing hot spot and shear band ignition mechanisms in high explosive shock initiation.

*Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

12:27PM B03.00005: Multi criteria decision model for design of advanced energetic materials with tailored properties

MAIJA M KUKLA (Presenter), ROMAN TSYSHEVSKIY, University of Maryland, College Park — The search for new high energy density materials (HEDMs) with targeted high performance, low toxicity, and reliable stability remains challenging. New materials are typically developed by Edisonian trial and error approach that involves sophisticated synthesis protocols combined with extensive sensitivity characterization tests. Such efforts are time consuming and resource exhaustive while the successful outcomes are seldom guaranteed. A combination of ab initio, group additive methods, and statistical analysis represents a powerful tool for computational design and discovery of new advanced high energetic density materials. Here, we report a sophisticated approach for design of new HEDMs with tailored properties based on extensive state-of-the-art study of structure-property-function relationships of various classes of energetic and explosive materials. We also show how we use this approach for discovery and characterization of new linear and fused heterocyclic HDEMs with performance and stability parameters considerably superior to conventional O-, N- and C-nitro compounds such as PETN, RDX and TNT.

*This research was supported by ONR (Grant N00014-16-1-2069). R.T. acknowledges support from NSF XSEDE (DMR-130077), NERSC (DE-AC02-05CH11231), MARCC and UMD supercomputing resources.
12:39PM B03.00006: Transition and Optimization of Particle Impact Mitigation Sleeve Design between Munitions of Different Physical Parameters  
DANIEL PUDLAK (Presenter), KEVIN MIERS, Combat Capabilities Development Command - Armaments Center, US Army — Military munitions that fall within the NATO portfolio must be tested in accordance with Insensitive Munitions AOP-4496 Fragment Impact (FI) Testing. Under this test, a conical, steel cylinder is launched at the munition at 8300fps, and the response of the munition is evaluated for reactions ranging from violent detonation, to benign burning reaction. Standard practice to mitigate a violent detonation reaction from occurring is to develop barrier technologies (e.g. armor) that can reduce the velocity, and overall kinetic energy of the fragment to a level that will not produce a violent response of the munition. Previously, a technology known as Particle Impact Mitigation Sleeve (PIMS) that was developed for a specific munition, successfully reduced the munition's response from a detonation, to a benign burn. This PIMS design is currently being evaluated for application to a different munition. While these different munitions produce similar responses without the PIMS, their energetic content, munition physical parameters, and packaging materiel are different, which can substantially affect the response of the munition to FI. This paper will describe the transition and optimization of the PIMS design to successfully mitigate the new munition's response to the FI threat.

12:51PM B03.00007: Dynamic Compression of RDX Single Crystal and High Explosives*  
CHENG LIU (Presenter), CARL M CADY, KYLE RAMOS, BENJAMIN M MORROW, CHRISTOPHER MEREDITH, Los Alamos National Laboratory — Dynamic compression and failure of energetic RDX single crystals and high explosive PBX 9501 are studied experimentally using a miniature Split Hopkinson Pressure Bar (SHPB) combined with high-speed photography and optical digital image correlation (DIC) technique. In addition to the strain gages mounted at the center of the incident and transmitted bars, high-speed camera, running at the rate of 5 million frames per second, was used to capture the deformation process of the RDX single crystal and the PBX 9501. A random speckle pattern was also printed on the sample surface and optical DIC technique was applied to map out the displacement and the strain fields over the sample surface, as well as to capture the crack initiation and extension process. A technique was developed for quantitatively identifying crack, the motion of the crack tip, and extracting the fracture toughness of a brittle material in compression. Combined with the dynamic compression setup, we will be able to study the deformation and failure processes in much detailed and quantitative fashion.

*This research is supported by the LDRD program and the JMP Program.
Performance Evaluation Methodology for Materials Subjected to Explosively-Driven Highly Non-Radial Implosive Motion

LAWRENCE HULL (Presenter), STEVE M GILBERTSON, JONATHAN A HUDSTON, THOMAS A BEERY, Los Alamos Natl Lab — Non-radial implosive motion is experienced during the early stages of various important device formation processes, such a shaped charge jet. If the response of the material can be characterized during this initial stage of motion, then often the subsequent motion will be predictable. Diagnostics are either available or are under development, such as Modulation Based Ranging (MBR), to address this initial stage of motion. The use of velocimetry to evaluate material response when non-radial flow occurs is complicated by the non-colinearity of the velocity the surface normal, and non-colinearity with the laser beam. The result is that ordinary velocimetry results in an incomplete measurement, that of the component of velocity in the direction of the laser beam. We introduce a method, MBR, that measures the position that any object that intersects the laser line as a function of time, approximately closing the measurement system and enabling the application of the velocity-based evaluation methodologies. We describe our use of simultaneous Photon Doppler Velocimetry (PDV) and MBR along with radiography to characterize and compare the response two geometrically identical hemispherical shells that were manufactured differently.

*Supported by Laboratory Directed Research and Development

Shock-induced paracrystallinity in PPTA

PAULO BRANICIO (Presenter), SUBODH TIWARI, SUNGWOOK HONG, DANIEL SHEBIB, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Univ of Southern California — The outstanding strength-to-weight ratio of para-aramid fibers, such as Kevlar and Twaron, is largely attributed to their high content of crystalline p-phenylene terephthalamide (PPTA). Atomistic simulations of shock loading on PPTA are performed along the [100] and [010] crystallographic directions, using reactive molecular-dynamics simulations. The reactive forcefield utilized is fitted to PPTA properties using first principles data and the results are validated by *ab-initio* molecular dynamics (QMD) simulations. Simulation results reveal an anisotropic shock response displaying elastic, crosslinking, and phase transformation from crystalline to para-crystalline phases. While QMD simulations show elastic to amorphous planar transformation for shocks along [010] direction, long time simulations accessible by reactive molecular dynamics indicate the formation of a para-crystalline phase initiated by an amorphous planar transformation, which displays H-bond scission and rotation of chains. The rotation process reorients the polymer chains such that vdW interactions dominate chain-chain interactions leading to the formation of local domains where new H-bond interaction forms leading to the para-crystalline phase.
1:27PM B03.00010: Experiment and Numerical Simulation Study on Near-field Underwater Explosion of Aluminized Explosive  
YUANXIANG SUN (Presenter), State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, China — Aluminized explosive can improve the energy output structure and power of detonation products. The application of aluminized explosive to underwater explosion enhances the brisance and damage capability of underwater weapons significantly. The near-field underwater explosion experiments of aluminized explosive RL_F and TNT were carried out using PVDF pressure sensor based on electrical measurement method, and Coupled Eulerian-Lagrangian (CEL) method was used for simulation. The numerical results agreed well with experimental and empirical ones. The results show that CEL method can be used to simulate the propagation process of near-field underwater explosion shock wave of TNT and aluminized explosive accurately if reasonable boundary conditions, calculation parameters and finite element model are adapted. Near-field underwater shock wave pressure attenuation of aluminized explosive is slower than TNT. Then, the approximate regression formulas of near field underwater explosion shock wave peak pressure of TNT within 6 times of charge radius and aluminized explosive in a certain distance range are obtained by fitting the simulation results.

1:39PM B03.00011: Thermal transport across diamond/copper interface functionalized by self-assemble monolayer  
BIN XU, SHIH-WEI HUNG, JUNHO CHOI, JUNICHIRO SHIOMI (Presenter), Univ of Tokyo — 
Copper and diamond composite is regarded as one of the most promising candidates for effective condensed heat dissipation. However, thermal boundary conductance (TBC) between copper and diamond becomes a key factor for deciding thermal conductivity. Interface functionalization using self-assemble monolayer (SAM) is a well-known method for enhancing TBC of a solid interface. While the underlying mechanism has been discussed in terms of strengthening the bonds or bridging of the lattice vibrational spectra, there is a need for more experiment-simulation coupled work on a well-defined system. In this sense, the copper and diamond system is ideal as the soft copper and hard diamond give rise to a large mismatch in the lattice vibration frequencies and the smoothness/uniformity. 
In this study, we measure the TBC of copper/SAM/diamond interface by the time-domain thermoreflectance method. By using ellipsometer, X-ray photo-electro spectroscopy, and Fourier transform infrared spectroscopy, morphology and the chemical bonding of the SAM on copper and diamond are clearly observed. In addition, molecular dynamics simulations are carried out to explain the measured dependence of TBC. We found that there is a comprehensive correlation between the chain length, functional group, and TBC.
B03.00012: Pressure- and Temperature-Dependent Structural Stability and Photoluminescence properties of LLM-105 Crystal  ZENGMING ZHANG (Presenter), ZILONG XU, JUNKE WANG, University of Science and Technology of China — Energetic material LLM-105 maintains its structure stability under high pressure below 30 GPa at room temperature or in the temperature range from 513 K to 5 K with ambient pressure. One structural phase transition occurs at about 30 GPa and is confirmed by pressure-dependent Raman and infrared spectra. The structure of LLM-105 crystal shows anisotropic compressibility under pressure. Debye temperature of 1225 K for this crystal is obtained. Raman and infrared spectra at extreme conditions suggest that the structure stability is contributed to the stronger inter- and intra-molecule hydrogen bonding networks within LLM-105 crystal. Photoluminescence, absorption spectroscopy and the DFT calculations were employed for LLM-105. With the pressure increasing, the luminescence first increases due to the limited molecular vibration, then over 9.0 GPa, the intensity decreases due to the lower electronic transfer efficiency. Results reveal that the band gap of LLM-105 crystal presents a strong pressure dependence. The high pressure phase transition has also been observed at about 30 GPa with a band gap suddenly decrease again. Moreover, the PV phase diagram has been completed.


Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B04 DCP DSOFT DPOLY DLS: Coherent Nonlinear Optical Microscopy I 109 - Marcus Cicerone, Georgia Inst of Tech - Tag(s): Focus

11:15 AM B04.00001: Coherent Nonlinear Optical Microscopy with Mid-infrared Radiation*
[Invited] DAVE KNEZ, RICHARD C. PRINCE, ADAM M. HANNINEN, ERIC POTMA (Presenter), University of California, Irvine — Fundamental vibrational modes are efficiently excited by mid-infrared (MIR) radiation, in a light-matter interaction that is many orders of magnitude stronger than vibrational excitation through the Raman effect. Despite this clear advantage, MIR microscopy is not ubiquitously used for imaging of biological samples due to practical limitations including low spatial resolution, the use of expensive cameras and the intrinsic limitation of absorption-based detection. Some of these limitations can be overcome when using nonlinear upconversion techniques to translate the driven MIR transition into a signal in the visible/NIR range of the spectrum. We will discuss several coherent nonlinear optical approaches that enable rapid laser-scanning microscopy in the MIR with high, three-dimensional resolution.

*National Institutes of Health, R01-GM132506
11:51AM B04.00002: Multidimensional spectroscopy on the microscale: Development of a multimodal imaging system incorporating 2D white-light spectroscopy, broadband transient absorption, and atomic force microscopy.* ANDREW JONES (Presenter), Los Alamos National Laboratory, NICHOLAS KEARNS, MIRIAM BOHLMANN KUNZ, JESSICA FLACH, MARTIN T ZANNI, Chemistry, University of Wisconsin — The dynamics of electronic transitions in solid-state materials are closely linked to microscopic morphology, but it is often challenging to simultaneously characterize their broadband spectral and temporal response with high spatial resolution. We present a combined coherent multidimensional spectroscopy and microscopy system using visible white-light supercontinuum pulses as a broadband light source. This system correlates ~nm scale sample morphology determined from atomic force topography measurements with broadband transient absorption hyperspectral images and ultrafast multidimensional spectra, all with a spatial resolution of ≤1 μm. We demonstrate the application of this technique to the mapping of spatial heterogeneity in the process of singlet fission within single microcrystals of an organic semiconductor material, TIPS-Pentacene. Here, we identify heterogeneity in the temporal and spectral response corresponding to presence of non-equilibrium molecular packing near edges and morphological defect structures.

*Air Force Office of Scientific Research (FA9550-19-1-0093); National Science Foundation (NSF CHE 1664110)

12:03PM B04.00003: Image Formation in Coherent Nonlinear Optical Microscopy* [Invited] LORA RAMUNNO (Presenter), Univ of Ottawa — Coherent nonlinear optical microscopy has allowed real-time visualization of objects and biological processes on small length scales, where molecule-specific imaging can be achieved without the use of labels. Given the coherent nature of the nonlinear processes involved (which includes, for example, coherent anti-Stokes Raman scattering, second and third harmonic generation), the images produced are complex and not always straightforward to interpret, especially when object sizes are much smaller than the focal volume. Images are subject to, for example, interference from multiple scatterers, interference due to competing nonlinear processes, and distortion due to inhomogeneities. This can lead to bright spots that appear in the wrong place or are 10x brighter than they should be, unexpected shadows, false dark and bright signals, spectral shifts that depend on the spatial position of objects along the laser axis, and signals that depend on the precise shapes and relative positions of sub-wavelength objects within the focal volume (rather than just the total number of molecules present), to name a few. I will discuss the origin of these strange effects, and review our work and others in this area over the last several years.

*Natural Sciences and Engineering Research Council of Canada; Canada Research Chairs; Canadian Foundation for Innovation; Ministry of Research and Innovation Ontario; Compute Canada; SOSCIP Smart Computing for Innovation
12:39PM B04.00004: Strong-field-driven dynamics and high-harmonic generation in interacting 1D systems*  
FERNANDO SOLS (Presenter), Univ Complutense de Madrid, IMDEA Nanociencia, SANDRA DE VEGA, ICFO (Barcelona), JOEL COX, Danish Institute for Advanced Study (Odense), JAVIER GARCIA DE ABAJO, ICFO (Barcelona), ICREA — We explore the role of electronic band structure and Coulomb interactions in solid-state HHG by studying the optical response of linear atomic chains and carbon nanotubes to intense ultrashort pulses. Specifically, we simulate electron dynamics by solving self-consistently the single-particle density matrix equation of motion in the presence of intense ultrafast optical fields and electron interactions. Our 1D model provides insight on the temporal evolution of electronic states in reciprocal space. We demonstrate that electron interactions play an important role in the HHG yield. This model further predicts that doped semiconductors generate high harmonics more efficiently than their metallic and undoped counterparts. To complement this idealized system we also show results for HHG in more realistic quasi-1D structures such as carbon nanotubes, whose behavior is found to be in good qualitative agreement with that of the atomic chains. Our findings apply directly to extreme nonlinear optical phenomena and can be extended to optimize existing platforms for HHG or identify new solid-state alternatives in the context of nonlinear plasmonics.


12:51PM B04.00005: Broadband Coherent Anti-Stokes Raman Scattering (BCARS) MicroSpectroscopy [Invited]  
CHARLES HENRY CAMP (Presenter), National Institute of Standards and Technology — The ability to noninvasively image the dynamic chemical composition within cells and tissues would revolutionize our understanding of biology and disease. Molecular vibrational imaging techniques detect the small oscillations between bonded atoms, providing dense spectral information about composition and state without the addition of fluorophores or dyes. Technologies, such as Raman and infrared microscopies, have offered this capability for over half a century, but significant limitations in speed, resolution, or sample preparation have prevented their ubiquity. Coherent Raman imaging (CRI) methods, proposed as the solution, have been practically confined to small increments of the vibrational spectrum with limited chemical specificity. Broadband coherent anti-Stokes Raman scattering (BCARS), a particular CRI modality, on the other hand, has demonstrated an unprecedented combination of speed, sensitivity, and spectral breadth, enabling full hyperspectral imagery in minutes rather than hours. Furthermore, as a coherent anti-Stokes Raman scattering (CARS)-based method, a coherent background is generated that is molecularly sensitive and can be used as a built-in internal reference at each pixel; thus, enabling directly comparable results between samples and spectra collected on different microscope systems.

In this seminar, I will present an introduction to BCARS microscopy from a theoretical and practical perspective. Specifically, covering the physics of signal generation and extraction of Raman signatures. Further, I will touch upon application space examples and our efforts towards quantitative imaging.
1:27PM B04.00006: Studying the photodynamics of FRET paired fluorescent molecules near gold nanogratings*  JENNIFER STEELE (Presenter), CHAE RAMNARACE, Physics and Astronomy, Trinity University, WILLIAM FARNER, Physics, Drexel University — The plasmonic properties of structured metal surfaces can be engineered to enhance the output of nearby quantum emitters through the manipulation of the local density of optical states (LDOS). Although metal enhanced fluorescence (MEF) has been well understood for decades, the influence of plasmonic modes in Förster resonance energy transfer (FRET) is still a debated issue. Gold nanogratings provide a unique plasmonic substrate to study the effects of altering the LDOS on FRET efficiencies. Gratings support narrow plasmon resonances at a range of wavelengths, allowing for the comparison of FRET efficiencies by increasing the LDOS at donor and acceptor emission wavelengths on a single substrate. Previous work has shown an increase in efficiency when the surface plasmon modes overlapped the acceptor emission spectrum. In this talk, ongoing work on the optimizing the increase in efficiencies will be discussed. Furthering the understanding of the application of MEF to FRET will aid developing methods for the enhancement of FRET, expanding its use in biological systems, photosynthesis, and photovoltaic devices.

*This work was supported by an award from the Research Corporation for Science Advancement and from the W.M. Keck Foundation Undergraduate Education Program.

1:39PM B04.00007: Geophotonics: Multimodal Nonlinear Optical Microscopy in Geology [Invited]  ADRIAN PEGORARO (Presenter), Univ of Ottawa — Nonlinear optical microscopy offers label-free contrast and enhanced depth penetration in heterogeneous media compared to more traditional optical microscopy techniques. These advantages make it a natural fit for biological imaging where optical microscopy is frequently the tool of choice. For geologic materials, where electron microscopy is much more prevalent than optical imaging, the utility of newly developed nonlinear optical techniques was less obvious. Nonetheless, we show that these techniques, such as second harmonic generation, coherent Raman microscopy, and pump-probe microscopy, provide complementary contrast mechanisms for a host of geological systems. For some applications, the ability to image rapidly in 3D reveals previously unseen spatial correlations. Even in opaque systems, nonlinear optical signals can achieve comparable contrast to electron microscopy techniques which are inherently confined to the surface. This allows for much more rapid screening of samples with less sample preparation. We believe that by leveraging ongoing developments in biophotonics, it is possible to offer new and improved imaging tools for many other systems that are not traditionally studied using optical microscopy.

Monday, March 2, 2020 11:15 AM - 12:27 PM

Session B05 DCP DCMP DPOLY: The Chemical Physics of Molecular Polaritons II. Photophysics II 111 - Luis Angel Martinez Martinez, University of California, San Diego - Tag(s): Focus
11:15AM B05.00001: First principles approaches to excited states chemistry under strong light-matter coupling  
JOHANNES FLICK (Presenter), Center for Computational Quantum Physics, Flatiron Institute, PRINEHA NARANG, John A. Paulson School of Engineering and Applied Sciences, Harvard University — In recent years, research at the interface of chemistry, material science, and quantum optics has surged and now opens new possibilities to study strong light-matter interactions at different limits [1]. In these limits, electrons, nuclei and photons have to be treated on the same quantized footing. Towards this goal, we have introduced a general time-dependent density-functional theory [2].

In this talk, we use a novel linear-response formulation [3] within a density-functional framework to study excited states of strongly light-matter coupled systems. We study how the potential-energy surfaces (PES) of a CO bond stretching in a formaldehyde molecule is modified and show the influence of strong light-matter coupling on avoided crossings. These results demonstrate the novel abilities to alter and open new chemical reaction pathways as well as to create new hybrid states of light and matter [4].

Our work opens an important new avenue in introducing ab initio methods to the nascent field of collective strong light-matter interactions.


11:27AM B05.00002: Communication between polaritonic and excitonic manifolds in an electronically strong coupled system* [Invited]  
COURTNEY DELPO, KYU HYUNG PARK (Presenter), BRYAN J KUDISCH, FRANCESCA FASIOLI, GREG SCHOLES, Department of Chemistry, Princeton University — Optically dark states, which arise from intermolecular exciton coupling, are a crucial component in understanding the optical properties of natural and artificial light harvesters. Dark states also constitute a major density of states in the energy manifold of a strong-coupled system, which is generated from the interaction between a cavity photon and molecular excitons. Unlike optically bright upper and lower polariton states, dark state wavefunctions contain no photonic excitation and therefore have been considered to retain molecular character. In this framework, dark states not only serve as a deactivation pathway but also can participate in excitation energy exchange to states that are not coupled to cavity photons. We test this view by following the excited-state dynamics of bright to dark state interconversion in an electronically strong-coupled cavity composed of 1,2,3,5-tetrakis(carbazol-9-yl)-4,6-dicyanobenzene (4CzIPN). We show that dark states have a lifetime longer than that of uncoupled molecules indicating a significant change in the state character. Discussion on the communication between the dark states and the exciton manifold of uncoupled 4CzIPN triplet states will be presented.

*This work is funded by the Gordon and Betty Moore Foundation.
Mixed Quantum-Classical Methods for Molecules in Cavities — Describing chemical processes that are strongly correlated with quantum light requires an accurate, flexible, and computationally efficient treatment of light-matter interactions. Thus, in order to develop ab-initio theoretical descriptions of cavity modified chemical systems, extensions to the traditional theoretical tool-kits for quantum optics and quantum chemistry are required. Here, we investigate the extension of mixed quantum-classical trajectory methods as well as the concept of time-dependent potential energy surfaces, both traditionally introduced for electron-nuclear problems, to the photonic degrees of freedom. Within our work we find that classical Wigner dynamics for photons can be used to describe quantum effects such as correlation functions, bound photon states and cavity induced suppression by properly accounting for the quantum statistics of the vacuum field while using classical/semi-classical trajectories to describe the time-evolution. Investigating the time-dependent potential energy surfaces for photons we find significant differences with the potential used in conventional approaches. Furthermore, we analyze the exact time-dependent potential energy surface driving the proton motion of a cavity-induced chemical suppression.

Mixed quantum-classical simulation of molecules in a cavity* — Photons in an optical cavity can strongly interact with electronic and vibronic state of molecules, which provides great promise to manipulate chemical reaction in cavity. Mixed quantum-classical methods, such as mean-field Ehrenfest, have been successfully applied to traditional photochemical reaction and provide many valuable insights into the reaction mechanisms. In this talk, we will present our recent results on how to generalize the mean-field Ehrenfest dynamics to the molecules in cavity by treating nuclei classically and other degrees of freedom quantum mechanically. The derived quantum force is general and can be used to include any number of electronic and photon states. As an example, we use our method to study the dissociation of LiF in cavity and compare the results with exact quantum simulation, which shows the reaction outcomes can be controlled by the coupling strength and the dipole self-energy term. Our approximate approach produces accurate results compared with exact quantum simulation, and can be broadly applied to investigate molecular reactions in the cavity.

*This work is supported by the National Science Foundation (NSF)"Enabling Quantum Leap in Chemistry" program under a Grant number CHE-1836546 and NSF CAREER Award under Grant No. CHE-1845747.
11:15AM B06.00001: A statistical ensemble approach to understanding adaptive immunity: using sequence data to quantify the extraordinary diversity, in both sequence and protective specificity, of the T- and B-cells cells that make up an individual human’s immune system.* [Invited] CURTIS CALLAN (Presenter), Princeton University — Individual T cells of the adaptive immune system recognize specific pathogens via a certain protein expressed on the surface of the cell. The gene for this protein undergoes random editing each time a new immune cell is created. As a result, any individual’s immune system is an ensemble of distinct T cell types (in fact about $10^9$ in number) created by a stochastic process. I will explain how high-throughput DNA sequencing has made it possible to develop a precise quantitative understanding of this stochastic process. I will then explain some consequences of this understanding: a) that the stochastic gene editing process is nearly universal across the human species, b) that the diversity of the process is so large that the overlap between T cell repertoires of two individuals is small, c) that the one-shot generation probabilities of specific T cell types range over nearly twenty orders of magnitude, and, as a corollary, d) that certain specific T cell types will be found in all individuals, while others have negligible sharing likelihood. I will then discuss how these developments bring into sharp focus the central biophysical question of adaptive immunity, namely: what is the diversity of pathogenic molecules that a single T cell can recognize, and is the diversity of the T cells present in one individual large enough so that the entire space of pathogenic molecules can be recognized? Implications of these developments for cancer immunotherapy will be briefly discussed. References for this talk are:


*The work of C. Callan is supported by NSF grants PHY-1607612 and PHY-1734030.

11:51AM B06.00002: Evaluation of nuclear reaction cross sections via proton induced reactions for the production of $^{72}$As: a potential entrant for theranostic pairs WARIS ALI (Presenter), Physics, GC University Lahore — Theranostic applications of radiopharmaceuticals have revolutionized present era specially, dealing with cancer diseases. Increase in the uses of radionuclides in nuclear medicine has resulted in the demands of optimized new radionuclides to be produced focussing on the economy, simplicity and maximum yield. Some arsenic radionuclides have wide range of positron-emission, half-lives ranging from an hour to weeks and have potential to be used for nuclear medicine. Present work will elucidate all over the production of $^{72}$As on Germanium (Ge) and Selenium (Se). The experimental results obtained by several nuclear reactions were compared with the results of nuclear model calculations using the codes ALICE-IPPE, EMPIRE 3.2 and TALYS 1.9. The thick target yields (TTY) of $^{72}$As were calculated from the recommended excitation functions. Analysis of radio-impurities was also discussed. A comparison of the various radio-impurities showed that to produce $^{72}$As, $^{72}$Ge(p, n)$^{72}$As and $^{76}$Se(p, x)$^{72}$As reactions in different energy ranges. We have identified the nuclear process which gives high yield with minimum impurities to make it as a potential candidate for theranostic applications and in particular in Positron Emission Tomography (PET).
12:03PM B06.00003: Improving blood vessel tortuosity measurements via highly sampled numerical integration of the Frenet-Serret equations*  
ALEX BRUMMER (Presenter), VAN M SAVAGE, University of California, Los Angeles — Measures of vascular tortuosity, how curved and twisted a vessel is, are associated with a variety of vascular diseases. Consequently, accurate measurements of vessel tortuosity are greatly needed yet have proven problematic. Some researchers do not measure it at all, and others' results have been mismeasured, null, or contradictory. We present a new method that ensures accurate measurement of vessel tortuosity from medical image data that relies on numerical integration of the Frenet-Serret equations. By reconstructing vessel coordinates from tortuosity measurements, our approach identifies a minimally-sufficient sampling rate based on vessel radius. This work further identifies a key failing in current practices of filtering asymptotic measurements, and also highlights inconsistencies between existing tortuosity metrics. We demonstrate the utility of our method on published data for a range of healthy human vessels including: cerebral and coronary vascular networks and individual carotid, abdominal, renal and iliac arteries. Preliminary application to disease data will also be discussed.

*NSF Grant #1254159

12:15PM B06.00004: Diffeomorphic morphometry of the tibio-femoral joint for quantitative assessment of osteoarthritis*  
NICOLAS CHARON (Presenter), ASEF ISLAM, WOJCIECH ZBIJEWSKI, Johns Hopkins University — We present an application of the framework of Large Diffeomorphic Deformation Metric Mapping (LDDMM) for statistical analysis of morphological variants of knee anatomy associated with osteoarthritis (OA). The LDDMM models the morphological variability by associating each population member – here, a tibial surface – with a diffeomorphic transformation that maps the shape of that member to a common template (mean shape). Compared to conventional Active Shape Models, LDDM has the significant advantage in that it does not require a priori point correspondences between the surfaces in the population. We also investigated an extension of LDDMM (functional shapes, fshapes) that jointly considers the variations in shape and variations in a function on the shape (signal) – here, the signal was a map of tibio-femoral joint space width. The diffeomorphic modeling was applied to 34 CT scans of normal and OA subjects. To validate that the resulting model captures the morphology of OA, we measured the accuracy of a Support Vector Machine (SVM) classifier using either only the shape features or the joint shape+signal features. We achieved correct classification (OA vs. normal) in 91% of subjects using shape features and in 85% of subjects using shape+signal.

*Partly supported by NIH R01 EB018896
12:27PM B06.00005: Probabilistic approach to treatment planning in radiation therapy*

PETER FERJANCIC (Presenter), ROBERT JERAJ, University of Wisconsin - Madison — Radiation therapy (RT) is a common treatment for cancer. Current RT planning uses binary tumor definitions and accounts for uncertainties by simply expanding target volume by margins. This approach has several limitations and oversimplifies complex processes that are not linear in nature.

Here, we present a probabilistic approach to RT planning. First, mapping of tumor occupancy probability density functions was performed by sampling existing segmentation methods. Voxel-based microscopic tumor infiltration likelihood was simulated using CT imaging-derived anatomical constraints and clinically measured ranges of cellular infiltration. Desired voxel-level ranges of RT dose were prescribed based on this infiltration likelihood and its uncertainty.

Realistic dose plans were created using an in-house treatment planning software modified to use minimax robust optimization over a range of uncertainty realizations. Finally, traditional and probabilistic dose plans were compared, and their performance quantified.

Using this approach, traditional expansion by margins was replaced with non-binary tumor maps and robust optimization, which more realistically represent treatment planning and delivery.

*Partially funded by the University of Wisconsin Carbone Cancer Center Support Grant P30 CA014520

12:39PM B06.00006: Evolutionary dynamics of cancer on complex stress landscapes*

YUSHA SUN (Presenter), KE-CHIH LIN, TRUNG PHAN, Princeton University, GONZALO TORGA, SARAH AMEND, KENNETH J. PIENTA, Johns Hopkins University, JAMES STURM, ROBERT AUSTIN, Princeton University — Understanding the evolutionary dynamics of cancer progression requires explicit consideration of both spatial and environmental heterogeneities. We have recently developed a purely diffusion-based cancer-on-chip microfluidic platform, enabling the quantitative study of various cell types on chemotherapeutic gradients on long time scales. In a co-culture of bone-metastatic prostate cancer cells (PC3-EPI) with bone marrow stromal cells (HS5), we found a marked transition in population dominance across a docetaxel gradient. To interpret these results, we employ evolutionary game theory (EGT) as a predictive framework for cancer-stroma dynamics. We generate a spatial interacting-agent EGT model comprised of interconnected habitats in various network topologies. Informed by our experimental findings, we explore distinct strategies utilized by populations under stress by considering system parameters as a function of both space and time as well as by modulating migrational probabilities. This model will be adapted to probe interactions between drug-resistant cancer subpopulations, stromal cells, and immune cells, providing clinical implications for therapeutic approaches.

*This work was supported by NSF PHY-1659940.
Doppler Spectroscopy of Intracellular Dynamics During Chemotherapy in Tumor Biopsies  ZHEN HUA (Presenter), JOHN TUREK, MICHAEL CHILDRESS, DAVID DOUGLAS NOLTE, Purdue Univ — Biodynamic imaging is a high-content optical imaging technology based on Doppler spectroscopy and digital holography that uses dynamic speckle as high-content image contrast to probe living tissue. Biomarkers from the living tissues were extracted using fluctuation spectroscopy from intracellular Doppler light scattering in response to the molecular mechanisms of action of therapeutic drugs that modify a range of intracellular motions. Biodynamic imaging measurements of canine B-cell cancer tissues with unknown outcomes were performed and the drug-response spectrograms were compared to results from tissues of 22 pre-clinical trial dogs with known outcomes. A machine learning classifier was constructed based on feature vector correlations and linear separability in high dimensional feature space. The prediction of resistance or sensitivity to chemotherapy for unknown patient clinical outcomes was demonstrated. These results point to the potential for biodynamic profiling to contribute to personalized medicine by aiding the selection of chemotherapy for cancer patients.

Quantifying Similarity in Histopathology Images Using Pathology-specific Deep-learned Features  QIAN CAO (Presenter), ASEF ISLAM, ZIHANG FANG, JAYLEN KANG, ALEXANDER BARAS, WOJCIECH ZBIJEWSKI, Johns Hopkins University — Interpretation of histopathology slides is often labor intensive and operator dependent. This work aims to support the pathologists by matching unknown slides with reference slides of similar characteristics (normal, benign, type of carcinoma, etc) from an annotated collection. We expand on prior efforts in this area by developing a set of pathology-specific deep-learned features for the similarity matching. The features were extracted from digitized breast histopathology slides using a convolutional autoencoder (CAE). For training, random patches of 256x256 pixel ROIs (tiles) were extracted from each slide and augmented with random affine transformations and perturbations in HSV color space to consider variability in orientation, magnification, staining and lighting conditions. Batch sizes of 128 were used in training for 2000 epochs. To assess the ability to detect similar images using the deep-learned features, we compared feature vectors of neighboring tiles of the same slide using a separate validation slide set. For inference, input tiles extracted from unknown slides are featurized with the encoder and a kNN search is performed on feature vectors derived from an annotated reference collection, returning similar tiles and corresponding slides for the pathologist.

Mathematical Models for Living Forms in Medical Physics Submodel 1: The Information Processing from Teeth to Nerves*  CHRISTINA POSPISIL (Presenter), Physics, Mathematics and Computer Science Student at University of Massachusetts Boston and Research Trainee at Harvard Medical School — This talk continues the presentations at APS March Meeting 2019 and APS April Meeting 2019. In this part of the project the first submodel is presented; The information processing from teeth to the nerves. Information processing is modeled via p-waves passing through the tooth layers enamel and dentin. Odontoblasts located in the liquid in the tubules of the tooth dentin layer perform finally the transformation into electrical information (an electrical signal) that passes along nerves.

* I fund the project currently on my own.
1:27PM B06.00010: Potential Efficacy of the Monte Carlo Dose Calculations of 6MV Flattening Filter-Free Photon Beam of M6™ Cyberknife® System  
TAINDRA NEUPANE (Presenter), Florida Atlantic University, CHARLES SHANG, Medical Physics, South Florida Proton Therapy Institute, WAZIR MUHAMMAD, THEODORA LEVENTOURI, Florida Atlantic University — Retrospective MapCheck measurements of 50 patient’s treatment plans have suggested that MapCheck could be effectively employed in routine patient specific quality assurance in M6 Cyberknife with beams delivered at different treatment angles. However, for smaller MLCs segments (< 8 mm) a correction of (-4 %) was used to match the planned dose with MapCheck. To generalize this correction, a Monte Carlo (MC) simulation is required for such types of treatment plans. In doing so, MC simulations were performed for the M6 Cyberknife using the EGSnrc program. A total of 2-5 and 10-20 millions of incident particles histories in BEAMnrc and DOSXYZnrc, respectively were simulated. Preliminary results showed dose uncertainties ≤ 3% for all the standard fields (7.6 x 7.7 mm² to 100 x 100 mm²). During the simulation, an incident electron beam of 7 MeV with a FWHM of 2.2 mm was used to match with the stated nominal energy by comparing the simulation and corresponding measurement results. Good agreements for the dose profiles (≤ 2%) and dose outputs (≤ 3%) were found between the simulations and measurements at 800 mm Source to Axis Distance (SAD).

1:39PM B06.00011: Thermal transport simulation in healthy and arthritic fingers*  
URBAN SIMONCIC (Presenter), University of Ljubljana, ELMAR LAISTER, Medical University Vienna, MATIJA MILANIC, University of Ljubljana — Infrared thermography can distinguish rheumatoid arthritic (RA) joints from healthy joints by measuring elevated skin surface temperature caused by the inflammation present in RA joints. However, infrared thermography is more sensitive for the assessment of small joints.
Thermal transport simulations of healthy and arthritic fingers were implemented by solving the bio-heat diffusion equation within joint models using finite elements method (FEM). FEM models were based on high resolution MR images. Arthritic joint models were simulated by increasing the metabolic heat generation of healthy joint models. Simulated thermographic images were compared to real images.
Our simulations confirmed that elevated internal joint temperature results in elevated surface temperature. Internal and surface temperature depended on internal heat generation, heat dissipation due to perfusion, joint geometry, and finger surface cooling. Patterns of finger surface temperature from simulation were similar to that in thermographic images.
Thermal transport simulations relate thermographic images of the finger, finger geometry, internal temperature distribution and internal heat sources or sinks. Understanding these relations facilitate better RA diagnostics with infrared thermography.

*ARRS: P1-0389, J2-8171
1:51PM B06.00012: A fast and effective denoising solution using deep learning for real time X-ray Acoustic Computed Tomography*  DAVID THOMAS (Presenter), FARNOUSH FORGHANI, ADAM MAHL, BERNARD JONES, Radiation Oncology, University of Colorado Denver, MARK BORDEN, University of Colorado, Boulder, MOYED MIFTEN, Radiation Oncology, University of Colorado Denver — The X-ray acoustic (XA) computed tomography has recently been proposed as a method for real-time 3D in-vivo patient dosimetry for radiation therapy. The XA effect follows the same principles as the photoacoustic effect: acoustic waves are induced due to the absorption of heat energy by the tissue from a pulsed photon beam. XA signals are small in amplitude and suffer from interference from RF noise generated by the Linear Accelerator electronics. For a real time dose reconstruction, a fast and effective denoising solution is required to increase the signal to noise in the measured XA signals. Here, we present a method to denoise the XA signals using deep learning neural networks. A Convolutional Neural Network (CNN) that operates on the spectral domain of XA signals is used. Given a noisy XA spectrogram, the CNN predicts clean XA signals. An advanced numerical model for time domain propagation of XA waves (kWave) is used to generate the training data for the CNN. Theoretical and experimental clean and noisy XA signals are obtained by megavoltage energy X-rays with long pulse width (4 us) generated from a clinical linear accelerator.

*This work is supported by American Cancer Society, Colorado Clinical and Translational Sciences Institute, and Cancer League of Colorado.

2:03PM B06.00013: Modeling polymer precursors for preparation of molecularly imprinted polymers for drug delivery and sensing  OLEKSANDR KOBRYN (Presenter), Nanotechnology Research Centre, National Research Council Canada — Molecularly imprinted polymers (MIPs) are synthetic receptors and are promising alternatives to natural receptors (e.g. antibodies) for a range of applications requiring specific and selective molecular recognition (e.g. sensing, drug delivery, sample clean and separation, etc.). In the absence of a rational approach to the design of MIPs, monomer selection is often made on the basis of previous experience or chemical intuition which can be time intensive and very expensive. Here, we present an example of a careful computational analysis of selected monomers with the main purpose to screen out the least suitable and identify the most appropriate ones. The modeling is based on the statistical mechanical theory of molecular liquids in terms of the Reference Interaction Site Model (RISM). With this instrument, we are be able to yield one- and three-dimensional distribution functions of interaction sites constituting the molecules and predict the solution structure and thermodynamics of its species on the nanometer scale. The recommendations for synthesis and subsequent experimental verification of selected monomers are based on visual examination of the solvent nanomorphology and quantitative analysis of their thermodynamic properties, both predicted by modeling.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B07 DQI: Electron and Hole Based Spin Qubits in Heterostructures 102 - Manuel Rispler, Delft University of Technology
**11:15AM B07.00001: Electric dipole-induced spin resonance of holes in Ge/Si nanowires**

FLORIAN FRONING, LEON CAMENZIND, University of Basel, ANG LI, Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology, ERIK BAKKERS, Applied Physics, Eindhoven University of Technology, DOMINIK ZUMBUHL, FLORIS BRAAKMAN (Presenter), University of Basel — Electric dipole-induced spin resonance (EDSR) forms a basic tool in quantum information processing with spin qubits. It enables electrically driven quantum gates and forms a way to accurately probe the energy spectrum of spin qubits. We demonstrate EDSR of hole spins confined in a double quantum dot in a Ge/Si nanowire. The spin-orbit interaction of hole spins in this system has a unique character, as it is predicted to be very strong, potentially enabling GHz Rabi oscillation frequencies, as well as electrically tunable. Recent experiments support this with a demonstration of a 30 nm spin-orbit length and Rabi frequencies exceeding 400 MHz.

Here we perform hole spin spectroscopy through the measurement of EDSR transitions between double dot spin states under various resonance conditions. In particular, we characterize the hole g-tensor as well as the direction of the effective spin-orbit magnetic field through an investigation of EDSR transitions as a function of the magnitude and orientation of an applied external magnetic field. Knowledge of these parameters allows tuning the system towards optimized Rabi oscillation frequencies and minimized decoherence.

*Supported by the Swiss National Science Foundation, the Swiss Nanoscience Institute, and the European Microkelvin Platform.

**11:27AM B07.00002: Electric control of the single hole g-factor by 400% in a silicon MOS quantum dot.**

SCOTT LILES (Presenter), FREDERICO MARTINS, Univ of New South Wales, DMITRY MISEREV, University of Basel, IAN THORVALDSON, MATTHEW RENDELL, FAY E. HUDSON, Univ of New South Wales, MENNO VELDHORST, University of Twente, OLEG SUSHKOV, ANDREW STEVEN DZURAK, ALEX HAMILTON, Univ of New South Wales — Holes in silicon quantum dots are attracting significant attention for their potential use as fast, highly coherent spin qubits [1]. However, there are still gaps in the understanding of the physics of hole spins. For example, the full effects of confinement and spin-orbit coupling on hole spin states remains an open problem. Studies of the Lande g-tensor are valuable for characterizing this underlying spin physics, however most studies of holes have been performed in an unknown orbital configuration where spin-orbit coupling can lead to complex non-trivial spin effects. Studies of a single hole in a known and reproducible orbital state can therefore provide valuable insight into the complex spin physics.

In this work we confine a single hole in a known orbital state [2] and study the Lande g-tensor using a 3D vector magnet. We compare the g-tensor for different confinement profiles and find the g-tensor can be strongly modulated and even rotated by up to 30 degrees. These results show that the anisotropy of the single hole g-tensor is due to symmetries in the tunable electric confinement. This tunability can be harnessed for further use of holes in spin qubit applications.

11:39AM B07.00003: Fast and tunable Rabi oscillations of hole spins in Ge/Si nanowires*

FLORIAN FRONING (Presenter), LEON CAMENZIND, University of Basel, ANG LI, ERIK BAKKERS, TU Eindhoven, DOMINIK ZUMBUHL, FLORIS BRAAKMAN, University of Basel — The strong confinement of holes to one dimension in Ge/Si core/shell nanowires gives rise to direct Rashba spin-orbit interaction which is predicted to be both very strong and electric field tunable. The full electrical control promises to switch the spin-orbit interaction either on, enabling fast qubit operations, or off, protecting the spin state in order to achieve an increased qubit lifetime. These properties make Ge/Si nanowires a very promising system for the implementation of hole spin qubits. Recent experiments have found a spin-orbit interaction length on the order of only 30 nm, paving the way to very fast spin manipulation by electric dipole spin resonance. This mechanism allows us to drive very fast Rabi oscillations above 400 MHz at a Larmor frequency of 3.4 GHz, thus entering the strong driving regime. Furthermore, we find the Rabi oscillation frequency as well as the g-factor to be highly tunable with small changes in gate voltages, indicating the feasibility to electrically control the spin-orbit interaction strength.

*Supported by Swiss NSF, Swiss Nanoscience Institute SNI, and European Microkelvin Platform EMP.

11:51AM B07.00004: Towards scalable hole spin qubits in silicon* RAMI EZZOUCH (Presenter), SIMON ZIHLMANN, ALESSANDRO CRIPPA, ROMAIN MAURAND, AGOSTINO APRÀ, ANTHONY AMISSE, XAVIER JEHL, BENOIT BERTRAND, LOUIS HUTIN, MAUD VINET, BENJAMIN VENITUCCI, JING LI, YANN-MICHEL NIQUET, CEA Grenoble, MATIAS URDAMPILLETA, TRISTAN MEUNIER, Institut Néel, CNRS, MARC SANQUER, SILVANO DE FRANCESCHI, CEA Grenoble — Since the first proof-of-concept demonstration of a silicon hole spin qubit based on industry-standard CMOS technology [1], our research efforts have focused on acquiring a better understanding of the mechanism for electric-field-driven hole-spin manipulation [2], as well as on the development of spin readout based on rf gate reflectometry [3]. All of these studies were carried out on p-type silicon-nanowire devices with two crossing gates in series. Here we report the first implementation of hole-qubit functionality in a face-to-face gate geometry [4]. This more scalable geometry can be regarded as the elementary building block of a one-dimensional chain of qubits were each qubit on the chain is read through a facing helper quantum dot via the Pauli spin blockade mechanism and rf gate reflectometry [5].

References:

*The work is supported by the EU's Horizon 2020 research and innovation program under grant agreement No. 688539 MOS-QUITO and the ERC Project No. 759388 LONGSPIN.
12:03PM B07.00005: Hole spin echo envelope modulations  PERICLES PHILIPPOPOULOS (Presenter), McGill University, STEFANO CHESI, Beijing Computational Science Research Center, JOE SALFI, University of British Columbia, SVEN ROGGE, University of New South Wales, WILLIAM COISH, McGill University — An anisotropic hyperfine coupling can give rise to a substantial spin-echo envelope modulation that can be Fourier-analyzed to accurately reveal the hyperfine tensor. We give a general theoretical analysis for hole-spin-echo envelope modulation (HSEEM), and apply this analysis to the specific case of a boron-acceptor hole spin in silicon [1]. For boron acceptor spins in unstrained silicon, both the hyperfine and Zeeman Hamiltonians are approximately isotropic leading to negligible envelope modulations. In contrast, in strained silicon, where light-hole spin qubits can be energetically isolated, we find the hyperfine Hamiltonian and g-tensor are sufficiently anisotropic to give spin-echo-envelope modulations. We show that there is an optimal magnetic-field orientation that maximizes the visibility of envelope modulations in this case. Based on microscopic estimates of the hyperfine coupling, we find that the maximum modulation depth can be substantial, reaching ~ 10%, at a moderate laboratory magnetic field, B < 200 mT.


12:15PM B07.00006: Effects of Valley-Orbit Coupling on the Exchange Interaction in a Si/SiGe Double Quantum Dots*  BILAL TARIQ (Presenter), XUEDONG HU, State Univ of NY - Buffalo — We investigate the effects of the phase and magnitude of the valley orbit coupling on the tunnel coupling matrix elements and the exchange interaction in a Si double quantum dot. Our results show that a difference in the phase between the two quantum dots modifies the single-electron tunnel coupling between different valley eigenstates. In particular, valley-blockade between the ground valleys of individual dots could be obtained when the valley phase difference between the dots is π. For the two-electron case, exchange interaction at the symmetric point (zero detuning) is suppressed when valley phase difference is finite, and reaches its minimum value when the phase difference is 180 degrees. The energy spectrum at finite detuning also depends on the magnitudes and phases of the valley orbit couplings of the two dots. Our results shed new lights on the controllability of Silicon based spin qubit for its application in quantum information processing.

*This work is supported by US ARO through grant W911NF1710257.
12:27PM B07.00007: Singlet-triplet splitting of two electrons in a Si/SiGe quantum dot*

EKMEL ERCAN (Presenter), University of Wisconsin - Madison, SUSAN NAN COPPERSMITH, University of Wisconsin-Madison, The University of New South Wales, MARK G FRIESEN, University of Wisconsin - Madison — We theoretically study the effects of quantum dot confinement strength on the singlet-triplet (ST) splitting of two-electron dots in Si/SiGe quantum wells. Our analysis includes valley effects and disorder at the quantum well interface by combining full configuration interaction (FCI) scheme with tight-binding (TB) calculations. While TB provides an accurate description of single-electron wave functions by taking microscopic effects like interface disorder into account, and captures the valley physics of silicon, FCI allows us to calculate multielectron energies and corresponding wave functions by including the effects of electron-electron interactions. We show that these interactions can have unexpectedly strong or unexpectedly weak effects on the ST splitting, depending on the confinement strength and anisotropy.

*This work was supported by the Vannevar Bush Faculty Fellowship program sponsored by the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering and funded by the Office of Naval Research through Grant No. N00014-15-1-0029, and by ARO through Award No. W911NF-17-1-0274.

12:39PM B07.00008: Operation of a four-qubit device in isotopically enriched Si/SiGe*

ANTHONY SIGILLITO (Presenter), MICHAEL GULLANS, JASON PETTA, Princeton University — Quantum processors based on electron spins in silicon are rapidly becoming a strong contender in the race to build a quantum computer. Over the past few years, quantum-dot spin qubits have been shown to offer high fidelity single-qubit [1] and two-qubit [2-5] control at levels approaching the fault tolerant threshold. However, most experiments have been conducted in one-qubit, or two-qubit devices. Recently, we have demonstrated operation of a four-qubit device in isotopically enriched Si/SiGe [6]. Here we outline improvements to our four-qubit device design and present new data on one- and two-qubit operation in the device including recent randomized benchmarking results.


*We thank L. F. Edge and M. Borselli of HRL Laboratories for providing the isotopically enriched heterostructure. Research sponsored by ARO grant No. W911NF-15-1-0149 and the Gordon and Betty Moore Foundation's EPIQS Initiative through grant GBMF4535. Devices were fabricated in the Princeton University Quantum Device Nanofabrication Laboratory.
12:51PM B07.00009: Coherent spectroscopy of a Si/SiGe double quantum dot molecule
JOELLE BAER (Presenter), JOHN DODSON, BRANDUR THORGRIMSSON, EKMEL ERCAN, MERRITT LOSERT, TREVOR KNAPP, NATHAN HOLMAN, THOMAS MCJUNKIN, SAMUEL NEYENS, EVAN R MACQUARRIE, RYAN H FOOTE, University of Wisconsin - Madison, LISA F EDGE, HRL Laboratories, LLC, MARK G FRIESEN, SUSAN NAN COPPERSMITH, MARK ALAN ERIKSSON, University of Wisconsin - Madison — We report the wideband microwave spectroscopy of a gate-defined double quantum dot qubit. The double quantum dot, operated with a total of five electrons, has a series of molecular energy levels that can be manipulated coherently. Working in the (4,1)-(3,2) charge configuration, we use a two-step Ramsey pulse sequence to characterize the energy levels of the (3,2) charge configuration as a function of the double-dot detuning. Using this procedure, we demonstrate differences in the dispersion for two closely spaced levels (<2GHz separation in energy). We present measurements of the broadband spectrum, discovering seven energy levels that can be addressed coherently, each with distinct Rabi oscillation characteristics. The double quantum dot is formed in an undoped Si/SiGe heterostructure using an overlapping gate architecture [1]. The measurements are acquired using a tunable latched measurement scheme similar to that in Ref. [2], made possible by the presence of independent reservoirs and corresponding tunnel barriers for each quantum dot.


1:03PM B07.00010: Towards coupled valley qubits in silicon* JOHN ROONEY (Presenter), BLAKE M FREEMAN, NICHOLAS PENTHORN, University of California, Los Angeles, LISA F EDGE, HRL Laboratories, LLC, HONGWEN JIANG, University of California, Los Angeles — Valley states in silicon are a promising candidate for encoding qubits in gate-defined quantum dots due to their protection against charge noise, fast operation times, and ability to operate without a magnetic field. Recently, two-axis quantum control of a valley qubit using gate pulse sequences with X and Z rotations, occurring within a fast operation time of 300 ps, has been demonstrated [1]. In this talk, we present our progress on coupling two such valley qubits. We have fabricated a device consisting of two double-quantum dots on a SiGe heterostructure for our experiments. We further measure the capacitive coupling between the two double dots in the few electron region, showing sufficiently large and tunable coupling. By exploiting this electrostatic interaction, we discuss our plan for employing the two coupled valley qubits to realize a two-qubit logic gate.


*This work is supported by U.S. ARO through Grant. No. W911NF1410346.
1:15PM B07.00011: Hyperfine effects in a single hole GaAs/AlGaAs double quantum dot device* SERGEI STUDENIKIN (Presenter), JORDAN DUCATEL, MAREK J KORKUSINSKI, D. G. AUSTING, PIOTR ZAWADZKI, ANDREW STANISLAW SACHRAJDA, National Research Council Canada, PERICLES PHILIPPOPOULOS, WILLIAM COISH, Department of Physics, McGill University, LISA A TRACY, JOHN RENO, TERRY HARGETT, Sandia National Laboratories — Hole spin qubits are attractive because, compared to electrons, they are predicted theoretically to have significantly weaker interactions with host nuclei, resulting in longer coherence times [1]. As a result it is more challenging to quantify hyperfine (hf) effects with holes. In Ref. [2], in a quantum point contact device, Dynamic Nuclear Polarization (DNP) through the hf interaction with holes was undetectable. In this work, we detect and explore small DNP effects in a single hole GaAs/AlGaAs gated DQD device using a modified EDSR technique [3]. As compared to our previous studies [3], the device is tuned to a much smaller inter-dot coupling regime to minimize spin-orbit effects and to make nuclear spin effects detectable.

[1] Philippopoulos, et al. PRB 100, 125402 (2019);

*Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

1:27PM B07.00012: A realistic GaAs-spin qubit device for a classical error-corrected quantum memory and beyond* MANUEL RISPLER (Presenter), Delft University of Technology, PASCAL CERFONTAINE, VEIT LANGROCK, JARA-FIT Institute Quantum Information Forschungszentrum Jülich and RWTH Aachen, BARBARA MARIA TERHAL, Delft University of Technology — Based on numerically-optimized real-device gates and parameters we study the performance of the phase-flip (repetition) code on a linear array of GaAs quantum dots hosting singlet-triplet qubits. We first examine the expected performance of the code using simple error models of circuit-level and phenomenological noise, reporting a.o. a 3% circuit-level depolarizing noise threshold. We then perform density-matrix simulations using a maximum-likelihood and minimum-weight matching decoder to study the effect of real-device dephasing, read-out error, quasi-static as well as fast gate noise. Considering the trade-off between qubit read-out time versus dephasing time (T2), we identify a sub-threshold region for the phase-flip code which lies within experimental reach.

*ERC grant EQEC No. 682726
1:39PM B07.00013: Developing atom-based solid-state quantum simulators: understanding charge-stability diagrams of dopant arrays in Si  
GARNETT BRYANT (Presenter), EMILY TOWNSEND, XIQIAO WANG, RICHARD SILVER, National Institute of Standards and Technology — Atomically precise fabrication of dopant arrays in Si provides exciting opportunities to perform quantum simulations and to study the dynamics of engineered quantum systems. Here we describe theoretical simulations done for two-dimensional arrays of dopants in Si used to implement an extended range Fermi-Hubbard model. Simulations are done with and without atom disorder, as a function of the electron-electron interaction to test the limits of weak and strong interaction, and with and without a spin/valley degree of freedom. Results are used to understand charge-stability diagrams, recently obtained for two-dimensional arrays of dopants in Si. The nature of transport through these arrays depends critically on the ratio of the inter-dopant tunneling to tunnel coupling of the dopants to the source and drain. We consider n x m arrays of different sizes to identify the array states that are probed in transport. We further consider the effect of array orientation relative to the source and drain on the tunnel coupling and on the capacitive coupling to side gates. Implications for using dopant arrays as a quantum lab on a chip are discussed.

1:51PM B07.00014: Controlling textured hole spins in InAs quantum dots with oscillating electric fields*  
ARTHUR LIN (Presenter), Joint Quantum Institute, University of Maryland, MATTHEW F DOTY, Department of Materials Science and Engineering, University of Delaware, GARNETT BRYANT, Nanoscale Device Characterization Division, National Institute of Standards and Technology — Recently, we have shown that hole spins in InAs quantum dots (QDs) exhibit spatially dependent texture, caused by the spin-orbit properties of the material and the geometry of the dot. Utilizing this spin texture, we demonstrated the ability to flip the overall hole spin by reversing the in-plane electrical bias across the dot. To fully capture the spin texture of the hole states, we used an atomistic tight-binding model that is able to resolve the wavefunction at the atomic level. However, atomistic tight-binding calculations are computationally expensive. Here, we present a reduced Hamiltonian capable of describing the evolution of the lowest hole state tight-binding wavefunctions, simulating the effect of oscillating electric fields, while fully preserving the effects of the spin texture. We calculate the timescale at which the spatial texture of the hole spin evolves, how the spin texture changes as the field oscillates, and how oscillating fields drive the overall net spin. We briefly discuss how our results can be used to design new control schemes for holes in QDs.

*This project is partially supported by the National Science Foundation (NSF) under DMR-1505628.

Monday, March 2, 2020 11:15 AM - 1:39 PM

Session B08 DQI: Programming and Compiling: the QC Stack session 104  
- Ali Javadi, IBM
11:15AM B08.00001: Extending Modern C++ for Heterogeneous Quantum-CLASSICAL Computing*  ALEXANDER MCCASKEY (Presenter), EUGEN DUMITRESCU, PAVEL LOUGOVSKI, SARAH POWERS, SHIRLEY MOORE, TIFFANY MINTZ, Oak Ridge National Lab — Software frameworks for quantum computing have progressed significantly over the past few years. Most approaches have put forward vendor-specific frameworks leveraging high-level languages like Python. As quantum hardware improves, we expect that these high-level approaches will detract from overall performance gains garnered from quantum computation. Tighter integration models will require low-level, system software and compilers extending commonly-used languages. We present QCOR, a C++ language extension specification with an associated compiler that enables the programming of quantum expressions alongside standard C++ in a single-source context. Our specification puts forward abstractions and concepts that are common to typical quantum-classical algorithmic workflows. We implement this language extension via light-weight extensions to Clang and build off the system-level, quantum-classical XACC framework. Our approach represents the state-of-the-art with regards to enabling quantum programming alongside standard languages leveraged in existing high-performance domain scientific computing.

*The authors acknowledge DOE ASCR funding under the QCAT program, FWP number ERKJ347. ORNL is managed by UT-Battelle, LLC, for the US Department of Energy under contract no. DE-AC05-00OR22725.

11:27AM B08.00002: OpenPulse: Software for Experimental Physicists in Quantum Computing  LAUREN CAPELLUTO (Presenter), THOMAS ALEXANDER, IBM TJ Watson Research Center — The quantum computing industry provides public access to superconducting qubit systems through open-source quantum computing frameworks such as Qiskit. Compilation techniques play a critical role in leveraging these small scale, noisy devices by driving down error rates in program execution. The compiler backend decomposes quantum operations into microwave pulses which aim to realize the desired quantum operations with the highest fidelity possible. We introduce OpenPulse, a pulse-level programming component of Qiskit, that hands over analog control of quantum computing systems to the user. Using OpenPulse, the user can specify the exact time dynamics of a program by scheduling arbitrary waveforms on control system resources, and can recover the time dynamics of the measured output. This is sufficient to allow the user to freely characterize, verify and validate the quantum system, and to explore gate optimization and error mitigation techniques to enhance system performance. OpenPulse enables the community to collectively push the field onwards towards practical computation.
11:39AM B08.00003: qupulse: A quantum computing pulse parametrization and sequencing framework

PASCAL CERFONTAINE (Presenter), SIMON HUMPOHL, LUKAS PREDIGER, PATRICK BETHKE, EUGEN KAMMERLOHER, LARS SCHREIBER, JARA-FIT Institute for Quantum Information, RWTH Aachen University, STEFANIE MEYER, Central Institute of Engineering, Electronics and Analytics ZEA-2, Forschungszentrum Jülich GmbH, BERNHARD RUMPE, Chair of Software Engineering, RWTH Aachen University, HENDRIK BLUHM, JARA-FIT Institute for Quantum Information, RWTH Aachen University — We present an open source python package for the operation of advanced qubit control experiments, which emerged from our experimental work on spin qubits. It allows for hierarchical definition of control pulses and pulse sequences with an arbitrary nesting depth in a hardware-independent way.

Pulses can be described in terms of symbolic parameters. Reparametrization by mathematical expressions, for example when combining or sequencing pulses, is possible. This enables the simple generation of parameter sweeps and the reuse of predefined pulses. qupulse also exploits the sequencing capabilities of different arbitrary waveform generators for efficient use of waveform memory. Furthermore, serialization to JSON allows for a straightforward documentation of experiments and simplifies exchanging pulses between researchers.

In order to automatically configure acquisition hardware and simplify the data analysis, measurements can be specified as part of the pulse definition. We designed qupulse to interact with different instrument control and data acquisition frameworks such as QCodeS, special-measure (currently implemented) and labber.

qupulse is available at github.com/qutech/qupulse or quantuminfo.physik.rwth-aachen.de/code, accompanied by extensive documentation.

11:51AM B08.00004: Compiled Quantum Optimization Algorithms in NISQ Processors*

DAVIDE VENTURELLI (Presenter), QuAIL, USRA, NASA, MINH DO, NASA Ames Research Center, BRYAN O’GORMAN, QuAIL, Berkeley University, NASA, ZHIHUI WANG, QuAIL, USRA, NASA, ELEANOR RIEFFEL, QuAIL, NASA, JEREMY FRANK, NASA Ames Research Center, RYAN M LAROSE, QuAIL, UMich, USRA, NASA, VANESA GOMEZ GONZALEZ, USRA — We discuss resource estimation and synthesis optimization results related to compilation of a variety of structured variational algorithms. Specifically, we look at software tools and methods for finding a swap network that allows the efficient execution of algorithms on different superconducting chips (Rigetti’s Aspen Chip, Google’s Sycamore, IBM’s Tokyo). Efficiency is measured in terms of the total temporal makespan of execution of the compiled quantum circuit. Examples include algorithms for scheduling and asset allocation with both soft and hard constraints. We address two different regimes: where near-optimal compilations can be found, and where only heuristics (e.g., temporal planning methods) are available.

*NASA NAMS NNA16BD14C and Advanced Exploration Directorate; AFRL Information Directorate F4HBKC4162G001; AFRL FA8750-19-3-6101; NSF SpecEES1824470
12:03PM B08.00005: Optimizing compiler for Fermion simulation circuits* QINGFENG WANG (Presenter), University of Maryland, College Park, YUNSEONG NAM, IonQ, CHRISTOPHER ROY MONROE, University of Maryland, College Park — Jordan-Wigner and Bravyi-Kitaev transformations are the two widely known examples of the Fermion → qubit operator mappings. There exist however at least $O(2^{n^2})$ possible such mappings. Thus, an appropriate choice of the mapping can result in the reduction of quantum resource cost in practice, such as two-qubit gate counts in Fermion-simulation circuits. In this talk, I will present a methodology that may be used to optimize these simulation circuits, leveraging the vastly large space from which a suitable mapping may be drawn. A series of heuristics will be explored to arrive at the post-optimization quantum circuits.

*This work is supported by the IARPA LogiQ program, the ARO MURI on Modular Quantum Systems, the ARL Center for Distributed Quantum Information, the NSF QIS program, the NSF PFCQC Program, the DOE BES QIS Program, the DOE HEP QuantISED Program, and the NSF Physics Frontier Center at JQI.

12:15PM B08.00006: Heuristics for Quantum Compiling with a Continuous Gate Set MARC DAVIS (Presenter), Physics, UC Berkeley, COSTIN IANCU, Lawrence Berkeley National Laboratory — Abstract
We present an algorithm for compiling arbitrary unitaries into a sequence of gates native to a quantum processor. As accurate CNOT gates are hard for the foreseeable Noisy-Intermediate-Scale Quantum devices era, our A* inspired algorithm attempts to minimize their count, while accounting for connectivity. We discuss the search strategy together with “metrics” to expand the solution frontier. For a workload of circuits with complexity appropriate for the NISQ era, we produce solutions well within the best upper bounds published in literature and match or exceed hand tuned implementations, as well as other existing synthesis alternatives. In particular, when comparing against state-of-the-art available synthesis packages we show $2.4 \times$ average (up to $5.3 \times$) reduction in CNOT count. We also show how to re-target the algorithm for a different chip topology and native gate set, while obtaining similar quality results. We believe that empirical tools like ours can facilitate algorithmic exploration, gate set discovery for quantum processor designers, as well as providing useful optimization blocks within the quantum compilation tool-chain.
Introducing Control Flow in Qubit Allocation for Quantum Turing Machines

MICHAEL CUBEDDU (Presenter), WILL T FINIGAN, PRINEHA NARANG, Harvard University; Aliro Technologies, VITALI VINOKOUR, Aliro Technologies — To make NISQ devices practical for quantum software engineers, novel programming tools with maximal flexibility have to be developed. Several proposed algorithms and error-correcting codes for near term devices require the ability to execute classical control statements based on quantum measurements. However, the unpredictable nature of control flow on a quantum device complicates the compilation process in the presence of variable noise. The functionality of control flow allows for expanded algorithmic power of the programming language in the form of conditional statements and loops, which a linearly-executed program is incapable of computing. In this work, we introduce a framework to reconcile the non-deterministic properties of quantum control flow when allocating virtual qubits from a given quantum circuit to physical qubits on a specific NISQ device in the pre-processing and compiling stage. We consider the respective connectivity and fidelity constraints, with the goal of reducing the expected error rate of the computation. Our protocols will allow for quantum developers and NISQ devices together to more efficiently exploit the compelling algorithmic power that the quantum Turing machine model provides.

*This work is supported by Harvard University OTD's PSE Accelerator Grant

Noise-Aware Qubit Allocation Techniques for NISQ Devices

MICHAEL CUBEDDU, WILL FINIGAN (Presenter), Harvard University; Aliro Technologies, VITALI VINOKOUR, Aliro Technologies, PRINEHA NARANG, Harvard University; Aliro Technologies — With a growing diversity in devices, control systems, topologies, programming languages, and applications, computation in the NISQ era needs to be navigated through adaptable cloud-based software. In order to provide the highest fidelity results to users, it is essential that this software employs hardware-aware optimizations at all levels of the stack, both in the pre-processing and post-processing stages. We present our work in pre-processing error mitigation through variation-aware qubit allocation techniques for gate-based quantum computers, with a focus on superconducting platforms. We formulate a description of the “allocation problem” and propose several solutions: a deterministic algorithm for finding the optimal solution as well as a more scalable and flexible randomized heuristic approach. We will present and validate the implications of these different techniques on various NISQ devices.

*This work is supported by Harvard University OTD's PSE Accelerator Grant.
12:51PM B08.00009: Benchmarking NISQ Devices Using qFlex*
SALVATORE MANDRA (Presenter), NASA Ames Research Center, BENJAMIN VILLALONGA, University of Illinois at Urbana-Champaign, DMITRY LIAKH, Oak Ridge National Lab, SERGIO BOIXO, Google Inc. — Quantum supremacy is the task to perform a quantum calculation on a Noisy-Intermediate Scale Quantum (NISQ) device that cannot be performed on the latest and most powerful supercomputer by using the best known classical simulator. To this end, the Google team has designed a series of benchmarks, based on the sampling of Random Quantum Circuits (RQCs), to challenge classical supercomputers. In a programming-like language, the RQC sampling corresponds to the first “Hello, World!” program in the quantum computing era. In my talk I will present qFlex, a fast and flexible software to simulate large RQCs to both verify and benchmark NISQ devices. qFlex is a NASA-Google-ORNL collaboration and it's now publicity available at https://github.com/ngnrsaa/qFlex. As part of my talk, I will show some live demos and present our latest results on benchmarking available NISQ devices.

*AFRL Information Directorate under grant F4HBKC4162G001. This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DEAC05-00OR22725. This research has been authored by UT-Battelle LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

1:03PM B08.00010: Characterization of State-dependent Noise in NISQ Processors*
RONALD J SADLIER (Presenter), he Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, Knoxville, TRAVIS HUMBLE, Quantum Computing Institute, Oak Ridge National Laboratory — Characterization of the quantum operations in current NISQ devices reveal noise spectra that are highly dependent on the underlying quantum state. These results indicate that a state-dependent noise model is needed to accurately control the behavior of quantum computing programs on today's noisy hardware. We develop a method for characterizing state-dependent errors based on classical truth tables for the gate operations, and we use these results to compute the amplitudes of the corresponding channel operators. Using this method, we characterize a 20-qubit fixed-frequency superconducting transmon processor to develop a noise model for this device. We then use this noise model to estimate the fidelity of quantum circuits executed on the hardware and compare these results with tomographic fidelities.

*This work was supported by the Department of Energy Office of Science Early Career Research Program.
1:15PM B08.00011: Strategies for reducing the number of controlled gates on noisy intermediate scale quantum circuits*  KOSUKE MITARAI (Presenter), KEISUKE FUJII, Graduate School of Engineering Science, Osaka University — We show that certain kind of controlled gates can be decomposed into a sequence of single-qubit operations when expectation values of some operators are needed. It is performed by decomposing the corresponding quantum channels into linear combination of single-qubit channels. Firstly, we discuss the usefulness of the presented method in variational algorithms which runs on quantum computer by showing that it can extract information about the derivatives of the parametrized state without adding ancilla qubit. It can also be applied for measuring the time correlation of observables in quantum simulations. Finally, we show that the method can decompose a large, in the number of qubits, quantum circuit into smaller ones. Although the runtime of this method scales exponentially in the number of decompositions performed, it reduces the requirement on the hardware by reducing the number of gates and qubits in the trade-off of increased runtime.

*KM thanks the METI and IPA for their support through the MITOU Target program. KM is also supported by JSPS KAKENHI No. 19J10978. KF is supported by KAKENHI No.16H02211, JST PRESTO JPMJPR1668, JST ERATO JPMJER1601, and JST CREST JPMJCR1673. This work is supported by MEXT Quantum Leap Flagship Program (MEXT Q-LEAP) Grant Number JPMXS0118067394.

1:27PM B08.00012: qubit-ADAPT-VQE: An adaptive algorithm for constructing hardware-efficient ansätze on a quantum processor*  HO LUN TANG (Presenter), Physics, Virginia Tech, HARPER GRIMSLEY, NICHOLAS J. MAYHALL, Chemistry, Virginia Tech, EDWIN BARNES, SOPHIA E. ECONOMOU, Physics, Virginia Tech — The variational quantum eigensolver, being a promising algorithm on near-term quantum devices, is extensively used for finding the ground state energy of molecular Hamiltonians. The classical and quantum resources needed by this algorithm, the number of variational parameters in the wavefunction ansatz and the depths of the state preparation circuits, critically depend on the choice of ansatz. Recently, an algorithm termed ADAPT-VQE was introduced to build system-adapted ansätze with substantially fewer variational parameters compared to other approaches. However, deep state preparation circuits remain a challenge. Here, we present a hardware-efficient variant of this algorithm called qubit-ADAPT. By numerical simulations, we show that with a well-designed operator pool, qubit-ADAPT can reduce the circuit depth by one order of magnitude while maintaining the same accuracy as the original ADAPT-VQE. This result highlights the promise of adaptive ansätze algorithms on near-term quantum devices.

*NSF Award No. 1839136

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B09 DQI: NISQ: Algorithms 106 - Hari Krovi, BBN Technologies
11:15AM B09.00001: Noise-resilient quantum algorithm design for adiabatic quantum computers  JIAN LIN (Presenter), XIAOPENG LI, Department of Physics, Fudan University — We have developed a novel architecture for automated design of quantum adiabatic algorithm by combining deep reinforcement learning and simulation annealing techniques. Through numerical test, we find that our architecture is adaptable for noise-resilient quantum algorithm design, which is of great current demand in the era of noisy intermediate-scale quantum computing. We show that in solving Grover search, our method automatically reaches the optimal performance in terms of time-complexity scaling. Our approach offers a recipe to make the noise-resilient adiabatic quantum computing, and is also generalizable to optimizing quantum simulations.

11:27AM B09.00002: Preserving symmetries in NISQ algorithms*  MICHAEL STREIF (Presenter), Quantum AI Lab, USRA and NASA Ames, ELEANOR RIEFFEL, Quantum AI Lab, NASA Ames Research Center, ZHIHUI WANG, Quantum AI Lab, USRA and NASA Ames — Many classical optimization problems display local or global symmetries. In the Quantum Alternating Operator Ansatz (QAOA), these symmetries can be used to design mixers which restrict the evolution of the system to a subspace which is exponentially smaller than the full Hilbert space [1,2]. However, in realistic scenarios, errors can break the symmetry and yield invalid solutions to the optimization problem. In this talk, we show an analysis of the probability of staying in the correct subspace under the influence of realistic noise models. Moreover, for the example of 3-coloring, we show that it is possible to exploit the natural redundancy of the qubit encoding to bring back the evolution into the correct subspace.


*We appreciate support from NASA Ames Research Center, NASA Advanced Exploration systems (AES) program, NASA Transformative Aeronautic Concepts Program (TACP), and the AFRL Information Directorate under grant F4HBKC4162G001. ZW is also supported by NASA Academic Mission Services (NAMS), contract number NNA16BD14C, and MS by USRA NAMS R&D Student program.
Using Grover’s search algorithm to test a three-level quantum system*

VASILY GEYKO (Presenter), ALESSANDRO CASTELLI, ILON JOSEPH, YUAN SHI, FRANK R GRAZIANI, STEPHEN BERNARD LIBBY, JEFFREY PARKER, YANIV J ROSEN, JONATHAN L DUBOIS, Lawrence Livermore Natl Lab — In the present work, Grover’s search algorithm is modified and studied for application to a three-level “qutrit” quantum device. The modified algorithm constructs the superposition of all states via the discrete Fourier transform instead of the standard Hadamard gate. Then, the analogous Grover’s diffusion operator is applied $m$ times. The probability of determining the correct answer as a function of $m$ is derived and shown to be very close to unity for specific choices of $m$. In a real device, the measured probability will deviate from theoretical predictions due to decoherence effects, and, since different energy levels of the qutrit have different decoherence properties, this can potentially affect the performance of the algorithm depending on the marked state. To address these issues, the algorithm has been specifically designed for implementation on the LLNL Quantum Design and Integration Testbed (QuDIT) hardware platform. This device is based on superconducting circuit architecture where the first three-levels of a transmon are used to define the qutrit.

*This work was performed under the auspices of US DOE by LLNL under Contract DE-AC52-07NA27344 and was supported by DOE FES under Project No. AT1030200-WA-OP SCW-1680 and LLNL-LDRD under Project No. 19-FS-072.

Utilizing NISQ devices for evaluating quantum algorithms*

ELEANOR RIEFFEL (Presenter), NASA Ames Research Center — With the advent of quantum supremacy, we have an unprecedented opportunity to explore quantum algorithms in new ways. The emergence of general-purpose quantum processors opens up empirical exploration of quantum algorithms. Classically, heuristic algorithms, empirically tested on benchmark and real-world problems, work well in practice. With the empirical evaluation NISQ hardware enables, we enter the era of quantum heuristics, where we can expect a broadening of established applications of quantum computing. What to run, and how best to utilize these still limited quantum devices, remain open research questions. We discuss opportunities and challenges for using NISQ devices to evaluate quantum algorithms, including in elucidating quantum computational mechanisms, in designing novel quantum algorithms, in compilation and error-mitigation, and in techniques for evaluating quantum algorithms empirically.

*We are grateful for support from NASA Ames Research Center, from the AFRL Information Directorate under grant F4HBKC4162G001, and from the Office of the Director of National Intelligence (ODNI) and the Intelligence Advanced Research Projects Activity (IARPA), via IAA 145483.

What we’ve learned from NISQ application experiments on Sycamore

RYAN BABBSH (Presenter), Google Inc. — Does implementing larger and more accurate examples of VQE, QAOA and the like actually teach us anything useful about quantum computing? Or are we wasting our time on refinements of these NISQ favorites if none of them are going to scale to the classically intractable regime without a significant breakthrough? In this talk, I will reflect on these questions in the context of Google’s recent application demonstration experiments on the Sycamore quantum processor.
12:15PM B09.00006: Sequential minimal optimization for quantum-classical hybrid algorithms*  
KEN M. NAKANISHI (Presenter), Graduate School of Science, The University of Tokyo, KEISUKE FUJII, Graduate School of Engineering Science, Osaka University, SYNGE TODO, Graduate School of Science, The University of Tokyo — We propose a sequential minimal optimization method for quantum-classical hybrid algorithms, which converges faster, is robust against statistical error, and is hyperparameter-free. Specifically, the optimization problem of the parameterized quantum circuits is divided into solvable subproblems by considering only a subset of the parameters. In fact, if we choose a single parameter, the cost function becomes a sine curve with period $2\pi$, and hence we can exactly minimize with respect to the chosen parameter. By repeatedly performing this procedure, we can optimize the parameterized quantum circuits so that the cost function becomes as small as possible. We perform numerical simulations and find that the proposed method substantially outperforms the existing optimization algorithms. This accelerates almost all quantum-classical hybrid algorithms readily and would be a key tool for harnessing near-term quantum devices.

*KMN thanks IPA for its support through MITOU Target program. The computation in this work has been partly done using the facility of the Supercomputer Center, Institute for Solid State Physics, The University of Tokyo. KF is supported by KAKENHI No.16H02211, JST PRESTO JPMJPR1668, JST ERATO JPMJER1601, and JST CREST JPMJCR1673. This work is supported by MEXT, Q-LEAP.

12:27PM B09.00007: Systematically Improving Quantum Approximate Optimization Algorithm with an Adaptive Ansatz*  
SOPHIA E. ECONOMOU (Presenter), LINGHUA ZHU, HO LUN TANG, GEORGE S. BARRON, EDWIN BARNES, Department of Physics, Virginia Tech, NICHOLAS J. MAYHALL, Department of Chemistry, Virginia Tech — The quantum approximate optimization algorithm (QAOA) is a hybrid variational quantum eigensolver (VQE) algorithm that uses a variational ansatz of an alternating form to minimize a classical (‘problem’) Hamiltonian. The two alternating operators are given by exponentiation of the problem Hamiltonian and by the ‘mixing’ layer, which in the original formulation of QAOA is a rotation of all the qubits about the x axis. It has been discussed in the literature that by using more general mixers the performance of QAOA can be improved. However, determining how to choose these mixers is an open question. Here we provide a solution by employing the recently introduced ADAPT-VQE\(^1\) algorithm, an iterative approach to creating ansatze for VQEs. We show that the performance of QAOA can be improved considerably by allowing more freedom in the single qubit gates and even further by allowing for entangling operations in the mixing layer.


*US Department of Energy (Award No. de-sc0019199)
US Department of Energy (Award No. de-sc0019318)
12:39PM B09.00008: Bounds on classical simulation of simple quantum models from quantum supremacy. PETER LOVE (Presenter), Tufts Univ — Quantum simulation is a central application of quantum computing. Quantum supremacy defines systems whose efficient classical simulation is unlikely given complexity-theoretic assumptions. We consider simple physically motivated quantum models that can display quantum supremacy and hence whose efficient simulation by classical means is unlikely. We consider quantum extensions of classical hydrodynamic lattice gas models. We find that the existence of local conserved quantities strongly constrains such extensions. We find the only extensions that retain local conserved quantities correspond to changing the local encoding of a subset of the bits. These models maintain separability of the state throughout the evolution and are thus efficiently classically simulable. We then consider evolution of these models in the case where any of the bits can be encoded and measured in one of two local bases. For quantum extensions of classical models that are computationally universal such quantum extensions can encode Simon’s algorithm and demonstrate quantum supremacy, thus presenting an obstacle to efficient classical simulation.


12:51PM B09.00009: Maximum weighted independent set and quantum alternating operator ansatz ZAIN SALEEM (Presenter), Argonne Natl Lab — We study the maximum weighted independent set problem of graph theory using the quantum alternating operator ansatz. We perform simulations on the Rigetti Forrest simulator and analyze the dependence of the algorithm on the depth of the circuit, initial states and the weights of the vertices. We point out that the probability distribution of observation of the feasible states representing maximum independent sets is asymmetric for the Maximum Independent Set problem unlike the MaxCut problem where the probability distribution of feasible states is symmetric. We also give a numerical comparison of the approximation ratios for the algorithm when we choose different initial states in our graph.

1:03PM B09.00010: Multi-block ADMM Heuristics for Mixed-Binary Optimization on Classical and Quantum Computers CLAUDIO GAMBELLA (Presenter), ANDREA SIMONETTO, IBM Research Ireland — Solving combinatorial optimization problems on noisy intermediate-scale quantum (NISQ) devices is currently being advocated for (and restricted to) binary polynomial optimization with equality constraints. This is achieved using, e.g., the variational quantum eigensolver (VQE), a hybrid quantum/classical heuristic approach. We present a decomposition-based approach to extend the applicability of current approaches to mixed binary optimization (MBO) problems, so as to solve a broad class of real-world optimization problems. In the MBO framework, we show that the alternating direction method of multipliers (ADMM) can split the MBO into a binary unconstrained problem (that can be solved via variational quantum approaches), and continuous constrained convex subproblems (that can be solved cheaply with classical optimization solvers). The validity of the approach is then showcased by numerical results obtained on several optimization problems via simulations with VQE on the quantum circuits implemented in Qiskit, an open-source quantum computing software development framework.
1:15PM B09.00011: Learning unitaries via gradient descent optimization  BOBAK KIANI, Mechanical Engineering, Massachusetts Institute of Technology, REEVU MAITY (Presenter), Physics, University of Oxford, SETH LLOYD, Mechanical Engineering, Massachusetts Institute of Technology — We study the learnability of unitary operations within the framework of the quantum alternating operator formalism using gradient descent method. Gradient descent algorithms are first order optimization methods which are of particular interest to the machine learning community due to their greater computational efficiency over second order techniques. However, the manifold of unitaries is non-convex in general and it is well known that gradient descent does not converge to the global minimum in such spaces. This motivates the question of how hard it is to learn a unitary with an alternating operator circuit using gradient descent. In this work, we find that gradient descent requires at least d^2 parameters in an alternating operator sequence to learn an arbitrary unitary in U(d) with a desired accuracy. The rate of convergence rapidly increases when gradient descent is performed in over-parameterized spaces greater than d^2. We heuristically argue the onset of a phase transition when gradient descent is performed on all d^2 parameters to learn a unitary. We present a greedy algorithm that can learn low-depth unitaries with much less than d^2 parameters in an alternating operator sequence. However, the success probability of the greedy algorithm is low.

1:27PM B09.00012: Practical demonstration of quantum approximate optimization on Google's superconducting qubit processor  MATTHEW HARRIGAN (Presenter), Google Inc. — The quantum approximate optimization algorithm (QAOA) has attracted significant interest as an algorithm suitable for noisy, intermediate-scale quantum (NISQ) computers. QAOA seeks to find approximate ground states of classical Hamiltonians, typically representing binary optimization problems. We demonstrate a practical implementation of QAOA on three problem families at various qubit counts and circuit depths. We show good performance at larger problem sizes and on more complicated problems than has been previously reported. We investigate practical considerations for implementing near-term quantum algorithms. QAOA is a hybrid algorithm involving a classical “outer-loop” optimizer to find optimal parameters. We profile traditional and novel classical outer-loop optimizers to minimize algorithm run-time in a real-world scenario.
Running large quantum circuits on small quantum computers

François-Marie Le Régent, Atos Quantum Lab, Argonne National Lab, Thomas Ayral (Presenter), Atos Quantum Lab, Zain Hamid Saleem, YuriAlexeev, Martin Suchara, Argonne National Laboratory — With the advent of NISQ computers, the question of running quantum programs whose number of qubits exceeds the capacity of today's small processors becomes pressing. In this work, we have implemented a recent theoretical proposal [1] consisting in splitting a large circuit into smaller fragments that can be run on smaller processors. As a test case, we have taken circuits used by the quantum approximate approximation algorithm (QAOA [2]) to solve combinatorial optimization problems. We have implemented, run and assessed the method on the IBM Poughkeepsie 20-qubit superconducting quantum processor, and have compared the obtained results with simulations in the presence of noise that we characterized via tomography.


Reverse engineering a pairwise entanglement witness for a near-term N-qubit computer

Nathan Thompson (Presenter), Nam Nguyen, Elizabeth Behrman, James Steck, Wichita State Univ — Designing and implementing new and general algorithms for the noisy intermediate scale quantum (NISQ) computers that will soon be available is not easy. In previous work we have suggested, and developed, the idea of using machine learning techniques to train a small quantum system such that the desired process is "learned," thus obviating the algorithm design difficulty. Here, we extend our results towards implementation on NISQ machines. We reverse engineer our learned two-qubit entanglement witness for implementation on Microsoft's Quantum Development Kit and IBM's Quantum Experience; and, using the machine learning technique called "bootstrapping", we infer the pattern for mesoscopic N from simulation results for three-, four-, five-, six-, and seven-qubit systems. The learned witness is robust to noise and decoherence. Our results suggest a fruitful pathway for general quantum computer algorithm design and computation.

Monday, March 2, 2020 11:15 AM - 12:39 PM

Session B10 GIMS: Advances in Scanned Probe Microscopy 2: High Frequencies and Optical Techniques

Christopher Lutz, IBM Research – Almaden - Tag(s): Focus
**11:15AM B10.00001: Measurement of fluorescent quantum yield using photothermal deflection spectroscopy**  
STEPHEN JOHNSON (Presenter), BRANDON T COUCH, ANDREW MEYER, BRANDON HELLER, Transylvania Univ — Photothermal deflection spectroscopy (PDS) is technique best known for its ability to measure weak optical absorptions various media. In this presentation we demonstrate an extended application for PDS, namely, measurement of the fluorescent quantum yield ($\Phi_f$) of fluorophores. Starting from first principles of energy conservation, a simple model for the photothermal deflection spectrum as a function of $\Phi_f$ is fit to the spectral data using $\Phi_f$ as a single fitting parameter. Using this method, extracted values of $\Phi_f$ for standard fluorophores such as Rhodamine 6G match closely with literature values. Given that this measurement technique requires no calibration standard, this method could potentially be used as a new standard procedure for determining $\Phi_f$ in fluorescent materials.

**11:27AM B10.00002: Imaging chiral optical excitations through inelastic electron-light scattering**  
TYLER HARVEY (Presenter), JAN-WILKE HENKE, OFER KFIR, CLAUS ROPERS, IV. Physicalisches Institut, University of Göttingen — Circular dichroism spectroscopy offers rich insight into biomolecular structure and nanoscale magnetic domain structure, but resolution is limited by the optical wavelength. We demonstrate a nanometer-resolution circular dichroism technique that employs electrons to probe optical near fields.

Electrons can exchange integer multiples of the photon energy with an optical field near a material [1,2]. The strength of the coupling between electron momentum states and photon number in the optical field depends on material structure and optical properties. Because sub-nanometer spotsize is routine in electron microscopes, this interaction can be employed to image optical fields with nanometer spatial resolution. By illuminating with left- and right-circularly polarized light and measuring the difference in coupling strength with electrons, we probe chiral optical near fields. This technique may enable the investigation of chiral optical and electronic states in plasmonic nanostructures, molecules and atoms with sub-nanometer spatial resolution.


*T.R.H. acknowledges support from the Alexander von Humboldt Foundation. The work is also supported by the German Science Foundation (DFG-SFB 1073/project A05).*
11:39AM B10.00003: Visualization of Surface Acoustic Wave by Transmission Mode Microwave Impedance Microscopy  LU ZHENG (Presenter), University of Texas at Austin, LINBO SHAO, Harvard University, QICHENG ZHANG, ALAN T JOHNSON, University of Pennsylvania, MARKO LONCAR, Harvard University, KEJI LAI, University of Texas at Austin — Surface acoustic wave (SAW) devices based on piezoelectric materials play a critical role in modern information technology and the research field of phononic metamaterials and quantum computing. High-resolution real-space mapping of the phononic modes is therefore of fundamental importance for the understanding of propagation, scattering, diffraction, and localization of the acoustic waves. However, it was challenging to image the GHz-range acoustic properties in piezoelectrics directly. Using a transmission-mode microwave impedance microscope (T-MIM), we demonstrate the ability to visualize SAW in multiple systems, including band-pass filter, resonator, and phononic crystals. Our results show that T-MIM can be used to locally probe acousto-electronic behaviors in various platforms with nanoscale spatial resolution.

11:51AM B10.00004: Experimental and numerical studies of near-field infrared phenomena at nanometer length scales*  P. MCARDLE (Presenter), D. LAHNEMAN, H. JIANG, M. M. QAZILBASH, Department of Physics, College of William and Mary, T. SLUSAR, H.-T. KIM, Metal-Insulator Transition Laboratory, Electronics and Telecommunications Research Institute, A. BISWAS, Department of Physics, University of Florida, F. KEILMANN, Fakultät für Physik & Center for NanoScience (CeNS), Ludwig-Maximilians-Universität, J. CHEN, Department of Chemistry and Biochemistry, University of Arkansas — Broadband near-field infrared spectroscopy is fast emerging as a valuable experimental probe of nanomaterials. Light-matter interactions in polaritonic materials at nanometer length scales can be probed effectively with this experimental technique. When there is strong coupling of light to the probe-sample system in highly polar materials such as insulating SrTiO₃, the phonon-polariton resonances should be described by detailed numerical simulations. More generally, experimental data needs to be accurately modeled to obtain optical properties at nanometer length scales in non-trivial geometries such as multilayered samples (for example, insulating SrTiO₃ crystal with metallic surface), and materials with physical boundaries comparable to the probe apex (for example, nano-platelets of Cu₂S). Near-field infrared spectra of materials with anisotropic dielectric function can also be modeled numerically (for example, rutile TiO₂). We will present our results on the materials described above, thereby establishing the efficacy of detailed numerical simulations for analyzing experimental spectra.

* M.M.Q. acknowledges support from ETRI and the National Science Foundation (NSF). Simulation work was performed, in part, using computing facilities at the College of William and Mary.

**Session B11 APS/SPS: Undergraduate Research III**

11:15AM B11.00001: Linear Optimum Filtering for Axion Dark Matter Search*

SUKHMANPREET SINGH (Presenter), Yale University — The Haloscope At Yale Sensitive To Axion CDM (HAYSTAC) Experiment is a microwave cavity search for cold dark matter (CDM) axions in the galactic halo. It attempts to detect a resonant photon signal produced by axion conversion in a magnetic field, the detection of which would provide useful insights on the nature of dark matter. Thus, the data acquisition from this experiment necessitates efficient filtering out of noise and other interfering signals, along with minimal scan times.

In this project, we present the theory and applications of linear optimum filters, namely the Wiener-Hopf and matched filters that minimize the mean-squared-error between processed and desired signals on MATLAB. By injecting random noise into an initially known signal, we present filtering techniques that allow us to perform the following three things: first, obtaining the best linear estimate of the desired signal \( d(n) \) from noisy data \( x(n) \); second, predicting a signal \( d(n+m) \) for \( m>0 \) from data \( x(n) \); and lastly, carrying out an a posteriori estimation of \( d(n+m) \) for \( m<0 \) from data \( x(n) \). By incorporating principles of optimization theory, this project helps speed up data analysis during the operation of the HAYSTAC experiment.

*I would like to thank Professor Steve Lamoreaux for funding this project.

11:27AM B11.00002: Simulation of Light Propagation Through CsI for the Mu2e Experiment

VICTORIA LLOYD (Presenter), Harvey Mudd College — The Mu2e experiment will search for charged lepton flavor violating neutrino-less conversion from a negative muon into an electron in the field of a nucleus. This reaction is extremely suppressed in the Standard Model of particle physics and an observation would be a clear sign of new physics. Mu2e plans to improve the current sensitivity on mu-to-e conversion by four orders of magnitude. The experiment relies on a crystal calorimeter to separate electrons from muons to reduce background. Using the Geant4 framework, we model the transit time taken by optical photons to reach the photomultiplier as a function of their origin for different crystal geometries. By cataloging these distributions, my project will improve the accuracy of the simulated time-of-flight data used to create the particle identification algorithms used in the experiment.
CONOR MCGIBBONEY (Presenter), ERIC BOOTH, Chemistry and Physics, Southeastern Louisiana University — The purpose of this research is to study the feasibility of Liquid Air Cycle Engines (LACE) and Air Collection and Enrichment System (ACES) for single stage to orbit (SSTO) space programs. Various thermodynamic properties such as Joule-Thomson, Para-to-Ortho with hydrogen, and general heat exchanger performance are used to determine feasibility on a fundamental theoretical level. For LACE we examined the condensation ratio (CR) kg air condensed by kg H\textsubscript{2} coolant used, and examined how much variations in pressure, as well as para-orthohydrogen conversion would aid heat-exchanger efficiency. No matter what is done, we cannot achieve a desired CR that is close to the needed stoichiometric ratio of 34.4. For ACES we examined CR with and without precooling with excess N\textsubscript{2}. Remarkably, precooling intake air with nitrogen worsens performance dramatically. The deficiency that causes ACES to be counterproductive is that, below 165 Kelvin, the proportional rise in the constant pressure heat capacity (Cp) of air is much greater than the proportional fall in the Cp of para-H\textsubscript{2}. Additionally, masses of system components needed for precooling and heat-exchange would need to be carried to space on the vehicle thus, further reducing efficiency.

11:51AM B11.00004: Search for Higgsino inside Large Hadron Collider via Vector Boson Fusion
CHENG TAO (Presenter), ALFREDO GURROLA, Physics, Vanderbilt University, ANDRES FLOREZ, NATHALIA CARDONA, Physics, University of Los Andes, PAUL DOUGLAS SHELDON, WILL JOHNS, Physics, Vanderbilt University — Supersymmetry (SUSY) is a theoretical extension of the standard model (SM) of particle physics that could describe the particle nature of Dark Matter (DM). In SUSY models assuming R-parity conservation, the lightest neutralino is neutral, stable, and interacts with SM particles in the early universe to give the DM relic density observed today. A Higgs-like neutralino (Higgsino) is known to be a promising candidate for DM. Current search methods for Higgsinos at the LHC mainly rely on Drell-Yan production mechanisms, however, are experimentally difficult in cases where the mass of the DM candidate is only slightly less than the masses of other neutralinos, making these so-called compressed spectrum Higgsino scenarios important search targets using new techniques. The focus of this talk is on the development of a search methodology for Higgsino DM at LHC using Vector Boson Fusion (VBF) processes, which offers an alternative and complementary search strategy. We combine the VBF topology with a final state of one and two soft leptons and large missing momentum. The requirement of one or two soft leptons combined with jets of large dijet mass can significantly reduce SM backgrounds, resulting in enhanced Higgsino discovery potential at the LHC.

*NSF Award PHY-1506406.
12:03PM B11.00005: Decoupling bosonic modes using sequential quantum transducers

SHOUMIK CHOWDHURY (Presenter), Yale University, MENGZHEN ZHANG, LIANG JIANG, Department of Molecular Engineering, University of Chicago — Quantum transducers are devices that can faithfully convert quantum signals from one mode to another. Building robust quantum transducers will be crucial to the development of hybrid quantum networks and scalable quantum computers. Previous studies have explored techniques to achieve perfect transduction using even imperfect transducers -- however, these methods either require infinite squeezing or apply only to the case of two modes. Here, we develop a new protocol that works for an arbitrary number of modes and requires only finite squeezing. Specifically, we show that by operating transducers in sequence, interspersed with appropriate single-mode operations, it is possible to decouple unwanted degrees of freedom and so reduce a three-mode transduction problem to the solved two-mode case. Furthermore, we investigate the dependence of the squeezing needed on the mode-coupling strength for a given transducer and propose some potential experimental setups.

*N/A

12:15PM B11.00006: Dark Count Reduction in Superconducting Nanowire Single Photon Detectors (SNSPDs)

HYUNSEONG KIM (Presenter), ANDREW MUELLER, Division of Physics, Mathematics and Astronomy, Caltech, BORIS KORZH, MATTHEW SHAW, Jet Propulsion Laboratory — Superconducting nanowire single photon detectors are the fastest single photon detectors with high detection efficiency, record time-resolution, and ultra-low dark count rate. However, for applications in dark matter search and quantum information, the dark count rate of SNSPDs must be further improved. In order to push these limits, we implemented a cryogenic differential bias-tee circuit, which filters high frequency noise from the current source and reduces electromagnetic noise coupling into the circuit thanks to a balanced architecture. We demonstrate that this differential architecture exhibits lower dark count rates compared to a single-ended device referenced to ground. We show, using a gaussian noise model, that the difference in dark counts for these two configurations can be attributed to electromagnetic noise.

*Caltech SURF Office, JPL Education Office, DOE, INQNET

12:27PM B11.00007: Etaloning Laser Interference Analysis Spectrometry (ELIAS)

JASON PORTER (Presenter), JAROM S JACKSON, DALLIN S. DURFEE, RICHARD SANDBERG, Brigham Young University — Many fields of research require precise wavelength measurement, but commercially available wavemeters are often too expensive, too large, or too fragile to be practical. We have designed and constructed a robust, compact, and inexpensive wavelength meter that analyzes the interference patterns caused by a series of etalon-like structures. Measuring this etaloning across a range of known wavelengths provides a set of wavelength-dependent reference functions which can be used to calculate an unknown wavelength within the same range. We present data showing that this device can measure a laser's wavelength with an average error less than a picometer, and a standard deviation less than 2 picometers.

*Funded by Brigham Young University.
**12:39PM B11.00008: Temperature dependence of the index of refraction of TOPAS cyclic olefin copolymer in the terahertz range**

TIMOTHY KRITZELL (Presenter), EVAN JASPER, YUFEI LI, NICHOLAS CRESCIMANNO, THUC MAI, REBEKAH SMITH, DANIEL HELIGMAN, MATTHEW T WARREN, Ohio State Univ - Columbus, FRANK C PEIRIS, Kenyon College, ROLANDO VALDES AGUILAR, Ohio State Univ - Columbus — Past measurements on the cyclic olefin copolymer TOPAS reveal a spectrally-flat refractive index within the terahertz range, giving the material exciting potential applications in optical apparatuses. Here we use THz spectroscopy to expand the understood frequency range, and as a probe to extract information regarding the temperature dependence of the refractive index, in which we find that the index of refraction increases with decreasing temperature. In hopes to understand this counterintuitive behavior, we report the temperature dependence of the reflectivity due to vibrational modes within the C-H band via Fourier-Transform Infrared Spectroscopy.

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**12:51PM B11.00009: Protonic Bipolar Semiconductor Melted Ice Periodic Lattice Model Explains the Abnormally High Electrical Mobility of Positive and Negative Ions in Pure Liquid Water.**

CINDY TIANHUI JIE (Presenter), Massachusetts Institute of Technology MIT, BIN JIE, CHIH-TANG SAH, Physics Department, Xiamen University — The mobility of positive and negative ions in pure liquid water are higher than impurity ions. This is not understood for 100+ years, but are accurately measured, tabulated in texts and manuals, and used in manufacturing. At the 2013 National Fall Meeting of the Chinese Physical Society, we proposed the melted-ice bipolar protonic semiconductor model to explain this high electrical mobility by drift-diffusion-generation-recombination-trapping of positive protons and negative prohols, including resolution of one protonic boson interacting with one protonic fermion. Our model extends the 1933 Bernal-Fowler Hexagonal Close Packed ice model, proven by 1935 Pauling residual entropy theory on Giauque specific heat measurements. Our 2013 idea arose from the many daily observed properties of nearly pure water, which suggest the persistent long-range-large-volume order when ice melts into liquid. This talk describes, in undergraduate language, the excellent agreement between our model and the three experimental properties of pure liquid water (the proton product or pH and the two protonic mobilities), by viewing the proton and prohol transport tracks through our atomic crystal lattice of pure water.

*TJ & BJ supported by CTSA.US, LLC, Florida, USA. BJ & CTS, partially supported by XMU.*
1:03PM B11.00010: Perturbation of Quantum Harmonic Oscillator and its effect on Quantum Electromagnetic Field Theory*  SANKARSHAN SAHU (Presenter), Indian Institute of Engineering Science and Technology, Shibpur — Here a special case of perturbation in quantum harmonic oscillator is studied. Here we assume the perturbed potential to be a Harmonic Oscillator that has been shifted in the position space. We construct the new creation and annihilation operators for the new Hamiltonian to find out its energy eigenstates. This paper mainly deals with why the coherent states provide a more complete picture of electric and magnetic field theory compared to just energy eigenstates. Here we find how our perturbation act as a coherent state generator and adds a new term in the Hamiltonian. The Perturbation is thought to arise from the only available interaction i.e. observation. The perturbation also explains how observation leads to coherence of photon states. We will find out how the new perturbation affects the time evolution of electromagnetic field. The Perturbation is also assumed to be instantaneous and time dependent such that sudden approximation can be applied in the time evolution of states. We also explain the results of the double slit experiment using our new mathematical model and thus try to come up with a new model for Quantum Mechanics.

1:15PM B11.00011: Revisiting the Wettability of Graphene*  CHRISTINA MCBEAN (Presenter), PRIYANKA MANCHANDA, PRATIBHA DEV, Howard University — Since its discovery in 2004, graphene has been the main focus of many researchers as they study its unique structure and properties. This two-dimensional, hexagonal carbon lattice has been proven to be a well-suited material for use in small molecule gas sensors, surface coatings, lubricants, etc. In studying the water wettability of graphene, studies first demonstrated that graphene is a hydrophobic material. However, more recent experiments have suggested that graphene is intrinsically hydrophilic. Based on the ambiguity of these conclusions, further studies must be done to find some clarity on the precise nature of the interactions between graphene and water. In this theoretical work, we use density functional theory to study the adsorption of water on graphene-based substrates and in the presence of ambient gases to determine surface water wettability of graphene.

*This work is supported by National Science Foundation under grant number DMR-1752840.

Monday, March 2, 2020 11:15 AM - 1:03 PM

Session B15 DFD DSOFT: Flow of Complex Fluids: Rheology, Structure, and Instabilities II  210/212 - Ehssan Nazockdast, Univ of NC - Chapel Hill
**11:15AM B15.00001: Cell nucleus as a microrheological probe to study the rheology of the cytoskeleton**  
EHSSAN NAZOCKDAST (Presenter), MOSLEM MORADI, Univ of NC - Chapel Hill —  
Mechanical properties of the cell are important biomarkers for probing its pathological changes, and are increasingly used for cancer diagnosis and detecting rare cells. Yet, determining the time-dependent contributions of different cellular components --including the cell membrane, the cell cytoskeleton and the nucleus-- to the mechanical response of the whole cell has remained challenging. We propose a novel method to decouple the mechanics of membrane and cytoskeleton, by analyzing the correlation between the membrane deformations that are induced by external microfluidic flows and nucleus displacements induced by those membrane deformations i.e. we use the nucleus as a microrheological probe to study the rheology of the interior cytoskeleton, independent of membrane rheology. To demonstrate the applicability of this method, we consider a proof of concept model consisting of a rigid spherical nucleus centered in a spherical membrane. We obtain analytical expressions for time-dependent nucleus velocity as a function of membrane deformations, when the interior cytoskeleton is modelled as a viscoelastic and a poroelastic material, and demonstrate how the nucleus velocity can be used to characterize the rheology of the cytoskeleton over a wide range of forces and time-scales.

**11:51AM B15.00002: The divergence-conforming immersed boundary method: Application to vesicles, capsules, and red blood cells under flow**  
HUGO CASQUERO (Presenter), YONGJIE JESSICA ZHANG, Carnegie Mellon Univ —  
The divergence-conforming immersed boundary (DCIB) method is presented to tackle a long-standing issue of immersed boundary (IB) numerical methods for fluid-structure interaction (FSI), namely, the challenge of accurately imposing the incompressibility constraint at the discrete level. In the DCIB method, the Eulerian velocity-pressure pair is discretized using divergence-conforming B-splines, which leads to \textit{inf-sup} stable, \textit{H}\textsuperscript{1}-conforming, and pointwise divergence-free Eulerian solutions. In order to discretize the higher-order derivatives that appear in vesicle and capsule formulations, we use \textit{C}\textsuperscript{2}-continuous cubic B-splines with periodic knot vectors and \textit{C}\textsuperscript{1}-continuous bi-cubic analysis-suitable T-splines in 2D and 3D settings, respectively. Non-negligible spurious changes of the fluid volume inside of closed co-dimension one solids is a well-known issue of IB methods. The DCIB method results in volume changes various orders of magnitude lower than conventional IB methods. Benchmark and application problems of vesicle, capsules and red blood cells are solved, including mesh-independence studies and comparisons with other numerical methods.

*PECASE Award N00014-16-1-2254 and NSF grant CBET-1804929*
12:03PM B15.00003: Flow-induced microstructural rearrangement and rheological consequences for model red blood cell suspensions in microvessels* YENG-LONG CHEN (Presenter), Inst of Physics Academia Sinica, CHIH-TANG LIAO, Engineering and System Science, National Tsing-Hua University — Flow-induced structural evolution of soft particle clusters in microflow is a key driver of non-Newtonian fluid response. We investigated how inter-particle attraction affect cluster and particle migration in microvessels, where the near wall particle depletion layers due to hydrodynamics significantly alters fluid viscosity. We found that strong particle aggregation correspond to structurally intact large clusters at low shear rates, resulting in large near wall depletion layer and low suspension viscosity. Shear-induced cluster break-up at moderate shear rates reduces the wall depletion layer, corresponding to viscosity increase akin to shear-thickening. At high shear rates, particle deformation and inter-particle ordering leads to shear-thinning.

*Ministry of Science and Technology, ROC
National Center for Theoretical Sciences, ROC
National Center for High Performance Computing, ROC

12:15PM B15.00004: Cross-stream migration of non-spherical particles in a second-order fluid SHIYAN WANG (Presenter), CHENG-WEI TAI, VIVEK NARSIMHAN, Purdue Univ — Particle migration in viscoelastic suspensions is vital in many applications in the biomedical community and the energy industries. Previous studies have provided insight on the motion of spherical particles in simple viscoelastic flows, yet the combined effect of more complex flow profiles and particle shapes is underexplored. Here, we develop approximate, analytical expressions for the polymeric force and torque on an arbitrary-shaped particle in a second-order fluid, subject to a general quadratic flow field. This model is exact for the case when the first and second normal stress coefficients satisfy \( \psi_1 = -2\psi_2 \). In shear driven flows, we observe that spheroidal particles adjust their orientation to align their longer axis along the vorticity direction, although significant deviations from slender body theories occur for finite aspect ratios. In pressure driven flows, we identify scaling theories to quantify how the particle lift depends on shape for a wide variety of shapes. We find that prolate particles slowly transition to a log-rolling state as they approach the flow center, with the lift initially being larger than that of an equal-volume sphere, but then becoming smaller as log-rolling emerges. Lastly, we extend our analysis towards more complicated systems (\( \psi_1 \neq -2\psi_2 \)).

12:27PM B15.00005: Vortices in 2D Colloids MYEONGGON PARK (Presenter), Ulsan Natl Inst of Sci & Tech, BO LI, Institute of Basic Science, STEVE GRANICK, Ulsan Natl Inst of Sci & Tech — Particles and molecules composing real materials generally contain anisotropic properties such as a spin or an electric dipole. To understand their roles in material phase states, we observed colloidal crystals comprised of Janus colloids whose anisotropic properties can be controlled. Here, we found a BKT transition by tuning an interparticle interaction and could see dynamics of topological defects in real time. We think that this model system can eventually give an insight to apprehend roles of molecular and atomic orientational dynamics in 2D crystal phases.
12:39PM B15.00006: On the mechanisms of superspreading*  PANAGIOTIS THEODORAKIS (Presenter), Institute of Physics, Polish Academy of Sciences, EDWARD SMITH, Mechanical and Aerospace Engineering, Brunel University London, ERICH A MÜLLER, Chemical Engineering, Imperial College London, RICHARD V CRASTER, Mathematics, Imperial College London, OMAR K MATAR, Chemical Engineering, Imperial College London — Superspreading is the rapid and complete spreading of surfactant-laden droplets on hydrophobic substrates, which is caused by certain surfactant molecules known as superspreaders. Despite significant experimental efforts, the precise mechanisms of this phenomenon and the characteristic properties of superspreading surfactants had remained elusive. Here, we report on extensive molecular dynamics simulations of a coarse-grained model based on the SAFT force-field. Our studies highlight the mechanisms of superspreading, the features of superspreading surfactants and a range of parameters that affect the spreading efficiency of surfactant-laden droplets. We anticipate that our investigations will pave the way for the design of molecular architectures tailored specifically for applications that rely on the control of wetting.

*This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No. 778104. E.A.M. acknowledges partial support from the Engineering and Physical Sciences Research Council (EPSRC) of the U.K. through grants EP/I018212, EP/J010502, and EP/R013152.

12:51PM B15.00007: Microfluidic flow-processing of soft matter systems  LIVA DONINA (Presenter), JOAO CABRAL, Imperial College London — Arguably one of the most striking properties of soft matter systems is the propensity to have a major response to minor perturbations. One of such perturbations is flow, which allows to induce phase changes and structural rearrangements. Here, two pseudo-quaternary systems containing sodium dodecyl sulfate (SDS) and medium to long chain alcohols as co-surfactants in a lamellar phase (Lα) are studied. The structural transformation from planar lamellar sheets to multilamellar vesicles (MLVs) is observed upon the application of shear stress to the solution. This transformation is characterised with nuclear magnetic resonance (NMR), rheology and small angle neutron scattering (SANS). Furthermore, the kinetics of the transformation is resolved with realtime measurements within a microfluidic device to obtain well-defined shear fields. Time-resolved kinetics are investigated by tracking the changes in birefringence pattern employing cross-polarised microscopy. The results point to MLV formation and indicate that it is a time-dependent and shear rate dependent process. The combination of microfluidics with high resolution spatio-temporal measurements allows characterisation of out-of-equilibrium transformations in complex surfactant mixtures.
11:15AM B16.00001: Readout of fluxonium qubits in circuit QED*  KONSTANTIN NESTEROV (Presenter), University of Wisconsin - Madison, LONG NGUYEN, AARON SOMOROFF, QUENTIN FICHEUX, IVAN PECHENEZHSKIY, University of Maryland, College Park, JEREMY STEVENS, NATHANAEL PIERRE COTTET, BENJAMIN HUARD, Ecole Normale Superieure de Lyon, VLADIMIR MANUCHARYAN, University of Maryland, College Park, MAXIM G VAVILOV, University of Wisconsin - Madison — In the idealized dispersive model of circuit QED, a single-shot heterodyne qubit measurement can be made as accurate as desired by increasing the power of the microwave drive. However, in realistic systems, populating the microwave cavity with photons can have many detrimental effects: in addition to nonlinear effects in the cavity itself, its photons can increase qubit relaxation and excitation rates, including excitations to noncomputational states. In addition, a high drive power can induce resonance transitions between qubit states. In this talk, we present the results of the simulation of the readout process in the fluxonium circuit and discuss how the qubit states and integrated readout signal are affected by the cavity occupation.

*We acknowledge funding from the U.S. Army Research Office (Grant No. W911NF-18-1-0146).

11:27AM B16.00002: Microwave-activated entangling gates for fluxonium qubits*  YINQI CHEN (Presenter), KONSTANTIN NESTEROV, University of Wisconsin - Madison, LONG NGUYEN, AARON SOMOROFF, QUENTIN FICHEUX, IVAN PECHENEZHSKIY, VLADIMIR MANUCHARYAN, University of Maryland, College Park, MAXIM G VAVILOV, University of Wisconsin - Madison — The main qubit transition of the superconducting fluxonium circuit in its flux sweet spot is characterized by a low frequency and very long coherence time, which reaches 500 μs [1]. At the same time, the transition between the first and second excited states of the fluxonium is comparable to those in transmons: it has an order of magnitude higher frequency and stronger coupling to a microwave field, but shorter lifetime. In this talk, we analyze and compare two-qubit gates between such qubits activated by driving different transitions in the two-qubit spectrum. In one scheme [2], the microwave drive is applied in resonance with a higher-frequency transition leading outside of the computational subspace. In the second scheme, which is similar to the cross-resonance gate with transmons [3], the microwave drive is applied at a low frequency to keep the system in the computational subspace. We calculate fidelity metrics for both gates with decoherence effects accounted for.


*We acknowledge funding from the U.S. Army Research Office (Grant No. W911NF-18-1-0146).

11:39AM B16.00003: Single-shot dynamics of fluxonium in the strong dispersive coupling regime  HAONAN XIONG (Presenter), YEN-HSIANG LIN, LONG NGUYEN, QUENTIN FICHEUX, AARON SOMOROFF, VLADIMIR MANUCHARYAN, University of Maryland, College Park — We report single-shot measurement of a fluxonium qubit in the strong dispersive regime with maximum coherence time T2>200usec. Our results set the stage for a variety of quantum optics experiments where a combination of very strong anharmonicity and long coherence is desirable. In particular, we investigate temporal dynamics involving multiple transitions of fluxonium in order to reveal new information about solid state decoherence mechanisms.
11:51AM B16.00004: Fluxonium two-qubit gate with simultaneous Raman transitions
JACOB BRYON (Presenter), ANDREI VRAJITOAREA, Princeton University, YIDAN WANG, PRZEMYSŁAW BIENIAS, REX LUNDGREN, RON BELYANSKY, ALEXEY V GORSHKOV, ALICIA KOLLAR, University of Maryland, ANDREW HOUCK, Princeton University — Quantum computing applications rely on high-coherence qubits with two-qubit gates to control them. The Fluxonium circuit is a superconducting qubit with favorable coherence properties, but unlike the transmon qubit, there has been no experimental demonstration of a two-qubit gate. We propose a new scheme using a cavity to couple two fluxonium qubits and drive a two-qubit swap gate. We report experimental progress towards driving simultaneous Raman transitions in the two qubits, utilizing the coupling cavity and the lambda energy level structure of fluxonium. This work expands the available coherent controls for the fluxonium circuit and increases its viability for quantum computing as well for interesting quantum simulation applications.

12:03PM B16.00005: High Coherence Fluxonium Qubits [invited] VLADIMIR MANUCHARYAN (Presenter), University of Maryland — Vlad Manucharyan has led the push to ever longer fluxonium coherence.

12:39PM B16.00006: Fast flux qubit gates on a heavy fluxonium* HELIN ZHANG (Presenter), SRIVATSAN CHAKRAM, NATHAN D EARNEST, YAO LU, University of Chicago, ZIWEN HUANG, DANIEL WEISS, JENS KOCH, Physics, Northwestern University, DAVID I SCHUSTER, University of Chicago — A capacitively shunted fluxonium qubit has both long life time and coherence time at the half-flux sweet spot. However, the suppressed matrix elements and low transition frequency make it challenging to perform fast fluxon gates via charge coupling. Here, we present schemes for state initialization, fast single-qubit flux gates, and plasmon assisted readout for a fluxonium qubit, demonstrating the feasibility of controlling a superconducting qubit at background temperatures much higher than the operating frequency. This scheme improves the quantum control of fluxonium qubits, making it a strong candidate for quantum information processing. We additionally present schemes for fluxonium two-qubit gates without using lossier higher levels.

*This work was supported by ARO Grant No. W911NF-15-1-0421; SUB0000079
Spectroscopy and logic gates in a strongly coupled two-fluxonium device*  
EBRU DOGAN (Presenter), DARIO ROSENSTOCK, Univ of Mass - Amherst, LONG NGUYEN, AARON SOMOROFF, VLADIMIR MANUCHARYAN, University of Maryland - College Park, CHEN WANG, Univ of Mass - Amherst — The fluxonium is one of the leading candidates as an upgrade to the mainstream transmon qubits in large-scale superconducting quantum processors: With stronger anharmonicity, longer coherence times and the ability to engineer selection rules, it has the qualities to in principle deliver better logic gate fidelity than transmons. Towards validating fluxonium as a viable qubit for scaling up, it is essential to go from one fluxonium to two or more; yet two coupled fluxoniums in various coupling regimes still remain to be better explored. Our experimental study focuses on two fluxonium qubits under strong capacitive coupling and we analyze the hybridization of computational states and higher excited states as a function of external flux bias. We also show that the ZZ coupling between two fluxonium qubits makes it straightforward to realize single and two qubit operations and report our progress on benchmarking single and two qubit gates.

*We acknowledge support from Army Research Office (ARO) Grant # W911NF1810146.

Fluxonium-like qubit design for improved coherence*  
PRANAV MUNDADA (Presenter), ANDREW HOUCK, ANDRAS GYENIS, Princeton University, ZIWEN HUANG, JENS KOCH, Northwestern University — Fluxonium qubits provide high anharmonicity and can offer states with disjoint support and large relaxation time. There has been significant progress in exploring different parameter regimes of the fluxonium for optimizing coherence times. However, in traditional fluxonium qubits, the external flux sweet spot is only present when external magnetic flux threading through the superconducting loop is either 0 or 0.5 flux quantum. Additional sweet spots can be achieved via the careful engineering of the Hamiltonian. We present experimental data on the implementation of such a fluxonium-like qubit architecture with extra sweet spots.

*Supported by Army Research Office Grant No. W911NF1910016

The Most Coherent Superconducting Qubit?  
AARON SOMOROFF (Presenter), LONG NGUYEN, YEN-HSIANG LIN, RAY MENCIA, NICHOLAS GRABON, QUENTIN FICHEUX, University of Maryland, College Park, KONSTANTIN NESTEROV, MAXIM G VAVILOV, University of Wisconsin - Madison, VLADIMIR MANUCHARYAN, University of Maryland, College Park — We report superconducting fluxonium qubits with coherence times limited by energy relaxation and reproducibly satisfying $T_2 > 100 \mu s$ ($T_2 > 400 \mu s$ in one device). Moreover, given the state-of-the-art values of the surface loss tangent and $1/f$ flux noise amplitude, coherence times can be further improved beyond 1 ms. Our results violate a common viewpoint that the number of Josephson junctions in a superconducting circuit - over $10^2$ here - must be minimized for the best qubit coherence. We outline how the combination of long coherence times and large anharmonicity unique to fluxonium can benefit both gate-based and adiabtic quantum computing.
Preparing and stabilizing entangled states is critical to many quantum information tasks, including autonomous quantum error correction. Inspired by previous dissipation-engineering schemes[1,2], we propose an autonomous protocol that prepares and stabilizes an arbitrary Bell state between a pair of superconducting qubits. This is achieved by parametrically coupling the superconducting qubits to each other, and to two dissipative baths that are made of low-Q resonators. The parametric couplings are engineered through the dynamical modulation of the qubit-qubit and the qubit-cavity interaction strengths at three different frequencies with appropriate phases. Numerical simulation shows that high fidelities of >95% are reached for all the Bell states, under realistic circuit parameters well-achievable by current circuit-QED technology. We further demonstrate how this scheme is fully compatible and can be experimentally realized on the VSLQ circuit[1].


*This work was supported by ARO Grant No. W911NF-17-S-0001.

We report our experimental progress towards the stabilization of an arbitrary Bell-state. We first describe our circuit implementation of the Very Small Logical Qubit [1] that substantially reduces operational complexity by reducing the number of RF drive lines and is fully compatible with the stabilization scheme. The circuit is composed of two superconducting qubits coupled through a small Josephson junction with a time-dependent flux bias and two low-Q resonators each coupled to the qubits. The experiment requires calibration of the static circuit parameters under DC flux biasing and mitigation of the flux cross-talks. Next, we demonstrate the generation of various sideband interactions required for the stabilization scheme by modulating the coupler using RF drives with appropriate frequencies, amplitudes, and phases. Finally, we compare our experimental results with the simulation and discuss the scope for further improvements. Our results pave the way towards the realization of the passively protected arbitrary logical qubit states from single-qubit error channels [1].


*This work was supported by ARO Grant No. W911NF-17-S-0001.
B16.00012: Towards high-fidelity quantum operations with fluxonium qubits: Part II—experimental progress  HSIANG-SHENG KU (Presenter), GENGYAN ZHANG, TENGHUI WANG, WENLONG YU, HAO DENG, JINGWEI ZHOU, YINGSHAN ZHANG, HANTAO SUN, ZHIJUN SONG, XIAOHANG ZHANG, CHENGCHUN TANG, RAN GAO, HUA XU, ZHISHENG LI, JIN QIN, XUN JIANG, XING ZHU, HUIHAI ZHAO, FENG WU, DAWEI DING, CHUNQING DENG, Alibaba Quantum Laboratory, Alibaba Group — Superconducting quantum circuits, controlled and readout by using RF electronics, have demonstrated the potential to outperform classical computers. The state-of-art multi-qubit superconducting circuits are capable of performing two-qubit gates with infidelity less than 1%. To further improve the precision of superconducting quantum processors, qubits with longer coherence times and larger anharmonicities are desirable. Fluxonium, created by introducing a large linear inductance, is a promising candidate for the next generation quantum processors. In this talk, we present the experimental progresses on developing fluxonium quantum processors. The fabrication process and measurement results on qubit operations and readout are discussed.

B16.00013: Towards high-fidelity quantum operations with fluxonium qubits: Part I—design and simulation  HSIANG-SHENG KU, GENGYAN ZHANG, TENGHUI WANG, WENLONG YU, HAO DENG, JINGWEI ZHOU, YINGSHAN ZHANG, HANTAO SUN, ZHIJUN SONG, XIAOHANG ZHANG, CHENGCHUN TANG, RAN GAO, HUA XU, ZHISHENG LI, JIN QIN, XUN JIANG, XING ZHU, HUI-HAI ZHAO (Presenter), FENG WU, DAWEI DING, CHUNQING DENG, Alibaba Quantum Laboratory, Alibaba Group — Superconducting quantum circuits, controlled and readout by using RF electronics, have demonstrated the potential to outperform classical computers. The state-of-art multi-qubit superconducting circuits are capable of performing two-qubit gates with infidelity less than 1%. To further improve the precision of superconducting quantum processors, qubits with longer coherence times and larger anharmonicities are desirable. Fluxonium, created by introducing a large linear inductance, is a promising candidate for the next generation quantum processors. In the talk, we present the design of fluxonium quantum processors. The simulation and optimization of the superconducting circuits and gates are discussed.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B17 DQI: Hybrid Systems - Electro-Optics, Superconductors, & Helium 203 - Joseph Kerckhoff, HRL Laboratories - Tag(s): Focus
**11:15AM B17.00001: Strong-coupling physics with semiconductor spin qubits** [Invited]  JASON PETTA (Presenter), Princeton University — Electron spins are excellent candidates for solid state quantum computing due to their exceptionally long quantum coherence times, which is a result of weak coupling to environmental degrees of freedom. However, this isolation comes with a cost, as it is difficult to coherently couple two spins in the solid state, especially when they are separated by a large distance. Here we combine a large electric-dipole interaction with spin-orbit coupling to achieve spin-photon coupling. Vacuum Rabi splitting is observed in the cavity transmission as the Zeeman splitting of a single spin is tuned into resonance with the cavity photon. We achieve a spin-photon coupling rate as large as $g_s/2\pi = 10 \text{ MHz}$, which exceeds both the cavity decay rate $\kappa/2\pi = 1.8 \text{ MHz}$ and spin dephasing rate $\gamma_s/2\pi = 2.4 \text{ MHz}$, firmly anchoring our system in the strong-coupling regime [1]. We next utilize spin-photon coupling to achieve a resonant spin-spin interaction between two spins that are separated by more than 4 mm [2]. An enhanced vacuum Rabi splitting is observed when both spins are tuned into resonance with the cavity, indicative of a coherent spin-spin interaction. Our results demonstrate that microwave-frequency photons can be used as a resource to generate long-range two-qubit gates between spatially separated spins.


*In collaboration with Felix Borjans, Guido Burkard, Xanthe Croot, Michael Gullans, Xiao Mi, Stefan Putz, Jacob Taylor, and David Zajac. Funded by ARO grant W911NF-15-1-0149 and the Gordon and Betty Moore Foundation's EPiQS Initiative through grant GBMF4535. Devices were fabricated in the Princeton University Quantum Device Nanofabrication Laboratory.*

**11:51AM B17.00002: Control and readout of superconducting qubits over optical fiber using cryogenic photonic links**  JOHN TEUFEL (Presenter), FRANKLYN QUINLAN, FLORENT LECOCQ, SCOTT ALAN DIDDAMS, JOSE AUMENTADO, National Institute of Standards and Technology Boulder — As superconducting quantum circuits continue to increase in size and complexity, one bottleneck for scaling becomes the large number of microwave signals lines that must connect room temperature electronics to the cryogenic environment of the device. Typical experiments require multiple coaxial cables per qubit, each heavily filtered and attenuated to ensure excess noise will not degrade qubit coherence, gate fidelity or measurement efficiency. An alternative to this brute force method is to use optical fiber and cryogenic high-speed photodetection as an optical-to-microwave converter, capable of generating shot-noise limited microwave signals directly at millikelvin temperatures. Leveraging the low thermal conductivity, low loss and large intrinsic bandwidth of optical fiber would allow for efficient, massively multiplexed delivery of coherent microwave control pulses. In this talk we will present recent experimental progress toward the control and readout of a superconducting qubit using microwave signals transmitted over optical fiber to the ultracryogenic environment (< 20 mK), and show proof of principle results that this novel method can meet the stringent requirements for superconducting quantum information processing.
12:03PM B17.00003: A Lithium Niobate Electro-Optic Transducer for Quantum Networks
TIMOTHY MCKENNA (Presenter), JEREMY WITMER, RISHI PATEL, JASON F HERRMAN, WENTAO JIANG, PATRICIO ARRANGOIZ-ARRIOLA, EDWARD A WOLLACK, RAPHAEL VAN LAER, AMIR SAFAVI-NAEINI, Stanford University —
In order to create a quantum network in which superconducting qubit processors are connected over kilometer-scale distances, transducers capable of converting quantum information between microwave and optical frequencies are required to allow for fiber optical networking. We present the design and experimental demonstration of an electro-optic photon converter to connect superconducting qubit-based systems with light. We fabricate lithium niobate racetrack resonators with superconducting circuits and demonstrate microwave-to-optical photon coupling rates over 1.5 kHz at cryogenic temperatures. We characterize our transducer with resolved sideband spectroscopy to measure the electro-optically generated Stokes and anti-Stokes optical sidebands which show an extinction ratio of ~30 dB.

12:15PM B17.00004: Microwave-to-optical transduction in a silicon-organic-hybrid platform
JEREMY WITMER (Presenter), TIMOTHY MCKENNA, PATRICIO ARRANGOIZ-ARRIOLA, EDWARD A WOLLACK, RISHI PATEL, RAPHAEL VAN LAER, AMIR SAFAVI-NAEINI, Stanford Univ — In order to realize long distance quantum networks in which superconducting quantum processors are connected by optical fiber links, it is necessary to transduce quantum signals from the microwave domain to the optical domain and vice versa. Here, we present progress towards electro-optic photon conversion using a silicon-organic hybrid photonic platform. Our device uses a high-Q photonic crystal cavity and superconducting microwave resonator to simultaneously confine optical and microwave electric fields. We achieve a room temperature electro-optic tuning rate of 3.7 pm/V and demonstrate microwave-to-optical photon conversion in a milliKelvin dilution fridge environment. Our device provides nearly 10 dB selectivity between the generated Stokes and anti-Stokes sidebands, which we can resolve using a heterodyne spectroscopy technique. Finally, we examine the deleterious effects of quasiparticle generation due to stray light and discuss techniques to mitigate this.
Dispersive sensing of electron tunneling between quantum dots in proximitized InAs nanowires

DAMA DE JONG (Presenter), DAAN WAARDENBURG, Delft University of Technology, NEJC BLAZNIK, Utrecht University, LIN HAN, FILIP MALINOWSKI, CHRISTIAN PROSKO, JASPER VAN VEEN, Delft University of Technology, PETER KROGSTRUP, Center for Quantum Devices and Microsoft Quantum Lab Copenhagen, Niels Bohr Institute, University of Copenhagen, LEO P KOUWENHOVEN, WOLFGANG PFAFF, Microsoft Quantum Lab Delft, Delft University of Technology — Dispersive gate sensing (DGS) is a powerful technique that has enabled novel ways for probing condensed matter systems and reading out solid-state quantum bits, such as Josephson or spin qubits. DGS has also been proposed for the measurement of topological qubits based on Majorana zero-modes (MZMs). Such a measurement can be realized by detecting parity-dependent electron tunneling through a superconducting island hosting MZMs at its ends. Here, we demonstrate tunneling between two quantum dots separated by a superconducting island realized in an InAs nanowire, partially proximitized by Al. Using multiplexed coplanar waveguide resonators with tailored circuit parameters we can simultaneously detect tunneling between multiple quantum dots with high SNR to correlate tunneling events with sub-microsecond resolution. The resonator response depends -via the tunneling rate between the quantum dots- on the superconducting spectrum, and in particular on the presence of MZMs in the island. Importantly, dispersive readout allows the system to be probed in the floating regime without transport channels. This will be crucial for fast, non-invasive detection of the topological state of superconducting islands and parity readout of topological qubits.

A gate-tunable, field-compatible fluxonium*

MARTA PITA-VIDAL (Presenter), ARNO BARGERBOS, QuTech, Delft University of Technology, CHUNG-KAI YANG, DAVID J. VAN WOERKOM, WOLFGANG PFAFF, Quantum Lab Delft, Microsoft, NADIA HAIDER, Netherlands Organisation for Applied Scientific Research (TNO, PETER KROGSTRUP, Quantum Materials Lab Copenhagen, Microsoft, LEO P KOUWENHOVEN, GIJS DE LANGE, ANGELA KOU, Quantum Lab Delft, Microsoft — Hybrid superconducting circuits, which integrate non-superconducting elements into a circuit quantum electrodynamics (cQED) architecture, expand the possible applications of cQED and provide new insights into mesoscopic superconductivity. Extending the capabilities of hybrid flux-based circuits, which provide access to current-phase relations, to work in magnetic fields would be especially useful both as a probe of spin-polarized Andreev bound states and as a platform for topological qubits. Here, we present a new hybrid circuit: a magnetic-field compatible fluxonium with an electrostatically-tuned semiconducting nanowire as its non-linear element. We demonstrate in-situ gate-control of the Josephson energy of the fluxonium over more than an order of magnitude. We also operate the fluxonium in magnetic fields up to 1T, where we observe the anomalous Josephson effect. This combination of gate-tunability and field-compatibility opens avenues for the exploration and control of spin-polarized phenomena using superconducting circuits and enables the use of the fluxonium as a readout device for topological qubits.

*Research co-funded by the allowance for Top consortia for Knowledge and Innovation (TKI’s) from the Dutch Ministry of Economic Affairs and the Microsoft Quantum initiative.
The physics of conventional and exotic superconductors can be probed through their microscopic quasiparticle excitations. Recent advances in mesoscopic superconductor-semiconductor devices have created the opportunity to measure and control such excitations, such as Majorana zero modes in a topological superconductor regime. Here, our mesoscopic device is a Josephson element with an InAs nanowire weak link. Due to spin-orbit coupling in the nanowire, the spin states of a single quasiparticle trapped in the junction’s Andreev levels exhibit microwave-accessible energy splittings without an applied magnetic (Zeeman) field. This “superconducting spin” is readily coupled to a microwave resonator via its spin-dependent supercurrent. We will present our experimental platform demonstrating large spin-dependent dispersive shifts of a microwave resonator. We achieve single-shot, quantum-non-demolition readout of the spin as well as coherent manipulation of the quasiparticle state. We will discuss the real-time dynamics of the quasiparticle, which have implications for Majorana devices and Andreev spin qubits. In this first part of a joint presentation, we will present the background, experimental setup, and a theoretical model for our system.

*Work supported by: ARO, ONR, NSF, and AFOSR.
**1:03PM B17.00008: Dynamics and manipulation of a trapped, superconducting quasiparticle: Part 2/2**

MAX HAYS (Presenter), VALLA FATEMI, Applied Physics, Yale University, DANIËL BOUMAN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, KYLE SERNIAK, SPENCER DIAMOND, TOM CONNOLLY, GIJS DE LANGE, Applied Physics, Yale University, PETER KROGSTRUP, JESPER NYGÅRD, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, ATTILA GERESDI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, MICHEL H. DEVORET, Applied Physics, Yale University — The physics of conventional and exotic superconductors can be probed through their microscopic quasiparticle excitations. Recent advances in mesoscopic superconductor-semiconductor devices have created the opportunity to measure and control such excitations, such as Majorana zero modes in a topological superconductor regime. Here, our mesoscopic device is a Josephson element with an InAs nanowire weak link. Due to spin-orbit coupling in the nanowire, the spin states of a single quasiparticle trapped in the junction's Andreev levels exhibit microwave-accessible energy splittings without an applied magnetic (Zeeman) field. This “superconducting spin” is readily coupled to a microwave resonator via its spin-dependent supercurrent. We will present our experimental platform demonstrating large spin-dependent dispersive shifts of a microwave resonator. We achieve single-shot, quantum-non-demolition readout of the spin as well as coherent manipulation of the quasiparticle state. We will discuss the real-time dynamics of the quasiparticle, which have implications for Majorana devices and Andreev spin qubits. In this second part of a joint presentation, we will describe the experimental data and discuss its outlook.

*Work supported by: ARO, ONR, NSF, and AFOSR

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**1:15PM B17.00009: Resonant phenomena in a microchannel-confined Wigner solid**

NIYAZ BEYSENGULOVA (Presenter), JUSTIN LANE, Michigan State Univ, DAVID G REES, EeroQ Inc., KOSTYANTYN NASYEDEKIN, TARYN V STEFANSKI, MARK DYKMAN, JOHANNES POLLANEN, Michigan State Univ — Collective excitations of an electron solid on the surface of liquid helium coupled to a bosonic field of surface capillary waves (ripplons) manifest in pronounced radio-frequency (RF) resonances that are detectable via transport. Theses coupled plasmon-ripplon resonances are modified in the presence of strong transversal confinement of the electron system, which can be realized in microchannel devices. We present new experimental results on the resonant response of electrons on helium confined in a single microchannel device and subjected to RF irradiation. The RF excitation causes heating of the electron system, which leads to a weakening of the Bragg-Cherenkov mobility limit. Additionally, we find that the nonlinear electron transport is modulated by the RF driving field and gives rise to a series of new resonant features. The origin of these resonances will be discussed. Understanding of the electron-ripplon dynamics and decoherence mechanisms in these hybrid devices will be essential for quantum information processing with electrons on helium.

*This work was supported by the NSF under Grant no. DMR-1708331.
**1:27PM B17.00010: Dynamical coupling of surface acoustic waves to electrons on helium**

HEEJUN BYEON (Presenter), KOSTYANTYN NASYEDKIN, NIYAZ BEYSENGULOV, JUSTIN LANE, BAOKANG BI, JOHANNES POLLANEN, Michigan State Univ — We report on the dynamical coupling between high-frequency piezoelectric surface acoustic waves (SAWs) and a two-dimensional (2D) system of electrons floating on liquid helium. This coupling leads to a reduction in the velocity of the SAW and attenuation of SAW energy, which reflects the high-frequency, wavevector-dependent conductivity of 2D electron sheet. In our device, a piezoelectric substrate incorporates a micro-channel array filled with superfluid helium above which a 2D ensemble of electrons are trapped. Underlying electrodes capacitively couple to the electron system and are used to control the areal density of electrons. Employing pulsed time-of-flight SAW techniques, we measure the attenuation and the velocity shift of SAWs as function of electron density at \( T = 1.5 \) K where the electron system is in liquid state. We also present SAW response near the phase transition regime from the electronic liquid to the Wigner crystal.

*This work is supported by the NSF (Grant no. DMR-1708331).

**1:39PM B17.00011: Dispersive readout of qubit states: towards realizing spin qubits using electrons on helium**

ERIKA KAWAKAMI (Presenter), ASEM ELARABI, DENIS KONSTANTINOV, Okinawa Inst of Sci & Tech — Electrons on the surface of liquid helium present an extremely clean two-dimensional electron system. Thanks to its cleanness, the quantum states of the electrons on helium are expected to have a long relaxation time, which provides a perfect platform to realize qubits with [1]. In particular, spin states are expected to have an extremely long relaxation time: \( T2 \sim 100 \) s [2].

Recently, we propose and experimentally demonstrate a new readout technique for the hydrogen-like quantized states (Rydberg states) of many electrons on helium [3]. This new technique was inspired by the dispersive readout technique used in semiconductor quantum dots [4] and in Penning traps [5]. Currently, we are working on the measurement of the relaxation time of the Rydberg state of the electrons on helium using this technique. We also show that this technique can potentially be used to detect spin states of a single electron by introducing an interaction between the Rydberg states and the spin states.

Superfluid helium is an extremely low-loss dielectric, an excellent thermal conductor, and harbors many unique collective excitations, making it an attractive candidate to incorporate into superconducting qubit systems. We controllably immerse a three-dimensional superconducting transmon qubit in superfluid 4He and measure the spectroscopic and coherence properties of the system. We find that the cavity, the qubit, and their coupling are all modified by the superfluid, which we analyze within the framework of circuit quantum electrodynamics (cQED). At temperatures relevant to quantum computing experiments, the energy relaxation time of the qubit is not significantly changed by the presence of the superfluid, while the pure dephasing time modestly increases, which we attribute to improved thermalization of the microwave environment via the superfluid.

*The Michigan State portion of this work was supported by the Cowen Family Endowment and by the NSF (Grant no. DMR-1708331). The Washington University portion of this work was also supported by the NSF (Grant no. PHY-1607156 and PHY-1752844 (CAREER)).

**Monday, March 2, 2020 11:15 AM - 2:15 PM**

**Session B18 DBIO FED: Bringing Together Biology, Medicine, and Physics in Education** 205 - Phil Nelson, University of Pennsylvania - Tag(s): Careers, Education, Invited, Undergrad Friendly
11:15AM B18.00001: What do 21st century biology students need to know and be able to do? The view from biology education research* [Invited] MICHELINE SMITH (Presenter), Cornell University — Many STEM undergraduate students take biology and physics courses, so it is important for both disciplines to understand what is happening in the other classrooms. When people picture undergraduate biology classrooms, they often think about students memorizing disconnected bits of information and repeating classic findings in cookbook labs. However, biology education is undergoing a revolution and today's classrooms look different from this stereotypical view. Transformed biology classes are emphasizing core concepts and skills that are described in reports supported by the major funding agencies and biological professional societies. Concepts are being integrated across subfields of biology and instructors are encouraged to explore them along a continuum from a single cell to a whole ecosystem. Laboratory courses have also changed; undergraduate students are exploring novel research questions and contributing data to advance the field. New assessment instruments that span multiple time points, including across the entire duration of the undergraduate program, are being used to motivate faculty to discuss and come to agreement on the essential learning outcomes of their program and consider how students will achieve these outcomes regardless of the specific courses they take. Notably, instructors are publishing their innovative lessons in peer-reviewed journals such as CourseSource and contributing to broader discipline-based education research questions. In this talk, I will explore what transformed biology education looks like and discuss connections with the skills learned in undergraduate physics classrooms. I will also explore how research on critical thinking conducted in undergraduate physics classrooms is directly affecting how we are studying the student experience in undergraduate biology field courses.

*This material is based on work supported by the National Science Foundation under grant nos. DUE-1725130 and DUE-1909602
11:51AM B18.00002: Transform and Thrive: Large-Scale Change in Introductory Physics for the Life Sciences* [Invited] LAURIE MCNEIL (Presenter), Univ of NC - Chapel Hill — The number of undergraduate degrees in biological sciences awarded each year exceeds the number of degrees awarded in physical sciences and engineering combined, so teaching introductory physics for the life sciences (IPLS) is a substantial part of a physics department’s responsibilities. Before Fall 2012 my department taught a very traditional (and not very effective) IPLS lecture/lab sequence that covered the same topics as our physical science sequence but in less depth. By Fall 2015 we were teaching a new sequence that incorporates physics education research (PER) findings and includes a range of physics topics important to the life sciences, such as diffusion, non-linear stress/strain, and nerve signal propagation. We accomplished this with a team of PER experts, PER users, biologists, chemists, and grad students (plus funding from NSF and AAU). We now teach all ~600 students who enroll in IPLS each semester this way, with much more success. The sequence is fully institutionalized, and faculty members routinely rotate through it. I will describe how we accomplished this transformation, the benefits (and difficulties) it affords, and offer advice to departments contemplating a similar reformation.

*Funding: NSF DUE-1323008 and AAU Undergraduate STEM Education Initiative

12:27PM B18.00003: Pre-health students may not know what physics is. [Invited] ALISON SWEENEY (Presenter), Department of Physics, Yale University — Unlike in introductory chemistry or biology courses, pre-health students in introductory physics courses often don't know the premise or purpose of the discipline. Popular stories about, e.g., black holes and quantum computing don't provide a route for lay observers to understand how these topics share fundamental rules about forces and energies, expressed mathematically. About half of U.S. high schools don't offer physics courses, and many that do exist teach a qualitative version of the subject rather teaching than the process of physical abstraction. As high-resource universities and physics departments continue the necessary work of diversifying their student bodies, it is important for us to recognize this divide, potentially new to our classrooms, and learn to teach to it. The traditional approach of diving into mathematically-motivated formalism at the beginning of the course will often leave the least-prepared students, who are most important to reach, bewildered and alienated. This talk discusses my experience and possible insights from reforming a traditional pre-health physics course, to teach the conceptual core of physics to students completely inexperienced with physics. For example, explicitly addressing questions such as "what is an equation in physics, and what is it for?", and initially prioritizing form equally with content in student work, have been helpful measures.
The Purpose of Homework Problems is Insight, Not Numbers: Crafting Exercises for an Intermediate Biological Physics Class [Invited]  
BRADLEY ROTH (Presenter), Oakland University — Richard Hamming famously said “The purpose of computing is insight, not numbers.” This view is true also for homework problems in an intermediate-level physics class. I constantly tell my students “an equation is not something you plug numbers into to get other numbers; it tells a story.” I will use examples from courses in Biological Physics and Medical Physics to illustrate this idea. A well-formed homework problem must balance brevity with storytelling. Often the problem is constructed by creating a “toy model” of an important biological system, and analysis of the toy model reveals some important idea or insight. A collection of such problems becomes a short-course in mathematical modeling as applied to medicine and biology, which is a skill that needs to be cultivated in biology majors, pre-med students, and anyone interested in using physical and mathematical tools to study biology and medicine.

Essential data science instruction for biophysicists [Invited]  
JUSTIN BOIS (Presenter), Division of Biology and Biological Engineering, Caltech — Biological physicists, along with researchers across nearly all biological sciences, obtain quantitative data in their experiments. Much of our training of students focuses on theoretical modeling of the phenomena underlying the measurements, often with state-of-the-art physics. As a necessary complement to this training, we should teach students how to manage their data sets and perform statistical inference using state-of-the-art techniques from the rapidly developing fields of data science and applied statistics. In this talk, I will discuss what I view as essential data science principles we should teach students. These are:

**Software development**: Modern principles including version control and test-driven development.

**Validation**: Ensuring that a data set from the data source meets expectations (format, missing values, etc.).

**Wrangling**: The process of converting data from the source to a more readily usable format.

**Preservation and sharing**: Strategies for long-term storage and easy sharing of data.

**Visualization**: Construction of instructive plots and interactive data displays.

**Bespoke statistical modeling**: Statistical inference custom built for the specific experiment, as opposed to off-the-shelf techniques.

I will discuss my approach to teaching these topics using hands-on, team-based analyses of real biological data sets.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B19 GMAG: Skyrmions in Oxide Materials and Heterostructures 207 - Kai Liu, Georgetown University - Tag(s): Invited
11:15AM B19.00001: Harsh condition scanning probe microscopy vs. imaging detection of new magnetic structures and their topological protection [Invited]  QINGYOU LU (Presenter), University of Science and Technology of China — The scanning probe microscope has atomic resolution, which is a revolution in microscopy. But, it is sensitive to even weak vibration or sound (V/S) and requires well designed V/S isolation. However, many important researches must be performed in harsh conditions such as in ultra-strong water-cooled magnet (WM), cryogen-free (dry) superconducting magnet, dilution refrigerator or reactive solution. To this end, we have achieved high quality atomic resolution images in harsh and ultra-harsh conditions. Finally, we are successful in obtaining high clearance atomic resolution images in a WM [Ultramicroscopy 205(2019)20], dry magnet [Nano Res. 8(2015)3898] and active/reactive solution [Nano Res. 9(2016)2551; Nanoscale 8(2016)15142]. We will report these achievements as well as their applications in the imaging detections of new and weak magnetic structures with topological protection such as magnetic skyrmions in ultra-thin (only 5 layers of unit cells) oxide heterostructures BTO/SRO [Nature Mater. 17(2018)1087], artificially fabricated skyrmions [Adv. Funct. Mater. (2019)1907140], structural domain walls [Adv. Mater. 30(2018)1805353], multiply ordered electronic crystals [ACS Appl. Mater. Inter. 10(2018)20136] and phase competition in re-entrance process [Nature Comm. 6(2015)8980].


12:27PM B19.00003: Spin-Hall topological Hall effect in highly tunable Pt/ferrimagnetic-insulator bilayers* [Invited]  FENGYUAN YANG (Presenter), Ohio State Univ - Columbus — Electrical detection of topological magnetic textures such as skyrmions has been limited to conducting materials. Magnetic insulators offer key advantages for skyrmion technologies with high speed and low loss. We observe a prominent topological Hall effect in Pt/Tm$_3$Fe$_5$O$_{12}$ bilayers, where the pristine Tm$_3$Fe$_5$O$_{12}$ epitaxial films down to 1.25 unit cell thickness allow for tuning of topological Hall stability over a broad range from 200 to 465 K through atomic-scale thickness control [1]. Although Tm$_3$Fe$_5$O$_{12}$ is insulating, the topological magnetic textures can be detected through a novel phenomenon: “spin-Hall topological Hall effect” (SH-THE), where the interfacial spin-orbit torques allow spin-Hall-effect generated spins in Pt to experience the unique topology of the underlying skyrmions in Tm$_3$Fe$_5$O$_{12}$. This novel electrical detection phenomenon paves a new path for utilizing a large family of magnetic insulators in future skyrmion technologies.


*This work was primarily supported by DARPA under Grant No. D18AP00008. Partial support was provided by the Center for Emergent Materials, an NSF-funded MRSEC, under Grant No. DMR-1420451 for the bulk synthesis and film growth of TmlG.
1:03PM B19.00004: Observation of room temperature polar skyrmions

RAMAMOORTHY RAMESH (Presenter), University of California, Berkeley — Complex topological configurations are a fertile playground to explore novel emergent phenomena and exotic phases in condensed-matter physics. For example, the recent discovery of polarization vortices and the associated complex-phase coexistence and response under applied field in superlattices of (PbTiO3)n/(SrTiO3)n suggests the presence of a complex, multi-dimensional system capable of exotic physical responses. I will describe the discovery of polar skyrmions in a lead-titanate layer confined by strontium-titanate layers by atomic-resolution scanning transmission electron microscopy (STEM). Phase-field modeling and second-principles calculations reveal that the polar skyrmions have a skyrmion number of +1 and resonant soft X-ray diffraction experiments show circular dichroism confirming chirality. Such nanometer-scale polar skyrmions exhibit a strong signature of negative permittivity at the surface of the skyrmion, which is furthermore highly tunable with an electric field. They are a new state of matter and electric analogs of magnetic skyrmions, and may be envisaged for potential applications in information technologies. I will attempt to describe the exciting observations we have made through many collaborations.

*This work is supported by the US Department of Energy, Office of Science, Basic Energy Sciences.

1:39PM B19.00005: Nonequilibrium Skyrmion Dynamics under Oscillating Magnetic Fields

CHRISTINA PSAROUDAKI (Presenter), Physics, California Institute of Technology, DANIEL LOSS, Physics, University of Basel — We extend earlier studies on the quantum propagation of a skyrmion in chiral magnetic insulators [1], to include the effects of time periodic magnetic field gradients on skyrmion dynamics [2]. The unavoidable coupling of the external field to the magnons gives rise to time-dependent dissipation for the skyrmion, with measurable consequences on the skyrmion path. These ac fields act as a net driving force on the skyrmion via its own intrinsic magnetic excitations. We generalize the standard quantum theory of dissipation to include the stochastic effects of the driven bath on the skyrmion dynamics. We address the stochastic effects of the quantum driven bath on the skyrmion propagation [3], and provide a generalized version of the nonequilibrium fluctuation-dissipation relation for externally driven reservoirs. We also predict a novel fast thermal activation for the mean-square displacement that scales quadratically with temperature in the experimentally accessible low-temperature regime.


Monday, March 2, 2020 11:15 AM - 1:51 PM

Session B20 DBIO DCOMP: Physics of Proteins: Progress on Structure-Function Relationships II 301 - Wouter Hoff, Oklahoma State University-Stillwater - Tag(s): Focus
Proteins are commonly believed to be insulators, consistent with their appearance and the results of simple measurements. This is in line with the expected behavior of a disordered, wide bandgap solid with strong vibronic coupling. Yet some soil bacteria transfer electrons via thin protein filaments with near-metallic conductivities. Are they a special case? Motivated by calculations that indicate that many proteins have evolved towards a quantum critical structure\textsuperscript{1} we decided to measure the conductance of single molecules of proteins chosen precisely because they lack redox centers and lack any known electron transfer function. Unique to our approach is the use of specific chemical bonding between proteins and electrodes to minimize the effects of contact resistance.\textsuperscript{2} We find that nS conductances over distances of many nm are common. The conductance is limited by contacts, with very long electronic decay lengths inside the protein.\textsuperscript{3} What biological pressure could drive evolution towards this unlikely state? We have studied a functioning DNA polymerase, finding large changes in its internal conductance as it undergoes functional changes in conformation. This suggests a possible role for delocalized states in function. It also points to a new method for DNA sequencing based on direct electrical measurement of enzyme function.\textsuperscript{4}


*This work was supported by grants HG006323 and HG010522 from the National Human Genome Research Institute, by Recognition AnalytiX Corp and the Edward and Nadine Carson Endowment.

Nearly 150,000 of protein structures have been reported using X-ray crystallography, NMR technologies, and more recently cryogenic electron microscopy (Cryo-EM). Many of these structures played indispensable roles in our understanding of protein function. Then why do we need time-resolved infrared structural biology for proteins? Infrared structural biology is an emerging technology that offers unique advantages. Based on the 3D structure of a protein, can the functional mechanism of this protein be fully explained? In my talk, I will discuss important challenges we are facing in protein structural biology, and how to overcome some of these challenges using time-resolved infrared structural biology of proteins. More importantly, time-resolved infrared structural biology can bring new insight to the study of many proteins.

*Financial supports from National Science Foundation (DBI 1338097) and Oklahoma Center for the Advancement of Science and Technology (HR10-078) are greatly appreciated.
12:27PM B20.00003: Domain Swapping in Crystallin Proteins Can Drive Early Stages of Cataract Formation  GOVARDHAN PATLURI (Presenter), Indian Institute of Science — Crystallins (Crys) are densely packed, long-lived eye lens proteins responsible for the ocular functions of the lens. Physicochemical perturbations in the cellular environment disrupt the native state stability of Cry proteins and populate aggregation prone misfolded states. These misfolded states gradually accumulate to produce high molecular weight amorphous aggregates, which scatter visible light resulting in lens opacity or cataract. The molecular mechanism of cataract formation or structure of these aggregation prone precursors remain elusive to date. Using molecular dynamics simulations and coarse-grained protein model of human γC and γD Crys, we identified the aggregation prone misfolded states present in the unfolding pathways of these proteins. We further show that these partially misfolded conformations readily undergo dimerization by domain swapping revealing the early stages of aggregation leading to cataract formation.

12:39PM B20.00004: Evaluating molecular simulations of protein dynamics using novel experimental data  LAUREN MCGOUGH (Presenter), University of Chicago, JUSTIN KIM, EUGENE KLYSHKO, University of Toronto, RAMA RANGANATHAN, University of Chicago, SARAH RAUSCHER, University of Toronto — Proteins are evolved molecular machines that carry out the essential chemical reactions necessary for life. Like machines designed by humans, proteins execute their functions through an orderly set of motions and fluctuations - their “reaction coordinate”. However, proteins are also marginally stable, with the expectation that functional dynamics are embedded in a small subspace of a high dimensional pattern of overall motions and configurational changes. One approach to studying intramolecular fluctuations is computational simulation of atomic trajectories using molecular dynamics. Recent advances in experimental protein dynamics now open up the ability to test, validate, and possibly improve the process of molecular dynamics (MD) simulations through direct comparisons between computational predictions and data. We present a comparative analysis between MD and experiment using data from X-ray diffraction studies reporting electric field-stimulated excited state motions. The analysis develops methods for simulating a protein crystal while carrying out rigorous evaluations of structural conformation ensembles, atomic strain, force field differences, and more. This work represents an opportunity for MD and initiates a path towards understanding the physics of protein function.
12:51PM B20.00005: Effects of artificial mutations on topological features of proteins
HARU NEGAMI (Presenter), Engineering department, The University of Tokyo — Relationship between the mutations of the proteins and its physiological activities is an important research area for many reasons. One reason is that bacteria or viruses acquire their resistance to existing drugs by mutations. The conformational changes due to the mutations have a significant role on the affinity to their ligand.

To understand the relationships, we focus on a topological method called “Fatgraph models of proteins” [1]. Fatgraph models of proteins are topological two-manifold with boundary components (surface) which have one to one correspondence with three-dimensional protein structures listed on Protein Data Bank (PDB) [2] with only a few exceptions. Topological invariants represent geometrical features, and thus they are effective method to grasp the effects of local mutations on three dimensional structures of the proteins as a whole.

In this research we investigated the topological features of artificial proteins and showed the topological traits of mutants which have a drug resistant to antibiotics.

http://www.rcsb.org/

1:03PM B20.00006: Using Molecular Dynamics to Improve Molecular Docking
CONNOR MORRIS (Presenter), DENNIS DELLA CORTE, Brigham Young Univ - Provo — We have been developing an improved method of protein-ligand docking. In our study of an intrinsically disordered protein, SNAP25B, we discovered that docking on a single rigid protein structure alone does not give us complete information on how the protein-ligand pair would interact in vivo, since intrinsically disordered proteins can form multiple 3D structures. A docking-predicted binding pose on this rigid structure may not exist in vivo due to the tendency of the 3D structure of the protein to change under different conditions. However, running the protein through a molecular dynamics (MD) simulation and collecting multiple 3D protein structures gives information about how the protein structure changes in solution. Docking on these MD-derived 3D protein structures increases the probability of finding an accurate ligand binding position using molecular docking that matches in vivo interactions.
1:15PM B20.00007: Marburg VP24 Protein K-loop Cysteine Interactions with the Human Keap1 Protein  NISHA BHATTARAI (Presenter), BERNARD S GERSTMAN, PREM P CHAPAGAIN, Physics, Florida International University — Marburg and Ebola viruses are pathogenic viruses that belong to the Filovirus family and have up to 90% fatality rates. The Marburg VP24 protein (mVP24), has been found to bind with the Human Keap1 protein, which allows the nuclear accumulation of Nrf2, activating the antioxidant response elements during the viral life cycle. In this work, we investigate the molecular level details of the interactions between Marburg and Ebola VP24 proteins and Keap1 using molecular dynamics simulation. Sequence alignment of Ebola and Marburg VP24 reveals that two cysteine residues are present in mVP24 protein but absent in the Ebola VP24 protein (eVP24). Our results show that the presence of cysteine residues in the K-loop region of Marburg VP24 protein makes binding with Keap1 stronger, forming hydrogen bonding and pi-interactions. These cysteine residues are absent in eVP24 protein, which does not bind with Keap1. These computational results provide insights into how Marburg but not Ebola, is able to bind with Keap1 protein and activate antioxidant response pathways.

1:27PM B20.00008: Anomalous kinetics on low-fouling surfaces*  DIEGO KRAPF (Presenter), MOHAMMADHASAN HEDAYATI, MATT J KIPPER, Colorado State University — Protein-surface interactions were probed in terms of adsorption and desorption on a low-fouling surface using single-molecule localization microscopy. Strikingly the experimental data show anomalous kinetics, evident as a surface dwell time distribution that exhibits a power-law distribution, i.e. a heavy-tailed rather than an exponential distribution. As a consequence, the average desorption rate depends upon the time scale of the experiment and the surface protein concentration does not reach equilibrium. Further analysis reveals that the observed anomalous desorption emerges due to the reversible formation of a small fraction of soluble protein multimers, such that each one desorbs from the surface at a different rate. The overall kinetics can be described by a series of elementary reactions, yielding simple scaling relations that predict experimental observations. This work reveals a mechanistic origin for anomalous adsorption/desorption kinetics that can be employed to define design principles for non-fouling surfaces and to predict their performance.

*This work was supported by the National Science Foundation (award number 1511830).
1:39PM B20.00009: Single polypeptide antibody functionalized electrochemical probe development for enterovirus detection* YI-XIANG LU (Presenter), CHIA-YU CHANG, Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, Taiwan, WEN-BIN FAN, JYH-YUAN YANG, Department of Health, Research and Diagnostic Center, Centers for Disease Control, Taipei, Taiwan, CHIA-CHING CHANG, Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, Taiwan — Enterovirus 71 affects global public health and causes the millions of infections in human via oral and respiratory infection every year. Conventional detection approaches are through cell culture and PCR assay processes. However, these processes are time consuming. Therefore, a rapid, sensitive detection of enterovirus is required. Electrochemical impedance spectroscopy (EIS) is widely used for antigen-antibody interaction to measure the impedance change of the bio-sensing probe. However, conventional antibody is not stable for EIS probe. We have developed a single polypeptide antibody for enterovirus 71 detection. This single polypeptide antibody can conjugate with EIS electrode directly via self-assembly process. Moreover, this functionalized sensing probe can bind with EV71 sensitively and selectively within a few minutes by EIS. This single polypeptide antibody is relatively stable to detect enterovirus and may reduce the risk of enterovirus outbreak.

*This project was supported by MOST grant MOST 107-2112-M-009-016-MY3. This work is particularly supported by the Ministry of Education through the SPROUT Project-Center for Intelligent Drug Systems and Smart Biodevices (IDS²-B) of NCTU, Taiwan.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B21 GERA: Energy Storage - Electrolyte Physics 302

11:15AM B21.00001: High Ionic Conductivity Composite Solid-State Electrolytes* ERNESTO MARINERO (Presenter), ANDRES VILLA, JUAN CARLOS VERDUZCO, School of Materials Engineering, Purdue University — We report on the development of a solid-state electrolyte (SSE) with high ionic conductivity, having physical properties that allow their ready integration into current battery devices whose fabrication is amenable to large scale manufacturing. The prototype Composite SSE reported comprises a polymer-Li-salt matrix embedded with super-ionically conducting garnet nanoparticles. We employ polyethylene-oxide (PEO) + LiTFSI (salt) as a matrix incorporating Bi-doped lithium lanthanum zirconium oxide (LLZBO) ceramic nanoparticles (~350nm diameter). We study the role of Bi-aliovalent substitution in LiLaZrO on the microstructure and the ionic conductivity of the ceramic garnet material. We successfully reduce the synthesis temperature of LiLaZrO by Bi-additions utilizing sol-gel reactions. Additions of very small amounts (5% weight load) of the garnet nanoparticles to the polymer-salt matrix result in over two-orders of magnitude increments of the ionic conductivity of the polymer-salt matrix. This composite SSE is amenable to large-scale fabrication and integration into battery devices, furthermore given the small amount of ceramic particles needed, it is cost-competitive.

*Work supported by Purdue University and Mexico’s CONACYT partial support for A. Villa and J. C. Verduzco.
11:27AM B21.00002: Understanding ionic diffusivity in (meta)stable (un)doped solid state electrolyte from first principles: A case study of LISICON (Li$_4$SiO$_4$)  

DEEPIKA GILL (Presenter), Physics, IIT Delhi, India —
Solid electrolyte is expected to be an alternative to liquid electrolyte in Li-ion batteries. The former is believed to be safer, capable of delivering higher energy density, faster recharging, higher voltage capability and longer cycle life. Here, we have studied ionic diffusion and its correlation with dopants/defects by taking LISICON (Li$_4$SiO$_4$) as a test case. As a first step, using density functional theory (DFT), we compute the formation energies of different defects in LISICON to determine the thermodynamically stable configurations. Following this, we have performed ab initio Molecular Dynamics (AIMD) simulation on (meta)stable (un)doped systems to study the diffusion and ionic conductivity of Li-ions. Our results reveal that jumps between different planes are not same, leading to anisotropy in ionic conductivity. We observe that interplanar jumps are minimum in $bc$ planes that limits the ionic conductivity. We report that the limited jump rate can be enhanced at room temperature by point defects, viz. Li-vacancy and substitution at Si-sites with different elements viz. P, Ge, Al.

11:39AM B21.00003: Design of the sodium ionic conductor for all-solid-state battery

KAZUYUKI KAWAHARA (Presenter), SATOSHI HEGURI, Osaka Inst of Tech — The high ionic conductivity of solid electrolyte plays a key role in the performance of all-solid-state batteries. Therefore, the crystal structure is very important in the design of solid ionic conductor. Recently, various solid electrolytes for all-solid-state lithium-ion batteries, especially lithium thiophosphate system, have been reported. These materials generally exhibit high ionic conductivity and can be obtained by easy preparation methods. Kandagal et al. theoretically predicted a new sodium-ion conductor having same crystal structure of lithium thiophosphates [1]. To date, however, it has been not experimentally demonstrated. In the present study, we synthesize a new sodium-ion conductor using a mechanochemical technique and subsequent optimized thermal treatments. The details of the crystal structural analysis and characterization of the AC impedance will be discussed.

11:51AM B21.00004: First-principles study on electrode-contact chemical stability and Na ion dynamics of Na$_3$SbS$_4$ solid electrolyte for all-solid-state Na ion batteries*  RANDY JALEM (Presenter), YOSHITAKA TATEYAMA, Center for Green Research on Energy and Environmental Materials & Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute — To enhance safety, the replacement of the combustible organic-/liquid-based electrolyte in sodium ion batteries with a ceramic-based solid electrolyte has been sought. In this talk, we present our results on thermodynamic and ion dynamics analyses of Na$_3$SbS$_4$ solid electrolyte using first-principles calculations. Based from the calculated chemical potential diagram when Na$_3$SbS$_4$ is in contact with possible layered cathode compounds Na[TM]O$_2$ (where TM = {V, Cr, Mn, Fe, Co, Ni}), sulfur has the driving force to migrate across the electrolyte-cathode interface which may partly explain the experimentally observed formation of interface reaction layer in such all-solid state battery interfaces. From space-time correlation analysis of molecular dynamics trajectory, we determined a concerted migration behavior for Na ions which can explain for the material's superionic conductivity behavior (>10$^{-3}$ S/cm). The effects of halide doping on the conductivity behavior of Na$_3$SbS$_4$ will also be discussed.

*R.J.le is thankful for the JST Precursory Research for Embryonic Science and Technology (PRESTO) program for the financial support. This research has been supported by MEXT, Japan under “Elements Strategy Initiative for Catalysts and Batteries (ESICB)” and “Priority Issue (No. 5) on Post K computer.

12:03PM B21.00005: Tracking structural dynamics in operando sodium ion batteries*  OLEG GOROBTSOV (Presenter), Cornell University, HAYLEY HIRSH, Univeristy of California San Diego, DANIEL WEINSTOCK, RYAN BOUCK, Cornell University, DINA SHEYFER, Argonne National Laboratory, ZIYI WANG, Cornell University, MINGHAO ZHANG, Univeristy of California San Diego, WONSUK CHA, ROSS HARDER, Argonne National Laboratory, SHIRLEY MENG, Univeristy of California San Diego, ANDREJ SINGER, Cornell University — Sodium ion batteries are promising candidates for storage of energy produced by solar and wind sources. Alternative energy sources are by nature intermittent, and require storage facilities to compensate. Lithium ion batteries, while ubiquitous, are too expensive to satisfy this need. Sodium ion batteries promise to be a cheaper alternative to produce in mass. However, they currently suffer from much faster degradation than Li-ion batteries and often degrade after just a few charge-discharge cycles. Defects in the nanoparticles in lithium ion batteries have been studied by coherent diffraction imaging at X-ray sources (CXDI). We have applied CXDI to sodium ion batteries in operando and obtained information about the evolution of planar and linear defects in the nanoparticles in Na-ion battery cathodes, offering insights in how to improve the performance of Na-ion batteries.

*This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.
**12:15PM B21.00006: Prediction and analysis of a sodium ion electrolyte: Li$_2$Na$_2$P$_2$S$_6$**

YAN LI (Presenter), Department of Physics, Wake Forest University, ZACHARY D HOOD, Electrochemical Materials Laboratory, Massachusetts Institute of Technology, NATALIE A HOLZWARTH, Department of Physics, Wake Forest University — Recent experimental results of Hood et al.$^1$ show that Na$_4$P$_2$S$_6$, which crystallizes in the based-centered monoclinic structure C2/m (#12), has significant Na ion conductivity ($3 \times 10^{-6}$ S/cm) at room temperature. Using density functional theory and density functional perturbation theory within the harmonic phonon approximation, we predict that the Na ion conductivity can be enhanced by alloying this electrolyte with Li to form Li$_2$Na$_2$P$_2$S$_6$ having the same C2/m structure with compacted $a$ and $b$ lattice constants. The calculation of Helmholtz free energies suggests that the alloy material is stable for a range of temperatures at and above room temperature in terms of the energy difference $F$(Li$_2$Na$_2$P$_2$S$_6$ + 2Na) $-$ (F(Na$_4$P$_2$S$_6$ + 2Li) $\leq$ −0.35 eV. Molecular dynamics simulations indicate that Li$_2$Na$_2$P$_2$S$_6$ has larger Na ion conductivity than does Na$_4$P$_2$S$_6$ and therefore is promising as a possible solid-state electrolyte for all-solid-state Na ion batteries.

$^1$Z. D. Hood et al. to be published.

*Supported by NSF grant DMR-1507942.

**12:27PM B21.00007: Mg ion conducting solid polymer electrolyte for advanced energy storage system**

MEETA TRIVEDI (Presenter), HAMAD ALBEHAIJAN, THEIN KYU, Univ of Akron — Magnesium (Mg) batteries have the potential to replace the Li-ion technology because of superior safety and high abundance of Mg metal. However, the commercialization is hindered due to lack in development of electrolyte and cathode systems. A novel highly conductive, solvent-free, solid state polymer Mg ion electrolyte for advanced energy storage application is developed. Mg-ion conducting solid state polymer electrolytes (SPE) comprised of polyethylene glycol diacrylate (PEGDA) prepolymer, magnesium bis(trifluoromethanesulfonyl) imide (Mg(TFSI)$_2$) salt, and succinonitrile (SCN) plasticizer were systematically examined. Optimization of composition for solid polymer electrolyte to achieve superionic conductivity was performed in the isotropic region guided by ternary phase diagram. Addition of plasticizer decreases $T_g$ of the system, but it increases the ionic conductivity. By using various plasticizers and mixed Mg/Li salts in the development of SPE, the effect of plasticization and salt composition on the ionic conductivity, electrochemical stability window, thermal stability and mechanical properties will be demonstrated.

*Support by NSF-DMR 1502543.
AC conductivity studies of polyethylene oxide-garnet-type Li$_7$La$_3$Zr$_2$O$_{12}$ hybrid composite solid polymer electrolyte films

PARISA BASHIRI (Presenter), T. PRASADA RAO RAO, Physics and Astronomy, Wayne State University, VAMAN NAIK, Natural Sciences, Univ of Michigan - Dearborn, GHOLAM ABBAS NAZRI, RATNA NAIK, Physics and Astronomy, Wayne State University — We have investigated both AC dielectric permittivity and ionic conductivity of hybrid composite solid polymer electrolyte (CSPE) films (~100 mm) comprised of sub-micron sized aluminum substituted cubic Li$_7$La$_3$Zr$_2$O$_{12}$ (LLZO) particles dispersed in polyethylene oxide-LiClO$_4$ (PEO-LiClO$_4$) matrix with [EO]:[Li] = 15:1. The complex AC permittivity and conductivity were determined using the measured electrical impedance spectra in the range of 1 Hz to 300 kHz and analyzed using generalized power-law that accounts for the effect of electrode polarization. The ionic and segmental relaxation times obtained from fitting the experimental data indicate a strong coupling between the ionic motion and segmental dynamics. Further, the observed temperature dependent conductivity follows the Vogel-Tammann-Fulcher (VTF) behavior implying a close correlation between ionic conductivity and segmental relaxation in these polymer electrolytes. The VTF model yields an activation energy of 0.32 eV for PEO-LiClO$_4$ film, and 0.07 eV for PEO-LLZO-LiClO$_4$ composite film, consistent with the observed enhancement in conductivity by two orders of magnitude at 30 °C upon the addition of LLZO particles. Details preparation of CSPE films and the analyses will be presented.

A solid 3D Li-S battery design via stacking 2D conductive microporous coordination polymers and amorphous Li-S layers

GUOPING GAO (Presenter), Lawrence Berkeley National Laboratory — In order to make a Li-S battery practical, not only high gravimetric energy capacity is important, high volumetric energy capacity will also be required. The currently explored Li-S cathode designs often deploy systems with liquid electrolyte infiltration, hence with relatively low volumetric capacity. In the current study, we theoretically test a compact solid 3D design (more like a Li-ion battery cathode than a conventional Li-S cathode) consisted of a sandwich structure alternating between the 2D Mn-HAB layer and amorphous Li-S layer. We study the theoretical limits for both its gravimetric and volumetric energy capacity, as well as its structural stability and Li diffusion within the cathode system. In order to study the Li diffusion within an amorphous system, we also develop a pull-atom molecular dynamics (PA-MD) to calculate the barrier heights of such disordered systems. We reveal the mechanism which determines the Li diffusion in the amorphous layer of the system. Overall, we find such 3D solid Li-S cathode can be practical, with sufficient large gravimetric and volumetric energy capacity, as well as the Li diffusion constant. It also solves many other common Li-S cathode problems, from Li polysulfide dissolution, to electrical insulating, and structure instabilities.
1:03PM B21.00010: First Principles Study of Electrolyte Interactions in Calcium Ion Batteries

JOSHUA YOUNG (Presenter), Chemical and Materials Engineering, New Jersey Institute of Technology, PETER KULICK, TAYLOR JURAN, MANUEL SMEU, Physics, Binghamton University — Multivalent ion batteries, which use species such as Ca as the working ion, are gaining increasing attention. Compared to other multivalent ions, Ca exhibits a reduction potential close to that of Li, high volumetric capacity, and faster diffusion. However, the breakdown of organic electrolytes causes a passivating layer (the solid electrolyte interphase, or SEI) to form on the electrode surface, blocking Ca diffusion and preventing reversible plating and stripping of the Ca anode. In this work we use density functional theory (DFT) and ab initio molecular dynamics (AIMD) calculations to study the interaction of these solvents, including ethylene carbonate (EC), propylene carbonate (PC), and tetrahydrofuran (THF), with Ca ions and investigate their breakdown on the anode surface. [1,2] We find that Ca forms a large first solvation shell with EC and PC and a slightly smaller one in THF. We then compute the diffusion coefficient of Ca in each solvent using AIMD, and find that it diffuses fastest in THF, and slower in EC and PC. Finally, we use AIMD to study the decomposition of EC on Li, Ca, and Al surfaces and identify the principle components of the SEI on each.


1:15PM B21.00011: Proton conductivity mechanism of liquid imidazole - an ab initio molecular dynamics study

ZHUORAN LONG (Presenter), New York Univ NYU, AUSTIN ATSANGO, JOE ANTHONY NAPOLI, THOMAS E MARKLAND, Stanford University, MARK E TUCKERMAN, New York Univ NYU — Imidazole, as a fundamental organic compound, exhibits high proton conductivity comparable to water at similar temperatures relative to the melting point. Its potential application in fuel cells has motivated numerous experimental research efforts. However, details of the proton conductivity mechanism are still ambiguous. Using multiple time-step ab initio molecular dynamics simulations, we were able to accumulate trajectories totaling 1 ns in length. The predicted proton diffusion coefficient of imidazolium is 0.52 Å²/ps at 384K, and structural diffusion is the dominant mechanism. The proton transfer event is local and must go through a geometrically restricted Zundel-type transition state at a sub-picosecond time scale. Long hydrogen-bonded chains were detected in our liquid imidazole system within which the imidazolium defect undergoes frequent identity changes from individual proton transfer events. Chain diffusion is controlled by the dynamic hydrogen bond forming and breaking via rotational reorientation at a time scale of ~30ps. The decoupling of local proton transfer and chain diffusion together explains the fast proton hopping rate and relatively large diffusion coefficient of the charge defect.
**1:27PM B21.00012: Smart power system: Tuning energy storage by electrophoretic repositioning of TiO\(_2\) nanoparticles in electrolytes.** BIPALV ACHARYA (Presenter), CAITLIN M SEED, JACQUELINE KRIM, North Carolina State University — An effective strategy for efficient use of power is to deliver variable energy whose level depends on the fluctuating demand. Electric double layer capacitors are regarded as one approach suitable for such power management systems. Prior investigations of TiO\(_2\) nanomaterials have primarily focused on how they can be incorporated into a system's electrodes and not its electrolytes. We demonstrate here that TiO\(_2\) nanoparticles (NPs) dispersed directly into an electrolyte may also be an approach to smart energy storage applications. Cyclic voltammetry measurements are employed to explore charge storage capabilities and, together with repositioning of the TiO\(_2\) and Al\(_2\)O\(_3\) NPs in the electrolyte. TiO\(_2\) NPs are revealed to be actively positioned to form a transient film on the electrode surface, significantly enhancing the system's energy storage capabilities. In contrast, minimal enhancement is observed for the Al\(_2\)O\(_3\). This study shows that TiO\(_2\) NPs are intrinsically capable of being a component of a “smart power” system, designed to deliver variable power commensurate with a fluctuating demand.

*National Science Foundation Award Number DMR1535082

**1:39PM B21.00013: Ab Initio Study of the Discharge Mechanism of Bi- and Cu- Modified MnO\(_2\)/Zn Rechargeable Batteries.** BIRENDRAG ALE MAGAR (Presenter), NIRAJAN PAUDEL, TIMOTHY N. LAMBERT, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003, TIMOTHY N. LAMBERT, Department of Materials, Devices, and Energy Technologies, Sandia National Laboratories, Albuquerque, New Mexico 87185, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003 — Bi and Cu additives have a great influence on the performance of rechargeable Zn/MnO\(_2\) batteries, however, the mechanism by which these additives affect the rechargeability and cyclability of the MnO\(_2\) electrode has not been explained in detail. We applied first-principles computational methods based on density functional theory to study the discharge mechanism of Bi- and Cu-modified \(\delta\)-MnO\(_2\) electrodes in rechargeable Zn/MnO\(_2\) batteries. Our calculations show the possibility of formation of Bi-Mn and Cu-Mn oxides in Bi/Cu-modified \(\delta\)-MnO\(_2\) cathodes during battery cycling. The results of our study suggest that the formation of intermediate Bi-Mn and Cu-Mn oxides could reduce the rate of accumulation of irreversible redox reaction products in the MnO\(_2\) electrode.

*This work was supported by the LDRD program at Sandia National Laboratories and by the U.S. DOE OE Energy Storage Program.
1:51PM B21.00014: Ab initio Analysis of Membrane Stability in Alkaline Environments: a Joint Density Functional Theory (JDFT) Study*  MARIEL TADER (Presenter), WEI YOU, GEOFFREY COATES, TOMAS ALBERTO ARIAS, Cornell University — Improving membrane stability in alkaline environments is crucial to the development of alkaline fuel cells (AFCs). Ab initio studies using the nudged elastic band (NEB) method, combined with a detailed transition-state theory analysis, allow us not only to predict quantitative lifetimes of alkali-stable membrane polymers, but also to uncover unexpected mechanisms for improving membrane lifetime. In this later regard, we find that the choice of a first-principles joint-density functional theory (JDFT) description of the solvent and consideration of the impact of the hydrophobic regions of the membrane are critical to understanding the polymer degradation process. This work is foundational to computation-enabled searches for yet more stable AFC membranes.

*This research is supported as part of the Center for Alkaline Based Energy Solutions (CABES) an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award No. DE-SC0019445.

2:03PM B21.00015: Enhancement of Quaternized Ammonium Polyaromatic Anion Membrane Performance in Alkaline Fuel Cells by Deposition of Graphene Oxide and Catalyst Ink Optimization*  AVINASH RAO (Presenter), MICHAEL HAN, CARTER BIAN, MIRIAM RAFAILOVICH, STOYAN BLIZNAKOV, Stony Brook University — To bolster the performance of polyaromatic ionomer membranes in alkaline fuel cells (AFCs), two major modifications were made. First, catalyst ink composition was optimized to yield the maximum power performance for the low platinum loading (0.6 mg/cm²). From the tested compositions, an 80:20 (catalyst:ionomer) ratio produced the greatest results for quaternary ammonium biphenyl membranes, yielding an improved 66 mW/cm² power density despite reduced back-pressure. In addition to determining an optimal ink composition, partially reduced graphene oxide (PRGO) was deposited onto catalyst-loaded electrodes. The membrane electrode assembly (MEA) reached a power density of 66 mW/cm² at a low back-pressure of 50 kPa; likewise, the current density of 400 mA/cm² was unprecedented for this particular polyaromatic membrane in prior tests. By varying the composition of the catalyst ink, we demonstrated a 453% increase in power per milligram platinum (PPMP) from 58% ionomer by mass to 20% ionomer by mass. Through the direct application of PRGO to the gas diffusion electrode surface, we achieved the highest recorded PPMP membrane — 0.97 W/mgPt in MEA 6.

*We acknowledge support from the Louis Morin Charitable Trust and NYS Department of Economic Development.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B22 DBIO: Biofluid Dynamics; Biological Pattern Formation; Biological Oscillators  303 - Ofer Kimchi, Harvard University
11:15AM B22.00001: Flow due to chirality in suspensions of magnetotactic bacteria
ANDREJS CEBERS (Presenter), Univ of Latvia — Phenomena due to chirality are observed in suspensions of magnetotactic bacteria. As a particular example that is simple enough for analysis we consider a layer of magnetotactic bacteria suspension with thickness h and width 2d above a solid wall. The torque dipoles of the bacteria are oriented by an oblique magnetic field, leading to torques distributed on the free interface of the layer. As a result a boundary value problem for the 2D Stokes equation is formulated with a jump of the fluid velocity on the free interface and a no-slip condition on the solid wall. It is solved by the known methods of complex analysis where the flow field is defined by two analytical functions. The solution shows fluid motion perpendicular to the plane defined by the normal to the solid wall and the oblique magnetic field. The numerical value of the velocity and its dependence on the angle of the field inclination is in good agreement with the experimental data [1].

11:27AM B22.00002: Active depinning of bacterial droplets due to gravity* HARSHITHA SHANKAR KOTIAN (Presenter), AMITH ZAFAL ABDULLA, HITHYSINI K. N., VARSHA SINGH, MANOJ M VARMA, Indian Institute of Science — A bacterial culture on a nutrient rich agar plate exhibits swarming motility. Many species of swarming bacteria collectively extract water from the underlying agar and produce surfactants to enhance the spreading of the bacterial droplet to colonise the entire plate. When the agar plate is placed on an incline, this bacterial droplet de-pins to slide down the surface. This de-pinning has so far been presumed to be due to the reduction in surface tension of the droplet by the surfactants produced by the bacteria. Contrary to this belief, we present experimental evidence that motility of the individual bacteria and the stiffness of the agar dominates the de-pinning dynamics to an extent that de-pinning can happen even in mutant strains incapable of producing surfactants. We also present a fluid dynamical model to describe this active de-pinning mechanism of droplets containing surfactant producing bacteria such as Pseudomonas aeruginosa and Bacillus subtilis.

*This study was funded by DST-ICPS programme.
**11:39AM B22.00003: Optimal Geometry of Perfusion in Flow Networks**

TATYANA GAVRILCHENKO (Presenter), ELENI KATIFORI, University of Pennsylvania — In organ capillaries, oxygen detaches from red blood cells and diffuses through a porous membrane into the nearby tissue, eventually getting absorbed by tissue cells. Motivated by this system, we study networks where flow is laden with nutrients able to diffuse out of the vessels and into the surrounding faces. In a uniform network with a single flow source and sink, the nutrients become depleted far from the source, forming a gradient of nutrient density that may leave some tissue undersupplied. Nonetheless, organs have developed capillary bed networks that avoid tissue starvation. In anticipation of engineering networks for artificial organs, we explore theoretical network designs for uniform perfusion over an extended area. Here, we first propose an algorithm with rules to induce local topological changes in a flow network, which serves to generate a wide range of network topologies. We then use vertex model dynamics to tune the vertex positions in a way that equalizes nutrient distribution. Ultimately, we hope to use this uniformly perfusing network ensemble to identify topological features that serve to dissipate an undesirable nutrient gradient.

*We gratefully acknowledge support from the National Science Foundation and the Burroughs Wellcome Fund.

**11:51AM B22.00004: Confined Diffusion of a Colloidal Particle Between Two Parallel Walls: Quantifying Diffusing Diffusivity**

GARY W. SLATER (Presenter), MAXIME IGNACIO, LE QIAO, Univ of Ottawa — "Anomalous yet Brownian" diffusion has been observed in numerous physical and biological systems over the last few years, both experimentally and in simulations. The concept of Diffusing Diffusivity, which we proposed to explain such phenomena, has also been studied extensively. As shown by the Bechhoefer group (PRE 96, 042604, 2017), the simplest experimental system is possibly that of a particle confined to a slit since its diffusion coefficient does depend on the distance to a wall. We revisit this problem using Lattice Boltzmann simulations of a particle between two walls in the absence of external forces, a simpler situation since no external force is present. Instead of using the Kurtosis as a measure of the non-ideality of the diffusion motion, we introduce a new empirical fitting function with a tunable exponent and a critical time scale. We test our results with an alternative Monte Carlo simulation and discuss the implications.

*The authors acknowledge funding from NSERC and the China Scholarship Council.
12:03PM B22.00005: Fluid flow dynamics in networks of compliant vessels  
SEAN FANCHER (Presenter), ELENI KATIFORI, Department of Physics and Astronomy, University of Pennsylvania — Flow networks appear in a wide variety of natural and artificial contexts, and as such, a significant number of works have aimed to study their properties. However, most of these previous efforts have focused on continuous and dynamically invariant flow through networks of rigid vessels. Here, we develop a theoretical model of pulsatile flow using compliant vessels that interact with the flow and are capable of storing material and elastic energy. Pressure pulses can propagate, dissipate and scatter in such a fluidic network, and the system can support complex and rich dynamics. We solve for the flow and pressure profiles at any point within the network as a function of the properties of the input and output pressure or current waveforms, and we study the sensitivity of the dynamic flow profile to alterations or complete removal of single vessels. We use this to calculate not only the necessary power needed to maintain such a flow profile but also the power required to alter the profile, and show how a network can be optimized with respect to both. Finally, we explore possible applications of this work to biological systems such as the human vasculature network.

12:15PM B22.00006: Optimization of solute dissemination in complex flow networks  
GEORGIOS GOUNARIS (Presenter), MIGUEL RUIZ GARCIA, ELENI KATIFORI, University of Pennsylvania — Flow networks efficiently transport nutrients in many physical systems, such as plant and animal vasculature. In the case of the animal circulatory system, the oxygen and nutrient distribution are crucial for the survival of tissue. Homogeneity of the nutrient distribution provides a fitness advantage as waste is minimized while all tissue gets enough nutrients to survive. Can biological flow networks self-organize and remodel to optimally perfuse the tissue? We propose a local adaptation rule for the vessel radii that is able to equalize perfusion, while minimizing energy dissipation to circulate the flow and a cost constraint. These different objective functions compete to produce complex network morphologies including hierarchy and asymmetry between the network input and output.

12:27PM B22.00007: Probing in-mouth texture perception with a biomimetic tongue  
ALEXIS PREVOST (Presenter), Sorbonne University, Laboratoire Jean Perrin CNRS UMR8237, Paris, France, JEAN-BAPTISTE THOMAZO, Sorbonne University, Laboratoire Jean Perrin CNRS UMR8237, Paris France & Nestlé Dairy Center, Lisieux, France, JAVIER CONTRERAS PASTENES, Sorbonne University, Laboratoire Jean Perrin CNRS UMR8237, Paris, France, CHRISTOPHER J PIPE, BENJAMIN LE RÉVÉREND, Nestlé Research Center, Lausanne, Switzerland, ELIE WANDERSMAN, Sorbonne University, Laboratoire Jean Perrin CNRS UMR8237, Paris, France — An experimental biomimetic tongue– palate system has been developed to probe human in-mouth texture perception. Model tongues are made from soft elastomers patterned with fibrillar structures analogous to human filiform papillae. The palate is represented by a rigid flat plate parallel to the plane of the tongue. To probe the behavior under physiological flow conditions, deflections of model papillae are measured using a novel fluorescent imaging technique enabling sub-micrometer resolution of the displacements. Using optically transparent Newtonian liquids under steady shear flow, we show that deformations of the papillae allow their viscosity to be determined from 1 Pa s down to the viscosity of water (1 mPa.s), in full quantitative agreement with an elastohydrodynamics model.
Towards a synthetic post-translational protein oscillator

Ofer Kimchi (Presenter), Carl Goodrich, Agnese Curatolo, Harvard University, Alexis Courbet, Nick Woodall, Dmitri Zorine, David Baker, University of Washington, Michael Phillip Brenner, Harvard University — Synthetic protein circuits have the potential to significantly change the landscape of biomimicry engineering. While synthetic gene circuits have already borne fruit over the past several decades, post-translational circuits engineered to bypass transcription/translation machinery can offer more immediate responses and more direct coupling to endogenous systems. However, engineering dynamic phenomena such as oscillations in these circuits remains an outstanding challenge. Only a few known biological systems, such as the KaiABC system regulating the circadian clock in cyanobacteria, offer examples of post-translational oscillators, creating a need for theoretical work to fill in the gaps. Here, we develop two distinct post-translational oscillators, each using a small number of components which interact only through reversible binding and phosphorylation/dephosphorylation reactions. Our designed oscillators rely on the self-assembly of two protein species into multimeric functional enzymes which respectively interfere with and enhance this self-assembly. We will describe the systems, the intuition behind them, and their dependence on the (few) kinetic parameters.

*O.K acknowledges the NSF-Simons Center for Mathematical and Statistical Analysis of Biology at Harvard, award #1764269

Protein recruitment through indirect mechanochemical interactions

Andriy Goychuk (Presenter), Atul Mohite, Erwin A Frey, Ludwig Maximilian University of Munich — Some proteins have the ability to recruit other proteins from the cytosol to phospholipid membranes. This binding cooperativity plays a major role for the formation of protein patterns, which provide spatiotemporal control over many cellular processes. For example, Min oscillations guide the positioning of division axis in E. coli, and members of the Rho family of GTPases control contractility and migration of eukaryotic cells. However, the physical basis for this recruitment is still unclear. We suggest a generic feedback mechanism that explains how cooperativity can directly arise from mechanochemical coupling between the membrane and proteins. Such a mechanochemical coupling leads to membrane deformation, which in turn affects the affinity of proteins for the membrane, leading to a positive feedback in the protein binding rates. Our theory predicts that the mechanical properties of the membrane strongly affect protein recruitment, and therefore also protein pattern formation.

*E.F. acknowledges financial support from the Deutsche Forschungsgemeinschaft (DFG) via the Collaborative Research Center (SFB) 1032 (project B2). A.G. is supported by a DFG fellowship through the Graduate School Quantitative Biosciences Munich (QBM).
Modelling the Ear with Electronic Oscillators: The Wien Bridge Oscillator as a Physical Analogue for the Hair Cell

COURTNEY FLEMING (Presenter), RANDALL TAGG, MASOUD ASADI-ZEYDABADI, University of Colorado, Denver — The hair cell is the sensory organ of the human ear. In the vestibule, hair cells allow us to detect linear accelerations and rotations of the head. In the cochlea, patterns of hair cell activation along the dynamic basilar membrane allow us to encode information about complex sounds such as speech and music. A particularly important feature of hair cells is their intrinsic nonlinearity which gives rise to both a quiescent and oscillatory regime. This nonlinearity has been approached in the literature by treating the hair cell as a Hopf-type oscillator, wherein cochlear hair cells are poised just below the bifurcation point. In our research, we sought to construct and model a simple physical system that exhibited this same Hopf-type nonlinearity. We chose as our model system the Wien bridge electronic oscillator, an affordable and relatively simple circuit which mimics many of the essential features of the hair cell. We will introduce our theoretical model for nonlinearity and resonance within the Wien bridge oscillator based on experimental results, and discuss parallels between the dynamics of the Wien bridge oscillator and the dynamics of the hair cell.

Bulk-surface coupling reconciles Min-protein pattern formation in vitro and in vivo

FRIDTJOF BRAUNS (Presenter), Ludwig Maximilian University of Munich, GRZEGORZ PAWLIK, Department of Bionanoscience, TU Delft, JACOB HALATEK, Microsoft Research (Cambridge), JACOB KERSSEMAKERS, Department of Bionanoscience, TU Delft, ERWIN A FREY, Ludwig Maximilian University of Munich, CEES DEKKER, Department of Bionanoscience, TU Delft — The Min system of E. coli exhibits a rich variety of protein patterns whose phenomenology differs qualitatively and quantitatively between in vitro and in vivo settings. Here, we combine experiments and theory to show that this variety of patterns originates from distinct pattern-forming mechanisms (oscillation modes) that operate at different ratios of cytosolic volume to membrane surface area. Experiments in vitro, using laterally wide microchambers show qualitatively distinct patterns at different bulk heights, from standing waves, and sustained large-scale oscillations, to traveling waves. Our theoretical analysis shows that in vitro patterns at low bulk height are driven by the same lateral oscillation mechanism as in vivo pole-to-pole oscillations. Two distinct vertical oscillation modes – anti-phase oscillations between the opposite membrane surfaces and membrane-to-bulk oscillations – set in at larger bulk heights, marking the transition from the in vivo to the in vitro regime. We predict and experimentally confirm vertical pattern-synchronization (in-phase and anti-phase) between the microchambers' top and bottom surface and multistability of patterns in the transition regime.
HECTOR VELASCO PEREZ (Presenter), FLAVIO H FENTON, Georgia Inst of Tech — Our understanding of cardiac dynamics is frequently limited by our lack of knowledge of the ionic interactions at the microscopic level and how they drive the macroscopic phenomena. This has generated a series of complex models that are computationally demanding, inflexible and not generalizable. Nevertheless, there are characteristics or patterns that consistently show up in all of them, such as traveling waves and spiral waves. These patterns turn out to be low dimensional structures in an optimal basis, and optimal frame of reference. Here, we will focus on the study of traveling waves with alternans, that is, the change in the action potential wave length and/or amplitude in time. It is known that alternans are one of the main contributors to the initiation of fibrillation, which can be lethal if not attended. I will illustrate the derivation and properties of two types of reduced order models of cardiac tissue exhibiting various levels of alternans. These model reductions are based on proper orthogonal decomposition and sparse regression methods. We will compare the properties of both models and discuss the applications to other systems.

*Funding: NSF #1028261 and #1489420

DAIBHID O MAOILEIDIGH (Presenter), Stanford University, YUTTANA ROONGTHUMSKUL, Physics, Chulalongkorn University, AJ HUDSPETH, Rockefeller University — Our ears emit sounds spontaneously, known as spontaneous otoacoustic emissions (SOAEs). It is unclear, however, why some animals emit sounds with identical frequencies from their two ears. In most nonmammalian tetrapods, acoustic coupling between the eardrums through the head cavity might influence SOAE production.

We record SOAEs simultaneously from the two ears of the tokay gecko and find several synchronized SOAEs. A model describing the eardrums as acoustically coupled, stochastic, active oscillators also produces synchronized SOAEs. In agreement with our experimental observations, the model captures the frequency-dependent phase differences between ears, the complex alterations in emissions upon suppression of the contralateral ear by static pressure, the change in emission frequency as the contralateral oscillator’s peak frequency is varied, the synchronization of emissions as the peak frequencies converge, and the dependence of some SOAEs on the emission strength of the contralateral ear.

Moreover, the model predicts that the ears’ activities enhance the localization of weak sound sources. The two ears of a gecko evidently function together as a single active system that is sensitive to the location of weak sound sources.
Patterns make patterns: how hierarchical self-organization couples cell shape to biochemical dynamics

TZER HAN TAN (Presenter), Massachusetts Institute of Technology MIT, MANON WIGBERS, FRIDTJOF BRAUNS, Ludwig Maximilian University of Munich, ZACHARY SWARTZ, Massachusetts Institute of Technology MIT, ERWIN A FREY, Ludwig Maximilian University of Munich, NIKTA FAKHRI, Massachusetts Institute of Technology MIT — Many biological processes rely on the precise positioning of proteins on the membrane to perform complex tasks. Such protein patterns are susceptible to cell shape changes, raising the question of how these patterns can be robust in a mechanically dynamic environment. Here, we elucidate a mechanism that pattern protein localization on the membrane robustly despite cell shape deformations. By combining experiments in starfish oocytes with mathematical modelling, we find that cell shape information encoded in a cytosolic gradient can be decoded by a bistable front of a RhoA regulator. In turn, this bistable front precisely positions RhoA by locally triggering excitable dynamics. We posit that this hierarchical coupling between a biochemical gradient and protein self-organization provides mechanochemical feedback for cell shape sensing and control.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B23 DBIO DSOFT: Cellular Biophysics: structure, mechanics, and dynamics

11:15AM B23.00001: “Cellular Stokesian Dynamics“: a computational model for biological cells

ROSEANNA ZIA (Presenter), DREW ENDY, AKSHAY MAHESHWARI, EMMA DEL CARMEN GONZALEZ GONZALEZ, ALP M SUNOL, Stanford Univ — The frontier in operational mastery of biological cells arguably resides at the interface between biology and colloid physics: cellular processes that operate over colloidal length scales, where continuum fluid mechanics and Brownian motion underlie whole-cell scale behavior. It is at this scale that much of cell machinery operates and is where reconstitution and manipulation of cells is most challenging. This operational regime is centered between the two well-studied limits of structural and systems biology: the former focuses on atomistic-scale spatial resolution with little time evolution, and the latter on kinetic models that abstract space away. Colloidal hydrodynamics modeling bridges this divide by unifying the disparate length and time-scales of solvent-molecule and colloidal dynamics, and may hold a key to numerous open questions in biological cell function. I will discuss our physics-based computational model of a biological cell, where biomolecules and their interactions are physically represented, individually and explicitly. With it, we study a model process: translation elongation. We find that Brownian self-diffusion alone is insufficient to recover experimentally measured elongation rates but accounting for other colloidal forces improves agreement.
11:27AM B23.00002: The roles of patchy attractions and Brownian motion in fundamental biological processes in a model cell* JENNIFER HOFMANN (Presenter), ROSEANNA ZIA, Department of Chemical Engineering, Stanford University — Microscopic forces and physical phenomena at the colloidal scale are involved with fundamental processes inside living cells [Maheshwari et al., Phys. Rev. Fluids, 2019]. Examples of such phenomena include Brownian motion, confinement within the boundary of a cell membrane or wall, and hydrodynamic & electrostatic interactions between constituents of the cellular milieu (e.g. proteins). In the case of electrostatic interactions, isotropic inter-particle potentials are often insufficient to reproduce experimental results due to anisotropic charge distributions on protein surfaces [Bucciarelli et al., Sci. Rep., 2018]. To connect these microscopic forces to whole-cell functions, we examine the interplay between these colloidal-scale phenomena in dynamic simulations. Specifically, we use coarse-grained, patchy simulations to study the biological process of translation elongation in a model prokaryotic cell. Here, we present our results investigating the structure and dynamics of these coarse-grained systems, probing the inseparable connection between colloidal-scale transport and biological function.

*The authors gratefully acknowledge funding through the NSF Graduate Research Fellowship Program and use of computing resources from the Stanford Research Computing Center.

11:39AM B23.00003: The structure of tubular organelle networks can accelerate diffusive transport and kinetics AIDAN BROWN (Presenter), ELENA KOSLOVER, University of California, San Diego — Diffusion is an important, and often dominant, mode of transport for molecules inside cells. Many cell processes occur within specialized organelles with a variety of internal geometries, notably the tubular networks of the endoplasmic reticulum and mitochondria, which form a complex meshwork of loops spanning much of the cell. We describe how the structure of these tubular network organelles controls diffusive search times and kinetic rates, using both analytical calculation and computational simulation of diffusive first-passage times on organelle structures extracted from yeast and mammalian cells. We find that total network length alone is not a good predictor of search time. However, total length combined with the number of loops robustly determines search times. Strikingly, increasing the number of loops substantially accelerates diffusive search and reaction kinetics. Mitochondrial mutant networks deficient in fusion and fission have many fewer loops than wild-type networks. By comparing these two network types we show wild-type networks can nearly double diffusive reaction rates for sparse reactants, compared to mutant networks. Overall, we find that the looped structure of organelle networks can function to accelerate diffusive processes.
11:51AM B23.00004: Elucidating mechanics of vascular regression in *Botryllus schlosseri* using image analysis* ROOPA MADHU (Presenter), Univ of Denver, DELANY RODRIGUEZ, CLAUDIA GUZIK, SHAMBHAVI SINGH, ANTHONY TOMASO, Department of Molecular, Cellular and Developmental Biology, University of California Santa Barbara, MEGAN VALENTINE, Department of Mechanical Engineering, University of California, Santa Barbara, DINAH LOERKE, Univ of Denver — Epithelial tubules form critical structures in various body tissues; however, due to experimental inaccessibility, their architecture and dynamics are not well understood. We examined epithelial tube remodeling in vivo using a novel model system: *Botryllus schlosseri* vasculature. In *Botryllus*, blood vessel retraction can be triggered through disrupting (i) collagen crosslinking in the basement membrane using β-aminopropionitrile (BAPN); or (ii) integrin pathway through inhibition of focal adhesion kinase (FAK)(Rodriguez D et al. 2017). We performed stereographic projections of 3-dimensional confocal scans to ‘unwrap’ the blood vessels to enable quantitative analysis of morphology. In normal vessels, the cells are axially elongated with circumferentially aligned actin bundles. While we found no differences in morphology between normal and BAPN treated vessels, FAK-inhibited vessels have significantly smaller cells with circumferential cell orientation. Our results demonstrate the feasibility of *Botryllus* for imaging-based studies of the mechanics of epithelial tube remodeling; in addition, they suggest a critical role of integrin in the maintenance of epithelial morphology.

*2016 Scialog award from RCSA and Moore Foundation
Mathers Foundation Grant SB170066
NSF MRI Grant DBI-1625770

12:03PM B23.00005: Vesicle formation processes on the Golgi significantly altered by overexpression - Duel FRAP investigation* GARETT C SAGER (Presenter), Physics, Univ of Alabama - Birmingham, ELIZABETH S. SZTUL, Cell, Developmental and Integrative Biology, Univ. of Alabama - Birmingham, RYOICHI KAWAI, Physics, Univ of Alabama - Birmingham — Overexpression of a target protein is commonly used in fluorescence-based experiments, such as fluorescence-recovery-after-photobleaching (FRAP), to boost the fluorescence intensity. Since the order of magnitude of protein concentration is artificially altered, the biochemical processes under investigation might be altered as well. We have studied how overexpression could affect the way we understand vesicle formation using FRAP experiments and kinetic Monte Carlo simulation based on continuous-time random walk. Specifically, we are investigating two proteins that are vital during initial vesicle formation on the Golgi (GBF1 and Arf1). Traditionally, either GBF1 or Arf1 would be overexpressed during FRAP, but we also performed dual FRAP where both proteins are overexpressed and measured simultaneously. Comparing the single versus dual FRAP measurements with the computer simulation and a simple mathematical model, we show a significant difference between the two cases. More importantly, the difference would affect the way vesicle formation is understood in cell biology. This shows overexpression can affect biochemical dynamics enough to alter our conclusion(s) from the data.

*This work was supported by NSF (MBC-1615607).
**12:15PM B23.00006: Probing force balance in the S. pombe mitotic spindle by laser ablation**

PARSA ZAREIESFANDABADI (Presenter), MARY ELTING, Physics, North Carolina State University — A microtubule-based machine called the mitotic spindle segregates chromosomes when eukaryotic cells divide. In the fission yeast *S. pombe*, which undergoes closed mitosis, the spindle forms a single bundle of microtubules inside the nucleus. During elongation, the spindle extends via antiparallel microtubule sliding by molecular motors. These extensile forces from the spindle resist compressive forces from inside the nucleus. We probe the source of this force balance via laser ablation of spindles at various stages of mitosis. We find that spindle pole bodies collapse toward each other following ablation, but that spindle geometry is often rescued, allowing spindles to resume elongation. While this basic behavior has been previously observed [1,2], many questions remain as to the timing, mechanics, and molecular requirements of these phenomena. Here, we quantify the time scales of both the relaxation and rescue responses and probe their molecular requirements. We test the possible mechanical roles of nuclear envelope-, centrosome- and microtubule-based forces.


**12:27PM B23.00007: Theoretical framework for the description of transmembrane receptor cluster coalescence in cells**

KATHRIN SPENDIER (Presenter), University of Colorado, Colorado Springs, VASUDEV M KENKRE, University of New Mexico — Moving boundary problems that appear in many fields of science are notoriously difficult to formulate and solve. Due to their complexity, approximation methods play an important role and are widely used to analyze such systems. We present an approximation method for moving boundaries or traps in reaction-diffusion processes that is applied to investigate coalescence of receptor clusters in mast cells. To handle the complexity, which stems from boundary growth due to particle melding, the study is divided into three parts. The first is about stationary trapping problems investigated by the standard defect technique, and the second is about a validity study of an adiabatic approximation for moving boundaries. In the last part, a coalescence theory is developed, which is based on a completely self-consistent approach. Finally, the developed theoretical framework is applied to study the kinetics of immunoglobulin E receptors (FcεRI) cluster coalescence in rat basophilic leukemia cells.
Animal cells and bacteria are enveloped and sealed by lipid membranes and mechanically protected by cortical polymer networks. Cells typically actively maintain a small (eukaryotic cells) or large (prokaryotic cells) positive osmotic pressure against their environment. Volume and shape regulation impact the mechanical properties of cells. The mechanical properties of cells can be probed by exerting external force and measuring cell response. To interpret micro-mechanical optical trapping experiments with suspended rounded eukaryotic cells, we developed finite element simulations and modeled cells as pressurized elastic shells. During deformation, competition between osmotic pressure resulting from compression of the cytosol and the elastic stretching of the actin cortex determines the cell response. The finite element simulations suggest that (eukaryotic) cell deformations are essentially isovolumetric.

When cells divide, a microtubule-based machine called the mitotic spindle delivers chromosomes to two new daughter cells. Microtubule bundles called kinetochore-fibers (k-fibers) attach chromosomes to the spindle, and forces transmitted through k-fibers ultimately segregate chromosomes. Thus, the mechanical integrity of the k-fiber is critical to accurate chromosome segregation, which in turn is essential for cell and organismal health. Yet, the k-fiber itself as a mechanical object is not well understood. We do not fully understand how or where k-fiber microtubules attach to each other along their lengths, nor what molecules mediate these connections. To address these questions, we are probing the mechanics of the k-fiber by severing it via laser ablation, and by using single-molecule speckle microscopy to analyze intra-k-fiber microtubule movements. Speckle microscopy suggests that k-fiber microtubules move poleward together as a single mechanical unit. However, splaying of the k-fiber in response to laser ablation demonstrates that these intra-k-fiber connections can be disrupted. Furthermore, initial evidence suggests more splaying after perturbation of the molecular motor kinesin Kif15, supporting its role as an inter-k-fiber crosslinker.
1:03PM B23.00010: 3D particle diffusion in Escherichia coli cells. [1] DIANA VALVERDE MENDEZ (Presenter), BENJAMIN P BRATTON, JOSEPH P SHEEHAN, ZEMER GITAI, JOSHUA SHAEVITZ, Princeton University — We use Genetically Encoded Multimeric nanoparticles (GEMs) to probe the microrheology of the Escherichia coli cytoplasm. We reconstruct three-dimensional trajectories from optical microscopy images obtained with a custom-built biplane microscope. The use of different sized GEM particles enables us to explore diffusion of objects ranging in size from 20 to 50 nm, similar in scale to ribosomes and other macromolecular complexes in the cell. We also vary the total charge of the fluorescent proteins from -17 e to +48 e and investigate the effect on diffusion. Using specific small molecule drug treatment, we show progress towards understanding the effects of the nucleoid and cell metabolic state on the 3D diffusion of particles inside bacterial cells.

*This work was supported by the NSF Center for the Physics of Biological Function PHY-1734030 CPBF.

1:15PM B23.00011: Opto-genetic control of gene regulation in living fly embryos[2] ANAND SINGH (Presenter), PING WU, ERIC WIESCHAUSS, JARED TOETTCHER, THOMAS GREGOR, Princeton University — Gene regulation is a hallmark of most processes in biology, in particular for cell fate decisions and patterning during early development of an organism. Precise and highly coordinated dynamic gene activity dictates the functional output in the context of complex genetic networks. In order to construct causal relationships in the programs underlying gene regulatory networks and transcription, we developed a light-inducible system to directly interfere with these programs and to quantitatively measure the cellular response in living fly embryos. Our approach allows us to precisely control transcription factor (TF) levels and their immediate response in gene expression. We show how nuclear concentration and TF residence times affect the kinetic rates and expression levels of downstream gene targets, and we test the limits of natural expression patterns by altering the shapes and strengths of the input patterns and measuring their genetic responses. The following questions will be asked: How cells utilize the differential levels of TF to make cell fate decisions? How do downstream genes respond to spatially and temporally modulated doses of TF input concentration?

*Funding: NSF Center PHY–1734030, NIH R01 GM097275
NMR and small-angle neutron scattering examination of dynamics and structure in a polymer-colloid model system directed at understanding macromolecular crowding in cells

SWOMITRA PALIT, Physics & Physical Oceanography, Memorial University of Newfoundland, LILIN HE, Biology and Soft Matter Division, Oak Ridge National Laboratory, WILLIAM A HAMILTON, Instrument and Source Division, Oak Ridge National Laboratory, ARUN YETHIRAJ, Chemistry, University of Wisconsin - Madison, ANAND YETHIRAJ (Presenter), Physics & Physical Oceanography, Memorial University of Newfoundland — The inside of a living cell is crowded (30 - 40% volume fraction) with many macromolecular components, so that each individual macromolecule is not necessarily highly concentrated. This unique system calls for a colloidal perspective to tease out the competing roles of size, shape, flexibility, charge, hydrodynamic interactions, and chemical specificity.

In this work[1], we study long-time self diffusion (using pulsed-gradient NMR) and size (via small-angle neutron scattering) of a linear polymer, polyethylene glycol (PEG, radius of gyration $R_g$, and a more compact crowder (polysucrose, radius $R_c$) of varying size ratio $R_g/R_c$. We find that polymer diffusion exhibits a universal exponential concentration dependence at all polysucrose volume fractions, suggestive of an entropic origin[2]. The crowder exhibits reversible clustering at a volume fraction of 5 - 10%, depending on crowder charge. In the crowding limit, the flexible PEG is up to 100 times mobile than the compact Ficoll.


*This work is funded by the Natural Sciences and Engineering Research Council (Canada).
Analysis and simulations of Bcl10 self-assembly and degradation in activated T cells - LEONARD CAMPANELLO (Presenter), University of Maryland, College Park, MARIA TRAVER, BRIAN SCHAEFER, Uniformed Services University, WOLFGANG LOSERT, University of Maryland, College Park — The adaptive immune system serves as a potent and highly specific defense mechanism against pathogens. A component of this system, the effector T cell, provides rapid pathogen-clearing responses upon detecting pathogen-associated signals. Stimulation of the T cell receptor leads to a signaling cascade resulting in pathogen eradication. Bcl10, a key regulatory protein in this cascade, rapidly assembles into filaments that form the core of the signal transduction machinery; simultaneously, Bcl10 is targeted for slow degradation to ensure tight control of immune activation. Despite the importance of Bcl10 for an effective immune response, the mechanisms and timescales of its assembly and degradation are poorly understood. Here, we will provide insights into Bcl10 filament formation and degradation via image analysis and Monte Carlo simulations. Using image-based bootstrapping, we show that Bcl10 preferentially colocalizes with autophagosomes and that the spatial organization of this complex is significant for immune function. Using stochastic Monte Carlo simulations, we shed light on key Bcl10 filament dynamics, including nucleation, growth, and degradation. Together, these data provide key insights into important mechanism that regulate adaptive immunity.

Investigating the eukaryotic CO2-fixing phase-separated organelle, the pyrenoid - GUANHUA HE (Presenter), SHAN HE, MARTIN JONIKAS, NED WINGREEN, Princeton University — In most eukaryotic algae, an organelle called the pyrenoid helps concentrate CO2 to enhance carbon fixation by the enzyme Rubisco. We recently found that in Chlamydomonas reinhardtii, the pyrenoid has liquid-like behavior including rapid condensation and dissolution during cell division. Our data suggests that the matrix is primarily composed of Rubisco and a linker protein, EPYC1. Rubisco and EPYC1 each have multiple binding sites for the other, allowing the two proteins to form a multivalent phase separation system. We showed that Rubisco and EPYC1 are sufficient to phase separate in an in vitro reconstitution experiment. Here, we measure the phase boundary in terms of concentration of both proteins, which is in the uM range. We use microscale thermophoresis (MST) to determine the dissociation constant (Kd) of EPYC1-Rubisco binding. And we use fluorescence correlation spectrometer (FCS) to determine the protein particle sizes. Combined together, our results suggest the existence of small oligomer complexes composed of EPYC1 and Rubisco in the dilute phase. Our work reveals that the stoichiometry of oligomer complexes is a key factor that regulates phase separation, which might be a general principle in multivalent phase separation system in biology.

China Scholarship Council
2:03PM B23.00015: Dynamics of Self-Organized Organelle Transport in a Developing Macroscopic Single-Celled Organism*  
ELDAD AFIK (Presenter), Division of Biology and Biological Engineering, California Institute of Technology, ELLIOT M. MEYEROWITZ, Howard Hughes Medical Institute, California Institute of Technology — Caulerpa is a marine green alga exhibiting differentiated organs resembling leaves, stems and roots; while individuals can exceed a meter in size, each one is comprised of a single multinucleated giant cell. Thus, according to current understanding, the distinction between the cellular and organismal levels in Caulerpa does not exist. In turn, this challenges our intuition that morphogenesis on large scales necessitates division into cells. It has been hypothesized that active transport plays a key role in the development of the alga. Yet, the most recent reports studying organelle transport in Caulerpa are over three decades old. We have designed an imaging system based on the affordable Raspberry-Pi and its camera module. The system allows us to track over weeks the morphogenesis of tens of samples in parallel, each one in a separate well. Our observations of chloroplasts redistribution on whole-organism scales over hours reveal a pulse-like behavior. We further explore this macroscopic manifestation of the self-organized transport through perturbations, such as alternating illumination protocols and application of an external electric field. In this work we seek to establish a framework to study the dynamics of homeostasis and its stability.

*Zuckerman STEM Leadership Program

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B24 GSNP: Systems Far from Equilibrium 401 - John Bechhoefer, Simon Fraser University

11:15AM B24.00001: Thermodynamic uncertainty relations and fluctuation theorems for Bayes nets*  
DAVID WOLPERT (Presenter), Santa Fe Inst — The pioneering paper [1] analyzed the non-equilibrium statistical physics of a set $S$ of multiple interacting systems whose joint discrete-time evolution is specified by a Bayesian network. Their major result was an integral fluctuation theorem (IFT) governing the sum of two quantities: the entropy production (EP) of an arbitrary single one of the systems, $v \in S$, and the transfer entropy from $v$ to the other systems in $S$. Here I derive a detailed fluctuation theorem (DFT) for an arbitrary subset of the systems in $S$ (including the full set). I then derive an IFT for an arbitrary subset of the systems in $S$, extending the IFT in [1]. I also derive thermodynamic uncertainty relations for the precision of probability currents among joint states of the systems, and for the precision of the work performed by the full set of systems. Rather than the EP generated by a single system in $S$ and the transfer entropy from it to the other systems, these results involve the sum of the EPs generated by all of the systems in $S$ and the change in the multi-information of the joint system as it evolves.


*This work was supported by the Santa Fe Institute and Grant No. CHE-1648973 from the NSF.
A characteristic feature of nonequilibrium steady states is their ability to maintain nonzero fluxes in steady state. Here I will discuss mass fluxes in a class of nonequilibrium systems characterized by driving at the level of individual particles. By constructing an explicit mathematical representation of the full nonequilibrium steady state, I am able to quantitatively connect mass fluxes in the bulk with the boundary conditions. In particular, the emergence of nonzero mass fluxes is tied to the breaking of detailed balance at the boundaries.

We acknowledge support from the Brandeis Center for Bioinspired Soft Materials, an NSF MRSEC, DMR-1420382 (CGW, AB, MFH), NSF DMR-1149266 and BSF-2014279 (CGW and AB), and DMR-1855914 (MFH). Computational resources were provided by the NSF through XSEDE computing resources (MCB090163) and the Brandeis HPCC which is partially supported by the Brandeis MRSEC.

We introduce a new technique to bound the fluctuations exhibited by a physical system, based on the Euclidean geometry of the space of observables. Through a simple unifying argument, we derive a sweeping generalization of so-called Thermodynamic Uncertainty Relations (TURs). We not only strengthen the bounds but extend their realm of applicability and in many cases prove their optimality, without resorting to large deviation theory or information-theoretic techniques. In particular, we find the best TUR based on entropy production alone and also derive a novel bound for stationary Markov processes, which surpasses previous known bounds. Our results derive from the non-invariance of the system under a symmetry which can be other than time reversal and thus open a wide new spectrum of applications.


Project NanoThermo ERC-2015-COG agreement no. 681456 and FNR INTER mobility program.
**11:51AM B24.00004: Non-Gaussian diffusion and energy balance of a Brownian particle in active baths**  
JIN TAE PARK (Presenter), Department of Physics, Ulsan Natl Inst of Sci & Tech, GOVIND PANERU, Center for Soft and Living Matter, Institute for Basic Science, CHULAN KWON, Department of Physics, Myongji University, STEVE GRANICK, HYUK KYU PAK, Center for Soft and Living Matter, Institute for Basic Science — We present a minimal model to generalize the iconic feature of active matter that Brownian particles diffusing in a harmonic potential are kicked by external forces to engender mobility beyond that attributable to thermal energy. The wide time and length scales of usual active matter systems are mapped onto the generic concept of a single Brownian diffusion time (a particle diffusing in a harmonic potential) and kicks from external forces that arrive at random intervals with a defined, programmable, duration time for each kick. Our experiments using an optical trap agree in showing enhanced diffusion that is Gaussian only if the kick duration time is larger than the Poisson interval time. In addition, we conclude that maximum energy dissipation occurs at the time-scale of the geometric mean of the kick duration time and the particle thermal equilibration time. Usual active matter systems do not allow this independent variation of thermal motion, active motion, and the relative time scales of both. In this streamlined system they are varied independently, allowing one to rapidly prototype the limits of various stochastic thermodynamic models.

*This work was supported by the taxpayers of South Korea through the Institute for Basic Science, project code IBS-R020-D1.

**12:03PM B24.00005: Periodic driving in a two-dimensional Brownian ratchet**  
TODD GINGRICH (Presenter), NILS STRAND, RUEIH-SHENG FU, Northwestern University — Brownian dynamics on a fixed potential landscape generates no steady-state current, but currents can be obtained by periodically switching between multiple landscapes. Even more interesting than the existence of such ratcheted currents is that the direction of the current can depend on the frequency of the switching. I will present numerical work on the behavior of current reversals in a two-dimensional system. I will discuss our efforts to make sense of the system by conditioning a time-periodic Markov process for a coarse-grained model. Interestingly, the low-frequency asymmetry between leftward and rightward motion appears at the level of typical events, but the high-frequency asymmetry only emerges for atypical events.
12:15 PM B24.00006: Equation of State for a Far-from-equilibrium Thermodynamic System with Emergent Scales at Steady-state  ATANU CHATTERJEE (Presenter), GERMANO SIANNACCHIONE, Department of Physics, 100 Institute Road, Worcester Polytechnic Institute — One of the hallmarks of soft-condensed matter systems is their ability to exhibit emergent order - spanning a wide range of length and time-scales - when driven out-of-equilibrium. Some of these patterns emerge and disappear at sub-nanosecond scales while some are large enough that they can be physically measured. We present a field theoretic formalism by defining the Lagrangian density as a function of a generic thermodynamic scalar. Our definition of the thermodynamic Lagrangian density involves two components, the internal work or the coherent part which gives rise to emergent order, and the internal dissipation or the incoherent part which acts as the internal sink. The salient feature of this formulation is that it takes into account the spatial and temporal gradients of the generic thermodynamic scalar as the system is driven out-of-equilibrium. On minimizing the action and solving the Euler-Lagrange equations, we obtain a generalized thermodynamic equation of state.

12:27 PM B24.00007: Thermodynamic Analysis of Non-Ergodic and Asymmetric Dimension  YU QIAO (Presenter), University of California, San Diego — We report an interesting Monte Carlo simulation result of a Billiard-type model system, wherein two larger ergodic areas are separated by a small non-ergodic barrier. The two ergodic areas have different heights in a gravitational field. In-plane pressure does work to the lower “plain” when the plain area varies, and gravitational force does work to the upper “plateau” when the plateau height changes. The steady-state is defined by the macroscopic variables measured from the system surface. The simulation results indicate that the particle density ratio spontaneously follows a non-Boltzmann distribution and remarkably, in an isothermal cycle the produced work is significantly greater than the consumed work. The non-ergodic barrier, referred to as the non-ergodic and asymmetric dimension (NEAD), is not “Maxwell's demon”. Its operation does not require detailed knowledge of system microstate. The particle motion is unmonitored, unforced, and random. The explanation of the system performance should be unrelated to the physical nature of information. The concept of NEAD is also being investigated experimentally, through the measurement of the cross-influence of chemical potential and electric potential of large ions confined in small nanopores.

12:39 PM B24.00008: Bounds on current fluctuations for periodically driven systems  KAREL PROESMANS (Presenter), Simon Fraser Univ — The thermodynamic uncertainty relation, in its original form, bounds the amount current fluctuations can be suppressed in terms of the dissipation in a mesoscopic steady-state system. We extend such bounds to systems with time-periodic driving, where they lead to a bound for the hysteresis of any thermodynamic flux. Our results are illustrated on the work fluctuations of an expanding gas.
12:51PM B24.00009: Entropy production bounds under Hamiltonian and rate matrix constraints* ARTEMY KOLCHINSKY (Presenter), DAVID WOLPERT, Santa Fe Inst — Entropy production (EP) is a fundamental measure of the thermodynamic inefficiency of a physical process. If there are no constraints on the rate matrices and Hamiltonians available to a driving protocol, one can transform a system from any initial Hamiltonian and state distribution to any final Hamiltonian and state distribution with zero EP. We investigate the minimal EP that must be incurred to implement such a transformation, if there are constraints on the set of allowed Hamiltonians and rate matrices. Our first result is that zero EP can be achieved even when the Hamiltonian has only a single controllable degree of freedom, as long as there are no constraints on the rate matrix (beyond detailed balance). We then derive non-trivial bounds on the EP that arise from the presence of simultaneous constraints on the Hamiltonian and the rate matrix. These bounds are determined by an effective non-equilibrium free energy, which reflects the work value of a distribution and Hamiltonian under a set of constraints.

*Grant No. CHE-1648973 from the U.S. National Science Foundation.

1:03PM B24.00010: Pre-Cooling Strategy Can Generate Exponentially Faster Heating* OREN RAZ (Presenter), AMIT GAL, Weizmann Institute of Science — What is the fastest way to heat a system which is coupled to a temperature controlled oven? The intuitive answer is to use only the hottest temperature available. However, we show that in some cases it is possible to achieve an exponentially faster heating, and propose a strategy to find the optimal protocol. Surprisingly, this protocol can have a pre-cooling stage: cooling the system before heating it shortens the heating time significantly. This approach can be applied to many-body systems, as we demonstrate in the 2D antiferromagnet Ising model.

*O.R. is the incumbent of the Shlomo and Michla Tomarin career development chair, and is supported by a research grant from Mr and Mrs Dan Kane and the Abramson Family Center for Young Scientists.

1:15PM B24.00011: The solution of the Metropolis dynamics on a complete graph with applications to anomalous thermal relaxations* MARIJA VUCELJA (Presenter), ISRAEL KLIICH, Univ of Virginia — We find analytically the complete set of eigenvalues and eigenvectors associated with Metropolis dynamics on a complete graph. As an application, we use this information to study an unusual relaxation phenomenon, called the Mpemba effect. This effect describes situations when, upon performing a thermal quench, a system prepared in equilibrium at high temperatures relaxes faster to the bath temperature than a system prepared at a temperature closer to that of the bath.

*The NSF grant DMR-1508245 supported the work of IK. This research was supported in part by the National Science Foundation under Grant No. NSF PHY-1748958.
1:27PM B24.00012: Out-of-equilibrium chemical networks: dissipation shapes selection

DANIEL MARIA BUSIELLO (Presenter), SHILING LIANG, PAOLO DE LOS RIOS, Ecole Polytechnique Federale de Lausanne — Life has most likely originated as a consequence of processes taking place in non-equilibrium conditions (e.g. in the proximity of deep-sea vents) selecting states that would have been otherwise unfavorable at equilibrium. Here we present a simple chemical network in which the selection of states is driven by the dissipation rate, as previously suggested in the literature: states participating to faster reactions dissipate faster and are the most populated ones in non-equilibrium steady-state conditions. Building upon these results, we show that, as the complexity of the chemical network increases, the velocity of the reaction path leading to a given state determines its selection, giving rise to phenomena of global localization in state space. A byproduct of our studies is that, in the presence of a temperature gradient, thermophoresis-like behavior inevitably appears depending on the transport properties of each individual state, thus hinting at a possible microscopic explanation of this intriguing and long-standing phenomenon.

1:39PM B24.00013: Isometric uncertainty relations

HADRIEN VROYLANDT (Presenter), Northwestern University, KAREL PROESMANS, Simon Fraser University, TODD R GINGRICH, Northwestern University — We generalize the link between fluctuation theorems and thermodynamic uncertainty relations by deriving a bound on the variance of fluxes that satisfy an isometric fluctuation theorem. The resulting bound, which depends on the system's dimension $d$, naturally interpolates between two known bounds. The bound derived from the entropy production fluctuation theorem is recovered for $d=1$, and the original thermodynamic uncertainty relation is obtained in the $d \to \infty$ limit. We show that our result can be generalized to order parameters in equilibrium systems, and we illustrate the results on a Heisenberg spin chain.

1:51PM B24.00014: Quantum Thermodynamics of a Spin one System

MULUGETA BEKELE (Presenter), Addis Ababa Univ — We take a collection of large non-interacting spin one particles, each having an electric dipole of magnitude $m$ in contact with a heat reservoir at temperature $T$. We apply a strong static electric field, $E_z$, to the system along a $z$-axis causing three level split energy values. In addition to the strong electric field, we apply a weak AC electric field in the $xy$-plane. This weak field induces transitions between the three levels. Through a given protocol $\lambda(t)$, the system is taken from an initial state $F(T,\lambda_i)$ to a final non-equilibrium state with parameter $\lambda_f$. We analytically obtain the expressions for the probability amplitudes for a transition from one particular initial state to the other two final states. This will enable us to find the work distributions of a finite-time process of taking the system from one initial state to other final states. This finite-time non-equilibrium process will then enable us to extract equilibrium thermodynamic quantities like free energy from non-equilibrium process, which is what we call Jarzanski equality and its relation to the second law of thermodynamics.

*ISP Uppsala University, Uppsala, Sweden for the financial support
B24.00015: Stochastic Thermodynamics with both Even and Odd Controlling Parameters*  
ZHANCHUN TU (Presenter), Beijing Normal Univ — Shortcuts to isothermality inspired development of stochastic thermodynamics with both even and odd controlling parameters, was developed to understand nonequilibrium phenomena of small systems. It is found that the definition of heat and the microscopically reversible condition are incompatible for small systems with odd controlling parameters. Such a contradiction also leads to a revision to the fluctuation theorems and nonequilibrium work relations. By introducing adjoint dynamics, we find that the total entropy production can be separated into three parts, with two of them satisfying the integral fluctuation theorem. Revising the definition of heat and the microscopically reversible condition allows us to derive two sets of modified nonequilibrium work relations, including the Jarzynski equality, the detailed Crooks work relation, and the integral Crooks work relation.

Reference  

*National Natural Science Foundation of China (Grants No. 11675017)

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B25 GSNP DPOLY: From Responsive Matter to Actuated Structures 402 - Dong Yan, Ecole Polytechnique Federale de Lausanne - Tag(s): Focus

11:15AM B24.00001: Decentralized reinforced learning of emergent behavior in robotic matter [Invited]  
GIORGIO OLIVERI, LUUK CAROLUS VAN LAAKE, JOHANNES OVERVELDE (Presenter), AMOLF — Soft robots have the potential to be more robust, adaptable, and safer for human interaction than traditional rigid robots. State-of-the-art developments push these soft robotic systems towards applications such as rehabilitation and diagnostic devices, exoskeletons for gait assistance, and grippers that can handle delicate objects. However, despite these exciting developments, their inherent non-linear response limits the number of actuators that can be accurately controlled simultaneously, especially in complex or unknown environments. To enable modularly scalable and autonomous soft robots we have developed a new type of soft robot that is assembled from identical 1D building blocks with embedded pneumatic actuation, position sensing and computation. In this robotic system, motility might emerge from local interactions, rather than from a central brain. Here we shows that we are able to implement decentralized learning in this system. Using a stochastic optimization approach, each building block individually adjusts its actuation phase continuously, in order to find the fastest way to move in a predefined direction. We show that even for larger number of modules, this robotic system is still capable of learning. As a result, the system is robust to damage, as it will adjust its behaviour accordingly.
11:51AM B25.00002: Collective behavior of BOBbots, a robotic active matter system
SHENGKAI LI (Presenter), BAHNISIKHA DUTTA, DANA RANDALL, DANIEL I GOLDMAN, Georgia Inst of Tech — We introduce BOBbots (Behaving, Organizing, Buzzing Robots, named to honor the late Bob Behringer), a custom low-cost active matter system composed of disk-shaped “granular” robots. The robots are equipped with controllable vibration that can react to light and stress. The vibration couples to two bristles on the base of the robot which generates translation and rotation. The robots can attract each other via loosely constrained magnets in cavities on a robot's circumference. We first investigate the clustering of the collective which results from a competition between the attraction and driving. In experiments and discrete element method simulations, increasing magnet strength leads to a rapid increase in steady-state cluster size which saturates for sufficient attraction. The dynamics of this nonequilibrium system resemble those in an equilibrium lattice model. An algorithm by which robots decrease drive upon increased stress increases clustering rate at fixed magnet strength. Formation of clusters enables the collective to perform a task no individual can: transport of a free obstacle.

12:03PM B25.00003: Smarticle glider: Locomoting, spontaneous excitations in a shape changing active matter system* AKASH VARDHAN (Presenter), SHENGKAI LI, Physics, Georgia Institute of Technology, YUNBO ZHANG, Computer Science, Georgia Institute of Technology, KURT A WIESENFELD, DANIEL I GOLDMAN, Physics, Georgia Institute of Technology — Smarticles or smart active particles are 3 link robots which change their shape periodically through the actuation of the arms. Limited individually in their ability to translate or rotate in the current experimental setting, they exhibit interesting collective behavior (directed locomotion) as a result of stochastic mechanical interactions (W, Savoie et al., Science Robotics 2019). The glider, which is a two smarticle bound excitation, is the fundamental building block for these phenomena. It has a lifetime of about 90 periods and moves about 4 body lengths before dissociating. We seek to understand the mechanistic principle behind the creation of these states and their ensuing dynamics with an iterative map. Simulations reveal that for these excitations to locomote, there must be fluctuations in the coefficient of friction. Since the smarticles only interact with each other via collisions, gliders are essential to keep a cloud of smarticles connected and hence harness their collective behavior.
Reference:

*School of Physics, Georgia Institute of Technology
12:15PM B25.00004: Photothermal actuation of a fluidic soft muscle*  LUKE GOCKOWSKI
(Presenter), Department of Mechanical Engineering, University of California, Santa Barbara, SERENA
SESHADRI, Department of Chemistry, University of California, Santa Barbara, JAEJUN LEE, Department of
Mechanical Engineering, University of California, Santa Barbara, MIRANDA SRODA, Department of
Chemistry, University of California, Santa Barbara, MATTHEW HELGESON, Department of Chemical
Engineering, University of California, Santa Barbara, JAVIER READ DE ALANIZ, Department of Chemistry,
University of California, Santa Barbara, ELLIOT W. HAWKES, MEGAN VALENTINE, Department of
Mechanical Engineering, University of California, Santa Barbara. — Despite innovations in materials and
fabrication schemes that have enabled impressive soft robotic structures and devices, most soft
robots remain tethered to cumbersome power sources (e.g., compressed gas) and/or require
unwieldy valving. Developing soft robots capable of untethered actuation and remote control
requires new methods of actuation. Compared to conventional power and control, visible light
offers several advantages—including wireless remote control, spatial (~200 nm) and temporal
(~ms) precision, and tunability (e.g., wavelength, intensity). Here, we exploit a novel class of
photoswitches, donor-acceptor Stenhouse adducts (DASAs), for the remote actuation of soft
muscles. Guided by studies of DASA’s unique photoswitching and photothermal properties, we
achieve the remote actuation of a soft muscle via controlled photothermal phase changes
without valves or internal controls. Further, we demonstrate the force output of this muscle and
its promise for actuation in multi-scale soft robots.

*Primary: USARO under W911NF-19-2-0026. Partial: NSF MRSEC through DMR-1720256, and ONR
MURI through N00014-18-1-2624. Views and conclusions are those of the authors and should not
be interpreted as representing official policies, either expressed or implied, of the U.S.
Government.
Programmable Photothermal Actuation using Novel Negative Photochromic Donor-Acceptor Stenhouse Adduct (DASA) Polymers* JAEJUN LEE (Presenter), Department of Chemistry, Department of Mechanical Engineering, University of California at Santa Barbara, MIRANDA SRODA, Department of Chemistry, University of California at Santa Barbara, YOUNGHOON KWON, Department of Mechanical Engineering, University of California at Santa Barbara, SARA EL-ARID, SERENA SESHADRI, Department of Chemistry, University of California at Santa Barbara, LUKE GOCKOWSKI, ELLIOT W. HAWKES, Department of Mechanical Engineering, University of California at Santa Barbara, JAVIER READ DE ALANIZ, Department of Chemistry, University of California at Santa Barbara, MEGAN VALENTINE, Department of Mechanical Engineering, University of California at Santa Barbara — Light-driven actuation has significant advantages including untethered operation, precise spatiotemporal activation, and the ability to operate in complex surroundings without significant modification. Here, we use a new class of molecular photoswitches, called donor-acceptor Stenhouse adducts (DASAs), to generate a novel but conceptually simple photoresponsive polymer bilayer actuator, capable of repeatedly lifting a load against the force of gravity. We will present a synthesis pathway for chemically attaching DASA conjugates to poly(hexyl methacrylate) through norbornadiene click chemistry, and will demonstrate actuator performance. Importantly, we can leverage the different time scales of photothermal and photochemical responses of DASAs to achieve dynamic material control, including the ability to switch on and off actuation. Our results highlight the promising benefits of high molar absorptivity, negative photochromism, and visible light absorption of DASAs for actuation.

*Primary: USARO under W911NF-19-2-0026. Partial: NSF MRSEC through DMR-1720256, and ONR MURI through N00014-18-1-2624. Views and conclusions are those of the authors and should not be interpreted as representing official policies, either expressed or implied, of the U.S. Government.
The realm of magnetorheological elastomers: experiments, theory and instabilities

KOSTAS DANAS (Presenter), CNRS, Ecole Polytechnique — In this talk, I will present a broad overview of our work on magnetorheological elastomers (MREs) including experiments, theory and numerical implementation. MREs are composite materials comprising metallic soft (e.g. iron) or hard (e.g. NdFeB) magnetic micron-sized particles. The latter have been called h-MREs. Out of these materials one can devise a number of interesting meso- and macrostructures, slender or not that can lead to a number of functionalities such as surface patterning, negative or positive swelling, network activation, negative Poisson ratio, evolving anisotropic magnetic properties, hierarchical buckling and others. The main idea lies in the ability to drive the systems by using two external loads, i.e. mechanical and magnetic ones and in particular to harness the resulting instabilities that are natural in magnetic structures. This allows, in turn, to reach a critically stable state by applying one of the fields (e.g. mechanical) and trigger patterning and instabilities at low energetic cost with the other (e.g. magnetic). As an example, we will discuss in more detail a recently obtained pattern, called crinkling. This pattern appears in slender magnetic structures such as MRE films bonded to soft (non-)magnetic substrates that are subjected to a combination of mechanical pre-compression and transverse to the film magnetic loads. In particular, the initial wrinkles evolve into crinkles, a bifurcation mode that is defined by the accompanied curvature localization and significant shearing of the side faces of the wrinkled geometry. Interestingly, the presence of the magnetic field prohibits the formation of creases and folds. The presentation will close with recent results on h-MREs and their potential ability to lead to unconventional responses mechanically and magnetically.

*ERC Starting Grant MAGNETO

Understanding the kinetic arrest in deswelling microgels

SVETOSLAV NIKOLOV, ALBERTO FERNANDEZ-NIEVES, ALEXANDER ALEXEEV (Presenter), Georgia Inst of Tech — Biofriendly microgels, like PNIPAM and dextran, find numerous applications as microscopic delivery agents for advanced therapies of cancer, diabetes, and bacterial infections. We use mesoscale computer simulations to model the deswelling kinetics of spherical microgels. Deswelling occurs as the result of gel-solvent phase separation, leading to the hydrogel network collapse and in certain conditions, to the formation of a dehydrated “skin layer” at the gel-solvent interphase. This dehydrated skin layer hinders solvent flow from the microgel interior which arrests the kinetics of the collapsing microgel. We examine the conditions at which the skin forms and probe how these conditions depend on the microgel size, porosity, and micromechanics. These findings can be useful for designing microgel based drug release systems with controlled release profiles, leading to more effective disease treatments.

*This work is supported by NSF DMR-1255288 and DMR-1609841. Simulations were done using the Extreme Science and Engineering Discovery Environment (XSEDE) supported by NSF ACI-1548562.
1:27PM B25.00008: Tunable buckling strength of magnetically active elastomeric shells
DONG YAN (Presenter), MATTEO PEZZULLA, Ecole Polytechnique Federale de Lausanne, LILIAN CRUVEILLER, Ecole Polytechnique, PEDRO REIS, Ecole Polytechnique Federale de Lausanne — It has long been recognized that the buckling of shell structures is highly sensitive to material or geometric imperfections, leading to observed critical loads that are significantly lower than classic predictions. In this class of problems, the knockdown factor is defined as the ratio between the experimentally measured critical load and the classic theoretical prediction. This knockdown is typically regarded as an intrinsic property of the structure since the type and distribution of defects are encoded into the shell during fabrication. Here, we demonstrate the ability to actively tune the knockdown factor of pressurized spherical shells. We fabricate our spherical shells with a magneto-rheological elastomer (MRE) using a coating technique. The shells are first magnetized and then loaded by pressure under a uniform magnetic field. We find that, by adjusting the strength and polarity of the field, the knockdown factor of the magnetically active shells can be increased or decreased up to a maximum change of 30%. As such, we can externally tune their intrinsic buckling strength, on-demand. An axisymmetric shell model is used to rationalize the experimental results on how the magnetic field interacts with the buckling of imperfect shells.

1:39PM B25.00009: Tailoring magneto-mechanical properties of NdFeB particle-filled soft elastomers*
DIPAYAN MUKHERJEE (Presenter), KOSTAS DANAS, LMS, CNRS, Ecole Polytechnique — This work investigates the possibilities of tailoring the magneto-mechanical properties of hard (permanent) magnetic NdFeB particle-filled soft magnetorheological elastomers by proposing novel microstructures. Our numerical computations for the mechanical response of various regular and chiral unit cells with a permanently magnetized elliptic inclusion show distinct features depending on the aspect ratio and the orientation of the inclusion. It is observed that the mechanical deformations are selectively preferred at certain directions, which make the magnetic inclusions align themselves along their easy axes, reducing the net magnetic moment. In particular, for the microstructural orientation angle of 30-60 degrees, the simple shear mode is observed to facilitate easy magnetic alignments and thus becomes energetically favorable over the uniaxial tension/compression mode. Moreover, the overall (effective) magnetic coercivity of these composites are found to reduce considerably with a softer elastomeric matrix, which, in turn, facilitate easy particle alignments.

*This work is supported by the European Research Council (ERC) grant agreement no. 636903—MAGNETO.
Magnetically triggered thin-film instabilities for surface pattern control*  
MATTHIAS RAMBAUSEK (Presenter), KOSTAS DANAS, Ecole Polytechnique — The study under consideration is concerned with instabilities of a thin magnetic film attached to a soft (magnetic) substrate under general biaxial precompression and transverse magnetic fields leading to complex two-dimensional surface patterns. This study builds upon previous experimental work on one-dimensional surface patterns through magneto-elastic loading. Our findings contribute a key ingredient for the design of haptic displays and more general applications of surface actuation. For the characterization of the instabilities of interest we conduct numerical studies using finite-element and Fourier discretizations for a wide range of in-plane prestresses and applied magnetic field. By virtue of these results we obtain stability maps which are an important input for subsequent numerical and experimental studies in the post-buckling regime.

*Funding: ERC Starting Grant MAGNETO

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B26 DBIO DSOFT DFD DPOLY: Mechanics of Cells and Tissues Across Scales II

Force generation and self-organization in mitosis* [Invited]  
MEREDITH BETTERTON (Presenter), University of Colorado, Boulder — Life on earth depends on cells’ ability to duplicate. In order to divide successfully, cells must solve fascinating physics problems. A key step in cell division is ensuring that each of the daughter cells inherits a single copy of the genetic material. In eukaryotes, a self-organized machine called the mitotic spindle physically move the chromosomes. The spindle is composed of microtubules, molecular motors, and associated molecules. We are using theory, simulation, and experiment to understand how the mitotic spindle self-assembles and achieves the correct size, and how the spindle organizes and moves chromosomes. This talk will discuss how force is generated by motors, crosslinkers, and chromosomes over time during mitosis to correctly assemble the spindle. Depending on the dynamics of spindle molecules and microtubule-chromosome attachments, overall spindle length can be relatively constant in time, or undergo large fluctuations. I will explain our current understanding of spindle length stabilization.

*NSF grants DMR-1725065, DMS-1620003. DMR-1420736; NIH grants K25GM110486, R01GM124371.
11:51AM B26.00002: Intrinsic time-scales of active forces control the dynamics of soft living matter  GRZEGORZ GRADZIUK (Presenter), GABRIEL TORREGROSA CORTÉS, CHASE BROEDERSZ, Ludwig Maximilian University of Munich — Living cells are crowded with active agents which consume energy and perform work on their surrounding environment, constantly keeping the system out of thermodynamic equilibrium. These locally exerted active forces are propagated to larger distances by the cytoskeleton and the cytoplasm. Such activity is believed to play an important role in vital intracellular processes such as transport. The active agents involved in these processes - molecular motors - are characterized by their intrinsic correlation time, typically of the order of seconds. While the significance of these correlation times is not well understood, we argue that they may be tuned to improve the efficiency of particular processes taking place in the cell. We investigate this by analyzing a model comprised of elastic network embedded in a viscous fluid and driven by a collection of stochastic, time-correlated forces. We show how the interplay between the correlation times of the active agents and the relaxation times of the system can lead to qualitatively different behaviors at different length scales.

12:03PM B26.00003: Mechanical properties of intermediate filament networks under compression*  BOBBY CARROLL (Presenter), MAHESH CHANDRASEKHAR GANDIKOTA, Syracuse University, IMAN ELBALASY, JOERG SCHNAUSS, JOSEF A. KAS, Leipzig University, JENNIFER SCHWARZ, ALISON PATTESON, Syracuse University — Cell motility is a fundamental process that contributes to building and maintaining tissues as well as the progression of diseases such as fibrosis and cancer. The material properties of cells and tissues are a central feature of this process. The mammalian cytoskeleton is made up of a network of (semi-)flexible biopolymers, including actin, microtubules, and intermediate filaments. While the mechanical responses of fibrous biopolymer networks to shear deformation have been studied in great detail, their response to uniaxial loading remains poorly understood. Here, we study the mechanical response of reconstituted polymer networks comprised of the intermediate filament proteins vimentin and keratin using a parallel-plate rheometer. Our results indicate that reconstituted vimentin and keratin networks stiffen under axial compression, with cation concentration mediating network crosslinking. This stiffening contrasts with other biopolymer networks which compression soften but coincides with the compression stiffening behavior of cells themselves. These results motivate future work in cytoskeletal mechanics as well as the general phenomenon of compression stiffening in biopolymer environments.

*We acknowledge partial support from NSF award number DMR-1832002.
12:15PM B26.00004: Cytoskeletal Regulation of Three-Dimensional Epithelial Cell Shape*
THERESA CHMIEL (Presenter), MARGARET GARDEL, University of Chicago — Three-dimensional force distribution within the actin cytoskeleton of epithelial tissue regulates cell shape. While two-dimensional cell shape has been well characterized and heavily studied, three-dimensional cell shape regulation is less well understood despite its critical role in large scale epithelial processes such as invagination. By examining the relationship between cell height, density and biological components of the actin cytoskeleton, we explore the mechanisms by which epithelial cells regulate shape and volume. We observe that while cell density is not a strong indicator of epithelial height, osmotic shock drastically decreases both tissue height and cell volume while leaving the lateral shape of cells in the tissue undisturbed.

*This research was supported by NIH RO1 GM104032 and the University of Chicago Materials Research Science and Engineering Center (NSF Division of Materials Research Grant 1420709)

12:27PM B26.00005: Physical limits to sensing material properties*
FARZAN BEROZ (Presenter), Univ of Michigan - Ann Arbor, DI ZHOU, Georgia Institute of Technology, XIAOMING MAO, DAVID LUBENSKY, Univ of Michigan - Ann Arbor — Constitutive relations describe how materials respond to external stimuli such as forces. All materials respond heterogeneously at small scales, which limits what a localized sensor can discern about the global constitution of a material. In this talk, I will present the limits to the precision of such constitutional sensing for sensors embedded in disordered media. Our results reveal how one can construct microscopic devices capable of sensing near these physical limits, e.g. for medical diagnostics. I will show how our theoretical framework can be applied to an experimental system by estimating a bound on the precision of cellular mechanosensing in a biopolymer network.

*This work was supported in part by the National Science Foundation Grants DMR1056456 (to D.K.L.), DMR 1609051 (to X.M.), EFRI-1741618 (to D.Z. and X.M.), a Margaret and Herman Sokol Faculty Award (to D.K.L.), and a Michigan Life Sciences fellowship (to F.B.).
The shape of an adherent cell spread on a surface depends upon the biophysical properties of the cytoskeleton. However these are controlled by biochemical circuits and ultimately by gene expression. While shape of a single cell is dynamic, enough evidence has accumulated that cells in the same state adopt shapes that are, in a statistical sense, similar to each other, and distinguishable from cells in different states. If we could understand the major determinants of cell shape, we may be able to infer aspects of cell state merely by observing cell shape. We have imaged thousands of cells in different experimental conditions and have developed a large number of morphological parameters to quantify cell shape and cytoskeletal morphology. Using these we show that quantifiers of cell shape and cytoskeletal texture can be used to discriminate between different cell states. Projections of the data to lower-dimensional shape space can be used to distinguish between similar and dissimilar changes in shape. Pharmacological drugs that perturb the cytoskeletal can help to identify some of the biochemical circuits that control cell shape. Linking results of our experiments and data analysis with previous molecular biology studies on cytoskeletal proteins that affect cell shape, coupled with mathematical modeling, allow us to deconstruct some of the determinants of cell shape.

*NSF PHY-1151454

During cancer cell migration, cells on a 2D surface experience uniform mechanical cues whereas in a fibrous 3D environment there exists heterogeneity at cellular and sub-cellular levels, leading to dramatically different invasion strategies. Here, we physically characterize morphodynamics (the temporal fluctuations of cell shape) rather than real-space migration alone. By studying morphodynamics, we show that 3D cell migration is accompanied by spontaneous and rapid shape changes regulated by the extracellular matrix (ECM), in contrast to 2D migration. We employ machine learning to classify cell shape into five different morphological phenotypes corresponding to different migration modes. We systematically characterize the phenotype evolutions including occurrence probability, dwell time, transition flux, and 3D migrational characteristics. By tuning ECM density, pore-size, and fiber-alignment, we show local mechanical influence on migration mode switching. We find mechanosensing mediated by rho-signaling is important to the resultant morphodynamics. We demonstrate cell morphodynamics as an information-rich biomarker that is directly regulated by cell mechanosensing and contributes critically to the cell motility.

*National Science Foundation, PHY-1844627
Switching between optimum substrate rigidity and focal adhesion reinforcement at the cell leading edge  

PARTHO SAKHA DE (Presenter), RUMI DE, IIISER Kolkata — It’s well known that substrate mechanical properties strongly influence cell behaviour and fate. There exists two well documented but contrasting responses of cells to substrate rigidity, namely the biphasic and the monotonic relationship of traction force and retrograde flow velocity with substrate stiffness. We have developed a theoretical model for the dynamics at the leading edge of a cell placed on a viscoelastic substrate, involving a pair of coupled reaction-diffusion equations. Motivated by experiments, the association and dissociation rates of focal adhesions are taken to be force dependent. Our model not only captures the experimentally observed stick-slip dynamics at the cell edge, but also can predict switching between both the biphasic relationship i.e. the presence of an optimum substrate stiffness where the retrograde flow is minimum and traction force is maximum; and the monotonic relationship between retrograde flow, traction force and substrate stiffness. Besides, our theory also elucidates the role played by substrate viscosity, predicts the presence of optimum viscosity as well as states the condition under which cellular rigidity sensing is lost.

Stick-slip dynamics of migrating cells on viscoelastic substrates  
P. S. De and R. De  

Mechanics of endocytosis under large osmotic pressure*  
RUI MA (Presenter), JULIEN BERRO, Molecular Biophysics and Biochemistry, Yale University — In this talk, I will discuss membrane deformations powered by a point force under the condition of high pressure and low tension, which is rarely studied but directly relevant for endocytosis in yeast cells with a cell wall. I will show that the force-height relationship of membrane deformations under this condition is drastically different from that under conditions of high tension and low pressure. In addition, the boundary conditions at the attachment points of the membrane with the cell wall have dramatic effects on the force-height relationship. In particular, if the membrane is allowed to freely rotate at the attachment points, proteins that induced membrane curvature can lift the membrane off the cell wall without any external forces. This result is in sharp contrast with the conclusion of a previous study which adopted boundary conditions that fix the angle between the membrane and the cell wall at the attachment points. I will also discuss possible ways to pull the membrane off the cell wall against the high osmotic pressure with a small amount of force that can be provided by actin polymerization.

*This research is supported by National Institutes of Health/National Institute of General Medical Sciences Grant R01GM115636.
1:51PM B26.00010: Plasticity in vertex model of epithelial tissues  MARKO POPOVIC (Presenter), VALENTIN DRUELLE, MATTHIEU WYART, École polytechnique fédérale de Lausanne — In order to properly develop living organisms are required to change and maintain shape. These properties exists in a class of materials called amorphous solids such as colloidal gels, emulsions and foams: they respond elastically when exposed to low external stress but at a critical value of stress they yield and permanently change shape, allowing them to retain the memory of past stresses. Could such plasticity play a role during biological morphogenesis? Motivated by this question in this work we study plastic properties of vertex model of epithelial tissues, in which mechanical properties of cells are prescribed and emerging tissue mechanics is obtained from their collective behaviour. We investigate mechanical properties of elementary plastic event, a so called T1 transition in which two pairs of cells exchange neighborship. We demonstrate that they are analogous to plastic events in amorphous solids and find that elastic interactions among T1 transitions lead to non-linear steady state rheology and mechanical stability in the vertex model that are the same as found in mesoscopic models of amorphous solids. Finally, we devise observables quantifying a ‘distance’ to the critical stress in flowing vertex model and epithelial tissues.

2:03PM B26.00011: Loops versus lines and the compression stiffening of cells  MAHESH CHANDRASEKHAR GANDIKOTA (Presenter), Syracuse University, KATARZYNA POGODA, Institute of Nuclear Physics, Polish Academy of Sciences, ANNE VAN OOSTEN, Leiden Academic Centre for Drug Research, Leiden University, TYLER ENGSTROM, Hobart and William Smith Colleges, ALISON PATTESON, Syracuse University, PAUL JANMEY, Institute for Medicine and Engineering, University of Pennsylvania, JENNIFER SCHWARZ, Syracuse University — Tissues exhibit a nonlinear phenomenon known as compression stiffening: an increase in moduli with increasing uniaxial compressive strain. Does such a phenomenon exist in single cells, which are the building blocks of tissues? One expects an individual cell to compression soften since the semiflexible biopolymer cytoskeletal network maintains the mechanical integrity of the cell. To the contrary, we find that mouse embryonic fibroblasts (mEFs) compression stiffen. To understand this finding, we uncover potential mechanisms for compression stiffening. First, we study a single semiflexible polymer loop modeling the actomyosin cortex enclosing a viscous medium modeled as an incompressible fluid. Second, we study a two-dimensional semiflexible polymer network interspersed with area-conserving loops, which are a proxy for vesicles and fluid-based organelles. Third, we study two-dimensional fiber networks with angular-constraining crosslinks. We find for the fiber network with area-conserving loops model that the stress-strain curves are sensitive to the packing fraction and size distribution of the area-conserving loops, thereby creating a mechanical fingerprint across different cell types. We make comparisons of these models with fibrin network experiments interlaced with beads.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B27 FIAP: Applications of Semiconductors, Dielectrics, and Complex Oxides 404 - Meeghage Perera, National Research Council
11:15AM B27.00001: Effects of residual stress on MEMS direction-finding sound sensors

MEEGHAGE PERERA (Presenter), RENATO RABELO, FABIO ALVES, GAMANI KARUNASIRI, Physics, Naval Postgraduate School — The hearing mechanism of the fly *Ormia Ochracea* has been studied and mimicked using micro-electromechanical system (MEMS) technology as an acoustic direction-finding sensor. A typical MEMS sensor consists of two wings connected by a bridge with the entire mechanical structure connected to a substrate. The sensors employed in this work were fabricated on a silicon-on-insulator (SOI) substrate using MEMSCAP’s SOIMUMPS process which found to generate a residual-stress induced curvature on the wings. This reduces the overlap between the wing and substrate comb fingers, which affects the electronic signal output. An in-depth study was performed to understand the stress dependence on geometry and substrate and device configurations. A set of sensors fabricated with different configurations were systematically studied using optical profilometry and scanning electron microscopy. The measured profiles show offsets between the edge of the wings and substrates as high as 40 um for metalized devices and as low as 10 um for non-metallized devices. The curvatures of the sensors were fitted using finite element models to provide the stress values for each configuration and designing parameters to minimize this effect in future designs.

*Supported by ONR and NRP

11:27AM B27.00002: Alloying hexagonal/orthorhombic Ga$_2$O$_3$ with Al$_2$O$_3$*  

SIERRA SEACAT (Presenter), Department of Physics & Astronomy, University of Kansas, JOHN LYONS, Center for Computational Materials Science, US Naval Research Laboratory, HARTWIN PEELAERS, Department of Physics & Astronomy, University of Kansas — Ga$_2$O$_3$ is a wide-band-gap semiconductor with promising applications in high-power devices and UV photodetectors. It occurs in several polymorphs, with monoclinic β-gallia the thermodynamically stable phase. Other polymorphs of Ga$_2$O$_3$ can be stabilized as well, but are less studied. The ε- and κ-polymorphs are of interest as they possess ferroelectric properties and exhibit large spontaneous electrical polarizations. Here we use density functional theory with hybrid functionals to elucidate how alloying with Al$_2$O$_3$ can be used to modify the structural and electronic properties of Ga$_2$O$_3$. We focus on tuning lattice constants and band gaps as a function of Al concentration. We also report the absolute alignments of valence and conduction bands. Our quantitative results can be used to guide experimental design of new devices.

*Work supported by the Office of Naval Research through the Naval Research Laboratory’s Basic Research Program.
11:39AM B27.00003: Nanomaterials-based Color-Detection via Machine-Learning Algorithms* DAVOUD HEJAZI (Presenter), SHUANGJUN LIU, AMIRREZA FARNOOSH, SARAH OSTADABBAS, SWASTIK KAR, Northeastern University — Some of the major challenges in optical spectrum estimation include the necessity to create an array of thousands of identical photodetectors, or intricate mechanical systems that make the estimation system bulky and expensive. Using the spectral transmittance of an array of 11 solution-processed nanomaterial thin film filters fabricated from two layered semiconducting materials, Molybdenum-Disulfide and Tungsten-Disulfide, we have estimated the wavelength of any incoming light in a wide spectrum range. By applying machine learning techniques we have used the variations in spectral transmittance of nanomaterials as the alternative method for optical spectrum estimation. We have studied the efficacy of various machine learning algorithms including k-nearest neighbors, artificial neural networks, support vector machines, and Bayesian statistics in spectrum estimation problem and identified the key advantages and limitations of each algorithm for real-time applications such as accuracy and speed. Furthermore, we have modeled the temporal drift of filters' spectral transmittance over a period of one year and showed that it is possible to overcome the drift-induced inaccuracies over time using a modeled drift function.

*NSF ECCS 1351424
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11:51AM B27.00004: SiGe Devices with High-k Dielectric Gates JENNIFER DEMELL (Presenter), GREGORY STEPHEN, CHOMANI K. GASPE, CHRISTOPHER RICHARDSON, ADAM FRIEDMAN, Laboratory for Physical Sciences — SiGe is an attractive material for future advanced electronic devices desired for beyond Moore’s law high performance computing. In particular, for spintronic devices, it offers extremely high mobilities that can lead to long spin diffusion lengths and a spin-orbit coupling that can be used to control spin relaxation in spin valves—a prerequisite for any spinFET device. Moreover, it is amenable to scaling and is compatible with most commercial device fabrication facilities in foundries. Here, we grow a compressively strained Ge quantum well with relaxed Si$_{0.2}$Ge$_{0.8}$ barriers using molecular beam epitaxy. We fabricate devices to determine the basic properties of the films using both charge and spin state variables. We perform a systematic study to create a method of growing high-quality high-k dielectrics (hafnia and alumina) by atomic layer deposition to allow gating of the devices. We present magnetotransport results for both the charge- and spin-based devices from 3-300 K at fields up to 2.5 T.
A bifurcation study of the dynamics of TaO memristors

YURIY PERSHIN (Presenter), Department of Physics and Astronomy, University of South Carolina, VALERIY SLIPKO, Institute of Physics, Opole University — Pulse-driven memristors (resistance-switching cells) are interesting from the dynamical system point of view. When driven by periodic alternating-polarity pulses, their time-averaged dynamics may converge to fixed-point attractors [1]. Recently, we have shown that the maximum number of stable fixed points in a broad range of popular memristor models is one [2]. Here, we analyze the pulse-driven dynamics of tantalum oxide memristors using a sophisticated device model developed in Ref. [3]. Our main finding is the identification of a driving regime when two stable fixed points exist simultaneously [4]. To the best of our knowledge, such bistability is identified in a single memristor for the first time. Bifurcation curves separating pulse parameter regions corresponding to 0, 1, or 2 stable fixed points have been found analytically. Our results can be tested experimentally and are expected to be useful in future memristor circuit designs.


Parametric Coupling in Aluminum Nitride Lamb Wave Devices Through a Nonlinear Elastic Modulus

JOSEPH SCHNEIDER (Presenter), TING LU, SIDHANT TIWARI, XIATING ZOU, AJIT MAL, ROBERT CANDLER, YUANXUN ETHAN WANG, GREG P CARMAN, University of California, Los Angeles — Parametric coupling was intensely studied in the 1950s where a time varying circuit parameter (i.e. capacitance or inductance) is used to provide frequency conversion, allowing energy supplied at one frequency to be converted to another. The main advantage of this process is its low noise characteristic and is a promising step forward for low noise radio frequency (RF) devices. However, the realization of small devices relying on a time varying circuit parameter is difficult for lower frequency applications (100MHz – 1GHz) due to the long electromagnetic wavelength. In this research, Aluminum Nitride (AlN) Lamb wave devices are investigated as an option for parametric coupling in acoustic waves, significantly reducing the size of devices in the desired frequency range.

AlN Lamb wave devices are modeled, fabricated, and tested. Results show successful parametric mixing in the devices at both an up converted frequency and down converted frequency. The output power of the mixed signal is linearly dependent on the carrier power until gain compression is reached. A circuit model developed closely matches the experimental data. These devices provide evidence for next generation RF components that are 5 orders in magnitude smaller than the current state of the art.

*EFRI NewLaw no. 1641128
Evidence for ferroelectric polaron in lead halide perovskites

XIAOYANG ZHU (Presenter), Columbia Univ — Lead halide perovskites are characterized by dielectric responses and phonon dynamics resembling those of liquids. We show that the dielectric function in the THz region in this class of materials may lead to dynamic and local ordering of polar nano domains by an extra electron or hole, resulting a quasiparticle which we call a **ferroelectric large polaron**, a concept similar to solvation in chemistry. Compared to a conventional large polaron, the collective nature of polarization in a ferroelectric large polaron may give rise to order(s)-of-magnitude larger reduction in the Coulomb potential. We show that the shape of a ferroelectric polaron resemble that of a Belgian waffle. Using two-dimensional coherent phonon spectroscopy, we directly probe the energetics and local phonon responses of the ferroelectric large polarons. We find that that electric field from a nascent e-h pair drives the local transition to a hidden ferroelectric order on picosecond time scale. The ferroelectric or Belgian waffle polarons may explain the defect tolerance and low recombination rates of charge carriers in lead halide perovskites, as well as providing a design principle of the “perfect” semiconductor for optoelectronics.

Surface structure and electronics of all-inorganic halide perovskites

**CsPbI\textsubscript{3}: A first-principles study of surface reconstructions**

AZIMATU SEIDU (Presenter), PATRICK RINKE, Applied Physics, Aalto University, JINGRUI LI, Xi'an Jiaotong University — The all-inorganic halide perovskite CsPbI\textsubscript{3} is emerging as a promising perovskite solar cell (PSC) material with a power conversion efficiency of 18%. To further improve the efficiency and stability of CsPbI\textsubscript{3}-based PSCs, better knowledge of the materials surface and interface properties is required. In this work, we use density-functional theory and atomistic thermodynamics to calculate the surface phase diagrams of the (001) surfaces of CsPbI\textsubscript{3} in the Pm-3m (α), P4/mbm and Pnma (γ) phases. We consider different add-atom and missing-atom reconstructions and investigate different growth regimes. For stable surface reconstructions in the surface phase diagram, we then calculate the electronic structure. Our results indicate that surfaces with CsI terminations, including the clean surface, are more stable. Surfaces with missing Pb atoms exhibit a unipolar self-doping behaviour with Cs and I atoms inducing transition energy levels in the valence and conduction bands, respectively. Even though the removal and addition of CsI and PbI\textsubscript{2} complexes leads to considerable surface reconstructions, they remain electronically neutral and do not donate charge to the valence or conduction band.

*1. Finnish Academy of Science and Letters
2. Academy of Finland
3. Novel Materials Discovery (NOMAD)*
12:51PM B27.00009: Local Magnetic Field Effect on InSb Nanowire Devices  
YIFAN JIANG (Presenter), Univ of Pittsburgh, VINCE VAN DE SANDE, ELINE DE JONG, SASA GAZIBEGOVIC, GHADA BADAWY, ROY OP HET VELD, ERIK BAKKERS, Eindhoven University of Technology, SERGEY M FROLOV, Univ of Pittsburgh — Devices based on InSb nanowires are platforms for various of experiments, including quantum point contacts, quantum dots and Majorana zero modes. In most of such experiments, when a magnetic field is necessary, a large superconducting solenoid magnet is used to produce a global field. However, this homogenous magnetic field may limit device architecture. Instead of producing a global magnetic field, we can produce magnetic field locally by placing micro-magnets beside nanowire devices. In our experiment, we fabricate CoFe micromagnets next to InSb nanowire devices which also have Ti/Au ohmic contacts. Hysteretic magnetoresistance with sharp switches is observed, indicating penetration of local magnetic field from CoFe micromagnets into the nanowire. We also estimate that the magnitude of the local magnetic field into the InSb nanowire is several tens of mT. This successful demonstration of local magnetic field effect may bring a new approach for scalable topological computing.

1:03PM B27.00010: Comparison of spin photocurrent in devices based on in-plane or out-of-plane magnetized CoFeB spin detectors  
PIERRE RENUCCI (Presenter), Institut National des Sciences Appliquees de Toulouse, XIAODI XUE, LAIPAN ZHU, WEI HUANG, YU LIU, YANG ZHANG, XIAOLIN ZENG, JING WU, BO XU, ZHANGUO WANG, YONGHAI CHEN, Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, Beijing Key Laboratory of Low Dimensional Semiconductor Materials, WEIFENG ZHANG, Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing 100083, China, XAVIER MARIE, Institut National des Sciences Appliquees de Toulouse, YUAN LU, Université de Lorraine, Institut Jean Lamour, UMR CNRS 7198, campus ARTEM, 2 Allée André Guinier, 54011, Nancy, France — We have measured a helicity-dependent photocurrent at zero external magnetic field in a device based on a semiconductor quantum well embedded in a \textit{p-i-n} junction. The device is excited under vertical incidence with circularly polarized light. The spin filtering effect is evidenced in the temperature range 77–300 K owing to a CoFeB/MgO spin filter with \textit{out-of-plane} magnetization in remanence. The helicity-dependent photocurrent is explored as a function of the temperature and bias. These characteristics are compared with those of a spin photocurrent device with \textit{in-plane} magnetized CoFeB/MgO spin filter, excited under oblique incidence with circularly polarized light. In contrast to the in-plane spin filter device, the circularly polarized light asymmetry of the photocurrent in the out-of-plane device depends weakly on the external bias. The two devices are sensitive to the spin filtering of either the in-plane ($S_x$) or out-of-plane ($S_z$) photogenerated electron spin in the semiconductor quantum well. The photocurrent results can be explained by the Dyakonov-Perel electron spin-relaxation mechanism. Our study reveals the large spin relaxation anisotropy in III-V zinc-blende quantum wells in the presence of a vertical electric field. [1] Phys. Rev. B 100, 045417 (2019)
1:15PM B27.00011: Characterization of quantum tunneling devices by controlled current pulses
EDGAR J PATINO (Presenter), LEONARDO RIOS E, University of the Andes — Quantum tunneling devices constitute a prominent research area due to their use in fundamental and applied research investigations such as superconducting, magnetic and spintronic devices. The main difficulties in fabrication of such devices relies on two fronts directly related with; tunnel barrier quality i.e. absence of pinholes or hot spots, and low dissipation within the tunnel barrier material. A good tunnel barrier quality usually requires an oxygen plasma with pronounced uniformity and long oxidation time. Regarding the minimization of dissipation, in the present work, we show the development of a characterization technique based on controlled current pulses, which significantly reduces heat dissipation and thus allows a significant increase in the Tunnel Junctions lifetime. Acquiring data this way permits to reach higher tunneling current values compared to the ones obtained by standard DC characterization techniques, which are customary used in tunnel junction experiments.

*This work was funded by“Programa Nacional de Ciencias Basicas” COLCIENCIAS(No.120452128168),“ConvocatoriaProgramas2012”Vicerrectoria de Investigaciones, and Departamento de física of Universidad de los Andes (Bogota,Colombia)

1:27PM B27.00012: Topology-optimized Metal-Semiconductor Hybrid Structures to obtain Optimal Extraordinary Magnetoresistance
DEBANIK DAS (Presenter), SATHWIK BHARADWAJ, L RAMDAS RAM-MOHAN, Department of Physics, Worcester Polytechnic Institute — Semiconductor wafer with metallic inclusions generates extraordinary magnetoresistance (EMR) response [1]. This effect has found applications in high sensitivity magnetic sensors, and smaller magnetic read heads. Since its inception, efforts have been made to increase magnetoresistance through different choices of materials, by altering location of contacts, filling factor, and shape of the device. However, a systemic study to optimize topology of the metallic inclusions has not been considered in the literature. Here, we employ a topology optimization scheme based on the level set function. For evolution of the level set curve, topological derivative is used as the sensitivity term in the Hamilton-Jacobi equation. In contrast to conventional homogenization based methods, this optimization scheme will not produce gray region in the metal-semiconductor boundary. We are also able to control the complexity of the structure to design realistic geometries for fabrication of the physical prototype. The optimized geometry is robust and independent of the initial configuration. When combined with material optimization, this algorithm manifests a potential for significant improvements in EMR technology.

ARCHIT DHINGRA (Presenter), Physics and Astronomy, University of Nebraska - Lincoln, PAVLO V. GALIY, Electronics, Ivan Franko L'viv National University, LU WANG, CAS Key Lab of Materials for Energy Conversion, University of Science and Technology of China, TARAS M. NENCHUK, Electronics, Ivan Franko L'viv National University, ANDREW J. YOST, Physics, Oklahoma State University-Stillwater, WAI-NING MEI, Physics, University of Nebraska-Omaha, PETER A DOWBEN, Physics and Astronomy, University of Nebraska - Lincoln — In₄Se₃ (001) is a novel n-type semiconductor with great potential for 2D material phototransistors and beyond CMOS electronics. X-ray photoemission spectroscopy (XPS) measurements indicate that In₄Se₃ (001) system terminates in In (and not Se). These results disagree with density functional theory, which indicates that the Se termination of In₄Se₃ (001) is more stable. The interface between In₄Se₃ (001) and evaporated Au indicates toward the existence of Schottky barrier. This is very different from the interface between Au and TiS₃ (001), which exhibits Ohmic behavior. Additionally, the shift in binding energy (due to a barrier height) shows up only in one of the In core level photoemission components that is nearest to the interface.

This research was supported by the National Science Foundation (NSF), through grants NSF-ECCS 1740136, as well as by the nCORE, a wholly owned subsidiary of the Semiconductor Research Corporation (SRC), through the Center on Antiferromagnetic Magneto-electric Memory and Logic task #2760.002.

CHANDRASEKAR SIVAKUMAR (Presenter), GANG-HAN TSAI, MON-SHU HO, Department of Physics, National Chung Hsing University — Resistive memory is one of the promising next generation nonvolatile memories with advantages over other emerging nonvolatile memories like DRAM, PCRAM, CBRAM etc. Dielectric thin films as the resistive switching material have been studied extensively through the scientific community. In this study, we have taken advantage of controlled electron flow in 2D and 1D materials to study the resistive switching. High-density single crystalline β-Ga₂O₃ 2D-nanoleafs and 1D nanowires on Si (100) substrate are grown by vapor-liquid-solid growth technique. The structural features are explored by SEM, TEM and XRD analysis. The elemental compositions and binding characteristics are confirmed by the EDS spectrum from FESEM and TEM analysis and XPS respectively. The photoelectrical property is studied by Raman spectroscopy and absorption spectroscopy. Here we have compared the resistive switching performance of a single 2D β-Ga₂O₃ nanoleaf and 1D β-Ga₂O₃ nanowire ReRAM devices. The switching mechanism of both 1D and 2D nanostructures are governed by the oxygen migration between two electrodes by the formation and rupture of conducting filaments.

Keywords: Resistive memory, β-Ga₂O₃, nanoleaf, nanowire, VLS growth

Innovation and Development Center of Sustainable Agriculture,NCHU and MOST, Taiwan.
11:15AM B28.00001: Flow of concentrated and highly polydisperse emulsions* [Invited] Eric Weeks (Presenter), Yonglun Jiang, Joaquim Clara-Rahola, Emory University — We study experiments and simulations of highly polydisperse emulsions under shear flow. By highly polydisperse, we mean with the largest droplet diameters being as much as ten times the smallest diameters. We’re studying how to best define and quantify non-affine motion in these highly polydisperse samples — motion where droplets move with displacements distinctly different from their neighbors, or from the overall imposed shear flow. The largest droplets typically move affinely, as if they are in a simple effective fluid formed by the other droplets. In contrast, the smallest droplets often move non-affinely. Additionally, we quantify how the non-affine motion diminishes as a function of droplet size. Our main conclusion is that highly polydisperse samples behave qualitatively differently than weakly polydisperse samples.

*NSF (CBET-1804186).

11:51AM B28.00002: Fingering in dense suspensions* [Invited] Sungyon Lee (Presenter), University of Minnesota — We experimentally inject silicone oil into the mixture of oil and non-colloidal particles inside a Hele-Shaw cell, to investigate the connection between miscible fingering and the flow structure that develops inside the dense suspension. Previous studies with pure fluids have demonstrated that the onset of miscible fingering coincides with the transition from a smooth tongue-like structure to a sharp front between invading and defending fluids inside the thin gap. Our current experiments with suspensions reveal the same general behavior at the onset of miscible fingering, which we capture qualitatively using a continuum model. However, beyond the onset, we observe distinctly different morphologies of miscible fingering, which depend on the ratio of the gap thickness to particle diameter. We present the new quantitative measurements that highlight these differences and discuss how the wall confinement may alter the particle dynamics and the resultant fingering patterns.

*National Science Foundation through the University of Minnesota MRSEC (DMR-1420013)
The mixing of a powder of 10- to 50-μm primary particles into a liquid to form a dispersion with the highest possible solid content is a common industrial operation. Building on recent advances in the rheology of such “granular dispersions,” we study a paradigmatic example of such powder incorporation: the conching of chocolate, in which a homogeneous, flowing suspension is prepared from an inhomogeneous mixture of particulates, triglyceride oil, and dispersants. Studying the rheology of a simplified formulation, we find that the input of mechanical energy and staged addition of surfactants combine to effect a considerable shift in the frictional jamming volume fraction of the system, thus increasing the maximum flowable solid content. We discuss the possible microscopic origins of this shift, and suggest that chocolate conching exemplifies a ubiquitous class of powder–liquid mixing.

*We thank Mars Chocolate UK Ltd. for initiating and funding part of this work. Other funding came from Engineering and Physical Sciences Research Council Grants EP/J007404/1 and EP/N025318/1. Research at New York University was supported partially by the Materials Research Science and Engineering Centers Program of the National Science Foundation under Award DMR-1420073.
Suspensions of non-Brownian particles in complex fluids (hereafter complex slurries) are relevant in industrial processes (e.g. waste disposal, concrete, drilling muds, metalworking chip transport, and food processing) and in natural phenomena (e.g. flows of slurries, debris, and lava). It is also relevant to mention that some biological and smart materials can be designed from various suspensions, drawing attention to applications in physiology, bio-locomotion and shock absorbers. This countless number of suspensions has a wide range of nonlinear rheological behaviors, such as shear thinning, shear thickening, shear banding, yield stress, and finite normal stress differences even when inertia is negligible.

This talk will introduce an array of experimental and modeling techniques that my research team uses to investigate rheological properties and fluid dynamical behavior of the complex slurries. The goal is to establish a continuum framework and refine it through a series of microstructure investigations. This continuum framework is formulated and explained via a mean field study, homogenization theory, as well as a computational study based on the Immersed Boundary Method. In addition, it will be presented that how confinement effects transition a suspension from one rheological behavior to another and how these observations can be explained beyond the framework of the mean field approaches. Finally, open questions will be disclosed, which must be answered in order to build a firm foundation for a long-term contribution to the area of complex slurries.

*NSF (Grant no. CBET-1554044-CAREER and Grant No. CBET-1641152), ACS PRF (Grant no. 55661-DNI9), NSERC (PDF-439036-2013), ANR-13-IS09-0005-01, ANR-17- CE07-0040-05

Force networks in shear thickening suspension [Invited] JEFFREY F MORRIS (Presenter), The City College of New York — From simulations shown to capture primary features of the shear thickening transition in suspensions -- with particles interacting through lubrication, short-range repulsive forces, and frictional contact forces -- we explore the microstructural development underlying this transition. In particular we study the statistics of the contact force network. Using methods of k-core analysis and persistent homology, we explore the role of the particle contact network connectivity, and will present signatures of the rheological transition in terms of both local and global measures of the connectivity.
11:15AM B29.00001: The Physics of Cold Active Matter: on how time-independent disorder affects the motion of self-propelled particles* [Invited] FERNANDO PERUANI (Presenter), University of Nice Sophia-Antipolis — Most examples of natural active matter systems, if not all, take place in heterogeneous media. Despite this, most experimental and theoretical efforts have focused on homogeneous media and the impact of environmental heterogeneities on individual and collective properties of active systems has remained, up to recently, unexplored. Here, we will see that the physics of active systems in heterogeneous media is fundamentally different from the one in homogenous environments. For instance, in heterogeneous environments, spontaneous particle trapping of particles and sub-diffusion can occur, while long-range order of two-dimensional polar active liquids is not possible. Furthermore, in the absence of dynamic noise, it is possible to show that when the equations of motion exhibit a Hamiltonian structure, particle trapping cannot occur, while the presence of attractors in these equations indicates the asymptotic convergence of particle trajectories to bounded areas in space, i.e. traps.

References:

*ANR project BactPhy, ANR-15-CE30-0002-01

11:51AM B29.00002: The motion of active colloids and their induced flow field at fluid interfaces MEHDI MOLAEI, NICHOLAS G CHISHOLM, JIAYI DENG, TIANYI YAO, JOHN CROCKER, KATHLEEN JOAN STEBE (Presenter), University of Pennsylvania — Colloid motion is altered by adsorption to fluid interfaces, allowing for boundary guidance or directed assembly. This is particularly interesting for colloidal motion driven by external fields (driven colloids) or for self-propelled objects (active colloids or swimmers). However, the influence of a fluid interface on these hydrodynamic phenomena and the 2-d flow field induced by the motion of these active colloids are relatively unexplored. Here we image the motion of passive tracer probes at the interface to discern displacement fields generated by (1) a microbead undergoing thermal motion, (2) a magnetic disk forced to translate at constant velocity, and (3) actively swimming bacteria. We also theoretically quantify the flows generated by interfacially trapped colloids by developing an appropriate flow singularity model for both driven and active colloids. We consider an ideal flat "clean" interface characterized solely by a uniform interfacial tension. We also consider an incompressible fluid interface, as can occur even for trace surfactant adsorption. Theoretical results are compared with experimental flow field. Our results will be useful in future work on the use of active colloids to direct and enhance transport at interfaces
12:03PM B29.00003: Hydrodynamic attraction of bacteria to gas and liquid interfaces*
ADIB AHMADZADEGAN (Presenter), SHIYAN WANG, PAVLOS P VLACHOS, AREZOO M ARDEKANI, Purdue Univ — Motile microorganisms often encounter solid and fluid boundaries. Understanding the underlying physics of their accumulation near these boundaries can impact a wide range of applications from biofilm formation to micro-robot design. We combine experiments and numerical simulations to investigate bacteria (Escherichia coli) attractions to various fluid-fluid interfaces. We show that the strongest cell accumulation occurs near the lowest viscosity ratio (gas interfaces). We develop a new theory based on Brownian dynamics including hydrodynamics and short-range physio-chemical interactions between bacteria and surfactant-laden interfaces and explain our experimental findings. We include higher order singularities in our hydrodynamic model and study their effects on bacterial orientations, trajectories, and accumulation.

*This work is partially supported by grants from the Gulf of Mexico Research Initiative and the National Science Foundation CBET-1604423.

12:15PM B29.00004: Non-Markovian active droplets*
ADRIEN IZZET (Presenter), Center for Soft Matter Research, New York University, RUBEN ZAKINE, ERIC VANDEN-EIJNDEN, Courant Institute, New York University, JASNA BRUJIC, Center for Soft Matter Research, New York University — Active droplets are a model system for the chemotactic dynamics of microbes. They propel themselves through solute-mediated interactions. Previously, we showed that the motion of small droplets (~30µm diameter) is akin to active rotational diffusion whose speed and persistence time can be tuned by changing the salt and surfactant concentrations, respectively (Izzet et al., arXiv:1908.00581, 2019). Here we show that the trajectories of larger droplets display complex non-Markovian behaviors, such as self-interacting dynamics, that require a more complicated model than rotational diffusion. These results indicate that our tunable swimmers are ideal candidates for the study of the departure from equilibrium to high levels of activity, on both the single-particle level and their collective behavior, including the motility-induced phase separation (MIPS).

*This work was supported by the Materials Research Science and Engineering Center (MRSEC) program of the National Science Foundation under Grants No. NSF DMR-1420073, No. NSF PHY17-48958, and No. NSF DMR-1710163.
12:27PM B29.00005: Stigmergy in active furrowers  MD IMARAN (Presenter), IITB-Monash Research Academy, RANGANATHAN PRABHAKAR, Monash University, RAGHUNATH CHELAKKOT, MANDAR M INAMDAR, Indian Institute of Technology Bombay — Stigmergy is the emergence of spatiotemporal coordination between agents through interactions mediated by their environment. Pheromone trail-following in ants is a well-known example. Recently, a mechanical form of stigmergy has been observed in colonies of motile bacteria that create networks of furrows as they advance over soft agar [Gloag et al., PNAS, 2015]. Vanguard rafts of bacteria mechanically deform the substrate to create a physical signal that other cells follow. Under certain conditions, extensive furrow networks emerge with a distinctive morphology that spans a broad range of length scales. It is possible that the formation of such a sparse network of furrows is a strategy to loosely colonize large areas with a small number of cells. We investigate the conditions under which extensive furrow networks emerge using simulations of self-propelled rods that furrow through a passive elastic or plastic medium. The structure of the furrow network appears to critically depend upon the clustering behaviour of active rods at the advancing edge, which, in turn, depends on substrate stiffness and the self-propulsion velocity of the rods. We attempt to explain our observations through a coarse-grained, but general, model of stigmergy.

12:39PM B29.00006: Slip and distance effects on the self-propulsion of catalytic microswimmers close to a wall  STEFANIA KETZETZI (Presenter), Leiden University, JOOST DE GRAAF, Utrecht University, RACHEL PAMELA DOHERTY, DANIELA JUTTA KRAFT, Leiden University — Catalytic microswimmers are typically found self-propelling parallel to substrates. Although experimental observations have so far hinted at non-negligible substrate effects on the swimmer velocity, a quantitative examination of the effect of the substrate is still lacking. In this talk, we will present quantitative measurements of the effect of the substrate on the velocity of Pt-coated model microswimmers. We will show that under otherwise fixed conditions the velocity depends on the substrate wetting angle, which in turn relates to the associated hydrodynamic slip length of the substrate. We will further demonstrate that our hypothesis on slip dependent velocities is not only supported by qualitative and scaling arguments, but also by our measurements on swimmer-wall separation distance.

Our findings provide further understanding on the swimming behavior of synthetic microswimmers. Such understanding is desirable for future applications that may require microscopic devices to self-propel in liquid environments in confinement and along boundaries.
12:51PM B29.00007: Measuring chaotic advection in a biological active nematic in viscous environments*  AMANDA TAN (Presenter), KEVIN A MITCHELL, LINDA S. HIRST, University of California, Merced — Active flows are commonly found in nature ranging from macro-scale (bird flocks and schools of fish), to the micro-scale (cytoplasmic streaming and bacterial colonies). The common theme among these active materials is the individual entities consume energy leading to large-scale collective motion and flows. A widely studied example is the microtubule/kinesin based active network which is highly tunable. When this non-equilibrium system is confined in 2D at the oil/water interface, active topological defects emerge generating chaotic flows where the microtubules are advected within the network. An avenue of interest in nonequilibrium systems is to observe the material's response to external changes in its environment. Prior research has shown that changing the viscosity of the oil in contact with the active network changes the velocity and morphology of the network. Increasing the viscosity increases the number density of defects and decreases the network velocity. We investigate how the external changes from viscosity affect various quantitative parameters from chaotic advection theory, such as local fluid stretching rates within the network and topological entropy calculated from defect braiding.

*NSF DMR 1808926
NSF MRSEC DMR 1420382
NSF-HRD-1547848

1:03PM B29.00008: Hydrodynamic interactions between passive colloids in an active bacterial bath*  SHREYAS GOKHALE (Presenter), JUNANG LI, Massachusetts Institute of Technology MIT, ALEXANDRE SOLON, Sorbonne University, JEFFREY GORE, NIKTA FAKHRI, Massachusetts Institute of Technology MIT — The dynamics of active particles has been a subject of intense scientific investigation owing to the complex nonequilibrium patterns observed in these systems. Nonequilibrium effects also have tangible consequences for interactions between active and passive objects, as evidenced by the spontaneous rotation of microscopic gears in suspensions of motile bacteria. Here, using video microscopy experiments and simulations, we show that motile bacteria have a profound impact on dynamical interactions between passive colloidal particles. By quantifying spatial velocity correlations and the short time pair diffusivity tensor for colloids, we show that bacterial motion leads to partial screening of long-ranged hydrodynamic interactions. Notably, for sufficiently dense bacterial suspensions, transverse velocity correlations develop a pronounced minimum at a characteristic length scale that is independent of the bacterial density, but depends on the bacterial species. We hypothesize that the observed length scale demarcates short-ranged interactions dominated by direct collisions between colloids and bacteria from long-ranged ones associated with hydrodynamics.

*S.G. thanks the Human Frontier Science Program (HFSP) for a cross-disciplinary postdoctoral fellowship
1:15PM B29.00009: Self-organization of swimmers drives long-range fluid transport in bacterial colonies*  XU HAORAN (Presenter), Department of Physics and Shenzhen Research Institute, The Chinese University of Hong Kong, JUSTAS DAUPARAS, DEBASISH DAS, ERIC LAUGA, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, YILIN WU, Department of Physics and Shenzhen Research Institute, The Chinese University of Hong Kong — Motile subpopulations in microbial communities are believed to be important for dispersal, quest for food, and material transport. Here, we show that motile cells in sessile colonies of peritrichously flagellated bacteria can self-organize into two adjacent, centimeter-scale motile rings surrounding the entire colony. The motile rings arise from spontaneous segregation of a homogeneous swimmer suspension that mimics a phase separation; the process is mediated by intercellular interactions and shear-induced depletion. Our findings present a unique form of bacterial self-organization that influences population structure and material distribution in colonies.

*We thank Howard C. Berg, Karine Gibbs, Daniel B. Kearns, Arnab Mukherjee, and Charles M. Schroeder for their kind gifts of bacterial strains, and Howard C. Berg for helpful comments. The work of H.X. and Y.W. was supported by the National Natural Science Foundation of China (NSFC 21473152; to Y.W.) and by the Research Grants Council of Hong Kong SAR (RGC Ref. No. GRF 14322316&14301915, CUHK Direct Grants 4053230&4053310; to Y.W.). This project has also received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement 682754 to EL).

1:27PM B29.00010: Linear instability and nonlinear dynamics of droplets and layers of active fluid*  DAVID STEIN (Presenter), Flatiron Institute, YUAN-NAN YOUNG, New Jersey Inst of Tech, MICHAEL JOHN SHELLEY, Courant Institute, New York University — Active suspensions are fluids with extra stresses from the energy-consuming activity of suspended particles. Coarse-grained continuum descriptions have successfully predicted instabilities and pattern formation observed in some experimental systems. In this work we focus on the effects of surface tension on the stability and nonlinear dynamics in droplets and layers of active fluid. Specifically we study the stability of a moving boundary between a viscous fluid and droplet- or layer-bound active suspension. Linear stability analyses predict parameter regimes for various dynamics such as rotation, self-propulsion, and chaotic dynamics. Weakly nonlinear analyses predict the equilibrium drop deformation as a function of activity magnitude in the suspension. Simulations of a small system of such active drops give insight into how the activity inside the drops dictates how they communicate with each other.

*Funding from Flatiron institute, part of Simons Foundation, is acknowledge.
1:39PM B29.00011: Swimming of active drops in confinements with external flows*  
RANABIR DEY (Presenter), CAROLA M. BUNESS, CHENYU JIN, CORINNA MAASS, Max Planck Institute for Dynamics and Self-Organization — Biological microswimmers commonly navigate through liquid flows in confinements, e.g. locomotions of spermatozoa in the reproductive tract and bacteria in blood vessels. Artificial microswimmers designed for drug delivery also swim in confinements having flows. So far, there are theoretical works explaining the dynamics of microswimmers in Poiseuille flow. However, there is little quantitative experimental data regarding swimming of active matter in confined microflows. Here, we elucidate the swimming behaviour of active drops in Poiseuille flow. The Marangoni stress dominated `self-propulsion' of these droplets serves as a model for studying the swimming hydrodynamics of microorganisms, specifically pushers like E. Coli. We quantitatively explain the upstream swimming and downstream tumbling motion of the active drops in externally imposed flows; we also provide a comparative analysis of the experimental data with the hydrodynamics based non-linear theory. We feel that understanding such swimming behaviour of active matter will make significant contribution towards better comprehension of certain important biological phenomena.

*DFG SPP 1726 "Microswimmers"; Max Planck Society

1:51PM B29.00012: Examining collective mechanical properties of fish schools using projected light fields*  
JAMES PUCKETT (Presenter), Physics, Gettysburg College, AAWAZ R POKHREL, Physics, Georgia Inst of Tech — Social animals including insects, fish, birds, and even humans exhibit self-organized collective behavior. Models have shown that simple local interactions between individuals gives rise to the emergent self-organized macroscopic states such as flocks, swarms, or schools. We investigate the material properties of laboratory fish schools by exploiting the negative phototaxicity of Rummy-Nose Tetra (Hemigrammus blehri). To do this, we use an overhead high speed camera to record individual fish trajectories in a quasi-two-dimensional tank. By projecting two dark regions moving in opposite directions, the school of fish is strained as individuals use both social and environmental information to determine their behavior. The school undergoes a large deformation before snapping back into one of the dark regions. Our results show that the school exhibits a stress-stain relationship similar to Hooke's law.

*This work is also supported by Gettysburg College and by the Cross-Disciplinary Science Institute at Gettysburg College (X-SIG).

Monday, March 2, 2020 11:15 AM - 12:51 PM

Session B30 DSOFT GSNP: Morphing Matter: from Soft Robotics to 4D Printing II  
502 - Pierre-Thomas Brun, Princeton University
11:15AM B30.00001: Encoding kirigami bi-materials to morph on target in response to temperature*  DAMIANO PASINI (Presenter), LU LIU, CHUAN QIAO, HAICHAO AN, McGill Univ — Shape morphing in response to an environmental stimulus, such as temperature, light, and chemical cues, is currently pursued in synthetic analogs for manifold applications in engineering, architecture, and beyond. Existing strategies mostly resort to active materials, whose responsiveness is controlled by the chemical composition and/or arrangement of their constituents, which is dispensed through a specific fabrication process. Here, we demonstrate that a pair of off-the-shelf passive solids, such as wood and silicone rubber, can be topologically arranged in a kirigami bi-material to engage temperature to collectively deploy into a geometrically rich set of periodic and aperiodic shapes that can shape-match a predefined target. The results highlight reversible morphing by mechanics and geometry, thus contributing to relax the dependence of current strategies on material chemistry and fabrication.

*Natural Sciences and Engineering Research Council of Canada

11:27AM B30.00002: Assembly Behaviors Design with Magnetic Handshake Materials
CHRISY XIYU DU (Presenter), Harvard University, RAN NIU, Cornell University, EDWARD P ESPOSITO, University of Chicago, PAUL L MCEUEN, ITAI COHEN, Cornell University, MICHAEL PHILLIP BRENNER, Harvard University — Inspired by nature’s ability of assembling intricate materials, we recently developed an assembly platform that can create specific binding by encoding magnetic dipole patterns into panel-like building blocks. With this platform, which we term magnetic handshake materials, we are able to achieve controlled polymerization, complementary binding strands and 3D folding from 2D nets. However, in order to perform more systematic materials design that can match nature's ability, we need to develop design protocols to more efficiently search through the parameter space. Here, I will demonstrate how to use computational methods to systematically probe the design space. With the help of molecular dynamics and inverse design techniques, I will show that we can predict self-assembly behaviors of arbitrary panels based on their local interaction and optimize for specific structures.
11:39AM B30.00003: Photothermally Reconfigurable Shape Memory Magnetic Cilia*  
JESSICA A.-C. LIU, Materials Science and Engineering, North Carolina State University, BENJAMIN A. EVANS, Physics, Elon University, JOSEPH TRACY (Presenter), Materials Science and Engineering, North Carolina State University — Functional artificial cilia usually require maintaining an applied stimulus or are programmed to perform one-way processes that cannot be reset. Reconfigurable artificial cilia are desirable, whose shape can be set, locked, unlocked, and reconfigured. Magnetic iron microparticles were dispersed in a thermoplastic polyurethane shape memory polymer matrix and formed into artificial, magnetic cilia that respond simultaneously to magnetic fields and light. Temporary shapes obtained through combined magnetic actuation and photothermal heating can be locked by switching off the light and magnetic field. Subsequently turning on the light without the magnetic field drives recovery of the permanent shape of the magnetic cilia. The permanent shape can also be programmed after preparing the cilia by applying mechanical constraints and annealing at high temperature. Spatially controlled actuation of magnetic cilia is demonstrated by applying a mask for pattern transfer into the array of magnetic cilia. Development of a theoretical model aids understanding the behavior of reconfigurable magnetic cilia and provides guidelines for their design and optimization.

*National Science Foundation CMMI-1663416 and CMMI-1662641

11:51AM B30.00004: Control of a Hydrogel Based Soft Robot Using Light*  
AAVEG AGGARWAL (Presenter), HANG YUAN, MONICA OLVERA DE LA CRUZ, Northwestern University — Soft robotics is an emerging field of research as robots built from soft materials can offer many advantages over conventional robots. Hydrogels are an interesting family of materials for realization of such soft robots as they can change their morphology by exchanging fluids with their environment. This further opens opportunities for biological applications. Remote control of these hydrogel robots with external stimuli such as light and magnetic fields can add useful functionality to them. Photo-responsive hydrogels provide an easy way to remotely control the shape of these robots by exposing them to light. This phenomenon can be exploited to design robots that can transit between multiple modes of operation by changing their geometry. To this end, we report our theoretical work on the light induced deformations in these robots and the corresponding changes in functionality.

*This work was supported by the Center for Bio-Inspired Energy Science (CBES), an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE) Office of Basic Energy Sciences (DE-SC0000989)
12:03PM B30.00005: Semiflexible origami and their many minima*  MARY ELIZABETH LEE-TRIMBLE (Presenter), JI-HWAN KANG, RYAN HAYWARD, University of Massachusetts, Amherst, CHRISTIAN SANTANGELO, Syracuse University — Self-folding origami structures, which allow flat materials to be deployed into three dimensional structures, have many engineering applications. These applications, however, require that the structures fold without error and robustly. For infinitely rigid origami, many configuration space components meet at the flat, unfolded state, so even when every fold is programmed to the desired equilibrium result, the structure can misfold into an undesired branch of configurations. Here, we show how to relax the rigidity of origami by allowing a small amount of stretching along the folds, which in turn allows Gaussian curvature at the vertices. We map the energy landscape for simple origami and explore the bifurcations of the energy landscape that lead to multiple minima. Furthermore, we explore how the basins of attraction of different energy minima affect the potential to misfold.

*This material is based upon work supported by the National Science Foundation (NSF) Graduate Research Fellowship under Grant No. 1451512 and under NSF Grant DMR-1822638.

12:15PM B30.00006: Morphing Colloidal Crystals with Active Additives  BRYAN VANSADERS (Presenter), SHARON C GLOTZER, Univ of Michigan - Ann Arbor — Active matter studies have focused mostly on homogenous systems where all elements are active. However, for dense systems the forces applied by small quantities of active matter can have far-reaching effects. Because the positions of particles in colloidal crystals are highly correlated, an active particle’s sphere of influence in such a medium can extend many particle diameters away. By controlling the creation and propagation of mobile defect species this range can be further extended. In this work we discuss how small clusters of active particles with variable diameter can cause long range shear displacement within a simulated colloidal monolayer. Such displacement can be confined to a single slip plane by the design of the embedded cluster. We approach the design of these heterogeneous active materials by focusing on the creation and migration of dislocation defects from the embedded cluster edges during expansion. We demonstrate the reconfiguration of large quantities of passive colloidal crystal with a small amount of active matter. Using a designed cluster shape with a single cyclic actuation mode, large plastic deformations can be accomplished over the course of many swell/shrink cycles, providing a new way of creating morphing matter for soft colloidal robotics.
12:27PM B30.00007: Generating multiple surfaces from a single inhomogeneous anisotropically deforming sheet* ITAY GRINIASTY (Presenter), ITAI COHEN, JAMES PATARASP SETHNA, Laboratory of Atomic and Solid State Physics, Cornell University — Can we make a flat sheet transform first into Rodin's thinker and then Michelangelo's David? Here, we derive a general solution to this inverse design problem for inhomogeneous, anisotropically deforming materials. Such actuating materials include 3D printed hydrogels that swell or "Baromorphing" pneumatic elastomers. In these materials local variations of the director field and deformation factors along and across the director field produce global shape changes. These multiple local degrees of freedom allow a single sheet to deform into multiple desired surface geometries in response to external actuation. Actuation by two external parameters, enables the sheet to cycle through a closed loop in conformation space to swim or do work. To solve the inverse problem, we use the curvatures of the target shapes to derive an integrable system of differential equations for the sheet's local degrees of freedom. We then provide an algorithm for integration of this system of equations that allows us to systematically find all solutions to the problem. This approach paves the way to find solutions optimized for different criteria including ease of manufacture, deformation pathway, and work efficiency.

*This work was supported by (ARO W911NF-18-1-0032).

12:39PM B30.00008: Morphing Surfaces for μ-Contact Printing* MITCHELL ANTHAMATTEN (Presenter), SOYOUN KIM, NAN LIU, ALEXANDER A SHESTOPALOV, Chemical Engineering, University of Rochester, JOHN LAMPROPOULOS, Mechanical Engineering, University of Rochester — Micro contact printing is an increasingly reliable technique to pattern various ink materials with microscale precision over large areas on flat or curvilinear substrates. The method involves contacting an elastomeric stamp to a transferable ink, pickup of the ink and transfer to a target substrate, and interfacial fracture to release the ink to a target substrate. Here, we employ shape-memory surfaces with thermo-mechanical programming to achieve large-area pattern transfer to multilayered films from donor substrates to receiving plates. We show that shape-memory can enable robust pattern transfer at higher resolution. New photolithography methods were applied to create patterns of SiO$_2$ microdiscs on a silicon wafer. High resolution pattern transfer of vapor deposited thin films was demonstrated by (i) pressing a shape-memory stamp against a donor substrate; (ii) cooling the system to encourage adhesion between the stamp and the ink; (iii) removing the stamp and pressing against a receiving substrate, and (iv) heating followed by stamp removal to transfer the material. Control experiments indicate that thermal mechanical programming is critical to successful pattern transfer.

*The authors acknowledge support from funding provided by the NSF under Grant ECCS-1530540.
11:15AM B31.00001: Viscous flows with thin, compliant boundaries* [Invited] DOMINIC VELLA (Presenter), University of Oxford — Viscous fluids flowing in channels with solid, but compliant, boundaries are common in a range of biological and industrial settings. The presence of such compliance can qualitatively alter the behaviour of such systems, forcing us to revisit the basic principles with which viscous flows are usually understood: the reversibility of Stokes flow no longer holds and the relationship between flux and driving pressure may be nonlinear. In other situations, the mere presence of boundary compliance, combined with capillarity is enough to spontaneously generate fluid motion. I will give examples of some of these unusual behaviours, focussing on situations in which the compliant boundary is in some sense thin, as well as discussing the validity of the different models of boundary compliance.

*ERC Starting Grant 637334

11:51AM B31.00002: Slicing Soft Materials STEVEN RHODES (Presenter), ERIC WEEKS, Emory University — We experimentally study the slicing of soft materials. We use a rheometer to press a circular cutting tool into these materials (a steel “cookie cutter”) at a controlled rotation speed and controlled speed in the normal direction. Typical rates are 100 rad/s angular speed and 10 microns/s normal speed. The rheometer allows us to measure the normal force and torque required to press the cutter through a material. The soft materials we use to experiment with are mainly Styrofoam and Clay. From examining the fluctuations of torque and normal force over time, we find that the most effective cutting occurs with slower normal speed, and that cutting is less sensitive to the rotation rate of the cutter.

12:03PM B31.00003: Valve Elasticity for Optimal Lymphatic Pumping* KI WOLF (Presenter), J. BRANDON DIXON, ALEXANDER ALEXEEV, Georgia Inst of Tech — The lymphatic system transports interstitial fluid, fatty acid, and immune cells and maintains this vital function by pumping the lymphatic fluid via networks of contracting lymphatic vessels and elastic valves. The interplay of peristaltic motion of the lymphatic vessels and valves achieve unidirectional flow against adverse pressure gradient while minimizing any backflow. Despite the significance, research into the lymphatic system has been limited, especially regarding the function of lymphatic valves. We use fully coupled, three-dimensional fluid-structure interaction model to study the performance of compliant lymphatic valves in the lymphatic vessel that undergoes peristaltic motion. Parameters such as adverse pressure gradient, contraction frequency, contraction amplitude, and elasticity of the lymphatic valves are varied to investigate their effects on the flow rate and pumping efficiency, which are compared against their valve-less counterparts. The results suggest that lymphatic valves significantly extend the range of operational adverse pressure gradients. Furthermore, the simulations reveal the optimum valve elasticity enhancing pumping performance.

*Financial support from the National Science Foundation (CMMI-1635133) is gratefully acknowledged.

VISHAL ANAND, IVAN CHRISTOV (Presenter), TANMAY C SHIDHORE, XIAOJIA WANG, Mechanical Engineering, Purdue University — The hydraulic resistance of conduits of any cross-section can be calculated from exact unidirectional flow solutions of the steady Stokes equations. Recently, however, experiments on internal flows in channels with soft boundaries have shown that wall deformation leads to a nonlinear relationship between the volumetric flow rate and the pressure drop. Thus, the soft hydraulic resistance is not simply a constant dependent on the cross-sectional shape. We propose a perturbative approach to solving soft hydraulics problems. The Stokes equations are coupled to the equations of linear elasticity. For a long and slender geometry, the flow problem is reduced to lubrication theory. The deformation of the elastic wall is reduced to a two-dimensional problem in each flow-wise cross-section. Closed-form solutions for the deformation (either from the full elasticity problem or through simplifications via plate theory) allow us to predict the resistance of soft hydraulic elements. Our theory compares favorably to microscale flow experiments, as well as to three-dimensional two-way coupled direct numerical simulations. The effect of non-Newtonian fluid rheology will also be addressed.

*Supported by the U.S. National Science Foundation under Grant CBET-1705637.

12:27PM B31.00005: Devising and characterizing a non-perturbative manipulator in 3D microfluidic channels

JEREMIAS GONZALEZ (Presenter), BIN LIU, Physics, UC Merced — Thanks to the lack of inertia of fluids, hydrodynamic forces in the Stokes regime, such as a microscale flow, are products of only flow pattern geometry. Consequently, an object entrained in a microfluidic flow cannot sense any variations if the surrounding flow remains uniform such that it is strain-free. This concept thus suggests the capacity of a microfluidic device for non-perturbative manipulations, which has not been fully explored. Here, we investigate the capability of such non-perturbative manipulations in a microscope-compatible 3D microfluidic device having vertically offset channels converging on a middle chamber. Using symmetry arguments, we illustrate a minimum of 6 channels are necessary to realize microscale manipulations along arbitrary directions, completely strain-free at the chamber center. By introducing two independent strain rate tensor invariants for characterizing flow perturbation, we demonstrate a finite volume with substantially low strain rate can be achieved around the strain-free center and can thus enable effectively non-perturbative manipulation over a spatial scale much greater than the size of the manipulated objects. We also fabricated such a microfluidic device and demonstrated its non-perturbative manipulation capabilities in experiments.
12:39PM B31.00006: The interaction of elastomeric coatings with viscous flows: how incompressible is PDMS?  THOMAS CHANDLER (Presenter), DOMINIC VELLA, University of Oxford — Elastic substrates bounding fluid flows are common in many experimental and industrial settings; their principal purpose is usually to drive or suppress the flow of fluid. In particular, PDMS is one of the most frequently used materials in microfluidic platforms, since it is easily designed into complex channel shapes. The deformation of such PDMS and other elastomeric layers is becoming increasingly recognised, but the model appropriate for describing its deformation depends on how close to incompressible the coating is. While the Poisson ratio is usually quoted as being in the range of 0.49 – 0.5, the precise value may change the behaviour of the coating and have knock-on consequences. We will present a model for thin, near-incompressible elastic foundations, and discuss how its application to examples of fluid-structure interaction problems at low Reynolds number can depend sensitively on how incompressible the coating is.

12:51PM B31.00007: Active Foam: Connecting Structure, Dynamics and Control*  LAUREL KROO (Presenter), Department of Mechanical Engineering, Stanford University, MATTHEW S BULL, Department of Applied Physics, Stanford University, MANU PRAKASH, Department of Bioengineering, Stanford University — By inflating and deflating voxels within a polydisperse 2-D air-liquid foam, we demonstrate a system where we perturb soft materials in a radially-symmetric manner. These cyclic perturbations can be coordinated spatially and temporally to encode (“write”) mechanical properties into the material. In addition to experiments, we will discuss a new simulation method used to test distributed local control strategies to achieve global behavior. We can estimate where regions of topological rearrangements occur by connecting microstructural mechanics with the dynamics of slowly oscillating sources and sinks in the material. We address the significant complexity that arises from polydispersity and initial topological disorder. The goal of this work is to understand fundamental principles of confluent tissues and develop functional synthetic analogs.

*This research received funding from NSF (GRFP, 1453190) and CZ Biohub.

1:03PM B31.00008: Active sieving : from flapping nano-doors to vibrating nanotubes  SOPHIE MARBACH (Presenter), NYU, Courant Institute of Mathematical Sciences, DAVID DEAN, France, Universite Bordeaux, LYDERIC BOCQUET, France, Ecole Normale Superieure — Filtering specific molecules is a challenge faced for several vital needs: from biomedical applications like dialysis to the intensive production of clean water. The domain has been boosted over the last decades by the possibilities offered by nanoscale materials. Filtration is however always designed according to a passive sieving perspective: a membrane with small and properly decorated pores allows for the selection of the targeted molecules. This inevitably impedes the flux and transport, making separation processes costly in terms of energy. Here we investigate alternative approaches to separation and filtration. We explore the possibility of non-equilibrium sieving, harnessing the difference in the molecular dynamics of particles to separate them across "active" nanopores.
1:15PM B31.00009: Fibre-reinforced microfluidic droplets* HERVE ELETTRO (Presenter), FRANCOIS GALLAIRE, Ecole Polytechnique Federale de Lausanne — Soft microfibers can be strongly bent by capillary forces and even be reversibly coiled inside fluid cavities. If present, hydrodynamic forces may compete with capillary forces, uncoil the microfiber and induce its deployment from its original coiled state. Here we fabricate a microfiber coiled within a droplet that is attached on the wall of a microfluidic channel. This is done by photocuring a thin liquid jet of hydrogel (PEG-DA) and transporting the resulting soft microfibre to the carefully prepared droplet for adequate coiling. The mechanical response of the hybrid system is then investigated under increasing flow rates. The present results open opportunities to form the building blocks of microfluidic elements with high on-off ratio that may be useful for the design of on-chip tunable circuits for bioengineering applications.

*We acknowledge funding from the Marie Sklodowska-Curie Actions Fellowship, project "El_CapiTun" n°750802.

1:27PM B31.00010: Pulp friction: lubricating properties of soft particle suspensions* JOSHUA DIJKSMAN (Presenter), Physical Chemistry and Soft Matter, Wageningen University, RAISA RUDGE, ELKE SCHOLTEN, Physics and Physical Chemistry of Foods, Wageningen University — Friction between two sliding surfaces is often reduced with a lubricant. Lubricants can contain particles that help mitigate dissipation. The mechanics of friction is complex, especially when soft substrates/particles and lubricating fluids are involved. We shine new light on the complex mechanics of particle based lubrication by evaluating the lubricating properties of particle suspensions. We synthesize custom soft micron-sized gel particles to create a soft particle suspension that acts as model lubricant. The suspension lubrication deviates from typical Striebeck behavior as we find four frictional flow regimes. These frictional regimes are influenced by the particle size, deformability and the amount of particles in suspension, which allows us to propose mechanisms for the different lubrication regimes. We verify some hypotheses by performing lubrication experiments with soft substrates and hard particles.

*This work was generously supported by graduate school VLAG
1:39PM B31.00011: Propagation and interactions of hydraulic fractures in model heterogeneous solids  STEFANO AIME (Presenter), DAVID A WEITZ, Harvard University — The propagation of cracks in heterogeneous environments is a very rich and complex scientific problem, with implications in many fields, from geology, to everyday life and industrially-relevant processes. Interactions of the propagating crack with material heterogeneities, defects, interfaces and other cracks ultimately determine the path that the crack follows, as well as the occurrence of crack branching and merging. Addressing such interactions in experiments is however extremely challenging, since it requires at the same time a fine control of the crack propagation and a detailed knowledge of the material response to the crack itself, which is typically nonlinear and dynamic. In this work we study the propagation of hydraulic fractures in model, well-controlled colloidal materials, using microfluidics coupled to an innovative dynamic light scattering technique providing time- and space-resolved information on the local strain and the microstructural damage caused in the material by the propagating crack. Our preliminary results suggest that combining such information with a fine control of the mechanical and structural properties of our model samples can pave the way for a more comprehensive understanding of crack propagation in heterogeneous media.

1:51PM B31.00012: Effect of the 3D swelling of microgels on their 2D phase behavior at the liquid-liquid interface*  STEFFEN BOCHENEK (Presenter), ANDREA SCOTTI, RWTH - Aachen, LUCIO ISA, ETH - Zurich, WALTER RICHTERING, RWTH - Aachen — We investigate soft, temperature-sensitive microgels at fluid interfaces and how changing temperature across the microgels' volume phase transition temperature, which leads to swelling/deswelling of the microgels in the aqueous phase, affects the phase behavior within the monolayer. We combine compression isotherms, AFM imaging, and ellipsometry. At low compression, the interaction between microgels is dominated by their highly stretched corona and the phase behavior of the monolayers is the same. The polymer segments within the interface lose their temperature-sensitivity. At high compression, the portions of the microgels located in the aqueous side of the interface become relevant and prevail in their interactions. These portions are able to collapse and, consequently, the isostructural phase transition is altered. Thus, the temperature-dependent swelling perpendicular to the interface (3D) affects the compressibility parallel to the interface (2D). Our results highlight the distinctly different behavior of soft, stimuli-sensitive microgels as compared to rigid nanoparticles.

*The authors acknowledge financial support from the SFB 985 "Functional Microgels and Microgel Systems" of Deutsche Forschungsgemeinschaft within Projects C4 and B8.
2:03PM B31.00013: Underactuated fluidic control of continuous multistable structures
OFEK PERETZ, Technion - Israel Institute of Technology, ANAND MISHRA, ROBERT SHEPHERD, Cornell University, AMIR GAT (Presenter), Technion - Israel Institute of Technology — This work addresses the challenge of underactuated pattern generation in continuous multistable structures. The examined structure is a slender membrane, actuated by a viscous fluid, which can concurrently sustain two different equilibria states, separated by transition regions. We first demonstrate the formation and motion of a single transition region and then sequencing of several such moving transition regions to achieve arbitrary patterns by controlling the inlet pressure of the actuating fluid. Finally, we show that non-uniform membrane properties, along with the transient dynamics of the fluid, can be leveraged to directly control any segment of the membrane.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B32 DPOLY: Polymer Networks, Gels, and Elastomers: Mechanics 504 - Saad Khan, North Carolina State University - Tag(s): Focus

11:15AM B32.00001: Multiaxial Stretching of Nearly Critical Gels with Extremely Low Modulus  TAKUMA AOYAMA (Presenter), NAOTO YAMADA, KENJI URAYAMA, Kyoto Inst of Tech — Linear dynamic viscoelasticity of the gelation systems near the critical point has been investigated intensively, but the large deformation behavior of nearly critical gels, which are obtained slightly beyond the gelation point, remains to be characterized. In contrast to matured gels, nearly critical gels have very low modulus due to the extremely sparse network structures. In this study, we have characterized the large deformation of the nearly critical gels by using a custom-made biaxial tensile tester optimized for very soft gels. Biaxial tensile data varying the strains in two directions independently provide a definite basis to discuss the whole aspects of the large deformation behavior. The biaxial tensile data have revealed that the nearly critical gels exhibit minimal cross-effect of strains which results only from volume conservation in contrast to the matured gels with finite cross-effect. The feature of the nearly critical gels is attributed to their extremely sparse network structures.
Soft viscoelastic polymers and gels are commonly used as biomaterials and soft actuators owing to their ability to accommodate large deformations. Their applicability is however often limited by their tendency to abruptly fracture in ways that cannot be predicted by conventional elastic fracture mechanics. Our understanding of the fracturing process in these networks has particularly been hindered by the complex interplay between the viscous dissipation in the bulk and the accumulated damage around the crack tip.

To tackle this question, we explore the condition for a crack to initiate and propagate in transient polymer networks. We used a recently developed Transient Network Theory (TNT) that provides a statistical evolution of a transient network whose topology change as a result of macroscopic deformation and chain reconfiguration via transient crosslinks. This approach is particularly amenable to determine macroscopic measures characterizing the crack driving force. Based on the crack geometry and external loading, we determine the conditions that lead to crack blunting and crack propagation. By determining the interplay of these two mechanisms, we are able to predict fracture process of transient polymer networks with comparison to experiments.

*NSF Award No. 1761918
11:39AM B32.00003: High-Rate Dynamics and Fracture Behavior of Model Swollen Polymer Network Characterized by Seeded Laser-Induced Cavitation*  SACCHITA TIWARI (Presenter), Mechanical and Industrial Engineering, University of Massachusetts, Amherst, IPEK SACLIGIL, Polymer Science and Engineering, University of Massachusetts, Amherst, YUE ZHENG, Mechanical and Aerospace Engineering, University of California, San Diego, CHRISTOPHER BARNEY, Polymer Science and Engineering, University of Massachusetts, Amherst, CAREY DOUGAN, Chemical Engineering, University of Massachusetts, Amherst, SHENGQIANG CAI, Mechanical and Aerospace Engineering, University of California, San Diego, ALFRED J CROSBY, Polymer Science and Engineering, University of Massachusetts, Amherst, SHELLY PEYTON, Chemical Engineering, University of Massachusetts, Amherst, GREGORY N TEW, Polymer Science and Engineering, University of Massachusetts, Amherst, JAE-HWANG LEE, Mechanical and Industrial Engineering, University of Massachusetts, Amherst — Mechanical characterization of soft materials at high strain rates is challenging due to their high compliance, slow wave speeds, and rate-dependent viscoelasticity. Swollen polymer networks are attractive model materials as they can be tuned to simulate the high-rate dynamics and damage mechanisms of soft tissues, such as the brain, under extreme mechanical stimuli. In this study, seeded laser induced cavitation (SLIC) is performed within polydimethylsiloxane gels containing a significant amount of solvent (50 - 80 wt.%), levels similar to those of soft tissues. Ultrafast stroboscopic observation of a laser-induced microscale cavity is exploited to characterize the viscoelastic response of the gels at strain rates of $10^6$ s$^{-1}$. By varying the molecular weight between crosslinks from 1.2 to 12 kg/mol, fracture initiation and post-cavitation characteristics of the gels are systematically controlled. The demonstrated SLIC framework can guide the development of tailored synthetic systems that precisely mimic the high-rate plastic behavior of soft tissues.

*This research was supported by the Office of Naval Research under contract N00014-17-1-2056.

11:51AM B32.00004: Chemical tools for investigating the topology of polymer networks* [Invited]  JEREMIAH JOHNSON (Presenter), Chemistry, MIT — All polymer networks have topological heterogeneities that span various length scales and dictate their bulk properties. Nevertheless, these features have traditionally been difficult to quantify and control. Informed by classical crossover experiments in physical organic chemistry, we have developed experimental methods for the precise counting of cyclic topologies (loops) in polymer networks. These studies have enabled new theoretical advances pertaining to elasticity and the gel point, and have inspired new stimuli-responsive materials that leverage topology as a design principle.

*National Science Foundation (DMREF CHE-1629358)
12:27PM B32.00005: Cavitation and Fracture of Soft Materials*  CHRISTOPHER BARNEY (Presenter), IPEK SACLIGIL, GREGORY N TEW, ALFRED J CROSBY, Univ of Mass - Amherst — Rapid expansion of soft solids subjected to a negative hydrostatic stress can occur through an elastic cavitation mechanism or an inelastic fracture mechanism. Balancing how these two mechanisms relate is important to applications in materials characterization, adhesive design, and tissue damage. Significant research effort has focused on understanding how these two mechanisms relate; however, the available experimental data in this area has been limited by both the techniques employed and materials considered. Experimental investigation into the transition between cavitation and fracture requires 1) knowledge of the initial cavity geometry and 2) a material system where both the elastic and fracture properties are independently characterized. In this work, recent improvements in needle-induced cavitation and independent characterization of elasticity and fracture in a set of model end-linked tetra-PEG gels are exploited to experimentally probe the relationship between the elasto-fracture length and cavitation and fracture. The results indicate that three distinct regimes exist where expansion occurs through either cavitation, cavitation-initiated fracture, or fracture.

*ONR grant number N00014-17-1-2056

12:39PM B32.00006: Role of Topological Defects on Fracture of Polymer Networks*  AKASH ARORA (Presenter), TZYY-SHYANG LIN, BRADLEY OLSEN, Massachusetts Institute of Technology MIT — Chemically crosslinked polymer networks often possess various types of topological defects such as loops and bridges, which are shown to have a noticeable effect on elastic properties of the material. In this work, we use theory and simulations to investigate the influence of such defects on the fracture of the material. A Monte Carlo algorithm is first used to generate a series of 3D periodic networks having varying concentration of defects. The respective networks are then subjected to tensile deformation with the bond breaking events modeled using a kinetic theory of fracture incorporating the experimentally-measured mechanochemical characteristics of covalent bonds. We discuss the effect of both the fraction of primary loops and their spatial distribution on the fracture toughness of the material. Additionally, we use the classical Lake-Thomas theory to estimate the ultimate strength of defects-containing networks, and compare the resulting predictions to simulation results. Using both theory and simulations, this work provides insight into the molecular origins of fracture in polymer networks.

*This work is supported by the Dow Chemical Company.
**12:51PM B32.00007: Indentation Rate Sensitive Relaxation of Soft Hydrogels**  
MOHAMMAD ISLAM (Presenter), MICHELLE L. OYEN, Department of Engineering, East Carolina University —  
Mechanical behavior of hydrogels is strongly time-dependent, often characterized as a combination of viscoelastic and poroelastic relaxation. Load-relaxation of hydrogels largely depends on gel composition. Here, we further demonstrate that mechanical loading conditions also influence load relaxation of hydrogels. Spherical indentation experiments are performed for agar, gelatin and polyacrylamide gels with a range of indentation rates. As expected, faster indentation results in more pronounced relaxation in all three gels. The rate-sensitivity is also indentation depth-dependent, such that the degree of relaxation decreases with depth for a constant rate. We interpret the findings within both viscoelastic and poroelastic frameworks. The theoretical analysis demonstrates that viscoelastic relaxation is more rate sensitive compared to poroelastic relaxation. Hydrogels become more viscous at higher indentation rates, indicating significant network reorganization at short time-scales. On the contrary, intrinsic permeability is observed to be largely indentation rate-independent, meaning solvent migration is not affected significantly. Overall, the findings emphasize the importance of loading conditions during mechanical characterization of hydrogels and hydrated biological materials.

**1:03PM B32.00008: Influence of polymer concentration and midblock length on the mechanical behavior of [ABA] triblock copolymer gels in a B-selective solvent**  
SATISH MISHRA, ROSA MARIA BADANI PRADO, Mississippi State Univ, THOMAS E. LACY, Mechanical Engineering, Texas A&M University, SANTANU KUNDU (Presenter), Mississippi State Univ — We present the effect of polymer concentration and midblock length on the large deformation behavior of [ABA] triblock copolymer gels in a midblock selective solvent. In our case, “A” represents poly(styrene) [PS], “B” represents poly(isoprene) [PI], and the solvent is mineral oil. The micellar microstructure of these gels consists of collapsed PS endblock aggregates acting as crosslinks, which are bridged by PI midblocks. The polymer concentration and polymer midblock lengths were varied to introduce midblock entanglement in the gels. Small-angle x-ray experiments capture the micellar microstructure of these gels. Tensile testing reveals a rate dependent moduli for the samples with entangled midblocks. The sample stretchability is governed by stretch rate, midblock length, and polymer concentration. Fracture experiments with a predefined crack reveal a linear dependence of energy release rate with the crack-tip velocity. Fracture in these gels occurs due to endblock pullout from the aggregates and we have estimated the theoretical energy release rate by considering all entropic and enthalpic processes.
1:15PM B32.00009: Fracture of Model End-Linked Networks*  
CHRISTOPHER BARNEY, Univ of Mass - Amherst, ZIYU YE, University of Pennsylvania, IPEK SACLIGIL, GREGORY N TEW, Univ of Mass - Amherst, ROBERT RIGGLEMAN, University of Pennsylvania, ALFRED J CROSBY (Presenter), Univ of Mass - Amherst — Advances in polymer chemistry over the last decade have enabled the synthesis of well-defined networks that exhibit homogeneous structure. These well-defined polymer gels create the opportunity to assess and verify novel and existing molecular models of network elasticity and fracture. A novel theory of network fracture that accounts for loop defects by drawing on recent advances in network elasticity is proposed. This loop modified Lake-Thomas Theory is tested against both MD simulations and experimental fracture measurements on model gels. Good agreement between the theory and measurement is obtained. These findings enable a priori estimation of fracture energy in swollen gels where chain scission becomes an important failure mechanism.

*ONR grant number N00014-17-1-2056

1:27PM B32.00010: Unveiling the effects of molecular topology on the viscoelasticity of entangled polymers under gelation  
WEIZHONG ZOU (Presenter), ALEXANDRA A. SOURAKOV, NATHAN REBELLO, TZYY-SHYANG LIN, BRADLEY OLSEN, JEREMIAH JOHNSON, Massachusetts Institute of Technology — When polymer molecules are constantly crosslinked during the curing process, the presence of intramolecular loops and tree-like hyperbranched structure make the prediction of viscoelastic properties rather complex due to the change of molecular topology. Based on the effective potential in primitive path fluctuations for the relaxation of star polymers [Milner & McLeish, Macromolecules 1997], we propose a novel strategy, i.e., by defining effective relaxation potentials at the “termini” of each polymer strand in a hierarchical manner, to determine the timely movement of the relaxation “front” [Read et al. Science 2011] between the fully relaxed outer layer and the unrelaxed inner core in an arbitrary molecular architecture. For monodisperse polymer systems with specified molecular structure, this model is shown to capture the stress relaxation quite well when compared to those from analytical theories and experimental data. By implementing a kinetic Monte Carlo method [Rui et al. PRL 2016] to access the topological information of crosslinked polymers, this model allows for the prediction of a change in the exponent of power law relationships for rheological moduli at intermediate frequencies with different conversions, which is consistent with the experimental measurements.
1:39PM B32.00011: Constitutive modelling of responsive and non-responsive polymer gels with limited compressibility* PRIYANKA NEMANI (Presenter), RAVI SASTRI AYYAGARI, PRATYUSH DAYAL, Indian Inst of Tech Gandhinagar — Design of futuristic synthetic materials to replicate biological mechanisms has been a challenge for science and engineering. Polymer gels that are intrinsically powered by self-oscillating Belousov Zhabotinsky (BZ) reaction are systems that utilize chemo-mechanical transduction to produce mechanical work from chemical energy. Here, we develop the chemo-mechanical theory for modelling these systems under isothermal conditions. Our approach harnesses the finite element framework to combine the reaction-diffusion phenomena with large elastic deformations of the non-gaussian compressible polymeric networks. In particular, we use Oregonator model to capture BZ kinetics while the modified Flory-Huggins theory is used to capture interactions between BZ-catalyst and polymer gel. Using our model we simulated the dynamics of BZ and non-responsive gels under equilibrium and transient conditions; we validated our results with the existing models and experimental results. In essence, we develop and establish a framework to design and study responsive materials with complex geometries. Moreover, we believe that by extending our methodology it is possible to capture large deformations akin to volume phase transitions in polymer gels under non-isothermal conditions.

*DST-SERB (EMR/2016/007778)

1:51PM B32.00012: New Insights into the Chain Dynamics and Microstructure of Highly Crosslinked Polymer Networks as a Function of Network Heterogeneity BRAD JONES (Presenter), TODD M ALAM, MATHIAS C CELINA, Sandia National Laboratories, SANGWOO LEE, Isermann Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute — Key physicochemical phenomena in polymer networks are critically impacted by the spatial distribution of crosslinks, i.e., network heterogeneity. Despite this fact, the chain dynamics and microstructure of heterogeneous networks, particularly bulk thermosets, have not been well characterized. To this end, we present a detailed investigation of novel photopolymerized thiol-ene networks. High glass transition temperatures and continuously tunable network heterogeneity were achieved by varying the stoichiometry between aromatic thiol and acrylate monomers. The chain dynamics and microstructure of these materials were characterized using a combination of dynamic mechanical analysis, solid-state nuclear magnetic resonance spectroscopy, and small angle x-ray scattering. We found that heterogeneous networks exhibited enhanced mobility deep in the glassy state, in contrast to their homogeneous counterparts. In addition, the heterogeneous and homogeneous networks were distinguished by their fractal structures. These new insights may help guide the future design of new crosslinked polymers with carefully controlled network heterogeneity.
Deformation of Inhomogeneous End-linked Polymer Networks

ZIYU YE (Presenter), ROBERT RIGGLEMAN, University of Pennsylvania — Polymer networks represent an important class of soft materials with a broad range of applications in adhesives, coatings, membranes and natural materials. In particular, synthetic end-linked polymer gels, where the network is swollen in solvent, has received growing attention in the biomedical field due to their structural and mechanical similarities to tissues. Failure of these materials during mechanical deformations is intimately tied to their elastic and fracture properties. Synthetic and natural gels have highly complex environments that contain defects and phase boundaries, and the interplay between these molecular structures and the elastic and fracture responses remains an open question. In this study, we use molecular dynamics simulations to prepare and characterize two-phase polymer networks with one glassy and one rubbery domain. We characterize their mechanical properties and how the strain localizes in the glassy and rubbery domains as a function of the polymer chain length. Our simulations reveal that structural features on multiple length-scales serve to localize the site of failure.

*ONR-40004251

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B33 DPOLY DSOFT GSNP: Polymer Nanocomposites: Interfaces

Designing Polymer Nanocomposites: Critical Role of the Interfacial Layer

ALEXEI SOKOLOV (Presenter), University of Tennessee, Knoxville — It is now well recognized that interfacial layer controls macroscopic properties in polymer nanocomposites (PNCs). In this talk we overview recent studies on structure and dynamics of the interfacial layer in various PNCs. We employ broad array of experimental techniques and MD-simulations that provide detailed characterization of the interfacial layer. These studies revealed a gradient in the interfacial layer dynamics, but no “glassy” or “dead” layer. The thickness of the interfacial layer increases upon cooling to Tg, and depends strongly on polymer rigidity, increasing from ~2nm in flexible polymers to ~5 nm in more rigid ones. We discuss a possible connection of the interfacial layer thickness to the dynamic heterogeneity length scale. We emphasize usually overlooked dynamic property of the interfacial layer – strong suppression of the amplitude of structural relaxation on time scale of segmental dynamics. At the end, we present a general picture how microscopic parameters control the interfacial layer, and how by tuning the interfacial layer we can tune macroscopic properties of polymer nanocomposites.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division
**11:51AM B33.00002: Dynamics in polymer and polymer-grafted nanocomposites: it's the interfacial zone after all**

EMMANUEL MAPESA (Presenter), DAYTON P. STREET, S. MICHAEL KILBEY II, JOSHUA SANGORO, University of Tennessee, Knoxville — Polymers exhibit deviations from their bulk physical properties in the vicinity of solid substrates due to changes in various properties arising in the interfacial regions. Broadband dielectric spectroscopy and differential scanning calorimetry are used to study molecular dynamics in poly(methyl methacrylate)/silica nanoparticle composites. By systematically examining nanocomposites based on non-functionalized Si NPs dispersed in PMMA matrices and on PMMA-grafted Si NPs in PMMA matrices, we investigate the effects of interfacial interactions and confinement in each of these cases on $T_g$ and the time-scales as well as breadth of the corresponding dielectric relaxations. We show that in addition to slower mobility, which is commonly reported in literature and assigned to interfacial relaxations, faster modes also arise due to confinement effects, and that these faster modes are more pronounced in nanocomposites with polymer-grafted nanoparticles. These faster relaxation modes are attributed to the increasing importance of chain wetting and packing in the interfacial zones around nanofillers.

*NSF through DMR-1905597 & CBET-1512221; DoE's Kansas City National Security Campus, operated and managed by Honeywell Federal Manufacturing & Technologies, LLC, Contract DE-NA-0002839.

**12:03PM B33.00003: Theory of coupled activated relaxation in dense polymer-particle mixtures: effects of size ratio, particle loading and interfacial attraction**

YUXING ZHOU (Presenter), KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Dense polymer-particle mixtures represent a wide range of systems including polymer nanocomposites, polymerized ionic liquids, and bio-related materials. Understanding and predicting the dynamical and mechanical properties of such hybrid systems is of practical importance and high theoretical interest. Here we study the dynamics of polymer nanocomposites using the Elastically Collective Nonlinear Langevin Equation (ECNLE) theory with structural correlations obtained from Polymer Reference Interaction Site Model (PRISM) approach. The latter captures the depletion, steric stabilization, and tight bridging states of structural organization. We focus on the effects of particle-segment size ratio, interfacial (cross) attraction strength, and particle loading on the segmental relaxation time, glass or gel like mechanical properties, and kinetic arrest. Cooperative motions of segments and particles is treated in a dynamically self-consistent manner, and compared to the limiting case of pinned particles. We find a rich dynamical behavior with both plasticization and anti-plasticization regimes, and a nanocomposite shear modulus which can be either softened or reinforced. The key physics relates to the interplay between geometric packing and physical bonding effects.
The interfacial zone around nanoparticles in polymer nanocomposites and in thin polymer films

WENGANG ZHANG (Presenter), National Institute of Standards and Technology, HAMED EMAMY, BEATRIZ PAZMINO BETANCOURT, FERNANDO VARGAS-LARA, FRANCIS STARR, Wesleyan University, JACK DOUGLAS, National Institute of Standards and Technology —

We perform coarse-grained simulations of polymer materials to quantify the range over which interfaces alter the structure and dynamics near the interface. We study the interfacial zone around nanoparticles (NPs) in polymer-NP composites with variable NP diameter, as well as the interfacial zone at the solid substrate and free surface of thin supported polymer films. These interfaces alter both the segmental packing and mobility in an interfacial zone. Variable NP size allows us to gain insight into the effect of boundary curvature, where the film is the limit of zero curvature. We find that the scale for perturbations of the density is relatively small and decreases on cooling for all cases. In other words, the interfaces become more sharply defined on cooling. In contrast, the interfacial mobility scale $\xi$ for both NPs and supported films increases on cooling and is on the order of a few nanometers, regardless of the polymer-interfacial interaction strength. Additionally, the dynamical interfacial scale of the film substrate is consistent with a limiting value for polymer-NP composites as the NP size grows. These findings are based on a simple quantitative model to describe the distance dependence of relaxation that should be applicable to many interfacial polymer materials.

**12:27PM B33.00005: Polymer NanoComposites, Interfaces and Data** [Invited]  
CATHERINE BRINSON (Presenter), Duke University — For polymer composites, nanocomposites and polymer thin film systems, the local properties of polymers can be altered by the chemical and physical interactions with substrates and embedded particles over a substantial length scale. In order to better understand and design nanocomposites, polymer coatings and electronic components, it is essential to develop better understanding and robust design strategies. Two key missing links are understanding of altered polymer properties near surfaces/particles and ability to quantitatively leverage prior data for these systems, predictively in a robust manner. Therefore there is great interest in utilizing scanning probe methods to quantify the local property changes in the polymer region near surfaces. Additionally, there is great need to harvest, record and be able to learn from the vast amount of data archived in journal articles. In this work, both experimental characterization and development of a data framework and infrastructure is presented. The ability of Atomic Force Microscopy (AFM) to characterize the local mechanical properties (elastic and viscoelastic) of the interphase region in model composites is presented and combined with numerical simulations to refine the analysis. A new platform for data, analysis tools and simulation portals for polymer nanocomposites will be presented: NanoMine. NanoMine utilizes a robust schema to hold the data in a software infrastructure with query, visualization and microstructure analysis tools. Case studies are demonstrated which connect the property-structure-property domains through a combination of machine learning and physics-based modeling, demonstrating the ability to identify the most critical features influence properties. Together this work illustrates a new approach to tackle materials design principles for the complex, high dimensional problems inherent in the multi-phase polymer space.

*NSF, AFRL
Chemical Heterogeneities and Architectures of Interfacial Layers in Polymer Nanocomposites

DI WU (Presenter), SIYANG YANG, PINAR AKCORA, Stevens Inst of Tech

Polymer coated nanoparticles have been widely used to achieve good dispersion in polymer matrices. Dynamics and glass-transition temperature of bound interfacial layers on nanoparticles of different sizes have been recently investigated to understand the effect of interfacial relaxations as they govern reinforcement in composites. We investigate the effect of chemical heterogeneities and varying chain architectures around nanoparticles on tuning the dynamics of interfacial polymers, hence the mechanical properties such as thermal-stiffening. Fe$_3$O$_4$ nanoparticles adsorbed or grafted with PMMA chains and dispersed in PMA matrices are prepared and their rheological behavior is characterized. Our findings show that short adsorbed chains lead to thermal-stiffening, whereas long adsorbed chains yield softening with increasing temperature. Conformations of adsorbed and grafted chains on the same particle sizes will be discussed together to reveal this unusual behavior which relies on the interfacial chemical heterogeneities in polymer nanocomposites. Further, other types of adsorbed chains of PA, P2VP, PMMA, with decreasing rigidity, are compared to understand the role of rigid chains on interfacial dynamics and relaxations.

*This work is funded by NSF-CMMI-MEP, Grant #1538725, 1825250.

Interfacial mechanics and viscoelastic properties of patchy graphene oxide reinforced nanocomposites

ZHAOXU MENG (Presenter), Clemson University

Graphene oxide (GO) is a promising building block for nanocomposites due to its excellent mechanical properties and tunable interfacial interactions with polymers. While experiments have shown that GO sheets consist of graphitic regions clustering into patches and oxidized regions constituting the remaining areas, the role that these heterogeneous patches play on interfacial and mechanical properties of GO reinforced nanocomposites have not yet been investigated. To address this issue at spatiotemporal scales beyond atomistic simulations, we employ recently developed coarse-grained models of GO sheet and polybutadiene to model patchy GO sheets and a representative GO/polybutadiene nanocomposite with GO sheets serving as fillers. We quantify how interfacial adhesion energy and polymer conformations depend on the size of patches and corroborate these findings with the viscoelastic behaviors of the nanocomposite. We find that heterogeneous patchy structures on GO sheets are responsible for variations in interfacial and viscoelastic properties of GO-based nanocomposites. Our study provides fundamental insights into the interfacial mechanisms of GO-polymer nanocomposites and the influence of heterogeneous functionalized surfaces on the mechanical properties of polymer nanocomposites.
1:27PM B33.00008: Theory and Simulation of Polymer Brushes - Interaction and Structure
SABIN ADHIKARI (Presenter), SANAT KUMAR, Chemical Engineering, Columbia University — Addition of polymer-grafted nanoparticles (NPs) to a polymer melt can result in hybrid materials with improved properties. Understanding of the structure and the interactions of polymer-grafted NPs in a melt is essential to improve their practical applicability. In this study, we focus on the fundamental aspects of the interactions and structure of polymer brushes in either a poor solvent (i.e., incorporating compressibility effects in the brush) or in a (compressible) polymer-matrix. First, we study two planar brushes in a poor solvent and then in a matrix-polymer melt by using theory and simulations. We study the dependence of monomer density distribution, brush height, and the interaction force between two brushes as a function of graft density and polymer chain length. Then we discuss the generalization of our results to a spherical geometry of relevance to the practically important testbed of polymer grafted nanoparticles.

1:39PM B33.00009: Aggregation of Grafted Nanoparticles in a Polymeric Matrix  CLEMENT KOH (Presenter), Columbia Univ, GARY GREST, Sandia National Laboratories, SANAT KUMAR, Columbia Univ — A common phenomenon for polymer-grafted nanoparticle (PGNP) systems is that NP aggregation spontaneously occurs at a specific ratio of the chain length $N_g$ of the grafted chains to the matrix chain length $N$. This aggregation is generally considered to be entropic in origin and can be attributed to the autophobic dewetting of the grafted chains. Here, we incisively probe the microscopic driving force governing PGNP aggregation through a series of large-scale multi-particle simulation studies. The matrix chain length, graft chain length, and volume fraction were varied. Analysis of our simulations indicate that aggregation take place only at unexpectedly low ratios of $N_g/N$. Further, simulations tuning the interaction mismatch between nanoparticles and polymer chains indicate that some form of enthalpic interplay between the polymer chains and NPs is significant in controlling the PGNP aggregation that is observed experimentally. These results suggest that entropy alone is probably not the only factor driving nanoparticle aggregation in nanocomposites.
Surface Segregation and Wetting of Nanoparticles in Polymer Nanocomposites

SHAWN MAGUIRE (Presenter), Materials Science & Engineering, University of Pennsylvania, JOHN DEREK DEMAREE, Weapons & Materials Research Directorate, Army Research Laboratory, CONNOR BILCHAK, Chemistry, University of Pennsylvania, NADIA KROOK, DuPont Co., Wilmington, DE, MICHAEL J. BOYLE, Materials Science & Engineering, University of Pennsylvania, ANDREEA-MARIA PANA, Chemical and Biomolecular Engineering, University of Pennsylvania, PATRICE RANNOU, MANUEL MARÉCHAL, UMR5819-SyMMES (CNRS/CEA/UGA), French National Centre for Scientific Research (CNRS), KOHJI OHNO, Polymer Chemistry, Kyoto University, RUSSELL COMPOSTO, Materials Science & Engineering, University of Pennsylvania — The segregation and wetting of polymer grafted nanoparticles (NP) to the free surface of a polymer nanocomposite film is driven by both surface energy and thermodynamic forces. Here, we probe these two contributions in a model system of PMMA grafted silica NPs in a poly(styrene-ran-acrylonitrile) (SAN) matrix using Rutherford backscattering spectrometry (RBS) and atomic force microscopy (AFM) as a function of thermal annealing temperature and time. Studies are performed above and below the critical point of this LCST system to decouple the thermodynamic and interfacial energy contributions. With increasing time, a monotonic increase in surface excess of PMMA grafted NPs is observed in the miscible regime, which is attributed to the difference in surface energies between the PMMA brush and SAN matrix. Upon annealing above the critical point, a much stronger increase in PMMA NP surface coverage is observed because of the thermodynamic driving force, namely the Flory-Huggins interaction parameter between the PMMA grafts and SAN matrix. Using the measured surface excess values of PMMA NPs at multiple annealing times and temperatures, we then extract the apparent diffusion coefficients of the particles and compare them to the systems homopolymer analogue.

*NSF PIRE - 1545884
2:03PM B33.00011: Initial Solvent-Driven Nonequilibrium Effect on the Adsorption Layer of Polymer Nanocomposites*

SOL MI OH (Presenter), Ulsan Natl Inst of Sci & Tech, MOZHDEH ABBASI, Martin-Luther University Halle-Wittenberg, TAE JOO SHIN, UNIST Central Research Facilities & School of Natural Science, KAY SAALWAECHTER, Martin-Luther University Halle-Wittenberg, SO YOUN Y KIM, Ulsan Natl Inst of Sci & Tech — There have been extensive efforts to characterize interfacial layers in polymer nanocomposites (PNCs), which determines the final structures and properties of PNCs. While tremendous studies have focused on intrinsic parameters of components such as size, shape, chemistry, an understanding for the variation of the structure and dynamics under different processing conditions is relatively lacking. In this work, we report that the initial dispersing solvent, which is not present in final PNCs, induces nonequilibrium effects on polymer chain dynamics at interfaces. By employing $^1$H NMR free induction decay, we probe that the quantity rather than the mobility of interfacial polymers can be changed depending on the initial solvent, which leads to a difference in thickness of interfacial layers. Accordingly, the particle microstructures and rheological properties are greatly influenced observed by small-angle X-ray scattering and oscillatory rheometry experiments. In addition, we reveal that the outcome of the nonequilibrium effect driven by the initial solvent becomes more prominent at effective range of particle volume fraction related to the polymer chain dimension.

*NRF-2015K2A9A2A18065964, NRF-2018R1A2B6008319, and DFG, Grant No. SA982/13-1, Project No. 316439043

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B34 DPOLY DSOFT: Confinement, Dynamics, and Ion Interactions in Ion-Containing Polymers II 506 - Bryan Beckingham, Auburn University - Tag(s): Focus
**11:15AM B34.00001: Ion Confinement in Self-Assembled Precisely Segmented Polyolefin Ionomers**

KAREN WINEY (Presenter), LU YAN, JINSEOK PARK, University of Pennsylvania, STEFAN MECKING, University of Konstanz — Confining ions within self-assembled nanoscale structures is demonstrated in a series of single-ion conducting segmented polyolefins, nominally multiblock copolymers. We report a series of precisely-segmented polyethylene-like ionomers containing sulfonate groups (PES) with Li+, Na+, Cs+, or NBu4+ counterions synthesized from step-growth polymerization. At room temperature, the PES ionomers with long methylene units are semicrystalline with well-defined nanoscale ionic layers with spacings influenced by the spacer length and cation type. In situ X-ray scattering measurements reveal that the layered ionic aggregates in some of these polymers transform, upon melting the PE segments, into gyroid morphologies. The gyroid structure can further evolve into hexagonal symmetry as T increases. The ion transport behavior of these polymers is strongly dependent on the ionic aggregate morphologies. Specifically, a 3D interconnected gyroid morphology exhibits higher ionic conductivity than the isotropic layered or hexagonal morphologies. This innovative and versatile molecular design of ionomers leads to unprecedented percolated gyroidal ionic aggregate morphologies that provide a continuous pathway for improved ion transport.

*National Science Foundation - DMR/Polymers

**11:27AM B34.00002: Unraveling how nanoconfinement and phase-separation affect the transport properties of ionomer membranes**

RUI ZHANG (Presenter), Department of Chemistry and Macromolecules Innovation Institute, Virginia Tech, YING CHEN, Physical & Computational Sciences Directorate, Pacific Northwest National Laboratory, DIEGO TROYA, LOUIS A MADSEN, Department of Chemistry and Macromolecules Innovation Institute, Virginia Tech — Transport of water and ions through ionic polymer membranes depends on multi-scale membrane structure. This talk will focus on the nano-scale structure-transport relations of ionomer membranes. We will present studies on the temperature dependence of diffusion as a function of water uptake in a perfluorosulfonic acid (PFSA) membrane. Using NMR diffusometry and MD simulations, we are able to probe the activation energy of water diffusion \( E_a \), which arises from molecular scale interactions and reflects the nano-scale environment of a water molecule. By comparing \( E_a \) in the PFSA membrane to \( E_a \) in a free liquid environment, we are able to identify two structural primary features of ionomer membranes, nanoconfinement and nano-scale phase separation, that affect membrane transport. Nanoconfinement alters local energetics of water molecules and can prompt formation of more ordered water structures. Nano-scale phase separation creates a local environment for water molecules that is closer to that of pure water, and thus gives rise to \( E_a \) values that approach that of pure water. These findings shed light on the fundamental aspects of structure-transport interplay in ionomer membranes.

*This work was supported by the National Science Foundation under Awards DMR 1507764.
11:39AM B34.00003: Polymeric Ionic Liquid-Ligand Gels Exhibiting Transient Gel Behavior and Multivalent Ion Conductivity  SEAMUS JONES (Presenter), Chemical Engineering, University of California, Santa Barbara, NICOLE MICHENFELDER-SCHAUSER, Materials, University of California, Santa Barbara, GLENN H FREDRICKSON, RACHEL A SEGALMAN, Chemical Engineering, University of California, Santa Barbara — The conduction of metal ions through solid polymeric electrolytes relies on favorable but highly dynamic interactions between mobile metal cations and polymer-bound solvating functionalities. Metal-ligand interactions have shown promise as solvating functionalities in solid polymer electrolytes due to their ability to strongly solvate metal salts while simultaneously conducting mono and multivalent metal ions in the solid state. These interactions simultaneously act as reversible cross-links, enhancing the storage modulus of the material over short timescales. Controlled poly(methyl acrylate)s with imidazole chain ends are synthesized as model polymers to investigate metal-ligand bond lifetimes and design rules for solid polymer electrolytes. Materials with a controlled number of imidazole ligands per chain are used to generate dynamic star-like and network topologies which relax to a disordered melt through metal-ligand bond dissociation. The network-forming materials are further used to probe the kinetics of cation-ligand association when the identity and valency of the metal cation is varied. Scaling arguments based on oscillatory rheology and electrical impedance measurements are used to support a hopping-type mechanism of ion conduction in metal-ligand coordinating polymers.

11:51AM B34.00004: Hydroxide conducting block copolymers* [Invited] YOSSEF ELABD (Presenter), Texas A&M Univ — Hydroxide ion conducting block copolymers have the potential to possess the multiple orthogonal properties required for anion exchange membranes to enable long-lasting alkaline fuel cell performance, and therefore can accelerate the advancement of the alkaline fuel cell, a low-cost alternative to the well-adopted commercial proton exchange membrane fuel cell. In this work, an overview of hydroxide ion transport (a property that is proportional to fuel cell performance) in block copolymers will be presented and the subsequent impact of block copolymer morphology on ion transport (conductivity), where the careful design of block copolymer chemistry and chain architecture can accelerate hydroxide ion transport and subsequently alkaline fuel cell performance.

*This work is supported in part by the National Science Foundation under award no. CBET-1703645.
Simulation of Ion Transport through Percolated Aggregates in Precise Sulfophenylated Polyethylene Ionomers

BRYCE THURSTON (Presenter), MARK STEVENS, Center for Integrated Nanotechnologies, Sandia National Laboratories, BENJAMIN PAREN, KAREN WINEY, Materials Science & Engineering, University of Pennsylvania, AMALIE FRISCHKNECHT, Center for Integrated Nanotechnologies, Sandia National Laboratories — Ionomers present an attractive potential alternative to standard electrolytes in Li ion batteries due to their capacity to function as single-ion conductors. When the spacing between adjacent pendant groups is precisely controlled, ionic groups within ionomers have been shown to self-assemble to form aggregates with well-ordered morphologies. The structure of these aggregates can have a significant impact upon ion conductivity. In order to gain greater understanding at the microscopic level, we perform fully atomistic molecular simulations to probe the assembled ionic aggregates of sulfophenylated polyethylene ionomers with a spacing of five carbon atoms between pendant groups (p5PhS), neutralized with a series of cations (Li, Na, and Cs). We find that the ionic aggregates form percolating clusters provided the polymers are neutralized with a sufficiently high fraction of cations. Li and Na aggregates take ribbon-like configurations, while Cs aggregates are more disordered. In each case the ions are able to slowly diffuse from sulfonate group to sulfonate group through the percolated aggregates, with larger ions exhibiting larger mean-squared displacements. Finally, structure factors computed from simulation agree reasonably well with experimental X-ray scattering data.

Mechanisms of Ion Transport in Block Copolymeric Polymerized Ionic Liquids

ZIDAN ZHANG (Presenter), University of Texas at Austin, JAKUB KRAJNIAK, KU Leuven, JORDAN R KEITH, VENKATRAGHAVAN GANESAN, University of Texas at Austin — We present the results of a multiscale simulation framework investigating the ion transport mechanisms in multicomponent polymerized ionic liquids. Three different classes of polymeric ionic liquid systems, viz., random copolymers, lamellae forming block copolymers and homopolymers are constructed at the coarse-grained scale, and their atomistic counterparts are derived by using a reverse mapping method. Using such a framework, we investigate the influence of morphology on ion transport properties of such polymerized ionic liquids. Our results for ion mobilities are in qualitative agreement with experimental observations. Further analysis of random copolymer and block copolymer systems reveal that the reduced ion mobilities in such systems arise from the influence of architecture and/or morphology on ion coordination and intramolecular hopping events.
Composition fluctuation in weakly heterogeneous dielectric medium containing ions*  

XIAN KONG (Presenter), KEVIN J HOU, JIAN QIN, Stanford Univ — Impacts of salt doping on morphological behavior of block polymers, though well-documented, remain poorly understood. Selective ion solvation has been identified as a driving force for ordering, and its effects studied using mean-field models. We present an analysis of the composition fluctuation that couples, through the heterogeneous dielectric profile, to the ionic solvation in the weakly heterogeneous regime. The free energy is mapped onto the Brazovskii form. The scattering peak is found to depend on salt-doping, as a result of the shift of the critical point and the pairwise Coulomb interaction. Phase diagrams are presented under different doping conditions, revealing the competition between selective solvation and fluctuation. The need of consistently parameterizing permittivity and dispersion interaction is discussed.

*J. Q. acknowledges the 3M Non-Tenured Faculty Award and the Hellman Scholar Award. This research has been supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U.S. Department of Energy through the Advanced Battery Materials Research (BMR) Program (Battery500 Consortium).

Permeation and copermeation behavior of methanol and acetate in cation exchange membranes*  

JUNG MIN KIM, BRYAN BECKINGHAM (Presenter), Auburn University — The permeation of solutes, molecules and ions, through hydrated polymer membranes is of critical importance for many applications. We utilize in situ ATR FTIR spectroscopy to quantify the multicomponent transport of molecules and polyatomic ions through ion exchange membranes. We examine the individual and co-permeation of methanol and acetate across commercially available membranes, Nafion 117, and synthesized polyether-based membranes of varied and tunable ion content and charge type. Membrane permeability and selectivity calculated from single component permeation experiments are compared to those calculated for solutes in multicomponent permeation experiments. In Nafion 117 and model cation exchange membranes we find distinct differences in transport behavior of the acetate anion while the behavior of methanol remains unchanged. We also find no difference in transport behavior for these solutes in uncharged polyether membranes. We attribute this emergent transport behavior of the acetate anion to specific solute-solute-membrane interactions which likely emerge from the electrostatic screening of interactions between the acetate anion and membrane-bound anions.

*The authors thank Auburn University Presidential Award for Interdisciplinary Research.
**1:15PM B34.00009: Percolated ionic aggregates in precise sulfophenylated polyethylene ionomers: Morphology and ion transport**

BENJAMIN PAREN (Presenter), University of Pennsylvania, BRYCE THURSTON, Sandia National Labs, JUSTIN G KENNEMUR, Florida State University, MARK STEVENS, AMALIE FRISCHKNECHT, Sandia National Labs, KAREN WINEY, University of Pennsylvania — We present a set of precise single-ion conducting ionomers that demonstrate decoupled transport of metal cations within self-assembled percolated aggregates in glassy polymer matrices. These precise ionomers consist of a polyethylene backbone with a sulfonated phenyl group pendant on every 5th carbon, that is fully neutralized by a counterion X (Li\(^+\), Na\(^+\), or Cs\(^+\)), p5PhSA-X. The morphologies of these ionomers are characterized with X-ray scattering, and the ion transport properties are characterized with electrical impedance spectroscopy. Both experiments are performed under vacuum, from room temperature up to 180°C. Atomistic molecular dynamics simulations elucidate that the structure of the aggregates in the ionomers is a percolated network. The characteristic length scales of these percolated aggregates as measured by X-ray scattering are ~2nm and independent of ion type. There is good agreement between simulations and experimental X-ray scattering data. The ionomers exhibit conductivity of \(10^{-7}\) to \(10^{-6}\) S/cm at 180°C and demonstrate Arrhenius behavior up to 180°C. This indicates that the ion transport is decoupled from the polymer backbone, which is consistent with a percolated aggregate within which ions travel.

*NSF DMR 1506726, NSF PIRE 1545884, and the VIEST at Penn.

**1:27PM B34.00010: Investigation of monomer segment distributions, chain conformations, and lithium salt solvation in self-assembled, tapered block polymer electrolytes**

PRIYANKA KETKAR (Presenter), Chemical and Biomolecular Engineering, University of Delaware, KUAN-HSUAN SHEN, LISA HALL, William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, THOMAS EPPS, Chemical and Biomolecular Engineering, University of Delaware — Tapered block polymers (TBPs) contain modified monomer segment distributions (e.g., gradient or random copolymer regions) at the chemical junction between two homogeneous blocks. Nanostructured polystyrene-\textit{block}-poly(oligo-oxoethylene methacrylate) (PS-\textit{b}-POEM) TBP electrolytes have exhibited improved ionic conductivities, shear moduli, and processabilities in comparison to their conventional block polymer analogues. In this work, we studied the microscopic characteristics of TBPs that impart these enhanced properties. The monomer segment distributions of lithium salt-doped normal-, inverse-, and non-tapered PS-\textit{b}-POEM TBPs were obtained \textit{via} X-ray reflectivity, and these distributions also were successfully modeled through coarse-grained molecular dynamics simulations that included strong ion solvation effects. This combined experimental-computational approach allowed the segregation strengths, chain conformations, and ion solvation energies of the salt-doped TBPs to be quantified as a function of taper sequence and salt concentration. By understanding how these polymer assembly and ion solvation behaviors affect ion transport, we can guide the rational design of higher-performance polymer electrolytes.
1:39PM B34.00011: Model single ion conducting polymer networks for understanding the impact of ion content, crosslink density, and side chain length on Li transport
CHRISTOPHER EVANS, University of Illinois at Urbana-Champaign, CHENGTIAN SHEN (Presenter), Chemistry, University of Illinois, Urbana-Champaign — Single ion conducting polymer networks were designed containing tethered anions of bis(trifluoromethane sulfonamide) (TFSI), an acrylic backbone, and ethylene oxide (EO) side chains and crosslinkers to develop fundamental structure property relationships. The crosslinking density was varied from 1-50 % mol of the starting monomers, while the crosslinker was an EO diacrylate with 11, 22, or 33 atoms between acrylate groups. The Li to EO ratio was set by the density of fixed TFSI sites and spanned 1:20 to 1:100, while the length of EO side chain on non-ionic monomers was 11 or 22 atoms is achieved. By systematically manipulating parameters, a 3 order of magnitude difference in ionic conductivity and a 70 C shift in Tg was observed indicating the importance of design in such networks. Conductivities approaching 10^{-5} S/cm are reported in dry, single ion conducting networks which is comparable to the state-of-the-art. Adding plasticizer further increases the conductivity. The observed structure-conductivity trends provide insight into the design of single ion conductors for a broad range of energy applications.

1:51PM B34.00012: Salt-tethered nanoparticles in solvent: A potential high conductivity, high lithium transference number electrolyte system* SANKET KADULKAR (Presenter), DELIA MILLIRON, THOMAS TRUSKETT, VENKATRAGHAVAN GANESAN, University of Texas at Austin — Improving the lithium transference number in electrolytes, while maintaining high ionic conductivity, is crucial for reliable and high-performing lithium-ion battery technologies. In this work, using computer simulations, we model a relatively new class of electrolyte system, reported in a recent work [Chem. Mater. 2013, 25, 6, 834-839], wherein nanoparticles cofunctionalized with polymeric ligands and tethered lithium salts, are dispersed in a solvent host. We employ a sequential combination of Molecular Dynamics and kinetic Monte Carlo simulations, to study ion transport in this system. Our results are qualitatively consistent with the experimental findings. Specifically, we explain the interesting dependence of ionic conductivity on nanoparticle composition and anion chemistry. Further, we predict significant improvement in conductivity with high dielectric constant solvents. These results suggest that such electrolyte systems can potentially exhibit high conductivity, along with high lithium transference number.

*Support for this research was provided by the National Science Foundation through the Center for Dynamics and Control of Materials: an NSF MRSEC under Cooperative Agreement No. DMR-1720595.
Cluster Cohesion Effects on Segmental Dynamics in Ionic Polymer Solutions: Molecular Dynamics Simulation Studies* CHATHURIKA KOSGALLANA (Presenter), Department of Chemistry, Clemson University, Clemson, SC, SIDATH I WIJESINGHE, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC, MANJULA SENANAYAKE, SUPUN SAMINDRA KAMKANAM MOHOTTALALAGE, Department of Chemistry, Clemson University, Clemson, SC, Piotr Zolnierczuk, Oak Ridge National Laboratory, Oak Ridge, TN, Gary Grest, Sandia National Laboratories, Albuquerque, NM, DVORA PERAHIA, Department of Chemistry/Department of Physics, Clemson University, Clemson, SC — A small number of ionizable groups tethered to a polymer backbone restricts their macroscopic dynamics. Here, using molecular dynamic (MD) simulations, the dynamics of sulfonated polystyrene (PSS) in toluene solutions are studied as the ionic domains are perturbed by small amounts of ethanol. The static and dynamic structure factors, S(q) and S(q,t) were calculated. S(q) exhibits a characteristic ionic domain signature that is affected by ethanol content. S(q,t), analyzed by KWW resolved two dynamic regions. At low ethanol concentrations, segmental dynamics increase, followed by constrained motion with increased alcohol concentration. Initially, the ionic domains swell, enabling segmental motion. Higher ethanol concentrations collapse the PS segments restricting the motion. These MD results are in excellent agreement with our neutron spin echo data.

*DOE DE-SC0019284

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B35 DPOLY: Directed Self-Assembly of Copolymers in Confined Geometry II 507 - Du Yeol Ryu, Yonsei University - Tag(s): Focus

In-Situ TEM Visualization of Pressure-Induced Ordering of Nanostructured Block Copolymer Thin Films RONG-MING HO (Presenter), CHEN-JUNG HUNG, SHIH-YI LI, JHENG-WEI LIN, HSIAO-FANG WANG, AUM SAGAR, YI-CHIEN LEE, Natl Tsing Hua Univ, AN-CHANG SHI, McMaster University, APOSTOLOS AVGEROPOULOS, University of Ioannina, FAN-GANG TSENG, Natl Tsing Hua Univ, FU-RONG CHEN, City University of Hong Kong — Here, we aim to suggest a facile and effective method for controlled orientation of block copolymer (BCP) thin films driven by pressure-induced ordering during thermal annealing. A novel chip with a built-up metal wire-based micro heater was fabricated utilizing microelectromechanical system (MEMS) technique to in-situ investigate the morphological evolution of free-standing polystyrene-block-polydimethylsiloxane (PS-PDMS) star-block copolymer thin films for demonstration of the suggested pressure-induced ordering. Owing to the high vacuum (~10^{-4} Pa) environment, the low pressure could transfer the extremely selective surface to weakly selective surface for the PDMS and PS, giving the neutral air surface for the formation of span-thru perpendicular cylinders with high-degree lateral ordering, as directly visualized by TEM. We believe that this finding will bring the new opportunities for the designs of polymeric materials in practical applications.
11:27AM B35.00002: Uncovering Hidden Structure in Polymer Films with Soft X-ray Reflectivity  
DANIEL SUNDAY (Presenter), JACOB THELEN, National Institute of Standards and Technology, CHUN ZHOU, IME, University of Chicago, R. JOSEPH KLINE, National Institute of Standards and Technology, PAUL F NEALEY, IME, University of Chicago — Studies on lamellar forming block copolymers (BCPs) organized parallel to a substrate are important for understanding assembly in confined conditions and the impact of surface effects. These have typically been conducted using either hard X-rays or neutron reflectivity where the contrast mechanism makes it difficult to distinguish depth dependent structural variations. Using soft X-rays the optical constants of a material can be controlled by varying the energy near an atomic absorption edge. As you approach the edge, the real and imaginary components can change dramatically as a function of functional group type, concentration and orientation. Additionally, unlike hard X-rays or neutrons, the absorption is no longer negligible and shifting energies can significantly change the depth profile of the electromagnetic field, providing additional control over sensitivity as a function of film depth. This technique is applied to two BCP multilayers with different affinities for a surface. Both systems show variations in interface width as a function of substrate proximity, where a strong surface affinity resulted in an increase in the interface width and a weak affinity resulted in a decrease. This type of surface induced behavior has important implications for BCP lithography.

11:39AM B35.00003: Mapping Self-Assembled Ternary Polymer Blend Phase Behavior Using Gradient Composition Libraries*  
GREGORY DOERK (Presenter), Brookhaven National Laboratory, KRISTOF TOTH, Yale University, CHINEDUM OSUJI, University of Pennsylvania, KEVIN YAGER, Brookhaven National Laboratory — Blending block copolymers (BCPs) with homopolymers, other BCPs, or nanomaterials is a simple yet powerful way to tune self-assembled structure. However, mapping the composition-dependent phase behavior of polymer blends experimentally is a slow, laborious process resulting in coarse data sets. In response, we have developed a first-of-its-kind user tool that combines electrospray deposition with programmable motor control and gradient solution pumping to generate three-component compositionally graded thin film libraries on single substrates. We describe the creation of thin film libraries featuring blends of polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) BCPs with PS and PMMA homopolymers, and demonstrate how synchrotron small angle X-ray scattering (SAXS) may be used to rapidly characterize the self-assembled domain morphology, spacing, and grain size as functions of blend composition and film thickness. This pairing introduces a high-throughput platform for autonomous characterization that promises to accelerate the discovery, design, and optimization of functional soft matter blends.

*Research performed at the CFN and NSLS-II, U.S. DOE Office of Science Facilities at Brookhaven National Laboratory under Contract No. DE-SC0012704.
11:51AM B35.00004: Rapid and Tunable Structuring of Block Copolymer Films using Controlled Solvent Swelling*  ANDREW SELKIRK (Presenter), ANNA TRUBETSKAYA, MICHAEL MORRIS, PARVANEH MOKARIAN, Department of Chemistry, Trinity College, The University of Dublin — We have studied the effect of the film swelling ratio on the phase separation of polystyrene-\(b\)-polyvinylpyridine (PS-b-PVP) block copolymer (BCP) nanopatterns by precisely controlling solvent uptake into the film. Using a custom-built annealing chamber with an inbuilt reflectometer, swelling ratios of up to 10x were achieved in a controlled vapor environment using a variety of solvents. The swelling behaviour of two different PVP molecular systems were studied, one of low molecular weight (~35 kg/mol) and another of high molecular weight (~800 kg/mol). Our results suggest that above a maximum swelling threshold, the ordering of BCP nanopatterns becomes extremely sensitive to slight variations in temperature and vapor pressure. By precisely controlling such variations, we successfully synthesized a surprisingly varied range of BCP morphologies from these individual systems, including highly sensitive metastable phases. Additionally, in comparison to conventional solvent vapor annealing methods we found that such highly ordered structures could be achieved in a matter of minutes rather than hours. A diffusion model is proposed to explain the kinetic effect, and the route to a rapid self-assembly process in BCP films.

*Enterprise Ireland (CF-2017-0638-P), Science Foundation Ireland

12:03PM B35.00005: Rapid Vertical Ordering of Lamellar Block Copolymer Films by Dynamic Thermal Gradient Annealing for Ion Conduction Membranes  MANINDERJEET SINGH (Presenter), WENJIE WU, Univ of Houston, MONALI N BASUTKAR, Intel Corporation, JOSEPH WALTER STRZALKA, Argonne National Laboratory, ALAMGIR KARIM, Univ of Houston — To achieve the full technological potential of block copolymers (BCPs) for use as electrolytes, filtration membranes, or in nanolithography, rapid ordering of BCPs with vertically oriented nanostructures on unmodified substrates is desirable. In this work, we demonstrate the rapid ordering of lamellar BCPs (< 40 s) by utilizing the effect of thermal gradient based Cold Zone Annealing (CZA) technique. The evaporation fronts during film casting results in poorly ordered yet vertically oriented BCP morphology. We demonstrate that CZA, by driving in-plane defect annihilation in such vertically oriented as cast BCP nanostructures, resulted in perpendicularly oriented and well-ordered morphology on a variety of substrates, at short time scales. The kinetics of lamellar grain size (x) evolution was observed to be much faster in CZA (x \(\sim t^{0.26}\)) as compared to oven annealing (x \(\sim t^{0.15}\)). Subsequent post-annealing integration of Ionic liquid (IL) as a penetrating additive was shown to selectively swell well-ordered lamellar domain by 100%, having potential use for mechanically robust ion-conducting channels in BCP membranes and electrolytes. Such highly swollen and vertically ordered lamellar nanostructures are not obtained by \textit{a priori} addition of IL to BCP solutions before film casting.
Directed self-assembly of block copolymer thin film with vertical lamellae by applying filtered plasma and repeated shear stress  

JINWOO OH (Presenter), JEONG GON SON, Korea Institute of Science and Technology — Directed self-assembly (DSA) of block copolymer (BCP) is a promising technology for nanolithography for semiconductors and nanodevices. Although defect-free BCP lamellar structure with vertical orientation nanopattern is necessary for the wide range of applications of BCP self-assembly, the formation of defect-free BCP lamellar nanostructures with vertical orientation in a large area is still a difficult challenge. In this study, we proposed a new approach of filtered plasma treatment and repeated shear stress on BCP film for directionally aligned and perpendicularly oriented lamellar BCP nanostructure. Shear induced ordering of BCP nanopatterns has been restricted to BCP with spherical and cylindrical nanopatterns because of the interfacial energy difference at surfaces. We introduced filtered plasma on the surface of the BCP thin film to produce crosslinked layer having neutral surface energy, and elastomer film was placed on the surface and subjected to shear stress to create a vertically oriented lamellae. To improve the quality of the alignment of BCP structures, the shear stress was repeatedly applied and defects of the nanopatterns were greatly reduced. Various types of BCP can be aligned with this strategy, and it suggests the potential for application in nanolithography.

Nanotubes from 6-arm star-shaped (PMMA-b-PS)$_6$ thin films*  

SO YEONG PARK (Presenter), CHUNGRYONG CHOI, EUNSEOL KIM, JUNHO JANG, YESEONG SEO, JINKON KIM, Department of Chemical Engineering, Pohang Univ of Sci & Tech — Fabrication of nanotube arrays has attracted much attention because of potential applications such as photo catalytic and sensors. Although nanotubes have been formed from core-shell cylindrical morphology in a triblock terpolymer, an appropriate solvent annealing should be done. Here, we obtained nanotube array by changing the chain architecture of block copolymers from linear to star shape. We synthesized 6-arm star-shaped poly(methyl metacrylate)-block-polystyrene copolymer [(PMMA-b-PS)$_6$] having a fixed volume fraction of PMMA with 0.50. When the film thickness was $nL_0$ ($n$ is integer and $L_0$ is the lamellar domain spacing), nanotube arrays were obtained after thermal annealing. We also investigated the surface reconstruction depending on film thickness, annealing time, and substrate.

*This work was supported by the National Creative Research Initiative Program, the National Research Foundation of Korea (2013R1A3A2042196)
**12:39PM B35.00008: Nanostructure sizes and interfacial roughness in blends of linear and cyclic block copolymers**  
AMY D GOODSON, MAXWELL RICK, JESSIE E. TROXLER, HANK ASHBAUGH, JULIE ALBERT (Presenter), Tulane Univ — Cyclic block copolymers (BCPs) are predicted to assemble into nanostructured domains up to 40% smaller than their linear analogues while exhibiting superior thin film stability and assembly dynamics, properties that are desirable for nanolithography. However, synthesizing large quantities of high purity cyclic BCPs is challenging. Thus, we employ dissipative particle dynamic (DPD) simulation to probe the self-assembly behavior of cyclic/linear BCP blends with the aim of answering two questions: How much impact do linear impurities have on cyclic BCP nanostructure size? Can cyclic BCPs be used as structure-directing agents to shrink the domains of linear BCPs in majority-linear blends? Our simulations indicate that up to 10% linear impurity in a cyclic BCP product has a negligible impact on domain spacing and interfacial width, suggesting that costly post-synthesis purification of cyclic BCPs to remove linear impurities may be unnecessary. In majority-linear BCP blends, we find that domain spacing decreases in direct proportion to the amount of cyclic BCP in the blend. These findings provide guidance to experimentalists wishing to utilize cyclic BCPs in nanolithography applications.

*National Science Foundation: NSF-CMMI 1825881; NSF-DMR-REU 1460637 & 1852274

**12:51PM B35.00009: Morphological Evolution of Poly(solketal methacrylate)-block-polystyrene in Thin Films**  
[Invited] THOMAS RUSSELL (Presenter), MINGQIU HU, DUK MAN YU, Univ of Mass - Amherst, DARREN SMITH, Chemistry, State University of New York, Buffalo, HYEYOUNG KIM, Univ of Mass - Amherst, JAVID RZAYEV, Chemistry, State University of New York, Buffalo — Driving the size scale of block copolymer (BCP) microdomains to the nanoscopic level poses numerous challenges in obtaining thin films with highly oriented, laterally aligned structures of large areas. Here, we used the morphological evolution of the lamellar microdomains in thin films of symmetric poly(solketal methacrylate-b-styrene) (PSM-b-PS) BCPs that are converted into poly(glycerol mono-methacrylate-b-styrene) (PGM-b-PS) BCPs by the use of a photoacid generator dissolved in the thin film. This simple hydrolysis, performed in the solid state, causes a marked increase in the segmental interaction parameter, converting a hydrophobic-hydrophobic BCP into a hydrophobic-hydrophilic BCP, wherein the segmental interaction parameter ($\chi$) increased from 0.035 to 0.438 at 25 °C. To orient the microdomains normal to the film surface a hydroxyl-terminated random copolymer (PSM-r-PS) where the fraction of the mers can be varied to tune the interfacial interactions with the substrate and where the (PSM-r-PS) is simultaneously transformed into PGM-r-PS along with the BCPs. The use of the photoacid generator alleviates the need to use toxic vapors and enables a transformation of the BCP in a gradient manner across the substrate that can be used to promote long-range lateral ordering. As the BCP period decreases, the film thickness also must be decreased. Consequently, the ability to use a fully hydrophobic significantly enhances the ability to prepare uniform thin films over large areas.

*This work was supported by the Air Force Office of Scientific Research under contract 16RT1602.*
**1:27PM B35.00010: Ordering and Defectivity in Sub-10 nm Perpendicular Lamellar Block Copolymer Thin Films**

ALVIN CHANDRA (Presenter), RYUICHI NAKATANI, TAKUMI UCHIYAMA, YUTA NABAIE, TERUAKI HAYAKAWA, Tokyo Inst of Tech - Tokyo — The self-assembled nanostructures of block copolymers (BCP) can be used to meet industrial demand for cost-effective methods for forming sub-10 nm lithographic patterns. By applying perpendicular lamellar BCP structures onto thin films, line and space patterns required for lithography can be obtained. However, there remain challenges that must be resolved prior to high-volume manufacturing; the development of strongly-segregating BCPs capable of forming sub-10 nm features, controlling the microdomain orientation into perpendicular structures, and reducing the nanostructure defectivity. Our lab has developed a strongly-segregating BCP, poly(methacrylyl polyhedral oligomeric silsesquioxane)-block-poly(2,2,2-trifluoroethyl methacrylate) (PMAPOSS-b-PTFEMA), that forms sub-10 nm perpendicular lamellae on thin films with ease. To work towards achieving zero defectivity, we studied the growth of ordered structures in PMAPOSS-b-PTFEMA thin films using combinatorial atomic force microscopy (AFM), grazing-incidence small angle X-ray scattering (GI-SAXS), and cross-sectional scanning electron microscopy (CS-SEM).

*This project was funded in part by NEDO, JSPS KAKENHI (17H03113, JP18H05482), and the Ogasawara Foundation for the Promotion of Science and Engineering.

**1:39PM B35.00011: Boundary-Directed Epitaxy of Block Copolymers**

ROBERT JACOBBERGER (Presenter), University of Wisconsin - Madison, VIKRAM THAPAR, Chonnam National University, GUANGPENG WU, Zhejiang University, TZU-HSUAN CHANG, National Taiwan University, VIVEK SARASWAT, AUSTIN J WAY, KATHERINE JINKINS, ZHENQIANG MA, University of Wisconsin - Madison, PAUL F NEALEY, University of Chicago, SU-MI HUR, Chonnam National University, SHISHENG XIONG, Fudan University, MICHAEL ARNOLD, University of Wisconsin - Madison — Historically, there have been two strategies—graphoepitaxy and chemoepitaxy—for directing the self-assembly of block copolymers (BCPs) into useful nanoscale patterns. We have recently discovered a third paradigm—termed “boundary-directed epitaxy”—in which templates consisting only of planar, low-resolution features are used to drive the formation of more complex BCP patterns with enhanced feature resolution. The templates are comprised of spatial boundaries separating regions on a surface with different composition, formed at the edges of isolated stripes on a background substrate. Vertical BCP lamellae are pinned by chemical contrast at each stripe/substrate boundary, align parallel to the boundaries, selectively form on the stripes (whereas horizontal lamellae form on the background substrate), and register to wide and incommensurate stripes to multiply the feature density. Isolated BCP line arrays with half-pitch of 6.4 nm are demonstrated on stripes wider than 80 nm. Boundary-directed epitaxy circumvents the need for topographic structures used in graphoepitaxy or ultra-narrow guiding features used in chemoepitaxy to direct assembly of sub-10 nm BCP features, and provides an attractive path towards nanofabrication beyond the resolution of conventional lithography.
Effect of chain architectures on the segregation degree of block copolymers*  
XIANWEN JI (Presenter), WEI-HUA LI, State Key Laboratory of Molecular Engineering of Polymers, Department of Macromolecular Science, Fudan Univ, Shanghai, China — The design of polymer architectures provides a possible route for lowering the domain spacing of block copolymers in the application of directed self-assembly (DSA). However, the change of segregation degree is always coupled with that of domain spacing. Therefore, we rescale the segregation degrees of different multiblock copolymers with reference to that of AB diblock using self-consistent field theory (SCFT), including [AB]_n linear multiblock, A_nB_n multi-arm star and A_d,nB_d,n dendron-like, such that their density profiles of the lamellar morphology are consistent. Then we compare the lamellar periods of these different copolymers under the condition of equivalent segregation degrees. We find that the star and dendron-like architectures can significantly lower the domain spacing relative to that of AB diblock, especially when the arm number or the generation number is large. Our work presents a simple scheme for quantitatively quantifying the reduction of domain spacing of a specific multiblock architecture relative to that of AB diblock and also provides a useful guide for the application of directed self-assembly.

*This work was supported by the National Natural Science Foundation of China (NSFC) (Grants No. 21774025).

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B36 DCOMP DCMP: Room temperature superconductivity in superhydrides at extreme pressures 601/603 - Renata Wentzcovitch, Columbia Univ - Tag(s): Invited
**11:15AM B36.00001: Clathrate Superhydrides Under High Pressure: A Class of Extraordinarily Hot Conventional Superconductors** [Invited] YANMING MA (Presenter), Jilin Univ — Room-T superconductivity has been a century long-held dream of mankind and a focus of intensive research. In an effort to search for Room-T superconductors, we proposed the first-ever sodalite-like clathrate superhydride CaH$_6$ suffer at extreme pressures that shows a potential of high superconductivity and is not captured at ambient pressure. We recently found a general phenomenon on the common formation of clathrate structures at high pressure in rare earth (RE) superhydrides having three stoichiometries of REH$_6$, REH$_9$, and REH$_{10}$, some of which exhibit high-T superconductivity$^2$. Subsequent experiments synthesized the predicted clathrate YH$_6$, YH$_9$, and LaH$_{10}$ with the measured $T_c$ values at 224, 243, and 260 K, respectively, setting up $T_c$ records among known superconductors. These discoveries open up the door of achieving Room-T superconductors.

In the talk, I will give an overview on the current status of research progress on superconductive hydrides, and then discuss the design principle for achieving Room-T superhydrides. As an example, our recent prediction on clathrate superhydride in Li-Mg-H ternary system$^3$ with a predicted $T_c$ at ~400 K will be discussed.

1Wang, et al., PNAS 109, 6463 (2012)
3Sun, et al., PRL 123, 097001 (2019)

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**11:51AM B36.00002: Road to Hot Hydride Superconductors** [Invited] MUHTAR AHART (Presenter), RAVHI KUMAR, Department of Physics, Univ of Illinois - Chicago, MADDURY SOMAYAZULU, HPCAT, X-ray Science Division, Argonne National Laboratory, RUSSELL HEMLEY, Departement of Physics and Chemistry, Univ of Illinois - Chicago — The realization of superconductivity in dense hydrides in the vicinity of room temperature dates back to predictions of very high $T_c$ in atomic metallic hydrogen and subsequently in doped metallic hydrogen alloys and compounds. Density-functional based structure-search methods calculations combined with BCS-type models predicted a series of dense hydride high $T_c$ superconductors (e.g., CaH$_6$, H$_3$S) at megabar pressures (>100 GPa), followed by the still higher $T_c$ superhydrides (e.g., LaH$_x$, YH$_x$, with $x > 6$). Using a variety of x-ray diffraction and transport measurements, we confirmed our predictions of the stability of LaH$_{10}$ and its $T_c$ to 260 K near 200 GPa as well as superconductivity in other La-H phases, results that were subsequently confirmed independently. Additional studies have been carried out on high $T_c$ hydrides of Se, Ca, Se-S, and other ternary systems. The results are consistent with conventional superconductivity, though the mechanism is likely affected by strong quantum effects in these systems. These efforts highlight the novel physics of metallic hydrogen-like materials, the success of ‘materials by design’ using high pressures, and the possibility of superconductivity well above room temperature as recently predicted.

*Supported by NSF (DMR-1933622, DOE-NNSA (NA-0003858; DE-NA0001974), and DOE-BES (DE-AC02-06CH11357).
MIKHAIL EREMETS (Presenter), Max Planck Institute for Chemistry — Room-temperature superconductivity is becoming realistic given progress in conventional superconductivity: the critical temperature $T_c = 203\, \text{K}$ has been discovered in $\text{H}_3\text{S}$ under high pressures $\sim 150\, \text{GPa}[1]$. Even higher, nearly room temperature superconductivity has been recently found in superhydride $\text{LaH}_{10}[2, 3]$ with $T_c \sim 250\, \text{K}$, following the theoretical predictions[4-6]. In this hydride, lanthanum atom is located at the center of the cage of hydrogen $\text{H}_{24}$ and acts as electron donor contributing to electron pairing, while the hydrogen atoms form weak covalent bonds with each other within the cage. This structure is different from that of $\text{H}_3\text{S}$, in which each hydrogen atom is connected by a strong covalent bond to the two nearby sulfur atoms. We will discuss prospects for further increase of $T_c$ to room temperature, which naturally is expecting for hydrides at high pressures. We will present recent studies on YH$x$, CaH$x$ and other compounds that are considered as potential room-temperature superconductivitors. We will consider various directions to explore high-temperature conventional superconductivity at low and ambient pressures.


*This work was supported by the Max Planck Society.*
1:03PM B36.00004: Electronic Structure and Superconductivity in Binary and Ternary Hydrides Under Pressure* [Invited] EVA ZUREK (Presenter), State Univ of NY - Buffalo — First principles calculations are employed to interrogate the electronic structure and bonding in two structures types that a priori crystal structure prediction methods have found for many compressed alkaline earth and rare earth metal binary hydrides: the $I4/mmm$ symmetry tetrahydrides, and the $Im-3m$ symmetry hexahydrides. We explore the relationship between their structure and electronic structure, as well as their propensity for superconductivity. Moreover, the XtalOpt evolutionary algorithm is used to predict the structures of novel stable and metastable ternary hydrides that could potentially be synthesized in high pressure experiments, and their superconducting critical temperatures are estimated.

*We acknowledge the NSF (DMR-1827815) and the National Nuclear Security Administration, through the Capital-DOE Alliance Center under Cooperative Agreement No. DE-NA0003858, for financial support.

1:39PM B36.00005: Superconductivity in Yttrium and Thorium Polyhydrides: a Route to Industrial Applications [Invited] DMITRII SEMENOK (Presenter), Material Science, Skolkovo Institute of Science and Technology, IVAN A TROYAN, FSRC Crystallography and Photonics, Shubnikov Institute of Crystallography, XIAOLI HUANG, College of Physics, Jilin University, ARTEM OGANOV, Material Science, Skolkovo Institute of Science and Technology — Recent blast growth in hydride superconductivity (SC) has resulted in the achievement of near-room critical temperatures ($\text{ThH}_{10}$: 161 K [1], $\text{H}_3\text{S}$: 203 K [2], $\text{YH}_6$: 226 K [3a-b], $\text{LaH}_{10}$: 250 K [4]) in centimeter-sized mini DACs. The logical final step in this sequence is achieving the room-temperature superconductivity. This progress would not be possible without the development of modern DFT methods and algorithms for crystal structure prediction (e.g. USPEX, CALYPSO, AIRSS). Thanks to these methods, the results of numerical simulations of new superconductors in La-H, Y-H, Th-H, Ce-H systems have been experimentally confirmed in recent years. This is probably the first such great success of computational material science in the field of high-$T_C$ SC.

Here we will present the latest results in high-pressure chemistry of Y, Ba, Sr, Eu superhydrides and measurements of their transport properties with targeted focus on ternary systems and doping of already known SC materials. Perspectives of hydride electronics in DACs, light and magnetic sensors, topology for superconducting storage rings and SQIUDs on diamonds will be discussed.

References:
[3] (a) arXiv:1908.01534; (b) arXiv:1909.10482

Monday, March 2, 2020 11:15 AM - 2:15 PM
In my lecture I will concentrate on accelerator-based light sources (with a focus on DESY). Here we will see novel particle accelerators in the next 10-15 years: (a) ring facilities with a revolutionary electron lattice exceeding the brilliance of previous synchrotron radiation sources by one hundred, (b) linear accelerators for X-ray laser sources which will routinely enable real-time imaging of molecular structures and processes in the femtosecond range, and disruptive developments in plasma accelerators with completely new fields of application, especially in medical technology.

11:51 AM B37.00002: THE EUROPEAN SPALLATION SOURCE [Invited]  
JOHN WOMERSLEY (Presenter), ESS — I will present an update on the European Spallation Source. The ESS is Europe's next-generation neutron scattering facility, and is under construction in Lund, with the data management and software centre hosted in Copenhagen. It will be the world's most powerful accelerator driven neutron source offering capabilities an order of magnitude beyond what currently exists. It is being built by a partnership of 13 European nations and has a total cost of roughly 2 billion Euros. Civil construction is nearing completion and operation of the first accelerator components is now starting. The initial suite of user instruments has been defined and we are making significant progress towards bringing the first three online in 2023. I'll describe progress on the project, outline the technical challenges and some of the science opportunities that ESS will offer. I'll also give an update on the work being done to understand and prepare for the start of operation of the facility in the coming decade.
The ASU Compact XFEL Project — We are pursuing phased development of a very compact XFEL (CXFEL) based on inverse Compton scattering (ICS) from a nanopatterned electron beam. In Phase 1 a compact x-ray light source (CXLS) is currently in commissioning and will demonstrate stable generation of femtosecond hard x-rays with properties similar to undulator radiation (not yet an XFEL). Results from CXLS commissioning will be presented.

In addition to commissioning results, we are designing the Phase 2 CXFEL that converts the undulator-like x-ray emission to fully coherent x-ray laser properties. CXFEL depends on a novel method to produce transform-limited x-ray output in all dimensions, i.e., with all photons in a single degenerate quantum state. This method avoids the noise amplification of SASE by imprinting a well-defined coherent modulation on the electrons via diffraction in a thin crystal grating. We will present experimental results demonstrating the first steps in this method.

The spatial pattern in the diffracted electrons is converted to a temporal pattern using sophisticated electron optics that exchange the transverse and temporal phase space dimensions. The result is a nano-patterned electron beam that can be tuned for wide range of applications. The method allows for coherent control of the phase, frequency, bandwidth, pulse length and amplitude of the x-ray pulses, and enables a variety of multi-color experiments with precisely tunable femtosecond delays for pump-probe experiments, and perhaps even sub-cycle phase-locking of the multiple colors. The output will cover the photon energy range from 100 eV to 8 keV. The CXFEL pulse energy is expected to be tens of nJ due to its small size and low beam energy. For experiments that require higher pulse energies or harder photons, CXFEL presents an excellent seed source that can transfer its unique phase control to large XFELs.

*This work is supported by NSF awards 1935994 (Bio) and 1632780 (Physics).
As we push the frontier of particle physics to higher particle energies, conventional accelerator techniques are attaining their limits. The use of an ionized gas —or plasma— circumvents the most significant barrier of conventional techniques by increasing the energy gained per unit length by several orders of magnitude. One class of plasma accelerators, relevant for high energy physics and light source applications, consists in using a particle beam, «the driver», to excite a plasma wave, that can then accelerate the main particle beam. These beam-driven plasma accelerators have made considerable progress in the past few years, with groundbreaking results such as the high-efficiency acceleration of an electron beam [1], the multi-gigaelectronvolt acceleration of positrons [2], and proton-driven electron acceleration [3].

Here we report on progress made in plasma-based accelerators using particle beam drivers from conventional RF accelerators as well as from novel laser-driven accelerators. First, we will present results on the successful acceleration of positron beams in plasma-based accelerators, and discuss intrinsic limitations, from experimental measurements and from theory and simulations. Second, we will show the first proof-of-principle demonstration of a plasma-based accelerator powered by laser-accelerated electron beams, and will discuss new possibilities opened by these results, from the direct optical imaging of the accelerating structure to the generation of bright beams beyond the state of the art.

Finally, we will discuss the perspectives of the field and the key physics challenges for plasma accelerators that need to be tackled in the future.


*The work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Miniature beam-driven Plasma Accelerators project, Grant Agreement No. 715807).
Electron beams are vital tools for scientific discovery, providing unique probes, sources of radiation and opening windows into the realm of high energy physics. To achieve these feats, accelerator physicists aim to improve beam brightness, spatial and temporal coherence, and achieve higher energies on smaller scales. The use of THz radiation to manipulate and accelerate electron beams is dramatically changing what is possible with the next generation of accelerators. We aim to explore new accelerating structures designed to withstand high gradients, power them with the newest generation of THz sources and lay the foundation for THz accelerator technology. This research will provide answers to fundamental questions about the limits of accelerating gradients and improve understanding for the role of frequency, pulse length and stored energy in plasma breakdown. In this presentation, we will review recent results, report on high gradient tests with metallic structures, explore advanced manufacturing techniques for structures and discuss near-term applications for THz accelerator technology.

*This work was supported by Department of Energy contract DE-AC02-76SF00515. This work was also supported by NSF grant PHY-1734015.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B38 GSNP: Heineman/Faculty/Greene Prize Session

11:15AM B38.00001: The Hofstadter's butterfly: from playing with numbers to studying quantum materials (Dannie Heineman Prize for Mathematical Physics talk)* [Invited]
SVETLANA JITOMIRSKAYA (Presenter), University of California, Irvine — We discuss some results on the Harper’s operator - the model behind the Hofstadter's butterfly: metal-insulator transitions of two kinds, the Ten Martini problem, the proof of Thouless' conjecture from the early 80s: that Hausdorff dimension of the spectrum is bounded by 1/2 for all irrational fluxes, as well as the discovery of self-similar (reflective-)hierarchical structure of eigenfunctions throughout the localization regime.
Partially based on joint works with S. Becker and R. Han, I. Krasovsky, and W. Liu.

*NSF
Many people are familiar with the atomic force microscope, but fewer have experience using its capabilities to do more than image the topography of a sample, usually in air. In this talk, I'll present three different subfields of research that all involve the atomic force microscope. The “force curve” enables the measurement of mechanical properties, including Young’s modulus and adhesion. Normally, the tip is brought into contact with a surface, and the force required to push into the sample is measured. We have used the AFM to image natively adhered bacteria to surfaces in fluid and perform force curves on individual bacteria. We have also grown the biofilm on a cantilever and brought it into contact with different surfaces, to study the early stages of adhesion. Magnetic force microscopy (MFM) may be a familiar technique that can reveal the magnetic state of nanostructures. In rings of the correct size, there is a vortex state in which all moments lie circumferentially in plane, creating a closed-flux state that does not have any MFM contrast in a perfectly symmetric ring. It is challenging to experimentally control the clockwise or counterclockwise circulation of this vortex state with a uniform external applied field. Instead, we pass a current through a solid platinum AFM tip in order to create a local circular Oersted field to probe the magnetic behavior of rings and discs. Finally, I'll present our current efforts using Kelvin probe force microscopy (KPFM) to image real-time charge motion in organic semiconductors. All of this work was completed in my lab at Mount Holyoke College, where I have mentored 50 undergraduate women over the past thirteen years.
The properties of quantum materials are dominated by electronic correlations, which often lead to novel emergent phenomena and spontaneous symmetry breaking at low temperatures or material interfaces. The underlying correlations are encoded in the collective excitations out of the ground state, which are sometimes unfortunately hidden from most experimental techniques. One example is the collective modes that transform as a pseudovector, e.g. the $A_{2g}$ representation of the $D_{4h}$ and $D_{3d}$ groups. Here, we use polarization resolved Raman scattering to directly probe the collective modes with $A_{2g}$ symmetry in two examples. In the heavy fermion metal, URu$_2$Si$_2$, the $A_{2g}$ collective mode uniquely couples to the reflection symmetry breaking ground state in the low temperature phase -- a chirality density wave that was hidden from other spectroscopic tools in the past [1,2]. Whereas on the surface of the 3D topological insulator, due to the strong Rashba spin orbit coupling, the electrons acquire chiral spin textures that results in novel collective modes and composite particles. In the example of Bi$_2$Se$_3$, we observed an $A_{2g}$ mode as the collective spin excitation from the surface states [3], and circularly polarized photoluminescence from chiral excitons [4].

Main References:

*NSF Grant DMR-1709161
Delafossite oxides: natural, ultra-pure metal-insulator heterostructures

VERONIKA SUNKO (Presenter), Max Planck Institute For Chemical Physics of Solids — Delafossite oxides are layered compounds, which can be thought of as natural heterostructures of triangularly coordinated metallic sheets and transition metal oxide blocks. A fascinating range of electronic states can be found both in their bulk and on their surfaces, including extremely high conductivity in PtCoO$_2$ and PdCoO$_2$ [1], maximal Rashba-like spin-splitting on the transition metal terminated surfaces of PtCoO$_2$, PdCoO$_2$ and PdRhO$_2$ [2], Stoner ferromagnetism on the Pd-terminated surface of PdCoO$_2$ [3] and, perhaps most remarkably, an intertwined spin-charge response due to a Kondo coupling between metallic and Mott insulating layers in PdCrO$_2$ [4]. Our group has investigated these states experimentally with angle resolved photoemission, and theoretically with first principles calculations and model Hamiltonians, where applicable.

Concentrating on the metal/Mott insulator heterostructure and the Rashba-like surface states, I will show how the simplicity of the materials allows us to pinpoint to the underlying cause for the remarkable electronic behaviour, and in turn to use delafossites as model systems to understand complex phenomena.


*Max Planck Society and UK EPSRC through grant EP/L015110/1

Hybridizing Spin, Charge and Photon on a Quantum Chip

XIAO MI (Presenter), Google — As we witness the transition of quantum information science from the singular objective of quantum supremacy to the eclectic world of NISQ algorithms, the metrics for success have become rapidly more complex. The simultaneous need for long coherence times, fast gates, accurate readout and high connectivity has both highlighted the respective advantages of various quantum hardwares and accentuated their shortcomings. Hybrid device developments, where technologies across different qubit incarnations are combined to compensate for their inherent physical limitations, have enjoyed much success in recent years. In this lecture, I will review one such example where the technique of circuit quantum electrodynamics (cQED) was successfully grafted from superconducting qubits to semiconductor quantum-dot spin qubits. We will cover the physics and technical developments that have led to the first observations of strong-coupling between a single electron charge in gate-defined quantum dots and a microwave photon [1] and strong-coupling between a single electron spin and a single photon [2]. As time permits, applications of the hybrid device to valley physics in silicon will also be covered [3, 4].

11:15AM B39.00001: Many-body effective energy theory: photoemission at strong correlation [invited] STEFANO DI SABATINO (Presenter), Université Toulouse - Paul Sabatier — Photoemission is a powerful tool to obtain insight into the electronic structure and excitations in materials. From the theoretical point of view, Many-Body Perturbation Theory, within the so-called GW approximation to electron correlation, is the method of choice for calculations of photoemission spectra of many materials. However, GW suffers from some fundamental shortcomings, and, in particular, it does not capture strong correlation, unless one treats the system in a magnetically ordered phase. In this talk, we illustrate some of these problems and efforts to overcome them [1-3]. In particular, we focus on a many-body effective-energy theory (MEET) that gives many-body spectral functions in terms of reduced density matrices (RDMs) [4]. We show that simple approximations, which require the knowledge of the lowest n-body RDMs only, can provide accurate photoemission spectra in model systems in the weak as well as strong correlation regime. With the example of several transition metal oxides, we show that our method yields a qualitatively correct picture both in the antiferromagnetic and paramagnetic phases, contrary to mean-field methods, in which the paramagnet is a metal [4,5].


11:51AM B39.00002: Stochastic Many-Body Perturbation theory beyond the GW approximation VOJTECH VLCEK (Presenter), University of California, Santa Barbara — I will present new stochastic approaches for the computation of electronic excitations within the many-body perturbation theory. The new methods go beyond the popular $G_0W_0$ approximation and include non-local vertex corrections in the screened Coulomb interaction ($G_0W_0^{tc}$) as well as in the self-energy ($G_0W_0^{tc} \Gamma_X$). I will discuss a stochastic implementation in real-time and space which scales linearly with the number of electrons. I will demonstrate that the vertex corrections predominantly affect unoccupied states and that they are crucial for predicting of the corresponding quasiparticle energies.
**12:03PM B39.00003: Stochastic resolution of identity to second order Green's function: ground-state and quasi-particle properties.** WENJIE DOU (Presenter), University of California, Berkeley, TYLER TAKESHITA, Mercedes-Benz Research and Development North America, MING CHEN, University of California, Berkeley, ROI BAER, The Hebrew University of Jerusalem, DANIEL NEUHAUSER, University of California, Los Angeles, ERAN RABANI, University of California, Berkeley — We develop a stochastic resolution of identity approach to the real-time second-order Green's function (real-time sRI-GF2) theory, extending our recent work for imaginary-time Matsubara Green's function (J. Chem. Phys. 151, 044114 (2019)). The approach provides a framework to obtain the quasi-particle spectra across a wide range of frequencies as well as predict ionization potentials and electron affinities. To assess the accuracy of the real-time sRI-GF2, we study a series of molecules and compare our results to experiments and to a many-body perturbation approach based on the GW approximation, where we find that the real-time sRI-GF2 is as accurate as self-consistent GW. The stochastic formulation reduces the formal scaling to $O(N^3)$, where $N$ is the number of electrons. This is illustrated for a chain of hydrogen dimers, where we observe as lightly lower than cubic scaling for systems containing up to $N=1000$.

**12:15PM B39.00004: Effects of electron-hole interactions in single-particle excitations within the $GW$ approach** MENG WU (Presenter), ZHENG LU LI, STEVEN LOUIE, Department of Physics, University of California at Berkeley and Lawrence Berkeley National Laboratory — There are a number of schemes in the literature to do “self-consistent” $GW$ calculations at different levels going beyond the $G_0W_0$ approximation. For single-particle excitations (e.g., the quasiparticle bandgap in semiconductors), a straightforward self-consistent update of both the single-particle Green's function $G$ and the screened Coulomb interaction $W$ generally gives less satisfactory results than those from the $G_0W_0$ approach as compared to experiment, which is due to an under-screening introduced and accumulated in the treatment of dielectric screening at the random phase approximation (RPA) level, where electron-hole interactions are neglected. In this work, we investigate the importance of electron-hole interactions in modifying $W$ and hence the $GW$ self-energy, as well as in reshaping single-particle excitations at the $GW$ level. We present our theoretical formalism, along with first-principles results for several conventional semiconductors.

*This work was supported by the Theory of Materials Program and the C2SEPEM at LBNL funded by the U.S. DOE under Contract No. DE-AC02-05CH11231, and by the National Science Foundation. Computational resources have been provided by NERSC and XSEDE.*
12:27PM B39.00005: Core-Level Spectra for Disordered Systems from GW*  DOROTHEA GOLZE (Presenter), PATRICK RINKE, Department of Applied Physics, Aalto University — We apply our recently developed GW core-level method to predict highly accurate X-ray photoelectron spectra (XPS) of disordered carbon-based materials, which require model sizes of more than 100 atoms. GW has become the method of choice for the computation of valence excitations [1]. We recently showed that GW can be also used for core excitations, even though it requires computationally more accurate techniques for the frequency integration of the self-energy than for valence states [2]. In addition, partial self-consistent schemes and relativistic corrections are crucial. For a benchmark set of small molecules, we find that GW-computed absolute and relative core-level binding energies deviate only 0.3 and 0.2 eV from experiment, respectively. Core-level spectroscopy is one of the few techniques that can be used to characterize disordered materials, such as functionalized amorphous carbon, which shows potential as coating and electrode material. However, the experimental spectra are difficult to interpret. We show that our method provides reliable computational references to support the peak assignment in experimental XPS spectra of amorphous carbon.


*Academy of Finland Grant No. 316168

12:39PM B39.00006: Core and valence electron excitations in SrTiO$_3$ and MgO: a first-principles study including many-body effects*  VIJAYA BEGUM (Presenter), MARKUS ERNST GRUNER, ROSSITZA PENTCHEVA, Universität Duisburg-Essen — Using density functional theory calculations combined with many-body perturbation theory we investigate the optical and XAS spectra of two paradigmatic oxides, SrTiO$_3$ and MgO. For both systems taking into account quasiparticle (GW) and in particular excitonic effects (Bethe-Salpeter equation) is decisive to obtain good agreement with experiment. For the cubic phase of SrTiO$_3$ [1], the theoretical optical spectrum shows a prominent excitonic peak at 6.58 eV which involves interband transition between O-2$p$ and Ti-$e_g$ states. The main effect of the tetragonal distortion below 105 K is observed around this peak due to splitting of the $e_g$ bands. The optical spectrum of MgO shows the best agreement with experiment using a hybrid exchange-correlation functional. Furthermore, the x-ray absorption spectra of the O and Mg K-edge are in good agreement with experiment. The analysis of the origin of the peaks in $k$-space indicates a strong hybridization of the respective unoccupied $p$ and $d$-states, whereas the real space visualization of the exciton wavefunction illustrates its localization and bound nature.


*Funding by DFG- CRC1242, project C02 is gratefully acknowledged.
12:51PM B39.00007: Cumulant expansion of the exciton Green's function: A unified approach for many-body intrinsic, extrinsic, and interference effects in XAS\textsuperscript{*} JOSHUA KAS (Presenter), JOHN REHR, University of Washington, JOHN VINSON, NIST, Gaithersburg, MD — Recently, a real-time cumulant approach has been successful in describing many-body effects in x-ray photo-emission and absorption spectra in a variety of systems.\textsuperscript{1} While the results for XAS are promising, intrinsic and extrinsic effects are not treated on the same footing, with the intrinsic excitations calculated via real-time TDDFT, while extrinsic/interference effects are calculated in a frequency space approach. In addition, extrinsic and interference effects are based on a model of free electrons interacting with plasmons, most appropriate for the alkali metals. Here we present a unified approach which treats satellites in terms of the real-time density response to the sudden appearance of an exciton, which is in turn described by solutions of the Bethe-Salpeter equation at a specific energy. We apply the method to the K-edge XAS of SrTiO3 and analyze the energy dependence of extrinsic and interference effects.\textsuperscript{1,2}

\textsuperscript{1}Kas et al, Phys. Rev. B \textbf{94}, 035156 (2016)
\textsuperscript{2}Vinson et al, Phys. Rev. B \textbf{83}, 115106 (2011)

\textsuperscript{*}J. K. and J.R. acknowledge support by DOE Office of Science BES Grant DE-FG02-97ER45623.

1:03PM B39.00008: Computational characterization of the RIXS Raman-to-fluorescence crossover in BaFe\textsubscript{2}As\textsubscript{2} KEITH GILMORE (Presenter), JONATHAN PELLICIARI, Brookhaven National Laboratory, THORSTEN SCHMITT, Paul Scherrer Institute — Resonant inelastic X-ray scattering (RIXS) studies have significantly enhanced our understanding of correlated materials. However, experimental and computational efforts have largely focused on insulating materials. We recently collected RIXS data on metallic BaFe\textsubscript{2}As\textsubscript{2} at the Fe L\textsubscript{3} edge, which exhibits a Raman-to-fluorescence crossover as the absorption threshold is traversed. By combining core and valence level Bethe-Salpeter solvers, we evaluate the RIXS cross section of BaFe\textsubscript{2}As\textsubscript{2} from first principles. Our calculations capture the Raman-to-fluorescence crossover as well as the main loss features observed in the experiment. By \textit{i)} considering additionally the absorption and non-resonant emission spectra, \textit{ii)} invoking the threshold singularity theory of Nozières and Abrahams \textsuperscript{[1]}, \textit{iii)} recognizing the role of the intermediate state lifetime, and \textit{iv)} decomposing the orbital character of the intermediate and final excitonic states, we are able to quantitatively and qualitatively separate simpler band structure contributions from more complex many-body effects in the RIXS spectra of BaFe\textsubscript{2}As\textsubscript{2}. This analysis is applicable to other strongly correlated metals.

Electronic structure of 3d-transition metal dioxide clusters from GW calculations*  

MEISAM REZAEI (Presenter), SERDAR OGUT, Univ of Illinois - Chicago — Transition metal oxide clusters are not only scientifically interesting, but they are also challenging systems to model using first principles approaches due to strong electron correlations and their open-shell character. These challenges are particularly noteworthy when modeling their excited state properties. The GW approximation using atom-centered localized basis sets has recently emerged as a reliable method for studying excited state properties of confined systems. Here, we investigate various flavors of the GW method (one-shot, eigenvalue self-consistent) with different starting points when applied to quasiparticle spectra of 3d transition metal dioxide cluster anions ScO$_2^-$, TiO$_2^-$, VO$_2^-$, CrO$_2^-$, MnO$_2^-$, FeO$_2^-$, NiO$_2^-$, and CuO$_2^-$. We compare predictions from different levels of theory with each other and with experimental photoelectron spectra.

*Work supported by DOE Grant No. DE-SC0017824

Importance of long-range correlations in transition metal compounds: First-principle studies using the the multitier GW+EDMFT approach*  

FREDRIK NILSSON (Presenter), Lund Univ/Lund Inst of Tech, FRANCESCO PETOCCHI, PHILIPP WERNER, Physics, University of Fribourg, FERDI ARYASETIAWAN, Lund Univ/Lund Inst of Tech — Transition metal compounds exhibit a wide range of intriguing properties, such as high temperature superconductivity and colossal magnetoresistance. The standard method to describe these materials is density functional theory + dynamical mean-field theory (DFT+DMFT), which can treat the strong onsite correlations between the 3d electrons to all orders but omits the long-range intersite correlations. In this talk I discuss the recently developed multitier combination of the GW-approximation and dynamical mean-field theory [1], a parameter-free ab-initio method which yields a fully self-consistent description of both long- and short-range correlations. A systematic study of the cubic perovskites Sr(V,Mo,Mn)O3 reveal that the long-range correlations, which are typically ignored for this class of materials, can have a profound influence on the interpretation of the spectra. Specifically spectral features previously interpreted as Hubbard bands are reinterpreted as plasmon satellites originating from long-range charge fluctuations.


*This work was supported by the Swedish Research Council (VR).
1:39PM B39.00011: Dynamically Screened Excitons in Heteropolar Semiconductors: The Case of Halide Perovskites* MARINA FILIP (Presenter), Molecular Foundry, Lawrence Berkeley National Laboratory, JONAH HABER, Physics, University of California, Berkeley, JEFFREY B NEATON, Lawrence Berkeley National Lab — The interaction between photogenerated electron-hole pairs in semiconductors is screened by their dielectric environment. In heteropolar semiconductors, dielectric screening originates with both electrons and polar phonons. State of the art GW/BSE methods for prediction of excitons typically only include the static electronic contribution to the screening. However, prior studies report on the importance of dynamical lattice contributions to screening from polar phonons for excitons in halide perovskites [1,2]. Here, we develop an extension of the BSE approach to include both electronic and lattice contributions to the dielectric screening. We show that in heteropolar semiconductors, lattice effects can significantly reduce the electron-hole interaction, even when the exciton binding energy is much larger than the characteristic phonon frequency. We demonstrate the importance of dynamical lattice screening for excitons in halide perovskites, and generalize our findings by extending the Wannier model to include lattice polarization effects, clarifying the relevance of this effect for general classes of heteropolar semiconductors.


*Work supported by the DOE within the C2SEPEM center, using resources at NERSC.

1:51PM B39.00012: GW calculations and ultraviolet photoelectron spectroscopy of gas phase ion pairs - a window into the electronic structures of ionic liquids JUHAN MATTHIAS KAHK (Presenter), Imperial College London, IVAR KUUSIK, VAMBOLA KISAND, Institute of Physics, University of Tartu, JOHANNES LISCHNER, Imperial College London — Room temperature ionic liquids have extremely low equilibrium vapor pressures, but in ultrahigh vacuum vapors consisting of neutral ion pairs can be detected. Spectroscopic measurements of these ion pairs, the fundamental building blocks of ionic liquids, can yield insights into the electronic structures of these unusual and technologically important materials. From a theoretical perspective, the description of these ion pairs is challenging due to the presence of long range charge transfer. For example, in density functional theory different exchange correlation functionals can produce qualitatively different ground state electronic structures. In this study, it is shown that the GW method yields a consistent description of the gas phase ion pairs that is only weakly dependent on the mean field starting point. The effect of different levels of self-consistency in the GW calculations is analyzed. Theoretical valence level photoelectron spectra are calculated, and it is found that G0W0 at a hybrid DFT starting point yields excellent quantitative agreement with experiment. In one instance, GW calculations highlighted the presence of a contaminant in the experimental spectrum that had not been previously recognized, and corroborated its assignment to a decomposition product.
Low-cost alternatives to the Bethe-Salpeter equation: a simple hybrid functional for excitonic effects in solids*  

JIUYU SUN (Presenter), CARSTEN A. ULLRICH, Univ of Missouri - Columbia — The Bethe-Salpeter equation (BSE) is the standard computational method for optical excitations in solids, including excitonic effects. We reduce the computational cost of the BSE by simplifying the dielectrically screened Coulomb interaction: instead of calculating the dielectric function from first principles, we replace it by a momentum-dependent model dielectric function or just by a single parameter. Combined with a semilocal exchange-correlation kernel, this defines a new hybrid functional for solids within generalized TDDFT. We perform a systematic assessment of these simplified approaches, and find that they yield optical absorption spectra and exciton binding energies of semiconductors and wide-gap insulators in close agreement with standard BSE. We also present applications to more complex systems.

*This work was supported by NSF Grant No. DMR-1810922

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B40 DCOMP DCMP DAMOP DCP: Building the bridge to exascale: applications and opportunities for materials, chemistry, and biology II 705 - Anouar Benali, Argonne Natl Lab - Tag(s): Focus
11:15AM B40.00001: Accelerating Large-Scale GW Calculations on Hybrid GPU-CPU Systems

MAURO DEL BEN (Presenter), Lawrence Berkeley National Laboratory, CHARLENE YANG, National Energy Research Scientific Computing (NERSC), STEVEN LOUIE, Department of Physics, UC Berkeley, JACK RICHARD DESLIPPE, National Energy Research Scientific Computing (NERSC) — Large-scale GW calculations are state-of-the-art to accurately describe excited state phenomena in materials, which is critical for the design of novel new devices based on complex materials with applications in many fields. Application of the GW method to complex systems is often perceived as being limited due to high computational cost. Reduced time to solution can be achieved through novel methods, algorithms and optimal implementations on modern HPC systems. In particular accelerators such as GPU’s can speed-up by order of magnitudes conventional CPU-only implementations and additionally reduce the energy per flop consumption. However, porting a large scale HPC code to hybrid GPU-CPU systems and achieve best performance is non-trivial and faces several challenges. This talk showcases the various techniques used to accelerate the Material Science code BerkeleyGW on hybrid architectures targeting to accelerate large scale simulations with thousands of atoms. These techniques include the efficient use of accelerated libraries, pinned host memory, asynchronous memory transfer, streams, batched operations, shared memory, and the overlapping of MPI communication and GPU computation. We achieve good strong- and weak-scaling on thousands of GPUs, and a 16x improvement is obtained on FLOPs/Watt efficiency compared to the CPU-only implementation. We show in this way that GW calculations on systems made of thousands of atoms can be performed with excellent time to solutions, of the order of minutes, even running on a moderate number of hybrid nodes.

*This work was supported by the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) at the Lawrence Berkeley National Laboratory, which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231, as part of the Computational Materials Sciences Program.

11:51AM B40.00002: Accuracy limits of quantum Monte Carlo in the weak-interaction limit

ROMAN FANTA (Presenter), MATUS DUBECKY, Department of Physics, University of Ostrava — Fixed-node diffusion Monte Carlo (FNDMC) method with single-determinant (SD) trial wave functions gains popularity as a scalable benchmark approach suitable for large noncovalent systems. The talk will summarize recent improvements and accuracy limits of the best available bias-cancellation-based SD FNDMC computational protocol suitable for a large class of noncovalent systems.

*We acknowledge financial support by the Czech Science Foundation (18-24321Y), University of Ostrava (IRP201826, SGS 02/PrF/2019), and, Slovak Research and Development Agency (APVV-18-0161).
12:03PM B40.00003: Simulating realistic features of chemical and materials systems with massively parallel many-body perturbation theory calculations*  DEREK VIGIL-FOWLER (Presenter), National Renewable Energy Laboratory, JACOB CLARY, CHARLES MUSGRAVE, Department of Chemical and Biological Engineering, University of Colorado, Boulder, AARON M HOLDER, National Renewable Energy Laboratory — With experiments obtaining increasingly fine resolution in time, energy, and position, there is a growing need for high-fidelity calculations that can match this rapidly improving resolution. Many-body perturbation theory is one approach that has had significant successes in the accurate simulation of the optoelectronic properties of many materials classes and also of surface chemistry. These methods have traditionally been applied to comparatively simple materials with relatively small numbers of atoms and atom types in a simulation cell, but increasing computing power allows for calculations on systems with hundreds and evens thousands of atoms in a simulation cell. In this talk we will discuss our work on simulating the electrochemical oxygen reduction reaction (ORR) on a system of FeN\textsubscript{4}clusters in graphene using the many-body random phase approximation (RPA) and including the effects of zero-point energy, vibrational entropy, solvation, and applied bias. We will also discuss calculations using the many-body GW-Bethe Salpeter equation (GW-BSE) approach to calculate the optoelectronic properties of complex materials including double perovskites.

*This work was funded by the AOP for the ElectroCat EMN and the NREL Computational Science Center.

12:15PM B40.00004: Large temperature sensitivity of optical emission via synergy of Raman and photoluminescence effects in BaTiO\textsubscript{3}-based phosphor*  ARNAB DE (Presenter), RAJEEV RANJAN, Dept. of Materials Engineering, Indian Institute of Science — The growing interest in luminescence-based optical thermometry in recent years is motivated by the prospect of designing phosphor materials capable of exhibiting large temperature sensitivity of the emission spectrum. The prevalent material design strategies predominantly rely on ascertaining temperature sensitivity using fluorescence intensity ratio (FIR) of the Stark lines in the photoluminescence (PL) emission spectrum of rare-earth(s) doped materials. This approach has yielded temperature sensitivity in the range 0-5%. Here we propose a new strategy for achieving high temperature sensitivity by considering a twin combination of Raman and PL spectrum of the phosphor material, and by introducing Raman-PL-intensity ratio (RPIR) as a parameter for measuring relative temperature sensitivity($S_r$). The effectiveness of this concept is demonstrated on Eu/Er-doped BaTiO\textsubscript{3} wherein a large $S_r$ range (-3 % to +6 %) and large color tuning (red to green) was achieved by exploiting the mechanisms which resulted in a contrasting effect of temperature on Raman and the PL part of the total spectra.

*Authors acknowledge the Science and Engineering Research Board (SERB) of the Ministry of Science and Technology (Grant no. EMR/2016/001457) Government of India for financial support.
12:27PM B40.00005: NWChemEx – Computational Chemistry for the Exascale Era*
HUBERTUS VAN DAM (Presenter), Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, EDOARDO APRA, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, RAYMOND BAIR, Computational Science, Argonne National Laboratory, JEFFERY S BOSCHEN, Chemistry, Iowa State University, ERIC J. BYLASKA, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, WIBE A DE JONG, Computational Chemistry, Materials and Climate Group, Lawrence Berkeley National Laboratory, THOMAS H DUNNING, Advanced Computing, Math & Data, Pacific Northwest National Laboratory, NIRANJAN GOVIND, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, ROBERT J HARRISON, Institute for Advance Computational Science, Stony Brook University, KRISTOPHER KEIPERT, Nvidia, KAROL KOWALSKI, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, SRIRAM KRISHNAMOORTHY, SURAJ KUMAR, ERDAL MUTLU, BRUCE PALMER, AJAY PANYALA, High Performance Computing, Pacific Northwest National Laboratory, BO PENG, Computational Engineering, Pacific Northwest National Laboratory, RYAN M RICHARD, Chemical & Biological Sciences, Ames Laboratory, T P STRAATSMAN, Oak Ridge National Laboratory, EDWARD F VALEEV, Department of Chemistry, Virginia Tech, MARAT VALIEV, Biosystems Dynamics & Simulation, Pacific Northwest National Laboratory, DAVID B WILLIAMS-YOUNG, CHAO YANG, Scalable Solvers Group, Lawrence Berkeley National Laboratory, THERESA L WINDUS, Chemistry, Iowa State University
— NWChemEx is an ECP project for computational chemistry that builds on the success of NWChem. NWChem is an early co-design project started in 1992, to address distributed memory parallel computers. The code's modular design, the Global Arrays for distributed data handling, and code generation using the Tensor Contraction Engine, provided a platform for building scalable chemistry capabilities. Key capabilities of the code are MD, DFT methods, and coupled cluster. The science challenges targeted by the NWChemEx are accurate simulations of catalytic reactions and biomolecular complexes. Such calculations require next generation computers that are very different from those NWChem was designed for. Hence, NWChemEx re-engineered the concepts, models and implementations for future computers. We focus on overcoming the limitations of NWChem's design. This involves platform enhancements like execution schedule aware tensor frameworks, composable simulations, code generation for accelerator hardware, and exploiting emerging sparsity. The required changes in the key methods will be discussed.

*This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.
12:39PM B40.00006: Accessible and collaborative web interface for HPC materials simulations TIMUR BAZHIROV (Presenter), Exabyte Inc. — High Performance Computing (HPC) predictive capabilities are of key importance to chemical and materials sciences and engineering, contributing to the goal of the Materials Genome Initiative for enhancing the rate of breakthroughs in complex materials chemistry and materials design. However, recent advances in theory, algorithms, and HPC hardware for materials and chemical sciences, especially aimed at the exascale, are yet to be widely available to the majority of scientifically and technically capable communities in the United States [1]. We outline the concept for the creation of a web-enabled infrastructure for predictive theory and modeling [2] able to facilitate access to, coordination and sharing of information and data produced by scalable codes adapted for exascale computing. In addition, we explain how our web-based infrastructure can help promote universal standards for data inputs and outputs in the multitude of codes and methodologies and discuss the use cases.


12:51PM B40.00007: Large-scale many-body perturbation theory calculations on leadership class facilities* MARCO GOVONI (Presenter), Argonne Natl Lab, HE MA, FRANCOIS GYGI, GIULIA GALLI, University of Chicago — Many-body perturbation theory (MBPT) has been shown to provide an accurate description of excited state properties for the simulation of spectroscopic signatures of materials and molecules. The advent of exascale computing offers the appealing opportunity to expand the applicability of MBPT methods to systems of unprecedented size and complexity, e.g. to thousands of electrons. We will discuss methodological advances implemented in the WEST code [http://west-code.org] for both GW and BSE calculations. We will present new functionalities enabled by the concurrent use of WEST and the Qbox code [http://qboxcode.org], with focus on interoperability paradigms. We will discuss the advantages of developing interoperable software, and we will present results for the calculation of spectroscopic properties of defective insulators and semiconductors hosting optically addressable spin-defects.

*This work was supported by MICCoM, as part of the Computational Materials Science Program funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.
Electronic density and atomic forces in solids by plane-wave auxiliary-field quantum Monte Carlo

SIYUAN CHEN (Presenter), Department of Physics, College of William & Mary, MARIO MOTA, Division of Chemistry and Chemical Engineering, California Institute of Technology, FENGJIE MA, Department of Physics, Beijing Normal University, SHIWEI ZHANG, Center for Computational Quantum Physics, Flatiron Institute — We present accurate electronic densities for several prototypical solids, including the ionic crystal NaCl, covalent-bond semiconductor Si, and metallic Cu. These results are obtained using ab initio auxiliary-field quantum Monte Carlo (AFQMC) method working in a plane-wave basis with multiple-projector, norm-conserving pseudopotentials. AFQMC has been shown to be an excellent many-body total energy method. Computation of observables and correlation functions other than the ground-state energy requires back-propagation, which we have implemented in this work in the plane-wave basis AFQMC framework. Our (near-exact) results are used to benchmark several density functionals, which can be useful in constructing improved density functionals. Besides density, we have also implemented the calculation of atomic forces, which paves the way for geometry optimization in solids.


*Siuyuan Chen acknowledges funding and support from Simons Foundation.

A pseudo-BCS wavefunction from density matrix decomposition - application in auxiliary-field quantum Monte Carlo

ZHI-YU XIAO (Presenter), Department of Physics, College of William & Mary, HAO SHI, SHIWEI ZHANG, CCQ, Flatiron Institute, Simons Foundation — We present a method to construct BCS-like (pseudo-BCS) wave functions from the one-body density matrix. The resulting many-body wave function reproduces the density matrix and has the form of a particle number-projected BCS wave function (or antisymmetrized germinal power), which can provide a better Ansätze in correlated fermion systems than a single Slater determinant or a linear combination of Slater determinants (for example from a truncated active space calculation). We apply the pseudo-BCS wave function to auxiliary-field quantum Monte Carlo (AFQMC) as a trial wave function. Using the two-dimensional Hubbard model as an example, we show that it leads to improved results as a constraint. Further, the pseudo-BCS wave function allows a fully self-consistent constraint via the density matrix.

*We acknowledge the support from Simons Foundation.
1:27PM B40.00010: Electronic band gaps from Quantum Monte Carlo methods*  YUBO YANG (Presenter), University of Illinois at Urbana-Champaign, VITALY GORELOV, Université Paris-Saclay, CARLO PIERLEONI, University of L’Aquila, DAVID CEPERLEY, University of Illinois at Urbana-Champaign, MARKUS HOLZMANN, Univ. Grenoble Alpes — We develop a method for calculating the fundamental electronic gap of semiconductors and insulators using grand canonical Quantum Monte Carlo simulations. We discuss the origin of the bias introduced by supercell calculations of finite size and show how to correct the leading and sub-leading finite size errors either based on observables accessible in the finite-sized simulations or from DFT calculations. Our procedure is applied to solid molecular hydrogen and compared to experiment for carbon and silicon crystals. arXiv: 1910.07531

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*DMC and YY were supported by DOE Grant NA DE-NA0001789. VG and CP were supported by ANR France HyLightExtreme.

1:39PM B40.00011: RuCl$_3$ electronic structure by quantum Monte Carlo*  ABDULGANI ANNABERDIYEV (Presenter), North Carolina State University, CODY MELTON, RAYMOND C CLAY, LUKE SHULENBURGER, Sandia National Laboratories, GUANGMING WANG, LUBOS MITAS, North Carolina State University — The alpha phase of RuCl$_3$ crystal consists of 2D stacked honeycomb layers coupled with van der Waals interactions. Both bulk and multi/single layers of bonded RuCl$_6$ octahedra have been produced and exhibit several promising electronic, magnetic and structural properties. The ground state is a magnetic insulator with several possible magnetic states that are energetically very close. Furthermore, the material allows for a formation of putative spin liquid phases and other unconventional magnetic states due to Ru spin-orbit coupling and favorable orbital occupations. We study these systems using fixed-node quantum Monte Carlo (QMC) with averaged spin-orbit as well as with recently developed fixed-phase spin-orbit QMC that is based on two-component spinors formalism. In particular, we attempt to understand the role of electron correlations as they affect the ground and excited states. We carry out calculations for the low-lying magnetic states vs non-magnetic state and attempt to reveal the impact of explicit spin-orbit effects on magnetic and electronic properties.

1:51PM B40.00012: Heavy-atom systems in quantum Monte Carlo: pseudopotentials and beyond*  GUANGMING WANG (Presenter), ABDULGANI ANNABERDIYEV, North Carolina State University, CODY MELTON, Sandia National Laboratories, MICHAEL BENNETT, Oak Ridge National Lab, LUKE SHULENBURGER, Sandia National Laboratories, LUBOS MITAS, North Carolina State University — We study the electronic structure of selected systems with heavy atoms such as Ru, Ir, Pb, Bi and I, using quantum Monte Carlo (QMC). This is motivated by expanding real space QMC to systems with strong spin-orbit interactions and significant correlation effects. Such studies require accurate effective core potentials (ECPs), the ability to obtain accurate spinors and the eventual inclusion of multi-reference expansions of trial wave functions. We start by assessing the accuracy of ECPs and their impact on the most basic quantities such as the lowest energy excitations and binding in atomic and molecular systems. Moreover, we try to assess the errors caused by averaged vs. explicit spin-orbit interaction using the recently developed two-component spinor fixed-phase QMC method. We study also the corresponding biases that stem from the fixed-node vs fixed-phase approximations. Furthermore, we try to explore the cases where spin-orbit and correlation are of the same magnitude and can impact important quantities such as band gaps and magnetic states in periodic materials.


2:03PM B40.00013: Mitigating the Sign Problem Through Basis Rotations*  RYAN LEVY (Presenter), BRYAN CLARK, University of Illinois at Urbana-Champaign — Quantum Monte Carlo simulations of quantum many body systems are plagued by the fermion sign problem. The cost of overcoming the sign problem (and its overall existence) is basis dependent. In this talk, we show how to use sign-free quantum Monte Carlo simulations to minimize the effect of the sign problem by optimizing over the choice of basis on large two-dimensional systems. This can be done despite the fact that the sign problem makes it difficult to even compute the average sign of such a simulation. We numerically illustrate these techniques by decreasing the ‘badness’ of the sign problem through single-particle basis rotations on one and two dimensional Hubbard systems.

*This research is part of the Blue Waters sustained petascale computing project and made use of the Illinois Campus Cluster.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B41 GMAG: Electron Transport in Magnetic Materials 707 - Kyung-Jin Lee, Korea Univ
11:15AM B41.00001: Transport spin polarization of Pt/ferromagnetic insulator bilayers*
MICHAEL OSOFSKY (Presenter), JOSEPH PRESTIGIACOMO, United States Naval Research Laboratory, PENG LI, YURI SUZUKI, Dept. of Applied Physics, Stanford University — It has been shown that the anomalous Hall effect can be observed in platinum films deposited on a ferromagnetic insulator which implies the existence of a magnetic proximity effect. One of the key features of ferromagnetic metals is a net spin polarization of the carriers at the Fermi energy which enable the functionality of spintronic devices. In this presentation we show that spin polarized carriers are indeed present in Pt films of various thicknesses that were deposited on magnesium aluminum ferrite (MAFO) using point contact Andreev scattering. The results were obtained by extracting conductance vs. voltage data from I-V curves taken through contacts formed by driving a sharpened superconducting Nb tip into the Pt/MAFO samples. The resulting spectra were then analysed using a modified BTK theory of supercurrent conversion at a normal/superconductor interface to obtain the values of the transport spin polarization.

*The authors acknowledge the support of the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering under the Laboratory University Collaboration Initiative (LUCI) and Vannevar Bush Faculty Fellowship (funded by the Office of Naval Research through grant N00014-15-1-0045).

11:27AM B41.00002: Strong transverse spin current generation in bulk ferromagnetic materials*
ROHIT NAIR (Presenter), KRITI GUPTA, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, ZHE YUAN, The Center for Advanced Quantum Studies and Department of Physics, Beijing Normal University, GERRIT BAUER, Institute for Materials Research & WPI AIMR & CSRN, Tohoku University, PAUL KELLY, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente — The intrinsic spin Hall effect (SHE) is widely studied in non-magnetic metals and semiconductors. Recent studies have reported the observation of an inverse SHE (ISHE) in 3d ferromagnetic alloys where the underlying spin currents that generate the ISHE are oriented along the magnetization direction of permalloy (Py) [1]. Subsequent studies report a non-trivial SHE in Py [2,3] where the spin-polarization is not oriented along the magnetization; its origin in a 3d magnetic alloy is not known. To shed some light on the intrinsic SHE in magnetic materials we calculate transverse spin currents as a function of concentration $x$ for fcc $\text{Fe}_x\text{Ni}_{1-x}$ alloys within a first-principles DFT-LDA scattering framework. For Py we find a spin Hall angle (SHA) of 4.8% compared to a value of 5% we calculate for platinum at room temperature [4]. We find a surprisingly large transverse spin current that is polarized along the same direction that could be useful in field-free switching applications.

*Computational sciences for energy research - Joint initiative by Shell and NWO-I
11:39AM B41.00003: Electric current control of spin helicity in an itinerant helimagnet

NAN JIANG (Presenter), Univ of Tokyo, YOICHI NII, HIROKI ARISAWA, Tohoku University, EIJI SAITO, Univ of Tokyo, YOSHINORI ONOSE, Tohoku University — The mechanism of homochirality in biological objects and other materials has been attracting great attention. The longitudinal helical magnetic structure is the chiral magnetic object, in which the ordered direction of the magnetic moment spatially rotates in the plane perpendicular to the propagation vector and the sense of rotation denoted as helicity determines the chirality. The robust magnetic degree of freedom may provide a new concept of magnetic memory if it can be electrically controlled and detected. Here we show that the helicity can be controlled by the magnetic field and electric current, and probed by the second-harmonic resistivity, which is sensitive to the chiral symmetry breaking, in an itinerant longitudinal helimagnet MnP. While the helicity can be controlled by the electric field in insulating multiferroic helimagnets, we have achieved the helicity manipulation in the conducting helimagnet compatible with electric circuits. The controllability may pave a new route to the spintronics.

11:51AM B41.00004: Experimental tests of spin transport models in organic semiconductors*

HENNA POPLI (Presenter), JINGYING WANG, XIAOJIE LIU, EVAN LAFALCE, TANIYA HANSIKA TENNAHEWA, HANS MALISSA, VALY VARDENY, CHRISTOPH M BOEHME, Department of Physics and Astronomy, University of Utah — It has been a long-standing question whether spin-transport and charge-transport in organic materials occur via the same electronic processes [1, 2], i.e. via charge excitations such as polaron states. If so, then the spin current that is produced by spin-pumping through Ferromagnetic resonance (FMR) excitation in an inverse spin-Hall-effect (ISHE) experiment on a NiFe/Alq_3/Pt device [3] must be diminished under electron paramagnetic resonance (EPR) excitation of the charge carriers [4]. We have executed such experiments and do not observe such quenching, which shows that spin-transport is neither due to propagation of charge carriers nor due to spin-transfer between weakly coupled charge carriers. However, these observations are consistent with the idea of exchange mediated transport. We discuss the implications of our experimental results as well as various control experiments that have been done to scrutinize our results. [1] M. Groesbeck et al. (unpublished); [2] Z. Yue et al., Phys. Rev. B 92, 045405 (2015); [3] S.W. Jiang et al., Phys. Rev. Lett. 115, 086601 (2015); [4] D. R. McCamey et al., Nature Mat. 7, 723 (2008).

*This work has been supported by the National Science Foundation, NSF-DMR #1701427.
**12:03PM B41.00005: Magneto-transport in half metallic CrO$_2$ nanowires with spin texture**

LIJUAN QIAN (Presenter), WENZHE CHEN, GANG XIAO, Brown University — Magneto-transport in ferromagnetic metals (FM) is influenced by spin textures. In this work, we study the magneto-transport of spin textures in epitaxial half-metallic CrO$_2$ nanowires. We quantitatively define the spatial non-uniformity of spin textures as spin curvature. We design geometric notches along the edges of the 300nm-width wires to introduce the spin curvature. The magnitude of the spin curvature is controlled via both the depth of notches and the magnetic fields. Through micromagnetic simulations and magneto-transport measurements, we uncover an empirical relation between the spin curvature and the magnetoresistance. This provides a quantitative method to predict the magneto-transport behavior of any spin texture. The thermal effect is studied from 10K and 250K. Results show that the thermal magnons worsen the spin asymmetry and suppresses the spin curvature induced resistivity at temperatures much lower than the ferromagnetic ordering temperature $T_c$.

*The work was supported by King Abdullah University of Science and Technology (KAUST) under the Sensor Initiative.

**12:15PM B41.00006: Non-local voltage measurements with wide F/I/N tunnel contacts are strongly affected by generation of circular electric currents**

YAROSLAW BAZALIY (Presenter), University of South Carolina, REVAZ RAMAZASHVILI, Laboratoire de Physique Theorique, IRSAMC, Universite de Toulouse, CNRS — Electric spin injection is routinely tested by non-local voltage measurements in lateral spin-valves. The advantage of this method is the absence of electric current entering the part of the device where the detecting F/N contact is located. Ideally this leads to the independence of the measured Johnson-Silsbee voltage from the contact size and shape. However, it was predicted [1] that if the detecting contact is wide enough, then circular electric currents are excited in it, altering the non-local voltage and making it dependent on the device geometry. Calculations [1] were performed in the regime of highly transparent F/N boundary. At the same time, modern measurements often use low transparency F/I/N tunnel contacts, in which circular currents should be strongly suppressed. Thus it seems that tunnel contact measurements should conform to the classic Johnson-Silsbee formula. Here we show that while circular electric currents are indeed suppressed by the tunnel barrier, the voltage modifications persist, may be significant, and have to be accounted for in the data analysis.


*Ya. B. is grateful to the Laboratoire de Physique Theorique, Toulouse, and to CNRS for funding the visits.
Magnetotransport in amorphous cobalt silicon and amorphous cobalt germanium thin films

CHRISTOPHER FUCHS (Presenter), University of California, Berkeley and University of Wurzburg, DINAH SIMONE BOUMA, University of California, Berkeley and Lawrence Berkeley National Laboratory, ZHANGHUI CHEN, Lawrence Berkeley National Laboratory, FRANK BRUNI, ARNOUD EVERHARDT, PAUL CORBAE, University of California, Berkeley, NEAL REYNOLDS, University of California, Berkeley and Lawrence Berkeley National Laboratory, LIN-WANG WANG, Lawrence Berkeley National Laboratory, FRANCES HELLMAN, University of California, Berkeley and Lawrence Berkeley National Laboratory — The transition-metal group IV compounds iron germanium and iron silicon show ferromagnetic properties in amorphous Fe\(_x\)(Ge,Si\(_{1-x}\)) films [1], and the recently shown non-trivial topology in crystalline CoSi [2] suggests a study of amorphous cobalt silicon (a-Co\(_x\)Si\(_{1-x}\)) and cobalt germanium (a-Co\(_x\)Ge\(_{1-x}\)) might lead to advances in the field of topological materials. A comparative study of a-Co\(_x\)Si\(_{1-x}\) and a-Co\(_x\)Ge\(_{1-x}\) thin films has been performed for 0.4<x<0.7. At low temperatures, a-Co\(_x\)(Ge,Si\(_{1-x}\)) shows no magnetism for x<0.6 and weak ferromagnetism above x≈0.6, well over an order of magnitude smaller than in a-Fe\(_x\)(Ge,Si\(_{1-x}\)). While the Fe-based alloys show hole carriers, the Co-based alloys show electron carriers. Resistivity measurements show that \(\rho_{xx} \geq 150\mu\Omega\text{cm}\) and dependents mainly on the carrier concentration, which is characteristic for amorphous metals. Hall measurements probe whether the anomalous Hall effect stems from the intrinsic (Berry curvature) mechanism, equal to the integral over occupied energy states of the density of Berry curvature, which is the sum of the spin-orbit correlations of local orbital states [1].


*Funded by the U.S. DOE, MSD, Contract No. DE-AC02-05-CH11231 (NEMM, MSMAG).

Two transient time in the charge and spin current

SUNG PO CHAO (Presenter), NARASIMHA RAJU CHEBROLU, Physics, Natl Kaohsiung Normal Univ — Using magnetic tunnel junction formed by two leads made of ferromagnetic metals and a thin insulating barrier, we study its time depedent charge and spin current following a square voltage pulse. Magnetic fluctuations in the tunnel junction is modeled as magnons, and its influence on the tunneling is treated as a local bosonic mode described by the spinful Anderson-Holstein model. We compute the time dependent spin and charge current perturbatively with Lang-Frisov transformation to handle the strong local electron-magnon or electron phonon interaction at finite temperature. Two transient behaviors are seen in the charge and spin currents. Those two time scales due to different spin and charge responses within one junction could be useful for parallel computing within a single unit.

*We acknowledge the funding support by Taiwan’s MOST (Grant No. 106-2112-M-017 -002 -MY3).
**12:51PM B41.00009: Sublattice Magnetization Driven Planar and Anomalous Hall Effect in β-W/Gdx(FeyCo1-y)1-x Heterostructures**

ANTHONY JOHNSON, EZANA NEGUSSE, DAN ANYUMBA, DEANDRE MCAMONT, RAMESH BUDHANI (Presenter), Morgan State Univ — The antiferromagnetic coupling between 4f and 3d spin sublattices in amorphous films of GdFeCo alloys is known to affect the temperature dependence of magnetization and magnetic anisotropy dramatically. Multilayers of these alloys also reveal non-trivial spin textures driven by dipolar and chiral exchange interactions. Here we present measurements of anomalous Hall (AH) and planar Hall (PH) voltages in β-W/Gdx(FeyCo1-y)1-x bilayer films across the sublattice magnetization compensation point and the temperature at which the magnetic anisotropy changes from in-plane to out-of-plane configuration. We observe a robust planar Hall Effect in these samples that tracks the behavior of magnetization measured with vibrating sample magnetometry. The magnetization switching fields extracted from the PH data allow calculations of anisotropy energy as a function of temperature and 4f/3d moment ratios in the films. The anomalous Hall data in the reversible and irreversible regimes of response are analyzed to extract the Berry phase and spin orbit torque contributions to Hall resistivity.

*This research is supported by the Office of Naval research (USA) Award No. N00014-17-1-2794

**1:03PM B41.00010: Chirality-induced Spin Selectivity in a Two-terminal Semiconductor Device**

TIANHAN LIU (Presenter), Physics, Florida State University, XIAOLEI WANG, HAILONG WANG, Institute of Semiconductors, Chinese Academy of Sciences, GANG SHI, FAN GAO, HONGLEI FENG, Institute of Physics, Chinese Academy of Sciences, HAOYUN DENG, LONGQIAN HU, ERIC LOCHNER, PEDRO SCHLOTTMANN, STEPHAN VON MOLNAR, Physics, Florida State University, YONGQING LI, Institute of Physics, Chinese Academy of Sciences, JIANHUA ZHAO, Institute of Semiconductors, Chinese Academy of Sciences, PENG XIONG, Physics, Florida State University — Electrical generation of spin polarization in semiconductors is of great interest for the device potential in spintronics. One such mechanism is chirality-induced spin selectivity (CISS), with which structural chirality leads to different electric conductivities for electrons of opposite spins. CISS has been widely reported for chiral molecule assemblies on metal surfaces. However, theoretical understanding of the microscopic mechanism and manifestation of CISS in specific device structures remain controversial. Here, we report direct evidence of CISS in two-terminal devices of heterojunctions of (Ga,Mn)As/AHPA-L molecules/Au. The (Ga,Mn)As layer acts as a spin analyzer for electrons injected from the Au electrode through the AHPA-L monolayer. The CISS of AHPA-L and spin injection into the (Ga,Mn)As are manifested as sharp changes in the junction conductance at the coercive fields of the (Ga,Mn)As. The observations provide a definitive signature of CISS-induced spin valve effect in a two-terminal device. Theoretical implications of the effect and its bias dependence will be discussed.


*Work supported by NSF grant DMR-1905843.
1:15PM B41.00011: Resistivity Minimum in Dilute Itinerant Magnets  ZHENTAO WANG, CRISTIAN BATISTA (Presenter), University of Tennessee, Knoxville — Resistivity minima are commonly seen in itinerant magnets and they are often attributed to the Kondo effect. However, recent experiments are revealing an increasing number of materials showing resistivity minima in absence of the Kondo singlet formation. In a previous work, we demonstrated that the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction can produce a classical spin liquid state at finite temperature, whose resistivity increases with decreasing temperature. In this work, we investigate the robustness of the RKKY-induced resistivity upturn against site dilution. By series expansions and molecular dynamics simulation, we show that site dilution competes with thermal fluctuations and further stabilizes the upturn, which applies to both 2D and 3D dilute itinerant magnets. Under a magnetic field, the resistivity upturn is reduced due to suppression of the electron-spin scattering.

1:27PM B41.00012: Nonequilibrium noise measurements using hBN tunnel barriers  XUANHAN ZHAO (Presenter), LIYANG CHEN, PANPAN ZHOU, DOUGLAS NATELSON, Rice Univ — Spin-orbit coupling, a relativistic effect coupling the spin angular momentum of an electron with its orbital angular momentum, has shown its significance for potential “spintronic” device applications. Nonequilibrium noise (or “shot”) noise, which comprises the inherent fluctuations in the electrical current of system driven out of equilibrium, is predicted to be an outstanding experimental probe for underlying physics in the spin-orbit coupling, since predictions shows the tunneling shot noise will be modified in the presence of spin accumulation. Here we report initial nonequilibrium charge current noise measurements in a variety of tunnel junctions prepared using hBN as monolayer tunnel barriers and strong spin hall angle materials as electros. We will also report flicker noise found during low-frequency noise measurement in Au/hBN/Au tunneling structures due to the presence of thermally excited dynamic defects.

1:39PM B41.00013: Theory of nonlinear Hall effects: modified semiclassics from quantum kinetics*  CONG XIAO (Presenter), University of Texas at Austin, ZONGZHENG DU, Southern University of Science and Technology, QIAN NIU, University of Texas at Austin — We propose a modified Boltzmann nonlinear electric-transport framework which differs from the nonlinear generalization of the linear Boltzmann formalism by a contribution that has no counterpart in linear response. This contribution follows from the interband-coherence effect of dc electric-fields during scattering and is related to the interband Berry connection. As an application, we demonstrate it in the second-order nonlinear Hall effect of the tilted massive Dirac model. The intuitive Boltzmann constructions are confirmed by a quantum kinetic theory, which shows that arbitrary $n$th-order nonlinear dc response up to the first three leading contributions in the weak disorder potential is handled by the same few gauge-invariant semiclassical ingredients.

*Q.N. is supported by DOE (DE-FG03-02ER45958, Division of Materials Science and Engineering) on the transport formulation in this work. C.X. is supported by NSF (EFMA-1641101) and Welch Foundation (F-1255).
1:51PM B41.00014: Spin valves with exfoliated 2D materials: MoS$_2$ MARTA GALBIATI (Presenter), FLORIAN GODEL, AYMERIC VECCHIOLA, VICTOR ZATKO, CNRS/THALES, SERGIO TATAY, Instituto de Ciencia Molecular, University of Valencia, REGINA GALCERAN, CNRS/THALES, SAMUEL MAÑAS-VALERO, Instituto de Ciencia Molecular, University of Valencia, MAËLIS PIQUEMAL-BANCI, MARIE-BLANDINE MARTIN, CNRS/THALES, ALICIA FORMENT-ALIAGA, EUGENIO CORONADO, Instituto de Ciencia Molecular, University of Valencia, BRUNO DLUBAK, PIERRE SENEOR, CNRS/THALES — In the last years 2D materials have attracted a huge attention for spintronics thanks to the amazing properties that arise when thickness approaches the single layer level and thanks to the large number of functionalities that they offer. The recent introduction of 2D materials in magnetic tunnel junctions (2D-MTJs) offers very promising properties such as atomically defined interfaces, spin filtering, perpendicular anisotropy and spin-orbit torques modulation. Nevertheless, the difficult integration of exfoliated 2D materials in spintronic devices has limited so far their exploration and performances, maintaining experimental results still far from theoretical expectations [1]. Here, we will show successful fabrication of NiFe/MoS$_2$/Co MTJs thanks to an in-situ fabrication process leading to the highest results reported so far for MTJs based on TMDCs 2D family [2]. Moreover, we will further discuss a path to alleviate fundamental technological and physics issues encountered for the integration of 2D-MTJs [2,3].


B41.00015: Coherent Resonant Tunneling through Double Metallic Quantum-Well States YUAN LU (Presenter), Institut Jean Lamour, Nancy, France, BINGSHAN TAO, CAIHUA WAN, PING TANG, JIAFENG FENG, HONGXIANG WEI, XIAO WANG, STÉPHANE ANDRIEU, Institute of Physics, Chinese Academy of Sciences, Beijing, China, HONGXIN YANG, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, China, MAIRBEK CHSHIEV, SPINTEC, University of Grenoble, Grenoble, France, XAVIER DEVAUX, THOMAS HAUET, FRANCOIS MONTAIGNE, STEPHANE MANGIN, MICHEL HEHN, DANIEL LACOUR, Institut Jean Lamour, Nancy, France, XIUFENG HAN, Institute of Physics, Chinese Academy of Sciences, Beijing, China — Study of resonant tunneling through multi-metallic quantum well (QW) structure is not only important for the fundamental understanding of quantum transport, but also for the great potential to generate advanced functionalities of spintronic devices. However, it remains challenging to engineer such structure due to the short electron phase coherence length in metallic QW system. Here, we demonstrate the successful fabrication of double-QW structure in a single fully epitaxial MTJ heterostructure, where two Fe QW layers are sandwiched between three MgAlOx tunnel barriers. We show clear evidence of the coherent resonant tunneling through the discrete QW states in the two QWs. Compared to the single QW structure, the resonant tunneling in double-QW MTJ produces strong conductivity oscillations with much narrower peak width (about half) owing to the enhanced energy filtering effect. This study presents a comprehensive understanding of the resonant tunneling mechanism in MTJ with multiple QWs, which is essential for future development of new spintronic devices operating in the quantum tunneling regime.
11:15AM B42.00001: Electronic Relaxation Rates in Clean Metallic Ferromagnets  JAMES AMAREL (Presenter), DIETRICH BELITZ, Univ of Oregon, THEODORE KIRKPATRICK, Univ of Maryland — In clean metallic ferromagnets at asymptotically low temperature the magnon-exchange contribution to the single-particle and transport relaxation rates is exponentially suppressed due to the exchange gap [1]. The power-law prefactor of the exponential term is difficult to determine since the gap provides an energy scale in addition to the temperature. To answer this question we present an asymptotically exact evaluation of the Kubo formula. Our solution also clarifies the relation between the integral equation inherent in the Kubo formula and the Boltzmann equation.


11:27AM B42.00002: Latent state in time-resolved nonlinear magnon scattering in thin films  TAO QU (Presenter), ANEESH VENUGOPAL, JAMES M. ETHERIDGE, PAUL CROWELL, RANDALL H. VICTORA, University of Minnesota — The physics of nonlinear magnon scattering has been exploited in nonlinear microwave devices for wireless and satellite communication applications. The latent state, which is the time delay in the response to a microwave pulse, is required to be reduced for fast information communication. We have studied the latent state in time-resolved nonlinear magnon scattering in thin films, in both theory and experiment. The experiment is performed using phase-sensitive time-resolved heterodyne ferromagnetic resonance. The theory is a hybrid time-resolved model which uses an analytical equation of motion based on the Holstein-Primakoff transformation, and realistic micromagnetic simulation, in order to capture the magnon number change caused by the scattering. From the experiment, we find the latent state is a function of power, frequency, and material properties, which indicates the delay time scale is tunable by specific design. The origin of the latent state is the magnon redistribution, in that the uniform magnon mode (wavevector $k=0$) takes time to scatter into non-uniform magnon modes $k\neq0$, which is reflected in the time-resolved magnon number of these modes.

*We thank DARPA, XSEDE and the SMART center (funded by SRC and NIST) for support of this project.
11:39AM B42.00003: A semi-analytical approach for studying the dynamics of magnetic vortices with Dzyaloshinskii-Moriya interactions* CARLA QUISPE FLORES (Presenter), Colorado State University, KAREN LIVESEY, Physics, University of Colorado Colorado Springs, KRISTEN S. BUCHANAN, Physics, Colorado State University — The magnetic vortex provides a convenient system to investigate the effects of the Dzyaloshinskii-Moriya interactions (DMIs) on the dynamics of patterned magnetic structures in confined geometries. Here we introduce a Landau-Lifshitz based diagonalization (LLD) method to calculate the effects of the DMI on radial-type modes in circular disks. The LLD method is a semi-analytical approach which diagonalize the magnetostatic kernel, exchange and DMI contributions to extract the system eigenfrequencies and eigenmodes. Our calculations show that the DMI leads to a frequency shift that is comparable to what is observed for extended films, however, only the down-shifted mode is observed. The excitation amplitudes are enhanced near the core and the structure edges, and modes with even symmetry that would normally be suppressed for a spatially uniform excitation field are present.

*This work is supported by NSF DMR 1709525.

11:51AM B42.00004: Theory for the unconventional dynamics of ferrimagnets [Invited] SE KWON KIM (Presenter), Univ of Missouri - Columbia — Title: Theory for the unconventional dynamics of ferrimagnets

Ferrimagnets have recently emerged as versatile platforms for spintronics owing to their unique tunability of material parameters. In particular, they offer the independent control of the spin density and the magnetization, which are impossible to achieve in more conventional magnets such as ferromagnets and antiferromagnets and thereby offer unprecedented opportunity to discover novel spin physics and realize highly tunable spintronic devices. In this talk, we will discuss the recent theoretical progress on the ensuing novel dynamics of ferrimagnets. The topics will include the dynamics of topological solitons such as domain walls [1,2], skyrmions [3,4], and vortices [5] within the framework of the generalized Landau-Lifshitz-Gilbert-like equations for ferrimagnets. Also, the novel properties of ferrimagnetic magnons such as the tunable g-factors, which can change the sign as well as the magnitude, will be discussed. The talk will be concluded by providing a future outlook on ferrimagnetic spintronics and by discussing some fundamental questions that we are facing to understand the non-equilibrium properties of ferrimagnets [6].

**12:27PM B42.00005: Local spin current probe of the global electrodynamics of ultrathin magnetic heterostructure electrofoils**  
DAVID MAYES (Presenter), MAXWELL GROSSNICKLE, MARK I LOHMANN, JUNXUE LI, VIVEK AJI, JING SHI, University of California, Riverside, JUSTIN SONG, Nanyang Technological University, NATHANIEL GABOR, University of California, Riverside — Spin current - the flow of angular momentum mediated by electrons - is a unique probe of non-trivial phases in ultrathin magnetic heterostructures. Electron spin, however, is highly sensitive to nearby electric and magnetic fields; thus, it is important to characterize nonlocal effects in spintronic devices. The high spin-orbit coupling of platinum in conjunction with ferrimagnetic insulator Yttrium Iron Garnet (YIG) provides an optimal platform for evaluating spin current as a robust probe. Here, we demonstrate the first technique capable of imaging the electric field using spin current as a local probe in Pt/YIG magnetic heterostructures. An imaging laser produces a localized thermal gradient that generates an out-of-plane spin current. In the Pt layer, this spin current scatters electrons in-plane and away from the external magnetic field, producing moving charges which interact with the local electric flux to generate a global voltage that we image in space. Electrofoil Pt/YIG devices, made with airfoil-shaped cutouts, are used to study several subtle nonlocal geometric effects, all of which are well described by the Shockley-Ramo theorem.

**12:39PM B42.00006: On the Field Dependence of Spin-Lattice Relaxation**  
JOHAN VAN TOL (Presenter), National High Magnetic Field Lab, Florida State Univ — Spin Lattice Relaxation (T₁) and spin-spin electron spin relaxation processes (T₂) are of importance for a variety of applications, like quantum information processing, quantum memory, spin cooling, and dynamic nuclear polarization. We studied the temperature dependence of the relaxation in the high magnetic field regime for a variety of paramagnetic spin systems. High frequency pulsed electron spin resonance at various fields and frequencies in the 3-14 T range was used to measure directly in the time domain. The low-temperature direct single-phonon spin lattice relaxation is found to have a strong field dependence (B²-B⁴) in the high frequency/field regime. A comparison is made between transition metal impurities in crystals, donor-bound electrons in semiconductors, and other systems of interest to quantum information processing. In spite of their small spin-orbit coupling, organic radicals in frozen solutions also show a marked field dependence of T₁. This is of importance to dissolution- and solid state dynamical nuclear polarization (DNP) for NMR and MRI studies. The experimental results are compared with existing theoretical models.

*The National High Magnetic Field Laboratory is supported by the National Science Foundation through NSF/DMR-1644779 and the State of Florida.*
12:51PM B42.00007: Spin dynamics in the density functional: problems and perspectives
VLADIMIR ANTROPOV (Presenter), Ames Laboratory, Ames, IA, 50011 — We discuss general dynamics in the charge-current-magnetization density functional theory. Starting from dynamics of one electron wave function we analyze transformation to coupled dynamics of charge, magnetization and current one electron densities. Further we concentrate on a coupled dynamics of total spin and spin current densities. From a methodical point of view we show a connection with the phenomenological Landau-Lifshitz dynamics, effective interactions of Heisenberg model and discuss major assumptions and key adiabatic approximations behind it. Practical expressions for the interatomic interactions parameters of this coupled dynamics are shown also in a standard long wave approximation. Realistic applications of such ab-initio coupled dynamics have been performed for spin excitations and exchange interactions in 3d ferromagnetic metals where “spin current enhancement” of spin waves appears as a perturbation. Several opposite examples of strongly coupled and non adiabatic spin dynamics have been found in 122 family of iron pnictides.

1:03PM B42.00008: Nonclassical magnetization reversal by quantum spin torque of many-electron pulse: A time-dependent density matrix renormalization group study* MARKO PETROVIC (Presenter), PETR PLECHAC, Department of Mathematical Sciences, University of Delaware, ADRIAN FEIGUIN, Department of Physics, Northeastern University, BRANISLAV NIKOLIC, Department of Physics & Astronomy, University of Delaware — Using the time-dependent density matrix renormalization group (tDMRG) method, we study nonclassical effects in the spin-transfer torque (STT) exerted by the spin-polarized electron current on a one-dimensional quantum Heisenberg ferromagnetic chain. Unlike standard STT induced dynamics of magnetization viewed as a classical vector of fixed length, quantum STT allows for the establishment of quantum entanglement between spins. Magnetization reversal driven by quantum STT is nonclassical in the sense that no rotation from its initial state occurs. We extend the findings of Ref. [1], which dealt with single electron wave packets impinging onto many quantum spins. In contrast, the tDMRG method allows us to tackle a problem of many quantum electrons coupled to many quantum spins. The quantum local spins, initially oriented along the negative z-axis, undergo a reversal into the positive z-axis direction after interaction with the spin-up polarized current.


*MDP and PP were supported by ARO MURI Award No. W911NF-14-0247. AEF acknowledges support by DOE-BES grant number DE-SC0019275, and BKN is supported by NSF Grant No. ECCS 1922689.
1:15PM B42.00009: Efficient Method for the Simulation of high-temperature Spin Dynamics* GRIGORII STARKOV (Presenter), Theoretical Physics 3, Ruhr Universitat Bochum, BORIS FINE, Skolkovo Institute of Science and Technology — The measurements of nuclear free induction decays (FIDs) can be used to extract microscopic information about solids such as the distances between nuclear spins or electronic spin susceptibility. At the same time, the first-principles calculation of solid FIDs, which is important for such an extraction, is a long-standing problem. We propose a new hybrid quantum-classical method for the first-principles calculation of solid FIDs, which is based on simulating a large quantum spin lattice by a small cluster of quantum spins coupled to an environment of interacting classical spins via a correlation-preserving scheme. The hybrid method is applied to the computation of FIDs in real materials, such as: CaF$_2$, $^{29}$Si-enriched crystalline silicon and fluorapatite. In all the cases, excellent agreement with the experiment is observed.

References:

*This work was supported by a grant of the Russian Science Foundation (Project No. 17-12-01587).

1:27PM B42.00010: Physical realization of complex dynamical pattern formation in magnetic spinwave active feedback rings* JUSTIN ANDERSON (Presenter), Colorado Sch of Mines, PRAVEEN JANANTHA, Physics, Colorado State University, DIEGO ALCALA, Colorado Sch of Mines, MINGZHONG WU, Physics, Colorado State University, LINCOLN CARR, Colorado Sch of Mines — We report the clean experimental realization of cubic-quintic complex Ginzburg-Landau physics in a single driven, damped system. Five numerically predicted categories of complex dynamical behavior and pattern formation are identified for bright and dark solitary waves propagating around an active magnetic thin film feedback ring: (1) periodic breathing; (2) recurrence; (3) spontaneous spatial shifting; (4) intermittency; and (5) interactions of multiple solitary waves. These non-transient, long lifetime behaviors are observed in microwave spinwave envelopes circulating within a dispersive, nonlinear Yttrium-Iron-Garnet wave guide operating in a ring geometry where net losses are directly compensated for via linear amplification on each round trip (~100 ns). The behaviors exhibit periods ranging from 10s to 1000s of round trip times (~ 1 ms) and are stable for 1000s of periods (~1 s). We find these dynamical behaviors span the experimentally accessible ranges of attractive cubic nonlinearity, dispersion, and external field strength that support the self-generation of backward volume spinwaves in a four-wave mixing regime.

*Funded by NSF
1:39PM B42.00011: An efficient method of spin dynamics for long-range interacting systems*  
TAICHI HINOKIHARA (Presenter), Physics, Univ of Tokyo, MUNETAKA SASAKI, Engineering, Kanagawa university, SEIJI MIYASHITA, Physics, Univ of Tokyo — We developed an efficient method for dynamical simulation, TQMC+SCO, which is useful for classical spin systems with long-range interactions. The method incorporates the stochastic cutoff method (SCO), which is originally specialized for simulating equilibrium state, into the time quantified Monte Carlo (TQMC) method. By using TQMC+SCO, the computational time for the spin-update process is proportional to $O(\beta N \log N)$ no matter how complicated the lattice structure is. We analytically proved that TQMC+SCO gives the same time evolution of the magnetization distribution as the stochastic Landau-Lifshitz-Gilbert (s-LLG) equation. In addition, we simulated a magnetization reversal process and confirmed that the result obtained by TQMC+SCO is in good agreement with that obtained by s-LLG. In this presentation, we introduce TQMC+SCO and discuss why this method works. We also present several examples, where TQMC+SCO can be a strong tool.

*This work is supported by the Elements Strategy Initiative Center for Magnetic Materials (ESICMM) under the outsourcing project of MEXT.

1:51PM B42.00012: Mechanism for a chemical potential of nonequilibrium magnons in parametric parallel pumping*  
NAOYA ARAKAWA (Presenter), Toho Univ — I present a new theory of parametric parallel pumping for a ferrimagnet and demonstrate a mechanism by which a chemical potential of nonequilibrium magnons is generated [1]. In the parametric parallel pumping, two magnetic fields parallel to each other are used; one is static, and the other is time-periodic. By using this pumping, we can achieve a nonequilibrium state in which the magnon distribution function is approximated by the Bose distribution function with a finite chemical potential. However, its mechanism has been unclear. In this talk, I will discuss how nonequilibrium magnons in the parametric parallel pumping acquire a finite chemical potential [1].


*This work was supported by JSPS KAKENHI Grant Number JP19K14664.
Spin transport at metallic interfaces is an essential ingredient of various spintronic device concepts, such as giant magnetoresistance, spin-transfer torque, spin-orbit torque, spin Hall magnetoresistance, and spin pumping. Spin-orbit coupling plays an important role in many such devices. In particular, spin current is partially absorbed at the interface due to spin-orbit coupling. Here, we develop a general magnetoelectronic circuit theory and generalize the concept of spin mixing conductance accounting for various mechanisms responsible for spin-flip scattering. For the case when exchange interactions dominate, we give a simple expressions for the spin mixing conductance in terms of contributions responsible for spin memory loss, spin torque, and spin precession, where all contributions are amenable to ab initio treatment. We observe that in general there is no straightforward relation between the spin torque part and the spin memory loss part, where the latter is often expressed in terms of the spin loss parameter, δ.


Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B43 DCOMP DAMOP DCMP: Precision many-body physics II: Dynamics of 1D quantum systems 702 - Guy Cohen, Tel Aviv University - Tag(s): Focus

11:15AM B43.00001: Quantum Phase Transitions Go Dynamical [Invited] VICTOR GURARIE (Presenter), Department of Physics and Center for Theory of Quantum Matter, University of Colorado, Boulder — Just like a thermal partition function can be a nonanalytic function of temperature, the trace of the evolution operator of a quantum system can be a nonanalytic function of time, the phenomenon referred to as dynamical quantum phase transitions. These singularities which occur at certain points in time in the evolution of a quantum system are the subject of this talk. Interestingly, they can even appear in systems which do not undergo conventional thermal or quantum phase transitions, although precise criteria when they are expected to occur are not yet known. While there might be no obvious way to measure the trace of the evolution operator directly, it is possible to observe the “return probability”, the probability that a system which underwent a quantum quench and subsequently evolved for some time finds itself back in its original state. Sharing some similarity with the trace of the evolution operator, this probability can also be singular at certain times. In the context of quantum quench dynamics these singularities were already observed experimentally. Interpreting the trace of the evolution operator in terms of spectral form factors allows to further narrow down the class of quantum systems which could feature these singularities. In particular, they can be seen in integrable and many body localized systems which can have appropriate spectral form factors, although they are not limited to these types of systems. In the absence of a comprehensive theory of these singularities, their numerical study is often the only tool at our disposal to identify relevant systems where they may be present.
11:51AM B43.00002: Information measures for local quantum phase transitions: Lattice bosons in a one-dimensional harmonic trap  
YICHENG ZHANG (Presenter), Department of Physics, Pennsylvania State University, LEV VIDMAR, Department of Theoretical Physics, J. Stefan Institute, Slovenia, MARCOS RIGOL, Department of Physics, Pennsylvania State University — We study ground-state quantum entanglement in the 1D Bose-Hubbard model in the presence of a harmonic trap. We focus on two transitions that occur upon increasing the characteristic particle density: the formation of a Mott insulating domain with site occupation one at the center of the trap (lower transition), and the emergence of a superfluid domain at the center of the Mott insulating one (upper transition). These transitions generate discontinuities in derivatives of the total energy and have been characterized by local (nonextensive) order parameters, so we refer to them as local quantum phase transitions. We show that while a second derivative of the total energy is continuous with a kink at the lower transition, it is discontinuous at the upper transition. We also show that bipartite entanglement entropies are order parameters for those local quantum phase transitions. We use the density matrix renormalization group, and show that the transition points extracted from entanglement measures agree with the predictions of the local density approximation in the thermodynamic limit. We discuss how to determine the transition points from results in small systems, such as the ones realized in recent optical lattice experiments that measured the order-2 Renyi entanglement entropy.

12:03PM B43.00003: Low-energy physics in the critical phase of the bilinear-biquadratic spin-1 chain*  
MORITZ BINDER (Presenter), THOMAS BARTHEL, Duke University — We use an efficient density matrix renormalization group (DMRG) algorithm to compute precise dynamic structure factors for the bilinear-biquadratic spin-1 chain with Hamiltonian $H = \sum_i [\cos\theta (S_i \cdot S_{i+1}) + \sin\theta (S_i \cdot S_{i+1})^2]$. Here, we focus on explaining the physics in the extended critical phase ($\pi/4 \leq \theta < \pi/2$) of the model. The phase transition from the Haldane phase to the critical phase is marked by the SU(3)-symmetric ULS point ($\theta = \pi/4$), where the elementary excitations are spinons that can be obtained from the Bethe ansatz solution. As we move deeper into the critical phase, the spinon continua contract, and new striking features appear at higher energies. In the vicinity of the transition point from the critical to the ferromagnetic phase, a dispersion with a surprisingly simple functional form emerges, suggesting integrability of the model in the limit $\theta \to \pi/2^-$.  

*Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0019449.
12:15PM B43.00004: Entanglement decomposition for the simulation of quantum many-body dynamics*

THOMAS BARTHEL (Presenter), Duke University — Nonequilibrium dynamics in quantum matter are at the frontier of current research. Efficient and precise simulation techniques are needed to improve our understanding of equilibration and thermalization, dynamical phase transitions, decoherence effects, quantum transport etc. A major obstacle is the growth of entanglement with time which generally implies an increased complexity of the quantum state. For instance, the computation costs of simulations based on tensor network states generally grow rapidly in time, limiting the maximum reachable times. I will show how this problem can be addressed through entanglement decomposition. We can follow the dynamics, starting from an initial state, until the entanglement has grown to a point where our simulation resources are exhausted. We then decompose the current state into lower entangled components and continue by simulating the evolution of these components, decomposing them again when needed. I will demonstrate a specific entanglement decomposition scheme for matrix product state simulations and discuss its efficiency for the study of dynamics in quantum magnets.

*Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0019449.

12:27PM B43.00005: Energy resolved many-body localization emulated with a superconducting quantum processor

CHEN CHENG (Presenter), Lanzhou University, QIUJIANG GUO, Zhejiang University, ZHENGHANG SUN, Chinese Academy of Sciences, RUBEM MONDAINI, Beijing Computational Science Research Center, HENG FAN, Chinese Academy of Sciences, HAOHUA WANG, Zhejiang University — Many-body localization (MBL) describes the regime where isolated matter in disorder environments is able to retain local quantum information at arbitrarily long times, evading thermal equilibrium that naturally occurs in generic quantum systems under their own dynamics. In most experimental studies, MBL has been investigated in various highly-controlled environments, ranging from ultracold atoms in optical lattices, trapped ions to, more recently, quantum processors implemented via superconducting qubits. In this work, taking advantages of the large degree of tunability of the latter platform and using up to 19 qubits, we report on an energy resolved MBL transition. Specifically, by preparing generic product states with different energies and monitoring the persistence of local information in real time dynamics, we are able, for the first time, to investigate the MBL transition at different energy densities, and show an energy resolved experimental MBL phase diagram. While controversies on the existence of many-body mobility edge still exist, due to the system finiteness amenable to classical computers, our investigation potentially opens a path to the final answer by direct quantum simulations.
**12:39PM B43.00006: Exact two-spinon contribution to the longitudinal dynamical structure factor of the anisotropic XXZ model with comparison to DMRG simulations**  
ANDREAS WEICHSELBAUM (Presenter), IGOR ZALIZNYAK, Brookhaven National Laboratory, ISAAC P. CASTILLO, UNAM, Mexico City, JEAN-SÉBASTIEN CAUX, University of Amsterdam, The Netherlands — Motivated by inelastic neutron scattering experiments on quasi-one dimensional XXZ systems such as Yb$_2$Pt$_2$Pb, an exact formula for the two-spinon contribution to the dynamical structure factor is developed based on the quantum group (QG) approach. The results provide a QG derivation of the Baxter formula for the T=0 ordered spin. They are consistent with sum rules, and in excellent agreement with Density Matrix Renormalization Group (DMRG) simulations.

*DOE Grant No. DE-SC0012704, and UNAM-DGAPA-PAPIIT-IN106219.

**12:51PM B43.00007: Nonequilibrium steady state of quantum impurities: A numerically-exact tensor-network approach**  
MATAN LOTEM, School of Physics and Astronomy, Tel Aviv University, FRAUKE SCHWARZ, Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität, ANDREAS WEICHSELBAUM, Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, JAN VON DELFT, Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität, MOSHE GOLDSTEIN (Presenter), School of Physics and Astronomy, Tel Aviv University — The accurate description of the nonequilibrium steady state properties of qubits coupled to different environments, or "quantum impurities" (such as an interacting quantum dot, e.g., in the Kondo regime, under the application of a finite bias voltage) is a central open problem in condensed matter physics. In order to study such systems, we employ a novel approach where the impurity is coupled to a finite number of lead levels, which in turn are incoherently coupled to baths, resulting in a Lindblad master equation for the density operator of an effective 1D system describing the impurity and the finite leads. Numerically exact tensor-networks based methods are employed in order to target the Lindblad equation steady state. First, equilibrium NRG is used to find the relevant Hilbert subspace of the impurity and its vicinity. The full system is then evolved towards the steady state using a time dependent Matrix Product Density Operator algorithm. Our results show that the Lindblad dissipation, if appropriately tuned, can cut off the entanglement entropy growth, which otherwise is the limiting factor in tensor-networks methods, while at the same time giving rise to the correct infinite system steady state observables.
Anomalous transport and hydrodynamics in 1D quantum systems

ROMAIN VASSEUR (Presenter), UTKARSH AGRAWAL, Univ of Mass - Amherst, SARANG GOPALAKRISHNAN, Physics, CUNY, BRAYDEN WARE, Univ of Mass - Amherst — In this talk, I will explain how anomalous transport can emerge in one-dimensional quantum systems at finite temperature, due to hierarchies of quasiparticle excitations. I will describe how to attack this problem using a combination of analytical (generalized hydrodynamics) and numerical (matrix product operators) techniques.

This work was supported by the National Science Foundation under NSF Grant No. DMR-1653271 (S.G.), the US Department of Energy, Office of Science, Basic Energy Sciences, under Early Career Award No. DE-SC0019168 (U.A. and R.V.), and the Alfred P. Sloan Foundation through a Sloan Research Fellowship (R.V.).

Universal scrambling in gapless quantum spin chains

SHUNSUKE NAKAMURA, University of Tokyo, EIKI IYODA (Presenter), Tokai Univ, TETSUO DEGUCHI, Ochanomizu University, TAKAHIRO SAGAWA, University of Tokyo — Information scrambling, characterized by the out-of-time-ordered correlator (OTOC), has recently attracted much attention, because it sheds new light on chaotic dynamics on quantum many-body systems. As an important feature of OTOC, its decay rate has an upper bound, which is referred to as the chaotic bound. The scale invariance, which appears near the quantum critical region in condensed matter physics, is considered to be important for the fast decay of OTOC.

In this study, we focus on the one-dimensional spin-1/2 antiferromagnetic XXZ model and investigate the relationship between scrambling and the scale invariance. As an indicator of the scrambling, we adopt the averaged OTOC, which is related to the operator space entanglement entropy (OSEE). We numerically calculate time-dependence of the OSEE in the early-time region in the thermodynamic limit by using the infinite time-evolving block decimation method. Our numerical results suggest that the scale invariance leads to a universal behavior of the OTOC that is independent of the anisotropic parameter, which reflects the universality of the two-dimensional conformal field theory with the conformal charge c=1 at low temperatures.

Reference
1:27PM B43.00010: Asymmetry in Forward/Backward Transition Times in Multi-Particle System with Interactions*  
JAEOH SHIN (Presenter), ANATOLY BORIS KOLOMEISKY, Rice Univ — Transition time is a fundamentally important property of various non-equilibrium processes, including biological transport and diffusion through channels that reflect the underlying microscopic dynamics. For single particles moving in arbitrary free-energy landscapes, it is known that the forward and backward transition times are the same due to the microscopic reversibility. To understand how and in which condition the symmetry breaks down, here we investigate a non-equilibrium one-dimensional multi-particle system on the lattice with periodic boundary conditions where the particles interact only via hard-core exclusions. We found the asymmetry in forward/backward transition times for time-averaged situations when the transition events are analyzed from long-time trajectories. We developed a fully analytical theoretical analysis that can describe the observed results. The microscopic origin of these surprising observations is discussed.

*The work was supported by the Welch Foundation (Grant No. C-1559), by the NSF (Grant No. CHE-1664218), and by the Center for Theoretical Biological Physics sponsored by the NSF (Grant No. PHY-1427654).

1:39PM B43.00011: Entanglement and matrix elements of observables in interacting integrable systems*  
TYLER LEBLOND (Presenter), KRISHNANAND MALLAYYA, Pennsylvania State University, LEV VIDMAR, Jozef Stefan Institute, MARCOS RIGOL, Pennsylvania State University — We study the bipartite von Neumann entanglement entropy and matrix elements of local operators in the eigenstates of an interacting integrable Hamiltonian (the spin-1/2 XXZ chain), and contrast their behavior with that of quantum chaotic systems. Remarkably, our results suggest that the volume-law coefficient of the average entanglement entropy of eigenstates of the spin-1/2 XXZ chain (zero magnetization sector) is the same as, or very close to, the one for translationally invariant quadratic fermionic models. We also study matrix elements of local operators in the eigenstates of the spin-1/2 XXZ chain at the center of the spectrum. For the diagonal matrix elements, we show evidence that the support does not vanish with increasing system size, while the average eigenstate to eigenstate fluctuations vanish in a power law fashion. For the off-diagonal matrix elements, we show that their distribution is close to log-normal, and that their variance is a well-defined function of \( \omega = E_\alpha - E_\beta \) (\( \{ E_\alpha \} \) are the eigenenergies) proportional to \( 1/D \), where \( D \) is the Hilbert space dimension.

Nonequilibrium dynamics of static electron-phonon models from Monte Carlo simulations* MANUEL WEBER (Presenter), JAMES FREERICKS, Georgetown University — Electron-phonon interactions play an important role in the relaxation of strongly-correlated materials driven out of equilibrium. However, numerical simulation of microscopic models is often restricted to very small system sizes due to the unbound dimensions of the bosonic Hilbert space or requires approximative schemes (such as perturbation theory). In this talk, we present an exact Monte Carlo method to simulate the nonequilibrium dynamics of electron-phonon models in the adiabatic limit of zero phonon frequency. We show applications to the one-dimensional Holstein and Su-Schrieffer-Heeger models and probe the formation and destruction of the ordered Peierls phase as a function of initial temperature when the system experiences strong applied electric fields.

*This work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award DE-FG02-08ER46542.

Heating rates in periodically driven strongly interacting quantum many-body systems* KRISHNANAND MALLAYYA (Presenter), MARCOS RIGOL, Pennsylvania State University — We study heating rates in strongly interacting quantum lattice systems in the thermodynamic limit. Using a numerical linked cluster expansion, we calculate the energy as a function of the driving time and find a robust exponential regime. The heating rates are shown to be in excellent agreement with Fermi's golden rule. We discuss the relationship between heating rates and, within the eigenstate thermalization hypothesis, the smooth function that characterizes the off-diagonal matrix elements of the drive operator in the eigenbasis of the static Hamiltonian. We show that such a function, in nonintegrable and (remarkably) integrable Hamiltonians, can be probed experimentally by studying heating rates as functions of the drive frequency.

*NSF Grant No. PHY-1707482

Monday, March 2, 2020 11:15 AM - 1:39 PM

Session B44 DCOMP: Real-Space Methods for the Electronic Structure Problem II 704 - Amir Natan, Tel Aviv University - Tag(s): Focus
11:15AM B44.00001: Real space and real time electron dynamics simulations for attosecond physics in solids [Invited] SHUNSUKE SATO (Presenter), Center for Computational Sciences, University of Tsukuba, Japan — Real-space and real-time electron dynamics simulation based on the time-dependent density functional theory is a powerful tool to analyze complex and highly-nonlinear interactions of light with solids. To investigate laser-induced ultrafast electron dynamics in solids, we developed a numerical technique to simulate pump-probe experiments [1]. Recently, we applied the numerical pump-probe simulations for the attosecond transient absorption spectroscopy and studied the light-induced ultrafast electron dynamics in solids [2,3]: First, we investigated laser-induced electron dynamics in GaAs with the first-principles simulations. As a result, we found an important role of the light-induced intraband transition in transient optical properties of optically-driven semiconductors [2]. Then, we investigated ultrafast electron dynamics in Titanium, and the first-principles simulations provided microscopic insight into laser-induced electron-localization dynamics in transition metals [3].


11:51AM B44.00002: Speeding up real-space based first-principles methods for excited-states properties using interpolative separable density fitting* JAMES CHELIKOWSKY, WEIWEI GAO (Presenter), University of Texas at Austin — Density fitting methods are a class of algorithms that provide low-rank approximations for products of orbital pairs. However, most of its applications in first-principles codes are based on localized basis sets. A recently proposed interpolative separable density fitting (ISDF) method does not rely on predefined auxiliary basis and is formulated in real space representation. We employ the ISDF method to significantly reduce the cost of linear response time-dependent density functional theory (LR-TDDFT) and GW calculations. In our implementation, we exploit the symmetry property of a system to effectively reduce the number of auxiliary basis and thus the computational cost. Our benchmarks show the cost for constructing auxiliary basis and interpolation coefficients are negligible compared to the total computational cost. Compared to a conventional “brutal-force” approach, the cost for evaluating all kernel matrix elements in LR-TDDFT and GW calculations is reduced by up to three orders of magnitude. The accuracy of our implementation is benchmarked with the GW100 set.

*Our work is supported by a subaward from the Center for Computational Study of Excited-State Phenomena in Energy Materials at LBNL, which is funded by the U.S. DOE under Contract No. DE-AC02-05CH11231.
12:03PM B44.00003: Ab initio stochastic time-domain formulation of the Bethe-Salpeter equation*  
CHENCHEN SONG (Presenter), Physics, University of California, Berkeley, ROI BAER, Fritz Haber Center of Molecular Dynamics and Institute of Chemistry, The Hebrew University of Jerusalem, DANIEL NEUHAUSER, Chemistry and Biochemistry, University of California, Los Angeles, JEFFREY B NEATON, Physics, University of California, Berkeley, ERAN RABANI, Chemistry, University of California, Berkeley — We present a reduced scaling formulation of the Bethe-Salpeter equation (BSE) through a combination of a time-dependent approach and stochastic representations, which allows efficient *ab initio* calculations of optical absorption spectra for semiconductor nanoparticles. The linear response of the system to external fields is simulated by propagating quasiparticle orbital dynamics in real time, followed by Fourier transforming the dipole-dipole correlation function to obtain the absorption spectrum. The spatially dependent screening of the system is described within the random phase approximation (RPA) and combines several efficient stochastic techniques, including factorization with stochastic representations, and time-dependent Hartree propagation of stochastic occupied orbitals. The computational cost of the new BSE formulation is quadratic scaling with respect to system size, which is a significant improvement compared with the conventional symplectic eigenvalue representation of the BSE. We discuss preliminary results from the applications of the method to silicon and CdSe nanocrystals.

*This work is supported by the Department of Energy through the Computational Materials Science Center C2SEPEM at Berkeley Lab; computational resources provided by NERSC.

12:15PM B44.00004: Fast real-time time-dependent density functional theory calculations using higher-order finite element methods  
BIKASH KANUNGO (Presenter), VIKRAM GAVINI, Univ of Michigan - Ann Arbor — We present a computationally efficient approach to solve the time-dependent Kohn-Sham equations in real time using higher order finite-element spatial discretization, applicable to both pseudopotential and all-electron calculations. To this end, we develop an apriori mesh adaption technique, based on the semidiscrete (discrete in space but continuous in time) error estimate on the time-dependent Kohn-Sham orbitals, to construct an efficient finite-element discretization. Subsequently, we obtain the full-discrete error estimate to guide our choice of the time step. Importantly, for the all-electron case, we present an efficient mixed basis, termed as enriched finite element basis, that combines the efficiency of atomic-orbitals-type basis to capture the sharp variations of the electronic fields closer to the atoms along with the completeness and spatial-adaptivity of the finite element basis. We demonstrate significant savings afforded by our approach over the finite-difference and Gaussian basis based approaches, for pseudopotential and all-electron calculations, respectively. Additionally, we discuss schemes to accelerate the time-evolution by constructing dynamic subspace based approaches, informed by time-dependent perturbation theory.
12:27PM B44.00005: Recent Advances in the Development of the Octopus Code for GPUs
SEBASTIAN OHLMANN (Presenter), Max Planck Computing and Data Facility — Since the end of Moore's law, using state-of-the-art supercomputers has become more and more difficult because simulation codes need to expose more and more parallelism to benefit from larger machines. Moreover, supercomputers have become heterogeneous as the increase in CPU performance has slowed down: all of the first three exascale machines to be built in the US will heavily rely on GPUs to achieve their compute performance. Thus, simulation codes in all areas, also real-space DFT codes, will need to utilize GPUs efficiently in order to use these next-generation machines. In this contribution, we report on recent advances in the development of the real-space DFT code Octopus for GPUs. Those developments include porting more algorithms to GPUs, both for ground-state and time-dependent calculations, improving the data handling when copying data to and from the GPU and improving the overlap of communication with computation. We will show how these advances improve the speed of the code and its scalability and apply the code to some larger problem sizes on GPUs.

12:39PM B44.00006: Excitonic effects from real-time parameter-free hybrid functions
NICOLAS TANCOGNE-DEJEAN (Presenter), ANGEL RUBIO, Max Planck Inst Structure & Dynamics of Matter — Hybrid functionals are known to provide excellent band-gap of semiconductors compared to local and semi-local functional. Because hybrid functionals can be constructed to include the long-range part of the screened Coulomb interaction, they contain the basic ingredients that can produce the bound excitons in optical spectra of semiconductors and insulators. So far, the construction of such parameter-free functional requires complex procedures such that optimally-tune parameters [], or fitting of the band-gap on GW calculations []. This hampers the predictive power of such a functional and anchors it to the realm of optical properties of materials at equilibrium.

Because real-time time-dependent density functional theory (TDDFT) does not rely on perturbation theory, it has the capability to study materials out of their equilibrium or perturbed by strong fields. It is therefore of tremendous importance to find hybrid functionals that do not require auxiliary calculations to adjust parameters, in order to bring their predictive power to nonlinear and out-of-equilibrium optical properties.

**12:51PM B44.00007: Ab-initio photo-ionization dynamics without continuum states**

UMBERTO DE GIOVANNINI (Presenter), Max Planck Inst Structure & Dynamics of Matter — Photo-ionization underpins a range of spectroscopies central to the study of structural and dynamical properties of matter in the gas and solid phases. In solid state physics angular resolved photoelectron spectroscopy (ARPES) and time-resolved (tr) ARPES are the most prominent techniques. Leveraging the flexibility offered by real-space methods we developed a technique, based on the real-time formulation of time-dependent density functional theory (TDDFT), to simulate ARPES and tr-ARPES ab-initio without explicit reference to continuum states [1]. I will present the theory, the algorithm involved in the implementation and some of the most representative applications and predictions.


**1:03PM B44.00008: Efficient electromagnetic potential calculations within ground state and time dependent density functional theory.**

DOR GABAY (Presenter), Department of Physical Electronics, Tel Aviv University, ALI YILMAZ, Electrical and Computer Engineering, University of Texas at Austin, VITALIY LOMAKIN, Electrical and Computer Engineering, University of California at San-Diego, AMIR BOAG, AMIR NATAN, Department of Physical Electronics, Tel Aviv University — Electromagnetic potentials play a fundamental role in ground and excited state calculations of Density Functional Theory (DFT). One method for the calculation of such potentials is to directly solve their corresponding differential equations. In this work, the equivalent integral expressions of those potentials are evaluated within their spectral representation. Such integral expressions play a critical role in handling problems ranging from hybrid functionals to the calculation of retarded potentials within the time-dependent Kohn-Sham equation. The simplest of these are FFT procedures used to evaluate the static Poisson integral within ground-state calculations. We extend the use of these integral expressions to time-dependent retarded electromagnetic potentials in both the Lorenz and Coulomb gauges and demonstrate the efficiency of the approach. We use this method for the calculation of several electronic structures using a real-time real-space TDDFT approach. Finally, the various gauge-fixing conditions are compared to assure alignment in the limit of small magnetic fields and the advantages of the Lorenz gauge are outlined.

*This research was supported by the United States-Israel Binational Science Foundation (BSF), Jerusalem, Israel, under BSF grant numbers 2014426 & 2018182.*
1:15PM B44.00009: Real-space approach to the calculation for ionization potentials, exciton, and biexciton binding energies in quantum dots using explicitly-correlated electron-hole interaction kernel method*  PETER MCLAUGHLIN, NICOLE SPANEDDA, ARINDAM CHAKRABORTY (Presenter), Syracuse University — Inclusion of unoccupied states is the leading computational bottleneck for calculation of excited states for large chemical systems. In this work, we present the geminal-screened electron-hole interaction kernel (GSIK) method to address this problem. The GSIK is a real-space r12 method that avoids unoccupied orbitals for constructing the electron-hole interaction kernel by performing an infinite-order diagrammatic summation of particle-hole excitations and deriving a renormalized real-space electron-hole correlator operator. The GSIK method also bypasses the computational expensive AO-to-MO integral transformation by computing all integrals directly in the real-space numerically using permutation sampling Monte Carlo method. These two features allow GSIK method to be used for chemical systems where inclusion of a large number of unoccupied orbitals will be computationally prohibitive. In this work, the GISK method was applied to investigate exciton binding energies, biexciton binding energies, and ionization potentials for large semiconductor (Pb$_{140}$S$_{140}$, Pb$_{140}$Se$_{140}$, Cd$_{144}$Se$_{144}$) nanoparticles. The results from these calculations demonstrate the efficacy of the GSIK method for capturing electron-hole correlation in large clusters and nanoparticles.

*Supported by NSF CHE-1349892 grant

1:27PM B44.00010: Recent developments in the Octopus code for strong light-matter coupling  MICAELOLIVEIRA (Presenter), Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — The Octopus code [1,2] is a finite-differences real-space code designed to fully take advantage of the flexibility and versatility of real-space grids and provide developers with a framework to easily implement and test new ideas and methods in the field of electronic excited states properties and dynamics, while ensuring optimal execution performance and parallelization.

In this talk I will give an overview of the recent advances in the Octopus code regarding several novel approaches in the field of strong light-matter interactions [3]. Such new methods are essential to correctly describe the coupling of light to chemical systems, quantum materials, or nanoplasmmonic systems, among others, when the electron-photon interaction has to be considered explicitly.


Monday, March 2, 2020 11:15 AM - 2:15 PM
11:15AM B45.00001: Sound Scattering and Plasticity in Amorphous materials* [Invited] ANNE TANGUY (Presenter), HAOMING LUO, PAUL DESMARCHELIER, ANTHONY GRAVOUIL, LaMCoS, INSァ Lyon, YAROSLAV BELTUKOV, Ioffe Institute, St Petersburg, FERNANDO LUND, universidad de chile, Santiago de chile — Plastic deformation in amorphous materials results from a succession of local irreversible rearrangements at the nanometric scale known as Transformation Zones. From a numerical point of view, these Transformation Zones are well described within the theory of Eshelby inclusions. In this talk, we will compare sound scattering in amorphous materials in the presence of inclusions. We first remind the signature of structural disorder on acoustic attenuation. We will then detail the role of heterogeneous elastic inclusions on sound attenuation and thermal transfers. Finally we will focus on the effect of Eshelby like inclusions on sound attenuation.


*We are thank to ECOS-chile for the financement C17E02, the 2018 Metchnikov fellowship of the French Embassy in Russia, and the french ministry of research for the PhD fellowship provided ED MEGA.
11:51AM B45.00002: Energy Dissipation in Amorphous Solids during Elastic Deformation*
JAN GRIESSER (Presenter), LARS PASTEWKA, Departement of Microsystems Engineering, University Freiburg — Excitation of atomic vibrational modes is an important mechanism for energy dissipation in friction phenomena. In crystalline materials, the vibrational modes can be represented as plane waves, i.e. the phonons. This is in general not possible in amorphous solids due to structural disorder, which gives rise to different types of vibrational modes. Energy dissipation is related to the lifetime of these vibrational modes. Here we use large-scale molecular dynamics simulations to investigate energy dissipation mechanisms in a model amorphous solid and compare it to a crystalline solid. While the lifetimes of phonons show universal scaling $\omega^{-2}$ in the limit of low frequencies $\omega$, vibrational modes in the amorphous system show different scaling that depends on the type of the vibrational mode. We also carry out cyclic deformation of the amorphous solid in the elastic regime. In this limit, energy dissipation can be traced back to non-affine deformation. We demonstrate that the energy dissipation can be predicted by knowledge of the lifetimes and the non-affine displacement field.

*The authors acknowledge support by the DFG (Grant PA 2023/2). Simulations were carried out on NEMO cluster in Freiburg (DFG grant INST 39/963-1 FUGG).

12:03PM B45.00003: Local excitations in re-heated ultrastable glasses  WENCHENG JI (Presenter), TOM W. J. DE GEUS, MARKO POPOVIĆ, EPFL, EDAN LERNER, University of Amsterdam, MATTHIEU WYART, EPFL — Quasilocalised modes are local excitations present at low frequency vibrational spectrum in glasses. We numerically study their frequency density $D_{\text{loc}}(\omega)$ evolution under thermal cycles at different temperatures $T$, starting from ultrastable glass configurations where these excitations are gapped. The latter are prepared by an algorithm where individual particles can "breathe", modelling the effect of the swap algorithm in a grand-canonical ensemble. We find that a quartic behavior $D_{\text{loc}}(\omega)=A_4 \omega^4$ always appears at any finite $T$. The prefactor $A_4$, which characterizes the number of quasilocalised modes, can increase by a factor of thousands with growing $T$ in our numerical observations. Moreover at small $T$, $A_4$ follows an Arrhenius behaviour: $A_4 \sim \exp(-E_a/T)$ where $E_a$ is atypical energy that depends on the magnitude of the gap initially present. We provide arguments for this dependence. Overall, our result support that true gaps never exists at finite temperature in finite dimensions, and suggest that in some equilibrated super-cooled liquids $A_4$ may decrease exponentially at low $T$. 
12:15PM B45.00004: Cluster-flip colloidal and atomistic algorithms with background potentials*  JARON KENT-DOBIAS (Presenter), JAMES PATARASP SETHNA, Cornell University — We introduce an extension to cluster algorithms of colloidal and atomistic models that naturally incorporates nonuniform background potentials. Simulations of these systems are important for studying the statistical mechanics of fluids and myriad liquid, solid, and glassy phase transitions. Nonuniform background potentials like gravitational or trapping fields are typically present in experiments and can reveal new features of the statistical mechanics at play due to, e.g., nonuniform chemical potential. This method takes existing cluster methods and incorporates background potentials without adding a rejection step by treating the orientation of the system as a dynamical degree of freedom. We assess its efficiency in several applications and explore connections with the celebrated swap Monte Carlo for glasses.

*NSF DMR-1719490

12:27PM B45.00005: Accelerated relaxation in amorphous materials under cyclic loading with alternating shear orientation*  NIKOLAI PRIEZJEV (Presenter), Wright State Univ — The effect of alternating shear orientation during cyclic loading on the relaxation dynamics in disordered solids is examined using molecular dynamics simulations. The model glass was initially prepared by rapid cooling from the liquid state and then subjected to cyclic shear along a single plane or periodically alternated in two or three dimensions. We showed that with increasing strain amplitude in the elastic range, the system is relocated to deeper energy minima. Remarkably, it was found that each additional alternation of the shear orientation in the deformation protocol brings the glass to lower energy states. The results of mechanical tests after more than a thousand shear cycles indicate that cyclic loading leads to the increase in strength and shear-modulus anisotropy.

*National Science Foundation (CNS-1531923)

12:39PM B45.00006: Mesoscale models of amorphous solids under cyclic shear: emergence and character of limit cycles.  KAREEM ABDELSHAFY (Presenter), Northeastern University, BOTOND TYUKODI, Physics, Brandeis University, DAMIEN VANDEMBROUCQ, PMMH, ESPCI Paris, CRAIG E MALONEY, Northeastern University — Amorphous solids (amorphous metallic alloys, glassy polymers, foams, emulsions, pastes, compressed granular packings, etc.) respond in complex ways to imposed shear. In steady shear, the response depends on preparation and shear may or may not localize upon yielding. In cyclic shear, if the amplitude of cycling remains below the yielding threshold, the system may either exhaust all plastic behavior and become purely elastic, or lock into a periodic orbit where plasticity is reversed after one or many cycles and the system returns to its previous configuration. These complex limit cycles have been observed in experiments and particle-based simulations. Here, we show that a simple mesoscale model which treats the material as a mosaic of yielding plaquettes is able to capture the complex limit cycles with orders of magnitude less computational time than particle-scale models. We use the mesoscale model to study the limit cycles at various strain amplitude.
Comparison of yielding behaviour in model network and atomic glasses

HIMANGSU BHAUMIK (Presenter), Theoretical Sciences Unit, Jawaharlal Nehru Centre For Advanced Scientific Research, Bangalore, India, GIUSEPPE FOFFI, Laboratoire de Physique des Solides, Universite Paris-Sud, France, SRIKANTH SASTRY, Theoretical Sciences Unit, Jawaharlal Nehru Centre For Advanced Scientific Research, Bangalore, India — Yielding in a model atomic glass (Kob-Andersen binary mixture) has been studied recently through athermal quasi-static shear deformations [1], revealing a sharp yielding transition accompanied by strain localisation [2]. We investigate the manner in which such a transition is manifested in a model network glass, the BKS model of silica [3]. Silica exhibits a fragile-to-strong cross over a function of temperature, and we investigate the manner in which yielding and the accompanying strain localisation differs in glasses prepared initially in the strong and fragile regimes. We find qualitative differences in the yielding behaviour, and in the details of structural changes accompanying yielding. We compare these results to the aforementioned atomic glass with comparable changes in the degree of annealing, and recent results regarding the effect of annealing in the yielding behaviour of glasses [4].

References:


*Indo-French (IFCPAR) project no. 5704-1

Molecular Dynamics Study on Mechanical and Rheological Properties of Bulk Metallic Glass around Glass Transition Temperature

JI WOONG YU (Presenter), Seoul Natl Univ, S. H. EBRAHIMNAZHAD RAHBARI, Korea Institute for Advanced Study, WON BO LEE, Seoul Natl Univ — Bulk Metallic Glasses (BMG) or amorphous alloys usually contain more than two kinds of atoms. These materials have been central in both material engineering and material physics ever since their first appearance in 1960s, and posses superior material properties (e.g. tensile yield stress). However, the mechanical properties of BMG are not well understood due to nonequilibrium nature of the glass transition, and dramatic slow-down of the dynamics around the glass transition temperature. Using large scale computational power, we investigated the mechanical properties of the celebrated Kob-Andersen mixture, a model BMG, using active microrheology in molecular dynamics (MD) simulations. Moreover, we systematically compared results of the active microrheology with those obtained from global shearing. With strong evidence, we conclude superiority of the either method.
1:15PM B45.00009: Computational generation of voids in a-Si and a-Si:H by cavitation at low density
ENRIQUE GUERRERO (Presenter), DAVID STRUBBE, University of California, Merced —
Hydrogenated amorphous Si (a-Si:H) has seen a renewed interest for its application in heterojunction with intrinsic thin-layer (HIT) solar cells. Known deficiencies in this material's photovoltaic properties are limited hole mobilities and the Staebler-Wronski effect, a light-induced degradation of efficiency which may be in part due to voids within the structure. Simulations of voids in a-Si typically involve atomic removal, but these methods require an a priori idea of the bonding structure near the void. Instead, we generate voids within a-Si and a-Si:H using a fast, unbiased approach: the Wooten-Winer-Weaire classical-potential Monte Carlo method where we vary the density and replace some Si-Si bonds with Si-H bonds. At low density, voids form (like cavitation in a liquid), maintaining 4-coordination but increasing bond angle deviation, reducing medium-range order, and altering local structure within 4 Å of the void. This work provides a set of void structures for further studies of their effects on degradation, hole mobility, two-level systems, thermal transport, and elastic properties. (ArXiv: 1907.01327)

1:27PM B45.00010: Molecular Dynamics Simulation of Amorphous Oxides
RUI ZHANG (Presenter), JUN JIANG, MAHER YAŻBACK, ALEC MISHKIN, HAI-PING CHENG, Physics, University of Florida — Amorphous oxides has been used as coating material of interferometers for gravitational wave detection. To optimize their performance, efforts have been devoted to determining diffusive behavior of amorphous pure Ta$_2$O$_5$ as well as Ta$_2$O$_5$ with various dopants by classical molecular dynamics (MD) simulations. Furthermore, empirical pair potentials aiming at reproducing elastic properties of GeO$_2$ and doped GeO$_2$ have been constructed. The new potentials are applied to examine the thermodynamic properties of such material. Also, the vibrational density of states and Raman spectra of amorphous oxides have been demonstrated using MD simulation.

*This work is supported by the NSF through grants PHY-1707870 and PHY-1404110.
We study two 2D systems known to support an open-packed Kagome phase[1]. Both systems have repulsive pair potentials, one designed by Piñeros, Baldea, and Truskett and another by Zhang, Stillinger, and Torquato[2-3]. Using the aperture cross-correlation function (ACCF), we identify structured fluctuations in the liquid phases approaching the Kagome-liquid transition[4]. These Kagome-like fluctuations may be distinguished from hexagonal ones by calculating the ACCF at two different wavevector magnitudes along the second diffraction ring. Fluctuations near a string-Kagome transition involve transient structures that are different for different potentials. We find congruencies in the sequence of phases along an isotherm for many different 2D systems of Hertzian, Lennard-Jones-Yukawa, Core-Corona, and Daoud–Cotton particle potentials. These similarities suggest a universal mechanism among the phase transitions of 2D systems supported by central repulsive potentials.


We thank the University of Chicago MRSEC, NSF Grant No. DMR-1420709, for funding this research.

Record Dynamics (RD) describes the ubiquitous relaxation phenomenology known as "aging" that ensues after a hard quench in terms of a log-Poisson process. According to RD, a nonequilibrium system after a quench relies on fluctuations that randomly generate a sequence of irreversible record-sized events (quakes or avalanches) that allow the system to escape ever-higher barriers of metastable states within a complex energy landscape. Only the activation over such barriers allows the system to relax while tumbling into the next meta-basin that is marginally more stable. Within this picture of RD, a clear distinction can be drawn between the coarsening dynamics of, say, an Ising ferromagnet and the aging of the spin glass, which are often put in the same category. To that end, we use Ising spin models that interpolate between the spin glass and ferromagnet by varying the admixture of anti-ferromagnetic bonds from 50% to zero. Indeed, the accumulation of record events grows logarithmically with time in the glassy regime, with a sharp transition at a specific admixture in the ferromagnetic regime where such activations saturate quickly. We show this effect both for the Edwards-Anderson model on a cubic lattice as well as the Sherrington-Kirkpatrick (mean-field) spin glass.
Many-body localization to spin glass phase transition in disordered spin-chain system

ZEYANG LI (Presenter), PAI PENG, Massachusetts Institute of Technology — Disorder in a strongly correlated spin-chain system can give rise to novel phases of matter, such as many-body localization (MBL) phases or spin-glass (SG) phases. The two phases share similar non-thermalizing properties due to the existence of extensive set of local integrals of motion (LIOMs), and the SG phases feature in other properties such as a SG order parameter as well as the doubly degenerate eigenstates.

We consider a disordered Heisenberg XXZ model with on-site random field and random anisotropy. By changing the relative strength between these two disorders, we numerically observe the phase transition from MBL to SG, using numerically constructed LIOMs. We also obtain a scaling property of this transition, which elucidates the phase diagram of this system in the thermodynamic limit.
Due to the exotic quantum phenomena of the frustrated quantum magnets, investigating the related ground states has caught a lot of attention. The two-dimensional Spin-1/2 triangular-lattice antiferromagnet (TLAF) is a typical example: the quantum fluctuations could interfere the spin states, such as the disordered liquid and glass phases, and keep them with the complicated interactions among the geometric frustration, low dimensionality, and small spin. \( \text{Ba}_3\text{CoSb}_2\text{O}_9 \) is the first spin-1/2 equilateral TLAF without the Dzyaloshinskii-Moriya interaction, and the magnetic \( \text{Co}^{2+} \) triangular layers are well separated by the non-magnetic clusters of the \( \text{Sb}_2\text{O}_9 \) bioctahedra and \( \text{Ba}^{2+} \) ions. The strong quantum effects were observed from a non-collinear 120° spin structure in zero magnetic field into a collinear up-up-down (uud) state in a finite range of applied magnetic field [1, 2]. Through the experimental and theoretical studies, we found that the Linear Spin-Wave + 1/S treatment was inadequate to explain our experimental observation and the interlayer interaction could not be ignored in the system [3, 4]. In order to study the interlayer interactions and magnetic moments dependence on the quantum effect, the work has been extended to the other TLAFs of the multi-layered perovskite compounds with \( S=1 \) and \( 5/2 \). Moreover, the non-magnetic \( B' \)-site ions of the \( \text{A}_m\text{BB}'_{m-1}\text{O}_{3m} \) were discussed.

References:

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11:51AM B46.00002: Effect of quenched disorder on an equilateral triangular lattice antiferromagnet Ba$_3$CoSb$_2$O$_9$* QING HUANG (Presenter), HAIDONG ZHOU, University of Tennessee, Knoxville, TAO HONG, Oak Ridge National Lab, EUN SANG CHOI, National High Magnetic Field Lab, JIE MA, Shanghai Jiao Tong University, LU LI, University of Michigan, COLE D MAUWS, University of Manitoba, CHRISTOPHER WIEBE, University of Winnipeg — Ba$_3$CoSb$_2$O$_9$ is one of few prototypical materials for the two-dimensional equilateral triangular lattice antiferromagnet. We present a systematic study on effect of quenched disorder on magnetic properties in the Sr doped single-crystalline sample of Ba$_{2.8}$Sr$_{0.2}$CoSb$_2$O$_9$ by means of DC and AC susceptibilities, specific heat and advanced neutron scattering. DC susceptibility in Ba$_{2.8}$Sr$_{0.2}$CoSb$_2$O$_9$ confirms an antiferromagnetic ordering below 2.8 K with an easy-plane anisotropy. AC susceptibility as a function of magnetic field measured at 0.02 K indicates a phase transition around 8 T. Evolution of the transition temperature as a function of field was determined by specific heat measurements in Ba$_{2.8}$Sr$_{0.2}$CoSb$_2$O$_9$. We will also discuss effect of side disorder on the magnetic structure in Ba$_{2.8}$Sr$_{0.2}$CoSb$_2$O$_9$ using the single-crystal neutron diffraction technique.

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Go student program ORNL

12:03PM B46.00003: Universal scaling of the heat capacity in a quantum spin liquid state of 1T-TaS$_2$ HINAKO MURAYAMA (Presenter), YUKI SATO, TOMOYA TANIGUCHI, RYO KURIHARA, HIROKI SUZUKI, XIANZHUO XING, WENKAI HUANG, SHIGERU KASAHARA, YUICHI KASAHARA, Physics, Kyoto University, ITAMAR KIMCHI, Physics, University of Colorado, MASARO YOSHIDA, CEMS, RIKEN, YOSHIHIRO IWASA, Applied Physics, the University of Tokyo, MARCIN KONCZYKOWSKI, Laboratoire des solides irradiées, L'École Polytechnique, YUJI MATSUDA, Physics, Kyoto University — To elucidate the nature of quantum spin liquid (QSL), it is important to understand the effect of randomness on QSL. Here, we have investigated the low energy excitations on pure, Se-substituted and electron-irradiated 1T-TaS$_2$, a QSL candidate material with spin-1/2 on a triangular lattice[1, 2], by measuring low-temperature thermal conductivity and heat capacity. Finite residual linear terms of thermal conductivity, $\kappa/T(T\to0)$, in pure 1T-TaS$_2$ indicates the presence of itinerant gapless excitations. The magnetic contribution of the heat capacity of 1T-TaS$_2$ and 1T-TaS$_{2-x}$Se$_x$ well obeys a universal scaling relation, consistent with a theory that assumes the presence of localized orphan spins forming random singlets[3]. These results capture a microscopic picture of the QSL, in which localized orphan spins induced by disorder are surrounded by itinerant spinon that forms Fermi surface. On the other hand, electron irradiation in 1T-TaS$_2$, which introduces strong quenched disorders in Ta-layers, changes the scaling function dramatically, suggesting a possible new state of spin liquid.

12:15PM B46.00004: Magnetic Excitations and Q-dependent magnon lifetime in Non-collinear Metallic Antiferromagnet CrB$_2$  
PYEONGJAE PARK (Presenter), KISOO PARK, TAEHUN KIM, Department of Physics and Astronomy, Seoul National University, YUSUKE KOUSAKA, JUN AKIMITSU, Research Institute for Interdisciplinary Science, Okayama University, TOBY G. PERRING, ISIS Pulsed Neutron and Muon Source, Rutherford Appleton Laboratory, MICHEL KENZELMANN, Paul Scherrer Institute, JE-GUEN PARK, Department of Physics and Astronomy, Seoul National University — Frustration and non-collinear magnetic ordering can introduce a wide variety of interesting physics; like a quantum spin liquid phase in insulators or topological band structures in metals, to name a few. Many studies have been made on the nature of magnetic excitations in non-collinear insulating magnets, while few experimental data exist for non-collinear metallic magnets. Using an inelastic neutron scattering technique, we report the magnetic excitation spectra of single crystal CrB$_2$; a metallic magnet in which magnetic moments of Cr on triangular lattice form incommensurate spiral magnetic order with the propagation vector $k = (0.285, 0.285, 0)$. Severely damped magnons are observed along with clear phonons which are as sharp as the instrumental resolution, yet most of them can be explained by Heisenberg Hamiltonian and a linear spin wave theory (LSWT). By excluding the effects of instrumental resolution, we mapped the intrinsic magnon linewidth $\Gamma(q, E)$ which shows some unusual behavior. We discuss the origin of the magnon decay by calculating 2-magnon density of states (DOS) and Stoner continuum DOS. Our work will be a rare comprehensive study on the spin dynamics of non-collinear metallic magnets; the 1st observation of 2-magnon effect in metallic magnets.

12:27PM B46.00005: Terahertz study of the frustrated triangular Ising magnet FeI$_2$*

ANAELLE LEGROS (Presenter), DIPANJAN CHAUDHURI, Johns Hopkins University, XIAOJIAN BAI, ZHILING DUN, MARTIN MOURIGAL, Georgia Institute of Technology, PETER ARMITAGE, Johns Hopkins University — 2D antiferromagnetic (AF) triangular lattices are of great interest due to their geometric frustration, which may lead to the absence of a long-range magnetic order at $T=0$. FeI$_2$ is part of the ferrous halides family, in which the Fe$^{2+}$ ions are distributed on hexagonal planes and spontaneously order in an AF phase below $T_N \sim 9$K [1]. Contrary to other ferrous halides, the spins in the ordered phase of FeI$_2$ form triangular AF sheets (instead of antiparallel ferromagnetic sheets), giving rise to a more complex magnetic structure. In this peculiar ground state, the spins (S=1) generate several types of magnetic excitations, including a mysterious two-magnon bound state that should be prevented by selection rules [2]. Moreover, when an external magnetic field is applied along the c-axis at $T<T_N$, successive magnetic transitions occur, including a phase without evidence of long-range order [3]. We present the results from in-field time-domain terahertz spectroscopy on FeI$_2$. These experiments give insight into the diverse magnetic excitations of this triangular AF lattice.


*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331.
**12:39PM B46.00006: Synthesis and frustrated magnetism of the triangular lattice \( \text{ARESe}_2 \) single crystals**

JIE XING (Presenter), LIURUKARA D SANJEEWA, Oak Ridge National Laboratory, JUNGSOO KIM, GREGORY RANDALL STEWART, University of Florida, MAOHUA DU, FERNANDO REBOREDO, RADU CUSTELCEAN, ATHENA S. SEFAT, Oak Ridge National Laboratory — We have successfully synthesized \( \text{ARESe}_2 \) (\( A = \text{Alkali metal}, \ RE = \text{rare-earth} \)) single crystals by the salt flux. These crystals stabilize in either the trigonal (\( R-3m \)) or hexagonal (\( P6_3/mmc \)) crystal systems depending on the \( RE \), containing the ideal triangular \( RE^3+ \) layers. We have characterized them through magnetization and heat capacity down to 0.4 K. Antiferromagnetic interactions with large magnetic anisotropy is observed, while no long-range order is found indicating frustrated magnetism. Yb-based crystals present a two-peak feature in the heat capacity below 10 K, while the magnetic plateau is found at 4 T when the magnetic field is applied in the \( ab \) plane. The 112 system is found to be particularly interesting for the study of frustrated magnetism and its potential for quantum spin liquid behavior.

*Work at ORNL was supported by U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Science and Engineering Division. The X-ray diffraction analysis by RC was supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division. Work at Florida by J. S. Kim and G. R. S. supported by the US Department of Energy, Basic Energy Sciences, contract no. DE-FG02-86ER45268.

**12:51PM B46.00007: Measurement of a 1/2 magnetization plateau in a frustrated antiferromagnet**

SHANNON HALEY (Presenter), NIKOLA MAKSIMOVIC, University of California, Berkeley, ERAN MANIV, Lawrence Berkeley National Lab, DANIEL PARKER, University of California, Berkeley, JOHN SINGLETON, Los Alamos National Laboratory, JOEL MOORE, JAMES ANALYTIS, University of California, Berkeley — Frustrated magnetic systems lend themselves to a wealth of nontrivial behaviors. Among these are plateaus in magnetization with the application of an external field, resulting from quantum fluctuations stabilizing particular spin states. The existence of these plateaus at specific fractions of the saturated magnetization has been observed in a handful of systems with distinct physics. This talk will discuss our recent discovery of a \( \frac{1}{2} \) magnetization plateau in a frustrated antiferromagnet on a triangular lattice using fields up to 65T. This directly confirms recent theoretical predictions in frustrated magnets.

*This work was supported by the Gordon and Betty Moore Foundation EPiQS Initiative through Grant No. GBMF4374.

A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1644779, the State of Florida, and the U.S. Department of Energy.
1:03PM B46.00008: Novel Excitations near Quantum Criticality in Geometrically Frustrated Antiferromagnet CsFeCl$_3$ [Invited] TAKATSUGU MASUDA (Presenter), SHOHEI HAYASHIDA, Institute for Solid State Physics, Univ of Tokyo, MASASHIGE MATSUMOTO, Shizuoka University, MASATO HAGIHALA, High Energy Accelerator Research Organization, NOBUYUKI KURITA, HIDEKAZU TANAKA, Tokyo Institute of Technology, SHINICHI ITOH, High Energy Accelerator Research Organization, TAO HONG, Oak Ridge National Laboratory, MINORU SODA, Ochanomizu University, YOSHIYA UWATOKO, Institute for Solid State Physics, Univ of Tokyo — The investigation of materials that exhibit quantum phase transition provides valuable insights into fundamental problems in physics. We present neutron scattering under pressure in a triangular-lattice antiferromagnet that has a quantum disorder in the low-pressure phase and a noncollinear structure in the high-pressure phase [1]. The neutron spectrum continuously evolves through critical pressure; a single mode in the disordered state becomes soft with the pressure and it splits into gapless and gapped modes in the ordered phase. Extended spin-wave theory reveals that the longitudinal and transverse fluctuations of spins are hybridized in the modes because of noncollinearity, and novel magnetic excitations are formed. We report a new hybridization of the phase and amplitude fluctuations of the order parameter near a quantum critical point in a spontaneously symmetry-broken state.


1:39PM B46.00009: Evidence of one-dimensional magnetic heat transport in the triangular-lattice antiferromagnet Cs$_2$CuCl$_4$* ERIK SCHULZE, STEVAN ARSENIJEVIC, LARS OPHERDEN, ALEXEY PONOMARYOV, JOACHIM WOSNITZA, Helmholtz-Zentrum Dresden-Rossendorf, TOSHIO ONO, Osaka Prefecture University, HIDEKAZU TANAKA, Tokyo Institute of Technology, SERGEI ZVYAGIN (Presenter), Helmholtz-Zentrum Dresden-Rossendorf — We report on low-temperature heat-transport properties of the spin-1/2 triangular-lattice antiferromagnet Cs$_2$CuCl$_4$. Broad maxima in the thermal conductivity along the three principal axes, observed at about 5 K, are interpreted in terms of the Debye model, including the phonon Umklapp scattering. For thermal transport along the $b$ axis, we found a pronounced field-dependent anomaly, close to the transition into the three-dimensional long-range-ordered state. No such anomalies were observed for the transport along the $a$ and $c$ directions. We argue that this anisotropic behavior is related to an additional heat-transport channel through magnetic excitations, that can best propagate along the direction of the largest exchange interaction. Our observations strongly support the quasi-1D spin-liquid scenario with spinons as elementary excitations, proposed for this frustrated antiferromagnet. Besides, peculiarities of the heat transport of Cs$_2$CuCl$_4$ in magnetic fields up to the saturation field and above are discussed.

*This work was supported by the Deutsche Forschungsgemeinschaft (DFG), through ZV 6/2-2, the excellence cluster ct.qmat (EXC2147, project-id 39085490), and SFB 1143, as well as by the HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).
1:51PM B46.00010: Torque equilibrium spin wave theory study of anisotropy and Dzyaloshinskii-Moriya interaction effects on the indirect K- edge RIXS spectrum of a triangular lattice antiferromagnet  TRINANJAN DATTA (Presenter), Chemistry and Physics, Augusta University, SHANJIAN JIN, LUO CHENG, DAO-XIN YAO, School of Physics, Sun Yat-Sen University — We apply the recently formulated torque equilibrium spin wave theory (TESWT) to compute the 1/S-order interacting K-edge bimagnon resonant inelastic x-ray scattering (RIXS) spectra of an anisotropic triangular lattice antiferromagnet with Dzyaloshinskii-Moriya (DM) interaction [1]. We extend the interacting torque equilibrium formalism, incorporating the effects of DM interaction, to appropriately account for the zero-point quantum fluctuation that manifests as the emergence of spin Casimir effect in a noncollinear spin spiral state. Using inelastic neutron scattering data from Cs₂CuCl₄ we fit the 1/S corrected TESWT dispersion to extract exchange and DM interaction parameters. We compare, and contrast the effects of spatial anisotropy and DM interaction on the RIXS spectra at various points across the magnetic Brillouin zone. We highlight the key features of the bi- and trimagnon RIXS spectrum at the roton like points whose behavior is quite different from an isotropic triangular lattice system [2]. Our calculation offers a practical example of how to calculate interacting RIXS spectra in a non-collinear quantum magnet using TESWT. [1] Jin et. al. Phys. Rev. B 100, 054410 (2019); [2] Luo et. al. Phys. Rev. B 92, 035109 (2015).

2:03PM B46.00011: A New Yb-based Spin-1/2 Triangular Lattice Magnet*  SHU GUO (Presenter), ROBERT J. CAVA, Princeton University — Very recently, two rare earth (R)-based triangular lattice (TL) materials, YbMgGaO₄ and NaYbO₂, are proposed to be quantum spin liquid candidate. From the structural point of view, the magnetic R atoms of these two compounds display a “ABCABC” stacking form in c axis. However, seldom research is focused on the “AA” cubic stacking R-based TL materials. Here, we present a cubic stacking Yb-based TL magnet. The centimeter-size single crystals of Yb-based TL magnet were grown by the flux method. In the crystal structure, the Yb-Yb separation (8.06 angstroms) between layers is larger than the in-plane Yb-Yb separation (5.63 angstroms). The absence of long-range ordering was confirmed by the magnetization (down to 1.8 K). Specific heat measured down to 0.3 K at zero field also confirmed the absence of long-range ordering. For applied field above 3 T, there is still no evidence of long-range magnetic ordering, but instead, a broad peak appears. This broad hump is associated with Schottky anomaly that shifts to higher temperatures at higher fields.

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences under Award No. DESC0019331.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B47 GMAG: Interfaces, Coupling, and Ultra-Thin Materials
710/712 - Nathan Satchell, Univ of Leeds - Tag(s): Focus
XIAOQIAN CHEN, Lawrence Berkeley National Laboratory, JUSTIN WOODS, University of Kentucky, ROLAND KOCH, Lawrence Berkeley National Laboratory, BARRY W FARMER, University of Kentucky, CLAUDIO MAZZOLI, WEN HU, Brookhaven National Laboratory, RAJESH V CHOPDEKAR, Lawrence Berkeley National Laboratory, WAI-KWONG KWOK, Argonne National Laboratory, LANCE ERIC DE LONG, University of Kentucky, SUJOY ROY, Lawrence Berkeley National Laboratory, JEFFREY HASTINGS (Presenter), University of Kentucky — Artificial spin lattices (ASLs), including artificial spin ices, consist of patterned magnetic nanostructures that mimic Ising spins. Here we show that a permalloy, square ASL with a double edge dislocation exhibits an ordered antiferromagnetic ground state, unlike square ASLs with a single dislocation.¹ We demonstrate that soft x-rays resonantly scattered from this magnetic texture carry orbital angular momentum. Moreover, x-ray OAM from these samples can be modulated using and temperature and applied magnetic fields. X-ray beams carrying orbital angular momentum (OAM) have potential applications in nanoscale imaging, spectroscopy, and manipulation, but current means of generating x-ray OAM are difficult to modulate or reconfigure.² Scattering from ASLs may offer a potential path to flexible control of x-ray OAM.


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Advanced Light Source, DOE DE-AC02-05CH11231
National Synchrotron Light Source II, DOE DE-SC0012704
National Nanotechnology Coordinated Infrastructure, NSF ECCS-1542164
Center for Nanoscale Materials, DOE DE-AC02-06CH11357
11:27AM B47.00002: Enhancement of magnetoelectric coupling by insertion of Co atomic layer into Fe$_3$Si/BaTiO$_3$(001) interfaces identified by first-principles calculations

YASUNARI HAMAZAKI (Presenter), YOSHIHIRO GOHDA, Tokyo Inst of Tech - Yokohama — Magnetoelectric (ME) coupling of Ferromagnetic(FM)/ferroelectric(Fe) interfaces is stronger than those of single phase multiferroic materials. Especially, interface ME effect caused by bonding effect between interfacial atoms has been reported in many FM/FE interfaces and observed at room temperature. In this study, we examine interface ME coupling at Fe$_3$Si/Co/BaTiO$_3$ heterostructures by using first-principles calculations based on density functional theory to clarify the influence of atomic-layer insertion on the ME effect. D0$_3$-type Fe$_3$Si has only 0.1 % lattice mismatch with tetragonal BaTiO$_3$ (001), and it is considered as promising to emerge the interfacial ME effect. We construct several interface structures and compare the energy of each structure. Comparing the Fe$_3$Si/BaTiO$_3$ interface with the Fe$_3$Si/Co/BaTiO$_3$ interface, it is found that the interface ME effect is greatly increased when Co is inserted. We also clarify the differences in ferroelectric displacement and magnetic properties between Fe$_3$Si/BaTiO$_3$ and Fe$_3$Si/Co/BaTiO$_3$.

*This work was supported in part by CREST-JST Grant No. JPMJCR18J1, ESICMM Grant No. 12016013.

11:39AM B47.00003: Long-range exchange coupling in Co/Nb/Co trilayers

VICTOR GONZÁLEZ (Presenter), University of the Andes, NICOLAS M VARGAS, UC San Diego, S MERCONE, LSPM-CNRS UPR-3407, Université Paris, EDGAR J PATINO, University of the Andes, IVAN K. SCHULLER, UC San Diego, JUAN RAMIREZ, University of the Andes — Long-range interlayer exchange coupling (IEC) in multilayers has been a topic of extensive research, both experimental and theoretical. IEC can be induced by two ferromagnetic (FM) layers spaced by a thin non-magnetic (NM) material. In this work, we performed vector model Vibrating Sample Magnetometer (V-VSM), Magneto-optic Kerr effect and magnetoresistance (MR) measurements as a function of temperature from 1K up to room temperature. Interestingly, we observed an oscillatory behavior of the magnetic coercive field usually associated with IEC without fully antiferromagnetic compensation of the ferromagnetic layers at all temperatures. This may suggest an additional Long-range exchange coupling mechanism beyond the direct exchange.

*This is highly collaborative research. The Moke and preliminary VSM measurements were done at UCSD under DOE grant # DE FG02 87ER-45332, the experiments were designed and the work was analyzed by all authors. The authors also acknowledge support from Colciencias grant 120471250659. The V-VSM measurements were done at the facilities of University of Paris-VII with sponsorship from grants of the Île-de-France region.
Reduced exchange interactions in thin perpendicularly magnetized magnetic tunnel junction free layers and spin-transfer reversal mechanisms* [Invited]

JAMILEH BEIK MOHAMMADI (Presenter), Loyola University New Orleans, BARTEK KARDASZ, GEORG WOLF, Spin Memory Inc, YIZHANG CHEN, New York University, MUSTAFA PINARBASI, Spin Memory Inc, ANDREW KENT, New York University — Perpendicularly magnetized magnetic tunnel junctions (pMTJs) are being widely developed for spin-transfer torque magnetic random-access memories for data storage and embedded memories. The magnetic properties of the pMTJ free layer affect the dynamic properties of the free layer, such as the spin-torque switching efficiency and the switching speed, and therefore the device performance.

The magnetic exchange constant is one of the most important yet hard to measure properties of the free layer, as the layer is very thin and embedded in a pMTJ layer stack that includes a magnetic reference layer coupled to a synthetic antiferromagnet. The exchange constant sets the length scale for spatial variations of the magnetization. In perpendicularly magnetized tunnel junction devices, the exchange constant can also set the energy barrier for thermally activated reversal [1].

I will present the results of a systematic experimental study of the exchange constant of CoFeB free layers with perpendicular anisotropy. We have used vibrating sample magnetometry to determine the temperature dependence of the magnetic moment, and therefore the magnon population density [2] of the free layer. In particular, I will show that when a thin W insertion layer is introduced into a 2.3 nm thick CoFeB free layer to increase the perpendicular magnetic anisotropy of the layer, the exchange constant of the free layer is significantly reduced.

I will also present a micromagnetic study that shows that the spin-transfer reversal nucleates at the center of the element and completed by domain wall motion in elements larger than a critical size set by the exchange constant, magnetization and perpendicular magnetic anisotropy.


*Research supported by Spin Memory Inc.
12:27PM B47.00005: Strain-driven spin-Hall antiferromagnetic memory for 180° switching*

ARUN PARTHASARATHY (Presenter), NIKHIL RANGARAJAN, Electrical and Computer Engineering, New York University, Brooklyn, NY 11201, SHALOO RAKHEJA, Holonyak Micro and Nanotechnology Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801 — Antiferromagnets exhibit ultrafast spin dynamics with response times in the picosecond range, produce negligible stray fields, and are promising to design high-density nonvolatile memories. NiO is an antiferromagnetic insulator whose Néel order can be switched by 90° using electric current in the spin-Hall system NiO/Pt [1], or piezoelectric strain in Ni/NiO/PMN-PT [2]. Although these switching schemes allow storage of information, the 90° state is thermally metastable.

We propose 180° reversal of the Néel order by leveraging both piezoelectric strain and spin-Hall effect in PMN-PT/NiO/Pt system. The reversal is accomplished by first realizing strain-induced perpendicular reorientation, followed by an electric current pulse that provides the antidamping torque necessary to tip the Néel order to the reversed easy-axis orientation. The antiferromagnetic state is read via exchange-bias-coupled magnetic tunnel junction. Modeling shows that the strain-driven NiO memory can switch under 100 ps, while consuming < 300 aJ/bit switching energy.


*This work was supported in part by the SRC and NSF through ECCS 1740136, and from the MRSEC Program of the NSF under Award Number DMR-1420073.

12:39PM B47.00006: Inter-particle magnetic correlations and fluctuations in assemblies of Fe3O4 nanoparticles

KARINE CHESNEL (Presenter), JOHNATHON RACKHAM, COLBY WALKER, BRITTNI PRATT, DALTON GRINER, ROGER HARRISON, MARK TRANSTRUM, Brigham Young Univ - Provo — Magnetite (Fe3O4) nanoparticles (NPs) are increasingly used in biomedical applications such as drug & gene delivery, hyperthermia, or MRI. While the structural and magnetic properties of bulk Fe3O4 is well known [1], knowledge is still lacking about the spatio-temporal magnetic behavior of collections of Fe3O4 NPs. We here investigate the inter-particle magnetic correlations within the NP assembly throughout the superparamagnetic transition using x-ray resonant magnetic scattering (XRMS) [2]. By exploiting the light polarization, we extract the local inter-particle magnetic order. We show a dependence on particle size, suggesting an enhancement of magnetic couplings for bigger particles. [3] Additionally, we show a model based on NP chains, which we use to fit the XRMS data, suggesting ferromagnetic ordering at high external magnetic field, and the emergence of antiferromagnetic ordering near remanence. [4] Finally we investigate the slow dynamics of magnetic fluctuations between NPs by using photon correlation spectroscopy and show a drastic change through the superparamagnetic transition.

[1] Verwey, Nature 144, 327 (1939);
Magnetic nanoparticles are increasingly used in nanotechnologies and biomedical applications, such as drug targeting, MRI, and bio-separation. Magnetite (Fe3O4) nanoparticles stand to be effective in these roles due to the non-toxic nature of magnetite and its ease of manufacture. To be more effective in these applications, a greater understanding of the magnetic behavior of the individual magnetite nanoparticles is needed when a collection of them is used. This research seeks to discover the local magnetic ordering of ensembles of magnetite nanoparticles occurring at various stages of the magnetization process. To complete this study, we use resonant x-ray magnetic scattering, which provides information about the magnetic orders in the material. Here we discuss the modeling of the magnetic scattering data using a one-dimensional chain of nanoparticles with a mix of ferromagnetic, anti-ferromagnetic, and random order and the model's validation against empirical gaussian fits. The model utilizes twelve variable parameters and we used a Levenberg-Marquardt algorithm to find the best fit parameters. By fitting the model to the experimental data, we extracted information about the magnetic correlations in the nanoparticle assembly.
Coupling of ferroelastic and ferromagnetic order parameters in materials offers a means to achieve novel multiferroic applications. In this talk, we report strong coupling between the structural degree of freedom and spin state transition in the LaCoO$_3$ (LCO) thin films and heterostructures. Three major results will be present, 1) symmetry transition from a pseudocubic to a monoclinic structure happens in the LCO films as increasing the layer thickness, leading to the nonlinear behavior of magnetization vs. thickness; [1] 2) the observation of one-dimensional ferroelastic domains in LCO thin films that are intimately linked to magnetization. Unidirectional structural modulation is achieved by selective choice of substrate or growth plane, which produces broken in-plane rotational symmetry; [2] 3) the interfacial symmetry mismatch triggers the nonuniformed crystallographic parameters, thus the structural modification within a single LCO layer. The magnetization exhibits a reduced magnetization but an enhanced atomic density, whereas the film's interior (i.e., its film bulk) shows the opposite trend. This assertion is tested by systematic application of hydrostatic pressure during the polarized neutron reflectivity experiments. The magnetization can be controlled at a rate of −20.4% per GPa. [3] These results provide unique insights into mechanisms driving FM in strained LCO films while offering a tantalizing observation that tunable deformation of the CoO$_6$ octahedra in combination with the ferroelastic and ferromagnetic order parameters.

References

*Er-Jia Guo acknowledges the support from Young talent program of China and Chinese Academy of Sciences.
1:39PM B47.00009: "Boundary Conditions in Granular Magnetic Nanostructures with Dzyaloshinski-Moriya Interactions"* AHSAN ULLAH (Presenter), BALAMURUGAN BALASUBRAMANIAN, WENYONG ZHANG, DAVID SELLMYER, RALPH SKOMSKI, Department of Physics and Astronomy, NCMN, University of Nebraska - Lincoln 68588-0299, USA — Magnetic nanostructures such as compacted ensembles of metallic nanoparticles and melt-spun ribbons often but not always yield a topological Hall-effect contribution caused by the Berry phase of the conduction electrons. Among the experimental systems recently investigated in our group are MnSi, NiMnGa, NiMnIn, and Co-Si, The Berry-phase effect depends on the spin structure, which is strongly affected by real-structure feature such as easy-axis orientation and grain boundaries. Chemical inhomogeneities at grain boundaries yield $\nabla A$ terms in the materials equations (partial differential equations), where $A$ is the exchange stiffness. For sharp interfaces, this term corresponds to Erdmann-Weierstrass (EW) boundary conditions. In the presence of Dzyaloshinski-Moriya interactions ($D$), there are $\nabla D$ terms and modifications to the EW condition. The effect of the boundary conditions on spin structure and Berry phase is far-reaching and epitomized by the contrast between Bessel and modified Bessel functions in grains with cylindrical symmetry.

*This research is supported by DOE BES (DE-FG02-04ER46152)

1:51PM B47.00010: The effect of x-ray illumination on magnetic domain memory in [Co/Pd] / IrMn multilayers* COLBY WALKER (Presenter), MASON L PARKES, Brigham Young Univ - Provo, DAVID J KEAVNEY, Advanced Photon Source, Argonne National Laboratory, ERIC FULLERTON, Center for Memory and Recording research, UCSD, KARINE CHESNEL, Brigham Young Univ - Provo — We are studying the effect that illumination by coherent x-rays may have on magnetic domain memory (MDM) in a [Co / Pd] / IrMn multilayers. MDM is the ability of the magnetic domains to retain their exact same domain topology upon field cycling. Earlier studies have suggested that under higher dose of x-ray illumination, the material may lose its existing MDM. To investigate this potential effect, we have used both x-ray resonant magnetic scattering (XRMS) along with magneto-transport measurements to track the exchange bias while the sample is illuminated with x-rays. Magneto-transport is here used to measure the hysteresis loop of our multilayers material from which we can measure the exchange bias and its possible alteration. A loss of exchange bias would indicate that the x-rays illumination dose may alter the strength of the exchange couplings and ultimately the amount of MDM. Knowing if a loss of exchange bias has occurred requires collecting magneto-transport data as well as XRMS data and correlating the observed changes under various dose of x-ray illumination.

*We would like to thank BYU for funding our research.
Quantification of mixed Bloch/Néel character in a Co/Pd DMI multilayer thin film with Lorentz transmission electron microscopy.

JOSEPH GARLOW (Presenter), Brookhaven National Laboratory, SHAWN D. POLLARD, National University of Singapore, MARCO BELEGGIA, Technical University of Denmark, HYUNSOO YANG, National University of Singapore, YIMEI ZHU, Brookhaven National Laboratory — Chiral magnetic order stabilized by the Dzyaloshinskii-Moriya interaction holds promise for a range of spintronic device applications such as for magnetic-based memory and logic. Yet, direct methods for the quantification of their exact structure remains a challenge and is crucial towards understanding the fundamental physics associated with their ordering and manipulation. Here, we present an approach to quantify the mixed Bloch-Néel character of domain walls stabilized by the Dzyaloshinskii-Moriya interaction in Co/Pd multilayers. Analysis of the observed intensities under varied imaging conditions yield vital parameters that dictate their stability and properties, namely, the degree of mixed Bloch-Néel character \( \eta = 56^\circ \pm 5^\circ \), the domain wall width \( w = 10 \pm 2 \text{ nm} \), the strength of the Dzyaloshinskii-Moriya interaction \( D = 1.0 - 1.1 \text{ mJ/m}^2 \), and the exchange stiffness \( A = 23 - 30 \text{ pJ/m} \). This approach provides the necessary framework to quantify the magnetic structure for a broad array of topological spin systems using Lorentz phase microscopy.

Monday, March 2, 2020 11:15 AM - 1:51 PM

Session B48 DCMP: Superconductivity in Low Dimensional Systems

High Ballroom 1A - Hongchao Xie, Univ of Michigan - Ann Arbor

11:15AM B48.00001: Quantum spin-liquid and chiral superconductivity in TaS\(_2^*\)

AMIT KANIGEL (Presenter), AMIT RIBAK, Technion - Israel Institute of Technology, RONI MAJLIN SKIFF, Tel Aviv University, MARK H FISCHER, Zurich University, JONATHAN RUHMAN, Bar Ilan University, YORAM DAGAN, Tel Aviv University — Van der Waals (vdW) materials offer unprecedented control of electronic properties via stacking of different types of two-dimensional materials. A fascinating frontier, largely unexplored, is the stacking of strongly correlated phases of matter. We study 4Hb-TaS\(_2\), which naturally realizes an alternating stacking of 1T-TaS\(_2\) and 1H-TaS\(_2\) structures. The former is a well-known Mott insulator, which has recently been proposed to host a gapless spin-liquid ground state. The latter is a superconductor known to also host a competing charge density wave state. This raises the question of how these two components affect each other when stacked together. We find a superconductor with a \( T_c \) of 2.7 K and anomalous properties, of which the most striking one is a signature of time-reversal-symmetry breaking, abruptly appearing at the superconducting transition. This observation is consistent with a chiral superconducting state.

\*The Israel Science Foundation 320/17 and 382/17
11:27AM B48.00002: Blockade of vortex flow by thermal fluctuations in atomically thin clean-limit superconductors  
AVISHAI BENYAMINI (Presenter), Columbia Univ, DANTE KENNES, Institut fur Mathematische Physik, Technische Universitat Braunschweig, EVAN TELFORD, Columbia Univ, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ANDREW MILLIS, JAMES C HONE, CORY DEAN, ABHAY NARAYAN, Columbia Univ — Resistance in superconductors arises from the motion of vortices driven by flowing supercurrents or external electromagnetic fields and may be strongly affected by thermal or quantum fluctuations. The common expectation borne out in previous experiments is that as the temperature is lowered, vortex motion is suppressed, leading to a decreased resistance. A new generation of materials provides access to the previously inaccessible regime of clean-limit superconductivity in atomically thin superconducting layers. We show experimentally that for few-layer 2H-NbSe$_2$ the resistance below the superconducting transition temperature may be non-monotonic, passing through a minimum and then increasing again as temperature is decreased further. The effect exists over a wide range of current and magnetic fields but is most pronounced in monolayer devices at intermediate currents. Analytical and numerical calculations confirm that the findings can be understood in a two-fluid vortex model, in which a fraction of vortices flow in channels while the rest are pinned but thermally fluctuating in position, effectively controlling the mobility of the free vortices. The findings provide a new perspective on fundamental questions of vortex mobility and dissipation in superconductors.

11:39AM B48.00003: Supercurrent detection of topologically trivial zero-energy states in nanowire junctions*  
OLADUNJOYE AWOGA (Presenter), JORGE CAYAO, ANNICA M BLACK-SCHAFER, Department of Physics and Astronomy, Uppsala University — In this work we investigate phase-biased transport in SNS junctions based on nanowires, with strong Rashba spin-orbit coupling and magnetic field, strongly coupled to 2D conventional $s$-wave superconductors. We find that all the nanowire parameters are renormalized, in a manner dependent on the width of the superconductor. In particular, we show that the finite width of the superconductor induces a finite energy shift, or effective chemical potential, in the nanowire sectors coupled to the two superconductors, thus leading to a natural formation of a quantum dot at the junction. Remarkably, under these conditions, the junction supports the emergence of a pair of zero-energy states in the trivial phase, i.e. false Majorana fermion states. We demonstrate that this effect is highly tunable by the superconductor width, and suggest this as an explanation for the formation of trivial zero-energy states reported in recent experiments. Most importantly, we show that these zero-energy states produce a $\pi$-shift in the phase-biased supercurrent. This gives access to a simple tool for their unambiguous detection, thus ruling out any Majorana-like interpretation. See Phys. Rev. Lett. 123, 117001 (2019) for further details.

*The Swedish Research Council (Vetenskaprådet)
Quantum disoliton as a one-dimensional linear potential system

GEUNYONG KIM (Presenter), JINHO YANG, ILKYU YANG, Department of Physics, Pohang University of Science and Technology, DIRK WULFERDING, Institute for Condensed Matter Physics, TU Braunschweig, JINYOUNG YUN, Department of Physics, Pohang University of Science and Technology, ROMAN MOVSHOVICH, MPA-CMMS, Los Alamos National Laboratory, GILYOUNG CHO, KI-SEOK KIM, JEEHOON KIM, Department of Physics, Pohang University of Science and Technology — Disoliton as a bounded soliton system appeared initially in a swimming pool in the form of half vortex ring. Subsequently, it turns out to be a universal phenomenon at all length scales. Despite the discovery of several disoliton systems, their underlying physics such as nature of an interaction potential remains elusive due to the lack of a model system allowing controllability and repeatability. Here we report on a quantum disoliton (QDS) created as a U-shape quantum flux tube in a superconducting Nb film. A systematic control on a single QDS reveals the purported 1D linear potential, i.e. distance-independent force. The QDS will provide a novel platform for exploring 1D phase transition, quantum transport, and non-Abelian statistics.

Andreev bound states in hybrid full-shell Al/InAs nanowire devices

MARCO VALENTINI (Presenter), MATTHIAS BRAUNS, ANDREA HOFMANN, Institute of Science and Technology Austria, PETER KROGSTRUP, Center for Quantum Devices and Microsoft Quantum Lab–Copenhagen, GEORGIOS KATSAROS, Institute of Science and Technology Austria — Hybrid superconductor-semiconductor nanowire (NW) devices have attracted widespread interest as they can host Majorana zero modes (MZMs). While most of the previous experiments dealt with semiconductor NWs partially covered by a superconductor, a recent theory proposal [1] suggests to fully cover the semiconductor NWs with a superconductor. One of the main advantages of having a superconducting full-shell is that MZMs should arise at a very precise magnetic field, namely in the odd lobes of the Little-Parks effect. A first result [2] showed the presence of a zero bias peak (ZBP) in the first lobe, suggesting the presence of MZMs in such NWs. However, also Andreev bound states (ABS) could arise in such experiments. Hence, it is important to study them and especially their evolution in a magnetic field. Here, we present low temperature magnetotransport data using InAs NWs fully covered by Al [3]. We investigate ABS in the Little-Parks regime; we show that ABS can merge at zero bias in the first lobe, mimicking MZMs behaviour. Furthermore, we suggest how to discriminate ZBPs arising from MZMs and from ABS.

**12:15PM B48.00006: Gate-tunable superconductivity in layered β-MoTe$_2$**  
APOORV JINDAL  
(Presenter), Department of Physics, Columbia University, DANIEL A RHODES, Department of Mechanical Engineering, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, Tsukuba, Ibaraki 305-0044, Japan, CORY DEAN, Department of Physics, Columbia University, JAMES C HONE, Department of Mechanical Engineering, Columbia University, ABHAY PASUPATHY, Department of Physics, Columbia University — van der Waals heterostructures of mechanically-exfoliated crystalline materials are a platform to observe quantum phenomena in the low-disorder limit. Of special interest are materials with low carrier density, where the use of electrostatic doping and electric field tuning of bandstructure gives us easily accessible experimental tuning knobs. Twisted graphene and TMD superlattices, and monolayer WTe$_2$ are a couple of striking recent examples. In monolayer WTe$_2$, the use of gate potentials has been shown to tune between a topological insulator and a superconducting phase. In this talk, we describe transport measurements on a closely related material, β-MoTe$_2$. We show that β-MoTe$_2$ exhibits robust gate-tunable superconductivity in the few-layer limit. hBN encapsulated devices in the monolayer exhibit a superconducting critical temperature of ~ 6 K, a nearly hundred-fold enhancement over the bulk value. Using a dual-gated device structure, we also observe a strong dependence of superconducting properties on carrier density and displacement field. In this talk, we will fully characterize the layer, carrier density, displacement field, and magnetic field phase diagrams of this material.

**12:27PM B48.00007: Non-linear $I$/$V$ characteristics in two-dimensional superconductors: Berezinskii-Kosterlitz-Thouless physics vs inhomogeneity**  
LARA BENFATTO (Presenter), GIULIA VENDITTI, Univ of Rome La Sapienza, JOHAN BISCARAS, Sorbonne Universite, Paris, France, SIMON HURAND, NICOLAS BERGEAL, JEROME LESUEUR, ESPCI, Paris, France, ANJANA DOGRA, National Physical Laboratory, New Delhi, India, RAMESH BUDHANI, Morgan State University, Baltimore, USA, MINTU MONDAL, School of Physical Sciences, Kolkata, India, JOHN JESUDASAN, PRATAP RAYCHAUDHURI, TIFR, Mumbai, India, SERGIO CAPRARA, Univ of Rome La Sapienza — One of the hallmarks of the Berezinskii-Kosterlitz-Thouless (BKT) transition in two-dimensional superconductors is the universal jump of the superfluid density, that can be indirectly probed via the non-linear exponent of the current-voltage $I$/$V$ characteristics. Here, we compare the experimental measurements of $I$/$V$ characteristics in two cases, namely NbN thin films and SrTiO$_3$-based interfaces. While the former display a paradigmatic example of BKT-like non-linear effects, the latter do not seem to justify a BKT analysis. Rather, the observed $I$/$V$ characteristics can be well reproduced theoretically by modelling the effect of mesoscopic inhomogeneity of the superconducting state. Our results offer an alternative perspective on the spontaneous fragmentation of the superconducting background in confined two-dimensional systems.

Two-dimensional superconductivity and violation of Pauli paramagnetic limit in MBE-grown Al nanofilms*  

CHI-TE LIANG (Presenter), CHING-CHEN YEH, GUAN-MING SU, ANKIT KUMAR, BIYI WU, Physics, National Taiwan University, YEN-TING FAN, SHENG-DI LIN, Electronics Engineering, National Chiao-Tung University, LEE CHOW, Physics, University of Central Florida — We have performed low-temperature transport measurements on Al nanofilms on GaAs substrates prepared by molecular beam epitaxy (MBE) with as-grown thicknesses of 3 nm, 3.5 nm, and 4 nm. Such MBE-grown nanofilms all show the Berezinskii-Kosterlitz-Thouless transition, which is compelling evidence for two-dimensional superconductivity, with enhanced transition temperatures (≈2.3 K) compared to that of bulk Al (1.2 K). When the magnetic field is applied parallel to the plane of the Al nanofilms, we measure the upper critical magnetic field $H_{c\parallel}$ by the mid-points of resistive transitions at different temperatures $T$. In this way, we can estimate $H_{c\parallel}(T=0)$. It is found that $H_{c\parallel}(T=0)$ increases with decreasing film thickness. Interestingly, for the thinnest device, $H_{c\parallel}(T=0)$ exceeds the Pauli paramagnetic limit. Such experimental results can be ascribed to spin-orbit coupling effects on superconductivity, even though Al has a low atomic mass.

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Superconducting Nanostructures Grown by He$^+$-Focused Ion Beam Induced Deposition (FIBID)  

ROSA CÓRDOBA, ICMOL, Universitat de València, PABLO ORÚS, ICMA, CSIC-University of Zaragoza (Spain), DOMINIQUE MAILLY, C2N, CNRS, GREGOR Hlawacek, HZDR, JOSE MARIA DE TERESA NOGUERAS (Presenter), ICMA, CSIC-University of Zaragoza (Spain) — W-C superconducting nanostructures have been grown by He$^+$-Focused Ion Beam Induced Deposition (He$^+$-FIBID), which allows superb lateral resolution as well as the capability for creating three-dimensional nanostructures. First, results on in-plane W-C superconducting nanowires grown by He$^+$-FIBID will be presented, where the long-range vortex transport has been investigated by means of non-local measurements; and we will compare them with previous research on in-plane nanostructures grown by Ga$^+$-FIBID [1]. Secondly, results on the growth and superconducting properties of out-of-plane nanotubes with well-controlled inner and outer diameter grown by He$^+$-FIBID will be shown [2]. Lastly, results on the growth and superconducting properties of nanohelices grown by He$^+$-FIBID with tailored dimensions will be presented. Here, remarkable vortex and phase-slip phenomena have been found and explained by the corresponding numerical simulations [3]. In summary, a better understanding of nanosuperconductivity is expected to occur in W-C nanostructures grown by the He$^+$-FIBID technique.

1:03PM B48.00010: Magnetotransport properties of layered quasi-one-dimensional superconductor Ta2PdS5† ENZE ZHANG (Presenter), Fudan Univ, JINHUA ZHI, Peking University, YICHAO ZOU, The University of Queensland, ZEFANG YE, LINFENG AI, JIACHENG SHI, CE HUANG, SHANSHAN LIU, Fudan Univ, NING KANG, HONGQI XU, Peking University, WEI WANG, LIANG HE, Nanjing University, JIN ZOU, The University of Queensland, JINYU LIU, Tulane University, ZHIQIANG MAO, The Pennsylvania State University, FAXIAN XIU, Fudan Univ — Ternary Ta2PdS5 is a newly discovered low-dimensional superconductor with typical quasi one-dimensional chain structure, which has attracted a great deal of research attention owing to its intriguing physical properties. Here we report the systematic study of magnetotransport properties of Ta2PdS5 nanowires exfoliated from its bulk material. The superconducting critical field of system shows strong anisotropic behavior and violation of the Pauli limit when the magnetic field is along the b-axis. I-V measurements show a series of multiple voltage steps in transition to normal state and systematic hysteresis between the up and down sweeps, indicating a typical quasi-one dimensional nature in its superconductivity. Surprisingly, the nanowire undergoes a superconductor-metal transition with increasing perpendicular magnetic field. Upon approaching the zero-temperature quantum critical point, the system uncovers the signature of the quantum Griffiths singularity state arising from enhanced quenched disorders, where the dynamical critical exponent becomes diverging rather than being constant.

†Enze Zhang acknowledges support from China Postdoctoral Innovative Talents Support Program

1:15PM B48.00011: Superconductivity at the LaAlO3/SrTiO3 1D Zigzag Nanowires† YUN-YI PAI (Presenter), MEGAN BRIGGEMAN, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNG-WOO LEE, Department of Materials Science and Engineering, University of Wisconsin at Madison, XIAOXING CHENG, Department of Materials Science and Engineering, Pennsylvania State University, MUQING YU, MENGCHEN HUANG, JIANAN LI, Department of Physics and Astronomy, University of Pittsburgh, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin at Madison, LONG Q. CHEN, Department of Materials Science and Engineering, Pennsylvania State University, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — LaAlO3/SrTiO3 exhibits electron pairing far outside of the superconducting state [1]. The superconducting state of LaAlO3/SrTiO3 also exhibits an intrinsic 1D nature [2] which has been linked to ferroelastic domain structure in the SrTiO3. We further explore the role of ferroelastic domain patterns on superconductivity by creating a series of “zig-zag” nanowire structures. We find that straight nanowires are comparatively more resistive, both in their normal and superconducting state, than channels that have a zig-zag structure. We discuss possible interplay between the charge degree of freedom and the structural domains and employ state-of-the-art phase-field modeling to simulate the relevant domain morphologies.


†J.L acknowledges support from a Vannevar Bush Faculty Fellowship (N00014-15-1-2847). C-BE acknowledges DOE Office of Science, Office of Basic Energy Sciences (DE-FG02-06ER46327).
1:27PM B48.00012: Frictional drag between two LaAlO$_3$/SrTiO$_3$ superconducting nanowires*  
YUHE TANG (Presenter), Department of Physics and Astronomy, University of Pittsburgh, JUNG-WOO LEE, Department of Materials Science and Engineering, University of Wisconsin-Madison, ANTHONY TYLAN-TYLER, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOOK LEE, Department of Materials Science and Engineering, University of Wisconsin-Madison, MICHELLE TOMCZYK, MENGCHEN HUANG, Department of Physics and Astronomy, University of Pittsburgh, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — We report frictional drag measurements between two superconducting LaAlO$_3$/SrTiO$_3$ nanowires. In these experiments, current passing through one nanowire induces a voltage across a nearby electrically isolated nanowire. The frictional drag signal contains both symmetric and antisymmetric components. The antisymmetric component arises from the rectification of quantum shot noise in the drive wire due to asymmetries in the drag wire. The symmetric component is ascribed to rectification of thermal noise in the drive wire during superconducting-normal transition. The absence of symmetric drag resistance between a normal drag wire and a superconducting drive wire suggests a higher electron-hole asymmetry in the superconducting LaAlO$_3$/SrTiO$_3$ nanowire arising from the 1D nature of superconductivity at LaAlO$_3$/SrTiO$_3$ interface.

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1:39PM B48.00013: Interface superconductivity in La$_{2-x}$Sr$_x$CuO$_4$ heterostructures*  
WENJIE GONG (Presenter), LARISSA LITTLE, JASON HOFFMAN, JENNIFER E. HOFFMAN, Harvard University — The lossless flow of current and the high, stable magnetic fields permitted by superconductor technology have led to advances in fields ranging from transportation to medical imaging. However, the low $T_c$ of conventional superconductors—often below 30 K—has limited their commercial applicability. Previous work has demonstrated high-$T_c$ superconductivity at interfaces between thin films of non-superconducting materials, such as between insulating and metallic La$_{2-x}$Sr$_x$CuO$_4$ [1]. Here, we aim to grow high-quality heterostructures of underdoped and overdoped La$_{2-x}$Sr$_x$CuO$_4$ on SrTiO$_3$ and LaSrAlO$_4$ with atomic layer-by-layer molecular beam epitaxy (MBE). We assess the samples grown with atomic force microscopy (AFM) and high-resolution x-ray diffraction (HRXRD). We then perform transport measurements on the La$_{2-x}$Sr$_x$CuO$_4$ heterostructures to examine the possible mechanisms behind $T_c$ enhancement at atomic interfaces.


*This work supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319, the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant No. GBMF4536, Office of Naval Research, Grants N00014-18-1-2691 and N00014-19-1-2622, and the Harvard Herchel Smith Fellowship.
B48.00014: Microscopic theory of in-plane critical field in two-dimensional Ising superconducting systems*  HONGCHAO LIU (Presenter), School of Physics, Peking University, HAIWEN LIU, Department of Physics, Beijing Normal University, DING ZHANG, Department of Physics, Tsinghua University, XINCHENG XIE, School of Physics, Peking University — We study the in-plane critical magnetic field of two-dimensional Ising superconducting systems, and propose the microscopic theory for these systems with or without inversion symmetry. Protected by certain specific spin-orbit interaction which polarizes the electron spin to the out-of-plane direction, the in-plane critical fields largely surpass the Pauli limit and show remarkable upturn in the zero temperature limit. The impurity scattering and Rashba spin-orbit coupling, treated on equal-footing in the microscopic framework, both weaken the critical field but in qualitatively different manners. The microscopic theory is consistent with recent experimental results in stanene and Pb superconducting ultra-thin films.

*This work was financially supported by the National Basic Research Program of China (Grants No. 2017YFA0303301, No. 2015CB921102), the National Natural Science Foundation of China (Grants No. 11674028, No. 11534001, No. 11504008), and the Fundamental Research Funds for the Central Universities.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B49 DCMP: Superconductors: Complex Compounds, Borides, Organics, and Others  Mile High Ballroom 1B - Rongying Jin, Louisiana State University

11:15AM B49.00001: Plasmon-Polaron Superconductivity in Strontium Titanate*  ALEXANDER EDELMAN (Presenter), PETER B LITTLEWOOD, University of Chicago and Argonne National Laboratory — Strontium titanate (STO) is a bulk insulator that becomes a semiconducting superconductor at remarkably low carrier densities - below $10^{17}$ cm$^{-3}$ - with a characteristic superconducting dome as a function of doping which peaks at $T_c \sim 300$ mK, all in very close proximity to a ferroelectric quantum critical point. We investigate a scenario of superconductivity mediated by coupling to a strongly anti-adiabatic longitudinal optic phonon by extending a simple Engelsberg-Schrieffer theory of electron-phonon coupling to include the effects of electronic Coulomb interactions. For the carrier densities of interest, we find that the plasmon hybridizes strongly with LO mode with one of the resulting coupled modes inheriting the low energy scales of the softening ferroelectric mode. Working within the cumulant expansion, we calculate the spectral signatures of this unusual regime of coupling compare to experiment photoemssion[1] and tunneling[2] experiments, as well as the superconducting phase diagram including self-energy effects beyond one loop.


*Work at Argonne is supported by DOE Office of Science Basic Energy Sciences, Materials Science and Engineering under contract DE-AC02-06CH11357.
Recently the copper(II) benzenehexathiolate coordination polymer $[\text{Cu}_3(\text{C}_6\text{S}_6)_n]$ (Cu-BHT) attracts significant interests as the first superconductor in metal-organic frameworks (MOFs) with a superconducting transition temperature $T_c \sim 250$ mK. Since Cu-BHT has a perfect 2D Kagome structure formed by $S = 1/2$ spins of Cu$^{2+}$, unconventional superconductivity related to quantum fluctuations is expected. Although we have already reported that our magnetic penetration depth measurements suggest unconventional superconductivity in Cu-BHT, fundamental superconducting and normal state properties, such as dimensionality, magnetism, and the Fermi energy, which are important to elucidate the superconducting mechanism, are still unrevealed. In this study, therefore, we measured the angle-resolved upper critical field, magnetoresistance, electron spin resonance (ESR), and optical conductivity. By comparing the ratio of $T_c$ to the Fermi temperature with other unconventional superconductors, we revealed that Cu-BHT is possibly a member of strongly correlated electron systems.
11:39AM B49.00003: Exploring superconductivity using muon spin resonance in chiral noncentrosymmetric superconductors.* DANIEL MAYOH (Presenter), MATTHEW PEARCE, KATHRIN GOETZE, Physics Department, University of Warwick, Coventry, CV4 7AL, United Kingdom, ADRIAN HILLIER, ISIS facility, STFC Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Oxfordshire OX11 0QX, United Kingdom, GEETHA BALAKRISHNAN, MARTIN LEES, Physics Department, University of Warwick, Coventry, CV4 7AL, United Kingdom — Unconventional superconductivity remains one of the most interesting problems in condensed matter physics. For all superconductors, the topology of the electronic band structure, along with the underlying crystal structure, play vital roles in determining the superconducting properties of the material. Systems lacking a centre of inversion exhibit a nonuniform lattice potential, giving rise to a Rashba-type antisymmetric spin-orbit coupling which allows for an admixture of singlet and triplet pairs. This may give rise to exotic superconducting band structures and magnetoelectric effects such as upper critical fields that exceed the Pauli limit. The discovery of two noncentrosymmetric superconductors with chiral structures, TaRh$_2$B$_2$ and NbRh$_2$B$_2$ [1], has added a new twist to an already exciting area of superconductivity. Here we present our investigation into the superconducting order parameter using muon spin resonance techniques in TaRh$_2$B$_2$ and NbRh$_2$B$_2$ [2, 3].


*This work is funded by the EPSRC, UK (EP/M028771/1) and the European Research Council (ERC) (Grant No. 681260).

11:51AM B49.00004: Magnetism and superconductivity in alkali metal doped 2,2'-bipyridine from near room temperature synthesis† DI PENG (Presenter), RENSHU WANG, XIAO-JIA CHEN, CEP, HPSTAR (Beijing) — Organic superconductors have long been the major players in the development of modern physical chemistry. So far, many cases of introducing charge into π-electron networks in organic superconductors with Meissner effect have been found. However, most of them lack pivotal zero resistance measurements because of the high synthesized temperature leading to the decomposition of organic materials and forming non-homogeneous phases. To avoid this tendency, a design principle for low temperature synthetic reaction process is indispensable.

We report a development method for doping alkali metals into organic materials and forming a homogeneous phase together with the experimental discoveries of superconductivity in sodium potassium alloy doped 2,2'-bipyridine. We successfully detected superconductivity from the observed Meissner effect and zero resistance effect. The work demonstrates that low temperature synthetic reaction process is of great significance for producing organic superconductors.

*National Key R&D Program of China (Grant No. 2018YFA0305900).
12:03PM B49.00005: Superconductivity in an organobismuth molecule*  RENSHU WANG (Presenter), LIUCHENG CHEN, XIAO-JIA CHEN, HPSTAR (Beijing), HUI YANG, MINGAN FU, JIA CHENG, XIAOLIN WU, YUN GAO, ZHONGBING HUANG, Hubei University — Recently, novel quantum phenomena such as topological insulators and superconductors were suggested in organobismuth compounds. However, evidence for superconductivity from the zero-resistivity state in any organometallic compound has not been achieved yet, though much effort has been made. Here, we report the experimental realization of superconductivity in a critical temperature of 3.6 K in potassium-doped tri-o-tolylbismuthine, with evidence of both the Meissner effect and the zero-resistivity state through dc and ac magnetic susceptibility and resistivity measurements. The superconducting phase and its composition are determined by combined studies of X-ray diffraction and theoretical calculations as well as Raman spectroscopy measurements. These findings enrich the applications of organometallic compounds in superconductivity and add a new electron-acceptor family of organic superconductors.

*National Key R&D Program of China, Grant No. 2018YFA0305900. National Natural Science Foundation of China, Grants No. 11574076, 11674087, and 91221103.

12:15PM B49.00006: Li$_{2x}$BC$_3$: a two dimensional MgB$_2$-like superconductor*  YUNDI QUAN (Presenter), WARREN PICKETT, University of California, Davis — Though most superconductors can be grouped into distinct structure classes, MgB$_2$ remains in a class of its own almost two decades after its discovery. Previous efforts to design superconductors in the same structure class as MgB$_2$ have been unsuccessful due to various complications. Recently, experimentalists are able to stabilize Li$_{2x}$BC$_3$ [1], a layered compound with Li sandwiched between alternating C-C and B-C honeycomb sheets similar to MgB$_2$. By carrying out linear response calculations, we find that at half occupation (i.e. x= 0.5), Li$_{2x}$BC$_3$ is a phonon mediated superconductor with a $T_c$ of around 45 K. Further increasing Li occupation (x) weakens electron-phonon coupling, thus lowering $T_c$. At occupation levels below 0.5, crystal structure of Li$_{2x}$BC$_3$ becomes dynamically unstable due to increased electron-phonon coupling. Electronic structure, Fermi surfaces and electron-phonon couplings etc of Li$_{2x}$BC$_3$ will be presented to help understand the origin of strong electron-phonon coupling.


*This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562.
12:27PM B49.00007: Inhomogeneity of superconductivity in a disordered charge density wave material Pd-intercalated ErTe$_3$ measured using scanning SQUID microscopy  YUSUKE IGUCHI (Presenter), JOSHUA A STRAQUADINE, JOHN ROBERT KIRTLEY, ANISHA SINGH, IAN FISHER, KATHRYN ANN MOLER, Department of Applied Physics, Stanford University — The rare-earth tri-tellurides RTe$_3$ (R=La-Pr, Sm, Gd-Tm) are quasi-2D metals that show unidirectional incommensurate charge density wave (CDW) states. Pd intercalation introduces significant disorder to the crystal lattice, suppressing the CDW formation and leading to a superconducting ground state. The material presents an opportunity to explore in detail the interplay between superconductivity (SC) and CDW formation in the presence of disorder. Here we study the spatial variance of the superfluid response as a function of Pd concentration in Pd$_x$ErTe$_3$ (0<x<0.06) by using a scanning SQUID microscope with sub-micron spatial resolution. We quantify the inhomogeneity of the emergent superconductivity as the CDW is progressively disordered by the Pd intercalation. Our results clarify how the superconducting state emerges from the disordered CDW.

12:39PM B49.00008: In-plane anisotropy of the c-axis magnetoresistance for BiCh$_2$-based superconductor  KAZUHISA HOSHI (Presenter), YOSHIKAZU MIZUGUCHI, YOSUKE GOTO, TATSUMA D. MATSUDA, Tokyo Metropolitan University, MOTOI KIMATA, Institute for Materials Research, Tohoku University — BiCh$_2$-based (Ch = S, Se) superconductor was discovered in 2012, the crystal structure is similar to that of high temperature superconductor, such as cuprate superconductor and iron-based superconductor. The pairing mechanisms of the superconductivity has not been completely understood. However, theoretical calculation, ARPES, and isotope effect suggest that unconventional superconductivity is essential for BiCh$_2$-based superconductor.

We have investigated the in-plane anisotropy measurement of the c-axis magnetoresistance for BiCh$_2$-based superconductor LaO$_{0.5}$F$_{0.5}$BiSSe single crystals. We observed the two-fold symmetry of the magnetoresistance in the $ab$-plane for LaO$_{0.5}$F$_{0.5}$BiSSe in superconducting states while the conducting plane possessed a tetragonal square plane with the four-fold symmetry. This results show that the BiCh$_2$-based superconductor may be nematic superconductor. Furthermore, more recently, we have investigated anisotropy measurement of the c-axis magnetoresistance for other BiCh$_2$-based superconductor NdO$_{0.7}$F$_{0.3}$BiS$_2$ single crystals. Two-fold symmetry was observed for NdO$_{0.7}$F$_{0.3}$BiS$_2$ above $T_c$, which is different behavior for LaO$_{0.5}$F$_{0.5}$BiSSe. We are going to report this latest result for the NdO$_{0.7}$F$_{0.3}$BiS$_2$ single crystals.
12:51PM B49.00009: Superconductivity at 262 K in Yttrium Superhydride at High Pressures*

ELLIOT M SNIDER, Department of Mechanical Engineering, University of Rochester, NATHAN M DASEN BROCK-GAMMON, Department of Physics, University of Rochester, RAYMOND MCBRIDE, Department of Mechanical Engineering, University of Rochester, RANGA DIAS (Presenter), Department of Physics and School of Engineering and Applied Sciences, University of Rochester — Superconductivity has been one of the most profound quantum phases in condensed matter physics. Efforts to identify and develop room temperature superconducting materials are an intensive area of research, motivated by both fundamental science and the prospects for applications. We report the synthesis and superconductivity in Yttrium superhydride with highest Tc of 262K at 183 GPa. The Tc is the highest ever recorded at this pressure. The superconductivity in Yttrium superhydride arises from clathrate based hydrogenic lattices. The electrical resistance measurements and magnetic field dependence transport measurement shows the clear indication of the observed superconductivity. Based on the Raman spectra, we suggest that YH6, is responsible observed superconductivity, which is in good agreement with recent theoretical studies. The hydrogen-rich materials are in the vicinity of achieving room temperature superconductivity.

*The NSF grant DMR-1809649 supported this research.

1:03PM B49.00010: Anisotropic energy gap in single crystals of isotropic superconductor SrPt$_3$P*

KYUIL CHO (Presenter), SERAFIM TEK NOWIJOYO, ELIZABETH KREN KEL, MAKARIY A TANATAR, RUSLAN PROZOROV, Ames Laboratory and Iowa state University, Ames, USA, NIKOLAI D ZHIGADLO, CrystMat Company, Zurich, Switzerland — Antiperovskie pnictide SrPt$_3$P shows the highest superconducting transition temperature, T$_c$, among the 5d element - based compounds, possibly with somewhat strong coupling, 2\(\Delta_0 / T_c\) ~5. While the material itself is quite isotropic, its energy gap structure and pairing state remain uncertain due to the lack of single crystals. Here we report directional measurements of electrical resistivity and London penetration depth in single crystals SrPt$_3$P. Surprisingly, our results show highly anisotropic nature of the superconducting energy gap.

*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract # DE-AC02-07CH11358.
Non-centrosymmetric superconductors (NCSs) lack inversion center in their crystal structure, and consequently one of the typical symmetries for the formation of Cooper pairs. The absence of inversion symmetry strongly influences the Cooper pairing states possible in these materials. Here we report a muon spin rotation/relaxation (μSR) study of LaNiC$_2$ single crystals, a non-magnetic, NCS with weak electronic correlations and a superconducting transition temperature, $T_c \sim 2.7$ K. Previous zero-field μSR measurements on a pressed pellet of LaNiC$_2$ powder revealed the onset of spontaneous magnetic fields at $T_c$. This finding signifies time-reversal symmetry breaking (TRSB) in superconducting phase, which is compatible with a non-unitary triplet-pairing state. However, other kinds of experiments have provided evidence for conventional BCS $s$-wave pairing, point nodes in the gap function and even two-gap superconductivity. Our new μSR investigation of LaNiC$_2$ provides a fresh perspective on the nature of the superconducting pairing state, by yielding the temperature and magnetic field dependencies of the magnetic penetration depth and vortex core size in the mixed state and through a new test of TRSB.

*Acknowledged support from NSERC and JSPS KAKENHI with grant nos. JP15K05156 and JP15KK0149
1:27PM B49.00012: Superconductivity in Cu-doped TiSe$_2$: A first-principles calculation

OBINNA UZOH (Presenter), TAE-HO PARK, HAN-YONG Choi, Sungkyunkwan Univ — We present the superconducting properties of Cu-doped TiSe$_2$ materials based on first-principles calculations. Experimental study of Cu intercalated 1T-TiSe$_2$ under various copper doping concentrations ($x = 0.04$ – $0.10$) has been investigated extensively. Such study has shown that as doping concentrations increase charge density wave is steadily suppressed until about $x = 0.04$ where a dome-shaped superconductivity emerges with maximum $T_c$ of $4.15$ K at $x = 0.08$ [1]. In order to understand this observation theoretically, we perform first-principles calculations based on density functional theory and density functional perturbation theory incorporated with maximally localized Wannier functions. We calculate the electronic structures at various doping concentrations by modeling doping using virtual crystal approximation. Also, we estimate the superconducting $T_c$ by calculating the electron-phonon coupling and the Eliashberg spectral function. Further, we analyze all possible phonon modes in Cu$_x$TiSe$_2$ and ascertain dominant modes contributing to the superconductivity.

Reference

1:39PM B49.00013: Strain-stabilized superconductivity in RuO$_2$ JACOB RUF (Presenter), HANJONG PAIK, NATHANIEL SCHREIBER, HARI NAIR, LUDI MIAO, JASON KAWASAKI, JOCIENNE NELSON, BRENDAN FAETH, YONGHUN LEE, BERIT GOODGE, BETUL PAMUK, CRAIG FENNIE, LENA FITTING KOURKOUTIS, DARRELL SCHLOM, KYLE M SHEN, Cornell University — The rational control of superconductivity and the possibility of deterministically enhancing the superconducting transition temperature ($T_c$) by design, rather than by serendipity, has been an elusive and long sought-after goal in solid-state physics. Here, we report the first instance of transmuting a normal metal into a superconductor through the application of epitaxial strain. We demonstrate that synthesizing RuO$_2$ thin films on TiO$_2$(110) substrates stabilizes superconductivity under strain, having $T_c$s up to $2$ K; by contrast, RuO$_2$ thin films grown on TiO$_2$(101) substrates are non-superconducting down to the lowest measured temperatures ($T_c < 0.4$ K), consistent with the behavior of bulk RuO$_2$. Using a comprehensive combination of characterization techniques—including electrical transport, x-ray diffraction, scanning transmission electron microscopy, angle-resolved photoemission spectroscopy, and density functional theory—we reveal the primary electronic mechanism underlying this strain-stabilized superconductivity: the anisotropic strains redistribute the carriers amongst the manifold of 4$d$ states near the Fermi level ($E_F$), partially depopulating flat bands with $d_{||}$ orbital character, and thereby increase the density of states at $E_F$. 
1:51PM B49.00014: Physical Properties of New Alkaline Earth Tantalum Sulfides*
SHERMANE BENJAMIN (Presenter), MICHAEL SMITH, JOHN J NEUMEIER, Montana State University, Bozeman — Transition-metal sulfides serve as an interesting class of compounds for comparison to transition-metal oxides. They also often demonstrate properties such as metal-insulator transitions, superconductivity, and magnetism. In this work, single crystals of $\text{CaTa}_5\text{S}_{10}$, $\text{Sr}_3\text{Ta}_5\text{S}_{10}$ and $\text{BaTa}_{10}\text{S}_{10}$ samples were synthesized via chemical vapor deposition. $\text{CaTa}_5\text{S}_{10}$, $\text{Sr}_3\text{Ta}_5\text{S}_{10}$ and $\text{BaTa}_{10}\text{S}_{10}$ superconduct at $T_{\text{C, onset}} = 3.25$ K, 3.8 K and 2.8 K, respectively. The magnetic properties, specific heat, electrical resistivity, structural analysis, and compositional analysis will be discussed.

*Work at Montana State University was conducted with financial support from the US Department of Energy (DOE) DE-SC0016156.

B49.00015: Coexistence of superconductivity and weak ferromagnetism in Rb-doped triphenylbismuthine and tri-$p$-tolylbismuthine* ZHONGBING HUANG (Presenter), Physics, Hubei University, REN-SHU WANG, JIA CHENG, Materials Science, Hubei University, MING-AN FU, HUI YANG, Physics, Hubei University, YUN GAO, Materials Science, Hubei University, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research, Shanghai — By using a two-step method - ultrasound treatment and low temperature annealing, we successfully synthesize Rb-doped triphenylbismuthine and tri-$p$-tolylbismuthine. The dc magnetic measurements show a coexistence of superconductivity at 4.0 K and weak ferromagnetism at 35 K in all synthesized samples, which is strongly supported by the resistivity measurements. The calculated electronic structure indicates that superconductivity is realized by transferring electron from rubidium to carbon atom, and the weak ferromagnetism is produced by nonparallel arrangement of magnetic moments on the phenyl rings. Our study provides a new platform for understanding the interplay between superconductivity and ferromagnetism.

*We acknowledge financial support from the National Natural Science Foundation of China under Grants Nos. 11674087 and 11574076.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B50 DCMP: Correlated F-Electron Materials Mile High Ballroom 1C - Kaya Wei, Florida State Univ
11:15AM B50.00001: Phase stabilization by electronic entropy in plutonium*  NEIL HARRISON (Presenter), JONATHAN B BETTS, MARK WARTENBE, FEDOR BALAKIREV, SCOTT RICHMOND, MARCELO JAIME, PAUL H TOBASH, Los Alamos Natl Lab — Plutonium metal undergoes an anomalously large 25% collapse in volume from its largest volume δ phase (δ-Pu) to its low temperature α phase, yet the underlying thermodynamic mechanism has largely remained a mystery. Here we use magnetostriction measurements to isolate a previously hidden yet substantial electronic contribution to the entropy of δ-Pu, which we show to be crucial for the stabilization of this phase. The entropy originates from two competing instabilities of the 5f-electron shell, which we show to drive the volume of Pu in opposing directions, depending on the temperature and volume. Using calorimetry measurements, we establish a robust thermodynamic connection between the two excitation energies, the atomic volume, and the previously reported excess entropy of δ-Pu at elevated temperatures.

*The work was performed under the Los Alamos National Laboratory LDRD program: project `20180025DR." Measurements were performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation, Florida State and the Department of Energy. N. H. thanks John Wills, Jianxin Zhu, Angus Lawson, Jason Lashley, Albert Migliori, Boris Maiorov and John Joyce for insightful discussions.

11:27AM B50.00002: Physical Properties of 1-Dimensional 4f/5f-electron Heavy Fermion Materials*  ERIC BAUER (Presenter), T. ASABA, SEAN THOMAS, JOE D THOMPSON, PRISCILA ROSA, FILIP RONNING, Los Alamos Natl Lab — Quantum criticality has been an organizing principle to explain the behavior of many families of quantum materials including the high-temperature cuprate and iron-based superconductors and f-electron heavy fermion compounds. A central, unresolved issue is the effect on the dimensional character of the quantum fluctuations has on the properties of the system. Most work to date has focused on quantum criticality with two-dimensional (2-D) and three-dimensional (3-D) fluctuations. Strong quantum fluctuations are expected in quasi-1-D materials. Furthermore, these 1-D systems may be treated exactly by theoretical tools such as Density Matrix Renormalization Group, providing robust and accurate methods for accounting for the strong correlations in 1-D f-electron materials. In this talk, I will describe the thermodynamic and transport properties of several 4f and 5f quasi-1D heavy fermion materials.

*This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
Probing the local 4f-orbital symmetry in heavy fermion systems by linearly polarized angle-resolved core-level hard x-ray photoemission spectroscopy

AKIRA SEKIYAMA (Presenter), Hidenori Fujiwara, Satoru Hamamoto, Yuina Kanai-Nakata, Graduate School of Engineering Science, Osaka University, Shin Imada, Ritsumeikan University, Arata Tanaka, Hiroshima University, Kenji Tamasaku, Tetsuya Ishikawa, RIKEN SPring-8 Center — Ground-state (GS) orbital symmetry determined by the local effective crystalline electric fields (CEF) in strongly correlated electron systems play crucial roles in their functional properties such as superconductivity and multipolar ordering. We have found that the CEF-split GS 4f-orbital symmetry can be probed by linear dichroism (LD) in angle-resolved core d-level hard x-ray photoemission owing to the selection rules in the optical process [1]. We have applied this technique to Ce, Pr, and Yb-based heavy fermion systems, where the $\Gamma_7$ states with $J_z = \pm \frac{3}{2}$ and the $\Gamma_8$ states in the CEF-split GS 4f symmetry have been established for tetragonal YbRh$_2$Si$_2$ [2] and cubic YbB$_{12}$ [3]. Mutually different LDs reflecting the different orbital symmetry have been seen for cubic PrBe$_{13}$, PrB$_6$, and PrIr$_2$Zn$_{20}$ [4,5]. This technique has also revealed the CEF-split GS 4f wave functions for a pressure-induced superconductor CeCu$_2$Ge$_2$ [6].


Pressure effect on the chiral helimagnetic order in YbNi$_3$Al$_9$

YOSHIHIKO OTA (Presenter), Kazunori Umeo, Takumi Otaki, Yudai Arai, Taka Hiro Onimaru, Hiroshima Univ, Shota Nakamura, Shigeo Ohara, Nagoya Institute of Technology — YbNi$_3$Al$_9$ crystalizes in the trigonal ErNi$_3$Al$_9$-type structure with a space group of R32. This compound undergoes the chiral helimagnetic (CHM) order at $T_M = 3.4$ K. According to the chiral sine-Gordon model, the CHM order is realized by the competition between the Dzyaloshinskii-Moriya interactions and the ferromagnetic (FM) interactions, both of which work along the helical axis. By applying magnetic field perpendicular to the helical c-axis, the magnetic phase transition to the forced FM state manifests itself at $B_c = 0.1$ T in association with the divergence of the helical pitch.

In this work, we have studied pressure effect on the CHM order in YbNi$_3$Al$_9$ by measuring magnetization, electrical resistivity, and magnetoresistance under hydrostatic pressures. Both of $T_M$ for 0 T and $B_c$ for 0.3 K monotonically decrease by applying pressures up to 2.5 GPa in the ratios of $-0.22$ K / GPa and $-0.013$ T / GPa, respectively. By the application of pressures, the ordered moment increases and the Kondo scattering is suppressed, suggesting that the Ruderman-Kittel-Kasuya-Yosida interaction dominates the Kondo effect. Based on these results, we attribute the reduction in $T_M$ and $B_c$ to the destabilization of helical structures owing to the development of the FM correlations.
12:03PM B50.00005: Quadrupolar fluctuations of heavy-fermion metal YbRu$_2$Ge$_2$* MAI YE, Department of Physics and Astronomy, Rutgers University-New Brunswick, ELLIOTT W ROSENBERG, IAN FISHER, Department of Applied Physics, Stanford University, GIRSH BLUMBERG (Presenter), Department of Physics and Astronomy, Rutgers University-New Brunswick — Long-range order of electric quadrupole moments is one characteristic phenomenon in the family of multipolar Kondo systems. The heavy-fermion metal YbRu$_2$Ge$_2$ enters a ferro-quadrupolar (FQ) phase below $T_{FQ}$=10K, in which the $B_{1g}$-symmetry quadrupole moments at Yb$^{3+}$ sites order at zero wave vector [Proc. Natl. Acad. Sci. U.S.A. 116, 7232 (2019)]. This FQ phase is a realization of electronic nematic states since the electronic properties spontaneously break the four-fold rotational symmetry of the tetragonal crystal. We study the quadrupolar fluctuations of this compound by Raman scattering [Phys. Rev. B 99, 235104 (2019)]. The electronic Raman susceptibility in quadrupolar symmetry channels exhibit nearly Curie-law behavior, indicating weak exchange interactions between local quadrupoles. It is the relatively strong coupling between the quadrupole moments and the lattice strain fields in the $B_{1g}$ symmetry channel, analogous to cooperative Jahn-Teller effect, that enhances the vanishingly small Weiss temperature to the temperature of quadrupolar phase transition at $T_{FQ}$.

*M.Y. and G.B. was supported by NSF DMR-1709161. E.W.R. and I.R.F. was supported by the Gordon and Betty Moore Foundation Grant GBMF4414.

12:15PM B50.00006: Thermodynamic and transport properties of Kondo lattice YbCuAs$_2$ single crystals* EUNDEOK MUN (Presenter), DAVID EVANS, SYMPHONY HUANG, Physics, Simon Fraser Univ — YbCuAs$_2$ compound crystallizes into a tetragonal ZrCuSi$_2$-type structure. Magnetic susceptibility measurements for the YbCuAs$_2$ polycrystalline sample showed an antiferromagnetic phase transition below 4 K. However, the neutron powder diffraction measurements of this sample didn't show any additional Bragg peaks down to 1.5 K, indicating either there is no magnetic ordering down to 1.5 K or the ordered moment of Yb ions is smaller than the current experimental limit. We succeeded in growing single crystals of YbCuAs$_2$ by high temperature ternary melt. Thermodynamic and transport properties were investigated by measuring the magnetization, electrical resistivity, and specific heat. In this talk, I will present thermodynamic and transport properties of Kondo lattice YbCuAs$_2$ single crystals.

*This work was supported by the Canada Research Chairs program, the Natural Science and Engineering Research Council of Canada, and the Canadian Foundation for Innovation.
Dynamical Scaling of Charge Responses at a Kondo Destruction Quantum Critical Point*  STEFAN B. KIRCHNER (Presenter), Zhejiang University, HAOYU HU, ANG CAI, Rice University, ZUODONG YU, Zhejiang University, QIMIAO SI, Rice University — An overarching question on quantum criticality is whether and how it goes beyond the Landau framework of order-parameter fluctuations. In the studies of heavy fermion metals, the notion of Kondo destruction has been developed to address this issue [1]. Microscopically, it captures how the inter-local-moment singlet formation dynamically competes with the Kondo-singlet formation at the quantum critical point (QCP). An exciting recent surprise is that charge dynamics is also singular and shows omega/T scaling at the prototype antiferromagnetic QCP of YbRh2Si2 [2]. We study prototype models for Kondo destruction QCP, and find that both the charge and spin responses are singular and obey omega/T scaling [3,4]. The criticality of the charge dynamics originates from an f-electron delocalization-localization across the Kondo destruction QCP. Broader implications of our results are discussed, both for the beyond-Landau quantum criticality in general and for the exotic excitations and unconventional superconductivity of strongly correlated metals.


*NSF (DMR-1920740) & Welch Foundation (C-1411)

Itinerant Nature of Ce in CeCo5*  RENU CHOUDHARY (Presenter), DURGA PAUDYAL, Ames Lab — Due to the high uniaxial anisotropy and abundant nature of Ce, CeCo5 has attracted the attention of scientists for developing an excellent permanent magnet. Here, we discuss the itinerant nature of Ce in CeCo5 using density functional theory (DFT). Ce based intermetallic compounds show interesting magnetism because of the mixed-valence 4f state. The 3+ valence would have provided 1.0 µB/Ce 4f; however, in either case with and without employing on-site electron correlation parameter, we obtain 4f spin moment less than 1.0 µB/Ce 4f. Also, the 3d-5d hybridization in CeCo5 is strong enough to overlap 4f states below the Fermi level and form a 3d-5d-4f hybridization thereby indicating the itinerant nature of Ce 4f in CeCo5. This assessment allows us to consider CeCo5 as an itinerant magnetic material system suitable to treat by standard DFT. Further, the 4f spin moment of CeCo5 is partially canceled by the orbital counterpart and the Co moment is reduced by the stronger 3d-4f hybridization in the spin-down channel.

*This work is supported by the Critical Materials Institute, an Energy Innovation Hub, funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.
12:51PM B50.00009: The ground state and Fermi-surface nesting phenomenon in antiferromagnetic CeAuSb$_2$. JAEKYUNG JANG (Presenter), JOO YULL RHEE, Department of physics, Sungkyunkwan Univ — Recently, it was reported that, under an external magnetic field (≤ 3T) along the c-axis, the in-plane wave vector of the spin-density wave (SDW) is ($\eta$, $\eta$, ½) with $\eta \approx 0.136$ for CeAuSb$_2$ compound. To elucidate this SDW and the ground state we investigate the electronic structure of antiferromagnetic (AFM) CeAuSb$_2$ using the full-potential linearized-augmented-plane-wave method. The results of volume optimize calculations and total energy show that 1 x 1 x 2 unit cell construction with $\uparrow\uparrow\downarrow\downarrow\downarrow$ AFM configuration is the ground state, which are well matched with experiments. Fermi surface (FS) on the $ab$-plane exhibit FS nesting along the (110) direction. The nesting vector $q = (\zeta, \zeta, ½) (2\pi/a)$ with $\zeta \sim 1/7$, is very similar to the results of experiment. To confirm the relation between this FS nesting and SDW we will calculate the generalized susceptibility $\chi(q)$.

1:03PM B50.00010: Microscopic Nature of Magnetic Ground State in CeAuSb$_2$* GEORGE YUMNAM, YIYAO CHEN, Univ of Missouri - Columbia, YANG ZHAO, Department of Materials Sciences and Engineering, University of Maryland, College Park, MD, A. THAMIZHAEL, SUDESH K. DHAR, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, DEEPAK K SINGH (Presenter), Univ of Missouri - Columbia — The synergistic investigation of ground-state magnetic correlation in the single-crystal heavy-fermion compound CeAuSb$_2$ using detailed neutron scattering measurements and density functional calculations is presented. Unlike previous reports of single antiferromagnetic transition at $T_N = 6K$, three successive transitions with distinct critical exponents at $T_N = 5.3, 4.46, 3.76$ K, respectively, are detected in CeAuSb. The low-temperature ground-state magnetic correlation is described by the spin density wave order in the basal plane with the propagation wave vector (0.135, 0.135, 0.5). The spin density wave order arises due to the nesting of hole pockets in the Fermi surface, with parallel surfaces being separated by the experimentally found propagation vector. The comprehensive investigation of magnetic ground-state properties is expected to provide new insights in understanding the emerging quantum magnetism in this system, including the debated quantum critical state and magnetic field-induced metamagnetic transitions at low temperatures.

*Department of Energy, Office of Science, Office of Basic Energy Sciences. Grant Number: SC0014461
Electronic and Magnetic Properties of EuNi$_{2-x}$Sb$_2$ Structural Variants

WILLIAM NELSON (Presenter), Physics, NHMFL, Florida State University, ASHINI JAYASINGHE, Chemistry, Florida State University, DAVID E GRAF, NHMFL, Florida State University, SUSAN LATTURNER, Chemistry, Florida State University, RYAN BAUMBACH, Physics, NHMFL, Florida State University — XRD, magnetic susceptibility, magnetization, heat capacity, and resistivity results are reported for single crystals of two structural variants of EuNi$_{2-x}$Sb$_2$. While the CaBe$_2$Ge$_2$-type structure forms with a stoichiometric ratio, the ThCr$_2$Si$_2$-type structure exhibits a Ni site vacancy of 18%. Both systems show Curie-Weiss temperature dependence at elevated temperatures, indicating an antiferromagnetic exchange interaction between the Eu$^{2+}$ ions. At low temperatures, the different structural environments give rise to distinct ordering behavior. The CaBe$_2$Ge$_2$-variant first orders antiferromagnetically near $T_{N2}$=6.9K and then undergoes a first order transition at $T_3$=4.6K. The ThCr$_2$Si$_2$-variant orders antiferromagnetically at $T_{N1}$=5.6K. The 4f entropy recovered by the antiferromagnetic ordering is consistent with the predicted J=7/2 Hund's rule multiplet values for the ThCr$_2$Si$_2$-variant, while it is reduced for the CaBe$_2$Ge$_2$-variant. Thus, EuNi$_{2-x}$Sb$_2$ emerges as a useful system in which to study the impact of structural variation on electronic correlations.

*This work was performed at the NHMFL which is supported by NSF Cooperative Agreement DMR-1644779 and the State of Florida. Synthesis and material characterization was supported by CAST, an EFRC funded by the US DOE under Award DE-SC0016568.

Magnetically-enhanced lattice instability in EuRh$_2$Si$_2$ under pressure

ANJANA KRISHNADAS (Presenter), Okinawa Institute of Science and Technology, STEPHEN ARMSTRONG, California Institute of Technology, WENLI BI, University of Alabama at Birmingham, JIYONG ZHAO, ESEN ALP, Argonne National Laboratory, RIKI KOBAYASHI, MASATO HEDO, TAKAO NAKAMA, YOSHICHIKA ONUKI, University of The Ryukyus, THOMAS F ROSENBAUM, California Institute of Technology, YEJUN FENG, Okinawa Institute of Science and Technology — The family of ThCr$_2$Si$_2$ structured rare-earth Eu intermetallics exhibits the coexistence of three different instabilities: the competing Kondo and RKKY exchange interactions in heavy-fermion magnetic materials, as well as an isostructural collapse of the lattice particular to this type of tetragonal structure. Moreover, there is a valence instability in Eu that connects the lattice and magnetic instabilities, as the Eu$^{3+}$ magnetic moment can vanish with an atomic volume reduction to a non-magnetic Eu$^{2+}$ state. Here, in a series of ThCr$_2$Si$_2$ structured Eu antiferromagnets, we explore the subtle interaction and cooperation between these instabilities under pressure, using synchrotron-based Mossbauer spectroscopy and optical Raman scattering to track the evolution of the magnetism and the lattice, respectively. Exemplified by two end members of this series, we observe that magnetism disappears in EuRh$_2$Si$_2$ by 1 GPa, while it persists in EuGa$_4$ to beyond 36 GPa at $T = 4$ K. With the assistance of the magnetic instability, the structural instability in EuRh$_2$Si$_2$ demonstrates a pressure dependence of its phase line $dT_s/dP$ nearly 100 times higher than that in EuGa$_4$. This dramatic contrast in behavior with applied pressure illuminates a cooperative, magnetically-enhanced structural instability.
Magnetic fluctuations in the itinerant ferromagnet LaCrGe3 studied by 139La NMR

Khusboo Rana (Presenter), Division of Materials Sciences & Engineering, Ames Lab and Iowa State University, Hisashi Kotegawa, Graduate School of Science, Kobe University, Rahim R. Ullah, Jeffrey S. Harvey, Department of Physics, University of California Davis, Sergey L. Bud'ko, Paul C. Canfield, Division of Materials Sciences & Engineering, Ames Lab and Iowa State University, Hideki Tou, Graduate School of Science, Kobe University, Valentin Taufour, Department of Physics, University of California Davis, Yuji Furukawa, Division of Materials Sciences & Engineering, Ames Lab and Iowa State University — Recently much attention has been paid to itinerant ferromagnetic (FM) compounds because of the observations of unconventional superconductivity (SC) as well as the avoidance of FM quantum critical point (QCP) under application of pressure (p) and magnetic field (H). In this context, the itinerant ferromagnet LaCrGe3 (Curie temperature of TC=85 K) is very unique. It exhibits an avoided FM QCP under pressure through both a modulated antiferromagnetic phase as well as tricritical wing structure in its temperature-pressure-magnetic field (T−p−H) phase diagram. In order to characterize the static and dynamical magnetic properties of this peculiar material, we carried out 139La nuclear magnetic resonance (NMR) measurements. Here we present our analysis of the NMR data using self-consistent-renormalization theory and provide a comparison of this system in the generalized Rhodes-Wohlfarth plot with other similar itinerant ferromagnets.

This work was supported by the USDOE, Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-07CH11358. Part of the work was supported by the Japan Society for the Promotion of Science KAKENHI Grant Numbers JP15H05882, JP15H05885, JP15K21732, and JP18H04321 (J-Physics).

Crystal field splitting and spin Hamiltonian of the quantum magnet YbCl3

Gabriele Sala, Matthew Stone, Binod Rai, Seunghwan Do, Andrew May, David Parker, Gabor Halasz, Pontus Laurell, Satoshi Okamoto, Oak Ridge National Laboratory, Nicholas Butch, National Institute of Standards and Technology, Yongqiang Cheng, G. Ehlers, Vasile O. Garlea, Qiang Zhang, Oak Ridge National Laboratory, Ganesh Pokharel, Hasitha Suriya Arachchige, David Mandrus, University of Tennessee, Mark D Lumsdon, Andy Christianson (Presenter), Oak Ridge National Laboratory — YbCl3 is a nearly ideal honeycomb lattice quantum magnet. Here we study YbCl3 with neutron scattering, magnetic susceptibility, and heat capacity measurements. We determine the crystal field Hamiltonian through simultaneous refinements of the inelastic neutron scattering and magnetization data. The ground state doublet of the crystal field Hamiltonian is well isolated and results in an effective spin-1/2 system with local easy plane anisotropy at low temperature. Cold neutron spectroscopy shows low energy spin waves peaked at 0.5 meV that can be understood through a Heisenberg model with a single nearest neighbor exchange interaction.
B50.00015: Quasi-1D Kondo chain in $\text{CeCo}_2\text{Ga}_8$  
YONGKANG LUO (Presenter), Huazhong University of Science & Technology — “Dimensions are critical”. This is because lower dimension means more phase space for long-wavelength fluctuations and a larger magnetic frustration parameter, the latter of which dictates the way that the system undergoes from a quantum ordered state to a disordered state: a conventional spin-density-wave (SDW) type quantum critical point (QCP) or an unconventional Kondo-destruction type QCP. Kondo destruction generically requires large spin fluctuations and thus favors lower dimension. In a limit where the Kondo coherence is realized in one dimension but fails in others, the Kondo lattice is reduced to a Kondo chain. Our recent study on the CeCo$_2$Ga$_8$ manifest that this compound is quasi-1D both electrically and magnetically, and most importantly, the Kondo scattering become coherent in c-axis but remains incoherent in both a- and b-axes. The anisotropy scattering mechanism and transport entropy are also investigated by thermopower and Nernst effect measurements.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B51 DCMP DMP: Graphene: Electronic Structure and Interactions Interactions: Moire, Correlations, and Topology  
Mile High Ballroom 1D - Onder Gul, Harvard University

11:15AM B51.00001: Ground State of Magic Angle Twisted Bilayer Graphene at Charge Neutrality II  
SHANG LIU (Presenter), Harvard University, NICK BULTINCK, University of California, Berkeley, ESLAM KHALAF, Harvard University, SHUBHAYU CHATTERJEE, University of California, Berkeley, ASHVIN VISHWANATH, Harvard University, MICHAEL ZALETEL, University of California, Berkeley — In magic angle twisted bilayer graphene (MATBG), interactions dominate over the kinetic energy, resulting in correlated insulating states and superconductivity whose origin remains a mystery. Here, using a combination of analytical arguments and numerical calculations we identify a family of candidate insulating ground states at charge neutrality and discuss how external perturbations such as the influence of the substrate or strain can alter the phase diagram.

Marginal Fermi liquid and dynamical symmetry breaking from Coulomb interaction in twisted bilayer graphene  JOSE GONZALEZ (Presenter), Instituto de Estructura de la Materia (CSIC), Spain, TOBIAS STAUBER, Instituto de Ciencia de Materiales de Madrid (CSIC), Spain — We investigate the effects of the strong Coulomb interaction near the magic angle of twisted bilayer graphene, focusing on the charge neutrality point and near half-filling of the highest valence band. In this latter instance, we predict the emergence of a marginal Fermi liquid, which can be traced back to the proximity to an extended van Hove singularity and the development of straight segments in the Fermi line. This leads to the linear scaling with energy of particle-hole excitations across the Fermi line, implying in turn the linear temperature dependence of the resistivity, logarithmic corrections to the heat capacity, and the consequent modification of the Wiedemann-Franz law. At the charge neutrality point, we show that the Coulomb interaction may be responsible for the opening of a gap through the condensation of particle-hole excitations about the Dirac nodes. We find in this case a direct competition between the dynamical breakdown of chiral symmetry (which prevails in the strong coupling regime) and the breakdown of time-reversal invariance (which has instead a stronger onset and leads to a Chern insulator phase at intermediate coupling).

Electrostatic gate-controlled fermi level dependent electronic band structure of graphene  RYAN MUZZIO (Presenter), Carnegie Mellon University, ALFRED JONES, Aarhus University, ROLAND KOCH, Advanced Light Source, DAVIDE CURCIO, DEEPNARAYAN BISWAS, JILL MIWA, PHILIP HOFMANN, Aarhus University, SIMRANJEET SINGH, Carnegie Mellon University, CHRIS JOZWIAK, ELI ROTENBERG, AARON BOSTWICK, Advanced Light Source, SØREN ULSTRUP, Aarhus University, JYOTI KATOCH, Carnegie Mellon University — The observation of electronic band structure in 2D material devices as they operate opens limitless opportunities to explore fundamental physics. The most robust technique to probe electronic structure is through angle-resolved photoemission spectroscopy (ARPES) and can now be used to investigate mesoscopic sized 2D materials and their heterostructures. Only being sensitive to filled states, ARPES measurements are restricted to states below the Fermi energy of the sample. Historically, chemical doping has been the preferred technique to manipulate the Fermi energy, but is difficult to control, introduces electronic states that are not intrinsic to the sample of interest, and can only be reversed through high-temperature annealing. Electrostatic doping, having none of these drawbacks, allows us to reversibly investigate the electron energy and momentum states of graphene far above the Dirac point. We will present our results on the electrostatic gate controlled electronic band structure of graphene using nanoARPES.
11:51AM B51.00004: Correlated states in magic angle twisted bilayer graphene under the optical conductivity scrutiny

*ELENA BASCONES (Presenter), MARÍA JOSÉ CALDERÓN, Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC — Moiré systems displaying flat bands have emerged as novel platforms to study correlated electron physics. There is evidence of correlation induced effects at the charge neutrality point (CNP) of twisted bilayer graphene which could originate from spontaneous symmetry breaking. We will show how optical conductivity measurements allow to distinguish different symmetry breaking states and to follow the evolution of the band distortions with doping. In the specific case of a nematic order, which breaks the discrete rotational symmetry of the lattice, we find that the Dirac cones tend to be displaced, not only in momentum space but also in energy, inducing a finite density of states and Drude weight at the CNP. The nematic order is revealed in a dc conductivity anisotropy with its sign depending on the degree of relaxation, the doping and the nature of the symmetry breaking.

*We acknowledge funding from Spanish Ministerio de Ciencia, Innovación y Universidades under Grant No. PGC2018-097018-B-I00

12:03PM B51.00005: Correlated states and tunable topological bands in twisted monolayer-bilayer graphene heterostructures

HRYHORIY POLSHYN (Presenter), University of California, Santa Barbara, JIHING ZHU, Department of Physics, The University of Texas at Austin, MANISH KUMAR, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute of Materials Science, Japan, ALLAN MACDONALD, Department of Physics, The University of Texas at Austin, ANDREA YOUNG, University of California, Santa Barbara — We experimentally investigate twisted van der Waals heterostructures of monolayer graphene rotated with respect to a bernal stacked graphene bilayer. We report transport measurements for devices with twist angles between 0.9 and 1.4°. The electric field allows efficient tuning of the width, isolation and the topology of the moiré bands in this system. By comparing magneto-resistance measurements to numerical simulations, we develop an understanding of the band structure. Finally, we observe correlated states at half- and quarter-fillings, which arise when narrow moire sublattice band is isolated by energy gaps from dispersive bands. We investigate the effects of in-plane and out-of-plane magnetic field on these states and discuss the implication for their spin- and valley- polarization.

12:15PM B51.00006: Hartree Fock study of insulating states in twisted bilayer graphene using hybrid Wannier basis

KASRA HEJAZI (Presenter), University of California, Santa Barbara, XIAO CHEN, University of Colorado Boulder, LEON BALENTS, University of California, Santa Barbara — In this work, the insulating behavior of twisted bilayer graphene and in particular the quantum anomalous Hall state has been studied; the effects of electron-electron interaction are taken into account by performing a Hartree-Fock analysis which is the standard approach for finding symmetry broken states. The model is truncated to the active relevant bands and the study is done using the basis of maximally localized Hybrid Wannier functions; this basis on the one hand respects important symmetries of the system, and on the other hand makes the interaction local at least in one direction. It also implies that the geometry of the system is that of a cylinder. Furthermore, by tuning the form/strength of the interaction, we are able to predict some other interesting phases which might potentially be found in the future.
12:27 PM B51.00007: Local electronic compressibility of magic angle twisted bilayer graphene* URI ZONDINER, ASAF ROZEN (Presenter), Weizmann Institute of Science, DANIEL RODAN, YUAN CAO, Massachusetts Inst of Tech-MIT, RAQUEL QUEIROZ, Weizmann Institute of Science, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute of Materials Science (NIMS), YUVAL OREG, Weizmann Institute of Science, FELIX VON OPPEN, Massachusetts Inst of Tech-MIT, ADY STERN, EREZ BERG, Weizmann Institute of Science, PABLO JARILLO-HERRERO, Massachusetts Inst of Tech-MIT, SHAHAL ILANI, Weizmann Institute of Science — Twisted bilayer graphene near the magic angle (MATBG) exhibits remarkably rich electron correlation physics, displaying insulating, magnetic, and superconducting phases. In this talk, we probe the local electronic compressibility of MATBG using a scanning single electron transistor. We find that when carriers are added into this system, they repeatedly refill the same bands, leading to a Dirac-like compressibility cascade near integer moiré fillings. Additionally, we present a clear compressibility asymmetry around the center of the conduction and valence bands, reflecting the evolution from low DOS at charge neutrality to high DOS at the band edges. A mean-field theory that includes this asymmetry reproduces the experimental results, and explains previous observations that were not yet fully understood. This cascade of Dirac revivals should thus serve as the starting point for understanding the unusual behavior in this system.

*We acknowledge support from the Helmsley Charitable Trust grant, the ISF (grant no. 712539), Sagol Weizmann-MIT Bridge program, and the ERC-Cog (See-1D-Qmatter, no. 647413)

12:39 PM B51.00008: Towards correlated electron states in trilayer-graphene Moiré band* KAN-TING TSAI (Presenter), XI ZHANG, University of Minnesota, ZIYAN ZHU, STEPHEN CARR, Harvard University, MITCHELL LUSKIN, University of Minnesota, PHILIP KIM, EFTHIMIOS KAXIRAS, Harvard University, KE WANG, University of Minnesota — The recent discovery of Moiré superconductivity in twisted-bilayer graphene (tBLG) and twisted-double bilayer-graphene (tDBG) systems [1][2][3] has generated a great amount of interest in the condensed matter community. Beyond this model system, this work focuses on studying a new Moiré platform based on the twisted trilayer-graphene. Preliminary magneto-transport measurements will be presented. Characterization of interlayer screening, band evolution with displacement field and Moiré periodicity will also be discussed.


*This research was supported by NSF DMREF 1922165 and the ARO MURI W911NF-14-0247.
12:51PM B51.00009: Band flattening in slightly twisted bilayers of Bravais networks
TOSHIKAZE KARIYADO (Presenter), Natl Inst for Materials Sci, ASHVIN VISHWANATH, Harvard University — Discovery of superconductivity in twisted bilayer graphene ignited the current intensive studies on stacked 2D materials with moire patterns, especially focusing on flat bands and associated correlated physics. Here, we demonstrate band flattening in twisted bilayers of generic but high symmetric 2D lattices, i.e., 2D Bravais networks [1]. We first show how symmetry of each network gives constraints on the effective potential governing low-energy physics in twisted bilayers. We further numerically demonstrate the band flattening due to the constrained potential using tight-binding models. From the generic theory, we can find an interesting possibility of anisotropic band flattening, in which quasi 1D band dispersion is generated from relatively isotropic original band dispersion. Rich physics is expected with the anisotropic band flattening, ranging from the valley dependent transport to the spin-orbital intertwined model in the strongly correlated limit.


1:03PM B51.00010: Twist disorder in twisted bilayer graphene
JUSTIN WILSON (Presenter), YIXING FU, Physics, Rutgers, SANKAR DAS SARMA, Physics, University of Maryland, JED PIXLEY, Physics, Rutgers — Recent experiments in twisted bilayer graphene have set off a flurry of work due to the observation of purportedly correlated phases at the so-called "magic-angle." The nearly pristine samples of graphene used in the experiment mainly have one significant source of disorder: the twist angle is not uniform throughout the sample. Current models in the literature are inadequate to fully capture this effect, so we introduce and study a new microscopic model in which the twist angle enters as a free parameter in real space. After benchmarking the results of the model with the continuum model, we simulate the effects of twist-angle disorder by constructing "patches" of uniform twist angle. We find that while the minibandwidth and gap are renormalized substantially, the Fermi velocity is not significantly altered. We discuss the implications of this for existing and ongoing experiments on twisted bilayer graphene.

1:15PM B51.00011: Higher-Order Topological Insulator in Twisted Bilayer Graphene
MOON JIP PARK (Presenter), Physics, KAIST, YOUNGKUK KIM, Sungkyunkwan University, GIL YOUNG CHO, Pohang University of Science and Technology, SUNGBIN LEE, Physics, KAIST — Higher-order topological insulators are newly proposed topological phases of matter, whose bulk topology manifests as localized modes at two-or higher-dimensional lower boundaries. In this work, we propose the twisted bilayer graphenes with large angles as higher-order topological insulators, hosting topological corner charges. At large commensurate angles, the intervalley scattering opens up the bulk gap and the corner states occur at half filling. Based on both first-principles calculations and analytic analysis, we show the striking results that the emergence of the corner states do not depend on the choice of the specific angles as long as the underlying symmetries are intact. Our results show that the twisted bilayer graphene can serve as a robust candidate material of two-dimensional higher-order topological insulator.

Topological flat bands without magic angles in massive twisted bilayer graphenes*

SRIVANI JAVAJI (Presenter), Department of Physics, University of Seoul, JIN-HUA SUN, Department of Physics, Ningbo University, JEIL JUNG, Department of Physics, University of Seoul — We show that in massive twisted bilayer graphenes, isolated nearly flat bands below a threshold bandwidth $W_c$ are expected for continuous small twist angles up to a critical $\theta_c$ depending on the flatness of the original bands and the interlayer coupling strength. The phase diagram of finite valley Chern numbers of the isolated moire bands expands with increasing difference between the sublattice selective interlayer tunneling parameters. The valley contrasting circular dichroism for interband optical transitions is constructive near 0° and destructive near 60° alignments and can be tuned through electric field and gate driven polarization of the mini-valleys. Combining massive Dirac materials with various intrinsic gaps, Fermi velocities, interlayer tunneling strengths suggest optimistic prospects of increasing $\theta_c$ and achieving correlated states with large $U/W$ effective interaction versus bandwidth ratios.

*This work was mainly supported by Samsung Science and Technology Foundation under project no. SSTF-BA1802-06, Korean NRF under grant number NRF-2016R1A2B4010105, the 2017 Research Fund of the University of Seoul, and NSFC (No. 11604166). This work was partly performed at the Aspen Center for Physics, which is supported by National Science Foundation grant PHY-1607611.

Attractive electron-electron interactions from internal screening in magic angle twisted bilayer graphene

ZACHARY GOODWIN (Presenter), ARASH A MOSTOFI, JOHANNES LISCHNER, Imperial College London — Twisted bilayer graphene (tBLG) has emerged as a new platform for studying electron correlations. tBLG exhibits correlated insulating and superconducting states at twist angles close to the largest magic angle, with the phase diagram resembling that of cuprates, which suggests an unconventional mechanism for superconductivity. We have studied the effect of internal screening on electron-electron interactions and Hubbard parameters in undoped tBLG, within the random phase approximation (RPA) and constrained RPA (cRPA). Near the magic angle, the flattening of bands drastically increases the RPA dielectric constant of tBLG and the abrupt change in the band velocity as function of the band energy gives rise to attractive regions in the RPA screened interaction in real space, which could be intimately connected to the reported correlated-insulator and superconducting phases. The cRPA polarizability was used to parametrize a twist-angle-dependent Keldysh model which exhibits a dramatic enhancement with decreasing twist angle, and to calculate the extended Hubbard parameters of a downfolded Hamiltonian. We find that the extended Hubbard parameters depend sensitively on the twist angle and the on-site Hubbard $U$ is not simply a linear function of twist angle.
1:51PM B51.00014: Twistorics in bilayer graphene and other systems

SUJAY RAY (Presenter), Indian Institute of Science — The discovery of twisted bilayer graphene initiated the idea that a novel platform with unprecedented tunability can be garnered with a simple relative twist between two layers. For graphene systems, this technology has generated a versatile system where flat band, superconductivity and magnetism are intertwined. We present our work on the theory of Wannier pair in twisted bilayer graphene. For comparisons, we also study graphene on boron-nitride (GBN) possessing a different Moire pattern, and single-layer graphene (SLG) without a Moire pattern. We will also present novel properties emanating from similar bi-layer systems.


*The work is supported by the Science and Engineering Research Board (SERB) of the Department of Science & Technology (DST), Govt. of India for the Start Up Research Grant (Young Scientist), and also benefited from the financial support from the Infosys Science foundation under Young investigator Award.

BS1.00015: Symmetry breaking states at commensurate fillings of the Moire bands of the twisted bilayer graphene

YI ZHANG (Presenter), Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, KUN JIANG, ZIQIANG WANG, Department of Physics, Boston College, FUCHUN ZHANG, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences — We study the twisted bilayer graphene system with the continuous model together with the long-range Coulomb interaction. Within the Hartree Fock approximation, we are able to find some symmetry breaking ground states at commensurate fillings of the Moire bands, which will gap out the Dirac points at the reduced Brillouin Zone that are otherwise protected by the symmetry.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B52 DCMP: Complex Oxide Films, Surfaces, and Interfaces I

High Ballroom 1E - Matthew Brahlek, Oak Ridge National Lab
**11:15AM B52.00001: Growth of the Transparent Correlated Metal SrVO$_3$**

LISHAI SHOHAM (Presenter), MARIA BASKIN, Andrew and Erna Viterbi Department of Electrical Engineering, Technion—Israel Institute of Technology, MYUNG-GEUN HAN, YIMEI ZHU, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, LIOR KORNBLUM, Andrew and Erna Viterbi Department of Electrical Engineering, Technion—Israel Institute of Technology —

The ongoing search for earth-abundant transparent conduction oxides (TCOs) has spread across a wide variety of research fields, highlighting the correlated metal SrVO$_3$ as a potential candidate. SrVO$_3$ displays high conductivity and transparency in the visible. Moreover, SrVO$_3$ is an attractive candidate for future electronics. A major hurdle for the synthesis of high quality SrVO$_3$ is to mitigate the formation of defects throughout the thin film. These defects can cause electron scattering and result in high resistivity and obscure some of the interesting physics. Film growth was done with molecular beam epitaxy (MBE), providing a scalable and industry-compatible fabrication process. In this work we present low defect SrVO$_3$ films with residual resistivity ratios exceeding 10 and room temperature resistivities in the order of 30 $\mu\Omega$ cm. Careful analysis of the structural and electronic properties of the SrVO$_3$ films paves the way towards further improvement of their quality and their implementation as TCO in optoelectronics and renewable energy devices.

*This work was funded by the Israeli Science Foundation (ISF Grant 375/17).*

**11:27AM B52.00002: Magnetic properties in strained PrVO$_3$ thin films**

WILFRID PRELLIER (Presenter), CRISMAT, CNRS — Transition metal oxides often having a perovskite structure form a wide and technologically important class of compounds. In these systems, ferroelectric, ferromagnetic, ferroelastic, or even orbital and charge orderings can develop and eventually coexist. These orderings can be tuned by external electric, magnetic, or stress field, and the cross-couplings between them enable important multifunctional properties, such as piezoelectricity, magneto-electricity, or magneto-elasticity. Here, a series of high quality epitaxial PrVO$_3$ (PVO) thin films were grown, by Pulsed Laser Deposition (PLD) technique, as a function of thickness on various substrates inducing different types of strains. Using a battery of techniques, I will show how the strains modify the magnetic properties and structural characteristics of the layers. At the end, I will propose a model based on dead layer to explain the data.

*Thanks to ANR, CNRS and Region Normandie*
Phase transformation by superoxygenation in cuprate and iridate thin films

CHAO C ZHANG (Presenter), HAO ZHANG, Department of Physics, University of Toronto, NICOLAS GAUQUELIN, SHAOBO CHENG, GIANLUIGI BOTTON, Canadian Centre for Electron Microscopy and Department of Materials Science and Engineering, McMaster University, CHRISTOPHER MCMAHON, DAVID GEOFFREY HAWTHORN, Department of Physics and Astronomy, University of Waterloo, PATRICK CLANCY, SAEHWAN CHUN, Department of Physics, University of Toronto, AMBROSE SEO, Department of Physics and Astronomy, University of Kentucky, YOUNG-JUNE KIM, JOHN Y.T. WEI, Department of Physics, University of Toronto — High-pressure O$_2$ has previously been used to hole-dope and stabilize high-oxidation phases of cuprates. We extend this superoxygenation technique to materials in thin film form since they are more reactive due to their large surface-to-volume ratio. YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) thin films grown by PLD are annealed in up to 700 atm O$_2$ and then characterized by TEM, XRD and XAS. The annealed films show phase conversion to Y$_2$Ba$_4$Cu$_7$O$_{15-\delta}$ and Y$_2$Ba$_4$Cu$_8$O$_{16}$, as well as regions well as regions of YBa$_2$Cu$_5$O$_{9-\delta}$ and YBa$_2$Cu$_6$O$_{10-\delta}$. Epitaxial thin films of Sr$_2$IrO$_4$ are subjected to extended high-pressure annealing and similarly characterized. The post-annealed films show up to 3 order-of-magnitude drop in room temperature resistivity and an evolution towards semi-metallic behaviour. Furthermore, as film thickness is reduced, the annealed films show a structural transformation towards a quasi-cubic phase. Our results demonstrate the potential of using superoxygenation to stabilize exotic phases of transition metal oxides not achievable in bulk form and to create novel materials by selectively transforming constituent layers in multilayer films. [1]


*Work supported by NSERC, CFI-OIT and the Canadian Institute for Advanced Research
**11:51AM B52.00004: Coupling lattice instabilities across the interface in ultrathin oxide heterostructures**

THIERRY VAN THIEL (Presenter), Delft University of Technology, JENNIFER FOWLIE, University of Geneva, CARMINE AUTIERI, MagTop, NICOLA MANCA, MAKARS SISKINS, DMYTRO AFANASIEV, Delft University of Technology, STEFANO GARIGLIO, University of Geneva, ANDREA CAVIGLIA, Delft University of Technology — The resistivity of ultrathin SrIrO3 films grown epitaxially on SrTiO3 displays an anomaly at the temperature corresponding to the cubic-tetragonal transition of the substrate. We investigate its origin through synchrotron X-ray diffraction measurements, electronic transport and ab-initio calculations. The effect is ascribed to a redistribution of orthorhombic structural domains, driven by the cubic-tetragonal transition of SrTiO3. The compressive strain induced by the substrate is found to force the in-phase octahedral rotation axis of the film to lie in-plane, giving rise to a twofold degenerate domain structure that couples to SrTiO3 tetragonal domains. Transport measurements in van der Pauw devices reveal that a strong anisotropy of the longitudinal resistivity develops below the transition temperature. The strong structure-property relationships in the iridates makes these compounds particularly suitable for static and dynamic coupling at interfaces, providing a promising route towards realizing novel functionalities in oxide heterostructures.

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Netherlands Organisation for Scientific Research (NWO/OCW) as part of the Frontiers of Nanoscience program (NanoFront) and VIDI program.

**12:03PM B52.00005: Structure of SrRuO3 films on SrTiO3 (001) in the ultrathin limit**

PRAHALD SIWAKOTI (Presenter), MOHAMMAD SAGHAYEZHIAN, ZHEN WANG, Louisiana State University, Baton Rouge, YIMEI ZHU, Department of Energy Science and Technology, Brookhaven National Laboratory, E WARD PLUMMER, JIANDI ZHANG, Louisiana State University, Baton Rouge — The observation of unconventional anomalous Hall effect in SrRuO3 films on SrTiO3 has been suggested as the signature for the existence of topologically non-trivial magnetic structures driven by Dzyaloshinskii – Moriya (DM) interaction [1,2]. However, experimental evidence for RuO6 distortion, which should be directly correlated with DM interaction, is far from clear. We have carried out a study on the evolution of lattice structure and its relation to the magneto-transport properties of SrRuO3 films with thickness in the ultra-thin limit (< 10 unit-cells) utilizing in-situ Low Energy Electron Diffraction, ex-situ High Resolution Scanning Transmission Electron Microscopy and transport measurements. We discuss the lattice distortion effect on the Dzyaloshinskii – Moriya interaction in the system.


*Supported by U.S.NSF under Grant No. DMR1608865
Electronic and lattice coupling in thin films of Nd$_{1-x}$La$_x$NiO$_3$*  JENNIFER FOWLIE (Presenter), BERNAT MUNDET, Univ of Geneva, ALEXANDRU BOGDAN GEORGESCU, Flatiron Institute, CLARIBEL DOMINGUEZ ORDONEZ, Univ of Geneva, MARTA GIBERT, Univ of Zurich, JEAN-MARC TRISCONE, Univ of Geneva — The solid solution Nd$_{1-x}$La$_x$NiO$_3$ spans a range of materials properties. From NdNiO$_3$ (x = 0), a low temperature antiferromagnetic insulator with monoclinic symmetry to LaNiO$_3$ (x = 1) a metallic paramagnet with rhombohedral symmetry [1]. Using an intermittent sputtering technique, we grow high quality epitaxial thin films of this solid solution on various substrates and, in this way, achieve an analog control of the composition. We report here of an unexpected discontinuous electronic behaviour - an abrupt change from an insulating to a metallic groundstate - and establish a connection to the symmetries of the system. Our work sheds light on a little-explored area of the rare earth nickelate phase diagram.


*This work was supported by the Swiss National Science Foundation through Division II. The research leading to these results has received funding from the European Research Council under the European Union’s Seventh Framework Program (FP7/2007-2013)/ERC Grant Agreement 319286 (Q-MAC).
12:27PM B52.00007: Co valence transformation in isopolar LaCoO$_3$ / LaTiO$_3$ perovskite heterostructures via interfacial engineering* GEORGIOS ARAIZI-KANOUTAS (Presenter), Van der Waals-Zeeman Institute for Experimental Physics, Institute of Physics, University of Amsterdam, JAAP GEESSINCK, MESA+ Institute, Faculty of Science and Technology, University of Twente, NICOLAS GAUQUELIN, Electron Microscopy for Materials Science, University of Antwerp, STEEF SMIT, XANTHE VERBEEK, SHRAWAN MISHRA, Van der Waals-Zeeman Institute for Experimental Physics, Institute of Physics, University of Amsterdam, PETER BENCOK, Diamond Light Source Ltd, Diamond House, Harwell Science & Innovation Campus, CHRISTOPH SCHLUETER, PETRA III, DESY Photon Science, TIEN-LIN LEE, Diamond Light Source Ltd, Diamond House, Harwell Science & Innovation Campus, DILEEP KRISHNAN, JO VERBEECK, Electron Microscopy for Materials Science, University of Antwerp, GUUS RIJNDERS, GERTJAN KOSTER, MESA+ Institute, Faculty of Science and Technology, University of Twente, MARK GOLDEN, Van der Waals-Zeeman Institute for Experimental Physics, Institute of Physics, University of Amsterdam — Charge transfer up to a single electron per interfacial unit cell across the non-polar heterointerface consisting of the Mott insulator LaTiO$_3$ and the charge-transfer insulator LaCoO$_3$ was studied in multi-layered films grown by PLD, using element-specific soft X-ray absorption, magnetic dichroism, TEM and hard X-ray photoemission spectroscopies.

We provide robust evidence of systematic and controllable conversion of trivalent to divalent cobalt that occurs within an interfacial region of three unit cells in LaCoO$_3$ as a direct result of the ensuing Fermi energy mismatch, without the presence of dopants or structural modification, in agreement with the theoretical prediction. Through the excellent control of the growth process, the average Co valence is tuned at the nanoscale via a proper choice of the number of LaTiO$_3$ | LaCoO$_3$ interfaces and the thickness of LaCoO$_3$. Notably, the insertion of an ultrathin LaAlO$_3$ ‘break’ layer interrupts the charge transfer, highlighting its interfacial nature.

Besides the strong enhancement of the magnetic polarizability due to formation of divalent Co, this technologically-relevant guiding principle illustrates the efficacy of O2p-band alignment for property design in oxide heterointerfaces.

*This research is part of the NWO research programme DESCO.
Long-range ordered domain walls in MBE-grown BiFeO$_3$ thin films and manipulation of their electrical properties

YONGJIAN TANG (Presenter), Department of Physics, Cornell University, ANTONIO B MEI, Department of Materials Science and Engineering, Cornell University, JÜRGEN SCHUBERT, Peter Grünberg Institute, SAHAR SAREMI, Department of Materials Science and Engineering, University of California, Berkeley, LUDI MIAO, Laboratory of Atomic and Solid State Physics, Cornell University, LANE WYATT MARTIN, Department of Materials Science and Engineering, University of California, Berkeley, DARRELL SCHLOM, DANIEL RALPH, Department of Materials Science and Engineering, Cornell University — Multiferroic BiFeO$_3$ thin films can allow electrical control of magnetism at room temperature and potentially magnetic control of electric polarization. We have investigated the use of adsorption-controlled molecular-beam epitaxy to grow BiFeO$_3$ thin films, as an alternative to the more commonly-used pulsed laser deposition or sputtering. We demonstrate unprecedentedly long-range domain periodicity of domain walls in commensurately strained BiFeO$_3$/SrRuO$_3$/DyScO$_3$(110)$_0$ epitaxial heterostructures. We observe two domain variants under piezoresponse force microscopy (PFM), which form alternating 140-nm-wide striped domains. Conductive AFM shows that the domain walls exhibit enhanced conductivity relative to the bulk and electrical rectification. For applications, ion irradiation can be used to reduce the through-film leakage without increasing the coercive field for ferroelectric switching. Doping with lanthanum is effective in reducing the strength of ferroelectric polarization, a necessary step to enable magnetic control of the polarization.

*This work was supported by the Semiconductor Research Corporation (SRC) as nCORE task No. 2758.003, NSF under the E2CDA (ECCS 1740286), MRI (Grant No. 1338010) programs and NSF MRSEC program (Grant No. DMR-1719875).
12:51PM B52.00009: Properties of the BiVO\(_4\) (010) surface in single crystals and epitaxially grown samples: A joint first-principles and experimental effort*  WENNIE WANG (Presenter), Pritzker School of Molecular Engineering, The University of Chicago, PATRICK STROHBEEN, Materials Science and Engineering, University of Wisconsin-Madison, DONGHO LEE, Department of Chemistry, University of Wisconsin-Madison, CHENYU ZHOU, Department of Chemical Engineering, Columbia University, JASON KAWASAKI, Materials Science and Engineering, University of Wisconsin-Madison, KYOUNG-SHIN CHOI, Department of Chemistry, University of Wisconsin-Madison, MINGZHAO LIU, Center for Functional Nanomaterials, Brookhaven National Laboratory, GIULIA GALLI, Pritzker School of Molecular Engineering, The University of Chicago — As a prototypical oxide for water photocatalysis, BiVO\(_4\) has many advantageous optoelectronic properties, including strong absorption in the visible and a favorable band alignment with water. However, its use as a photo-absorber is limited by its inefficient charge dynamics, especially at interfaces. Here, we present an integrated experimental and computational study aimed at an atomistic understanding of the surface morphology and electronic properties of BiVO\(_4\) as a function of oxygen vacancy concentration.

We carried out first-principles calculations with Quantum Espresso (www.quantum-espresso.org/) and XPS/UPS measurements to obtain work functions and band alignments with vacuum. We show that oxygen vacancies at the surface behave differently from their bulk counterpart, in terms of formation energy and transport of small polarons. We also compare single-crystalline and epitaxially-grown samples, with focus on the relation among oxygen vacancies, electronic structure, and growth techniques. Finally, based on a combined study of measured and STM microscopy images, we propose how varying surface termination may help tune the photoelectrochemical performance of BiVO\(_4\).

*This work was supported by the National Science Foundation (NSF) through grant CHE-1764399.

1:03PM B52.00010: Multi-level ionic conductivity in Ca-doped BiFeO\(_3\) thin films  JEONGHUN SUH (Presenter), JI SOO LIM, HEUNG-SIK PARK, CHAN-HO YANG, Department of Physics & Center for Lattice Defectronics, KAIST — Ca-doped bismuth ferrite is a promising material for studying collective ionic migration in solids [1]. We conduct impedance analysis with different magnitudes of AC voltage to understand the ionic conduction mechanism of this material. To suppress the electronic contribution to the conductivity, we annealed the sample in a reducing condition at elevated temperatures before the measurement. By using the mixed conductor equivalent circuit model [2], we obtain ionic conductivity, which shows a multi-level feature. This result shows consistency with the observation from electroforming experiments with DC voltages. This work provides useful insight into the ionic conduction mechanism in solids.
1:15PM B52.00011: Observation of anisotropic filamentary conduction pathways in Cadoped bismuth ferrite thin films  HEUNG-SIK PARK (Presenter), JI SOO LIM, JEONGHUN SUH, CHAN-HO YANG, Department of Physics & Center for Lattice Deflectronics, KAIST — Ionic migration is a key ingredient for applications such as oxide electrolytes and resistive switching memories. We investigate the evolution of the ionic conduction pathways based on optical contrast in an epitaxial Bi$_{0.7}$Ca$_{0.3}$FeO$_{3-\delta}$ thin film where oxygen vacancies are spontaneously produced.[1] We visualized electroforming processes in the hundreds-micron-scale material channels between coplanar electrodes with a constant electric bias at an elevated temperatures, systemically varying the channel orientation with respect to the crystal axis.[2] At the initial stage of electroforming, conducting filaments are created and propagate nearly along the crystal axes $<100>$, thereby making orthogonal self-similar networks. We also find that the filament-type ionic conduction is abruptly transformed to the bulk conduction around the time when the filament pathways connect both electrodes. These results offers useful insight into collective ionic migration in crystalline solids.


1:27PM B52.00012: Charge transport and distribution at the interfaces of SrTiO$_3$/LaAlO$_3$/SrTiO$_3$ (100) (STO/LAO/STO (100))  AKHILESH KUMAR SINGH, Inst of Physics Academia Sinica, C.P. SU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan, T.C. WU, M.C. CHEN, M.Y. SONG, Inst of Physics Academia Sinica, Y.C. LAI, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan, GUANG-YU GUO, Department of Physics, National Taiwan University, M.-W CHU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan, WEI-LI LEE (Presenter), Inst of Physics Academia Sinica — The existence of a quasi-2-dimensional hole gas (q2DHG) in STO/LAO/STO (100) has been revealed by several groups. In this report, the STO(6-uc)/LAO(t-uc)/STO (100) samples with $t = 5$ and $3$ were grown using oxide MBE technique. From magneto-transport measurements at low temperatures and difference gate voltages ($V_g$), a clear signature for the existence of q2DHG was uncovered from rigorous two band model fittings to magneto-conductance data. At $T = 2K$ and $V_g = +100V$, the sheet density for q2DHG is as large as $1.47 \times 10^{13}$ per cm$^2$. Intriguingly, both the sheet densities for q2DEG and q2DHG increase with increasing positive $V_g$, which supports for a spatially separated electron-hole bilayer at the interfaces [1]. On the other hand, STEM-EELS measurements with atomic scale resolution across the interfaces were performed. The suppressed q2DHG in STO/LAO/STO (100) in the ultra-thin LAO limit can be attributed to the depolarization field within the LAO layer, arising from the strain-field interference across the two closely-spaced interfaces [2]. In principle, q2DHG can emerge by compensating the depolarization field, which is achievable either by increasing the LAO thickness or by electrical gating. [1] Singh et al., PRM 2, 114009 (2018). [2] Su et al., PRM 3, 075003 (2019).
1:39PM B52.00013: Observation of polar domains in a relaxor La-substituted BiFeO$_3$ thin film  YOUNGKI YEO (Presenter), YONG-JIN KIM, MUJIN YOU, CHAN-HO YANG, Department of Physics & Center for Lattice Defectronics, KAIST — Relaxor ferroelectrics have been widely studied because of their unique physical properties including high permittivity, high piezoelectric effects, etc. The existence of polar nanoregions (PNRs) is believed to be responsible for relaxor behaviors [1]. However, there is a lack of studies on PNRs linked to the flexoelectric effect. In this work, we report the direct observation of PNRs within tetragonal BiFeO$_3$ near morphotropic phase boundaries (MPBs) which are expected to involve large strain gradient. Heavily La-substituted BiFeO$_3$ thin films (BLFO) grown on LaAlO$_3$ (001) have been employed to explore the PNRs with the aid of an angle-resolved lateral piezoresponse force microscopy [2]. BLFO has been thought to be isotropic monoclinic energies [3]. the flexoelectric effect on tetragonal BLFO near MPBs stabilizes various monoclinic phases. The frequency-dependent dielectric anomalies and diffuse x-ray scattering have been confirmed to identify that our system shows the typical relaxor behaviors. Our findings will offer valuable information to study the role of the flexoelectric effect on the formation of PNRs.

References

1:51PM B52.00014: The linear electro-optical effect in thin oxide films*  ALEXANDER DEMKOV, ALI HAMZE (Presenter), WENTE LI, THERESE PAOLETTA, KURT D FREDRICKSON, University of Texas at Austin — The linear electro-optical (EO) effect, also known as the Pockels effect, has been the subject of increasing interest due to its potential for use in silicon photonic applications. As such, it is necessary to find materials that have a strong EO response in thin film form, which is essential for low power and small footprint devices. In this talk we will discuss general design rules for developing strong Pockels materials inferred from first principles theory. We will discuss the Pockels effect in BaTiO$_3$, strained SrTiO$_3$, LiB$_3$O$_5$ (LBO) and CsB$_3$O$_5$ (CBO) and use these materials as prototypical examples of where conventional wisdom breaks down. We analyze how the EO response is related to the optical phonon frequencies, Raman susceptibility and mode polarization and elucidate the underlying physical phenomena behind the large Pockels effect.

*This work is supported by the Air Force Office of Scientific Research under Grant FA9550-18-1-0053.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B53 DCMP: Device engineering of 2D materials  Mile High Ballroom 1F -
Guangyi Chen, Peking University
11:15AM B53.00001: Optical Phase Transitions in 1T'-MoTe$_2$ from Thin Film Strain Engineering AHMAD AZIZIMANESH (Presenter), TARA PENA, ARFAN SEWAKET, STEPHEN M WU, Electrical and Computer Engineering, University of Rochester — MoTe$_2$ has been shown to have the ability to undergo a semimetallic to semiconducting phase transition induced by strain. In this work, we explore this phase change in 1T'-MoTe$_2$ through static strain induced by thin film stress capping layers, analogous to the ones used in industrial strained silicon processes. The optically transparent stressor film is chosen to be e-beam evaporated Al$_2$O$_3$/MgF$_2$/Al$_2$O$_3$. This film carries a controlled amount of tensile thin film stress depending on MgF$_2$ film thickness. Al$_2$O$_3$ is used as both an adhesion layer to MoTe$_2$, and as a protective capping layer for the MgF$_2$ from the environment. Significant optical contrast change in the few layered MoTe$_2$ flakes is observed after stressor film deposition, which is confirmed to be a phase change with Raman spectroscopy. Al$_2$O$_3$ capped control samples eliminate the possibility that this effect originates from defect formation during device fabrication process. Increasing thin film stress, changes the phase of a larger number of layers from the top of each MoTe$_2$ flake, resulting in thinner flakes to show larger proportional contrast change. Stress is a well-known technique to induce a phase change in MoTe$_2$ and potentially other 2D materials, which may lead to interesting applications in 2D electronics and optics.

11:27AM B53.00002: Versatile multiscale envelope function formalism to study electron transport in lateral transition-metal dichalcogenide heterostructures SATHWIK BHARADWAJ (Presenter), Department of Physics, Worcester Polytechnic Institute, Worcester, MA, ASHWIN RAMASUBRAMANIAM, Department of Mechanical & Industrial Engineering, University of Massachusetts, Amherst, MA, L RAMDAS RAM-MOHAN, Department of Physics, Worcester Polytechnic Institute, Worcester, MA — Accurate determination of carrier transport properties is critical to design high-performance optoelectronic devices and quantum information platforms. Although, first-principles calculations effectively determine the atomistic potentials associated with heterointerfaces, defects, and impurities, they are ineffective for direct modeling of carrier transport properties at length scales relevant to device applications. Here, we develop a multiscale formalism to investigate electron transport in two-dimensional (2D) materials. We integrate $k.p$ perturbation theory, informed from ab-initio electronic structure calculations, with a novel non-asymptotic quantum scattering theory using the method of sources and absorbers [1]. Our approach fully accounts for the crucial contributions of evanescent solutions that arise in multi-band scattering across heterointerfaces. We apply this method to study electron transport in lateral transition-metal dichalcogenide heterostructures, and discuss the implication of interface patterns on enhancing the thermoelectric power factor of the system. This new formalism provides a versatile variational description, first-principles-informed modeling of electron transport in 2D materials.

11:39AM B53.00003: Characteristics of the localization of massless pseudospin-1 Dirac particles in 2D in a short-range correlated random one-dimensional potential* SEULONG KIM (Presenter), KIHONG KIM, Ajou Univ — We study theoretically the characteristics of Anderson localization of two-dimensional massless pseudospin-1 Dirac particles in a correlated random one-dimensional potential. These potentials include both scalar and vector potentials. Using the invariant imbedding method, we calculate the localization length in a numerically precise manner and derive the analytical expressions for the localization length in strong and weak disorder limits. We investigate the dependencies of the localization length on incident angle, disorder correlation length, disorder strength, energy and average potential for the cases with random scalar and/or vector potentials. Disorder correlations affect the scaling dependencies of the localization length on the disorder strength and the particle energy. We explain these dependencies and the crossovers between different scaling regimes using the analytical formulas.

*This research was supported by the Basic Science Research Program through a National Research Foundation of Korea Grant (NRF-2019R1F1A1059024) funded by the Ministry of Education.

11:51AM B53.00004: Strong two-body correlations in WS$_2$ – MoSe$_2$ Heterojunction Tunnel Diodes JEDEDIAH KISTNER-MORRIS (Presenter), TREVOR ARP, NATHANIEL GABOR, University of California, Riverside — Owing to the strong Coulomb interaction between electrons and holes, electron tunneling between individual layers of a van der Waals heterostructure may give rise to highly unusual phenomena not observed in conventional materials. Here we report on optoelectronic transport of encapsulated WS$_2$ – MoSe$_2$ tunneling heterojunctions, in which we observe anomalous photoconductance and strong rectification. Using Multi-Parameter Dynamic Photoresponse Microscopy, we generate $\sim 10^X$ photocurrent images of the heterostructure photoresponse as a function of source-drain voltage, gate voltage, and temperature. Alongside strong rectifying behavior, we observe an anomalous reduction in the interlayer conductance that is tunable with gate voltage and temperature. This behavior becomes significantly enhanced with optical illumination, allowing us to assess the interactions of electrons and holes at the heterostructure interface. Our measurements indicate that strong two-body correlations arise precisely at the onset to a reduction in tunneling conductance, which we speculate is a signature of the crossover from free electron to bound interlayer exciton state.
12:03PM B53.00005: Transfer-print of graphene, boron nitride and gold patterns onto polymeric materials  EVGENIYA LOCK (Presenter), United States Naval Research Laboratory, GABRIELLA GONZALEZ-PASCUAL, University of Puerto Rico, DANIEL CHOI, National Research Council, SANDRA VILLANUEVA RODRIGUEZ, University of Puerto Rico, RAY AUYEUNG, HEUNGSOO KIM, United States Naval Research Laboratory, KARTHIK SRIDHARA, Texas A&M university, BORIS FEYLGELESON, United States Naval Research Laboratory — Two dimensional (2-D) materials such as graphene, hexagonal boron nitride (h-BN), black phosphorene (BP), molybdenum disulfide (MoS₂) have intriguing electrical, optical and chemical properties, which may enable next generation flexible sensors and photodetectors fabrication. However, placement of 2D materials on polymers to produce large scale 2D material/polymer heterostructures and the following metal deposition remains challenging. In this work, we show a multistep approach towards realization of 2D heterostructures on flexible substrates using a dry transfer-print approach based on differential adhesion. First, plasma treatment of the polymeric materials was performed. Then, organic molecular linker layer was attached for increased polymer adhesion. Then, the polymers and the 2D materials were placed in a nanoimprinter at specified conditions (pressure, temperature and time) and mechanically separated after print. Similarly, gold patterns were transferred to polymers. Optical, chemical, electrical and structural characterization of the samples before and after print was performed. Based on our results, we believe that our 2D material transfer-print approach will allow for large scale fabrication of the next generation 2D/flexible hybrid electronics devices.

12:15PM B53.00006: A Novel Type of Water Desalination Technology Using MoS2-Based Thin Films for Selective Ion Transport.  GABRIEL MARCUS (Presenter), Wake Forest Univ — Molybdenum disulfide (MoS₂) is a widely studied transition metal dichalcogenide with a range of potential applications including next-generation electronics, hydrogen evolution, and catalysis. It can also be used as a thermoelectric, exploiting the Seebeck effect to generate an electric voltage in response to a temperature gradient. Additionally, lithium intercalated MoS₂ is known to undergo a transition from the 1T to 2H phase. Together, these two properties make this material suitable as a novel desalination technology that relies on selective ion transport. To assess MoS²'s capabilities for ion transport, two types of experiments were conducted. The first set of experiments investigated changes in electric potential resulting from dropwise contact of various salt solutions with an MoS₂ membrane. Droplet test data displayed abrupt changes in electric potential followed by an exponential decay representing ion movement over time. A second set of experiments measured ion concentration changes over time using an MoS₂ film in contact with separated DI water and salt solutions. Significant changes in solution ion osmolarities were recorded after a duration of one week. Results are promising for future development of a thermoelectric desalination device.
**12:27PM B53.00007: Substrate-Induced Dynamical Anti-Screening of Excitons in Quasi-2D Materials: Renormalization of Quasiparticle and Optical Excitations***

CHIN SHEN ONG (Presenter), FELIPE H. DA JORNADA, DIANA QIU, STEVEN LOUIE, University of California, Berkeley — It is now well established that screening from substrates can strongly reduce the many-electron interactions in quasi-2D insulating materials, and renormalize both the quasiparticle bandgap and exciton binding energy in such systems. However, for metallic substrates, the frequency dependence of screening plays a paramount role that is often ignored. Here, we show that the frequency dependence of metallic substrate screening can induce a strong anti-screening effect in the quasi-2D insulator and lead to anomalously non-hydrogenic exciton energy levels, i.e., there are dramatic additional changes that go beyond the q-dependent static screening of quasi-2D materials. A systematic first-principles study of renormalizations by a wide range of experimentally motivated substrates is carried out, and our calculated results provide conceptual and quantitative explanation of experiments.

*This work was supported by NSF Grant No. DMR-1508412 and the DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.*

**12:39PM B53.00008: Hydrodynamic Anomalous Transport in Interacting Noncentrosymmetric Metals***

RIKI TOSHIO (Presenter), Department of Physics, Kyoto University, KAZUAKI TAKASAN, Department of Physics, University of California, Berkeley, NORIO KAWAKAMI, Department of Physics, Kyoto University — In high-conductive metals with sufficiently strong momentum-conserving scattering, the electron momentum is regarded as a long-lived quantity, whose dynamics can be described by an emergent hydrodynamic theory. In this work, we propose a hydrodynamic theory for noncentrosymmetric metals, where a novel class of electron fluids is realized by lowering crystal symmetries and the resulting geometrical effects. Starting from the Boltzmann equation, we introduce the effects of the Berry curvature to electron hydrodynamics and formulate a *generalized Euler equation* for noncentrosymmetric metals. We show that this equation reveals a variety of novel anomalous nonlocal/nonlinear transport phenomena; *chiral vortical effect, quantum nonlinear Hall effect, thermal-gradient induced anomalous Hall effect, etc.*, whose transport coefficients are described by geometrical quantities such as *Berry curvature dipole* [1]. Furthermore, we give a symmetry classification of these coefficients and compare the results with existing hydrodynamic materials. In the presentation, we would like to discuss what phenomena are predicted to be observed in experiments in noncentrosymmetric materials, including bilayer-graphene and transition metal dichalcogenides.

12:51 PM B53.00009: Engineering the electronic, thermoelectric, and excitonic properties of 2D group-III nitrides through alloying \((Al_{1-x}Ga_xN, Ga_{1-x}In_xN, B_{1-x}Al_xN)\)\(^*\)  

DANIEL WINES (Presenter), FATIH ERSAN, CAN ATACA, Univ of Maryland-Baltimore County — Recently, two-dimensional (2D) group-III nitride semiconductors such as h-AlN, h-BN, h-GaN, and h-InN have attracted attention due to their exceptional electronic, optical and thermoelectric properties. It has also been demonstrated, theoretically and experimentally, that properties of 2D materials can be controlled by alloying. In this study we performed density functional theory (DFT) calculations to investigate 2D \(Al_{1-x}Ga_xN\), \(Ga_{1-x}In_xN\), and \(B_{1-x}Al_xN\) alloyed structures. We also calculated the thermoelectric properties of these structures using Boltzmann transport theory based on DFT and the optical properties using the GW method and the Bethe Salpeter equation (BSE). Fundamental band gaps were also calculated with quantum Monte Carlo (QMC) methods for benchmarking purposes. We find that by changing the alloying concentration, the band gap and exciton binding energies of each structure can be tuned accordingly, and for certain concentrations, a high thermoelectric performance is reported with strong dependence on the effective mass of the given alloyed monolayer. With the ability to control such properties by alloying 2D group-III nitrides, this work presents new novel possibilities to engineer the electronic, optical and thermoelectric properties of 2D materials.

\(^*\)NSF DMR-1726213

1:03 PM B53.00010: Intrinsic gap and temperature collapse of the electric conductivity in bilayer graphene\(^*\)  

MOHAMMAD ZARENIA (Presenter), GIOVANNI VIGNALE, Univ of Missouri - Columbia — Recent experiments have reported signatures of electron-hole scattering in the electric conductivity of suspended bilayer graphene near charge neutrality. According to these experiments, plots of the electric conductivity as a function of \(\mu/k_B T\) (chemical potential scaled with temperature) obtained for different temperatures in the range of \(10K<T<50K\) collapse on a single curve independent of \(T\). This puzzling observation has been taken as an indication that the relevant scattering mechanism (besides electron-hole scattering) is not electron-impurity but electron-phonon scattering. Here we demonstrate that the collapse can be explained without invoking electron-phonon scattering by taking into account the fact that the suspended bilayer graphene is not a truly gapless system. In the presence of a small gap the intrinsic Coulomb resistivity acquires a temperature dependence that compensates for the temperature dependence of the impurity resistivity. Our theory produces excellent agreement with the observed conductivity collapse over the full reported range of temperatures, with a gap of 5 mev.

\(^*\)This work was supported by the U.S. Department of Energy (Office of Science) under grant No. DE-FG02-05ER46203.
1:15PM B53.00011: Negative Differential Resistance in MoS\textsubscript{2} Esaki Diodes\textsuperscript{*} ADAM BRUCE (Presenter), YUN-PENG WANG, SHUANGLONG LIU, HAI-PING CHENG, University of Florida — Two dimensional MoS\textsubscript{2} is a semiconducting system valued for its potential application as a programmable material. In addition to its direct bandgap in a single layer, an external electric field allows for interlayer band-to-band tunneling in bilayer configuration, which raises the prospect of applications in nanocircuitry. Using a first principles approach via DFT+NEGF, we probe the electronic properties of MoS\textsubscript{2} p-i-n junctions. We show both the IV characteristics of our junctions as well as the corresponding partial density of states at biases of interest. By comparing the band alignment of the electrodes and the transmission of our junction, we establish a criterion for band to band tunneling. Finally, we discuss mitigating edge effects on electronic structure and the possible applications of our p-i-n junctions.

\textsuperscript{*}Funding is provided by DOE BES under Contract No. DE-FG02-02ER45995. Additionally, computing resources are supplied by UFRC and NERSC.

1:27PM B53.00012: Electrochemical intercalation of organometallic molecules in HfS\textsubscript{2}-based van der Waals material\textsuperscript{*} CHINEDU EKUMA (Presenter), Department of Physics, Lehigh University, Bethlehem, PA 18015, SINA NAJMAEI, ADAM A WILSON, ASHER LEFF, MADAN DUBEY, Sensors and Electronic Devices, U.S. Army Research Laboratory, Adelphi, MD 20783 — van der Waals (vdW) materials designed with atomic layers of 2D-based materials exhibit a broad set of novel properties that are highly desirable for enabling heterogeneous device concepts such as neuromorphic and quantum computing. Because of their flexible electronic structure, both carrier dynamics and charge injection are easily tunable with chemical or electrical doping. Using a combined computation and experiment, we demonstrate the feasibility of intercalating electronically active organometallic molecules of two of the family of metallocene: cobaltocene and chromocene into the vdW gap of HfS\textsubscript{2}-based prototype vdW materials. We achieve high tunability of the electronic and vibrational properties of the hybrid material. Our findings demonstrate a unique approach, leveraging the flexible structural properties of layered materials to create an organic/inorganic interface that tunes and tailor the properties of host materials for distinctive device applications.

\textsuperscript{*}This work is supported by the U.S. Army Research Laboratory and Lehigh University Start-up fund.
Electronic States at Lateral Interfaces in Transition Metal Dichalcogenides

KAELYN FERRIS (Presenter), SERGIO E ULLOA, Physics & Astronomy, Ohio Univ —

Lateral heterostructures of two-dimensional crystals have received attention as defect free interfaces are increasingly grown in experiments. These interfaces show excitations unlike those at the original materials, suggesting the robustness of the interface. Tight binding and first principles calculations show that electronic states along the interface lie within the band gap of the bulk structure and provide a platform for possible use as high performance thermoelectric materials, spin-valley filters without the need for external gating, excitonic solar cells, and photocatalysis [1]. In this work, we explore the appearance of interfacial states in continuum models of such massive Dirac systems at low energy. We use k*p models to characterize lateral interfaces of various 2D materials and analyze the results of appropriate boundary conditions on various types of interfaces. This approach is able to describe midgap interface states that appear under mass or band inversion, as well as sign changes in effective curvature across the two materials. The states exhibit complex dispersion curves with strong spin-orbit effects, while being localized along the interface with different features in different materials.


Advanced atomistic models to accurately simulate graphitic nanostructures, bio-interfaces, and aromatic molecules*

KRISHAN KANHAIYA (Presenter), JORDAN WINETROUT, MICHEAL NATHANSON, HENDRIK HEINZ, University of Colorado, Boulder —

Graphene and carbon nanomaterials are used in biosensors, batteries, renewable composites, and functional materials. We introduce new atomistic models for the simulation of graphitic nanostructures, bio-interfaces, and aromatic molecules using common energy expressions (CHARMM, AMBER, CVFF, OPLS-AA, PCFF). The model contain virtual π-electrons in graphene/benzene ring that significantly increase the reliability of computed properties. Benchmarking of the new model shows improvements in the reproduction of cation-π interactions, π-π stacking, and electrolyte interfacial properties by ~10 fold. Two dummy electrons are attached to carbon atom to add the multipoles due to π-electrons in the aromatic rings. This leads to columbic interaction in accordance with experiment, which is missing in the old models. The models can accurately predict binding free energies, adsorption sites and biomolecular recognition, binding orientations, surface diffusion, and competitive adsorption of molecules. Details of the validation include agreement with experimental lattice parameters (<0.5% deviation), surface energy (<5% deviation), elastic constants (<15% deviation), hydration energy (10% deviation), water contact angles (<10% deviation) and cation-π interaction (<15% deviation).

*ARFL
Effects of hydrogen, oxygen, and hydroxyl adsorption on the electronic properties of transition metal dichalcogenides

GEORGIOS KOPIDAKIS (Presenter), DAPHNE DAVELOU, ARISTEA E MANIADAKI, IOANNIS N REMEDIAKIS, Univ of Crete — The unique properties of 2D transition metal dichalcogenides (TMDs) attract a lot of interest for optoelectronics, catalysis and energy related applications. Strain, environment, nanostructuring, affect TMD electronic properties and intensive efforts focus on their controlled modification. We present DFT calculations for the stability and electronic structure of semiconducting MX$_2$ (M=Mo, W and X=S, Se) monolayers and nanostructures with several concentrations of adsorbed hydrogen, oxygen, and hydroxyl and compare our results with pristine systems. The metallic character of the edge states [1] is preserved for all TMD nanoribbons examined, albeit Fermi level shifts that depend on the adsorbed atoms. Tuning electronic properties with strain [2] for improved TMD catalysts [3] is briefly discussed.


*We acknowledge support from the R.C. University of Crete (KA 10120).

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B54 DCMP: Fractional Excitations in the Quantum Hall Effect
Mile High Ballroom 2A
11:15AM B54.00001: Fermionic parity stability and interference measurements of non-Abelian e/4 and Abelian e/2 quasiparticle braiding at 7/2 and 5/2 filling factors* ROBERT WILLETT (Presenter), Nokia Bell Labs, KIRILL SHTENGEL, U.C. Riverside, CHETAN NAYAK, Microsoft, LOREN PFEIFFER, EDWIN CHUNG, K. W. BALDWIN, KENNETH WEST, Princeton University — The 5/2 state is expected to have Abelian charge e/2 quasiparticles and non-Abelian charge e/4 quasiparticles; past interference measurements are consistent with this [1]. Recent [2] interferometer experiments present 3 new findings: 1) at 5/2 four dominant resistance oscillation periods are observed at the expected values for the full complement of braids of non-Abelian e/4 and Abelian e/2: e/2 braiding e/2, e/4 braiding e/2, and modulated oscillations specifically attributable to non-Abelian e/4 braiding e/4, the even-odd effect. Parameters controlling expression of these oscillations are delineated. 2) at 7/2 this full complement of e/4 and e/2 braiding oscillations is also observed, but at different periods as expected for that filling factor. 3) most importantly, the oscillations attributable to non-Abelian e/4 even-odd effect are stable against fermionic parity fluctuations over long times (hours) near 5/2 and 7/2; this observed stability strengthens the case for using non-Abelian e/4 quasiparticles for topological quantum computation.


*P.U.: Moore Foundation - Grant GBMF4420, NSF - MRSEC Grant DMR 1420541 (E.C.).

11:27AM B54.00002: Non-Abelian braiding statistics via Aharonov–Bohm interferometry KIRILL SHTENGEL (Presenter), UC Riverside, ROBERT WILLETT, Nokia Bell Labs, CHETAN NAYAK, Microsoft Station Q, LOREN PFEIFFER, EDWIN CHUNG, Princeton University, MILTON PEABODY, Nokia Bell Labs, K. W. BALDWIN, KENNETH WEST, Princeton University — One of the most striking consequences of the non-Abelian braiding statistics in the ν=5/2 quantum Hall state has been the so-called even–odd effect theoretically predicted over a decade ago. While signatures consistent with the theoretical prediction have been seen in quantum Hall Fabry–Pérot interferometers, the key ingredient – controlling the number of quasiparticles inside the interferometer – remains a challenging experimental problem. Fortunately, signatures of the non-Abelian statistics can emerge in a simpler setting, namely in Aharonov–Bohm-type experiments where interference patterns are produced solely by changing the magnetic field. This nucleates new quasiparticles inside the interferometer, and if those include non-Abelian particles, the Aharonov–Bohm oscillations are expected to have distinct spectral features that would be absent otherwise. This talk will focus on the theoretical predictions and their comparison with the recent observations [1], arguing that the preponderance of experimental evidence unmistakably points towards the non-Abelian nature of ν=5/2 and 7/2 quantum Hall states and provides strong evidence of non-Abelian braiding.

11:39AM B54.00003: Contacts and Equilibration in the ν=5/2 Quantum Hall Effect* HAMED
ASASI (Presenter), MICHAEL C MULLIGAN, University of California, Riverside — The thermal Hall
conductance $K_T$ of the fractional quantum Hall state at $\nu=5/2$ has recently been measured to be
$K_T \approx 2.5(\pi^2 k_B^2 T/3h)[1]$. The half-integer value of this result provides strong evidence for the
presence of a Majorana edge mode and a corresponding quantum Hall state hosting quasiparticles with non-Abelian statistics. Whether this measurement points to the realization of the
PH-Pfaffian state or the anti-Pfaffian state has been the subject of debate [2][3]. Here we
consider various edge-state scenarios which may explain the measured thermal conductance,
paying close attention to the role of contacts and edge-state equilibration. Through a study of the
kinetic equations describing the low-temperature transport in the anti-Pfaffian and PH Pfaffian
dge states, we determine regimes of parameter space, controlling the interactions between the
different edge modes, that agree with experiment. We also discuss how point-contact tunneling
can distinguish various edge-state scenarios.


11:51AM B54.00004: Patterns in paired electron additions to fractional quantum Hall edge
states in large GaAs quantum dots* RAYMOND ASHOORI (Presenter), AHMET DEMIR, NEAL
EDWARD STALEY, SAMUEL ARONSON, SPENCER TOMARKEN, Massachusetts Institute of Technology
MIT, K. W. BALDWIN, KENNETH WEST, LOREN PFEIFFER, Electrical Engineering, Princeton University —
In vertical tunneling into a large and low disorder 2D GaAs quantum dot, we observe
electrons entering edge states and an unusual and unpredicted pair tunneling of electrons
into the dot’s quantum Hall edge states, with double-height capacitance peaks and a
coincident $h/2e$ periodicity in magnetic flux through the dot. Remarkably, results from
interferometry experiments[1] at similar Landau level filling fractions also show this $h/2e$
periodicity over the nearly the same filling factor range where it is observed in these dot
experiments. Thus, in increasing the magnetic field through the dot by one flux quantum,
we observe that 4 electrons are added to the edge (2 double height peaks). While we
observe such pairing everywhere in the filling factor range from $\nu = 2$ to $\nu = 5$, the $h/2e$
periodicity applies near filling factor 5/2. Away from 5/2, the double-height peaks are not
uniformly spaced in magnetic field but instead themselves group into pairs. Fourier
transforms of the data reveal different unusual periodicities other than $h/e$ and $h/2e$,
particularly in the tunneling rates for the peaks.


*Funded by BES Program of the Office of Science of the US DOE, contract no. FG02-08ER46514,
and the Gordon and Betty Moore Foundation, GBMF2931
12:03PM B54.00005: Flux superperiods and periodicity transitions in quantum Hall interferometers*  
BERND ROSENOW (Presenter), Univ Leipzig, ADY STERN, Department of Condensed Matter Physics, Weizmann Institute of Science — For strongly screened Coulomb interactions, quantum Hall interferometers can operate in a novel regime: the intrinsic energy gap can be larger than the charging energy, and addition of flux quanta can occur without adding quasi-particles. We show that flux superperiods are possible, and reconcile their appearance with the Byers-Yang theorem. We explain that the observation of anyonic statistical phases is possible by tuning to the transition from a regime with constant chemical potential to a regime with constant particle density, where a flux superperiod changes to a periodicity with one flux quantum at a critical magnetic field strength.

*B.R. acknowledges support from the Rosi and Max Varon Visiting Professorship at the Weizmann Institute of Science, and from DFG grant RO 2247/8-1.
A.S. was supported by CRC 183 of DFG, the Israel Science Foundation, and the European Research Council (Project LEGOTOP)

12:15PM B54.00006: Probing the photon-assisted processes of anyons of charge e/3 and e/5 in the FQHE regime*  
CHRISTIAN GLATTLI (Presenter), IMEN TAKTAK, PREDEN ROULLEAU, CEA-Saclay — Recently, the microwave excitation of fractional edge channels at GHz frequency f have demonstrated time domain manipulation of e*=e/3 and e*=e/5 charged anyons in the FQHE regime [1]. The signature of anyons absorbing a single photon was observed a shot noise singularity when the applied voltage obeying the fractional Josephson relation e*V=hf. Going beyond these observations we analyze the amplitude of the microwave field propagating from the excited contact to a Quantum Point Contact. Using photon-assisted current, the microwave amplitude is shown to display interference when sweeping the frequency from 2 to 18GHz. We attribute these interference features to different propagation velocities of neutral and charged electron (or anyon) modes when several integer or fractional edge propagates in parallel. This study provide the necessary information to realize single anyon sources similar to Leviton [2] sources.


*The French National Agency funding ANR-16-CE30-0015-02 FullyQuantum and the FET-OPEN # 862683 UltraFastNano are acknowledged
12:27PM B54.00007: Sublattice resolved spin wave transport through graphene fractional quantum Hall states as a probe of isospin order  
HAOXIN ZHOU (Presenter), HRYHORIY POLSHYN, Department of Physics, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, ANDREA YOUNG, Department of Physics, University of California, Santa Barbara — High quality graphene heterostructures host an array of fractional quantum Hall isospin ferromagnets with diverse spin and valley orders. While a variety of phase transitions have been observed, disentangling the isospin phase diagram of these states is hampered by the absence of direct probes of spin and valley order. I will describe nonlocal transport measurements based on launching spin waves from a gate defined lateral heterojunction, performed in ultra-clean Corbino geometry graphene devices. At high magnetic fields, we find that the spin-wave transport signal is detected in all FQH states between $\nu = 0$ and 1; however, between $\nu = 1$ and 2 only odd numerator FQH states show finite nonlocal transport, despite the identical ground state spin polarizations in odd- and even numerator states. The results reveal that the neutral spin-waves are both spin and sublattice polarized making them a sensitive probe of ground state sublattice structure. Armed with this understanding, we use nonlocal transport signal to a magnetic field tuned isospin phase transition, showing that the emergent even denominator state at $\nu = 1/2$ in monolayer graphene is indeed a multicomponent state featuring equal populations on each sublattice.

12:39PM B54.00008: Microscopic theory of fractional excitations in gapless bilayer quantum Hall states: semi-quantized quantum Hall states*  
OGUZ TURKER, TOBIAS MENG (Presenter), Tech Univ Dresden — Recent experiments in quantum Hall bilayer systems have revealed a new strongly correlated state: the semi-quantized quantum Hall state. This state arises in a bilayer quantum Hall system with strong interlayer-interactions, has a quantized Hall resistance and vanishing longitudinal resistance, while at the same time featuring a gapless sector that allows this state to exist for a continuum of filling factors. In this talk, I will explain what a semi-quantized quantum Hall state is, and use a coupled-wire construction to predict possible future experiments in the already existing experimental platforms.

*We acknowledge financial support from the DFG via the Emmy Noether Programme ME 4844/1-1, SFB 1143 (project-id 247310070), and the Wurzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter - ct.qmat (EXC 2147, project-id 39085490)
Non-linear transport and noise measurements in reentrant integer quantum Hall states*  JIAN SUN (Presenter), JIASEN NIU, International Center for Quantum Materials, Peking University, PENGJIE WANG, Department of Physics, Princeton University, YANG LIU, International Center for Quantum Materials, Peking University, LOREN PFEIFFER, KENNETH WEST, Department of Electrical Engineering, Princeton University, XI LIN, International Center for Quantum Materials, Peking University — Two-dimensional electron gas (2DEG) system in strong magnetic field is an ideal platform to explore interesting physics such as reentrant integer quantum Hall (RIQH) effect in second and higher Landau levels. We have carried out non-linear transport and noise measurements in ultra-high mobility GaAs/AlGaAs 2DEG to study RIQH states in Corbino-geometry samples. By increasing the DC bias gradually, we found the insulating phase of RIQH states disappeared, and the depinning trace can be divided into three regions according to different DC bias values. The narrow-band noise only appears in the middle region.

*The work was funded by NBRPC (2017YFA0303301), NSFC (11674009), Gordon and Betty Moore Foundation (GBMF4420), National Science Foundation (DMR-1420541) and Keck Foundation.

Edge Mode Engineering and Interferometry in the Quantum Hall Regime

RAJARSHI BHATTACHARYYA (Presenter), MORDEHAI HEIBLUM, DIANA MAHALU, VLADIMIR UMANSKY, Department of Condensed matter Physics, Weizmann Institute of Science — The interference of fractional charges is a much sought after goal in a variety of electronic interferometers. It has been shown before in an electronic Mach-Zehnder interferometer that neutral modes, topological or non-topological (via edge-reconstruction), cause dephasing in the fractional quantum Hall effect regime [1]. Recently interference of fractional charges has been observed in an electronic Fabry-Perot interferometer [2], though anionic statistics was not revealed. Here, we have adapted a novel route of engineering edge channels away from the physical boundary in order to minimize edge reconstruction. First, we show that these engineered edge channels, especially fractional ones, can have different edge structures (with a different thermal conductance) compared to ubiquitous edge channels that have the same electrical conductance. We then used a modified Mach-Zehnder interferometer to interfere such synthetic edge modes, with initial promising results.

1:15PM B54.00011: Paired Electron Additions to Fractional Quantum Hall Edge States in Large GaAs Quantum Dots*  SAMUEL ARONSON (Presenter), AHMET DEMIR, NEAL EDWARD STALEY, SPENCER TOMARKEN, Massachusetts Institute of Technology MIT, KENNETH WEST, K. W. BALDWIN, LOREN PFEIFFER, Electrical Engineering, Princeton University, RAYMOND ASHOORI, Massachusetts Institute of Technology MIT — We measure capacitance signals from additions of single electrons to a large (0.8 μm) 2D GaAs quantum dot and thereby determine the energies required to add electrons to the dot. The dot is sandwiched inside of a “tunnel capacitor” in which electrons can tunnel from the dot to a nearby capacitor electrode. We observe single electron capacitance peaks to edge states over a wide range of filling factors. As a function of magnetic flux through the dot, between filling factors ν = 1 and ν = 2, these edge state peaks are regularly spaced, with periodicity h/e. Surprisingly, over the range ν = 2 to ν = 5, the peaks have double-height, and the periodicity is halved to h/2e. The pairing cannot be explained in the Coulomb blockade picture, in which the two electrons in a pair would instead be separated by a charging energy, and models involving electron rearrangements fail because they predict a suppression of tunneling rates that we do not observe. Instead the sequence of successive paired tunneling events behaves in the same way as tunneling of electrons into superconducting quantum dots.

*Supported by the DOE Office of Science BES, FG02-08ER46514, and the Gordon and Betty Moore Foundation, GBMF2931. S. Aronson is supported by NSF Graduate Research Fellowship Program, Grant No. 1122374.

1:27PM B54.00012: Fabry-Perot interferometry of fractional quantum Hall edge states  JAMES NAKAMURA (Presenter), SAEED FALLAHI, HARSAD SAHASRABUDHE, SHUANG LIANG, GEOFF C GARDNER, MICHAEL MANFRA, Physics, Purdue University — Electronic interferometry has been proposed as an experimental probe of the braiding statistics and quasiparticle charge in quantum Hall states. Two significant challenges in Fabry-Perot interferometers are Coulomb charging effects and poor phase coherence. We have overcome these challenges using a novel GaAs/AlGaAs heterostructure which utilizes auxiliary GaAs screening wells in addition to the primary quantum well in order to screen and suppress Coulomb charging effects. This heterostructure design has enabled measurements of robust Aharonov-Bohm interfere at the ν = 1/3 fractional quantum Hall state. A recent theoretical work has predicted a shift in the interference pattern at ν = 1/3 when the magnetic field is varied from the center of the plateau. We present experimental measurements of Aharonov-Bohm interference across the 1/3 plateau. These results represent progress towards direct observation of anyonic braiding statistics.
1:39PM B54.00013: Phase Diagram of Majorana Island

JIE SHEN (Presenter), Delft University of Technology, GEORG WOLFGANG WINKLER, Microsoft Station Q, University of California Santa Barbara, FRANCESCO BORSOI, Delft University of Technology, SEBASTIAN HEEDT, Microsoft Quantum Lab Delft, VUKAN LEVAJAC, Delft University of Technology, SASA GAZIBEGOVIC, ROY OP HET VELD, Eindhoven University of Technology, JOON SUE LEE, MIHIR PENDHARKAR, CONNOR DEMPSEY, CHRIS PALMSTROM, University of California Santa Barbara, ERIK P.A.M. BAKKERS, Eindhoven University of Technology, BERNARD VAN HECK, LEO P. KOUWENHOVEN, Microsoft Quantum Lab Delft — Scalable topological qubit proposals based on semiconductor-superconductor systems are built on Majorana islands hosting pairs of Majorana zero modes. Here, by systematically measuring the periodicity of Coulomb blockade oscillations of InSb/Al island, we reconstruct the ground state parity of the island over large ranges of magnetic field and plunger gate voltage (Vpg). The resulting phase diagram can be divided into three regimes compared with numerical simulations. For negative Vpg, sub-gap states are absent due to strong proximity effect, so the 2e to 1e-periodic transition happens at high B-fields, indicating the poisoning of the superconducting state. For positive Vpg, the 2e-1e transition happens instead at a constant but small B-field. The reason is un-proximitized states quickly disperse below the charging energy due to the orbital effect of the magnetic field. The two regimes are separated by an intermediate regime where the 2e-1e transition field varies smoothly with Vpg, which is the most promising for locating a robust topological phase according to simulations. In this regime, we observe correlated oscillating peak spacing and heights. This complete phase diagram of Majorana island can lead to a guideline to set up a topological qubit in more complicated devices.

1:51PM B54.00014: Wigner Crystal Melting Phase Diagram of GaAs Two-dimensional Holes

MENG MA (Presenter), KEVIN VILLEGAS ROSALES, HAO DENG, LOREN PFEIFFER, KENNETH WEST, K. W. BALDWIN, MANSOUR SHAYEGAN, Princeton University — In a strongly interacting two-dimensional (2D) electron system, when the Coulomb energy dominates over the kinetic energy, the electrons tend to arrange periodically and form a so-called Wigner crystal (WC) ground state. In a GaAs 2D electron system, a magnetic-field-induced quantum WC forms at very low temperature and high magnetic field near filling factor $v = 1/5$ when the kinetic (Fermi) energy is quenched and the Coulomb energy dominates. In an GaAs 2D hole system, on the other hand, the WC phase forms near $v = 1/3$ because of the significant Landau level mixing caused by the large hole effective mass. Despite the fact that the 2D hole system has been a subject of intense interest for many years, a WC melting temperature vs filling factor phase diagram has been missing. In this work, we map out such phase diagram using a newly developed technique which probes the melting of the WC via its screening efficiency. The phase diagram shows rich features of the WC phases at low fillings and a clear reentrant behavior around $v = 1/3$.

*Supported by the DOE BES (DE-FG02-00-ER45841) for measurements, and the NSF (DMR 1709076, ECCS 1906253, and MRSEC DMR 1420541), and the Gordon and Betty Moore Foundation (GBMF4420) for sample fabrication and characterization.

Monday, March 2, 2020 11:15 AM - 2:15 PM
**Session B55 DCMP: Dirac and Weyl semimetals: Experiment** Mile High

**11:15AM B55.00001: Transport properties of topological semimetal candidate ReSbTe (Re = Sm, Nd, Pr)**

RABINDRA BASNET (Presenter), KRISHNA PANDEY, AARON WEGNER, JIN HU, Univ of Arkansas-Fayetteville — The breakthrough in the discovery of topological semimetals provides opportunities to explore the exotic properties of relativistic fermions in condensed matter. Recently, the nonsymmorphic compound ReSbTe (Re = rare earth) has attracted interested owing to its non-trivial topological electronic state. Here we present the magnetic transport properties of these topological semimetal candidates that uncovers it's electronic and magnetic properties. The coupling of magnetism and electronic properties, plus the variation of magnetism for different rare earth compound, make this material family a tunable platform for investigating topological fermion physics and for further exploration of electronic and spintronic science and applications.

*We acknowledge support from DoE award DE-SC0019467*

**11:27AM B55.00002: Anomalous Hall effect in epitaxial WTe$_2$/VTe$_2$ heterostructures**

JASON TRAN (Presenter), JUNXUE LI, JING SHI, PENG WEI, Department of Physics and Astronomy, University of California, Riverside — The Td (orthorhombic) phase of WTe$_2$, a transition metal dichalcogenide (TMD), is a type-II Weyl semimetal (WSM) when a few monolayer thick. Topological semimetals with broken time-reversal symmetry have recently garnered attention due to the ability to manipulate Weyl nodes, causing interesting electro-magnetic responses. Realizing a magnetic WSM in the thin film form, however, is challenging. In this talk, we present our studies on the magnetic properties of WTe$_2$/VTe$_2$ thin film heterostructures. Using molecular beam epitaxy, we grow WTe$_2$ in its Td phase confirmed by in situ reflection high energy electron diffraction. Ultra-smooth film showing atomic terraces and Raman spectroscopy confirm film quality. We perform systematic transport measurements on WTe$_2$/VTe$_2$ heterostructures with vanadium doping to form (W$_{1-x}$V$_x$)Te$_2$, varying x from 0% to 20%. V-doping also changes the Fermi level in WTe$_2$ and induces a carrier type change. An anomalous Hall effect (AHE) signal is observed, whose magnitude varies with the doping level, reaching a minimum near the charge compensation point. The sign of AHE does not change with carrier type. The origin of the AHE will be discussed.

*Acknowledgement: Spins and Heat in Nanoscale Electronic Systems (SHINES), the DOE-EFRC center under Award # SC0012670.*
Surface chiral metal in the bulk half-integer quantum Hall effect of BaMnSb$_2$* Jinyu Liu, Tulane Univ, Jabin Yu, Pennsylvania State University, Jinliang Ning, Tulane Univ, Leixin Miao, Lujin Min, Kleyser E Agueda Lopez, Yanglin Zhu, Hemian Yi, Timothy Pillsbury, Pennsylvania State University, Yubo Zhang, Tulane Univ, Yubu Wang, Pennsylvania State University, Jin Hu, University of Arkansas, Huiibo Cao, Oak Ridge National Laboratory, Fedor Balakirev, Franziska Weickert, Marcelo Jaime, Los Alamos National Laboratory, Kun Yang, National High Magnetic Field Laboratory, Jianwei Sun, Tulane Univ, Nasim Alem, Venkatraman Gopalan, Cui-Zu Chang, Nitin Samarth, Chaoxing Liu, Pennsylvania State University, Ross McDonald, Los Alamos National Laboratory, Zhiqiang Mao (Presenter), Pennsylvania State University

The study of Quantum Hall effect (QHE) in two-dimensional (2D) systems such as 2D electron gas and graphene has led to important breakthroughs in the development of many new concepts in modern physics. Although the QHE is not generally expected for bulk materials due to the band dispersion along the magnetic field direction, bulk QHE has been observed in a few materials such as Cd$_3$As$_2$ (1), ZrTe$_5$ (2) and EuMnBi$_2$ (3). In this talk, we report a unique bulk half-integer QHE observed in a layered Dirac semimetal BaMnSb$_2$.

In the extreme quantum limit, its quantum Hall state is accompanied by two-dimensional chiral metal at the surface, which represents a novel quantum liquid, never observed in any other bulk single crystal materials [4]. This finding establishes a promising experimental platform which not only provides access to 3D interacting topological states, but also offers opportunities to investigate the novel physics of 2D chiral metal.

References:
4. J.Y. Liu et al., arXiv:1907.06318

*This work was supported by the US Department of Energy under grants DE-SC0019068 and DE-SC0014208
11:51AM B55.00004: Towards Weyltronics: Realization of epitaxial NbP and TaP Weyl Semimetal thin films  AMILCAR BEDOYA PINTO (Presenter), AVANINDRA PANDEYA, DEFA LIU, HAKAN DENIZ, KAI CHANG, HENGXIN TAN, HYEON HAN, JAGANNATH JENA, ILYA KOSTANOVSKIY, STUART PARKIN, Max Planck Inst Microstructure — Weyl Semimetals (WSMs), a recently discovered topological state of matter, exhibit an electronic structure governed by linear band dispersions and degeneracy (Weyl) points leading to rich physical phenomena, which are yet to be exploited in thin film devices. While WSMs were established in the monopnictide compound family several years ago, the growth of thin films has remained a challenge. Here, we report the growth of epitaxial thin films of NbP and TaP by means of molecular beam epitaxy. Single crystalline films are grown on MgO (001) substrates using thin Nb (Ta) buffer layers, and are found to be tensile strained (1%) and with slightly P-rich stoichiometry with respect to the bulk crystals. The resulting electronic structure exhibits topological surface states characteristic of a P-terminated surface and linear dispersion bands in agreement with the calculated band structure, along with a Fermi-level shift of -0.2 eV with respect to the Weyl points. The growth of epitaxial thin films opens up the use of strain and controlled doping to access and tune the electronic structure of Weyl Semimetals on demand, paving the way for the rational design and fabrication of electronic devices ruled by topology.

12:03PM B55.00005: Experimental electronic structure of the switchable, topological, antiferromagnet CuMnAs  ANDREW LINN (Presenter), KYLE GORDON, PEIPEI HAO, BRYAN BERGGREN, University of Colorado, Boulder, SONKA REIMERS, University of Nottingham, NATHANIEL SPEISER, DUSHYANT NARAYAN, University of Colorado, Boulder, LIBOR SMEJKAL, Johannes Gutenberg-Universität Mainz, TOMAS JUNGWIRTH, PETER WADLEY, University of Nottingham, DANIEL STEPHEN DESSAU, University of Colorado, Boulder — Electrical switching and read out of the AFM Néel vector orientation in tetragonal CuMnAs has been experimentally demonstrated to be scalable to THz speeds, far exceeding speeds in state-of-the-art memory devices today. Additionally, CuMnAs is predicted to host two Dirac points protected by a nonsymorphic, glide mirror plane symmetry, which may or may not exist depending on the orientation of the Néel vector, offering the possibility of opening and closing a gap at the Dirac point at THz speeds. Until now, we lacked experimental confirmation of the predicted electronic band structure, but here we report the electronic structure of tetragonal CuMnAs experimentally measured with ARPES, which we compare to DFT. We performed experiments on the (001) surface of tetragonal CuMnAs thin films, measuring Fermi surfaces, kz dispersion, and high symmetry cuts.
12:15PM B55.00006: Temperature dependent infrared spectroscopy of PrAlSi* CATALIN MARTIN (Presenter), AASHISH POUDEL, IHOR SYDORYK, Ramapo College of NJ, Mahwah NJ, 07430, RODICA M MARTIN, Montclair State University, Montclair NJ, 07043, HALYNA HODOVANETS, HYUNSOO KIM, JOHNPIERRE PAGLIONE, Maryland Quantum Materials Center, Department of Physics, University of Maryland-College Park, College Park, Maryland 20742 — PrAlSi has been shown recently to provide a new platform for studying Weyl fermions and related effects, such as the anomalous Hall effect. In order to better understand the electronic and magnetic properties of its ground state, we performed temperature dependent optical reflectance measurements of single crystals of PrAlSi. The reflectance was measured between 80 cm\textsuperscript{-1} to 50,000 cm\textsuperscript{-1}, at temperatures between 300 K and 5 K. The Drude peak sharpens with decreasing temperature, consistent with metallic behavior and in good agreement with dc resistivity measurements. From Kramers-Kronig analysis, we obtained various optical functions and here we focus in particular on the evolution of the spectral weight with temperature and energy in PrAlSi.

*This work is supported by the National Science Foundation through grant No. 1625882.

12:27PM B55.00007: Planar Hall Effect in the Magnetic Weyl Semimetal Co\textsubscript{3}Sn\textsubscript{2}S\textsubscript{2}† SHAMA MONGA (Presenter), RADHE GOPAL, YOGESH SINGH, IISER Mohali — We have done the detailed magneto-transport study on single crystals of magnetic Weyl Semimetal Co\textsubscript{3}Sn\textsubscript{2}S\textsubscript{2}. Recently Liu et al. (Nat. Phys. 14, 1125 (2018)) have observed large anomalous Hall Effect and chiral anomaly in this material which has been suggested to be related to the large berry curvature between the Weyl points. Another effect that is expected to result from the topological band structure of magnetic Weyl materials is the Planar Hall Effect (PHE). We observed this intrinsic effect in single crystals of Co\textsubscript{3}Sn\textsubscript{2}S\textsubscript{2}. Crucially, the PHE is observed for temperatures T < 74 K which is much smaller than the ferromagnetic ordering temperature T\textsubscript{C} = 175 K indicating non-magnetic origin. Furthermore, we found the large anomalous Hall conductivity, which supports the Topological character of Co\textsubscript{3}Sn\textsubscript{2}S\textsubscript{2}. Additionally, we have probed PHE and anomalous Hall conductivity in this Weyl semimetal as a function of the location of the chemical potential with respect to the Weyl nodes.

†We acknowledge the use of the x-ray and SEM facilities at IISER Mohali. We thank Dr. Suvankar Chakraverty from INST, Mohali for the use of his PPMS for some of our measurements.
12:39PM B55.00008: Giant magneto-optical effect in the magnetic Weyl semimetal \(\text{Co}_3\text{Sn}_2\text{S}_2\)

YOSHIHIRO OKAMURA (Presenter), JO MURAMOTO, Univ of Tokyo, SUSUMU MINAMI, Kanazawa University, YOSHIHIRO KATO, YUKAKO FUJISHIRO, Univ of Tokyo, YOSHIO KANEKO, RIKEN CEMS, RYOMA KANEKO, KENTARO UEDA, Univ of Tokyo, VILMOS KOCSIS, RIKEN CEMS, NAOYA KANAZAWA, Univ of Tokyo, YASUJIRO TAGUCHI, RIKEN CEMS, TAKASHI KORETSUME, Tohoku University, RYOTARO ARITA, Univ of Tokyo, YOSHINORI TOKURA, RIKEN CEMS, YOUTAROU TAKAHASHI, Univ of Tokyo — The search for the topological materials has rapidly developed and novel phase of matter has been extensively proposed in recent years. In particular, the discovery of the Weyl semimetal (WSM), which has a pair of the Wey points with intense Berry curvature, is the important advance in this field. While the WSM shows various giant/functional electromagnetic phenomena such as the nonlinear optical effects and anomalous Hall effect (AHE), the direct evidence that the Weyl point plays the decisive role for those phenomena is still lacking. In this presentation, we will report the magneto-optical study on the recently discovered magnetic WSM \(\text{Co}_3\text{Sn}_2\text{S}_2\) with the giant AHE. The magneto-optical Kerr effect (MOKE) and first-principles calculations reveal that the optical Hall conductivity spectra are significantly dominated by the interband transition upon the nodal ring structures and the Weyl points. This observation demonstrates that those electronic structures play the decisive roles for the giant intrinsic AHE. We will also discuss the MOKE, which is exceptionally large compared with the conventional ferromagnetic metals.

12:51PM B55.00009: Extreme Electron-Phonon Coupling in a New Weyl Semimetal

VINCENT PLISSON (Presenter), KEN BURCH, FAZEL TAFTI, Boston College — Weyl semimetals are topological systems that have generated considerable interest due to their transport properties. One of the mechanisms that may play an important role in the manifestation of these transport properties is electron-phonon coupling. Previous optical experiments done on various Weyl semimetals have already shown phonon linewidths deviating from the usual model of anharmonic decay. Here we report on Raman measurements performed on a new Weyl semimetal. Careful analysis reveals the lifetime is consistent with electron-phonon coupling far in excess of the anharmonic decay channels.
Doping induced topological phase transition in WTe2*  

ANTONIO ROSSI (Presenter), GIACOMO RESTA, Physics, University of California, Davis, SENG HUAT LEE, RONALD REDWING, MRI, Penn State University, CHRIS JOZWIAK, AARON BOSTWICK, ELI ROTENBERG, ALS, Lawrence Berkeley National Lab, SERGEY SAVRASOV, INNA VISHIK, Physics, University of California, Davis — WTe2 exhibits diverse phenomena including non-saturating magnetoresistance in its bulk with predicted type-II Weyl semimetal electronic structure, superconductivity under hydrostatic pressure, quantum spin hall insulator (QSHI) in its monolayer limit, and superconductivity in the gated monolayer. In many of these transformations, the tuning of the carrier density plays an important role. We report two non-monotonic changes in the electronic structure of WTe2 upon in-situ electron doping, realizing occupation near the chemical potential as a pathway for tuning structure and behavior of 2D materials. The first phase transition is understood in terms of the extra charge inducing a shear mode that triggers the recombination of the Weyl points, lifting the topological nature of the bands. This topological switching behavior is relevant for gate-controlled topological transistors or for producing lateral interfaces within a single material host via differential doping. The second phase transition is most consistent with a electrons in a 2D K-overlayer hybridizing with the WTe2 host, broadly relevant to understanding interactions with metallic contacts in devices constructed from 2D materials.

*UC Davis

Electronic Correlations in Nodal-line Semimetals  

YINMING SHAO (Presenter), Columbia University, ALEXANDER N. RUDENKO, Wuhan University, JIN HU, University of Arkansas, ZHIYUAN SUN, Columbia University, YANGLIN ZHU, Pennsylvania State University, SEONGPHILL MOON, National High Magnetic Field Laboratory, ANDREW MILLIS, Columbia University, SHENGJUN YUAN, Wuhan University, ALEXANDER I. LICHTENSTEIN, University of Hamburg, DMITRY SMIRNOV, National High Magnetic Field Laboratory, ZHIQIANG MAO, Pennsylvania State University, MIKHAIL KATSNELSON, Radboud University, DMITRI BASOV, Columbia University — Dirac fermions with highly-dispersive linear bands are usually considered weakly correlated, due to relatively large bandwidths (W) compared to Coulomb interactions (U). With the discovery of nodal-line semimetals, the notion of Dirac point has been extended to lines and loops in the momentum space. The anisotropy associated with nodal-line structure gives rise to greatly reduced kinetic energy along the line. However, experimental evidence for anticipated enhanced correlations in nodal-line semimetals is sparse. Here we report on prominent correlation effects in a nodal-line semimetal compound ZrSiSe through a combination of optical spectroscopy and density-functional-theory calculations. We observed two fundamental spectroscopic hallmarks of electronic correlations: strong reduction (1/3) of the free carrier Drude weight and of the Fermi velocity compared to predictions of density functional band theory. The renormalization of Fermi velocity can be further controlled with external magnetic field. ZrSiSe therefore offers the rare opportunity to investigate correlation-driven physics in a Dirac system.
Correlated Dirac Semimetal State with Highly Mobile Electrons in Perovskite $\text{CaIrO}_3$

RINSUKE YAMADA (Presenter), University of Tokyo, JUN FUJIOKA, University of Tsukuba, MINORU KAWAMURA, SHIRO SAKAI, MOTOAKI HIRAYAMA, RIKEN Center for Emergent Matter Science, RYOTARO ARITA, TATSUYA OKAWA, University of Tokyo, DAISUKE HASHIZUME, MANABU HOSHINO, YOSHINORI TOKURA, RIKEN Center for Emergent Matter Science — The interplay between electron correlation and quantum topology of Dirac electrons have been a subject of great interest. The perovskite $\text{AlIrO}_3$ ($A=$Ca, Sr, Ba) is a candidate of Dirac semimetal with the sufficiently strong correlation on the verge of Mott transition[1]. Although the Dirac band dispersion has been observed by the angle resolved photoemission spectroscopy[2], the quantum transport originating from highly mobile Dirac fermions has been rarely observed in this class of strongly correlated topological semimetals.

In this study, we report the unique quantum transport phenomena of correlated Dirac electrons in perovskite $\text{CaIrO}_3$ with the Mott criticality[3]. We found that the electron mobility exceeds 60,000 cm$^2$/Vs and the giant magnetoresistance emerges in the quantum limit of the Dirac electrons. Combined with ab-initio calculations, we conclude that the interplay between electron correlation and spin-orbit interaction causes the remarkable proximity of Dirac node to the Fermi energy, yielding the highly mobile electrons. In the presentation, the origin of the giant magnetoresistance will also be discussed.


Unraveling the Topological Phase of ZrTe$_5$ via Magneto-infrared Spectroscopy*

YUXUAN JIANG (Presenter), Natl High Magnetic Field Lab, JINGYUE WANG, School of Physics, Peking University, TIANHAO ZHAO, ZHILING DUN, School of Physics, Georgia Institute of Technology, QING HUANG, Department of Physics and Astronomy, University of Tennessee, Knoxville, XIAOSONG WU, School of Physics, Peking University, MARTIN MOURIGAL, School of Physics, Georgia Institute of Technology, HAIDONG ZHOU, Department of Physics and Astronomy, University of Tennessee, Knoxville, MYKHAYLO OZEROV, DMITRY SMIRNOV, Natl High Magnetic Field Lab, ZHIGANG JIANG, School of Physics, Georgia Institute of Technology — We have systematically studied the 3D band structure of ZrTe$_5$ up to its parabolic band components using magneto-infrared spectroscopy. By comparing the Landau level transitions in different magnetic field orientations, we find that the band velocities are highly anisotropic and the dominant contribution along the layer stacking direction is parabolic with a record-low band velocity. More interestingly, with such a low band velocity, we have both theoretically and experimentally demonstrated that the band inversion can lead to a second extremum (band gap), allowing for a direct probe of the material’s topological nature. Our work not only provides an alternative way to identify the band inversion in 3D layered topological materials, but also yields important implications for understanding the exotic behavior of ZrTe$_5$ as well as that in similar (layered) materials.

*The work at NHMFL was supported by the NSF Cooperative Agreement No. DMR-1644779 and the State of Florida, and DoE-BES DE-FG02-07ER46451.
1:51PM B55.00014: Observation of fractional states in the three-dimensional quantum Hall regime of HfTe$_5$

STANISLAW GALESKI (Presenter), Chemical Physics of Solids, Max Planck Institute, WENLIANG ZHU, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, SHASHANK HONNALI SUDHEENDRA, RAFAL WAWRZYNCZAK, NEETU LAMBA, ANASTASIOS MARKOU, CLAUDIA FELSER, Chemical Physics of Solids, Max Planck Institute, GENFU CHEN, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, JOHANNES GOOTH, Chemical Physics of Solids, Max Planck Institute

Interacting electrons in two dimensions can bind magnetic flux lines to form composite quasiparticles with fractional electric charge. Existence of such states manifests itself by the occurrence of the Fractional Quantum Hall Effect (FQHE). Although similar composite quasiparticles have been predicted to occur in three dimensions, their experimental realization remained elusive. In this talk, we report the observation of fractional plateaus in the Hall conductivity of the bulk semimetal HfTe$_5$. The plateaus are accompanied by Shubnikov-de-Haas minima of the longitudinal electrical resistivity. The height of the Hall plateaus is given by twice the Fermi wave vector in the direction of the applied magnetic field and scales with integer and particular fractional multiples of the conductance quantum. Our findings are consistent with the 3D FQHE, suggesting the existence of quasiparticles with fractional electric charge in a 3D crystal.

2:03PM B55.00015: Fermi Surface Topology and Evidence of Non-trivial Berry Phase in the Flat-band Semimetal Pd$_3$Pb*

MOJAMMEL ALAM KHAN (Presenter), NIRMAL GHIMIRE, TERENCE BRETZ-SULLIVAN, ANAND BHATTACHARYA, J SAMUEL JIANG, Argonne Natl Lab, PO-HAO CHANG, George Mason University, JOHN SINGLETON, Los Alamos National Laboratory, JOHN MITCHELL, Argonne Natl Lab — We present a study of the Fermi surface of the putative triple point topological semimetal Pd$_3$Pb carried out by measuring Shubnikov-de Haas (SdH) oscillations in fields of up to 60 T. A multi-sheet Fermi surface has been reconstructed from the oscillation data and is largely in agreement with DFT calculations, albeit with a Fermi level shifted slightly (~30 meV) by small electron doping. A Berry-phase analysis of the SdH oscillations reveals a non-trivial phase for two bands along high symmetry directions, confirming the topological nature of Pd$_3$Pb. Importantly, the phase of the oscillation shows an angular dependence with respect to the direction of the applied magnetic field. With the signature of a topological phase transition to a trivial phase, this angular dependence may signify a unique identity of the evolution of triple point fermionic states under field.

*Research was sponsored by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B56 DCMP GMAG: Kagome and Triangular Lattice Magnetism

Mile High Ballroom 2C - Gyanendra Dhakal, Univ of Central Florida
11:15AM B56.00001: Valence bond phases of herbertsmithite and related copper kagome materials*  
MICHAEL NORMAN (Presenter), Materials Science Division, Argonne National Lab,  
NICHOLAS LAURITA, DAVID HSIEH, Department of Physics, California Institute of Technology — Recent evidence from magnetic torque, electron spin resonance, and second harmonic generation indicate that the prototypical quantum spin liquid candidate, herbertsmithite, has a symmetry lower than its x-ray refined trigonal space group. Here, we consider known and possible distortions of this mineral class, along with related copper kagome oxides and fluorides, relate these to possible valence bond patterns, and comment on their relevance to the physics of these interesting materials.

*Work by MRN is supported by the US DOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. NJL acknowledges support from the Institute for Quantum Information and Matter Postdoctoral Fellowship.

11:27AM B56.00002: Evidence for a parity broken monoclinic ground state in the S = 1/2 Kagome antiferromagnet Herbertsmithite  
NICHOLAS LAURITA (Presenter), ALON RON, Institute for Quantum Information and Matter, California Institute of Technology, JEONG WOO HAN, JONGSEOK LEE, Department of Physics and Photon Science, Gwangju Institute of Science and Technology, ALLEN SCHEIE, Institute for Quantum Matter, Johns Hopkins University, JOHN P SHECKELTON, REBECCA SMAHA, WEI HE, JIAJIA WEN, YOUNG SANG LEE, Department of Applied Physics, Stanford University, MICHAEL NORMAN, Materials Science Division, Argonne National Laboratory, DAVID HSIEH, Institute for Quantum Information and Matter, California Institute of Technology — Nearest neighbor interacting S = ½ spins on the ideal Kagomé lattice have been predicted to form a variety of novel quantum entangled states, including quantum spin-liquid (SL) and valence bond solid phases. However, in real materials, the presence of additional perturbative spin interactions may greatly expand the variety of entangled states, which recent theoretical analyses have shown are identifiable through the spontaneous loss of particular discrete point group symmetries. Here we comprehensively resolve the ground state point group symmetries of the prototypical Kagomé SL candidate ZnCu$_3$(OH)$_6$Cl$_2$ (Herbertsmithite) using a combination of optical ellipsometry and wavelength-dependent multi-harmonic optical polarimetry. We uncover a subtle parity breaking monoclinic structural distortion well above the nearest neighbor exchange energy scale. Surprisingly, the parity-breaking order parameter is dramatically enhanced upon cooling and closely tracks the build-up of nearest neighbor spin correlations, suggesting that it is energetically favored by the SL state. The refined low temperature symmetry group greatly restricts the number of viable ground states, and, in the perturbative limit, points toward the formation of a nematic SL ground state, a SL analogue of a liquid crystal.
**11:39AM B56.00003: Magnetism on ideal triangular lattices in NaBaYb(BO$_3$)$_2$**  
ALIREZA GHASEMI (Presenter), Johns Hopkins University, SHU GUO, ROBERT J. CAVA, Chemistry, Princeton University, COLLIN LESLIE BROHOLM, Johns Hopkins University — In the search for compounds that have a stable spin liquid phase, the triangular lattice of Yb is of interest. Frustration combined with the quantum spin-orbital degree of freedom of Yb provides potentially favorable conditions for a quantum spin liquid. Here we study NaBaYb(BO$_3$)$_2$, which has two different triangular layers of Yb; one sandwiched between two layers of Na, the other between two layers of Ba. Here we discuss, the low-temperature heat capacity and susceptibility of this compound. Our high-field heat capacity data and susceptibility data indicate Yb$^{3+}$ has a Kramers doublet ground state. From lower field data where the Schottky anomaly moves to lower T, we infer the energy scale of inter-site interactions is similar to that of magnetic dipole interactions. While we find a small anomaly in the zero-field heat capacity at 0.41(2)K, most of the Rln2 magnetic entropy is retained to the lowest T=0.1 K accessed here [1].


*“This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331.”*

**11:51AM B56.00004: Magnetic and charge susceptibilities in the half-filled triangular lattice Hubbard model**  
SHAOZHI LI (Presenter), EMANUEL GULL, Univ of Michigan - Ann Arbor — The spin spectra of a triangular system have been studied extensively using the Heisenberg model. But for a correlated metallic triangular system, where the Heisenberg model is not valid, the spin properties are unknown. In this talk, I present momentum-dependent magnetic and charge susceptibilities of the half-filled two-dimensional triangular Hubbard model in the metallic, Mott insulating, and crossover regions of parameter space, using the dual fermion approach. In the insulating state, I find strong spin fluctuations at the K point at low energy corresponding to the 120° antiferromagnetic order. The spin spectra of the insulating state are consistent with the inelastic neutron spectra of the triangular compound Ba$_8$CoNb$_6$O$_{24}$. I also find that the spin fluctuations at the K point persist into the metallic phase and move to higher energy. These results are in agreement with the studies of spin-lattice relaxation times in k-(ET)$_2$Cu$_2$(CN)$_3$. Finally, I present charge susceptibilities in different areas of parameter space, which should correspond to momentum-resolved electron-loss spectroscopy measurements on triangular compounds.

*This work was supported by the National Science Foundation (NSF) under Grant No. DMR-1606348.*
12:03PM B56.00005: Topological flat bands in the 3d transition metal-based kagome lattices*  MIN GU KANG (Presenter), Massachusetts Institute of Technology MIT, SHIANG FANG, Department of Physics, Harvard University, LINDA YE, HOI CHUN PO, Massachusetts Institute of Technology MIT, JONATHAN DENLINGER, CHRIS JOZWIAK, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, Lawrence Berkeley National Laboratory, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University, JOSEPH G CHECKELSKY, RICCARDO COMIN, Massachusetts Institute of Technology MIT — Electronic flat bands in momentum space, arising from strong localization of electrons in real space, are an ideal stage to realize strong correlation phenomena as highlighted by the recent example of twisted-bilayer graphene. In certain lattice systems, electronic flat bands with nontrivial topology may naturally arise from the combination of geometrical frustration, spin-orbit coupling, and reduced dimensionality, while their experimental realization has been elusive so far. Here, we report the observation of topological flat bands in series of 3d transition metal-based kagome compounds. Using angle-resolved photoemission spectroscopy, we directly show how the dispersion of the flat bands is strongly quenched along all three momentum directions. Spin-orbit coupling opens a large gap at the quadratic band touching point between the Dirac and flat bands, endowing a nonzero $\mathbb{Z}_2$ topological invariant to the flat band. Our observation opens a promising route to engineer novel emergent phases at the crossroad between strong correlated and topological materials.

*This work was supported by the STC Center for Integrated Quantum Materials, NSF Grant No.DMR-1231319, Gordon and Betty Moore Foundation EPIQS Initiative, Grant No. GBMF3848, and ARO Grant No.W911NF-16-1-0034.

12:15PM B56.00006: Localized states of the topological flat bands in the 3d transition metal kagome compound*  SHIANG FANG (Presenter), Department of Physics and Astronomy, Rutgers University, MIN GU KANG, LINDA YE, HOI CHUN PO, Department of Physics, Massachusetts Institute of Technology, JONATHAN DENLINGER, CHRIS JOZWIAK, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, E. O. Lawrence Berkeley National Laboratory, JOSEPH G CHECKELSKY, RICCARDO COMIN, Department of Physics, Massachusetts Institute of Technology, EFTHIMIOS KAXIRAS, Harvard University — The kagome lattice can host both Dirac electrons and the flat band in the spectrum. With spin-orbit coupling, the flat band will acquire non-trivial topology. On the other hand, when the kinetic energy scale is quenched as with a flat band, the electron interactions could facilitate the formation of correlated phases. Hence, the kagome lattice system has the potential to open a door to study the interplay between topology and electron correlations. In synthesized kagome compounds, additional degrees of freedom such as the orbitals further enrich the physics. To elucidate the nature of the electronic structure, we perform the ab initio density functional theory calculations. We focus on the 3d transition metal kagome compound with topological flat bands, observed experimentally by angle-resolved photoemission spectroscopy. The effective Hamiltonians of these topological flat bands are investigated with the derivations of Wannier states. The implications of topological obstructions and crystalline symmetries are discussed. These localized Wannier functions with intricate spin and orbital texture in the real space reveal their origin from the frustrated kagome structure.

*This work was supported by STC CIQM, NSF Grant No. DMR-1231319.
**12:27PM B56.00007: Colossal transverse response from non-centrosymmetric kagome ferromagnets**

TOMOYA ASABA (Presenter), SEAN THOMAS, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory — The interest of the anomalous Hall effect (AHE) and anomalous Nernst effect (ANE) has been renewed since the discoveries of large values of the AHE and ANE due to topologically nontrivial origins, and their potential application to spintronics and efficient energy conversion. Good examples are kagome magnets Mn3Sn and Co2MnGa. Among topological materials, in particular, uranium compounds are one of the best candidates to find large responses of AHE and ANE due to the correlated, flat f-band feature and large spin-orbit coupling that is the key ingredient for topology. However, the study of AHE and ANE for uranium compounds has been very sparse with only a few superconducting exceptions. Here, we will present the giant transverse response from uranium kagome ferromagnets. Our results shed light on the potential of uranium compounds as new spintronic and energy-conversion materials.

**12:39PM B56.00008: Wigner solid of charge transfer excitons in Yin-Yang Kagome lattice**

GURJYOT SETHI (Presenter), Materials Science and Engineering, University of Utah, CONGJUN WU, University of California, San Diego, FENG LIU, Materials Science and Engineering, University of Utah — We demonstrate that photo absorption between two enantiomorphic topological flat bands, as hosted in a Yin-Yang Kagome lattice, provides a perfect platform for the realization of excitonic Wigner crystallization. By solving the Bethe Salpeter equation in Tamm Dancoff approximation within a tight-binding framework, we study the flat-band excitons in terms of their binding energy and dispersion. We show that they are charge-transfer excitons, characterized by a constant binding energy (dispersion-less) in momentum space and highly localized electron-hole pair distribution function in real space. By virtue of electronic and excitonic flat bands our results are indicative of excitonic Wigner crystallization. This would be the first-time realization of Wigner solid of charge-transfer excitons in a lattice model. Our findings open the door to further investigation of photo excitation and many-body physics of correlated electrons in multiple flat bands.

*This work was supported by U.S. DOE-BES (Grant No. DE-FG02-04ER46148)
12:51PM B56.00009: Three-colored quantum scars in the kagome quantum antiferromagnet*  Hitesh Chanrai (Presenter), Physics, Florida State University, Arijeet Pal, University College London — Non-equilibrium properties of quantum materials present many intriguing properties, among them athermal behavior, which violates the eigenstate thermalization hypothesis. Such behavior has primarily been observed in disordered systems. More recently, experimental and theoretical evidence for athermal eigenstates, known as "quantum scars", has emerged in non-integrable disorder-free models in one dimension with constrained dynamics. In this work we investigate quantum scar eigenstates and the associated dynamical properties for the two dimensional kagome antiferromagnet. The model we study was previously shown to harbor a special exactly solvable point with three-color ground states, which involves only nearest neighbor XXZ interactions [H. J. Changlani et al. Phys. Rev. Lett. 120, 117202 (2018)]. In particular, we demonstrate the occurrence of low entanglement states spread throughout the middle of the spectrum and show quantum revivals for appropriately chosen initial states. We also present natural generalizations of our ideas to higher dimensions.

*We acknowledge start-up funds from Florida State University and the National High Magnetic Field Laboratory which is supported by the National Science Foundation through NSF/DMR-1644779 and the state of Florida.

1:03PM B56.00010: A new quantum spin liquid candidate with Co-based triangular lattice  Ruidan Zhong (Presenter), Shu Guo, Princeton University, Guangyong Xu, Zhijun Xu, National Institute of Standards and Technology, Robert J. Cava, Princeton University — Currently under active study in condensed matter physics, both theoretically and experimentally, are quantum spin liquid (QSL) states. However, the existing QSL candidates all have their intrinsic disadvantages, and solid evidence for quantum fluctuations is scarce. Here, we report a previously unreported compound, Na2BaCo(PO4)2, a geometrically frustrated system with effective spin-1/2 local moments for Co2+ ions on an isotropic two-dimensional (2D) triangular lattice. Magnetic susceptibility and neutron scattering experiments show no magnetic ordering down to 0.05 K. Thermodynamic measurements show that there is a tremendous amount of magnetic entropy present below 1 K in zero magnetic field. The presence of localized low-energy spin fluctuations is revealed by inelastic neutron measurements. At low applied fields, these spin excitations are confined to low energy and contribute to the anomalously large specific heat. In larger applied fields, the system reverts to normal behavior as evident by both neutron and thermodynamic results. Our experimental characterization thus reveals that this material is an excellent candidate for the experimental realization of a QSL state.
1:15PM B56.0001

**SU(4) antiferromagnetism on the triangular lattice**

Anna Kesselman (Presenter), Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Lucile Savary, Laboratoire de physique, École Normale Supérieure de Lyon, Leon Balents, Kavli Institute for Theoretical Physics, University of California, Santa Barbara — In systems with many local degrees of freedom, high-symmetry points in the phase diagram can provide an important starting point for the investigation of their properties throughout the phase diagram. In systems with both spin and orbital (or valley) degrees of freedom, such as twisted multilayer graphene or transition metal dichalcogenides, such a starting point gives rise to SU(4)-symmetric models. Here we consider SU(4)-symmetric “spin” models, corresponding to Mott phases at half-filling, i.e. the six-dimensional representation of SU(4). In particular, we study the SU(4) antiferromagnetic “Heisenberg” model on the triangular lattice, both in the classical limit and in the quantum regime. Carrying out a numerical study using the density matrix renormalization group (DMRG), we argue that the ground state is non-magnetic. We then carry out a dimer expansion of the SU(4) spin model. An exact diagonalization study of the effective dimer model suggests that the ground state breaks translation invariance, forming a valence bond solid (VBS) with a 12-site unit cell. Finally, we consider the effect of SU(4)-symmetry breaking interactions due to Hund’s coupling, and argue for a possible phase transition between a VBS and a magnetically ordered state.

1:27PM B56.0001

**Stability of chiral spin liquid phase of the triangular lattice Hubbard model with hopping anisotropy**

Aaron Szasz (Presenter), Perimeter Institute for Theoretical Physics, Johannes Motruk, Lawrence Berkeley National Laboratory — In our previous work (arXiv:1808.00463), we showed using density matrix renormalization group (DMRG) simulations on infinite cylinders that the triangular lattice Hubbard model hosts a chiral spin liquid phase at intermediate interaction strength. However, the model we studied featured isotropic hopping, whereas real triangular lattice spin liquid candidate materials, such as $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, are not precisely isotropic. To better connect to experimental results in such spin liquid candidates, in this work we investigate the stability of the chiral spin liquid against anisotropy in the hopping and show that the phase survives, providing further support for the applicability of our findings to experiments.
1:39PM B56.00013: Dynamical DMRG study of spin excitation dynamics in triangular lattice spin-1/2 antiferromagnet  SHIGETOSHI SOTA (Presenter), TOMONORI SHIRAKAWA, SEIJI YUNOKI, RIKEN, TAKAMI TOHYAMA, Tokyo University of Science — Recently, the theoretical understanding of the ground state of frustrated two-dimensional spin-1/2 antiferromagnetic Heisenberg models has been dramatically progressed. In contrast, much less has been understood for the spin excitation dynamics. For example, it is well established by now that 120 degree Néel order appears in the ground state of the triangular lattice spin-1/2 antiferromagnetic Heisenberg model. However, the spin excitation dynamics is still under active debate. In fact, the spin excitations observed by recent neutron scattering for Ba$_3$CoSb$_2$O$_9$, modeled by the triangular lattice spin-1/2 antiferromagnetic Heisenberg model, cannot be explained by the linear spin wave theory. By using the dynamical DMRG method, here we investigate the spin excitation dynamics of the triangular lattice spin-1/2 antiferromagnetic Heisenberg model. We find that our results are in good agreement with the experimental results for Ba$_3$CoSb$_2$O$_9$, implying that the quantum fluctuations beyond the linear spin wave theory play an important role on the spin excitations dynamics of Ba$_3$CoSb$_2$O$_9$.

1:51PM B56.00014: Spin properties of triangular-lattice rare-earth compounds K$_2$CsYb(PO$_4$)$_2$ and K$_2$CsEr(PO$_4$)$_2$  LUWEI GE (Presenter), Physics, Georgia Institute of Technology, QING HUANG, Physics, University of Tennessee, Knoxville, ZHILING DUN, Physics, Georgia Institute of Technology, HAI DONG ZHOU, Physics, University of Tennessee, Knoxville, MARTIN MOURIGAL, Physics, Georgia Institute of Technology — On the way to discover frustrated magnetic materials that realize unconventional phases of matter such as spin liquids, recent attention has been devoted to triangular-lattice materials comprising lanthanoid atoms. Here we report our detailed study of two such rare-earth-based compounds K$_2$CsYb(PO$_4$)$_2$ and K$_2$CsEr(PO$_4$)$_2$, where the magnetic ions form equilateral triangular lattices and where site mixing/distortion effects are absent. In spite of the limited size of the single crystals that we could obtain, we conducted detailed thermomagnetic and inelastic neutron scattering (INS) studies unravelling the spin dynamics and crystal electric field effects in these systems. Our results indicate that exchange interactions are weak and magnetic excitations essentially accounted for by weakly coupled paramagnetic anisotropic effective spin degrees of freedom. We hope our research will benefit future efforts in this exciting line of research.

*The work at Georgia Institute of Technology was supported by NSF-DMR-1750186. The work at University of Tennessee, Knoxville was supported by NSF-DMR-1350002.
Imaging antiferromagnetic domains of $\text{PdCrO}_2$

(Presenter), Lawrence Berkeley National Laboratory, ARIELLE LITTLE, University of California, Berkeley, RITIKA DUSAD, Lawrence Berkeley National Laboratory, ELINA ZHAKINA, PHILIPPA MCGUINNESS, VERONIKA SUNKO, SEUNGYUN KHIM, CLIFFORD W. HICKS, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, JOSEPH ORENSTEIN, University of California, Berkeley — The layered antiferromagnet $\text{PdCrO}_2$ is an exceptionally pure system, providing an ideal platform for studying how magnetic frustration is relieved in a triangular lattice. Here we spatially resolve the antiferromagnetic domains of $\text{PdCrO}_2$ using a novel temperature-modulated birefringence imaging setup. The material undergoes a weakly first-order transition at the Néel temperature (38 K), forming three distinct types of antiferromagnetic domains that are oriented at 120 degrees from one other. The domain structure is observed to reorient after each cooling cycle (upon heating to sufficiently high temperatures), indicating that the domain walls are highly mobile under external perturbations. The effect of strain on the domain population and the phase transition will also be discussed.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B57 DMP DCOMP: 2D Semiconductors: Optical Spectroscopy

Manipulating the potential landscape of 2D materials through external dielectric screening [Invited] ARCHANA RAJA (Presenter), Molecular Foundry, Lawrence Berkeley National Laboratory — Atomically thin, quasi two-dimensional (2D) materials like semimetallic graphene and semiconducting transition metal dichalcogenide (TMDC) monolayers have been shown to have extraordinary optoelectronic properties, along with the possibility to tailor physical phenomena by assembling individual layers into novel heterostructures. The interaction between charge carriers in these 2D materials is strongly influenced by the local environment. By tuning the external dielectric screening, the band gap and exciton energies in 2D TMDCs can be modified to create lateral heterojunctions without modifying the material itself [1]. Using a combination of optical and angle-resolved photoemission spectroscopies with microscopic spatial resolution, we show that the band structure rigidly shifts in response to the change in local dielectric screening [2]. Furthermore, this environmental sensitivity can lead to a new type of disorder that leads to spatially inhomogeneous band gap and exciton energies as a consequence of spatial variations in the external dielectric screening rather than any material imperfections [3].

Nano-optical cavity imaging and control of interlayer exciton emission in WSe$_2$/MoSe$_2$ heterostructures

MOLLY A MAY (Presenter), Physics, Chemistry, and JILA, University of Colorado, Boulder, CHENFENG DU, Physics, University of Washington, TAO JIANG, KIYOUNG-DOUG PARK, Physics, Chemistry, and JILA, University of Colorado, Boulder, XIAODONG XU, Physics, University of Washington, MARKUS B. RASCHKE, MARKUS B. RASCHKE, Physics, Chemistry, and JILA, University of Colorado, Boulder — Long lived interlayer excitons in transition metal dichalcogenide heterobilayers hold promise for applications from high temperature exciton condensates to nano-lasers with extended spatial coherence and other 2D optoelectronic devices. However, fundamental properties of interlayer excitons, their relaxation processes, and the mechanism for their formation through interlayer charge tunneling are still poorly understood. Furthermore, new methods for control of interlayer exciton emission and the associated nonradiative decay pathways are desired to establish high temperature exciton condensation and coherent emission. Here, we use a configurable nano-optical cavity based on a plasmonic scanning probe tip to quantify the interlayer exciton lifetime of (39 +/- 8) ps and charge transfer rate of (80 +/- 20) fs at room temperature. Further, using tip-sample force perturbation with deep sub-nm precision, we actively control interlayer exciton formation and tune the competition between nonradiative charge transfer and Purcell enhancement. We discuss the extension of this tip nano-cavity approach to low and variable temperature modalities for nano-spectroscopy, imaging, and control from dark excitons to localized states.

Exciton valley depolarization in two-dimensional MoSe$_2$ and WSe$_2$

MIN YANG (Presenter), DINH VAN TUAN, Department of Electrical and Computer Engineering, University of Rochester, HANAN DERY, Department of Electrical and Computer Engineering & Department of Physics and Astronomy, University of Rochester — The valley degree of freedom is a sought-after quantum number in monolayer transition-metal dichalcogenides. Similar to the spins of electrons and holes, the valley degree of freedom is not a conserved quantity and excitons lose their original helicity over time. Valley depolarization of excitons in monolayer transition-metal dichalcogenides due to long-range electron-hole exchange typically takes a few ps at low temperatures. Exceptions to this behavior are monolayers MoSe$_2$ and MoTe$_2$ wherein the depolarization is much faster. We elucidate the enigmatic anomaly of these materials, finding that it originates from Rashba-induced coupling of the dark and bright exciton branches next to their degeneracy point. When photoexcited excitons scatter during their energy relaxation between states next to the degeneracy region, they reach the light cone after losing the initial helicity. The valley depolarization is not as fast in monolayers WSe$_2$, WS$_2$ and likely MoS$_2$ wherein the Rashba-induced coupling is negligible.

*This work is supported by the Department of Energy, Basic Energy Sciences, under Contract No. DE-SC0014349.
12:15PM B57.00004: Deciphering the rich photoluminescence spectrum of monolayer WSe$_2$. HANAN DERY (Presenter), University of Rochester — High-quality monolayer WSe$_2$ samples when gated and encapsulated by hBN exhibit unprecedented rich photoluminescence spectrum. In this talk, I will summarize what we (think we) already understand, identifying the signatures of dark and indirect excitons as well as of dark trions, along with their zone-center and zone-edge phonon replicas. I will then focus on the signatures of many-body interactions, proposing novel electron-assisted optical transitions of dark excitons and the brightening of these excitons when they are coupled to collective charge or spin excitations (plasmons and magnons). I will explain why these many-body interactions have the right conditions to manifest in the photoluminescence spectra of electron-doped tungsten-based monolayers.

*This work is supported by the Department of Energy, Basic Energy Sciences (DE-SC0014349)

12:27PM B57.00005: Candidates for the origin of many-body spectral features in monolayer WSe$_2$. DINH VAN TUAN (Presenter), HANAN DERY, University of Rochester — The combination of strong Coulomb interaction, spin and valley degrees of freedom give rise to multiple optical peaks in the spectrum of WSe$_2$. While the physics of many peaks has been identified, the origin of a strong low-energy peak in highly electron-doped WSe$_2$ remains elusive since its first observation in 2013 [1]. In this talk, we show possible explanations for the origin of this optical transition including the interaction of excitons with intervalley plasmons [2,3,4], or magnons induced by resident electrons. We explain why the proposed mechanisms are suitable for the peak to emerge in the spectrum of electron-doped WSe$_2$ while being absent in hole-doped regime or in the whole spectrum of MoSe$_2$ monolayer [5].


*This work is supported by the Department of Energy, Basic Energy Sciences (DE-SC0014349).
12:39PM B57.00006: Saddle-point Excitons and Their Extraordinary Light Absorption in Two-Dimensional beta-phase Group-IV Monochalcogenides*  
NANNAN LUO (Presenter), CHONG WANG, ZEYU JIANG, YONG XU, XIAOLONG ZOU, DUAN WENHUI, Tsinghua University — In two-dimensional (2D) materials, saddle-points in the electronic structure give rise to diverging density of states, which leads to intriguing physical phenomena useful for applications, including magnetism, superconductivity, charge density wave, as well as enhanced optical absorption. Using first-principles calculations, we show monolayer beta-phase of group-IV monochalcogenides are a new class of 2D materials that possess saddle-points. Due to the existence of saddle-points, a remarkable absorption peak within the fundamental gap is found in these materials. The properties of saddle-point excitons can be effectively tuned by both the strain and thickness of these materials. Importantly, the strong optical absorbance induced by saddle-point exciton absorptions and the appropriate band gap give ideal power conversion efficiencies as large as 1.11% for monolayer beta-SnSe, significantly higher than reported high-performance ultrathin solar cells using transition metal dichalcogenides. These results not only open new avenues for exploring novel many-body physics, but also suggest beta-phase MXs could be promising candidates for future optoelectronic devices.

*The National Natural Science Foundation of China (Grant Nos. 51788104, 11674188, and 11334006)

12:51PM B57.00007: Temperature dependent valley polarization in WS\(_2\) heterostructures*  
GEORGE KIOSEOGLOU (Presenter), Univ of Crete and IESL/FORTH, IOANNIS PARADISANOS, IESL/FORTH, KATHLEEN M MCCREARY, Naval Research Lab, AUBREY T. HANBICKI, LPS, LEONIDAS MOUCHLIADIS, IESL/FORTH, DAVOUD ADINEHLOO, VASILI PEREBEINOS, University of Buffalo, BEREND THOMAS JONKER, Naval Research Lab, EMMANUEL STRATAKIS, IESL/FORTH — The absence of degeneracy in the valley indices of monolayer-TMDs serves as an essential property for the development of valleytronic devices. One criterion for the realization of such a device is to attain high polarization at RT. We examine vertical WS\(_2\) heterostructures and show that the material type used, significantly influences the valley polarization of WS\(_2\). The interaction between WS\(_2\) and graphene has a strong effect on the T-dependent depolarization, with a polarization of 24% at RT under near-resonant excitation. This contrasts with hBN- encapsulated WS\(_2\), which exhibits a RT polarization of 11%. The low depolarization rate in WS\(_2\)/Graphene is attributed to a) rapid charge and energy transfer processes of the scattered excitons, b) absence of thermal dissociation of trions and thermally assisted dark-to-bright transitions and c) partial suppression of the T-dependent bandgap renormalization. Significant variations in the polarization are also observed at 4K. We propose that intervalley hole scattering in the VB proximity between the K and Γ points of WS\(_2\) is sensitive to the immediate environment, leading to the observed variations.

*This work is supported by the GSRT-Greece under the project FLAG-ERA II-JTC 2017-GRFAR-GRAPH-EYE and the SPIVAST Synergy-FORTH grant ΕΣΩ00118
Tunable Spontaneous Valley Coherence in Atomically Thin Semiconductors

MANDAR SOHONI (Presenter), MURALIDHAR NALABOTHULA, Physics, Indian Institute of Technology, Bombay, PANKAJ JHA, Applied Physics and Material Science, Califormnia Institute of Technology, TONY LOW, Electrical & Computer Engineering, University of Minnesota, ANSHUMAN KUMAR, Physics, Indian Institute of Technology, Bombay — An interesting feature of monolayer transition metal dichalcogenides (TMDCs) is the existence of two degenerate, but disparate, band extrema valleys in k space with different optical selection rules. In order to manipulate this “valley degree of freedom”, we should be able to control, and manipulate the coherence between the two valleys.

In this work we study the spontaneous valley coherence generated in a van der Waals heterostructure created by combining a TMDC with other two dimensional (2D) materials. First, we discuss general results on exploring the parameter space of the optical conductivity tensor of such a system to get the highest values of valley coherence and coherence times. Second, we analyze the spontaneously generated valley coherence for “hybrid” (a mixture of interlayer and intralayer) excitons in a system involving an anisotropic photonic metasurface and a TMDC heterostructure. We study the dependence of the coherence on external tuning knobs such as an electric field, and interlayer coupling in the heterostructure. Our analysis should help the community in designing heterostructures for maximum valley coherence, and help solidify the foundation of the valley degree of freedom as a qubit.

Valley-selective optical Stark shift of exciton-polaritons in a monolayer semiconductor

TREVOR LAMOUNTAIN (Presenter), JOVAN NELSON, ERIK J LENFERINK, AKSHAY MURTHY, VINAYAK D. DRAVID, NATHANIEL PATRICK STERN, Northwestern University — Light provides a high-speed coherent medium for measurement and manipulation of electronic quantum states. Exploiting the optical selection rules of transition metal dicalchogenide monolayers (TMDs), the optical Stark effect allows for valley-selective control of energy levels using sub-resonant optical pulses. Recent discoveries have revealed that microcavity exciton-polaritons in TMDs preserve valley features while also incorporating many of the favorable properties of light. Here, we use polarization-dependent transient reflectance to demonstrate that the optical Stark effect can also be used for valley-selective manipulation of energy levels in WS2 exciton-polaritons. In the reflectance spectra we observe a simultaneous shift of both polariton branches when pump and probe are co-polarized, and no appreciable shift when they are cross-polarized. We find excellent agreement between measured data and a Lorentz oscillator model over a wide range of experimental parameters. The extracted polariton shift confirms the expected linear power dependence of the optical Stark effect. The polarization-dependent Stark shift of TMD exciton-polaritons provides a new tool for state control in coherent valleytronics.

*This work was supported by DOE (DE-SC0012130) and ONR (N00014-16-1-3055).
1:27PM B57.00010: Anisotropic Optical Properties and Vibrational Characteristics of 2D Silicon Telluride Nanoplates* JIYANG CHEN (Presenter), ROMAKANTA BHATTARAI, XIAO SHEN, Univ of Memphis, JINGBIAO CUI, The University of North Texas, THANG HOANG, Univ of Memphis — The p-type semiconductor silicon telluride (Si2Te3) has a unique layered crystal structure with hexagonal closed-packed Te sublattices and Si-Si dimers occupying octahedral intercalation sites. The orientation of the silicon dimers leads to unique optical and electronic properties. Here, we report a combined experimental and computational study of the optical properties of individual Si2Te3 nanoplates (NPs). 2D Si2Te3 NPs with thickness of tens to hundreds of nanometers and diameter of tens of micrometers are synthesized by the chemical vapor deposition technique. Polarized reflection measurements at different temperatures show a 90-degree periodic change in the absorption coefficient, which indicates an anisotropic orientation of the Si-Si dimers and is in agreement with the theoretical calculation of the dielectric constants. Polarized and spatial Raman mapping measurements of single Si2Te3 NPs at different temperatures reveal various vibrational modes, which are in agreement with the Density Functional Theory calculation.

*This work was supported by National Science Foundation (DMR-1709528, DMR-1709612), Computational resources were provided by the NSF XSEDE under grants TG-DMR 170064 and 170076, and by the High-Performance Computing Facility at the University of Memphis.

1:39PM B57.00011: Anomalous photovoltaic effect in van der Waals heterointerface TOSHIYA IDEUE (Presenter), TAKATOSHI AKAMATSU, The University of Tokyo, LING ZHOU, Nanjing University, SOTA KITAMURA, MASARU ONGA, YUJI NAKAGAWA, The University of Tokyo, JOSEPH LAURIENZO, Case Western Reserve University, JUNWEI HUANG, Nanjing University, TAKAHIRO MORIMOTO, The University of Tokyo, HONGTAO YUAN, Nanjing University, YOSHIHIRO IWASA, The University of Tokyo — Van der Waals interfaces are unique platforms for novel properties and functionalities. In addition to being building blocks for functionalized devices such as p-n junctions or tunneling junctions, symmetry of the van der Waal interface has recently been attracting much attention, represented by Moiré physics in twisted interfaces [1-3] and pseudo landau level formation in graphene/black phosphorus heterostructures [4]. In this talk, I will focus on the effect of symmetry on the photovoltaic effect in van der Waals interface. The anomalous photovoltaic effect, which indicates the emergence of photo-induced spontaneous current without semiconductor p-n junction nor bias voltage, is observed at the symmetry engineered interface. A potential microscopic mechanism of the anomalous photovoltaic effect will be also discussed.

1:51PM B57.00012: Deep-Learning-Based Image Segmentation Integrated with Optical Microscopy for Automatically Searching for Two-Dimensional Materials*  
SATORU MASUBUCHI (Presenter), EISUKE WATANABE, YUTA SEO, IIS, Univ of Tokyo, SHOTA OKAZAKI, TAKAO SASAGAWA, Tokyo Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, Japan, TOMOKI MACHIDA, IIS, Univ of Tokyo — Deep-learning algorithms enable precise image recognition based on high-dimensional hierarchical image features. Here, we report the development and implementation of a deep-learning-based image segmentation algorithm in an autonomous robotic system to search for two-dimensional (2D) materials. We trained the neural network based on Mask-RCNN on annotated optical microscope images of 2D materials (graphene, hBN, MoS2, and WTe2). The inference algorithm is run on a 1024 × 1024 px optical microscope images for 200 ms, enabling the real-time detection of 2D materials. The detection process is robust against changes in the microscopy conditions, such as illumination and color balance, which obviates the parameter-tuning process required for conventional rule-based detection algorithms. Integrating the algorithm with a motorized optical microscope enables the automated searching and cataloging of 2D materials. This development will allow researchers to utilize unlimited amounts of 2D materials simply by exfoliating and running the automated searching process.

*This work was supported by the CREST (JST) Grant Nos. JPMJCR15F3 and JPMJCR16F2, and by JSPS KAKENHI under Grant No. JP19H01820.

B57.00013: Chiral phonon replicas of dark excitonic states in monolayer WSe2  
ERFU LIU (Presenter), JEREMIAH VAN BAREN, University of California, Riverside, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, YIA-CHUNG CHANG, Research Center for Applied Sciences, Academia Sinica, Taipei 11529, Taiwan, CHUN HUNG LUI, University of California, Riverside — We observe a set of replica luminescent peaks below the dark excitonic states (including excitons and trions) in monolayer WSe2. The replica redshift energies match the energies of the zone-center and zone-corner optical phonons. The phonon replicas exhibit parallel gate dependence and same g-factors as the dark excitonic states, but follow the valley selection rules of the bright excitonic states. Our results and symmetry analysis show that a K-valley dark excitonic state can decay into a left-handed chiral phonon and a right-handed photon, whereas a K'-valley dark excitonic state can decay into a right-handed chiral phonon and a left-handed photon. Such valley selection rules of chiral phonon replicas can be utilized to identify the valleys of the dark excitonic states and explore their chiral interactions with phonons.

Monday, March 2, 2020 11:15 AM - 1:39 PM

Session B58 DCP DCOMP DPOLY DCMP: DFT and Beyond II Mile High Ballroom
3B - Adam Wasserman, Purdue Univ - Tag(s): Focus
11:15AM B58.00001: On the Constrained Search-Coordinate Scaling Formulations in DFT

[Invited] MEL LEVY (Presenter), Chemistry and Quantum Theory, Tulane University — First, a review of the early history of DFT is given, including anecdotes, and the constrained-search formulation is presented within the context of this history. Then it is shown how this formulation leads to the derivation of key constraints for approximating density functionals. These constraints include those that involve the coordinate scaling of the total density, and of the individual up and down spin densities, where the use of spin-free wavefunctions for the derivations has very recently proven to be effective.

The utility of expressing the total energies of ground-states and excited states as simple sums of augmented orbital energies shall also be discussed. Then several open problems in DFT shall be presented.

11:51AM B58.00002: Essential difference between the machine learning and artificial Kohn-Sham potentials

RYO NAGAI (Presenter), Department of Physics, The University of Tokyo, KIERON BURKE, Departments of Physics and Astronomy and of Chemistry, University of California, Irvine, RYOSUKE AKASHI, OSAMU SUGINO, Department of Physics, The University of Tokyo — The Kohn-Sham density functional theory is widely used to predict physical or chemical properties of various materials with its practical accuracy and computational cost. Its accuracy depends on the exchange-correlation functional. Although there exist many approximations for the functional, its entire structure is yet elusive since the reference databases and physical conditions available are limited. On the other hand, we develop another strategy; the functional structure is represented with a flexible neural network and its parameters are trained with machine-learning algorithms[1]. The NN-based functional becomes transferable enough by training with the density, which contains abundant information in the 3D space.

Here, we analyze the properties of the machine-learning density functionals. We investigate essential differences between the machine-learned functionals and artificial functionals by comparing their performance using accurate densities and ones from artificial functionals as the training data.

12:03PM B58.00003: Machine learning accurate exchange and correlation functionals of the electronic density*  SEBASTIAN DICK (Presenter), MARIVI FERNANDEZ SERRA, State Univ of NY - Stony Brook — Density Functional Theory (DFT) is the standard formalism to study the electronic structure of matter at the atomic scale. The balance between accuracy and computational cost that DFT-based simulations provide allows researchers to understand the structural and dynamical properties of increasingly large and complex systems at the quantum mechanical level. In Kohn-Sham DFT, this balance depends on the choice of exchange and correlation functional, which only exists in approximate form. Here we propose a framework to create highly accurate density functionals by using supervised machine learning, termed NeuralXC. These machine-learned functionals are designed to lift the accuracy of local and semilocal functionals to that provided by more accurate methods while maintaining their efficiency. We show that the functionals learn a meaningful representation of the physical information contained in the training data, making them transferable across systems. We further demonstrate how a functional optimized for water can reproduce experimental results when used in molecular dynamics simulations.

*We acknowledge funding from DOE awards numbers DE-SC0001137 and DE-SC0019394. Sebastian Dick was supported by a fellowship from The Molecular Sciences Software Institute under NSF grant ACI-1547580

12:15PM B58.00004: Constrained Machine Learning de-orbitalization of meta-GGA exchange-correlation functionals*  KANUN POKHAREL (Presenter), JAMES FURNESS, JIANWEI SUN, Tulane Univ — Meta-generalized-gradient-approximation (mGGA) exchange-correlation functionals commonly take the orbital kinetic energy density $\tau(r)$ as an ingredient in their construction [1]. Such $\tau(r)$ dependent functionals have shown impressive performance for diverse problems, but orbital dependence of $\tau(r)$ complicates the exchange-correlation potential and increases computational cost. Recently, Rodriguez et.al. constructed a mGGA with laplacian $\nabla^2 n$ without significantly degrading accuracy [2]. This suggests an intriguing but unclear relationship between $\tau(r)$ and $\nabla^2 n$. We exploit this relationship using machine learning combined with exact constraints to explore how neural-network models can de-orbitalize functionals and model fundamental components of Kohn-Sham density functional theory.


*DOE #DE-SC0019350
ACS-PRF
**12:27PM B58.00005: Semiclassical Approximation to Sums of Eigenvalues with Application to DFT**

PAVEL OKUN (Presenter), KIERON BURKE, University of California, Irvine — I present a new mathematical framework developed by Kieron Burke and Michael V. Berry for estimating the sum of the lowest N eigenenergies of a one-dimensional potential. I apply this method to several model one-dimensional systems (harmonic oscillator, Poschl-Teller well, quartic oscillator, linear well, and exponential well). This new method gives the sum of the energies as a semiclassical series, which can be shown to reproduce the DFT gradient expansion for slowly varying densities, and also produces a correction to the gradient expansion for finite systems with a discrete spectrum. Explicit corrections to the gradient expansion of the kinetic energy are derived which in simple cases greatly improve accuracy. All work is done assuming a system of non-interacting identical fermions. This research is funded by the NSF (CHE 1856165).

*NSF Grant:CHE 1856165

**12:39PM B58.00006: Progress in the Development of Advanced Temperature-Dependent Free-Energy Density Functionals Beyond the Generalized Gradient Approximation**

DEYAN MIHAYLOV (Presenter), BRENDA MCLELLAN, VALENTIN V KARASIEV, SUXING HU, Laboratory for Laser Energetics, University of Rochester — Recently, it has been shown that explicit dependence on temperature in the exchange-correlation (XC) free-energy density functional is important in density functional theory studies of warm dense matter [1]. As a first approximation, in the attempt to include thermal effects into XC, the finite-T KSDT local spin-density approximation functional was constructed by the analytical parametrization of the XC free energy of the homogeneous electron gas. Consequently, the non-empirical KDT16 [2] generalized gradient approximation (GGA) functional, which captures nonhomogeneity effects and shows better agreement with experiments, has been constructed. Here, we present recent progress in going beyond the GGA by developing finite-T extensions to the PBE0 and SCAN-L (the de-orbitalized version of SCAN) XC functionals. We present preliminary results for optical reflectivity of shocked CH and warm dense He.


*This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856 and US National Science Foundation PHY Grant No. 1802964.
Symmetry-Breaking Polymorphous Descriptions for Correlated Materials without Interelectronic $U^*$

YUBO ZHANG, JAMES FURNESS, RUIQI ZHANG, Tulane Univ, ZHI WANG, ALEX ZUNGER, university of colorado, JIANWEI SUN (Presenter), Tulane Univ — Correlated materials with open-shell $d$- and $f$-ions having degenerate band edge states show a rich variety of interesting properties. The textbook view for the electronic structure of these materials is that mean-field approaches are inappropriate, as the interelectronic interaction $U$ is required to open a band gap between the occupied and unoccupied degenerate states while retaining symmetry. We show that the mean-field band theory can lift such degeneracies when nontrivial unit cell representations (polymorphous networks) are allowed to break symmetry, in conjunction with a recently developed non-empirical exchange and correlation density functional without an on-site interelectronic interaction $U$. We rationalize how density functional theory (DFT) in the polymorphous representation achieves band gap opening in correlated materials through a separate mechanism to the Mott-Hubbard approach. We show the method predicts magnetic moments and gaps for four classical $3d$ transition-metal monoxides in both the antiferromagnetic and paramagnetic phases, offering a highly-efficient alternative to symmetry-conserving approaches for studying a range of functionalities in open $d$- and $f$-shell complex materials.

*Work supported by DOE under grant DE-SC0235021 at Tulane and by DOE-BES-DM at CU

A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction*

RAJENDRA ZOPE (Presenter), YOH YAMAMOTO, CARLOS DIAZ, TUNNA BARUAH, University of Texas at El Paso, JUAN PERALTA, KOBLAR ALAN JACKSON, Central Michigan University, BISWAJIT SANTRA, JOHN P. PERDEW, Temple University — Self-interaction (SI) error, which results when exchange-correlation contributions to the total energy are approximated,limits the reliability of many density functional approximations. The Perdew-Zunger SI correction (PZSIC), when applied in conjunction with the local spin density approximation (LSDA), improves the description of many properties, but overall, this improvement is limited. Here we propose a modification to PZSIC that uses an iso-orbital indicator to identify regions where local SI corrections should be applied. Using this local-scaling SIC (LSIC) approach with LSDA, we analyze predictions for a wide range of properties including, for atoms, total energies, ionization potentials, and electron affinities, and for molecules, atomization energies, dissociation energy curves, reaction energies, and reaction barrier heights. LSIC preserves the results of PZSIC-LSDA for properties where it is successful and provides dramatic improvements for many of the other properties studied. Atomization energies calculated using LSIC are better than those of the Perdew, Burke, and Ernzerhof (PBE) generalized gradient approximation (GGA). LSIC also restores the uniform gas limit for the exchange energy that is lost in PZSIC-LSDA.

*U.S. DOE under grants DE-SC0018331 and DE-SC0006818.
1:15PM B58.00009: Kohn-Sham effective potentials from FLOSIC using Ryabinkin-Kohut-Staroverov method*  
CARLOS DIAZ (Presenter), LUIS BASURTO, RAJENDRA ZOPE, University of Texas, El Paso — Density functional or beyond methods are often used in combination with photoelectron spectroscopy to obtain physical insights about the electronic structure of molecules and solids. The Kohn-Sham eigenvalues are not electron removal energies except for the highest occupied one, but they often, though not always, provide good approximations to electron binding energies (EBEs). Eigenvalues of the range separated hybrid functionals using tuned separation parameter generally provide good approximations to EBEs due to mitigation of self-interaction (SI) errors. We adapt and implement the Ryabinkin-Kohut-Staroverov method to obtain effective local potentials from the self-interaction corrected Fermi-Lowdin orbitals and density in the FLOSIC code. The density of states and HOMO-LUMO gaps obtained using this approach show much closer agreement with experimental values compared to those obtained with a range of DFA or functionals.

*DE-SC0018331

1:27PM B58.00010: Performance of scaled self-interaction correction to semilocal functionals*  
PUSKAR BHATTARAI (Presenter), CHANDRA SHAHI, KAMAL WAGLE, BISWAJIT SANTRA, JOHN P. PERDEW, Temple Univ — Most semilocal functionals suffer from self-interaction error (SIE). Perdew and Zunger (PZ)\(^1\) applied self-interaction correction (SIC) to each delocalized Kohn-Sham orbital by subtracting the SIE from each occupied orbital. The Fermi-Lowdin orbital self-interaction correction (FLOSIC) uses size-extensive localized Fermi-Lowdin orbitals that improve the results for the properties like barrier heights that involves strong SIE, as in stretched bonds. However, it worsens the equilibrium properties such as atomization energies, as FLOSIC applied to a functional violates the exact constraints and the appropriate norms that the semilocal approximations satisfy\(^2\). Here, we apply a scaled PZ SIC to LSDA, PBE, and SCAN and calculated different properties such as electron affinity, ionization potential, barrier height, atomization energy, and bond length of some representative test sets. We find that the scaled SIC works well for both the equilibrium properties and for the features that involve stretched bonds or noded densities.


*This work was supported by NSF DMR-1607868 and DOE BES DE-SC0018331.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B59 DMP: Skyrmions and Topological Magnonics Mile High Ballroom 3C
11:15AM B59.00001: THz spectroscopy of topological magnon candidate CoTiO$_3$*  EVAN JASPER (Presenter), Ohio State Univ - Columbus, TIMOTHY DELAZZER, KATE ROSS, Colorado State University, ROLANDO VALDES AGUILAR, Ohio State Univ - Columbus — Recent advancements in topological band theory have predicted the existence of topologically-protected magnon excitations [1] with potential spintronic applications. CoTiO$_3$ is an Ilmenite-structure antiferromagnet with a Néel temperature of 38 K and magnon energies in the THz range. Previous work has also identified CoTiO$_3$ as a candidate to host topological magnons [2]. We follow up on that research by measuring the THz transmission and reflectivity of both single crystal and pressed powder samples of CoTiO$_3$ and we report the results including a large absorptions near 1 and 1.6 THz. We propose that the modes broaden with decreasing temperature or a new absorption appears below the Néel temperature with energy coinciding with a zone-center magnon excitation. We will discuss these possibilities together with the details of the THz polarization response.


*Funding at OSU for this research was provided by the Center for Emergent Materials: an NSF MRSEC under award number DMR-1420451, and at CSU by the CIFAR Quantum Materials program.

11:27AM B59.00002: Three-dimensional topological magnon systems*  HIROKI KONDO (Presenter), YUTAKA AKAGI, HOSHO KATSURA, Univ of Tokyo — Recently, magnonic analogs of spin Hall insulators in two dimensions have been proposed theoretically [1]. In our previous work, we defined a $Z_2$ topological invariant for them and proposed the first model of a magnonic analog of a spin Hall insulator without spin conservation [2]. Building on this previous work, in this study, we propose a concept of three-dimensional (3D) topological magnon systems characterized by a set of $Z_2$ topological invariants [3]. They can be thought of as magnonic analogs of 3D topological insulators. One of the models proposed is a bosonic counterpart of the Fu-Kane-Mele model, which is found to exhibit three distinct phases analogous to strong topological, weak topological, and trivial insulator phases. We also discuss a possible realization of the thermal Hall effect of surface Dirac magnons in the presence of a magnetic field.


*JSPS Grant-in-Aid for Scientific Research on Innovative Areas: No. JP18H04478 (H.Katsura) and No. 18H04220 (Y.A.)
11:39AM B59.00003: Chiral Magmonic Edge States in Ferromagnetic Skyrmion Crystals Controlled by Magnetic Fields  SEBASTIAN A DIAZ (Presenter), University of Basel, TOMOKI HIROSAWA, University of Tokyo, JELENA KLINOVJA, DANIEL LOSS, University of Basel — We show that an external magnetic field can drive a topological phase transition in the spin wave spectrum of a ferromagnetic skyrmion crystal. The topological phase transition is signaled by the closing of a low-energy bulk magnon gap at a critical field. In the topological phase, below the critical field, two topologically protected chiral magmonic edge states lie within this gap, but they unravel in the trivial phase, above the critical field. Remarkably, the topological phase transition involves an inversion of two magnon bands that at the Γ point correspond to the breathing and anticlockwise modes of the skyrmions in the crystal. Our findings suggest that an external magnetic field could be used as a knob to switch on and off magnon spin currents carried by topologically protected chiral magmonic edge states.


11:51AM B59.00004: Magnetic field control of topological magnon-polaron bands in two-dimensional ferromagnets*  PENGTAO SHEN (Presenter), SE KWON KIM, Univ of Missouri - Columbia — We theoretically study magnon-phonon hybrid excitations in a square lattice ferromagnet subjected to a magnetic field by varying the field direction. The bulk bands of hybrid excitations, which are referred to as magnon-polarons, are investigated by considering all three phonon modes: vertical phonon, transverse phonon, and longitudinal phonon. We show that the topological properties of three hybridizations are different in terms of the Berry curvature and the Chern numbers. We also find that the topological properties of the bands can be controlled by changing the direction of the magnetic field, exhibiting one or more topological phase transitions. The dependence of thermal Hall conductivity as a function of magnetic field direction is proposed as an experiment probe of our theoretical results. This work is posted on arXiv:1910.08603.

*This work is supported by the University of Missouri. S.K.K. acknowledges Young Investigator Grant (YIG) from Korean-American Scientists and Engineers Association (KSEA).

12:03PM B59.00005: Magnonic Su-Schiffer-Heeger Model in Honeycomb Ferromagnets  YUHANG LI (Presenter), RAN CHENG, University of California, Riverside — We study a collinear honeycomb ferromagnet with variable nearest-neighbor exchange interactions in the presence of the next nearest-neighbor Dzyaloshinskii-Moriya interaction. By examining the band topology and the associated chiral edge states, we find that varying the nearest-neighbor exchange interactions can induce topological phase transitions between trivial insulators with vanishing Chern number \( C=0 \) and magnon Hall insulators with \( C=1 \). Such a phase transition from topological trivial phase into a topological nontrivial one can be characterized by a sharp increase of the thermal Hall conductivity, which is attributed to the emerge of the topologically protected chiral edge states of magnons. Moreover, the magnon Hall state is robust against magnon-photon interactions. Possible materials realization is also discussed.
12:15PM B59.00006: Nonsymmorphic-symmetry-protected topological magnons in three-dimensional Kitaev materials  YONG-BAEK KIM (Presenter), WONJUNE CHOI, Univ of Toronto, TOMONARI MIZOGUCHI, Physics, University of Tsukuba — Topological phases in magnetic materials offer novel tunability of topological properties through varying the underlying magnetism. We show that field-induced canted zig-zag order of three-dimensional hyperhoneycomb Kitaev materials has gapless topological magnons protected by nonsymmorphic magnetic space group symmetries. The non-Hermitian nature of the bosonic magnons leads to unique topological protection that is different from their fermionic counterparts. We investigate how such topological magnons can be controlled by varying the strength of the spin-exchange interactions.

12:27PM B59.00007: Quantum field theory of topological spin dynamics*  PREDRAG NIKOLIC (Presenter), George Mason Univ — Topological magnetic materials are promising hosts for novel strongly correlated states. I will present a unifying quantum field theory of a wide range of such materials, which captures their universal and topological dynamics. All topological features arise from the continuum-limit gauge fields that one can calculate starting with a microscopic lattice model. Non-collinear incommensurate magnets are shaped by non-Abelian vector gauge fields, including the Dzyaloshinskii-Moriya interaction. Chiral spin couplings related to topological defects give rise to rank-2 antisymmetric tensor gauge fields. The spin-orbit coupling of mobile electrons is similarly described by non-Abelian gauge fields, including rank-2 tensors related to the 3D Berry flux. All gauge fluxes are generally exchanged between electrons and local moments through Kondo-type interactions. I will discuss applications of this theory to (i) spin-wave dynamics in the presence of Weyl electrons, (ii) instabilities of Weyl semimetals, (iii) fluctuations and temperature-dependence of the anomalous/topological Hall effect, and (iv) topological phase transitions involving monopoles and hedgehogs (which can fractionalize electrons).

*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331
12:39PM B59.00008: Polarization-resolved Raman spectroscopy of α-RuCl3 and evidence of room-temperature two-dimensional magnetic scattering  ANGELA HIGHT WALKER
(Presenter), THUC MAI, AMBER MCCREARY, National Institute of Standards and Technology, PAULA LAMPEN-KELLEY, Material Science and Technology Division, Oak Ridge National Lab, NICHOLAS BUTCH, National Institute of Standards and Technology, JEFFREY SIMPSON, Department of Physics, Towson University, JIAQIANG YAN, Material Science and Technology Division, Oak Ridge National Lab, STEPHEN E NAGLER, Neutron Scattering Division, Oak Ridge National Lab, DAVID MANDRUS, Material Science and Technology Division, Oak Ridge National Lab, ROLANDO VALDES AGUILAR, Department of Physics, The Ohio State University — Polarization-resolved Raman spectroscopy was performed and analyzed from large, high-quality, monodomain single crystal of α-RuCl3, a proximate Kitaev quantum spin liquid. Spectra were collected with laser polarizations parallel and perpendicular to the honeycomb plane. Pairs of nearly degenerate phonons were discovered and show either a fourfold or twofold polarization angle dependence in their Raman intensity, thereby providing evidence to definitively assign the bulk crystal point group as C2h. The low-frequency continuum that is often attributed to scattering from pairs of Majorana fermions was also examined and found to disappear when the laser excitation and scattered photon polarizations were perpendicular to the honeycomb plane. This disappearance, along with the behavior of the phonon spectrum in the same polarization configuration, strongly suggests that the scattering continuum is two-dimensional. We argue that this scattering continuum originates from the Kitaev magnetic interactions that survive up to room temperature, a scale larger than the bare Kitaev exchange energy of approximately 50 K. DOI: 10.1103/PhysRevB.100.134419

12:51PM B59.00009: Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures† YING SU (Presenter), Los Alamos National Laboratory, SATORU HAYAMI, Department of Physics, Hokkaido University, SHIZENG LIN, Los Alamos National Laboratory — Multiple-Q spin textures, such as magnetic bubble and skyrmion lattices, have been observed in a large family of magnets. These spin textures can be driven into motion by external stimuli and affects the electronic states. Here we show that to describe correctly the electronic dynamics, the momentum space needs to be transcended to higher dimensions by including the ancillary dimensions associated with phason modes of the translational motion of the spin textures. The electronic states have non-trivial topology characterized by the first and second Chern numbers in the high dimensional hybrid momentum space. This gives rise to an anomalous electric charge transport due to the motion of spin textures. By deforming the spin textures, a nonlinear response associated with the second Chern number can be induced. The charge transport is derived from the semi-classical equation of motion of electrons that depends on the Berry curvature in the hybrid momentum space. Our results suggest that the motion of multiple-Q spin textures has significant effects on the electronic dynamics and provides a new platform to explore high dimensional topological physics.

1:03PM B59.00010: Thermal-transport properties of chiral antiferromagnet CsCuCl$_3$

MASATOSHI AKAZAWA (Presenter), MASAAKI SHIMOZAWA, MINORU YAMASHITA, ISSP, Univ. of Tokyo, YUSUKE KOUSAKA, Department of Physics and Electronics, Osaka Prefecture University, JUN AKIMITSU, RIIS, Okayama Univ., NAOTO TSUCHIYA, KATSUYA INOUE, Department of Chemistry, Hiroshima Univ., JULIEN ZACCARO, ISABELLE GAUTIER-LUNEAU, CNRS, Institut NEEL, DOMINIQUE LUNEAU, Universite de Lyon — Recently, topological effects related to a Berry curvature dipole has been extensively studied in metals without inversion symmetry. On the other hand, these topological effects on charge-neutral bosonic excitations have yet to be clarified. To investigate this issue, we measured the longitudinal and transverse thermal conductivity of the chiral antiferromagnet CsCuCl$_3$, a high-quality homochiral single crystal of which becomes available very recently. We find a large enhancement of the longitudinal thermal conductivity in the ordered phase. This result suggests a large spin thermal conduction that could not be observed clearly in multi-domain crystals. We further find a sizable thermal Hall effect with a non-linear heater dependence even at zero magnetic field. We will discuss a possible origin for this non-linear thermal Hall effect.

1:15PM B59.00011: Intrinsic Quantized Anomalous Hall Effect in a Moiré Heterostructure, Part II: Temperature Dependence and Current Switching*

MAREC SERLIN (Presenter), CHARLES TSCHIRHART, HRYHORIY POLSHYN, YUXUAN ZHANG, JIACHENG ZHU, Physics, University of California, Santa Barbara, MARTIN E HUBER, Physics, University of Colorado, Denver, LEON BALENTS, Physics, University of California, Santa Barbara, KENJI WATANABE, TAKASHI TANIGUCHI, Physics, NIMS, ANDREA YOUNG, Physics, University of California, Santa Barbara — This is the second of three talks describing the observation and characterization of a ferromagnetic moiré heterostructure based on twisted bilayer graphene aligned to hexagonal boron nitride. I will compare the qualitative and quantitative features of this observed quantum anomalous Hall state to traditional systems engineered from thin film (Bi,Sb)$_2$Te$_3$ topological insulators. In particular, we find that the measured electronic energy gap of ~30K is several times higher than the Curie temperature, consistent with a lack of disorder associated with magnetic dopants. In this system, the quantization arises from spontaneous ferromagnetic polarization into a single spin and valley moiré subband, which is topological despite the lack of spin orbit coupling. I will also discuss the observation of current induced switching, which allows the magnetic state of the heterostructure to be controllably reversed with currents as small as a few nanoamperes.

* I would like to thank the MURI Program, AFOSR, Sloan Foundation, and the ARO for their generous support of this work.
We report the observation of a quantized anomalous Hall effect in a moiré heterostructure consisting of twisted bilayer graphene aligned to an encapsulating hBN substrate. The effect occurs at a density of 3 electrons per superlattice unit cell, where we observe magnetic hysteresis and a Hall resistance quantized to within 0.1% of the resistance quantum at temperatures as high as 3K. In this first of 3 talks, I will describe the fabrication procedure for our device as well as basic transport characterization measurements. I will introduce the phenomenology of twisted bilayer graphene and present evidence for hBN alignment as manifested in the hierarchy of symmetry-breaking gaps and anomalous magnetoresistance.

*I would like to thank the MURI program, Sloan foundation, AFOSR, and ARO for their generous support of this work.

This is the third of three talks describing the observation and characterization of a ferromagnetic moiré heterostructure based on twisted bilayer graphene aligned to hexagonal boron nitride. In this segment I will present scanning probe magnetometry data acquired using a nanoSQUID-on-tip microscope, which provides ~150 nm spatial resolution and a field sensitivity of ~10 nT/rtHz. We study the distribution of magnetic domains within the device as a function of density, magnetic field training, and DC current. Our data allow us to constrain the magnitude of the orbital magnetic moment of the electrons in the QAH state. Comparison with simultaneously acquired transport data allows us to precisely correlate single domain dynamics with discrete jumps in the observed anomalous Hall signal.

*I would like to thank the MURI program, Sloan foundation, AFOSR, and ARO for their generous support of this work. I would also like to thank the NSF GRFP and the Hertz foundation for their generous support of my graduate studies.
1:51PM B59.00014: The RKKY Interaction in Graphene Proximity Coupled to an Antiferromagnetic Insulator* JIA-JI ZHU (Presenter), JIN YANG, School of Science, Chongqing University of Posts and Telecommunications — We study theoretically the long-range Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction mediated by itinerant electrons of graphene between magnetic moments induced by proximity effect of an antiferromagnetic insulator. The antiferromagnetic insulators provides both broken time-reversal symmetry and spin-orbit coupling [1]. We find more spin-spin interaction terms which had not reported previously in other spin-orbit systems[2]. The additional terms could induce a spatially inhomogeneous spin order. We also find a rich texture of the total RKKY range function. With the Fermi energy residing in the band gap induced by the spin-orbit coupling, the RKKY interaction degenerates to the Bloembergen-Rowland (BR) interaction. The BR interaction is a short range exponentially-decay interaction mediated by virtual excitations. We show a possible transformation of anomalous Hall effect to quantum anomalous Hall effect while the RKKY interaction degenerating to the BR interaction.


*This work was supported by the NSFC (Grants No. 11404043).

B59.00015: Non-Spin-Wave type of Magnetic Excitations in a Well-characterized Nearest-Neighbor Triangular Antiferromagnet WEI BAO (Presenter), Physics, City University of Hong Kong —

The $S = \frac{3}{2}$ Mn$^{4+}$ ions of La$_2$Ca$_2$MnO$_7$ forms perfect triangular lattice in the ABC stacking. Therefore when the 120° antiferromagnetic order forms on the triangular lattice, interlayer magnetic interaction cancel out exactly. The two-dimensional long-range antiferromagnetic order develops below 2.8K, evidenced by the perfect Warren magnetic peak profile as well as in heat capacity and magnetic susceptibility data, substantially lower than the Weiss temperature of 25K. High temperature susceptibility data fitting to the Rushbrooke-Wood formulus yields a nearest-neighbor exchange constant which is identical to that derived from the low-energy stiffness of magnetic excitations, validating the nearest-neighbor magnetic interaction in plane. Different from magnetic excitation spectra previously reported in neutron scattering studies using samples with 3-dimensional long-rang 120° antiferromagnetic order, in our sample of 2-dimensional 120° antiferromagnetic order, the Spin-Wave spectrum definitely fails to describe our observed spectra. There are conflicting theories as to what kind of magnetic excitation beyond the Spin-Wave theory should be at the moment, ranging from the fractionalization of spin at the low dimensions to the mode-mode coupling decay of the spin-wave modes.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B60 DMP: Topological Materials: Weyl, Dirac, Chiral, and Other Semimetals Mile High Ballroom 4A - Gavin Osterhoudt, Boston College - Tag(s): Focus
We have shown that Kramers-Weyl fermions are a universal topological electronic property of all non-magnetic chiral crystals with spin-orbit coupling and are guaranteed by structural chirality, lattice translation and time-reversal symmetry. We determined that all point-like nodal degeneracies in non-magnetic chiral crystals with relevant spin-orbit coupling carry non-trivial Chern numbers. Kramers–Weyl materials can exhibit a monopole-like electron spin texture and topologically non-trivial bulk Fermi surfaces over an unusually large energy window [G. Chang et al. Nature Materials 17, 978-985 (2018)]. Among all the materials, we predicted the RhSi family to exhibit the ideal topological band structures, displaying the largest possible momentum separation of compensative chiral fermions, the largest proposed topologically nontrivial energy window, and the longest possible Fermi arcs on its surface [G. Chang et al. PRL 119, 206401 (2017)]. We present the theory of exotic nonlinear optical responses of topological chiral crystals, including quantized photogalvanic effect in RhSi and robust photocurrents from Fermi arc surface states [G. Chang et al. PRL 119, 206401 (2017) and arXiv:1906.03207 (2019)]. We also discuss the experimental discovery of RhSi as topological chiral crystals [D. S. Sanchez et al. Nature 567, 500-505 (2019)] and additional experiments that our discovery has enabled. (This work is in collaboration with D. S. Sanchez, I. Belopolski, T. A. Cochran, B. J. Wieder, F. Schindler, J. Yin, S. S. Zhang, S. Huang, B. Singh, T. Chang, A. Bansil, T. Neupert, S.-Y. Xu, H. Lin, and M. Zahid Hasan)

*This work at Princeton University is supported by the U.S. Department of Energy (DOE) under Basic Energy Sciences, grant no. DOE/BES DE-FG-02-05ER46200
11:51AM B60.00002: Unconventional Topological Fermions in Orthorhombic RhSi*  SHIRIN MOZAFFARI (Presenter), National High Magnetic Field Laboratory, NIRAJ ARYAL, Florida State University, RICO SCHOENEMANN, National High Magnetic Field Laboratory, KUAN-WEN CHEN, Florida State University, GREGORY MCCANDLESS, JULIA CHAN, University of Texas at Dallas, EFSTRATIOS MANOUSAKIS, Florida State University, LUIS BALICAS, National High Magnetic Field Laboratory — Topological semimetals with different types of band crossings, distinct from conventional Dirac and Weyl nodes, can give rise to novel fermionic excitations that may not have analogues in high-energy physics. Exotic multifold topological excitations have been predicted theoretically and observed in a family of transition metal silicides (e.g. β-RhSi). These compounds adopt the cubic FeSi structure type (space group No. 198), for which the calculations predict Chern numbers > 1 at specific high symmetry points within their Brillouin zone.

Through Density Functional Theory (DFT) calculations, we report that such multi degenerate fermions also exist in α-RhSi, which adopts an orthorhombic structure type (space group No. 62). Group symmetry analysis combined with DFT calculations indicate the coexistence of multiple types of multifold Dirac fermions at or near high symmetry points. Measurements of the angular dependence of the de Haas–van Alphen effect, indicate a Fermi surface whose topography is in reasonable agreement with the DFT calculations. We observe a pronounced anomaly in the magnetic torque of α-RhSi suggesting the possibility of topological phase-transitions.

*L.B. acknowledges supported from DOE-BES and S.M. from the FSU Provost Postdoctoral Fellowship Program.

12:03PM B60.00003: Ultrasound Studies of the Magnetic Weyl Semimetal Co₃Sn₂S  RUI XUE (Presenter), CANDICE KINSLER-FEDON, BRIANNA MUSICO, University of Tennessee, Knoxville, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, VEERLE M KEPPENS, DAVID MANDRUS, University of Tennessee, Knoxville — Co₃S₂Sn₂ is a magnetic Weyl semimetal that crystallizes in a shandite structure with the Co atoms forming a kagome lattice. It orders ferromagnetically at about 174 K with easy axis perpendicular to the kagome plane. Co₃S₂Sn₂ displays a giant anomalous Hall effect as well as other transport anomalies characteristic of Weyl semimetals. Here we present Resonant Ultrasound (RUS) measurements on single crystals of Co₃S₂Sn₂ as a function of temperature and magnetic field. RUS measures the mechanical resonances of the crystals and is highly sensitive to phase transitions and other thermodynamic irregularities in the sample.
Prototypical topological Weyl and Dirac semimetals are 3D crystal structures and are typically grown in the form of bulk. Discovering and engineering topological semimetals from the family of 2D TMDs could open the way for exploitation of their topological properties by fabricating thin epitaxial films and devices on suitable substrates. In this work, we show that using molecular beam epitaxy, single and few layers of HfTe$_2$[1] and ZrTe$_2$[2] can be grown epitaxially on AlN and InAs substrates. By combining ARPES and DFT calculations we provide evidence that they are type-I and type-II Dirac semimetals, respectively, with the Dirac point located at the Fermi energy. Dirac cones are maintained down to the single-layer, suggesting that they could be considered as the electronic analogues of graphene. Moreover, we report the first direct observation at room temperature of the orthorhombic Weyl semimetal phase of MoTe$_2$[3]. DFT calculations predict eight type-II Weyl nodes which are located just below the Fermi level, making them accessible to electronic transport, thus creating prospect for practical applications.


The Kagome lattice is hexagonal and composed of corner sharing triangles. Materials with layered Kagome lattice allow the interplay of topological properties and interactions in flat bands, and can give rise to spin liquids, skyrmions and other novel phases. There is broad interest in realizing high-quality topological semimetal materials such as Mn$_3$X (Sn, Ge and others) [1], FeSn [2] and Co$_3$Sn$_2$S$_2$ [3], in layered Kagome structure. Both angle-resolved photoemission spectroscopy (ARPES) and transport measurement indicate they are topologically nontrivial. Until now, most measurements are performed on bulk samples which can be a limitation for both physics and application. By using molecular beam epitaxy and sputtering, we synthesized Kagome structured FeSn and Mn$_3$Ge films. Both in-situ and ex-situ characterizations indicate these films are highly crystalline and c-axis oriented. Highly ordered atomic layers are captured by scanning transmission electron microscopy. Anomalous Nernst effect has been measured which can be related to non-vanishing Berry curvature.

*This work is supported by the Center for the Advancement of Topological Semimetals funded by the US DOE. Use of facilities at the CNM in Argonne was supported by the U.S. DOE, BES under Contract No. DE-AC02-06CH11357.
AHMAD IKHWAN US SALEHEEN (Presenter), RAMAKANTA CHAPAI, LINGYI XING, DONGLIANG GONG, ROSHAN NEPAL, DAVID P YOUNG, RONGYING JIN, Louisiana State University, Baton Rouge — We have investigated the magnetotransport properties of the transition metal trichalcogenide TaSe$_3$, which is a Dirac semimetal candidate. While the electrical resistivity exhibits metallic behavior at zero field, a magnetic field (H)-induced upturn is observed at low temperatures for $H > 4$ T, applied perpendicular to the current direction. The extremely large, non-saturating transverse magnetoresistance (MR) reaches $\sim 7000\%$ for $H = 14$ T at 1.9 K. For $H > 6$ T, Shubnikov-de Haas (SdH) oscillations are observed with frequencies $F_\alpha \approx 98$ T and $F_\beta \approx 186$ T. By constructing the Landau fan diagram for each oscillation, we calculated the Berry phase to be 1.1 $\pi$ and 0.2 $\pi$ for $F_\alpha$ and $F_\beta$, respectively. The underlying physics will be discussed.

*This work is supported by the U. S. Department of Energy under EPSCoR grant no DE-SC0012432 with additional support from the Louisiana Board of Regents.

ROBERT KEALHOFER (Presenter), JAMES ANALYTIS, University of California, Berkeley — Topological Weyl and Dirac semimetals have excited much research interest in the last few years. Much of the study of these materials has focused on the existence of exotic signatures of topology, such as Fermi arc surface states, nonlocal transport, and observations of boundary effects such as the quantum Hall effect. One feature shared by many of these materials is a low carrier density. Landau quantization in low carrier density topological semimetals in moderate magnetic fields produces large changes in the band structure of these materials, allowing the formation of tunable, strongly interacting correlated states. We present thermal and thermodynamic signatures of these strong correlations in the prototypical Weyl semimetal TaAs.

*R.K. is supported by the National Science Foundation (NSF) Graduate Research Fellowship under Grant No. DGE-1106400
Research supported in part by Gordon and Betty Moore Foundation: GBMF4374
1:03PM B60.00008: A non-linear Hall effect at zero field in a chiral nonmagnetic compound
KOHEI MATSUURA (Presenter), MINGWEI QIU, YUTA MIZUKAMI, KENICHIRO HASHIMOTO, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, The University of Tokyo, TEPPEI UENO, TAKESHI TAKAHASHI, Department of Physics, Okayama University, KAYA KOBAYASHI, Research Institute for Interdisciplinary Science, Okayama University, MASATOSHI AKAZAWA, SAKURAKO FUJII, JUN GOUCHI, MINORU YAMASHITA, YOSHIYA UWATOKO, Institute for Solid State Physics, The University of Tokyo, MASAAKI SHIMOZAWA, Department of Materials Engineering Science, Osaka University — The Hall effect arising from the Berry curvature is one of the most important topological phenomena. In the linear response regime, such a Hall effect appears only in the time-reversal symmetry breaking condition; this is well-known as an anomalous Hall effect. By contrast, the recent studies have proposed that in the nonlinear response regime, a Hall voltage can be observed due to the Berry curvature even in time-reversal invariant systems. These works demonstrate that the new-type of Hall effect is a powerful probe for investigating Berry physics in the nonmagnetic topological materials. However, experimental studies on this nonlinear Hall effect are still lacking.
Here, we report the observation of nonlinear Hall effect in a chiral nonmagnetic compound. We find that an electric current induces a nonlinear Hall voltage under time-reversal invariant conditions. The sign of the voltage at 4.2 K depends strongly on the direction of the chirality of crystal structure, which is consistent with the theoretical calculations. Furthermore, this nonlinear Hall effect becomes smaller at higher temperatures but is still observable even at room temperature.

1:15PM B60.00009: Topology Classification using Chiral Symmetry: Chiral Zak Phase and Spin Correlations
JINGWEI JIANG (Presenter), STEVEN LOUIE, Physics, University of California, Berkeley — Topology classification theory has been broadly applied to explain and gain deeper insight of many physical phenomena. On the other hand, the power of this theory for one-dimensional (1D) systems has not been as widely used. Quasi 1D graphene nanoribbons (GNRs) can now be synthesized with atomic precision via bottom-up molecular precursor techniques and are discovered to possess nontrivial topological properties, as predicted by Cao, Zhao and Louie under a $Z_2$ classification using time reversal and spatial symmetries. However, the use of these symmetries constrains the classification to nonmagnetic materials with symmetric unit cell. Here we develop another approach to use only chiral symmetry (based on chiral Zak phase) to classify 1D materials, which gives an $Z$ classification. Using bulk-edge correspondence, we connect the chiral Zak phase with an edge-index that predicts the characters of topology-induced states at junctions of two 1D materials belonging to different classes. Moreover, using the GNRs as an example, we investigate the spin-spin correlations between topologically protected junction states via first-principles calculations.

*This work is supported by the NSF and the Office of Naval Research under the MURI program, and computational resources from NERSC and XSEDE.
1:27PM B60.00010: Anisotropic thermoelectric properties of topological semimetal \textit{YbMnSb}_2 single crystal  
YU PAN, CHENGUANG FU, FENGREN FAN, YANGKUN HE, CLAUDIA FELSER (Presenter), Max-Planck Institute for Chemical Physics of Solids — Topological materials can be a suitable platform for the study of thermoelectric transport properties due to the high mobility and exotic transport behaviors. Some topological materials are also good thermoelectric materials, for example, Bi$_2$Te$_3$ alloys. In this work, we report the thermoelectric properties of topological semimetal \textit{YbMnSb}_2 single crystal. Although being a semimetal, \textit{YbMnSb}_2 still show promising Seebeck coefficient due to the much larger contribution of valence band than the conduction band. Large anisotropy is found in resistivity and thermal conductivity, while Seebeck is almost isotropic. Furthermore, we investigate the thermoelectric transport properties under magnetic field, wherein a maximum enhancement of the thermoelectric figure of merit ($zT$) reached 200\% at 100 K under 9 T. With further reduction of the thermal conductivity by alloying, microstructure engineering et al., we expect better thermoelectric performance. The present work can be instructive for the search of other new high-performing thermoelectric materials.

1:39PM B60.00011: STM/STS of Few-Layer Topological Semimetal \textit{NiTe}_2 at 78 K*  
STEPHANIE LOUGH (Presenter), Physics & Nanoscience Technology Center, University of Central Florida, DUY LE, Physics and Renewable Energy and Chemical Transformations Cluster, University of Central Florida, BRANDON BLUE, JESSE E THOMPSON, Physics & Nanoscience Technology Center, University of Central Florida, TALAT RAHMAN, Physics and Renewable Energy and Chemical Transformations Cluster, University of Central Florida, MASA ISHIGAMI, Physics & Nanoscience Technology Center, University of Central Florida — \textit{NiTe}_2 is a semimetal which has garnered interest due to recent observation of topological states and Dirac nodes near the Fermi level ($E_F$). Here, Au-assisted exfoliation of bulk \textit{NiTe}_2 is performed to generate a few-layer \textit{NiTe}_2 surface to better understand the evolution of the band structure as a function of film thickness. Scanning tunneling microscopy and spectroscopy measurements are performed at 78 K to probe the local density of electronic states (LDOS) at the surface and around defects. Multiple peaks in the LDOS are observed near $E_F$ and are compared to those obtained computationally from density functional theory (DFT) to reveal the nature of these features in the electronic structure.

* D.L. and T.S.R. are supported in part by U.S. Department of Energy Grant DE-FG02-07ER46354.
1:51PM B60.00012: Topological light meets topological semimetal  ZHURUN JI (Presenter), WENJING LIU, University of Pennsylvania, SERGIY KRYLYUK, National Institute of Standards and Technology, XIAOPENG FAN, ZHIFENG ZHANG, University of Pennsylvania, ANLIAN PAN, Hunan University, LIANG FENG, University of Pennsylvania, ALBERT DAVYDOV, National Institute of Standards and Technology, RITESH AGARWAL, University of Pennsylvania — A Weyl semimetal carries topological charges at the Weyl nodes; a light beam can also carry a topological charge, when it has an orbital angular momentum (OAM) from spatial phase and/or polarization gradients. Recently there has been a lot of interest in understanding how the spin angular momentum (SAM) of light interacts with materials to induce photocurrents (circular photogalvanic effect, CPGE), but not many studies have focused on photocurrents generated by the OAM of light. Here we report a unique orbital photogalvanic effect (OPGE) in a type-II Weyl semimetal WTe$_2$, featured by a photocurrent winding around the axis of OAM-carrying beams, whose intensity is directly proportional to the topological winding number of the light field, and can be attributed to a discretized dynamical Hall effect. In addition to obtaining new microscopic insights into light-matter interactions with topological light, these measurements show promise for fabricating on-chip photodetectors on Weyl semimetals capable of detecting OAM modes, which can be useful for building the next-generation, high-capacity optoelectronic circuits.

2:03PM B60.00013: Quenching of Relaxation Pathway In Weyl Semimetal TaAs  JIAYUN LIU (Presenter), LIANG CHENG, DAMING ZHAO, XIAOXUAN CHEN, Division of Physics and Applied Physics, Nanyang Technological University, Singapore, ZHILIN LI, XIAOLONG CHEN, Institute of Physics, Chinese Academy of Sciences, HANDONG SUN, EE MIN CHIA, Division of Physics and Applied Physics, Nanyang Technological University, Singapore — Following the topological classification of materials, Weyl semimetal has been predicted theoretically and has since been experimentally confirmed. Experimental investigation on Weyl semimetal shows promise in the field of optoelectronics due to its wide spectral response from visible to near infrared regime. However, the transient dynamics of Weyl semimetal has not been clearly established. In this work, we studied the ultrafast response of tantalum arsenide (TaAs) in the optical regime through transient reflection spectroscopy with varying pump fluence. We noted two relaxation pathways for the hot injected electrons in TaAs by the pump pulse. We identified the origin of these two relaxation pathways through pump fluence dependent study. We noticed that depending on the energy of the probing wavelength, one of the relaxation pathways is quenched. The understanding of this quenching mechanism provides a reliable way to study the transient dynamics in Weyl semimetal.

Monday, March 2, 2020 11:15 AM - 2:03 PM
Session B61 DMP DCMP DCOMP: Fe-Based Superconductors - Mayorana / Topological Mile High Ballroom 4B - Yanwei Ma - Tag(s): Focus
Majorana fermions can be realized as quasiparticle excitations in a topological superconductor, whose non-Abelian statistics provide a route to developing robust qubits. In this context, there has been a recent surge of interest in the iron-based superconductor, FeSe$_{0.5}$Te$_{0.5}$. Theoretical calculations have shown that FeSe$_{0.5}$Te$_{0.5}$ may have an inverted band structure which may lead to topological surface states, which can in turn host Majorana modes under certain conditions in the superconducting phase. Furthermore, recent STM studies have demonstrated the existence of zero-bias bound states inside vortex cores which have been interpreted as signatures of Majorana modes. While most recent studies have focused on Majorana bound states, more generally, akin to elementary particles, Majorana fermions can propagate and display linear dispersion. These excitations have not yet been directly observed, and can also be used for quantum information processing. This talk is focused on our recent work in realizing dispersing Majorana modes. I will describe the conditions under which such states can be realized in condensed matter systems and what their signatures are. Finally, I will describe our scanning tunneling experiments of domain walls in the superconductor FeSe$_{0.45}$Te$_{0.55}$, which might potentially be first realization of dispersing Majorana states in 1D.
11:51AM B61.00002: Longer-range exchange interaction in iron-based superconductors: First-principles studies* WEIGUO YIN (Presenter), Brookhaven National Laboratory — The nature of strong electronic correlations in iron-based superconductors (FeSCs) was shown to be kin to manganites where localized spins and itinerant electrons coexist and are coupled by Hund’s rule interaction, leading to fierce competition between superexchange antiferromagnetism and orbital-degenerate double-exchange ferromagnetism [1,2]. This implies that in a low-energy spin-only description of FeSCs where the itinerant-electron degree of freedom were integrated out, the effective exchange interactions would have been long ranged. The spin dynamics in FeSCs has been interpreted by using such spin-only Heisenberg models with exchange couplings extended to the third nearest neighbors, i.e., the J1-J2-J3 model. Here, we use first-principles calculations on the K2Fe4Se5 and KFeAgTe2 insulators to demonstrate the importance of J4 the effective exchange between the fourth nearest neighbors. We further reveal that the band gap of K2Fe4Se5 or KFeAgTe2 is not of Mott type but the gap of Hund's metal. Our findings shed a new light on the understanding of FeSCs and the puzzling strong magnetic fluctuations in FeSe in particular. [1] PRL 105, 107004 (2010); [2] PRB 86, 081106(R) (2012).

*This work was supported by US DOE Office of Basic Energy Sciences under contract DE-SC0012704.

12:03PM B61.00003: Quasiparticle self-consistent GW analysis in iron-based superconductors KATSUHIRO SUZUKI (Presenter), Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, TAISHI OGURA, Department of Physics, Ritsumeikan University, HIROFUMI SAKAKIBARA, TAKAO KOTANI, Department of Applied Mathematics and Physics, Tottori University, HIROAKI IKEDA, Department of Physics, Ritsumeikan University — Since the early theoretical study of iron-based superconductors, the density functional theory (DFT) has given great contributions to understand material properties, e.g. magnetic/orbital structure, pairing mechanism of superconductivity, etc. However, the LDA/GGA exchange-correlation potential in conventional DFT calculations is insufficient to describe the electronic state observed experimentally, such as in the angular resolved photoemission spectroscopy (ARPES) and de Hass van Alphen (dHvA) measurement [1-3]. In this study, we calculated the electronic band structure of iron-based superconductors with the quasiparticle self-consistent GW (QSGW) method. We found that the QSGW can improve the LDA/GGA band structure and Fermi surface in most cases. We will summarize the result and discuss the superconducting gap in the obtained QSGW band structure. [1] A. A. Kordyuk et al., Phys. Rev. B 83 134513 (2011). [2] K. Okazaki et al., Science 337 1314 (2012). [3] T. Terashima et al., J. Phys. Soc. Jpn. 79 053702 (2010).
12:15PM B61.00004: Search for evidence of quantum anomalous vortices in Iron-based Topological Superconductor Fe$_{1+y}$Te$_{1−x}$Se$_x$  LU LI (Presenter), LU CHEN, ZIJI XIANG, COLIN TINSMAN, Univ of Michigan - Ann Arbor, GENDA GU, Brookhaven National Laboratory — Topological superconductivity makes it possible for fault-tolerant quantum computations. Fe-based superconductors are a rich material family of intermetallic compounds for high-temperature superconductivity. The interplay between these two exciting fields creates an emergent new field, marked by recent discoveries of the superconducting Dirac surface state and Majorana bound states at the vortex cores in iron-based superconductors Fe$_{1+y}$Te$_{1−x}$Se$_x$. However, the direct electronic transport consequence is not clear out of these topological superconducting states. We are left wondering how to operate these novel excitations. We solve the problem by thermally drive ordinary superconducting vortices around these Majorana zero modes and search for a transverse electrical response. This scheme is the Nernst effect in the superconducting state. A finite Nernst signal is observed at zero fields in the superconducting states of Fe$_{1+y}$Te$_{1−x}$Se$_x$. This anomalous Nernst signal shows field-symmetric dependence on the external magnetic field. Our experiments provide the first evidence of broken time-reversal symmetry in topological superconductors and point to a new method to engage Majorana zero mode excitations in transport properties.

12:27PM B61.00005: The Triplet Resonating Valence Bond State and Superconductivity in Hund's Metals: I Concept and Symmetries*  PIERS COLEMAN (Presenter), YASHAR KOMIJANI, ELIO KOENIG, Rutgers University, New Brunswick — A central idea in strongly correlated systems is that doping a Mott insulator leads to a superconductor by transforming the resonating valence bonds (RVBs) into spin-singlet Cooper pairs. Here, we argue that a spin-triplet RVB (tRVB) state, driven by spatially, or orbitally anisotropic ferromagnetic interactions can provide the parent state for triplet superconductivity. One of the new features of the concept, is that triplet RVB bonds can resonate into the interior of an atom, where they are supported as Hund’s coupled triplet states between orbitals at the same site. Remarkably though, simple symmetry arguments due to P. W. Anderson, mean that such a process can only develop coherence with triplet pairs on the Fermi surface, if the there are two symmetry related atoms per unit cell, leading to a state that has staggered structure of onsite pair correlations that can be detected using Josephson tunneling. A natural candidate for this physics are the iron based superconductors, as will be described in the two following talks [1].


*  This work was supported by DOE Basic Energy Sciences grant DE-FG02- 99ER45790.
12:39PM B61.00006: Title: The Triplet Resonating Valence Bond State and Superconductivity in Hund's Metals: II Mean-field theory*  
PIERS COLEMAN, YASHAR KOMIJANI (Presenter), ELIO KOENIG, Rutgers University, New Brunswick — Triplet resonating valence bond (tRVB) states are entangled states that are produced in anisotropic magnetic environments [1], just like how singlet RVB states arise in frustated antiferromagnetic systems. A single Iron atom in a cubic environment contains miniature triplet states resonating between various t2g orbitals of the d-shell due to the large Hund's coupling. I will discuss how this can be used to derive a local inter-orbital triplet pairing applicable to Iron-based superconductors [2]. While the order parameter contains significant inter-band pairing, the projection on the Fermi surface appears as an odd-parity intra-band triplet pairing which enjoys a weak-coupling instability and gaps out the entire Fermi surface. In analogy with the RVB theory, a Gutzwiller projected variational mean-field is suggested for the ground state. Furthermore, we augment our mean-field theory using a Kotliar-Liu slave-boson approach to include the effect of intra- and inter-orbital interactions. 
Experimental signatures of the proposed triplet superconductor are discussed in the next talk.


*This work was supported by DOE Basic Energy Sciences grant DE-FG02-99ER45790.

PIERS COLEMAN, YASHAR KOMIJANI, ELIO KOENIG (Presenter), Rutgers University, New Brunswick — Based on the triplet Resonating Valence Bond concept introduced in the previous two talks, I will discuss the prospects and signatures of this theory in the context of iron based superconductors. I will explicitly concentrate on the spin-triplet, orbital antisymmetric pairing state as derived in part II and on four experimental techniques of fundamental interest: (1) nuclear magnetic resonance, (2) neutron scattering, (3) tunneling spectroscopy, (4) scanning Josephson tunneling microscopy.

First, I will demonstrate that this pairing state develops an anisotropic, partial suppression of the Knight shift and discuss existing experimental data on single crystals. Second and third, I will demonstrate that the relative sign between triplet d-vectors of electron and hole pockets crucially affects finite frequency spin-susceptibility and local density of states. I will discuss the consequences thereof for key experimental observables, i.e. a sharp subgap spin-resonance and characteristic quasi-particle interference patterns, that previously were interpreted as evidence for $s_\pm$ pairing. Finally, I describe experimental signatures of the staggered order parameter in scanning Josephson microscopy.

*This work was supported by DOE Basic Energy Sciences grant DE-FG02-99ER45790.
1:03PM B61.00008: Unconventional superconductivity and Hund's induced electron correlations: a Cooperative mechanism* LAURA FANFARILLO (Presenter), University of Florida, ANGELO VALLI, Institute for Solid State Physics, Vienna University of Technology, MASSIMO CAPONE, SISSA — The phenomenology of iron-based superconductors shows that the normal state is a bad metal characterized by orbital-selective correlations induced by the Hund's exchange coupling, suggesting an important role of the electron-electron interactions. On the other hand theories based on the exchange of bosons (e.g. spin fluctuations) describe correctly a variety of phenomena pointing towards a more standard pairing mechanism.

To overcome this dychotomy we study how a multiorbital superconducting pairing driven by a generic weak-coupling boson exchange is affected by the presence of correlations. The key novelty of the study is the inclusion of the dynamical properties that make a Hund's metal substantially different with respect to both a weakly interacting metal and to an ordinary correlated metal with a large effective mass renormalization. We unveil the crucial role of the redistribution of spectral weight of the Hund's metal to promote superconductivity and to enhance the orbital-selective character of the gap functions.


1:15PM B61.00009: Hund-enhanced electronic compressibility in LiFeP, LiFeAs and NaFeAs tuned by chemical substitution* PABLO VILLAR ARRIBI (Presenter), Argonne Natl Lab, LUCA DE MEDICI, ESPCI ParisTech — We study the electronic structure of LiFeP, LiFeAs and NaFeAs in their paramagnetic metallic phase including dynamical electronic correlations within a density functional theory + slave-spin mean-field framework. Our results show that the three compounds are next to the crossover between a normal and a Hund's metal, where a region of enhanced electronic compressibility that may be relevant for superconductivity is present in this type of systems. While LiFeP and LiFeAs lie in the normal metallic regime, with LiFeAs in the vicinity of the crossover, NaFeAs is in the Hund's metal regime, which explains the different behavior observed in these materials. Our findings correlate positively with the experimental trends for doping- and pressure-dependence of superconductivity in these compounds, as well as the predicted mass renormalizations and Sommerfeld coefficients.

* The authors are funded by the European Commission through the ERC-StG2016, StrongCoPhy4Energy, GA No724177
1:27PM B61.00010: Modified pairing structure due to momentum-dependent correlations in iron-based superconductors* SHINIBALI BHATTACHARYYA (Presenter), PETER HIRSCHFELD, University of Florida, THOMAS MAIER, Oak Ridge National Laboratory, DOUGLAS J SCALAPINO, University of California, Santa Barbara — We discuss the influence of momentum-dependent correlation effects arising from particle-hole interactions on the superconducting gap structure of iron-based superconductors. Within the Eliashberg formalism, we obtain a modified linearized gap equation arising from the spin-fluctuation interaction in the weak-coupling regime which includes self-consistent renormalizations of quasiparticle weights. The modification of the particle-particle interaction vertex by particle-hole processes modifies the superconducting gap structure, i.e. momentum-dependent enhancement or suppression of gap amplitude compared to traditional spin-fluctuation pairing calculations. We obtain good agreement with experimentally observed anisotropic gap structures in LiFeAs, indicating that inclusion of non-local correlation effects in the existing weak-coupling theories can account for observed signatures of the correlated iron-based superconductors.

*Shinibali Bhattacharyya acknowledges support in part through an appointment to the Oak Ridge National Laboratory ASTRO Program, sponsored by the U.S. Department of Energy and administered by the Oak Ridge Institute for Science and Education.

1:39PM B61.00011: Systematic derivation of ab initio effective Hamiltonians for iron-based superconductors* TAKAHIRO MISAWA (Presenter), KOTA IDO, YUICHI MOTOYAMA, KAZUYOSHI YOSHIMI, University of Tokyo, Institute for Solid State Physics — Iron-based superconductors have attracted much attentions since its discovery at 2008. Owing to huge amount of studies, more than a dozen iron-based superconductors including related compounds have been found. In this study, combining the first-principles calculations and accurate numerical methods for treating quantum lattice models [1], we systematically obtain and analyze first-principle effective Hamiltonians of more than 20 iron-based superconductor and the related compounds. We perform the band calculation using Quantum ESPRESSO [2], derive the ab initio effective Hamiltonians using RESPACK [3], and analyze the Hamiltonians using mVMC [4]. As a result, we show the materials dependence of the microscopic parameters/physical quantities, and their relations with the superconducting transition temperatures.

[3] https://sites.google.com/view/kazuma7k6r

*This research was conducted as a joint research with Toyota Motor Corporation.
Topological bands in Fe(Se,Te)*  

TAMAGHNA HAZRA (Presenter), Physics, Ohio State University, HIMANSHU LOHANI, AMIT RIBAK, YUVAL NITZAV, Physics, Technion - Israel Institute of Technology, HUIXIA FU, BINGHAI YAN, Condensed Matter Physics, Weizmann Institute of Science, MOHIT RANDERIA, Physics, Ohio State University, AMIT KANIGEL, Physics, Technion - Israel Institute of Technology — Bulk FeSe$_{0.45}$Te$_{0.55}$ has recently emerged as a promising candidate to host topological superconductivity on its surface, with experimental signatures for a Dirac surface state and Majorana bound states in vortex cores. However, ARPES measurements of the bulk band structure show essentially no $k_z$ dispersion, in apparent contradiction with DFT predictions for the significant $k_z$ dispersion that drives the band inversion.

We reconcile the observed lack of dispersion with the predicted band inversion using a tight binding model with strongly renormalized inter-layer hopping and reasonable values of spin-orbit coupling. We use symmetry arguments to identify a sharp signature of bulk band inversion in the photon energy dependence of the ARPES matrix elements. We test our prediction for the change in orbital character of the band using ARPES data with a wide range of photon energies covering several Brillouin zones along $k_z$. We thus provide direct evidence for the non-trivial topology of the bulk bands in Fe(Se,Te), where the band inversion occurs in a nearly flat band due to an interplay of strong correlations and topology.

*Work supported by US-Israel Binational Science Foundation grant 2014077 and Israeli Science Foundation Grant 320/17.

Monday, March 2, 2020 11:15 AM - 2:03 PM

Session B62 DMP: Nanostructures and Metamaterials II  

Mile High Ballroom 4C - Hou-Tong Chen, Los Alamos Natl Lab - Tag(s): Focus
11:15AM B62.00001: Nonlinear Optical Metasurfaces* [Invited] IGAL BRENER (Presenter), Center for Integrated Nanotechnologies, Sandia National Laboratories — Nonlinear optics is a decades-old, well-established discipline that normally relies on macroscopic media and propagation lengths that are much longer than the wavelength. Recent progress in artificially structured materials has enabled a resurgence of this field into new directions and phenomena. Examples are increased efficiencies using materials that were not useful for bulk nonlinear optics and complete relaxation of phase matching conditions. In this talk I will cover some of these new developments in nonlinear optical metasurfaces and hybrid nonlinear metasurfaces that include semiconductor quantum wells.

*This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering and performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

11:51AM B62.00002: Microwave hybrid resonance with an electromagnetic metasurface XIAONAN ZHANG (Presenter), PING SHENG, Hong Kong University of Science and Technology — Hybrid resonances were discovered in acoustics a few years ago. Here we demonstrate through full waveform simulations the realization of microwave hybrid resonance by using a simple H-fractal metallic metasurface, with unit cell's lateral dimension much subwavelength in size. With an extremely thin back cavity, the resonances of the metallic structure at different frequencies can be hybridized to generate a new mode near the anti-resonance frequency. The oscillator strength and dissipation power of the hybrid resonance can be easily tuned, with total absorption occurring when the surface impedance matches that of vacuum. Similar to the acoustic case, the local fields are found to be much larger than the incident wave amplitude while the surface averaged fields are comparable to the incident fields. The total thickness of the surface is less than the peak absorption wavelength by two orders of magnitude. And we also found this microwave hybrid resonance by using the metallic metasurface and its complementary structure, which is hard to achieve in acoustics.
12:03PM B62.00003: Regular sloshing modes in irregular cavity using metabathymetry
ADAM ANGLART (Presenter), Physique et Mecanique des Milieux Heterogènes (PMMH), AGNES MAUREL, Institut Langevin, ESPCI, PHILIPPE PETITJEANS, Physique et Mecanique des Milieux Heterogènes (PMMH), VINCENT PAGNEUX, Laboratoire d'Acoustique de l'Université du Maine — We demonstrate experimentally and numerically that metamaterials can be used to control water wave propagation and resonance properties of a closed cavity. The anisotropic medium, designed using coordinate transformation theory [1] and the homogenization of fully three-dimensional linear water wave problem [2], consists of a bathymetry with a layered structure at a subwavelength scale. Three cavities with bending angles of 15°, 30° and 45° are tested and compared to a reference case with flat bathymetry. Fourier Transform Profilometry [3] as well as Confocal Displacement Sensors are used for space-time resolved measurements of a water surface deformation. Experimental data show the capability of water-wave metamaterials to provide a robust anisotropic medium for wave propagation.

References

12:15PM B62.00004: Measurement of asymmetrical water waves wake due to an anisotropic bathymetry
LEO-PAUL EUVE, PHILIPPE PETITJEANS (Presenter), AGNES MAUREL, ESPCI Paris, VINCENT PAGNEUX, LAUM, Univ. du Maine, France — Metamaterials have the surprising property of modifying the wave propagation, and more precisely in our investigation, the waves forming the wakes. One example of wakes in metamaterials is the study of Luo et al [1] describing different behavior for the Cerenkov radiation in a photonic crystal. In our case, we consider ship wakes. This domain have received considerable attention over the last decade, even though this specific field of water waves has been studied for almost a century and a half, if we refered to the Lord Kelvin studies.

We show, experimentaly, that ship wakes can become highly asymmetrical when they propagate on an anisotropic metamaterial. In our study, the metamaterial is obtained with a periodic stratified bathymetry which varies at a subwavelength order. More precisely, vertical plates are placed in parallel on the bottom of a water tank, as in [2,3]. The experimental results can be numerically reproduced using a theory based on an anisotropic dispersion relation [3].

References
12:27PM B62.00005: High-index nanostructures and layered materials for light scattering control

VIKTORIIA BABICHEVA (Presenter), Electrical and Computer Engineering, University of New Mexico — Planar optical elements with efficient light control at the nanoscale can be designed based on transdimensional photonic lattices that operate in the translational regime between two and three dimensions. Such transdimensional lattices include 3D-engineered nanoantennas supporting multipole Mie resonances and arranged in the 2D arrays to harness collective effects in the nanostructure [1]. Optical antennas made out of van der Waals material with naturally-occurring hyperbolic dispersion is a promising alternative to plasmonic and high-refractive-index dielectric structures in the practical realization of nanoscale photonic elements. The antenna made out of hexagonal boron nitride (hBN) possesses different multipole resonances enabled by the supporting high-k modes and their reflection from the antenna boundaries. The full range of the resonances is demonstrated for the hBN cuboid antenna, a decrease of reflection from the array, and highly directional resonant scattering from antennas pairs. We show that transdimensional lattices consisting of resonant hBN antennas in the engineered periodic arrays have great potential to serve as functional elements in ultra-thin optical components and photonic devices. [1] V.E. Babicheva, MRS Advances 4, 713 (2019).

*AFOSR grant FA9550-19-1-0032.

12:39PM B62.00006: Towards perfect absorption via block copolymer designed metasurfaces

CIAN CUMMINS (Presenter), QUENTIN FLAMANT, ALEXANDRE BARON, Centre de Recherche Paul Pascal, University of Bordeaux, GEORGES HADZIOANNOU, GUILLAUME FLEURY, University of Bordeaux, VIRGINIE PONSINET, Centre de Recherche Paul Pascal, University of Bordeaux — Engineering light-matter nanoscale interactions has diverse applications for advancing optical nanodevices, sensors, and energy harvesting. An emerging route to realise perfect absorption is based on artificial ultrathin nanosurfaces, known as “metasurfaces”.1 We describe a versatile metasurface fabrication strategy based upon gold (Au) selective deposition in block copolymer (BCP) templates towards perfect absorption. Since BCPs can be patterned over large wafer scale areas (i.e. 300 mm) and are industry compatible, they offer a viable path towards realising nanophotonic devices.2 Here, we describe a Au−Al₂O₃−Au stack layer for perfect absorption at visible frequencies using BCP templating. Our approach opens up a flexible methodology to precisely tune Au nanostructure height, e.g. 5-30 nm and resulting absorption wavelength range. The ability to tailor Au features precisely is extremely appealing and surpasses various wet chemical approaches that cannot be processed in thin film form. We will present key experimental parameters guided by numerical simulations to show the effect of Au height and stack architecture on absorption properties.

12:51PM B62.00007: Femtosecond Polarization Pulse Shaping by Dielectric Metasurfaces

LU CHEN (Presenter), WENQI ZHU, National Institute of Standards and Technology, JUNYEOB SONG, Electrical and Computer Engineering, Virginia Tech, JARED H STRAIT, CHENG ZHANG, National Institute of Standards and Technology, WEI ZHOU, Electrical and Computer Engineering, Virginia Tech, HENRI J LEZEC, AMIT AGRAWAL, National Institute of Standards and Technology — Metasurfaces are ultra-thin, planar optical elements that have been successfully employed for a variety of spatial-domain wavefront manipulations[1]. Recently, the time-domain shaping of a large bandwidth, near-infrared femtosecond pulse was demonstrated using dielectric metasurfaces. Simultaneous and independent control of the phase and amplitude of frequency components of a pulse enables finely tailored pulse-shaping operations, including splitting, compression, chirping and higher-order distortion[2]. Here, we further exploit dielectric metasurfaces to control the temporal polarization state within a single pulse. Such an approach expands the versatility of the already fruitful metasurfaces, revealing new possibilities in the field of ultrafast science and technology.


*The authors acknowledge support under the Cooperative Research Agreement between the University of Maryland and the National Institute of Standards and Technology Physical Measurement Laboratory, Award#70NANB14H209, through the University of Maryland.

1:03PM B62.00008: Broadband Linear-to-Circular Polarization Conversion Enabled by Birefringent Off-Resonance Reflective Metasurfaces

DONGFANG LI (Presenter), CHUN-CHIEH CHANG, Los Alamos National Laboratory, ZHEXIN ZHAO, Stanford University, ANTOINETTE TAYLOR, Los Alamos National Laboratory, SHANHUI FAN, Stanford University, HOU-TONG CHEN, Los Alamos National Laboratory — Circularly polarized light in the terahertz (THz) regime is essential for a variety of scientific research and technological applications. However, it is challenging to achieve broadband circular polarization at these long wavelengths due to the dispersion of common birefringent materials. Here we propose and demonstrate the broadband linear-to-circular polarization conversion with up to 80% fractional bandwidth and near-unity power conversion efficiency based on the coupled-mode theory using reflective birefringent metasurfaces [1]. The arbitrary rotation of a linear polarization can also be achieved by leveraging the design parameters of the unit cell. This novel design approach can be further expanded to the mid-infrared and visible regimes by simply scaling the size of the structure. The realization of the polarization converter and rotator may significantly enrich the polarization-based optical probe of matter, including circular dichroism spectroscopy at THz regime and studies of the rising quantum materials.

1:15PM B62.00009: Constructing broadband multifunctional wave plates with stereo-metastructures*  
SIJIA SUN, XIANG XIONG (Presenter), YAJUN GAO, RUWEN PENG, MU WANG, 
Nanjing Univ — Polarization is one of the most important properties of light. Over the past few years, the development of metamaterials offers different approaches to manipulate the polarization state. Most designs are based on resonantly coupling. Due to the high losses and strong dispersion, their working frequency ranges are usually narrow. The multifunction design is another approach to integrating the element. Realizing different functionalities with one element can miniaturize the element. However, due to the uncontrollable electro-magnetic coupling between different parts, the multifunctional metastructures is difficult. Here we demonstrated two 3D broadband multifunctional wave plates. Simulated and experimental results indicate that half wave plate and quarter wave plate functions can be realized separately at lower and higher frequency with one metastructure. Moreover, coding and display depending on polarization were also proposed. Our work provides a new idea for design of highly compact metastructure and shows prospects for applications in display technology.

*National Natural Science Foundation of China(11474157, 11574141, 11634005, 11674155); Natural Science Foundation of Jiangsu Province (BK20160065, BRA2016350); National Key RD Program of China (2017YFA0303702)

1:27PM B62.00010: Optical properties of plasmonic metasurface with sub-nm gaps - Refractive index variation originating from electron transports -  
TAKASHI TAKEUCHI (Presenter), MASASHI NODA, KAZUHIRO YABANA, Univ of Tsukuba — Plasmonic metasurfaces consisting of two-dimensionally arrayed metallic nano-objects on a plane have drawn attention in terms of its exotic optical characteristics. Although investigations of metasurfaces conducted to date have focused on structures with sub-wavelength spatial scale, recent experimental studies have demonstrated those with much smaller size in which the gap distances between the nano-objects reach to sub-nm length where quantum mechanical effects becomes important. In our presentation, we theoretically and numerically investigate the plasmonic metasurface with sub-nm gaps in terms of the refractive index variation due to quantum mechanical effects. To take into account quantum mechanical effects in the analysis, we employ time-dependent density functional theory(TDDFT) treating the constituent nano-particles by a jellium model. Furthermore, to distinguish the importance of the quantum mechanical effects, another simulation based on conventional classical electromagnetism is also employed and compared with the TDDFT. SALMON(https://salmon-tddft.jp/) developed by our group has been used for those numerical calculations. We will show that drastic change of the refractive index starts around gap distances 0.2 nm where electron transports take an important place.
1:39PM B62.00011: Dynamic Switching between Surface Wave and Plane Wave with MEMS-based Metasurface* CHUNXU CHEN (Presenter), XIAOGUANG ZHAO, Boston Univ, KELSON KAJ, IAN HAMMOCK, University of California, San Diego, KE WU, Boston Univ, RICHARD AVERITT, University of California, San Diego, XIN ZHANG, Boston Univ — We present polarization-insensitive dynamic surface wave (SW) switching at terahertz frequencies utilizing a MEMS-based metasurface. Our MEMS-based metasurface consists of a micro-cantilever array, enabling dynamic tuning between a plane wave (PW) and a SW for normal incidence of terahertz radiation. Through individual control of the driving voltages on the cantilever unit cells, we achieve nearly 2π phase modulation with minimal reflection amplitude modulation. Coupled mode theory (CMT) is employed to design the metasurface device and agrees with full-wave electromagnetic simulations. Our demonstration paves the road for terahertz multifunctional metasurface devices for spatial light modulation, dynamic beam steering, focusing, and beam coupling.

*Research supported by National Science Foundation under Grant No. ECCS-1810252.

1:51PM B62.00012: Dynamically-tunable metastructures based on phase transition of vanadium dioxide RUWEN PENG (Presenter), F. Z. SHU, J. N. WANG, Nanjing University, China, YONGMIN LIU, Northeastern University, Boston, USA, MU WANG, Nanjing University, China — Tunable nanophotonic materials and devices are drawing intense attention with great promise for practical applications. In this work, we have experimentally demonstrated several dynamically-tunable metastructured devices based on phase transition of vanadium dioxide, which include dynamic plasmonic color generators, dynamically switchable polarizers, and dynamically tunable bowtie nanoantennas. First, we have fabricated periodic arrays of silver-nanodisks on a vanadium dioxide film to realize different colors, relying on the excitation of localized and propagating surface plasmons. Based on insulator-metal transition of vanadium dioxide, the plasmonic colors can be actively tuned by varying temperature. Second, we have demonstrated a system consisting of anisotropic plasmonic nanostructures with vanadium dioxide that exhibits distinct reflections subjected to different linearly polarized incidence at room temperature and in the heated state. Third, we have made the dynamically tunable bowtie nanoantennas integrated on a vanadium dioxide thin film. The investigations here can be applied in dynamic digital displays, optical data storage, and imaging sensors. References: 1) Adv. Opt. Mater.(2018) 6, 1700939; 2) Phys. Rev. Appl. (2018) 9, 034009; 3) Opt. Lett. (2019) 44, 2752.
Metasurfaces have enabled unprecedented control of the phase, amplitude, and polarization of optical wavefronts, providing new opportunities in areas such as negative refraction and optical cloaking. The fabrication of optical metasurfaces still requires complex processing techniques that include additive or subtractive methods. Here we electrically create metasurfaces in VO$_2$ thin film by using a resist layer with periodic boomerang-shaped orifices to strictly confine the metallic VO$_2$ antennas induced by ionic liquid gating within the insulating VO$_2$ matrix. The non-volatile insulator-to-metal transition in VO$_2$ is due to a tiny reduction of oxygen content of the VO$_2$ under ionic liquid gating. Such optical plasmonic metasurfaces, with metallic VO$_2$ feature sizes ranging from 100 to 500 nm, allow the complete phase control ($-\pi$ to $\pi$) and orthorhombic polarization switching of light in the mid infrared range. Our result represents a new paradigm for the fabrication and manipulation of optical metamaterials.

*We acknowledge partial funding from the EU H2020 program “Phase Change Switch”.

Monday, March 2, 2020 11:15 AM - 2:15 PM
Electronic Structure of Tetragonal CH$_3$NH$_3$PbI$_3$ * JEEHONG PARK (Presenter), DONGHEE KANG, JAEHYUN YANG, YOUNG WOO CHOI, Institute of Physics and Applied Physics, Yonsei University, SOONSANG HUH, Center for Correlated Electron Systems, Institute for Basic Science, HYOUNG JOON CHOI, Institute of Physics and Applied Physics, Yonsei University, CHANGYOUNG KIM, Center for Correlated Electron Systems, Institute for Basic Science, HYUNBOK LEE, Department of Physics, Kangwon National University, YEONJIN YI, Institute of Physics and Applied Physics, Yonsei University — Organic-inorganic halide perovskites (OIHP) have been highlighted in optoelectronics research area for the last decade. OIHPs exhibit long carrier diffusion length ($\lambda$) despite of its moderate-to-low mobility ($\mu$). In case of CH$_3$NH$_3$PbI$_3$, the highest value of reported $\lambda$ reaches beyond $\mu$m while the $\mu$ is about only <100cm$^2$s$^{-1}$V$^{-1}$. Several underlying mechanisms have been proposed in order to account for the unusual transport property. One of them is the suppression of charge-carrier recombination by formation of spin-polarized indirect bandgap due to the Rashba effect. However, experimental evidence of such effect is lacking so far and there are ongoing debates regarding its presence and effectiveness. In this presentation, we present our unprecedented high-quality ARPES results measured on single crystal CH$_3$NH$_3$PbI$_3$ (001) surface. We also show circular dichroism ARPES (CD-ARPES) from which we can exploit the information about spin-polarization of electronic structure and discuss the compatibility of the Rashba scenario. We believe our work provides important experimental evidence of one of the most debatable issues in OIHPs.

*This study was supproted by the NRF of Korea [NRF-2018R1D1A1B07051050, 2018R1A6A1A03025582 and 2017R1A5A1014862 (SRC program: vdWMRC center)]

Wavelength Dependent Photostability of Perovskite Thin Films * BEN ECKER (Presenter), KE WANG, YONGLI GAO, University of Rochester — In the ten years since their first reported use in a photovoltaic device, hybrid organic-inorganic perovskite solar cell's power conversion efficiencies have surpassed 25% and further research efforts have continued to improve their scalability and long-term operational stability. One stability that has to be thoroughly investigated is the long term photostability of the perovskite materials. Here we will present our recent in-situ wavelength-dependent photostability investigation on bare perovskite thin films. Pristine co-evaporated CH$_3$NH$_3$PbI$_3$ thin films were initially grown on pyrolytic graphite surfaces, and they were then illuminated for prolonged durations to approximately 1 sun (1mW/mm$^2$) of either blue (408 nms) or red (650 nms) laser light. The films were maintained under constant vacuum conditions, and x-ray photoemission spectroscopy measurements were taken after each exposure. The dichotomy of the behavior of the films while under either the red or blue light, is suggestive of a wavelength dependence to the degradation mechanisms.

*This work was supported by the NSF GR1903962.
11:39AM B63.00003: Excitonic behavior in hybrid halide perovskite for optoelectronic applications  
HYE RI JUNG (Presenter), WILLIAM JO, EWHA Woman's Univ — Organic-inorganic lead halide perovskites, \( \text{CH}_3\text{NH}_3\text{PbX}_3 \) (\( \text{X} = \text{Cl}, \text{Br}, \text{I} \)), have gained great attentions for their attractive optoelectronic properties and excellent performances in various optoelectronic devices. To resolve the remained issues and advance the optoelectronic application devices, understanding intrinsic properties of this material is significant. In particular, free carrier and excitonic behaviors play a crucial role to support the charge transport process which aids the advanced device design. We verified structural properties using temperature dependence photoluminescence and transmission spectra. Under 160 K as orthorhombic phase, unusual excitonic behaviors were found near band edge. We also determined surface potential distribution with and without external light source using Kelvin probe force microscopy. We described electronic band structures of halide perovskite effected by photovoltage. Since the large band gap energy about 3 eV, different photovoltages characteristics were displayed depending on the wavelength of the light source, and it is affected by the defect states on the band edges and the bound excitons on the band edge. Those results suggest that the identified perovskite structure and excitonic properties will apply to many optoelectronic devices.

11:51AM B63.00004: Recombination Dynamics of Chlorine Doped Hybrid Perovskite Single Crystals*  
LA MOYNE MIX (Presenter), MIN-CHEOL LEE, KENNETH O'NEAL, NICHOLAS SIRICA, JEREMY TISDALE, WANYI NIE, ROHIT P PRASANKUMAR, DZMITRY YAROTSKI, Los Alamos National Laboratory — Controlling the photo excited properties and behavior of hybrid perovskites by halide doping has the potential to impact a wide range of emerging technologies, including solar cells and radiation detectors. Crystalline samples of methyl ammonium lead bromide (MAPbBr) were substituted with varying levels of Cl at the c site and probed with transient reflectivity spectroscopy. MAPbBr perovskites exhibit an increase in transient reflectivity following photoexcitation, with electron-phonon relaxation on a few picosecond timescale and a triple exponential recombination dynamic which is not complete after 1.5 nanoseconds. The recombination dynamics strongly depend on pump fluences, while the electron-phonon relaxation remains unchanged. We also observed that the doping level affected the electron-phonon coupling within the conduction band, becoming stronger with increased percentage of Cl.

*Research presented in this report was supported by the Laboratory Directed Research and Development program of Los Alamos National Laboratory under project number 20180283ER. This work was performed at the Center for Integrated Nanotechnology user facility at Los Alamos National Laboratory.
12:03PM B63.00005: Ultrafast Carrier Dynamics of Dual Emissions from Methylammonium Lead Iodide Perovskites*  MARIA MUNOZ (Presenter), Florida International University, MICHAEL TITZE, Sandia National Laboratories, FEI CHENGBIN, Department of Physics, University of Miami, XUEWEN WANG, Florida International University, HE WANG, Department of Physics, University of Miami, HEBIN LI, Florida International University — Hybrid lead iodide perovskites have been attractive for its optical properties for many applications in different fields. One of the most promising applications is as a material for future generation of solar cells. The understanding of the photoexcitation dynamics is very important for improving their performance in solar cells and other applications. We implemented optical two-dimensional coherent spectroscopy to study the carrier dynamics and coupling of dual emissions in Methylammonium Lead Iodide film at 115 K. The sample was prepared by spin-coating perovskite precursor onto a glass substrate and successive annealing at 100 °C. From the 2D spectra we observed an ultrafast redistribution of the photoexcited carriers into the two emission resonances. The dynamics of carrier relaxation into the high energy and low energy resonance are different. The high-energy resonance is a short-lived transient state. The low-energy resonance has a longer lifetime and interacts with coherent phonons.

*M.T acknowledges FIUs DYF fellowship funding. The work at FIU is supported by ARO Grant No. W911NF-17-1-0497. C.F. and H.W. acknowledge support provided by the Air Force Office of Scientific Research (AFOSR) Award FA9550-17-1-0099.

12:15PM B63.00006: Third-order optical nonlinearities of lead halide perovskite single crystals*  KEIICHI OHARA (Presenter), TAKUMI YAMADA, HIROKAZU TAHARA, TOMOKO AHAREN, HIDEKI HIRONI, Kyoto Univ, HIDEKATSU SUZUURA, Hokkaido Univ, YOSHIHIKO KANEMITSU, Kyoto Univ — Lead halide perovskite semiconductors, MAPbX$_3$ (MA = CH$_3$NH$_3$, X = I, Br, and Cl), have attracted much attention as a new class of photonic device materials because of their excellent optoelectronic properties. Recently, we found unique nonlinear optical responses such as large optical modulation [1] and efficient higher-order harmonic generation [2] in MAPbX$_3$ perovskites. However, the origin of large nonlinear optical responses remains unclear. In this work, we determined the third-order nonlinear optical coefficients of the wide-gap semiconductor MAPbCl$_3$ single crystals by using the Z-scan method. We measured the excitation wavelength and polarization dependences of these coefficients. It is found that the absolute values of coefficients depended on the crystal orientation of perovskite single crystals. These excitation wavelength dependences can be quantitatively explained by a two-band model including the exciton effect and Kane’s kp theory. The Kane energy and the exciton reduced mass of MAPbCl$_3$ were determined [3].


*Part of this work was supported by KAKENHI (19H05465) and JST-CREST (JPMJCR16N3).
12:27PM B63.00007: Fine Features of Free and Bound Excitons in the Photoluminescence of Single Crystal MAPbI$_3$*  MATTHEW SHEFFIELD (Presenter), YUE YAO, ISAAC P BROWN HEFT, HESHAN HEWA WALPITAGE, University of Utah, YE LIU, ZHENYI NI, JINSONG HUANG, University of North Carolina at Chapel Hill, YAN LI, University of Utah — Understanding the photoluminescence (PL) characteristics and exciton properties of hybrid organic-inorganic perovskites (HOIPs) plays a key role in optimizing their performance in optoelectronic devices. In particular, PL is an important technique for the investigation of carrier-phonon interactions and quantification of defects in a system. However, these properties are inaccessible when important signatures are masked by the wide inhomogeneous broadening seen in polycrystalline films, which are commonly used in devices. Here, we study PL on high quality MAPbI$_3$ single crystals in the orthorhombic phase. The high crystalline quality and well controlled defect density allow us to obtain PL spectra with narrow features and reveal new ones that were not resolvable before. Temperature dependence and excitation intensity dependence data clearly show features of the free exciton and several bound excitons, with consistent energy levels verified among several samples. Assignment of each peak will be discussed, as well as exciton binding energy and exciton-phonon couplings. These newly resolved fine features on high quality single crystals will allow further in-depth studies of the intrinsic photophysics and defect properties related to growth conditions in HOIPs.

*DOE, EFRC CHOISE
12:39PM B63.00008: Spintronic Terahertz Emission by Ultrafast Spin-Charge Current Conversion in Reduced Dimensional Organic-Inorganic Hybrid Perovskites*  
KANKAN CONG, Advanced Photon Source, Argonne National Laboratory, ERIC VETTER (Presenter), Physics, North Carolina State University, YAN LIANG, Department of Chemistry, University of North Carolina at Chapel Hill, YI LI, Department of Physics, Oakland University, QI ZHANG, Advanced Photon Source, Argonne National Laboratory, YUZAN XIONG, Department of Physics, Oakland University, HONGWEI QU, Department of Electronic and Computer Engineering, Oakland University, RICHARD D SCHALLER, Advanced Photon Source, Argonne National Laboratory, AXEL HOFFMANN, Materials Science Division, Argonne National Laboratory, ALEXANDER F KEMPER, Physics, North Carolina State University, WEI YOU, Department of Chemistry, University of North Carolina at Chapel Hill, HAIDAN WEN, Advanced Photon Source, Argonne National Laboratory, WEI ZHANG, Department of Physics, Oakland University, DALI SUN, Physics, North Carolina State University — Reduced Dimensional Hybrid Metal Halides (RD-HMHs) are a new class of synthetic semiconductor prepared via low-temperature solution processing with a wide array of possible chemical and structural arrangements enabled by the versatility of their molecular cations. RD-HMHs have already been shown to possess remarkable photovoltaic, excitonic, and optoelectronic properties, but their rich spintronic functionalities have yet to be utilized. We report the successful observation of the inverse Rashba-Edelstein Effect (IREE) in a 2D HMH (BA)$_2$(MA)$_{n-1}$Pb$_n$I$_{3n+1}$ driven by spin pumping from an adjacent ferromagnetic Ni$_{81}$Fe$_{19}$ layer using femtosecond laser pulses. We observed spin-dependent THz radiation at room temperature. The phase of the THz field can be controlled by means of an external magnetic field. Circular polarization dependence of the THz radiation confirms the helicity-dependent directional THz radiation and reveals the Rashba states in the RD-HMH materials. This work opens the door for next generation, low-cost THz emitters with tunable functionalities.

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12:51PM B63.00009: Utrafast Spectroscopy Studies in Chiral Hybrid Perovskites*  
YAXIN ZHAI (Presenter), MATTHEW C BEARD, National Renewable Energy Laboratory — An organic–inorganic hybrid perovskite incorporating chiral organic molecules has been demonstrated as a new class of chiral semiconductors. Here we report our recent studies on the optical and spin properties in FAPbBr$_3$ nanoparticles with different ratio of chiral ligands by using the broadband ultrafast spectroscopy.

*This work was supported by the Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE) an Energy Frontier Research Center funded by the Office of Basic Energy Sciences, Office of Science within the U.S. Department of Energy. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.
1:03PM B63.00010: Exciton decoherence probed by magneto-photoluminescence in halide perovskite bulk single crystals* LIANG TAN (Presenter), Lawrence Berkeley National Laboratory, ALYSSA KOSTADINOV, EFRAT LIFSHITZ, Solid State Institute, Technion — Understanding the physics behind the high performance of lead halide perovskite compounds is an urgent objective of photovoltaics research. Due to the existence of large spin-orbit interactions, the investigation of spin properties in these materials has emerged as the primary consideration for using halide perovskites as building blocks in spin-electronic devices. Herein we report on a combined theoretical and experimental effort to probe spin dynamics in halide perovskites using magneto-optical measurements. We perform magneto-photoluminescence measurements of MAPbBr$_3$ high quality single crystals, observing luminescence intensity suppression and recovery at magnetic fields corresponding to cyclotron frequencies where triplet exciton thermalization is in competition with exciton spin precession into the singlet exciton state. Theoretical modeling of exciton dynamics provides evidence for the existence of an Overhauser effect, arising from spin exchange between the excitonic and nuclear spin systems.

*We acknowledge support from the Molecular Foundry at Lawrence Berkeley National Laboratory, supported by the Office of Science, Office of Basic Energy Sciences, of the US Department of Energy under contract No. DE-AC02-05CH11231.

1:15PM B63.00011: Investigating the Optical and Electrical Properties of Two-dimensional Organic-inorganic Hybrid Perovskite Multiple Quantum Wells via Electroabsorption Spectroscopy Studies* [Invited] LUISA WHITTAKER-BROOKS (Presenter), University of Utah — Despite the tremendous progress observed in the development of high-efficient 3D organic-inorganic halide perovskites (OIHPs) with power conversion efficiencies (PCEs) above 24%, there is still a significant challenge for the field related to addressing their poor stability towards extrinsic (i.e., moisture and oxygen) and intrinsic factors (ion migration, water intake, thermal instability). To ameliorate these notorious pitfalls that deleteriously affect PCEs and the long-term stability of OIHP solar cells, the photovoltaics field has shifted towards developing and understanding the properties of 2D OIHPs as the organic cation spacers comprising these layered systems do provide superb environmental stability to the structure. However, this increase in stability is often accompanied by a decrease in PCEs. Hence, the task posed by the field deals with increasing the PCEs of 2D OIHPs without compromising their stability. In this talk, I will discuss the role of excitons/free carries, sample heterogeneity, orientation, and bias stress effects on the photovoltaic performance of OIHPs. I will then discuss the exciton dynamics of 2D OIHPs and how phase and quantum well purity may affect exciton transitions and binding energies.

*This work is supported by the Department of Energy under grant# DE-SC0019041.
Visible and near-infrared emission properties of melt-grown Dy doped CsPbCl$_3$ perovskite crystals*  

SAMUEL UBA (Presenter), UWE HOMMERICH, ALIX ALLEN, Hampton University — Doping of lead halides perovskites with rare-earth metals ions has become of significant current interest for possible applications in optoelectronics. In this research, we studied the material preparation and the visible to near IR optical properties of Dy$^{3+}$ doped CsPbCl$_3$. The crystal was synthesized from purified starting materials and melt-grown by vertical Bridgman technique. Visible emission studies under resonant-intra-4f excitation at ~450nm revealed bright yellow emission centered at 575nm arising from the $^4F_{9/2}$ to $^4H_{13/2}$ transition of Dy$^{3+}$ ions. Additional emission bands arising from the $^4F_{9/2}$ excited states were centered at 485nm, 664nm and 752nm. The decay time of the $^4F_{9/2}$ level was non-exponential with an average lifetime of ~320 µs. Near-infrared emission studies were performed using a 808 nm diode lasers and revealed several IR bands located at 1.14 µm ($^6H_{7/2}$+$^6F_{9/2}$ ->$^6H_{15/2}$), 1.33 µm($^6H_{9/2}$+$^6F_{11/2}$ ->$^6H_{15/2}$), 1.55 µm ($^6F_{5/2}$ ->$^6H_{11/2}$), and ~1.7 µm ($^6H_{11/2}$ ->$^6H_{15/2}$) arising from lower excited states of Dy$^{3+}$ ions. More details of the emission spectra and dynamics of Dy:CsPbCl$_3$ as well as a comparison to Dy:KPbCl$_2$ will be presented at the conference.

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Improvement of luminescence properties of surface-passivated mixed-halide perovskites with CdSe/ZnS quantum dots  

IL-WOOK CHO (Presenter), MEE-YI RYU, Kangwon National University — CdSe/ZnS core-shell quantum dots (QDs) have been employed to enhance the optical properties of perovskite (PS). We investigated the luminescence properties of surface-passivated mixed halide perovskite (CH$_3$NH$_3$PbI$_2$Br) using photoluminescence (PL) and time-resolved PL spectroscopy. The integrated PL intensity and PL decay time of the QD/PS hybrid structure increased compared to those of the bare PS films, owing to charge transfer (CT) from the CdSe/ZnS QDs to the PS and reduced charge traps. The CT efficiency increased from ~7 to 63% for the QD/PS hybrid structure when the core diameter of the QDs decreased from 6.5 to 2.7 nm, respectively, which can be explained by the enhancement in the CT rate due to the control of energy level alignment of QDs. A shorter radiative lifetime was obtained in the QD/PS hybrid structures as compared to the bare PS film, which is attributed to the screening effects of the Rashba splitting and internal electric field due to the CT. These results allow us to understand fundamental mechanisms such as CT from QDs to PS as a function of the size of the QDs.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B64 DMP: Nickelate, Ferrite, and Cobaltate-Based Heterostructures: Metal-Insulator Transition, Magnetism, and Orbital Ordering  

Mile High Ballroom 4E - Divine Kumah, North Carolina State University - Tag(s): Focus
Effect of ordered oxygen vacancies on the electronic and magnetic structure of perovskite-derived LaNiO$_{3-\delta}$ nickelate  

YONGJIN SHIN (Presenter), JAMES RONDINELLI, Northwestern University — Rare-earth nickelates perovskites (RNiO$_3$, with R=rare earth) exhibit a plethora of electronic and magnetic phase transitions owing to the orbital structure of its trivalent Ni cations. Unlike other RNiO$_3$ compounds, LaNiO$_3$ is the only compound lacking a thermal metal-insulator transition. Nonetheless, oxygen-deficient LaNiO$_{3-\delta}$ exhibits interesting electronic/magnetic transitions with varying oxygen content $\delta$ owing to the reducibility of Ni$^{3+}$. Specifically, the metal-semiconductor-insulator transition occurs concurrently with paramagnetic (PM)-ferromagnetic (FM)-antiferromagnetic (AFM) transition in bulk materials as $\delta$ varies [1]. Here, we explain the LaNiO$_{3-\delta}$ phase transitions and their dependencies upon (ordered) oxygen vacancy formation using first-principles calculations. We find oxygen vacancies form along the (110)$_{pc}$ direction and transform NiO$_6$ octahedra to NiO$_4$ square planar units. The resultant NiO$_4$ unit is electronically and magnetically inactive, and this with the change in NiO$_6$ connectivity governs the phase transitions. We conclude with model interpretations of the transient states reported for LaNiO$_{2.5}$ and LaNiO$_3$, and their connection to experimental observations.


Length Scales and Symmetries in The Physics of Correlated Perovskite Oxides*  

ALEXANDRU BOGDAN GEORGESCU (Presenter), Center for Computational Quantum Physics, Flatiron Institute, CLARIBEL DOMINGUEZ ORDONEZ, JENNIFER FOWLIE, BERNAT MUNDET, University of Geneva, YAJUN ZHANG, ALAIN MERCY, University of Liège, SARA CATALANO, University of Geneva, DUNCAN T.L. ALEXANDER, École Polytechnique Fédérale de Lausanne, PHILIPPE R GHOSEZ, University of Liège, ANTOINE GEORGES, ANDREW MILLIS, Center for Computational Quantum Physics, Flatiron Institute, MARTA GIBERT, University of Zurich, JEAN-MARC TRISCOME, University of Geneva — An essential aspect in the study of correlated materials is the interplay of structural motifs and electronic degrees of freedom. This talk will describe how to design an oxide heterostructure composed of two different nickelates in order to provide insight into the length and energy scales involved in the metal insulator transition, as well as the resulting roles of the different structural motifs [1]. Then, I will explain how different aspects of the symmetry of the system can affect the interplay of correlations and kinetic energy. Specific results will be presented for heterostructures composed of different rare earth nickelate materials, and possible generalizations to other materials will be presented.


*The Flatiron Institute is a division of the Simons Foundation.
Effect of interfaces on band hybridization, orbital polarization, and helical magnetism in SrFeO$_3$/CaFeO$_3$ heterostructures* [Invited] STEVEN MAY (Presenter), Materials Science and Engineering, Drexel University — The alkaline earth ferrates exhibit an array of interesting physical phenomena such as metal-insulator transitions, strong Fe-O covalency, rapid redox reactions, and helical magnetism. In this talk, I will present how the Fe-O band hybridization and Fe 3$d$ orbital occupancy changes across interfaces in isoelectronic SrFeO$_3$/CaFeO$_3$ superlattices. A consequence of the strong hybridization in these materials is that their electronic configuration can be described as containing both d$_4$L$_0$ and d$_5$L$_1$ contributions, where L indicates a ligand hole. Using resonant soft x-ray reflectivity, we find a modulation of the Fe-O hybridization across the superlattice with SrFeO$_3$ hosting a larger ligand hole density than CaFeO$_3$.[1] We show that the Fe e$_g$ orbital polarization is correlated with the degree of d$_4$L$_0$ electronic character present in the layers. Results will also be presented on the stability of the helical magnetic order in (CaFeO$_3$)$_{20}$(SrFeO$_3$)$_n$ superlattices. Using resonant x-ray diffraction, we show that the helical magnetic order coherently propagates through superlattices with $n = 1$ but does not extend through the SrFeO$_3$ layer in a superlattice with $n = 6$.[2] We describe these results in context of recently reported multi-$q$ helimagnetism in metallic SrFeO$_3$, while our results support single-$q$ helimagnetism in insulating CaFeO$_3$.


*This work is supported by the Army Research Office (grant number W911NF-15-1-0133).
The construction of superlattices, unit-cell-scale layering of two or more materials at the nanoscale, allows one to access novel properties not possessed by the constituent materials. Here, we show that in superlattices consisting of strontium iridate and lanthanum nickelate, up to one electron can transfer from iridium to nickel at the interfaces, leading to Ni\(^{2+}\)(d\(^8\)) and the unusual oxidation state Ir\(^{5+}\)(d\(^4\)). Using density functional theory based calculations including a Hubbard U correction and spin-orbit coupling, we characterize the 1:1 superlattices with both (001) and (111) ordering, allowing us to explore the competition among Hund's coupling, the crystal field splitting and spin-orbit coupling. We find that the spin-orbit coupling present for iridium does not completely dominate the d\(^4\) configuration, which would result in a nonmagnetic state with a filled \(J_{\text{eff}} = \frac{3}{2}\) manifold, but competes with the Hund's coupling and crystal field splitting. In these superlattices, the surprising competition in the energy landscape results in Ir\(^{5+}\) with a non-zero magnetic moment.

*The authors acknowledge funding from ONR grant N000014-17-1-2770 and NSF grant DMR-1629059, as well as computational support from the DOD High Performance Computing Modernization Program for computational resources.

The degree of broken orbital degeneracy, which can be represented by the term \textit{orbital polarization}, can play a crucial role in the electronic and magnetic properties of transition metal oxides. Since spin, lattice, and orbital degrees of freedom are entangled, the fundamental origin and systematic understanding of the conditions leading to strong orbital polarization is lacking. Recently, we observed the strong orbital polarization of Co\(^{2+}\) in LaCoO\(_3\)+LaTiO\(_3\) (LCO+LTO) superlattice [1]. The orbital polarization of Co is particularly interesting, since Co\(^{2+}\) ion has multiple spin states and t\(_{2g}\) or e\(_g\) character is determined by these spin states. Here we systematically study the origin of the strong orbital polarization of Co\(^{2+}\) by considering the various structural phases of (LCO\(_1\)+LTO\(_1\) superlattice and La\(_2\)CoTiO\(_6\). While the symmetry reduction by forming a superlattice is the sufficient condition to break degeneracy of the e\(_g\) bands for the low-spin state, the polarization is greatly enhanced by Coulomb \(U\). The sign of the e\(_g\) polarization depends on \(U\), local octahedral distortion, and strain. For the high-spin state, the origin of the orbital polarization of t\(_{2g}\) bands is similar to e\(_g\) case.

12:39PM B64.00006: Ferromagnetism in ultrathin double perovskite La$_2$NiMnO$_6$ thin films
GABRIELE DE LUCA (Presenter), JONATHAN SPRING, UMAR BASHIR, Univ of Zurich, ANNA ZAKHAROVA, PSI, CLARIBEL DOMINGUEZ ORDONEZ, Univ of Geneva, MARTA ROSSELL, EMPA, CINTHIA PIAMONTEZE, PSI, MARTA GIBERT, Univ of Zurich — Double perovskite oxides with chemical formula A$_2$BB'O$_6$ possess the prototypical perovskite structure integrated by two different cations (B, B') ordered in a rock-salt fashion. In the R$_2$NiMnO$_6$ (RNMO) family, R being a rare-earth cation, the positive superexchange interaction between the Ni$^{2+}$ and Mn$^{4+}$ electronic states results in the coexistence of ferromagnetic order with insulating behaviour, a combination of features that is rarely found in nature. La$_2$NiMnO$_6$ (LNMO), in particular, has a bulk ferromagnetic Curie temperature of circa 280K. Although an insulating ferromagnetic oxide with near room temperature $T_C$ would be ideal for novel spintronic devices, only a few attempts of growing ultrathin LNMO films have been reported so far.
We grew LNMO films by RF off-axis magnetron sputtering and employed AFM, XRD, STEM and EDX for structural characterization. The results indicate high crystalline quality, sharp interfaces and minimal degree of antisite disorder. The valence state of the Ni and Mn ions has been also inferred by XAS. Bulk SQUID magnetometry and element sensitive XMCD reveal that the ferromagnetic order of our films is robust against epitaxial strain and is retained down to few unit cells (less than 2 nm).

12:51PM B64.00007: Probing the electronic ground states of thin film Ruddlesden-Popper ($R_{n+1}Ni_nO_{3n+1}$) nickelates*
GRACE PAN (Presenter), QI SONG, CHARLES BROOKS, SPENCER DOYLE, JAMES EHRETS, DAN FERENC SEGEDIN, Harvard University, HANJONG PAIK, Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM), Cornell University, JULIA MUNDY, Harvard University — The recent discovery of superconductivity in a hole-doped infinite layer nickelate has spurred the reexamination of how nickelate physics may be amenable to stabilizing new superconducting phases [1]. The nickelate identified is isostructural to the superconducting cuprates and lies squarely in the superconducting regime of the simple phase diagram by Zhang [2] but disentangling the electronic from the structural contributions presents a key challenge. We have stabilized, for the first time, the Ruddlesden-Popper nickelates (Nd$_{n+1}$Ni$_n$O$_{3n+1}$) in thin film form up to $n = 6$. We will discuss how tuning of the Ruddlesden-Popper order alters the electronic ground states of the system including the nickel 3$d$ occupancy and effects on the canonical metal-to-insulator transition.


*This work is supported by the National Science Foundation (Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)) under Cooperative Agreement No. DMR-1539918.
1:03PM B64.00008: Band Offset Induced Charge Redistribution in SrNiO$_3$/LaFeO$_3$

**Superlattices**

SCOTT CHAMBERS (Presenter), LE WANG, YANG ZHENZHONG, MARK BOWDEN, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, JOHN WILLIAM FREELAND, Advanced Photon Source, Argonne National Laboratory, SUSHKO PETER, DU YINGGE, Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory — Charge transfer at oxide interfaces can drive emergent phenomena that do not occur in the bulk, thereby significantly enriching our fundamental understanding of these material. We have synthesized a series of (SrNiO$_3$)$_1$/(LaFeO$_3$)$_n$ superlattices (SLs) by oxide molecular beam epitaxy on (LaAlO$_3$)$_{0.3}$(Sr$_2$AlTaO$_6$)$_{0.7}$ (001) substrates. Our structural characterization results indicate that cubic perovskite SrNiO$_3$ (SNO), which does not exist in the bulk, can be stabilized as a single unit cell level in SLs with LaFeO$_3$. Our *in-situ* X-ray photoemission spectroscopy and X-ray absorption spectroscopy measurements indicate that depending on the value of $n$, the Ni and Fe valences are either 3+ or 4+. The $n=1$ SL contains Ni$^{3+}$ and Fe$^{4+}$, while Ni$^{4+}$ and Fe$^{3+}$ are observed in the $n=5$ SL. These results are consistent with valence band offset measurements which indicate that a potential well for holes is present in the LFO (SNO) layers for $n=1$ (5). The insights gained from these spectroscopies shed considerable light on the associated two dimensional (2D) semiconducting transport behavior in these SLs, thereby positioning us to utilize these materials systems in new and novel electronic devices.

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1:15PM B64.00009: Role of interface polarity in the electronic reconstruction of infinite-layer vs. perovskite nickelate films on SrTiO$_3$(001)

** BENJAMIN GEISLER (Presenter), ROSSITZA PENTCHEVA, Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — Motivated by the recent observation of superconductivity in the infinite-layer nickelate NdNiO$_2$ on SrTiO$_3$(001) by Li *et al.* [1], we explore the effect of interface polarity on the electronic properties of NdNiO$_n$/SrTiO$_3$(001) and LaNiO$_n$/SrTiO$_3$(001) thin films $(n=2,3)$ by performing first-principles calculations including a Coulomb repulsion term. For infinite-layer nickelate films $(n=2)$, electronic reconstruction drives the emergence of a 2DEG at the interface due to a strong occupation of the Ti 3$d$ states. This effect is more pronounced than in the paradigmatic LaAlO$_3$/SrTiO$_3$(001) system and accompanied by a substantial reconstruction of the Fermi surface. We contrast our findings with results for the perovskite compounds $(n=3)$. Moreover, we analyze the topotactic reaction from a perovskite to an infinite-layer heterostructure and show why the reduction is confined to the nickelate film, whereas the SrTiO$_3$ substrate remains intact.


*Funding by the German Research Foundation (DFG) within CRC/TRR 80 (Projects G3, G8) is acknowledged.*
Spatial distribution of hole around LaNiO$_3$/LaMnO$_3$ interface

**MASATO ANADA** (Presenter), SATOSHI SAKAGUCHI, KAZUKI NAGAI, Osaka Univ, MIHO KITAMURA, High Energy Accelerator Research Organization, HIROSHI KUMIGASHIRA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku Univ, YUSUKE WAKABAYASHI, Department of Physics, Graduate School of Science, Tohoku Univ — The superlattice of LaMnO$_3$ and LaNiO$_3$ exhibits ferromagnetism as a result of charge transfer between Mn and Ni across the interface[1]. In case of bilayer of LaNiO$_3$ on LaMnO$_3$(NMT) and of LaMnO$_3$ on LaNiO$_3$(MNT) grown on SrTiO$_3$ (001) substrate, the former shows much larger magnetization [2]. Detailed structure and valence distribution of the interfaces were examined by non-resonant and K-edge resonant surface x-ray diffraction method. Bayesian inference was applied to derive the atomic positions [3] to derive local polarization. The spatial distribution of Mn$^{4+}$ was determined from the energy spectra of scattering. As a result, Mn$^{4+}$ was found mainly in the Ni-Mn mixture region, and the total amount of transferred electron in NMT(0.8±0.2e$^-$) is larger than MNT(0.5±0.2e$^-$), which is consistent with the larger magnetization in NMT.


Disentangled transitions in artificial rare-earth nickelates

**SRIMANTA MIDDEY** (Presenter), Indian Institute of Science, DEREK MEYERS, Oklahoma State University, MIKHAIL KAREEV, YANWEI CAO, XIAORAN LIU, Rutgers University, PADRAIC SHAFER, Lawrence Berkeley National Laboratory, JOHN WILLIAM FREELAND, J.-W. KIM, P. J. RYAN, Argonne National Laboratory, JAK CHAKHALIAN, Rutgers University — The observation of simultaneous metal-insulator transition, charge ordering transition, and structural transition in rare-earth nickelates hinders our understanding of the underlying mechanism. We have devised a series of new superlattices by combining EuNiO$_3$ and LaNiO$_3$ to form ultrashort period superlattices, which allow one to disentangle the simultaneous orderings. Tailoring an incommensurate heterostructure period relative to the bulk charge ordering pattern suppresses the charge order transition while preserving metal-insulator and antiferromagnetic transitions. Such selective decoupling of the entangled phases resolves the long-standing puzzle about the driving force behind the metal-insulator transition and points to the site-selective Mott transition as the operative mechanism.
1:51PM B64.00012: Structural Distortions and the Metal Insulator Transition in (111) LaNiO$_3$

Ultrathin Films  MARGARET KANE (Presenter), LAUREN RIDDIFORD, ARTURAS VAILIONIS, Stanford Univ, APURVA MEHTA, SLAC Natl Accel Lab, ALPHA T. N'DIAYE, ELKE ARENHOLZ, Adv Light Source LBL, YURI SUZUKI, Stanford Univ — LaNiO$_3$ (LNO) is unique among rare-earth nickelates in that it doesn't exhibit a temperature dependent metal-insulator transition (MIT) in bulk. A thickness dependent MIT can be seen in (001)-oriented LNO films at ~8 Å thick and has been ascribed to ligand-holes, oxygen vacancies and charge disproportionation. We observe a similar MIT in (111)-oriented LNO on LaAlO$_3$ in transport measurements, but at a greater critical thickness than in (001) LNO on LAO. Synchrotron x-ray diffraction data and dynamical analysis show an elongation of the out-of-plane lattice parameter to 2.4 Å near the (111) interface. As the film gets thicker, the lattice constant shrinks to 2.25 Å and the film exhibits bulk metallic behavior. This distortion in the [111] direction in the first 8 unit cells is distinct from strain accommodation in (001) films, where oxygen octahedra can more easily rotate to relieve strain. We correlate the insulating behavior to this distortion and an increase in Ni$^{2+}$, measured via x-ray absorption spectroscopy. Together these results imply that metallicity in LNO films is a balance among the charge, lattice and orbital degrees of freedom.

*Dept. of Energy, Director, Office of Science, Office of Basic Energy Sciences, Div. of Mat. Sci. and Eng., Contract No. DESC0008505 and NSF GRFP

2:03PM B64.00013: Bayesian inference of perovskite oxide interface structure based on surface x-ray diffraction data  KAZUKI NAGAI (Presenter), MASATO ANADA, Graduate School of Engineering Science, Osaka university, YOSHINORI NAKANISHI-OHNO, Graduate School of Arts and Science, University of Tokyo, MASATO OKADA, Graduate School of Frontier Sciences, University of Tokyo, YUSUKE WAKABAYASHI, Graduate School of Science, Tohoku University — Crystal truncation rod (CTR) scattering method is one of the approaches to determine the structure of ultrathin films. To perform structure refinement from CTR scattering data, a good initial model is needed to obtain the correct structure. Any surface electron density analysis requires to extrapolate the scattering data. We developed a robust structure refinement method for experimentally obtained CTR scattering data by using Bayesian inference with an exchange Monte-Carlo method. The exchange Monte Carlo method [2] enables us to search a wider parameter area in the parameter hyperspace, resulting in a better acceptance for the initial model. Our test analysis shows the structure of LaNiO$_3$ ultrathin film on LaAlO$_3$ was successfully refined from a simple LaAlO$_3$ structure as the initial model. The merit of using Bayesian inference is providing the degree of parameter uncertainty with a background of informatics. Proper estimation of uncertainty will be discussed.

Session B66 DCMP: Light-Induced Structural Control of Electronic Phases  

11:15AM B66.00001: Transient trapping into metastable states in systems with competing orders* [Invited]  
ANDREW MILLIS (Presenter), Physics/CCQ, Columbia University and Flatiron Institute — The use of tailored radiation pulses to control materials properties by guiding order parameters across a free energy landscape is an important goal of current research. Here we analyse the dynamics of systems with multiple competing or cooperative orders, focussing on situations where the radiation pulse drives the system to locally disordered states and considering the subsequent regrowth of the order. We show via a time-dependent Ginsburg Landau analysis how the distribution of fluctuations evolves and determine the circumstances under which the system may evolve into a metastable, rather than global, minimum of the free energy landscape. In the limit of small Ginsburg parameter a controlled theory of the evolution reveals generic features of the order parameter probability distributions. The theory is applied to pump problem experiments on charge ordered superconducting cuprates and to the dynamic interplay of magnetic and charge order in rare earth nickelates.

*This work was supported by the US Department of Energy under Grant DE-SC0018218.

11:51AM B66.00002: Atomic-scale dynamics of strongly correlated materials: driving and seeing coherence with light at THz to x-ray frequencies* [Invited]  
STEVEN JOHNSON (Presenter), Institute for Quantum Electronics, ETH Zurich — The broad range of strongly correlated and "quantum" materials often exhibit surprisingly strong interactions between electronic, magnetic and structural properties that can manifest as strong and complex responses to impulsive excitations. Recent advances in ultrafast technology spanning frequencies from THz to x-rays have enabled a new generation of experiments, where light can be tuned to selectively excite and probe different aspects of strongly correlated materials, giving a more complete and understandable picture of the interactions in both near-equilibrium and in a strongly driven regime. Here I give an overview of some of our recent work covering two directions of development in this area. The first direction is using low-frequency (THz) pulses to drive coherent vibrational dynamics in correlated systems with minimal electronic excitation. I will discuss recent examples of this in wide gap insulators and in low conductivity metals. The second direction, complementary to the first, is to use femtosecond hard x-ray scattering techniques to quantitatively measure coherent lattice dynamics in response to impulsive excitation. One recent example that will be discussed is the recent observation of and ultrafast manifestation of the Einstein-de Haas effect in a ferromagnetic system [1]. I will also discuss THz-driven dynamics in ferroelectric systems that represent the confluence of these two directions and shows the potential of these new methods.


*This research was supported by the NCCR MUST, funded by the Swiss National Science Foundation.
12:27PM B66.00003: Ultrafast spin-dynamics: TDDFT's killer app.* [Invited] SANGEETA SHARMA (Presenter), Max Born Inst — I will talk about all-optical switching of long-range magnetic order. The type of coupling between the constituent atoms of a magnetic solid, usually ferromagnetic (FM) or anti-ferromagnetic (AFM), is a fundamental property of any magnetic material. This coupling is governed by the exchange interaction, for which the time scale of a typical magnetic material is of the order of a few 100s of femtoseconds. In our work, using time-dependent density functional theory (TDDFT), we demonstrate that a rich control over magnetization at sub-exchange time scales (of the order of few tens of femtoseconds) is possible[1,2,3,4]. This even includes changing the magnetic order from AFM to FM[5]. By investigating a wide range of multi-sublattice magnetic materials we are able to formulate three simple rules that predict the qualitative dynamics of magnetization for ferromagnetic, anti-ferromagnetic, and ferri-magnetic materials on sub-exchange time scales.


*DFG TRR227

1:03PM B66.00004: Unraveling Momentum-Dependent Electron-Phonon Coupling and its Role in the Origin of Charge Density Wave Phases* [Invited] BRADLEY SIWICK (Presenter), MARTIN OTTO, JAN-HENDRIK PÖHLS, LAURENT RENÉ DE COTRET, MARK SUTTON, Department of Physics, McGill University — The nature of the couplings within and between lattice and charge degrees of freedom is central to condensed matter and materials physics. These interactions are essential to phenomena as diverse as superconductivity, charge density waves and carrier mobility in semiconductors and metals. Despite their fundamental role, detailed momentum-dependent information on the strength of electron-phonon coupling (EPC) and phonon-phonon coupling (PPC) across the entire Brillouin zone has proved elusive. This talk will describe a new technique, ultrafast electron diffuse scattering (UEDS), which provides such information. Specific applications of UEDS to 2D materials including graphite, TiSe2 and TaSe2 will be presented. These data demonstrate that UEDS patterns can separate the influence of the electronic susceptibility from the inelastic exchange of energy between the electron and phonon systems through the technique’ profound sensitivity to photoinduced changes to the phonon system. In TiSe2, this confirms key role of excitonic correlations to the phonon softening and CDW mechanism.

*Natural Sciences and Engineering Council of Canada (NSERC), Canada Foundation for Innovation (CFI), Canada Research Chairs (CRC), Fonds de Recherche du Québec – Nature et technologies (FRQNT)
Anton Burkov (Presenter), University of Waterloo — Weyl semimetal may be thought of as a gapless topological phase protected by the chiral anomaly, where the symmetries involved in the anomaly are the U(1) charge conservation and the crystal translational symmetry. The absence of a band gap in a weakly-interacting Weyl semimetal is mandated by the electronic structure topology and is guaranteed as long as the symmetries and the anomaly are intact.

The nontrivial topology also manifests in the Fermi arc surface states and topological response, in particular taking the form of an anomalous Hall effect in magnetic Weyl semimetals, whose magnitude is only determined by the location of the Weyl nodes in the Brillouin zone.

Here we consider the situation when the interactions are not weak and ask whether it is possible to open a gap in a magnetic Weyl semimetal while preserving its nontrivial electronic structure topology along with the translational and the charge conservation symmetries. Surprisingly, the answer turns out to be yes. The resulting topologically ordered state provides a nontrivial realization of the fractional quantum Hall effect in three spatial dimensions in the absence of an external magnetic field, which cannot be viewed as a stack of two dimensional states. Our state contains loop excitations with nontrivial braiding statistics when linked with lattice dislocations.

*This work was supported by Center for Advancement of Topological Semimetals, an Energy Frontier Research Center funded by the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences, through the Ames Laboratory under contract DE-AC02-07CH11358.
Nonlinear dynamic conductivity in structurally chiral Weyl semimetals [Invited] JOSEPH ORENSTEIN (Presenter), DYLAN REES, University of California, Berkeley and LBL, KAUSTUV MANNA, MPI, Dresden, BAOZHU LU, Temple University, HORST BORRMANN, CLAUDIA FELSER, MPI, Dresden, DARIUS TORCHINSKY, Temple University — WSMs are 3D versions of graphene, characterized by isolated band crossings which act as monopoles of the Berry curvature field. From the properties of the Berry curvature under time-reversal and inversion, it follows that breaking either $T$ or $I$ is necessary for a crystal to exhibit a WSM phase. $I$-breaking WSMs exhibit response functions that are forbidden in systems that possess a center of symmetry. We have investigated an important example of such responses: the second-order nonlinear conductivity, defined by $J_i = \sigma_{ijk} E_i E_j$. For monochromatic electric fields the nonlinear response generates dc currents whose direction is dependent on the polarization state of the electric field, giving rise to phenomena known as photogalvanic effects (PGEs). In this talk I will present results on PGEs in response to linear and circular polarized light (LPGE and CPGE, respectively) as probes of both the symmetry and topology of the WSM phase. RhSi is an ideal candidate for such a study, as point group symmetry predicts the simplest possible structure of $\sigma_{ijk}$, in which the only nonvanishing tensor elements are even and odd permutations of $xyz$. Furthermore, RhSi is structurally chiral (or handed), and the absence of mirror planes breaks the degeneracy of Weyl nodes of opposite Berry monopole charge. I will present results on the polarization selection rules and spectra of PGEs for light incident on 111 and 001 surfaces. On 111 we observe a CPGE current whose direction is parallel to the wavevector of the light and whose spectrum is consistent with photoexcitation across a Weyl cone. More surprising is that we observe in-plane CPGE and LPGE currents at normal incidence on the 001 surface, where the bulk point group predicts a null effect. I discuss the possibility that the current is allowed because truncation at the 001 surface breaks the nonsymmorphic (screw) symmetry and therefore may derive from helicoidal surface bands that give rise to Fermi arcs (see Chang et al. 1906.03207).

Universal plateau in the thermoelectric Hall conductivity of Dirac/Weyl semimetals [Invited] BRIAN SKINNER (Presenter), Ohio State Univ - Columbus, VLADYSLAV KOZII, Department of Physics, University of California, Berkeley, WENJIE ZHANG, Peking University, PEIPEI WANG, Southern University of Science and Technology, RAN BI, Peking University, CHANG-WOO CHO, Southern University of Science and Technology, RUIDAN ZHONG, JOHN SCHNEELOCH, Brookhaven National Laboratory, DAPENG YU, Southern University of Science and Technology, GENDA GU, Brookhaven National Laboratory, LIANG FU, MIT, XIAOSONG WU, Peking University, LIYUAN ZHANG, Southern University of Science and Technology — The three-dimensional Dirac and Weyl semimetals can exhibit thermoelectric properties that are not possible in conventional metals and semiconductors. Here I focus in particular on the thermoelectric Hall effect, which is the generation of a transverse heat current upon applying an electric field in the presence of a magnetic field. I show, in particular, that the thermoelectric Hall conductivity acquires a robust plateau in the extreme quantum limit, and that the plateau value is independent of the field strength, disorder strength, carrier concentration, or carrier sign. I then discuss recent experiments on the three-dimensional Dirac semimetal ZrTe$_5$, which clearly exhibit this plateau. Other thermoelectric coefficients in the material, such as the thermopower and Nernst coefficient, are greatly enhanced over their zero-field values even at relatively low fields.
1:03PM B67.00004: Pseudo-electromagnetic fields in topological semimetals [Invited]  RONI ILAN (Presenter), Tel Aviv University — Dirac and Weyl semimetals react to position- and time-dependent perturbations, such as strain or an inhomogeneous magnetisation, as if emergent electromagnetic fields were applied. Such pseudo-electromagnetic fields differ from external electromagnetic fields in their symmetries and phenomenology, and enable a simple and unified description of a variety of inhomogeneous systems. We review the different mechanisms for creating effective pseudo-fields and their observable consequences, which can be remarkably different from those resulting from external fields.

1:39PM B67.00005: Acoustics, Weyl, and chiral transport [Invited]  SEBASTIAN HUBER (Presenter), ETH Zurich — Weyl semimetals in an external field exhibit a number of interesting transport phenomena. Here we show how we can induce pseudo-magnetic and electric fields in acoustics, how they modify the transport of acoustic energy and what we can learn from these systems for electronic transport in Weyl semimetals. Moreover, we demonstrate on a concrete model how one can capitalize on Weyl physics to create platform 9 3/4 at King's Cross station.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B68 DPOLY: Machine Learning and Data in Polymer Physics

11:15AM B68.00001: Autonomous X-ray Scattering* [Invited]  KEVIN YAGER (Presenter), MASAFUMI FUKUTO, RUIPENG LI, GREGORY DOERK, Brookhaven National Laboratory, PAWEL W MAJEWSKI, University of Warsaw, MARCUS NOACK, Lawrence Berkeley National Laboratory — This talk will cover ongoing work to develop autonomous experimentation at a synchrotron x-ray scattering beamline. Deep learning (convolutional neural networks) is used to classify x-ray detector images, with performance improving when domain-specific data transformations are exploited ("physics-aware machine-learning"). These methods can be combining with customized data healing algorithms. To close the autonomous loop, we deploy a general-purpose algorithm that selects high-value experiments to conduct, attempting to minimize both uncertainty and experimental cost. Examples from recent autonomous experiments will be presented, including measuring nanoparticle ordering, combinatorial libraries of block copolymer materials, and realtime photo-thermal processing.

*This research used resources of the Center for Functional Nanomaterials and the National Synchrotron Light Source II, which are U.S. DOE Office of Science Facilities, at Brookhaven National Laboratory under Contract No. DE-SC0012704.
11:51AM B68.00002: Molecular Simulations Integrated Machine Learning Study of Bottlebrush Polymers* [Invited] SOUMIL JOSHI, SAMRENDRA SINGH, SANKET DESHMUKH (Presenter), Virginia Tech — Thermosensitive bottlebrush polymers (BBPs) are a type of graft polymers in which thermosensitive polymer side-chains are grafted to a polymer backbone. Most of these thermosensitive polymers with lower critical solution temperature (LCST) can undergo a coil-to-globule conformational transition with increasing temperature. This further results in a change in the overall shape of the BBPs, which is one of the most important properties needed in many biomedical applications including drug delivery, molecular actuators, etc. In this talk, I will discuss our recent coarse-grained (CG) molecular dynamics (MD) simulations study of poly(N-isopropylacrylamide) (PNIPAM; LCST= 305 K) BBPs of three different shapes: 1. Worm-like, 2. Cone-like, and 3. Dumbbell-like. The CG MD simulations were performed at 290 K (below LCST) and 320 K (above LCST) in the presence of explicit CG water for 500 ns. The analysis of simulation trajectories performed using in-house computer codes and data-driven machine-learning methods suggested that the shape of BBPs has significant impact on the conformations of side-chains as compared to other structural features (e.g. grafting density and side-chain length) and temperature.

*Sanket Deshmukh acknowledges the Virginia Tech Start-up Funds

12:27PM B68.00003: A Transfer Learning Framework for Improving Property Prediction, Interpretability, and Chemical Discovery from Scarce Datasets [Invited] BRETT SAVOIE (Presenter), Purdue Univ — Machine learning (ML) is being applied in virtually all areas of the chemical sciences to advance or complement activities that have traditionally been performed with physics-based methodologies. To sustain this progress and fulfill mounting expectations, ML must grapple with the intrinsic data scarcity of many applications. While datasets for image classification, object recognition, and some molecular properties may contain millions of samples, more typical chemical applications have access to only a few hundred to a few thousand samples. In data scarce scenarios, ML models can be severely underdetermined, exhibit limited transferability, and ultimately poor predictive power. Transfer learning addresses these data limitations with methodologies that utilize data across different domains, or data with mixed provenance and sparsity to augment and robustly train data scarce models. In this talk, I will discuss a flexible transfer learning approach to address data scarcity by using chemical latent space enrichment, whereby disparate data sources are combined in joint prediction tasks. I’ll show how this approach achieves three improvements over typical supervised learning approaches, including (i) increased property prediction accuracy from scarce data sets, (ii) increased model interpretability, and (iii) increased generative potential for use in the optimization and discovery of new chemistries. The talk will conclude with an outlook of current limitations, ongoing areas of improvement, and new applications.
1:03PM B68.00004: Optimization of organic molecules and macromolecules using machine learning* [Invited]  YAROSLAVA YINGLING (Presenter), Materials Science and Engineering, North Carolina State University — The number of applications of data driven materials discovery is rapidly growing. The large amount of available materials characterization and computational data, combined with high level statistical algorithms, is proving to be extremely useful in developing complex predictive models. However, in the field of soft matter, which includes complex materials such as polymers, liquids, emulsions, colloids, and gels, there is a slower adoption of informatics strategies than in adjacent fields mainly due to complexity of underlying processes and plethora of processing components that dictates the properties. In this talk, I will discuss the application of machine learning (ML) technique for optimization of ligand functionalized nanoparticles (NPs) and biopolymers. In our approach we use a combination of high throughput molecular dynamics simulations and data available from the literature to train the ML model. We address the uncertainty associated with MD simulations in the development of the model. Using this approach, we were able to design novel nanoparticle ligands capable specific desired properties driven by the specific optimization function. Our methods can significantly speed up the search for a new organic monomers (complex ligands or polymers) design based on experimental, in silico and available literature data.

*NSF CMMI-1763025 and CMMI-1727603

1:39PM B68.00005: Closed-loop, sequential learning for polymer systems [Invited]  KRISTOFER REYES (Presenter), State Univ of NY - Buffalo — Closed-loop, sequential machine learning has garnered an increasing amount of interest over the past few years in experimental science due to its ability to efficiently explore combinatorially large spaces of experimental parameters. Techniques in this new field can help accelerate scientific exploration of such spaces through the strategic selection of experiments whose outcomes could potentially yield a high amount of information. In this talk, we explore a few applications of such closed-loop, sequential design of experiments in the study of polymer systems, ranging from the optimization of polymer emulsions for use in drug delivery, to recent work in efficient phase mapping of polymerization phenomena and even real-time optimal control in driving block-copolymer evolution. While each example differs in application and experimental objectives, we will present a unified framework for the modeling and decision-making employed in each case. We will also present our work in the development of general-purpose tools designed to lower the barriers for applying these algorithms and techniques to other problems.

Monday, March 2, 2020 11:15 AM - 2:15 PM

Session B70 DPOLY DSOFT: Polymer Dynamics at the Nano-to Meso-Scale Revealed by X-ray and Neutron Spectroscopy II 208 - Tad Koga, State Univ of NY - Stony Brook - Tag(s): Focus
11:15AM B70.00001: Soft Matter Dynamics with Neutron Spin Echo Spectroscopy at the Spallation Neutron Source  PIOTR ZOLNIERCUZK (Presenter), Forschungszentrum Julich, LAURA-ROXANA STINGACIU, Neutron Scattering Division, ORNL, MICHAEL MONKENBUSCH, Forschungszentrum Julich —

Neutron spin echo spectroscopy is one of the most powerful techniques to study the dynamics of soft matter [1]. The SNS-NSE instrument [2] at the Spallation Neutron Source, Oak Ridge National Laboratory is the first, and to date the only one, instrument for high resolution NSE spectroscopy installed at a pulsed neutron source. The main advantage of the pulsed source NSE is the ability to resolve the neutron wavelength and collect neutrons over a wider bandwidth. This allows one to determine S(Q,t) on a flexibly chosen quasi continuous [Q,t] grid that can be selected a posteriori, trading statistical error with grid resolution.

We will show the capabilities of the SNS-NSE instrument and examples of soft matter experiments that have been performed using the SNS-NSE instrument. We will also present a new data reduction software called DrSPINE [3] that is capable to utilize all the available information contained in a series of experiments consistently in one step to yield a comprehensive representation of the intermediate scattering function S(Q,t).

References:

11:27AM B70.00002: Dynamics of multi-domain macro-molecules in the context of polymer physics  LAURA-ROXANA STINGACIU (Presenter), VOLKER URBAN, Oak Ridge National Lab —

Conformational ensembles of synthetic polymers and intrinsic disorder in proteins are both aspects of the varying degree of order and disorder that are crucial for the properties of macromolecules. Neutron scattering techniques, in particular small angle scattering and neutron spin echo, have an important contributions to understand conformation and dynamics of macromolecules with regards to polymer physics. The possibility for altering and defining accessible conformational spaces through localized or intermediate and long-range interactions of segments along a polypeptide chain are limited by chain stiffness and local hydrodynamic friction. Our research aims for a deeper understanding of this challenging topic. We will present the dynamics of several bio-molecular species based on results of neutron scattering and the comparison with secondary and segmental relaxations, Rouse and reptation dynamics in polymers, with emphasis on the significant difference between dynamics of random coil of synthetic polymers and the dynamics of globular proteins.

11:39AM B70.00003: WITHDRAWN ABSTRACT —
11:51AM B70.00004: Length-Scale Dependence of Block Copolymer Segmental Dynamics

DANIEL HALLINAN (Presenter), OLUWAGBENGA IYIOLA, Florida State University, KUNLUN HONG, MONOJOY GOSWAMI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, PIOTR ZOLNIERCZUK, LAURA-ROXANA STINGACIU, Jülich Centre for Neutron Science – SNS, Institute of Forschungszentrum Jülich GmbH, WILLIAM THOMAS HELLER, Neutron Scattering Division, Oak Ridge National Laboratory, KYOUNGMIN KIM, Florida State University — This work examines the effect of interface proximity and tethering on polymer segmental motion. Selectively deuterated block copolymers (BCPs) were studied with neutron spin echo (NSE) spectroscopy. A strongly segregated BCP was used as a model system in which a glassy deuterated polystyrene (dPS) block acted as the interface and the dynamics of a rubbery deuterated polyethylene oxide (dPEO) block was studied. The PEO block was selectively protonated as a label to examine the dynamics near the interface in one sample and near the chain end in another sample. A strong slowing of segmental dynamics in the sample with the protonated label tethered directly to the dPS was observed compared to the dynamics of the sample with the protonated label at the chain end, but with an unexpected length scale dependence. The slowing was only observed at length scales significantly larger than the characteristic PEO segment length (1 nm), and the disparity between interfacial and chain-end dynamics grew with increasing length. The novelty of examining polymer chain motion over a wide range of length scales is enabled by NSE of selectively deuterated BCPs and can impact BCP applications including batteries, water treatment, and gas separations.

*NSF Award 1751450
DOE Office of Science

12:03PM B70.00005: Investigating the effect of salt on polymer dynamics in block copolymer electrolytes through neutron spin-echo spectroscopy

WHITNEY LOO (Presenter), University of California, Berkeley, ANTONIO FARAONE, National Institute of Standards and Technology, NITASH BALSARA, University of California, Berkeley — Block copolymers have been studied for use in lithium metal solid-state batteries due to their ability to decouple ion transport and mechanical properties. While it is well known that the salt preferentially segregates into the conducting block, and that the motion of salt molecules is coupled to that of the polymer segments that solvate the ions, many questions about the nature of this coupling remain unanswered. Neutron spin-echo spectroscopy experiments were used to elucidate the nature of this coupling; the sample used was a mixture of a protonated and deuterated polystyrene-\textit{b}-poly(ethylene oxide) doped with a lithium salt. The isotopic labeling allowed for only the dynamics of the ion-containing block, poly(ethylene oxide), to be measured. We quantified the dynamics, corresponding to length scales of about 5 nm, by comparing the data to predictions based on the Rouse model at low times as well as the standard tube model at long times. The crossover time between these modes was determined as a function of salt concentration. The tube shrinks with added salt and the segments slow down due to this. There is a direct relationship between segmental dynamics measured on the monomer length scale and ion transport under an applied field on macroscopic length scales.
12:15PM B70.00006: Ion transport in solid polymeric lithium ion electrolytes
HANS-GEORG STEINRUECK (Presenter), CHRISTOPHER TAKACS, SLAC - Natl Accelerator Lab, DAVID MACKANIC, Department of Chemical Engineering, Stanford University, BENJAMIN HOLLADAY, Department of Physics, University of California, San Diego, HONG KEUN KIM, Argonne National Laboratory, CHUNTIAN CAO, SLAC - Natl Accelerator Lab, SURESH NARAYANAN, ERIC DUFRESNE, X-Ray Science Division, Argonne National Laboratory, YURIY CHUSHKIN, FEDERICO ZONTONE, BEATRICE RUTA, ESRF, JOHANNES WILL, Institute of Micro- and Nanostructure Research (IMN) & Center for Nanoanalysis and Electron Microscopy (CENEM), University of Erlangen-Nürnberg, OLEG BORODIN, Electrochemistry Branch, Sensor and Electron Devices Directorate, U.S. Army Research Laboratory, SUNIL K SINHA, Department of Physics, University of California, San Diego, VENKAT SRINIVASAN, Argonne National Laboratory, MICHAEL TONEY, SLAC - Natl Accelerator Lab — Understanding ion transport in solid polymeric electrolytes (SPEs) continues to be of interest concerning improving safety and energy density of lithium-ion batteries. Towards this end, we present an investigation of lithium ion transport in a baseline SPE consisting of lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) in Poly(ethylene oxide) (PEO) via a combination of x-ray photon correlation spectroscopy (XPCS), x-ray absorption microscopy (XAM), continuum modelling, and molecular dynamics (MD) simulations. Our experiments yield spatially resolved ion velocities (via XPCS) and ionic concentrations (via XAM) upon polarization of a Li/PEO-LiTFSI/Li symmetric cell, which we compare to our theoretical efforts. Particular interest lies in providing direct insight into the concentration dependent transference numbers, which can be challenging to accurately measure, but are essential to ionic transport. We realize this by variation of the input transport parameters, aided by MD simulations, within the continuum model, until a match with the experimental velocities and concentration profiles is achieved.

*This work was supported by the Joint Center for Energy Storage Research (JCESR).

12:27PM B70.00007: Diffusion of Lithium Salt in Block Copolymer
KYOUNGMIN KIM (Presenter), MICAH SILVERMAN, DANIEL HALLINAN, Florida State Univ — Salt-doped polymer electrolytes can replace the flammable liquid electrolytes enhancing safety and chemical stability. The challenges to apply the polymer electrolytes to commercial batteries are dendrite formation and the low ionic conductivity. Understanding the ionic transport is essential to design high-performance batteries. Limitations of the conventional electrochemical measurements arise as the system gets complicated. Accurate and straightforward way to measure the transport properties is required. We successfully applied the measurement technique using time-resolved Fourier Transform infrared - attenuated total reflectance (FTIR-ATR) spectroscopy to polymer electrolytes. The diffusion coefficients of lithium salt through a polystyrene-poly(ethylene oxide) block copolymer (SEO) electrolytes were investigated. Since the concentration gradient is the only driving force, the diffusion coefficient could be decoupled with the ionic conductivity and transference number. The results showed non-monotonic dependence of the diffusion coefficient on the salt concentration implying the polymer structure or ion dissociation plays a role in the diffusion in concentrated polymer electrolyte.

*This study is supported by NSF Award # 1804871.
12:39PM B70.00008: Unravelling the Interplay Between Structural Dynamics and Water Transport in Perfluorosulfonated Ionomer Nanocomposites Through the use of Neutron Scattering and Infrared Spectroscopy  
APOORVA BALWANI (Presenter), ALLISON B DOMHOFF, Clemson University, MADHUSUDAN TYAGI, ANTONIO FARAONE, NIST Center for Neutron Research, National Institute of Standards & Technology, ERIC M DAVIS, Clemson University — Ionomer nanocomposites are attractive as proton exchange membranes in redox flow batteries, as they combine the thermo-chemical resistance of perfluorosulfonated ionomers with the reduced vanadium ion transport due to the presence of silica nanoparticles (SiNPs). However, elucidating the impact of SiNPs on the structural ordering and transport properties of these nanocomposites is an ongoing challenge. In this study, neutron spin echo (NSE) spectroscopy and high flux backscattering (HFBS) spectroscopy were employed to probe changes in polymer segmental dynamics and water dynamics, respectively, while small-angle neutron scattering (SANS) was used to investigate the SiNP dispersion state. In tandem with these techniques, infrared spectroscopy was used to capture water transport and water-induced swelling of the ionomer nanocomposites. Data from this complementary set of techniques indicate that SiNPs inhibit both viscoelastic relaxations and segmental dynamics of the ionomer network. Further, ionomer swelling and water transport in these nanocomposites were found to be highly coupled, leading to a complex water transport mechanism in these membranes. Finally, SiNP surface chemistry was established as a handle for tunability for ionic transport in perfluorosulfonated ionomers.

12:51PM B70.00009: WITHDRAWN ABSTRACT

1:03PM B70.00010: Structure and dynamics of homogeneously and heterogeneously crosslinked PNIPAM microgels*  
TETYANA KYREY, JUDITH WITTE, Stranski-Laboratory, Technische Universitaet Berlin, LAURA-ROXANA STINGACIU, NScD, Oak Ridge National Laboratory, MARCUS WITT, REGINE VON KLITZING, Department of Physics, Technische Universitaet Darmstadt, STEFAN WELLERT, Stranski-Laboratory, Technische Universitaet Berlin, OLAF HOLDERER (Presenter), Forschungszentrum Juelich GmbH — Thermoresponsive poly(N-isopropylacrylamide) microgel particles have been largely studied in the past due to their interesting fundamental properties as well as their potential for application in drug delivery, sensor technology or biotechnology. In this contribution, microgel particles with homogeneous and heterogeneous crosslink distribution and different crosslinker concentrations will be studied with small angle neutron scattering (SANS) and neutron spin echo spectroscopy (NSE).

The segmental dynamics of polymer chains in solution, as described by the Zimm model, is modified in microgels due to the presence of crosslinks and the crowded environment inside the particle, both inducing heterogeneities, for example “frozen” inhomogeneities or density fluctuations. Such structural heterogeneities have an impact on the segmental chain dynamics, which makes NSE, the highest resolution neutron spectroscopy technique, the experiment of choice for accessing variations and changes induced by changes in crosslink distribution and crosslink density.

An outlook on interface effects on the internal structure and inhomogeneities of microgel particles will be given.

*Support of the DFG (grant number WE5066/3-1 (S. Wellert) and HO 5488/2-1 (O. Holderer) is acknowledged.
1:15PM B70.0001: Dynamics of polymeric additives in bicontinuous microemulsions adjacent to planar hydrophilic surfaces  HENRICH FRIELINGHAUS (Presenter), FREDERIK LIPFERT, OLAFF HOLDERER, STEFAN MATTAUCH, MICHAEL MONKENBUSCH, NIKOLAS AREND, DIETER OSWALD RICHTER, Forschungszentrum Juelich GmbH — Close to a planar surface, lamellar structures are imposed upon otherwise bulk bicontinuous microemulsions. Thermally induced membrane undulations are modified by the presence of the rigid interface. While it has been shown that pure membrane dynamics are accelerated close to the interface, we observed nearly unchanged relaxation rates for membranes spiked with large amphiphilic diblock copolymers with respect to the bulk. An increase of the polymer concentration by a factor of 2–3 for the first and second surfactant membrane layers was observed. We interpret the reduced relaxation times as the result of an interplay between the bending rigidity and the characteristic distance of the first surfactant membrane to the rigid interface, which causes the hydrodynamic and steric interface effects described in Seifert's theory. The influence of these effects on decorated membranes yields a reduction of the frequencies and an amplification of the amplitudes of long-wavelength undulations, which are in accordance to our experimental findings.

1:27PM B70.0001: High shear rate rheology in microcapillary flow with SANS* PAUL SALIPANTE, RYAN MURPHY, National Institute of Standards and Technology, VISHNU DHARMARAJ, Chemical Engineering, MIT, KATIE WEIGANDT, STEVEN HUDSON (Presenter), National Institute of Standards and Technology — The rheology of shear-banding wormlike micelle solutions, which exhibit polymeric viscoelasticity, is investigated at high shear rates using capillary rheometry, particle-streak velocimetry, and small-angle neutron scattering (SANS). The capillary entrance flow was examined so that results of fully developed flow are reported. Such results show shear-thinning power-law behavior for all channel geometries from shear rates of 1,000 /s to nearly 1,000,000 /s. Two distinct power-law behaviors with increasing shear rate indicate a structural change with corresponding broadening of neutron scattering. The transition between these two power laws shifts with changing surfactant concentration and temperature.

*NIST on a Chip, NIST Center for Neutron Research
1:39PM B70.00013: In-Situ/Operando X-ray Photon Correlation Spectroscopy Studies of Polymer Dynamics During 3D-Printing of Dual-Cure Polymer Epoxy [Invited] STANISLAS PETRASH (Presenter), Henkel Corporation — Synchrotron-based X-ray Photon Correlation Spectroscopy (XPCS) was used to probe the dynamic properties of soft matter at relevant size (submicrons) and time-scales (milliseconds). We combined XPCS with in-operando capabilities of synchrotron beamlines to shed light onto the unexplored dynamics of dual-cure (UV/thermal) industrial polymers for advanced 3D printing applications. We studied, in operando: a) the structural evolution and corresponding dynamics of the polymer during the extrusion phase of 3D printing, b) anisotropic structure formation & interfacial behavior during subsequent settling and UV curing, and c) the process of final thermal cure. The results revealed a) anisotropic polymer dynamics in different directions (printing (horizontal) vs. extrusion (vertical)) during printing and settling of the material, b) two-stage crosslinking dynamics during UV curing, and c) the chain dynamics near the polymer-polymer interface between 3D-printed filaments as a function of the distance from the interface. The present study shows that an in-situ/operando XPCS is not only an excellent technique for comprehensive, quantitative characterization of 3D printing processes, but also provides an unprecedented opportunity to perform studies of a wide variety of nonequilibrium phenomena of polymeric materials under external stimuli.

Monday, March 2, 2020 11:45 AM - 2:00 PM

Session C01 APS: Meet Your Future Hyatt Centennial D - Tag(s): Careers, Industry, Undergrad Friendly

11:45AM C01.00001: Meet Your Future — FIAP and APS Careers will host a special lunchtime session in which representatives from industry will briefly describe their career path and answer questions about physics careers in the private sector. Topics will include research opportunities for physicists in industry, strategies for successfully pursuing industrial jobs, and advice on how to thrive in this exciting and challenging work environment.

The panelists this year are:

Cameo Lance Rhea Space Activity Director of Physics Programs
Kate Raach HRL Laboratories Research Staff Member
Jie Ren Merck Senior Scientist
Anne Smith Siemens Healthcare Systems Engineer
Stefano Spagna Quantum Design Chief Technical Officer

Note that this session will be held in the Hyatt Hotel, not the Convention Center. Join us for a slice of pizza and gain many useful insights into this career path.

Monday, March 2, 2020 2:00 PM - 2:00 PM
C71.00001: Using GALFIT to Determine Galaxy Morphologies of Quasars* KAITLYN RAUB (Presenter), MARIANA LAZAROVA, Physics and Astronomy, University of Northern Colorado, GABRIELE CANALIZO, Physics and Astronomy, University of California Riverside, MARK LACY, National Radio Astronomy Observatory, National ALMA Science Center — Little is known about the morphologies of quasars. Quasars are the brightest of the active galaxies, in which a supermassive black hole is accreting material, creating an accretion disk that outshines the host galaxy. We model images obtained from the Hubble Space Telescope of 22 nearby quasars and the galaxies in their immediate neighborhood using the GALFIT software to determine how well they are fit by typical galaxy profiles. GALFIT is an image analysis algorithm which fits parametric functions to create light profiles from two-dimensional images. We fit the quasars using two main components - a Point Spread Function (PSF), which represents a point source object (the light of the accretion disk), and a Sérsic profile, which models galaxy structures, such as a disk or a bulge. We will present details on the models, including the types of components used in each fit as well as the residual maps after subtracting the model from the data.

*Support for this work was provided by the department of Physics and Astronomy at the University of Northern Colorado and by NASA through a grant from the Space Telescope Science Institute (Program GO-11557), which is operated by the Association of Universities for Research in Astronomy, Incorporated, under NASA contract NAS5-26555.

C71.00002: UNDERGRADUATE RESEARCH  —

C71.00003: SuperCDMS: Energy Calibration of a Cryogenic Ge HV Particle Detector* SALAMONG XIONG (Presenter), Physics & Astronomy, Macalester College — The goal of the SuperCDMS collaboration is to directly detect dark matter. Potential candidates for dark matter are Weakly Interacting Massive Particles (WIMPs). To detect WIMPs, it is important to be able to predict how a Ge/Si particle detector will respond to a dark matter signal. In particular, it is necessary to calibrate the recoil energy measured by these detectors. This paper presents the energy calibration spectrum of a SuperCDMS-HV Ge particle detector using Am-241 and a PuBe neutron source. Due to high event rate, criteria were developed to remove low-quality data arising from particle interactions that occur too soon after a previous interaction. Peaks in histograms of pulse amplitudes were identified as energy peaks from the various radioactive sources, and fits of these peaks formed the basis for generating an energy calibration function. The calibration function was used to generate the calibrated energy spectrum.

*This undergraduate summer research was funded by the TRIO McNair Scholars program at the University of Minnesota - Twin Cities.
C71.00004: Effect of polyethylene oxide on camphor sulfonic acid doped polyaniline thin film field effect transistor with ionic liquid gating*  LUIS M RIJOS (Presenter), ANAMARIS MELENDIZ, ROLANDO OYOLA, NICHOLAS PINTO, Univ of Puerto Rico - Humacao — Field effect transistors (FET) using camphor sulfonic acid (CSA) doped polyaniline (PANI) blended with several polyethylene oxide (PEO) concentrations were investigated via ionic liquid gating. The pure PANI-CSA FET could not be turned “off” and had an on/off ratio of 2. Blending with 22wt%-PEO retained a high “on” state throughput current and improved the mobility, while the on/off ratio increased by $10^3$. Superior film quality and PEO assisted electrostatic long range interactions with the PANi chains led to device parameter enhancement. For higher PEO concentrations the field effect was suppressed due to disorder. Analysis of the UV/Vis spectra polaron band peak area near 810 nm show an increase in the mobility with decrease in the peak area, consistent with the observed results. Enhanced device parameters, high throughput current and low operating voltages (±2V), make PANi-CSA/PEO blends attractive materials for use in low power consumption electronics.

*This work was supported in part by NSF under grants DMR-PREM-1523463 and DMR-RUI-1800262

C71.00005: Fabrication of femtosecond laser-induced crystals in lithium nioboSilicate 30: the effects of polarization angle on orientation and growth rate.*  RUTENDO JAKACHIRA (Presenter), Drew University, COURTNEY AU-YEUNG, Physics, Lehigh University, EVAN MUSTERMAN, HIMANSHU JAIN, Material Science, Lehigh University — Optical and Electron microscope inspections reveal a dependence of light polarization on the growth of crystals in glass using a femtosecond laser. Critical for these experiments is an algorithm based on a half-wave plate that insured constant laser intensity for varying polarization directions. Laser-induced crystallization is an effective way of fabricating crystals in glass and other transparent materials owing to the fact that the process is clean, precise and contactless. The crystals obtained are of interest because of their potential use in optical data transmission. The issue tackled in this paper was that of maintaining consistent power when the polarization angle was changed. For this work, LiNbO3 crystals were fabricated in Lithium NioboSilicate glass with 30 mol percentage of silicon dioxide in the glass. Cao et al observed that at moderate pulse energies, (0.5-0.9μJ/ pulse, 300kHz) textured nanocrystals are obtained with their polar axis perpendicular to the writing laser polarization direction[1].

CIS codes: 130.3730, 130.5296

References:

*Research funded by the National Science Foundation through Lehigh University Physics Department.
C71.00006: Ultrasonic Acoustic Probing Based on Gaussian Beam Analysis  EMILY LAPRIME  
(Presenter), SANICHIRO YOSHIDA, Southeastern Louisiana Univ — By analyzing differences in phase and amplitude of a signal, information about differing acoustic contrast between materials can be quantified. Prior methods used a scanning acoustic microscope which allowed for phase shifts to be identified by reflections but could not quantify phase shifts besides 0° or 180°. The new method uses a continuous signal to identify more precisely the phase and amplitude to analyze the transmitted signal. We have utilized the knowledge that the acoustic signal used behaves as a Gaussian beam travelling through a material. As the beam comes into contact with a defect, it is theorized to split into multiple source waves on either side which interfere as they travel across the plate to the receiver. By keeping the transmitter stationary and probing the receiver, we examine how the phase and amplitude change as the distance between transducers varies (transverse profiles). This approach potentially has a biological application because the acoustic contrast between healthy cells and cancerous cells is difficult to identify using current ultrasonic methods. This testing method could potentially gather more precise data with respect to the slightly differing contrasts between the cells and help better identify the presence and location of unhealthy cells.

C71.00007: Quantum Key Distribution Using Optimum Expectation Values of Maximally Entangled GHZ States*  COLLIN KESSINGER (Presenter), YE JIN HAN, QIAOREN WANG, Greenville Coll — We propose a new quantum key distribution scheme that is based on the optimum expectation values of maximally entangled Greenberger-Horne-Zeilinger states. Our protocol makes use of the degrees of freedom in continuously variable angles, thereby increasing the security of the key distribution. Outlined are two protocols that distribute a key from Alice to Bob using the above idea, followed by an extension that allows for the same key to be shared with Charlie. We show how this scheme provides for certain detection of any eavesdropper through absolute violation rather than the probabilistic violation used in many protocols.

*Cleveland University Science Founation

C71.00008: Temperature dependent charge transport in graphene with ferroelectric gating*  KELOTCHI FIGUEROA (Presenter), LUIS M RIJOS, NICHOLAS PINTO, Univ of Puerto Rico - Humacao, SRINIVAS MANDYAM, MENGQIANG ZHAO, ALAN T JOHNSON, University of Pennsylvania — CVD graphene was electrically characterized in a field effect transistor configuration with ferroelectric (FE) gating in the temperature range 300K < T < 350K. Saturated hysteresis loops of the FE co-polymer poly(vinylidene fluoride-trifluoroethylene)-PVDF-TrFE(75/25) showed that the memory window width decreased as temperature increased. Device trans-conductance (I-Vg) curves exhibit hysteresis behavior with two charge neutrality points (CNP) corresponding to the up/down polarization of the ferroelectric gate. Increasing the temperature decreased the change of the gate voltage and increased the change in the channel current measured between the two CNP’s. The electron mobility showed a steeper decrease compared to the hole mobility as temperature was increased. Desorption of O₂ and H₂O was used to explain these observations. Finally, non-volatile switching was realized using the charge storage property of the gate insulator.

*This work was supported by NSF under grants: DMR-PREM-1523463 and DMR-RUI-1800262
C71.00009: Developing a Method for Measuring the Optical Scattering of Silica Nanosprings*  
JEFFREY YODER (Presenter), Indiana Univ - South Bend, DAVID N MCILROY, Physics, Oklahoma State University — Nanosprings have been shown to have a variety of applications in medicine, industry and material science due to their unique nano-scale characteristics. Recent developments have vastly improved the ability to produce large quantities of high-quality silica nanosprings, making possible new avenues of research and applications. Current research includes applications in prosthetic-bone interfaces, detection of small quantities of gases, and the development of new composite materials. As such, there is a growing interest in better understanding their properties. The motivation for this work is to develop a method for studying the optical properties of these silica nanosprings. An apparatus for measuring the optical scattering of light off of the nanosprings has been constructed and measurements are ongoing. The first objective is to confirm visual observation of diffraction effects in nanosprings. The apparatus uses a visual microscope, a spectrograph, and illumination by a variety of lamps via fiber optics. A single nanospring is held by a micromanipulator; light (typically white) is then scattered off the spring and collected to produce spectra. This data is then analyzed for diffraction effects.

*Research conducted at Oklahoma State University and funded by NSF Grant #1757883.

C71.00010: Phase-Modulated Local Oscillator Effects on RF-DNA Fingerprints in IEEE 802.11a Wi-Fi Signals*  
WILLIAM MITCHELL (Presenter), Physics, Belmont University, KAITLIN HALL, Electrical and Computer Engineering, University of Utah, AHMED IBRAHIM `, DONALD REISING, THOMAS DANIEL LOVELESS, Electrical and Computer Engineering, University of Tennessee Chattanooga — With the increasing dependence on the internet in more and more consumer products, there is an urgent need to enhance existing digital security systems. RF-DNA fingerprints are one such approach to utilize discriminating waveform characteristics to augment the detection (rejection) of approved (unapproved) Wi-Fi devices. This work investigates a time-dependent approach to manipulate the RF-DNA fingerprints of a transmitting device through local oscillator phase modulation of the clocking system in Wi-Fi transmitters. Experimental results are used to investigate the ability for an unaffected receiver to detect a corresponding clock-modulated transmitter, as well as the changes of 802.11a Wi-Fi preambles of clock phase modulated transmissions. Changes in the waveforms are further analyzed using the Discrete Gabor Transform in the time-frequency domain. Analysis shows a predictable pattern of change over time, proportional in frequency to the phase-modulation frequency, and the ability for preamble structures to remain intact up to 30 kHz of phase modulation.

*This work was supported in part by the NSF through grant #1757777
C71.00011: Investigation of the Damage to Hydrophobic Self-Assembled Monolayers by Aqueous Salt Solutions  JULIANA SEBOLT (Presenter), CAYTON HORNBERGER, GRACE ROHaley, ADELE POYNOR, Allegheny Coll — When water is forced into contact with a hydrophobic surface, a depletion layer, or a low-density region of water, is formed. To study the depletion layer in more natural applications, we look at how aqueous salt solutions interact with hydrophobic surfaces made from self-assembled monolayers (SAMs) of octadecanethiol. In order to investigate this interaction we need smooth, homogeneous SAMs. Aqueous solutions can corrode the SAM, so we experiment salt molarity and cation size to eliminate this problem. The experimental methods include contact angle measurements, scanning electron microscopy, surface plasmon resonance.

C71.00012: Optimization of Microgel Imaging Using SEM*  SAMANTHA C TIETJEN (Presenter), PETRU STEFAN FODOR, KIRIL STRELETZKY, Cleveland State University — Microgels are polymer-based nanoparticles suspended in water that exhibit. The standard, noninvasive method for characterizing microgels is dynamic light scattering (DLS), which measures collective diffusion of microgels. While DLS provides reliable estimates for particle structure/dynamics, more direct methods of imaging are useful for studying polydisperse samples. Traditionally, scanning electron microscopy (SEM) uses an electron beam under high vacuum to characterize individual dried particles of dried. The dry microgel imaging suffers from two drawbacks: dehydrated particles collapse under vacuum and their dynamics is not observable. This project explored wet particle imaging in an ionic liquid stable under high vacuum. Particles were suspended in an ionic liquid film on a copper grid. Still images/movies were recorded to analyze microgel size distribution and dynamics. The average SEM size generally agreed with DLS both in ionic liquid and in water at room temperature. Variation was observed in individual particle sizes, but the average SEM size for both samples were close to the DLS size. Initial attempts at diffusion analysis using SEM particle tracking yielded mixed results as it requires tracing of many particles and further optimization.

*NSF REU Award #1659541, CSU USRA
C71.00013: Effect of cerium substitution on the superconducting state of $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$*

MOHAMED ESSAM NAWWAR (Presenter), BENJAMIN WHITE, Central Washington University — The superconducting compound $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$ has one of the highest critical temperatures ($T_c = 30$ K) of any non-cuprate oxide. In this study, we probed its superconducting properties by studying the impact of chemical substitution with Ce on the system $\text{Ba}_{0.6-x}\text{Ce}_x\text{K}_{0.4}\text{BiO}_3$. The objective of this study was to measure the effect of introducing magnetic moments by comparing the $x$-dependence of $T_c$ in $\text{Ba}_{0.6-x}\text{Ce}_x\text{K}_{0.4}\text{BiO}_3$ with the previously established behavior of $\text{Ba}_{0.6-x}\text{La}_x\text{K}_{0.4}\text{BiO}_3$. Our polycrystalline samples, synthesized using the molten salt technique, exhibited suppressed $T_c$ values compared with that of $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$; however, we were unable to observe a clear correlation between measured lattice parameter values and $x$, suggesting that the molten salt synthesis method we used is unable to finely control the Ce content of the samples. Additional measurements will be required to determine the exact stoichiometry of the samples and x-ray photoemission spectroscopy will be required to determine the oxidation state of Ce ions. In this poster, x-ray diffraction and magnetic susceptibility measurements will be presented and compared with results from $\text{Ba}_{0.6-x}\text{La}_x\text{K}_{0.4}\text{BiO}_3$.

*This project was funded by a Summer Undergraduate Research Experience grant from Central Washington University.

C71.00014: Fragmentation and Desorption of Surface-Immobilized DNA on PMMA and PAA Substrates for Sequencing Applications*

ELLEN GUO (Presenter), QINXI LIU, KATHY XING, KERUI YANG, LUISA PAN, JOCELYN ZHU, ANTHONY DEL VALLE, Stony Brook University, JOSEPH JENNINGS, Nassau Community College, JONATHAN CARL SOKOLOV, Stony Brook University — Producing ordered fragments of DNA would greatly simplify sequencing’s assembly problem. We studied the enzymatic cutting and desorption of surface-immobilized $\lambda$-DNA molecules on PMMA and PAA coated silicon wafers. Surfaces were dipped into 0.5-5.0 μg/mL DNA solutions and retracted at 1-10 mm/s speeds to stretch and immobilize (“molecularly comb”) DNAs on the surface. For PMMA, desorption was done in heated buffer solutions (DNase buffer, NEBuffer 3.1, pH-altered NEBuffer 3.1 (pH≈10) at 50-70°C). For PAA, which switches water-solubility by immersion in CaCl$_2$ or NaCl solutions, complete desorption into saline solution by PAA dissolution was observed. Relative to previous soft lithography methods, we employed a microfluidic method to improve DNA fragmentation. Holes in 1mm thick PDMS membranes were produced by piercing the PDMS with microneedles (d =250-400 μm) or by curing PDMS around the microneedles. PDMS layers with holes were pressed onto adsorbed DNAs and a DNase I cutting enzyme solution was deposited on top. By applying a vacuum (125 Torr) above the solution, the low-volume chambers fill with solution and efficiently cut the DNA, as confirmed by fluorescence microscopy.

*We acknowledge support from the Louis Morin Charitable Trust and NYS Department of Economic Development.
C71.00015: Observation on WSe$_2$/WS$_2$ hetero-bilayer spectroscopic and transport features*
ZHUOHANG YU (Presenter), Physics, Pennsylvania State University, FELIPE CERVANTES SODI, Physics and Mathematics, Universidad Iberoamericana Ciudad de México, NESTOR PEREA LOPEZ, ANA LAURA ELIAS ARRIAGA, TIANYI ZHANG, MAURICIO TERRONES, Physics, Pennsylvania State University — Semiconducting transition metal dichalcogenide (TMD) monolayers are one of the most promising materials for future optoelectronics. When two different TMD monolayers are brought together, the interlayer electronic coupling effects generate a new band structure inherent to the bilayer. We aim to fabricate hetero-bilayers comprising WSe$_2$ monolayer and WS$_2$ monolayer and analyze their optical spectroscopic and electronic transport features.
We synthesized WSe$_2$ and WS$_2$ monolayers on Si/SiO$_2$ substrates by chemical vapor deposition. After growth, both monolayers were sequentially transferred onto a pristine Si/SiO$_2$ substrate to have high quality overlapped areas of heterobilayers. The samples were then annealed to enhance the coupling between layers. Lastly, we patterned Au/Ti contacts on the bilayers by e-beam lithography for electrical property characterization.
The Raman and photoluminescence spectra of the bilayers were compared before and after annealing, and we found a significant decrease in the photoluminescence intensity for both WSe$_2$ and WS$_2$. Future work will include the analysis of the electronic transport data to obtain the carrier mobility as a function of stacking angle and possible tunability in the exciton energy emission.
*We thank the financial support from the NSF-MRSEC.

MICAH KARAHADIAN (Presenter), AUSTIN R SMITH, EMMA VAHLE, HEIDE M DOSS, Pt Loma Nazarene Univ — CR-39, a thermoset resin, is a well characterized integrative detector that, when etched, shows tracks created by energetic charged particles produced in nuclear reactions. It has been questioned whether this detection method can be used in Pd/D electrolytic cell environments. Of concern is whether the pyrophoric nature of hydrogen's interaction with palladium and its recombination with oxygen within the cell can create similar tracks. The validity of this detection method in an electrolytic cell environment is investigated. Additionally, track comparisons from detectors used in a Pd/D co-deposition experiments utilizing K-40 or Li-6 electrolytes were done to determine if Li-6 contributes to the observed tracks.
C71.00017: Topological Effects in Knotted Arrays of One-Dimensional Quantum Rings
COLIN RIGGERT (Presenter), KIERAN MULLEN, Homer L. Dodge Department of Physics and Astronomy, Univ of Oklahoma — Quantum ring arrays (QRAs) offer insight into the impact of topology in quantum systems, displaying phenomena which often have implications in quantum technology. We study the energy spectra and wavefunction behavior of small (two and three ring) QRAs by building up a model of tunnel-coupled one-dimensional quantum rings from existing models of crossed one-dimensional quantum wires. An ambiguity arises in how we connect the ends of these crossed wires, allowing us to create QRAs with the same tunnel coupling, but topologically distinct boundary conditions. We solve these systems numerically for various strengths of the tunnel coupling and find that topological differences in hole count manifest in observable differences in the single electron QRA energy spectrum in the absence of external fields. We also consider these QRAs in the presence of a uniform external magnetic field that induces an Aharonov-Bohm phase in the electron as it tunnels. By varying the induced phase, we explore magnetic phase commensuration effects in the QRA energy spectra and find that these QRAs have additional topological qualities that manifest in further differences in the energy spectra. We propose knot theory as the tool for distinguishing these systems and explaining phase commensuration effects.

C71.00018: Effect of transverse magnetic fields on an isotopically engineered diamond NV ensemble
JON CAMPAU (Presenter), PETER BRERETON, RAJRATAN BASU, US Naval Academy, DANIELLE BRAJE, MIT Lincoln Laboratory — The nitrogen vacancy (NV) in diamond is a leading candidate for quantum sensing applications such as magnetometry. Here, we study the effect of a transverse external magnetic field on the spin coherence of an ensemble of nitrogen vacancy (NV) centers in diamond with applications to high-sensitivity magnetometry. A transverse magnetic field has been shown to suppress electronic spin decoherence [1]. By utilizing 15N ions for implantation, the nuclear hyperfine interaction between the 13C spin bath and the defects is minimized. We utilize optically detected magnetic resonance and pulsed methods to explore this effect in isotopically engineered diamond films.


*This work is supported in part by the Office of Naval Research under grant N0001419WX00566 and the Admiral Frank Bowman Scholar Program.
C71.00019: Link Testing between the Data Formatter and Second Stage Boards for the Fast Tracker Trigger in the ATLAS Experiment at CERN* CHRISTINA PINO (Presenter), California State University, Sacramento — At CERN, link testing was performed between the Data Formatter (DF) board and the Second Stage Board (SSB). This was to advance the installation of the Fast Tracker Trigger (FTK) for the ATLAS collaboration by the end of the 2nd Long Shutdown (LS2). Link testing was performed in the Underground Service ATLAS hall (USA 15) where the FTK is located. Different combinations of the Data Formatter board and Second Stage Board were tested using Xilinx's Integrated Bit Error Ratio Tester (IBERT) to vary the transceiver and receiver settings between the boards. To analyze the bit error ratio between the boards, the IBERT core would generate eye scans and bathtub plots to get a visualization of the digital signal integrity.

*I would like to thank Dr. Joshua Moss (CSUS) for funding my research at CERN through the NSF Grant No. 1506502. I would also like to thank my mentors Jonathan Long (UIUC) and Stanislava Sevova (Stanford) for guiding me through the summer.

C71.00020: Highly non-stoichiometric amorphous oxide semiconductors: the structure and electronic properties of defects in a-InOx ELIZABETH CAPUTA-HATLEY (Presenter), JULIA MEDVEDEVA, Missouri Univ of Sci & Tech — Oxygen non-stoichiometry in crystalline In2O3 leads to formation of oxygen vacancies that play key role in carrier generation and transport in this transparent conducting oxide and have been well-studied both theoretically and experimentally. In contrast to the crystalline oxide, the structure and electronic properties of oxygen defects in amorphous indium oxide (a-InOx) are not understood and render to be fundamentally different due to the lack of lattice sites and periodicity as well as an increased number of degrees of freedom in disordered materials. Strikingly, the observed carrier concentration in a-InOx is two orders of magnitude higher than that in the crystalline oxide. Moreover, given the ionic nature of indium-oxygen bonding, it is possible to grow highly non-stoichiometric amorphous oxides that helps tune the properties over an extremely wide range. Here, we employ ab-initio Molecular Dynamics simulations and density-functional calculations to study the structural and electronic properties of a-InOx. Based on a thorough analysis of the interatomic distances, coordination, distortions, charge localization, and defect state energies, we derive a microscopic model of defects in disordered oxides and discuss their effect on the electrical and optical properties.
C71.00021: In situ ellipsometry of epitaxially grown bismuth antimony telluride on sapphire*  MOLLY MCDONOUGH (Presenter), Physics, Suffolk University, TIMOTHY PILLSBURY, ANTHONY R. RICHARDELLA, NITIN SAMARTH, Physics, Pennsylvania State University — Ellipsometry uses elliptically polarized light to characterize thin film and bulk materials. The light undergoes a change in polarization as it interacts with the sample structure. The measurement is typically expressed as two values: Psi (Ψ) and Delta (Δ). Bismuth telluride and its alloys are widely used as materials for thermoelectric and spintronic devices. This project uses in situ rotating compensator spectroscopic ellipsometer to measure properties of Bismuth Antimony Telluride ((BiSb)\textsubscript{2}Te\textsubscript{3}). If properties of bismuth antimony telluride such as thickness and composition can be determined by ellipsometry, it can be used as a tool to improve growth parameters in real-time, improving throughput and precision when growing these materials.

*This work was supported by NSF through the REU (DMR-1851987) and the 2DCC-MIP (DMR-1539916) programs.

C71.00022: Study of Optical Properties of composite layers of MEH-PPV nanopillars and PEDOT:PSS films  EVANGELINE BEECHING (Presenter), Slippery Rock Univ — Fabrication of MEH-PPV nanopillars was completed using porous Anodic Aluminium Oxide (AAO) templates. The diameter and height of the nanopillars was controlled by adjusting the dimensions of the template. The morphology of the nanopillars was studied using scanning electron microscopy. The absorption of light of MEH-PPV nanopillars plus thin film was greater than that of the thin film only, both being the same thickness. The dimensions of nanopillars are essential for carrier processes such as exciton generation, exciton diffusion and carrier dissociation and transport. As PEDOT: PSS can enhance hole collection and exciton diffusion, addition of PEDOT: PSS improves the performance of solar cells. The variation in optical properties of composite material consisting of MEH-PPV nanopillars and PEDOT:PSS films will be investigated using UV-Vis spectroscopy and fluorescence spectroscopy with change in height and diameters of the MEH-PPV nanopillars.

C71.00023: Modeling directed self-assembly of nanoparticles under perpendicular electric fields  ELISE BAKER (Presenter), MATTHEW WITHERS, DAN MAZILU, IRINA MAZILU, Washington & Lee Univ — We design and model an experiment to study the effect of electric bias on particle-coverage densities produced during ionic nanoparticle self-assembly. The experiment involves the application of a uniform external electric field parallel to a glass substrate during the self-assembly of silica nanoparticles. We refer to this procedure as directed self-assembly of monolayers (DSAM). In our theoretical analysis, we modify existing cooperative sequential adsorption models to account for diffusion under an applied electric field. We use the mean field approximation to solve for particle-coverage densities. To ascertain the validity of this method, we compare our solutions to Monte Carlo simulations of the system. We also discuss particular experimental implementations of an ionic self-assembled monolayer under the influence of perpendicular external electric fields.
**C71.00024: Nonlinear Magnon Scattering Observations Via The Magneto-Optical Kerr Effect**

* PAUL BAILEY (Presenter), Brigham Young Univ - Provo, PAUL CROWELL, University of Minnesota — Nonlinear Magnon Scattering is observed in Yttrium Iron Garnet (YIG) thin films. Nonlinearity is excited in the YIG thin films by high power microwave pumping. The magnetization of the films due to the microwave pumping is then observed through the Magneto Optical Kerr Effect (MOKE). The MOKE is of interest as a measurement technique because of its potential to observe magnon scattering in real time. Well-defined thresholds of the linear and nonlinear regimes are examined by ferromagnetic resonance measurements using this setup.

*This work is funded by the National Science Foundation REU grant 1757388.*

**C71.00025: Thermal metamorphism study of carbonaceous chondritic meteorites**

ROHIL KAYASTHA (Presenter), RAKA PAUL, AARON STOKKE, ANALÍA DALL'ASÉN, Physics and Astronomy, Minnesota State University, Mankato — Carbonaceous chondritic meteorites are some of the most primitive materials in our solar system. They did not experience melting or other processes on their parent bodies (e.g. asteroids) during their initial formation, and thus, they preserve information of physical and chemical mechanisms in the solar nebula, which can unveil evidence about the origin of the planets and their components. However, most carbonaceous chondrites are exposed to secondary processes on their parent bodies, such as thermal metamorphism and aqueous alteration, modifying the primary properties of the carbonaceous chondritic constituents. Hence, in order to understand how these relics formed, it is important to analyze the modifications they have experienced induced by these secondary processes. In this work, we study the thermal metamorphism of these chondrites examining their carbon composition by Raman spectroscopy. We analyze the Raman spectra of carbon allotropes to obtain specific parameters that we use for thermal metamorphism mathematical models. In addition, we correlate the Raman results with those acquired using SEM/EDS (Scanning Electron Microscopy/Energy Dispersive X-ray Spectroscopy), and we compare these findings with the results obtained from previously studied meteoritic samples.
We introduce dual-color differential dynamic microscopy (DDM) for detecting fast dynamics. DDM has been used extensively to measure the diffusive or ballistic motion of small particles, macromolecules and bacteria. Rather than localizing and tracking individual particles, DDM works by measuring the intensity fluctuations in images across a range of detectable spatial frequencies and provides data similar to that provided by dynamic light scattering. However, DDM is limited by the camera frame rate. Fast dynamics can be measured with high-speed cameras but those are typically expensive. We have developed a dual-color imaging setup which allows us to detect dynamics faster than the camera’s frame rate. We trigger blue and red light at well-defined times within a single image exposure. By analyzing each color channel separately and in combination we detect dynamics that are several times faster than the camera frame rate.

Research Corporation Cottrell Scholar award

C71.00027: Gradient-Based Algorithms for Characterizing the Structure of Fibrin Clots*
NOLAN ROTH (Presenter), High Point Univ — The human body's ability to close wounds through clotting is vital to everyday function—but irregular clotting can cause diseases like deep vein thrombosis, Von Willebrand disease, or hemophilia, which lead to hundreds of thousands of deaths each year. Understanding how various clotting mechanisms affect the mechanical and structural properties of a blood clot's fibrin fiber network is integral in working to prevent and treat these clot-related diseases. Two structural characteristics of the network, the average fiber diameter and branch point density, lend themselves to discovery by applying various computational image analysis techniques to images acquired using scanning electron microscopy or fluorescence microscopy. Algorithms using gradient-based thresholding were implemented in Python to minimize data loss from classic image analysis techniques and to quantify the network’s structural characteristics.

*Society of Physics Students for generous travel funding
C71.00028: Progress on the Development of a Magnetic Field Sensor*  KATHERINE GIFFORD
(Presenter), ZOYA SHAFIQUE, SEAN JAMES BENTLEY, Adelphi University — This project aims to
develop a magnetic field sensor by using the special properties of quantum entangled photons to
intensify the sensitivity of a Faraday effect based sensor. The Faraday effect occurs when the
polarization of light rotates as it passes through select materials in the presence of a magnetic
field. For our set up, we chose crystals with high Verdet constants: Cd0.57Mn0.43Te
andCd0.86Mn0.14Te. The introduction of a super magnet creates a measurable polarization
rotation in light passing through the selected crystals. Using a magnet in the shape of an annulus,
we experimented with a variety of geometrical configurations in an attempt to maximize the
rotation produced by the magnet and crystal. In the first set up, we mounted the magnet in close
proximity to the crystal. In later designs, we placed the crystal inside of the super magnet by 3-D
printing a structure to hold the crystal. Generating position-momentum entangled photons
through parametric down-conversion, our goal is to use the quantum nature of the photons to
create a highly sensitive magnetic field sensor.

*We would like to thank Adelphi University for funding.

C71.00029: Adsorption of CO$_2$ and N$_2$ on Graphite and Cone Grid*  EMILY KOIVU (Presenter),
Emory University, SILVINA GATICA, Howard University — Adsorption is the phenomenon that occurs
when a gas is in the presence of any material and is uniquely fit for different elements. Using
molecular dynamics simulations, the adsorption of a CO$_2$ and N$_2$ mixture on graphite is studied
at differing temperatures. Attempts to increase selectivity are made by introducing cones,
inverted and upright, on top of the graphite. Results show that at molecules are more easily
adsorbed at 300K than 400K and that the presence of the cones decreases selectivity, though
upright cones perform worse than inverted cones. Further study at different ranges of
temperature and strengths of interactions with the inverted cones should provide useful in
determining the most effective way to use adsorption to separate CO$_2$ and N$_2$.

*Financial support from the REU Site in Physics at Howard University NSF Award PHY 1659224 is
gratefully acknowledged.
C71.00030: The Effect of Si Nanoparticles and SiGe Nanoparticles on the Photovoltaic Conversion Efficiency CdS/CdTe Thin Film Solar Cells  JASMYNE EMERSON (Presenter), YUNIS YILMAZ, MEHMET ALPER SAHINER, Seton Hall Univ — The addition of embedded Si nanoparticles and SiGe nanoparticles in CdS/CdTe thin films deposited on ITO coated glass has been investigated in this study. We're testing the effects of Si nanoparticles and SiGe nanoparticles on the efficiency of CdS/ CdTe thin film solar cells and comparing the effects of different deposition times, particles sizes, and how they compare with each other. Si was originally tested in order to compare to the results of Au and Ag nanoparticles. SiGe nanoparticles are also being tested because Ge is likely to form more stable nanoparticles. SiGe alloys will have higher mobility as charge carriers than Si. In the process of creating these solar cells, CdTe and CdS are deposited onto ITO coated glass substrates using the method of Pulsed Laser Deposition. Si or SiGe nanoparticles were deposited between the CdS layer and the CdTe layer using the PLD method with various deposition parameters and durations to obtain variations in nanoparticles coverage at the interface. In order to characterize the Si nanoparticle embedded thin films, XRD, AFM, and SEM/EDX were used.

C71.00031: Engine of Life: Biophysics and Tyrosine*  JI KU (Presenter), Physics, Muhlenberg College, DEANNA LUNEAU, K. V. LAKSHMI, Chemistry, Rensselaer Polytechnic Institute — Carbon dioxide emissions have increased sharply within the last few decades, which has resulted in climate change and pollution. This has led to the search for alternative energy sources, using photosynthesis as an inspiration. Within photosynthesis, photosystem II (PSII) uses light energy to drive the energetically demanding four-electron oxidation of water to dioxygen. There are two symmetric redox-active tyrosine residues, Y_Z and Y_D, in the D1 and D2 protein subunits of PSII. While these tyrosine residues are chemically identical, they are functionally distinct. It is proposed that Y_Z is directly involved in the primary electron transfer pathway of PSII. In contrast, the Y_D residue is proposed to be involved in the assembly of the catalytic Mn_4Ca-oxo cluster. My research is focused on understanding the structure and function of the Y_Z and Y_D residues of PSII. In my presentation, I will describe the methodology of cyanobacterial cell cultures, isolation and purification of PSII and the application of pulsed electron paramagnetic resonance spectroscopy to study the Y_Z and Y_D radicals of PSII.

*This work was supported by the National Science Foundation via the Physics REU site at Rensselaer Polytechnic Institute. I would like to thank Lakshmi Lab for the research support.

C71.00032: Ideal Diode Behavior at the Graphene - WSe_2 Schottky Junction  COLLIN SANBORN (Presenter), JI UNG LEE, SUNY Polytechnic Institute — The metal-semiconductor interface is a core component of many nanoelectronic devices. The Schottky junction that can form at these interfaces is key to our understanding of device behavior. We have demonstrated that in graphene-silicon junctions, the current-voltage behavior based on bulk analysis no longer applies, and the diode is best characterized by the Landauer quantum transport formalism. We extend this analysis from silicon to transition metal dichalcogenides, a class of 2D semiconductors. We construct Van der Waals heterostructures of graphene and tungsten diselenide encapsulated in hexagonal Boron Nitride, and vary the geometry to analyze the physics of this new Schottky junction.
**C71.00033: Ferromagnetic Positron Beam Guidance for Single Shot Measurement in 2D-ACAR Spectrometers**  
MARTIN GROSSHAUSER (Presenter), University of Illinois at Urbana-Champaign  
— Angular correlation of electron-positron annihilation radiation (ACAR) is a technique to determine the electronic structure of solids. It is based on detecting the annihilation gammas' deviation from collinearity in order to measure the electron momentum before annihilation. This study deals with the experimental feasibility of single-shot ACAR measurements as a way of efficiently mapping the Fermi surface of crystals with a low electron momentum directions, corresponding to a quasi 2D electronic system.  
Single-shot measurements require the sample normal to be aligned with the detector axis, with the positron source being outside the field of view at the same time.  
A novel approach of ferromagnetically guiding positrons under high external magnetic field (1.0T) conditions is explored both in simulation and experimentally. Furthermore, new radiographic methods to quickly assay positron beams are evaluated.

**C71.00034: Symmetries of Two Atoms with Contact Interactions in a Ring Trap**  
ISABEL FERNANDEZ (Presenter), NATHAN L HARSHMAN, American University  
— We consider an idealized model of ultracold atoms in a ring-shaped optical trap with s-wave and p-wave contact interactions. The relative dynamics for two interacting particles are mapped onto a single particle traveling on a ring disrupted by zero-range delta-function barriers and delta-prime barriers. We categorize the symmetry groups of these potentials and find the exact solutions for stationary states. By classifying the energy spectrum in terms of the irreducible representations of the symmetry groups, we reveal that there are additional symmetries “hidden” in contact interactions.

**C71.00035: Measurements of the Size Variation of Optically Trapped Aerosol Water Droplets Using Cavity Enhanced Raman Spectroscopy (CERS)**  
DALTON ANDERSON (Presenter), LOWELL I MCCANN, University of Wisconsin-River Falls  
— Optical traps have numerous applications including the study of aerosol droplets. It has been observed that in a single beam optical trap, micro-meter sized aerosol droplets exhibit hysteretic axial motion in the direction of beam propagation. Two meta-stable positions have been observed and it is thought that the cause of this motion between positions may be due to morphology dependent resonances (MDRs). For this to occur, thermal expansion of the droplet from a varying laser beam power must occur. Using Cavity Enhanced Raman Spectroscopy (CERS) we can investigate the size of the droplet as the position of the droplet and the laser power varied.

*This research was supported by a UWRF URSCA Undergraduate Stipends and Expenses grant.*
C71.00036: Time-integrated Four-wave Mixing Measurements on Transition Metal Dichalcogenides in High Magnetic Fields*  ALEJANDRO VILLALOBOS (Presenter), DENIS KARAISKAJ, Physics, University of South Florida, STEPHEN A MCGILL, Physics, Florida State University, VARUN MAPARA, Physics, University of South Florida — Monolayer transition metal dichalcogenides are 2D materials with unique optical properties that make them potential candidates for use in optoelectronic devices and even quantum logic gates. We can observe changes in exciton dephasing rate in TMDs under high magnetic fields and use four wave mixing spectroscopy to better understand and manipulate exciton dynamics. Using the MONSTR apparatus, we took FWM measurements of a monolayer MoSe$_2$ sample, scanning from negative to positive delay signal to analyze the dephasing time of excitons. We applied magnetic fields up to 25T and altered the polarization scheme of the excitation pulses from cross-circular to co-circular to observe the dependence of exciton dephasing rate on these factors. The preliminary data suggests non-Markovian behavior, which can be seen in the broadening of the FWM signal. This may be a result of increased biexciton formation, which we learned may be tuned using a magnetic field. In the future, the application of a magnetic field onto heterostructure TMDs may also provide interesting insights, particularly into the dynamics of interlayer excitons.

*This work was supported by the National Science Foundation (NSF) grant DMR-1852269

C71.00037: The magnetic structure of a strongly correlated rare-earth based intermetallic system Au$_2$PrIn.*  SVETLANA DOROSHEVICH (Presenter), NAMI UCHIDA, Bergen Community College, KALANI HETTIARACHCHILAGE, Department of Physics, Seton Hall University, NEEL HALDOLAARACHCHIGE, Bergen Community College — The electronic structure of the rare-earth based intermetallic system, Au$_2$PrIn, is studied using computational methods. The material, a member of a large family of Heusler compounds, was recently discovered, and only crystallographic data was reported. The never reported Lanthanum version (Au$_2$LaIn) was also studied for the comparability of non-magnetic analogue. Both Au$_2$LaIn and Au$_2$PrIn show three-dimensional metallic nature with large band dispersion at Fermi level in electronic structure. Au $d$-electrons are dominated in the electronic band structure of La system, whereas rare-earth $f$-electrons are dominated in the electronic structure of Pr system. The study suggests that the magnetism develops as the $f$-orbital fills up from non-magnetic La-compound to magnetic Pr-compound. The electronic band structure of Pr compound shows local magnetism with $f$-electron bands near the Fermi level. Calculated magnetic moment is comparable with the expected magnetic moment of Pr. Calculated Curie temperatures are comparable with the stable magnetic structure predicted by spin polarized calculations. Detailed results of electronic and magnetic properties of Pr-system with the predicted magnetic structure will be presented.

*STEMatics Grant, Department of Education
C71.00038: MCG modelling and eccentricity calculations for Pb+Pb and Au+Au collisions at various $\sqrt{s_{NN}}$ — ANYA WOLTERMAN (Presenter), Physics and Astronomy, Macalester College — Glauber models provide insight into the initial state of nuclear collisions by treating them in terms of the interactions of the constituent nucleons, in accordance with theories about the scattering of composite particles. These phenomenological techniques are commonly used to determine various geometric quantities associated with such femtoscopic many-body systems. The Glauber Monte Carlo approach uses a random impact parameter and measured nuclear densities to investigate quantifiable properties such as the particle multiplicity and the average geometric eccentricity for heavy ion collisions. The former involves the incorporation of a particle production model to calculate the total transverse energy, a measure of centrality. The latter delves into the eccentricity of different event classes, which can be used to characterize various collision shapes for measurements of elliptic flow of heavy mesons. The results of both applications are then compared with analyses of data from the CMS and STAR experiments.

C71.00039: Utilizing Electronics to Extend the Life of Musical Instruments — REBECCA CALLAWAY (Presenter), MARY DYE, ADAM SCHOENE, Univ of Mary Washington — Musical instruments are often discarded when the cost of fixing an issue becomes an inconvenience. Millions of dollars worth of instruments are thrown away each year while communities around the country struggle with funding art and music programs. This causes music to become a privilege and for certain instruments to be only associated with certain socioeconomic classes. A new system needs to be designed where students and teachers can be exposed to musical instruments without having to worry about financial constraint. Instead of disposing of an expensive instrument and adding to landfills, mass produced electronic components can be used to extend its functionality as an educational tool. Affordable light sensors are used in place of the core sound producing material on the instrument. Software is combined with the light sensors in a manner to reproduce the sound it would make with original materials along with the ability to manually change the tone. Due to an electronic interface, performance can be easily recorded in notation software to keep track of progress and enhance the musicians understanding of music.
C71.00040: Study on the Spontaneous Elemental Lysis of an Electrolyte due to the presence of a Static Magnetic Field from contact with a so-called Permanent Magnet*  DEBOSMITA PATHAK (Presenter), Grinnell College, RAJATAVA MUKHOPADHYAY, Physics, IISER Thiruvananthapuram — This is a project to verify the results of a controversial experiment performed by Prof. Felix Ehrenhaft (1944). The absence of any constructive follow up research work for 74 years has motivated this work.

This experiment is focused on studying the effects of the static magnetic field due to standard laboratory and industrial grade AlNiCo bar magnets on a 0.1 M solution of CuCl$_2$. The deposition of copper granules begins near the south pole of the bar magnet and gradually progresses to cover the entire surface of the magnet. Gas bubbles form near the north pole of the magnet. This hints at the lysis of the CuCl$_2$ electrolyte. However, this happens without any external induced potential difference acting between the terminals, and only when a magnet is present, not otherwise. The study of the lysis of electrolytes in the presence of such a static magnetic field and the implications that this phenomenon presents are the aims of this experiment.

* We acknowledge the generous support of the Jagadis Bose National Science Talent Search (JBNSTS) Research Fund, Kolkata, India.
We also acknowledge the guidance of Dr. Joy Mitra, IISER Thiruvananthapuram, Thiruvananthapuram, India and Dr. Abhijit Kar, JBNSTS, Kolkata, India as mentors.

C71.00041: Synthesis and physical properties study of polar magnet HoFeWO$_6$*  CHRISTIAN BUCHOLZ (Presenter), DUY PHAM, Physics, Kennesaw State University, RAM C RAI, Physics, Buffalo state university, CHETAN DHITAL, Physics, Kennesaw State University — Polar oxides are important system to study due to their technologically relevant properties such as ferroelectricity, multiferroicity, piezoelectricity, magnetoelectricity. Recently, RFeWO$_6$ (R=Dy, Y, Tb, Eu) type polar oxides were synthesized and type-II multiferroic property was reported [1]. We have extended this series and successfully synthesized HoFeWO$_6$ in polar structure. We have also characterized this material using dielectric and magnetization measurements. We will present the synthesis method and the results from the dielectric, structural and magnetic measurements.


*This work is supported by mentor protege grant (432134) and SABAC through student physics society (SPS) Kennesaw State University.
**C71.00042: The Development of Four-Wave Mixing Spectroscopy to Measure Vibrational Spectra in the Low-Frequency Terahertz Range**

BENNY SCHUNDELMIER (Presenter), LASZLO JANOS UJJ, Univ of West Florida — We report the progress of developing four-wave mixing spectroscopy to measure vibrational spectra in the low-frequency terahertz range. The optical tabletop system, we have improved in the Laser Spectroscopy Lab at the University of West Florida is a multipurpose system [1], capable of executing a variety of spectroscopy methods such as e.g. Raman, Coherent Raman, and Laser-Induced Breakdown spectroscopy. For this project, our focus is on Coherent Raman Spectroscopy, through three-color two-beam broadband nonlinear frequency mixing. The three-color nature of the four-wave mixing signal allows for an effective non-resonant signal suppression relative to the polarized and depolarized Raman bands. This type of nonlinear four-wave mixing has not been fully utilized for ultrafast coherent Raman microscopy. To demonstrate the precision and merit of our modified system, we present measured and processed spectra of liquid and crystalline samples and provide a characterization of the critical components that constitute our system.


*OUR Award

**C71.00043: Thermal Analysis of Pr_{1-x}Nd_xOs_4Sb_{12} in Normal State**

MATTHEW CHAZLE BROWN (Presenter), YEH-CHIA CHANG, PEI-CHUN HO, Department of Physics, California State University, Fresno, M BRIAN MAPLE, Department of Physics, University of California, San Diego, TATSUYA YANAGISAWA, Department of Physics, Hokkaido University — At low temperatures, the filled-skutterudite compounds PrOs_4Sb_{12} and NdOs_4Sb_{12} exhibit states of unconventional heavy-fermion superconductivity (SC) and ferromagnetism (FM), respectively. Thus, we have interest in studying the doping system of Pr_{1-x}Nd_xOs_4Sb_{12} in order to identify the competing mechanisms between the two states. Because the multiband superconductivity in this system may still be influenced by the electron-phonon mechanism, the normal state properties may give us insight into the properties of conduction electrons and phonons. The molar specific heat of Pr_{1-x}Nd_xOs_4Sb_{12} is measured in the normal state 10K-300K, and the thermodynamic parameters are extracted by incorporating Debye Temperature, Einstein Temperature, and the electronic specific heat coefficient, which provide information about the lattice stiffness, rattling effect, and electron correlation, respectively. Our findings convey that the Debye and Einstein temperatures have a V shaped x dependence that decreases towards central values of x, following the trend in transition temperature of low temperature ordered state.

C71.00044: Ferromagnetic Resonance of All Oxide Core / Shell Nanoparticle Variants*  
N. SCHULZ (Presenter), Concordia College Moorhead, CORISA KONS, J. SHOUP, J. ROBLES, MANH-HUONG PHAN, HARIHARAN SRIKANTH, DARIO ARENA, Univ of South Florida — Core-shell magnetic nanoparticles (MNPs) are being considered for various applications in spintronics as well as in the bio-medical field. Ferromagnetic Resonance (FMR) is a widely-used technique for determining magnetic properties such as bulk magnetization and anisotropy, gyromagnetic ratio / g-factor, and damping. Broadband FMR using a co-planar waveguide (CPW) is well-suited for examining properties of thin film samples, but MNPs present some challenges. MNPs can have a wide distribution of sizes and crystalline orientation. Also, at room temperature MNPs are generally superparamagnetic, where the magnetic orientation is unstable against thermal fluctuations. This research sought to adapt the standard CPW-FMR methods for thin films to characterize the resonant responses of MNPs, starting with commercially available magnetite (Fe₃O₄) MNPs and progressing to more complex Fe₃O₄/CoFe₂O₄ core-shell nanoparticle variants. Protocols were developed for mounting the different MNPs onto substrates suitable for CPW-FMR. The temperature- and frequency-dependent resonant response of the MNPs was explored. The determination of specific sample properties extracted from the CPW-FMR methods will be discussed.

*This work was supported by the National Science Foundation (NSF) grant DMR-1852269.

C71.00045: Generation Optical Beating between Hyperfine levels in the Decay of Rb atoms Excited by Different Pulse Shapes.*  
OLIVIA CHIERCHIO (Presenter), CHARANPREET SINGH, ZAFIR MOMIN, JAMES P ST. JOHN, MATTHEW WRIGHT, Adelphi University — We are investigating quantum interference in the atomic decay signal in a dilute thermal atomic gas with an intense pulsed laser beam. A short pulse of laser light (~ 3 ns) is used to drive atoms from the ground state to an excited state hyperfine manifold of levels. We are exploring how quantum beating and other excitation properties depend on the shape of the driving frequency (e.g., cw, chirped, white-noise, etc).

*NSF Award #1803837
C71.00046: Analysis of Time Evolution Algorithms to be Utilized in Modeling Classical and Quantum Mechanical Systems*

KATHERINE HUDEK (Presenter), L RAMDAS RAM-MOHAN, Physics, Worcester Polytech Inst — Time evolution in classical and quantum mechanical systems has been the focus of research because the behavior of physical systems with time are determined by their initial conditions. Calculation methods for the system values as it changes throughout time have to be very accurate in order to have predictions that we can rely on. This is the challenge of time evolution and its modeling.

In this project several time evolution algorithms were implemented and evaluated according to criteria of accuracy, stability, and consistency. Several scalar algorithms were examined as well as a technique for matrix exponentiation. Results show that the matrix exponentiation technique has significant advantages and is suitable for use in extending the time evolution models for various systems.

*This project was funded by CCNS (Center for Computational Nanoscience) at Worcester Polytechnic Institute and the Clare Boothe Luce Scholarship.

C71.00047: Verifying 2D device potentials and conduction with Kelvin Probe Force Microscopy*

JOEL TOLEDO-URENA (Presenter), JOSEPH MURPHY, REBEKAH SMITH, JOSEPH SIMPSON, JENNIFER T HEATH, Linfield Coll — In a 2D field effect transistor (FET), the electrical properties of the channel are modulated using a gate voltage. The electrostatic doping of the channel and the contact resistance of the interacting layers both contribute to the overall device conductivity, which plateaus above a certain gate voltage. Other factors, such as surface cleanliness and microscopic details of the films also influence the conductivity as can be deduced from variations between multiple devices. In this study, we explore the ability of Kelvin probe force microscopy (KPFM) to separate out the different factors influencing overall device conductivity. By applying a potential bias to a simple device, we build confidence in the linear response and reproducibility of the KPFM technique. We then directly visualize the uniformity of the surfaces, the potential barriers between layers, and the characteristics of the WSe$_2$ film as a function of the applied voltage. These data deepen our understanding of device potentials and conduction in 2D FETs.

*Financial support from the National Science Foundation and the M.J. Murdock Charitable Trust is gratefully acknowledged.
C71.00048: Detecting topological superconductivity by using a dc-SQUID*  
BENJAMIN HAWN (Presenter), JOSEPH PAKIZER, ALEX MATOS ABIAGUE, Wayne State Univ — We theoretically investigate the current and phase response of a dc-SQUID composed of two Josephson junctions (JJs) in parallel. The JJs are exposed to an in-plane magnetic field and their chemical potential and Rashba spin-orbit coupling strength are tuned by top gates acting separately on each of the junctions. By tuning the system parameters, each JJ can individually be driven from the trivial to the topological phase and vice versa. We investigate the 3 possible dc-SQUID configurations: the two junctions are topological, one junction is trivial and the other topological, and the two junctions are trivial. We perform theoretical simulations of the phase difference and critical current of the dc-SQUID for the 3 different configurations, and by comparing them we identify the signatures of the topological superconducting phase and its dependence on junction transparency, magnetic field, and spin-orbit coupling.

*This work was supported by DARPA Topological Excitations in Electronics (TEE) Grant No. DP18AP90000 and US ONR Grant No. 000141712793.

C71.00049: Water and Carbon Dioxide in Hydrated Hyperbranched Polyethylenimine Membrane Using Molecular Dynamics Simulation and Density Functional Theory  
KYUNG IL KIM (Presenter), ROBIN LAWLER, Chemical and Biomolecular Engineering, Georgia Institute of Technology, SEUNG SOON JANG, Materials Science and Engineering, Georgia Institute of Technology — Since excessive use of fossil fuels is releasing large amounts of CO$_2$ and exacerbating global warming, developing efficient materials to capture CO$_2$ is crucial. In this study, we investigate the hydrated hyperbranched polyethylenimine (HB-PEI) membrane in the presence/absence of water and carbon dioxide using molecular dynamics (MD) simulation to characterize their distribution and reaction mechanism in the HB-PEI membrane. For this, we prepare a model HB-PEI molecule and construct a condensed HB-PEI phase in the amorphous phase with various concentration of water and carbon dioxide molecules. Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package is used in our MD simulations to establish the equilibrium state of HB-PEI membranes. Through our MD simulations, we obtain samples of the local structure of water/carbon dioxide nearby amine groups in HB-PEI membranes and scrutinize a possible molecular mechanism and corresponding energy barrier for carbon dioxide capturing, via density functional theory (DFT) approach.
C71.00050: An evaluation of methods for measuring thermomagnetic transport properties of bulk and thin film materials  
ANDREW JARYMOWYCZ, JASON PRUITT, KYLE THOMSON, AUSTIN TINKESS (Presenter), MATTHEW BEEKMAN, Department of Physics, California Polytechnic State University — In the “method of four coefficients,” experimental data for electrical conductivity, Seebeck, Hall, and Nernst coefficients are fit to models based on Boltzmann transport theory to estimate quantities such as the carrier effective mass, concentration, mobility, and scattering exponent. This powerful method provides experimental information about the electronic structure and charge carrier scattering mechanisms in solids, and has been used to understand enhanced performance in some thermoelectric materials. Nevertheless, there is relatively little literature available regarding descriptions of experimental apparatuses and methods of measurement of all four coefficients on a single sample in a single measurement cycle. We recently constructed a custom system for measurement of thermomagnetic properties from 8 K to 400 K. Here we report on a study of different approaches for experimentally measuring these four coefficients on both bulk and thin films samples. For example, we have investigated the effect of mounting the sample in a flat vs. vertical geometry, which can be important for adiabatic vs. isothermal Nernst measurements. Our results provide useful guidance for constructing such apparatuses to measure the thermomagnetic properties used in the method of four coefficients.

C71.00051: Analyzing Challenging Scientific Thoughts in a Christian Academic Setting*  
MASON POHLMAN (Presenter), Belmont Univ — Throughout a significant portion of history and within modern culture, the fields of science and religion appear to be competing for the same holds in a person’s belief system. Universities are where academics and the sciences are the prevailing held truth, while in churches, the Bible reigns as supreme authority. However, in a Christian academic setting, the predominate school of thought in belief systems might turn into a little more of a melting pot. By analyzing gathered personal data (via surveys and interviews), one can begin to piece together the predominate thoughts on the apparent conflict between religion and science at such a setting. Institutions such as this, while always diverse in thought, can present a cohesion between the two seemingly opposed parties in a way where neither side loses ground culturally. Data gathered on personal religious experience, beliefs and experiences gathered around evolution, creationism, the Big Bang, and other issues that fall from that have been collected to present an image of how science and religion might be in understanding at a Christian house of higher education.

*Belmont University Honors Program
C71.00052: Electronic and Structural Properties of Yb-based Materials  BRITNEY HOPGOOD
(Presenter), Department of Natural Sciences and Technology, Ana G Mendez University, CHINEDU EKUMA,
Department of Physics, Lehigh University — We have investigated the electronic, structural, and
optical spectroscopy of YbT$_2$Zn$_{20}$-based (T = Co, Rh, and Ir) 1-2-20 compounds using first-
principles calculations that account for the strong on-site-f-electron Coulomb interactions. We
observed the strong hybridization and screening of the f-levels by the itinerant conduction
electrons that led to massive electron behavior with an unenhanced electronic Sommerfeld
coefficient of over ~600 mJ mol$^{-1}$ K$^{-2}$. The optical spectroscopy exhibits renormalized Drude
response, a partial enhancement of the dynamical conductivity below ~1.0 eV, the emergence of
the midinfrared peak structures at ~0.46 eV, and low photon-energy dynamical effective mass
and scattering rate with nontrivial energy-dependent scattering resonances from free carriers.
Surprisingly, both the electronic and optical spectroscopy of YbT$_2$Zn$_{20}$ are distinctly different
from the rest of the studied materials, with characteristic features that support its closeness to
quantum criticality.

C71.00053: 395 GHz Sample Holder Waveguide for Dynamic Nuclear Polarization*  KIRSTY
SCOTT (Presenter), Florida State Univ, THIERRY DUBROCA, Condensed Matter Science, National High
Magnetic Field Laboratory — A major issue in nuclear magnetic resonance (NMR) is the low
sensitivity which can be achieved as a result of the small magnetic moment in nuclei. At the
MagLab, we exploit dynamic nuclear polarization (DNP), which increases NMR sensitivity through
a process in which electron spins transfer their larger polarization to the nuclei of interest, to
yield larger DNP signals at 14 T. For DNP experiments, our spectrometer uses a sample holder
which doubles as a waveguide for the microwave used to saturate the electrons in the sample
under study. The lack of axial symmetry in this sample holder limits our range of experiments.
To overcome this limitation, we are manufacturing axially symmetric sample holder-waveguides
by coating sample tubes with a conductive silver layer. The layer must have thickness and
conductivity such that it is transparent to a 600 MHz radio frequency, yet reflective to a 395 GHz
microwave. Our process consists of creating silver layer prototypes using various deposition
methods, characterizing the prototypes, replicating an optimized prototype on our sample tubes,
and implementing the final product in DNP experiments.

*Funding from the National Science Foundation (DMR-1644779) and the State of Florida is
gratefully acknowledged.
C71.00054: Effect of Post-deposition Thermal Treatment on the Structural and Electrical Properties of Oxygen Deficient Perovskite Metal Oxide Thin Films

BENJAMIN MOORE (Presenter), SKYLER KING, FRANCIS F WALZ, ANTON D WIGGINS, JOHN LEVENTIS, CHARLES J AY, GRACE YONG, DAVID SCHAEFER, GARY PENNINGTON, RAJESWARI KOLAGANI, Physics, Astronomy & Geosciences, Towson University — Thin films of perovskite metal oxides such as SrTiO3 (STO), La$_{0.67}$Ca$_{0.33}$MnO$_3$ (LCMO) and CaMnO$_3$ (CMO) exhibit many interesting electronic properties that are useful for technological applications. These properties are highly sensitive to the oxygen stoichiometry in the thin films, which can be varied by subjecting the thin films to heat treatment (annealing) after the film is deposited. We will discuss the results of our experiments to study changes in the lattice constants and electrical resistivity induced by post-deposition annealing in various gas ambients and in vacuum. We will also present the effects of annealing in the presence of a fluorine-containing polymer with the goal of incorporating fluorine in the film crystal structure. Thin films in this study are grown using pulsed laser deposition, lattice constants are determined using 4-circle x-ray diffraction and resistivity is measured using a 4-probe VanDerpauw technique.

*This work was supported by the NSF Grant DMR 1709781 & Fisher Endowment Grant from the Fisher College of Science and Mathematics at Towson University

C71.00055: Unsupervised Machine Learning for Rare Signal Detection in CMS Detector Data

LUC LE POTTIER (Presenter), Physics, University of Michigan, ANNAPAOLA DECOSA, Physics, University of Zurich — We present here a method for identifying high-$p_T$ beyond the Standard Model (BSM) signals, with no dependence on the expected physics signatures of these models. We do this by constraining our detector data to the expected signal region of a given model and training a deep neural autoencoder to 'recognize' jets belonging to the Standard Model (SM) background data. In this way, our models learn the background signature of SM jets in our signal region. We then evaluate this model on a mixture of SM and BSM jets, flagging jets with a high autoencoder reconstruction error as 'anomalous' or signal jets. This method of searching independently of any physics model is especially useful when the BSM model in question involves particles of unknown mass, branching fraction, etc. This is especially relevant in Dark Matter searches, such as the search for Semi-Visible jets in missing-$E_T$ events at the LHC. In these cases, our models are capable of flagging a range of BSM models with different parameters within our signal region, as opposed to a supervised model (such as a Boosted Decision Tree) which is only able to flag the exact signal it was trained on. We show that this technique is a promising method of identifying arbitrary BSM signals to high precision in LHC data.
HAO LI (Presenter), Harvard University, JAE-HO CHUNG, Korea University — Since the discoveries of robust two-dimensional ferromagnetism in CrI$_3$ [1] and Cr$_2$Ge$_2$Te$_6$ [2], many research interests have focused on thermal stabilities of magnetism on van der Waals monolayers. In this work, we investigated the thermal evolutions of classical spins on 2D ferromagnetic honeycomb monolayers during simulated cooling and/or annealing by using the Monte Carlo method. Using the Heisenberg Hamiltonian with parameters proposed for CrI$_3$ [3], we closely reproduce the experimentally observed temperature- and in-plane magnetic field-dependences of the magnetization including the size of the Curie temperature [1]. We also find that in zero-field cooling CrI$_3$ monolayers exhibit multiple domains with high densities of domain walls. We will present how the domains behave as the temperature or magnetic field is changed.


MATTHEW WITHERS (Presenter), ELISE BAKER, BENJAMIN WOOD ZEMAN, NOLAN ZUNK, CORY MORRIS, DAN MAZILU, IRINA MAZILU, Washington & Lee Univ — We design, model, and simulate an experiment to study the effect of electric bias on particle-coverage densities produced during ionic nanoparticle self-assembly. The experiment involves the application of a uniform external electric field parallel to a glass substrate during the self-assembly of silica nanoparticles. We refer to this procedure as directed self-assembly of monolayers (DSAM). In our theoretical analysis, we modify existing cooperative sequential adsorption models to account for diffusion under an applied electric field. We use the mean field approximation to solve for particle-coverage densities. To ascertain the validity of this method, we compare our solutions to Monte Carlo simulations of the system.
C71.00058: Correlating Multiphoton-Absorption-Induced Luminescence (MAIL) with Morphology in Noble-Metal Nanostructures*  ANNA GRAFOV (Presenter), XIAOYING LIN, University of Maryland, College Park, FARAH DAWOOD, Hamilton College, JOHN T FOURKAS, University of Maryland, College Park — The optical properties of nanostructured noble metals differ drastically from those of their bulk counterparts due to surface plasmon (SP) resonance. When incident light couples with the SPs of a noble-metal nanoparticle, it gives rise to strong, localized electromagnetic field enhancement. In particular, surfaces with high curvature experience especially strong field enhancement. Silver and gold SP absorption cross sections lie in the visible region, which make nanostructures of these metals ideal for studying optical phenomena. Multiphoton-absorption-induced luminescence (MAIL) is a nonlinear optical phenomenon that involves ultrafast pulses of light impinging on a nanostructured surface. The SP field enhancement allows for more efficient multiphoton absorption, and highly-efficient, broadband luminescence over the visible spectrum is produced as a result. We examine how the morphologies of noble-metal nanostructures correlate with their MAIL signals. Specifically, we focus on silver nanodendrites, synthesized from galvanic displacement reactions, and gold nanorings and nanotriangles, grown through colloidal synthesis. The absorption order, intensities, and spatial distribution of MAIL signals are examined for different morphologies.

*NSF Grant CMMI1449309

C71.00059: Characterizing the Mechanical Properties of 3D Printed Structures for Growth Plate Tissue Engineering  RACHEL HECHT (Presenter), A. CAMILA UZCATEQUI, VICTOR CRESPO CUEVAS, ROBERT R. MCLEOD, University of Colorado, Boulder — Stem cell differentiation is highly sensitive to the biochemical and mechanical environment. A major concern in tissue engineering is the need of a robust technique for producing structures with the precise amount of rigidity to guide stem cell differentiation. Damaged cartilage within the physis does not regenerate easily and can lead asymmetric growth arrest, making it an ideal model application. The physis has three distinct zones where cells evolve differently depending on the environmental conditions. Previous in vivo rabbit studies indicate that the mechanical properties of the 3D printed structures implanted in this area have an effect on stem cell differentiation in the area. In this work we use a solvent solution consisting of a multifunctional acrylate-based resin and ethanol to control the overall modulus of the structure. 3D printed pillar structures of varying solvent concentrations and backfills (air and a poly(ethylene glycol) diacrylate based hydrogel) were put through compression testing and we found that there was an apparent reduction in the modulus of higher concentrations of the solvent solution of over 30 percent. This work allows us to control the modulus of 3D printed structures, which can be applied to future stem cell differentiation studies.
C71.00060: The Effect of Short Range Attractions on Sequence Defined Polyelectrolyte Coacervation  
NATALIA MARKIEWICZ (Presenter), TYLER LYTLE, CHARLES SING, University of Illinois at Urbana-Champaign — Complex coacervation is the liquid-liquid phase separation of polyelectrolytes in aqueous salt solution into a polymer-dense phase, the coacervate, and a polymer-dilute phase, the supernatant. Previous work using Monte Carlo simulations demonstrated that changing the sequence of charged and neutral monomers on polyelectrolytes while keeping the charge fraction constant alters the extent of phase separation. However, previous data does not account for the hydrophobicity of different neutral monomers. To understand the coacervation of polymers with various chemical structures, van der Waals interactions at various strengths are included in Monte Carlo simulations to show hydrophobic effects in the system. Comparisons are made to existing Monte Carlo simulations and experimental data. Understanding these patterning effects will enhance the knowledge of biomacromolecule phase separation, as well as expand the understanding of sequence-dependent polymer physics.

C71.00061: All-Dielectric Nanophotonics Research Involving Undergraduates at Illinois State University*  
BRIGHTON COE, DANIEL EGGENA, Illinois State University, HIROSHI SUGIMOTO, Kobe University, MAHUA BISWAS, Millikin University, MINORU FUJII, Kobe University, UTTAM MANNA (Presenter), Illinois State University — Resonant excitation and manipulation of high-index dielectric nanostructures (such as Silicon, Germanium) provide great opportunities for engineering novel optical phenomena and applications. Here, we report selective excitation and enhancement of multipolar resonances, and non-radiating anapoles in silicon nanospheres using cylindrical vector beams (CVBs). Our approach can be used as a spectroscopy tool to enhance and identify multipolar resonances as well as a straightforward alternate route to excite electrodynamic anapoles at the optical frequencies.

*This material is based upon work supported by the National Science Foundation (NSF) under Grant No. ECCS-1809410. H.S. and M. F. acknowledge KAKENHI grant numbers 18K14092 and 18KK0141.
C71.00062: Silica Polypeptide Composite Janus Particles*  SEAN RONAYNE (Presenter), ALYSSA BLAKE, ELSA SAMANTARAY, JAMIE WOODING, MARK LASEGO, PAUL RUSSO, Georgia Institute of Technology — Janus particles are interesting materials due to their inherent dual face properties. The ability to be able to have different functionalization and properties on a single particle allows these materials to be used for drug delivery and interfacial chemistry. Silica polypeptide composite Janus particles are unique because they are stimuli-responsive particles containing an organic polypeptide shell with an inorganic colloidal silica core, half of which is coated in chromium. The responsive nature comes from the polypeptide shell consisting of the homopolypeptide, poly (ε-carbobenzyloxy-L-lysine) (PCBL), which is known to exhibit a reversible coil-helix transition when dissolved in m-cresol. The silica core particle can be removed from the particle via etching to retain a hollow polypeptide vesicle, potentially with the chromium still bound to part of the vesicle. These can be used to study the conformational transition of the polypeptides while being structured but without being tethered to a solid surface. This will help to better understand the polypeptides role as a drug delivery vesicle.

*National Science Foundation under Grant No 1505105 (DMR)

C71.00063: Arbitrary Super-Resolution Patterns Formed in Quantum Dots*  THOMAS DANZA (Presenter), RICHARD O MOURADIAN, MATEO MURILLO, SEAN JAMES BENTLEY, Adelphi University —

In this research, interference patterns were etched onto quantum nanoparticle thin-film samples using the second harmonic of a nanosecond Nd: YAG laser. By forming one interference pattern on a sample and then phase shifting the beam, we are able to produce patterns with twice the resolution due to the nonlinear nature of the quantum nanoparticles. By using the interferometric method with phase and amplitude masks arbitrary 1-D (with two beams) and 2-D (with four beams) patterns can be formed using this lithographic technique.

*Funded by Horace McDonell and Adelphi University
C71.00064: Using Depolarized Dynamic Light Scattering to Characterize Microgel Dependence on Synthesis Temperature* ANDREW SCHERER (Presenter), KIRIL STRELETZKY, Cleveland State University — Microgels formed by crosslinking polysaccharide polymer chains exhibit a thermally reversible volume phase transition due to the amphiphilic properties of the parent polymer. Specifically, the microgels deswell above a volume phase transition temperature, $T_v$. Microgel dynamics above and below $T_v$ has been studied extensively by dynamic light scattering (DLS) before. Here, the structure and dynamics of microgels synthesized at various temperatures are investigated through the use of depolarized dynamic light scattering (DDLS). The technique has previously been used in our lab to examine solely geometric anisotropies in non-spherical particles. It has also been used in the literature to study shape fluctuations in microgels that have a hard, polystyrene core and a soft, polymer shell. This research project looks into a possibility that the observed DDLS signal above $T_v$, for microgels synthesized at various temperatures, arises from microgel shape fluctuations.

*Cleveland State University 2019 USRA Program

C71.00065: Neutron Spectrum Unfolding with Deuterated Liquid Scintillator Detectors FABIO RIVERO (Presenter), JESUS F PERELLO, SERGIO J ALMARAZ-CALDERON, Florida State Univ — The detection of neutrons from nuclear reactions is becoming increasingly important in nuclear physics experiments. Neutron measurements are needed for understanding reactions that drive stellar explosions and provide insight into the behavior of exotic nuclei. Traditionally, neutron energies are obtained by the time-of-flight (ToF) method which consists in measuring the time that neutrons take to travel from the target to the detector. The quality of the measurements is limited by the distance traveled, the solid angle spanned by the detector array, and a background of gamma-rays and scattered neutrons. Pulse-shape-discrimination (PSD) allows one to distinguish, in certain detectors, neutron and gamma-ray interactions due to their decay times. A promising method in neutron research involves the use of deuterated liquid scintillators as neutron detectors where a unique correlation in the pulse-height (PH) information can also be extracted. In this work a method of unfolding neutron spectra will be presented. A response matrix is created from deuterated liquid scintillator detectors by combining PSD and PH data to obtain neutron energies alongside ToF. This method will enhance neutron studies relevant for nuclear structure and nuclear astrophysics research.
C71.00066: Gold-Aluminum Thin Films as an Alternative to Pure Metals for Plasmon Resonance Sensors*  ABDUL QADEER REHAN (Presenter), ROBERT MALCOLM KENT, MARIAMA REBELLO SOUSA DIAS, Univ of Richmond — Noble metal alloys have been widely investigated as an alternative to pure metals for improving the optical response of optoelectronic devices in the visible range of the electromagnetic spectrum. However, their use is hardly extended to the ultra-violet (UV) range. As an alternative, aluminum (Al)-based alloys could expand the functionality of photonic devices into the UV range. In this work, we fabricate and measure the dielectric constant of binary mixtures of gold (Au) and Al thin films. The films were deposited on a glass substrate via the co-sputtering method. The dielectric functions were measured using spectroscopic ellipsometry. We investigated how the optical response of the samples changed under a wide range of temperatures, from 25°C to 200°C. Also, we performed AFM, SEM, XRD, and EDS measurements. We demonstrate that, in all our cases, a bimetallic material outperforms their pure metal counterparts in the near-IR range after the temperature treatment, e.g., Al0.51Au0.49 shows an increased quality factor of its surface plasmon polariton (QSPP) than pure Au and Al. To verify our calculations, we measured the SPP of pristine and temperature treated samples.

*University of Richmond Arts and Science Summer Research Fellowship

C71.00067: Water Wheel Generator*  BRIGID LONG (Presenter), Ithaca Coll — The world continues to move toward eco-friendly renewable energy by creating new, more advanced technologies. Solar panels, wind turbines, and dams are some of our biggest contributors. This project takes a second look at the potential of bringing the vertical water wheel back into the limelight. Historically water mills have been crucial in the progress and growth of civilization by being a major source of strength and power. Combining this power with a continuously recycled water flow has the potential to create a constant source of renewable energy. Using the principles of water wheel designs that have been perfected over centuries and securing a small generator creates a viable configuration for a tabletop water powered generator. The goal is to create an enclosed system where a water wheel powers its own pump for recycling water flow and still outputs enough wattage to be used to charge batteries. This prototype has gone through rapid prototyping using 3D printed wheel designs for the optimization of electrical output. On a small scale this design can be a tabletop charger however, on a larger scale, this design could power homes and office buildings without the hazards of daming.

*This project is funded by the Ithaca College Department of Physics and Astronomy.
C71.00068: Reaction Kinetics and Mechanical Properties of Reversible Epoxies by Diels-Alder reaction
NICOLE PENNERS (Presenter), YOUNGMIN LEE, New Mexico Tech — Epoxies are an important class of thermosetting polymers for many long-term applications such as adhesives, structural materials, and coatings. Epoxies have durable and robust mechanical properties; but, they are difficult to remove, recycle and rework. Epoxies capable of reversible polymerization could solve these problems. In this experiment, reversible epoxies were synthesized by introducing the Diels-Alder reaction groups to epoxy monomers. 1,1’-(Methylenedi-4,1-phenylene) bismaleimide and furfuryl glycidyl ether were reacted to form a Diels-Alder cycloadduct. This cycloadduct was confirmed using Fourier Transform-Infrared (FTIR) Spectrometry. The forward and reverse Diels-Alder reaction was monitored by FTIR measurements at 90 °C and 110 °C as a function of exposure time. IR absorption peaks relevant to the reverse Diels-Alder reaction grew due to longer exposure time at 90 °C and 110 °C. The equilibrium shift was observed toward the reverse reaction dominant side at higher temperature by comparison of FTIR spectra at 90 °C and 110 °C. Mechanical properties of the reversible epoxies was examined to confirm two states of reversible epoxies: a durable network at lower temperature and soft segments at higher temperature.

C71.00069: Hyperentangled Bell-states analysis of two-photon 2n-degree-of-freedom system
CHUNZHEN LI (Presenter), Nankai University — It is known that it is impossible to unambiguously distinguish all the Bell states in one system using only linear optics even if you also use hyperentanglement. However, we can find out how many Bell states can be unambiguously distinguished with a given n in two-photon 2n-degree-of-freedom hyperentangled system. This work, based on the criterion of Peter van Loock and Norbert Lutkenhaus, uses the symmetric matrix to express Bell states and the number of distinguished Bell states can be obtained by the rank of a matrix made with all the Bell states. The results show that with the increase of n, the number of distinguished Bell states increases exponentially by $2^{n+1}-1$, while the efficiency of discrimination decreases exponentially by $1/2^{n-1}$. This work lays a foundation for Bell-state analysis of three-photon system.

C71.00070: Electronic Structure of Negative Trions in Semiconducting Quantum Dots
JAYDEN LEONARD (Presenter), QUE HUONG NGUYEN, Marshall Univ — A trion system is one that includes an exciton system pairing with either an electron (called a negative trion) or a hole (called a positive trion). Trions in bulks typically has infinitesimal binding energies, but recent research has shown that trions in quantum well have their binding energy increased by an order of magnitude, i.e. the confinement configuration supports the formation of trions. The measurements of the photoluminescence spectra of the trions in a single, self-assembled quantum dot also show the dependence of the photoluminescence lines on the size and geometry of the quantum dot. In this project, we will theoretically investigate the electronic structure of negative trions in a spherical quantum dot of a direct band gap semiconductor. The effect of an electric field on the trions will be considered to obtain the splitting of trion energy levels under the electric field. The respective wave functions of the resulting states have been obtained as well. The dependence of the electric field effect on the size of the dots will be investigated.
C71.00071: Floquet Engineering in 1D Non-Hermitian Model

HOUCHEN LI (Presenter), Nankai University — Topological properties of non-hermitian and periodically driven (floquet) systems have attracted great attention in recent years. Here, I find we can introduce robust topological edge state in 1D non-hermitian time-periodic system while its static counterpart is trivial. Also when we adjust the frequency of the outer driving within the regime around the bandwidth $\Delta$, topological phase transition of the system has a similar behavior with the Hermitian counterpart[1]. This will help us understand non-hermitian and floquet systems better.


C71.00072: Low-Pressure Plasma Device for Activation Bonding Polydimethylsiloxane(PDMS) to Glass

JACOB CARNEY (Presenter), KRISTA MCBRIDE, Belmont Univ — Surface activation of PDMS through plasma treatment is a common technique used in the fabrication of microfluidic chips for a strong bond between PDMS and glass. Plasma treatment can be done in an open lab or low-pressure environment, in which commonly produces more activated stronger bonds. The activation levels of plasma treatment of PDMS and glass can be measured using atomic force microscopy. A low-pressure plasma bonder is being built and tested in order to produce stronger microfluidic devices. The configuration and experimentation of the self-built low-pressure plasma generator will be presented.

*This research was supported by Belmont University, and the College of Science and Mathematics.

C71.00073: Electrocolonography: Non-Invasive detection of colonic cyclic motor activity from multielectrode body surface recordings

LAURA BRUCE (Presenter), JON ERICKSON, ANDREW TAYLOR, JACK RICHMAN, CONNOR HIGGINS, BETH REED, RIWAJ SHRESTHA, JACK ROBEY, UTKRIST THAPA, Washington & Lee Univ — Approximately 20% of Americans suffer from colonic motility disorders, including slow transit constipation (STC) and irritable bowel syndrome (IBS), with significant physical and social morbidity. Accurate clinical diagnosis is often challenging due to the non-specificity of symptoms. In addition, the only direct assessment tool available in current clinical practice is colonic manometry, which involves placing a small, flexible tube, or catheter, through the rectum and into the colon. There is a substantial need in both colon research and clinical practice for an accurate, non-invasive method to analyze colon motor activity. This work validates a novel non-invasive method to identify periods of cyclic motor activity in the colon using multichannel skin-surface electrical recordings on the lower abdominal region, termed electrocolonography (ECoLG). We also explore several spatial filtering techniques to identify wave propagation of the colon.

*We acknowledge the Lenfest Summer Research Grant, Washington and Lee University, Washington and Lee University Summer Research Scholar fund, the Levy Neuroscience Grant, Washington and Lee University, and we also thank the James Ramsay Project Grant, Royal Australasian College of Surgeons and the New Zealand Health Research Council.
C71.00074: Exploring the Memory Capacity of Embedded Synfire Chains* SARAH GREBERMAN (Presenter), YEVHEN TUPIKOV, DEZHE JIN, Department of Physics, Pennsylvania State University — Memory is a long-studied property of neural systems that is not well understood yet essential for the success of any animal. The synfire chain is a popular sequence generating model which has been hypothesized to represent a building block for neural computation and memory. Our research was conducted to explore what affects the storage capacity of memory networks composed of embedded synfire chains. Using computational modeling, we compared the memory capacity of two neuron models – Leaky Integrate-and-Fire (LIF) and Izhikevich – and systematically varied factors that showed to affect each network. In both cases, we used a simplified model of global inhibition to control run-away excitation. Our studies showed that the memory capacity for networks consisting of LIF neurons depends strongly on the inhibition, excitation, and width of the chains. The observed memory capacity was low and insufficient for practical applications. The memory capacity for networks consisting of Izhikevich neurons was considerably larger. More research needs to be done on this. Future directions would also explore more targeted models for inhibition in hope for achieving larger capacity for memory networks.

*NSF Award EF-1822476 and the Huck Institutes of Life Sciences at Pennsylvania State University

C71.00075: Enhancement of Nonlinear Optical and Piezoelectric Properties in Ferroelectrics from Symmetry-Breaking Strains* BAILEY NEBGEN (Presenter), Chemistry, University of Minnesota, RUI ZU, Materials Science and Engineering, Pennsylvania State University, WILLIAM NUNN, BHARAT JALAN, Chemical Engineering and Materials Science, University of Minnesota, VENKATRAMAN GOPALAN, Materials Science and Engineering, Pennsylvania State University — In the pursuit of lead-free piezoelectrics, recent studies have used temperature, pressure, applied voltage, and other methods to enhance piezoelectric properties in ferroelectrics. Here, we investigate changes in symmetry, polarization, and domain structure near phase boundaries in BaTiO3 crystals and BaTiO3-xBaSnO3 thin films in order to understand how property enhancement depends on external stimuli and replicate the property enhancements in versatile thin films. We use second harmonic generation (SHG) polarimetry to detect changes in point group symmetry and polarization direction, supplemented by scanning SHG microscopy, which reveals the domain structure and allows polarimetry of specific domains. We observe lower-symmetry monoclinic phases with SHG and piezoelectric property enhancements of up to 4 times near temperature phase boundaries and with applied voltage in BaTiO3 crystals. In addition, we observe similar symmetry lowering near a compositional phase boundary of BaTiO3-xBaSnO3 thin films, indicating the potential for similar property enhancements in the thin film system which is more easily integrable into a variety of devices.

*This work was supported by NSF grants DMR-1807768 and DMR 185-1987 as well as Penn State NSF-MRSEC Center for Nanoscale Science DMR 1420620.
C71.00076: Compaction and Creep in a Photoelastic Granular System*  EDNA OLVERA

(Presenter), Physics and Astronomy, Swarthmore College, NAKUL DESHPANDE, Earth and Environmental Science, University of Pennsylvania, CACEY STEVENS BESTER, Physics and Astronomy, Swarthmore College, DOUG JEROLMACK, Earth and Environmental Science, University of Pennsylvania — Creep is the subsurface, slow movement and deformation of constituents in a granular packing, such as sand or sediments, due to the applied stress and disordered nature of its grain-scale interactions. The phenomenon of creep in dense granular systems is relatively understudied, leaving many open questions. We explored creep through experiments in which we observed the influence of a controlled disturbance on rearrangements in a granular packing. Our granular system consists of disks that are made from a birefringent material; this allows us to use image acquisition to observe both the movement of the grains and the changing stress distribution within the system. In the experiment, we deliver disturbances via taps of a pendulum to one side of the chamber that contains the granular packing. The tapping strength is measured using an accelerometer. We tilt the chamber to varying slopes to observe changes in system response as we approach the critical slope for more rapid granular flow. Using image analysis, we examine grain rearrangements, changes in packing density, and stress redistribution as the grains creep due to these disturbances.

*We would like to thank the Swarthmore College and University of Pennsylvania Provost's Offices for their funding support towards this project.

C71.00077: Influence of Spin-coating Speed and Mixing Ratio on Polymer-Fullerene Films*  SEBASTIAN VALBUENA (Presenter), CHARITY DIAMONON, CAMERON M PROSSER, PROF WEINING WANG, Seton Hall Univ — Due to increasing environmental concerns and depletion of nonrenewable resources, different forms of renewable energy must be studied. Organic solar cells are a very popular and promising form of renewable energy; however, they are still relatively new and not as well studied in comparison to traditional silicon solar cells. Thus, it is important to gain more knowledge on how those organic solar cells could be enhanced in different areas. Among the organic solar cells (OSC), OSC based on polymer-fullerene bulk heterojunctions have attracted much attention due to their low cost and easy processing conditions. The most common polymer-fullerene bulk heterojunction is poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61 butyric acid methyl ester (PCBM).

In this work, we show our studies on how the characteristics of P3HT:PCBM films depend on spin coating speed and mixing ratios. By varying the ratio of PCBM:P3HT as well as using different spin coating speeds, the impact on the absorbance spectrum of the films were studied. The results help us choose the optimum processing conditions for P3HT:PCBM films to be used in bulk heterojunction solar cells.

*New Jersey Space Grant Consortium - NASA
C71.00078: The Durability of a Chiral Auxetic Structure  ANNA REPESH (Presenter), XIN DU,  Physics, Aquinas College —  Metamaterials are bulk objects with special mechanism properties defined by their repetitive inner structures, rather than the materials they are made of. One of the special mechanisms is `auxetic behavior`: when the materials are stretched in one direction, unlike conventional materials, they will also expand in the lateral direction. In this project we studied the dependence of Poisson's Ratio on the geometric parameters of a chiral auxetic structure. This chiral auxetic structure can be potentially applied in deployable antennas. We used 3-D printer to efficiently design and produce the chiral auxetic structures. With an innovative experimental setup and image analysis techniques, we were able to study the durability of the chiral auxetic structures with various geometric parameters.

C71.00079: Thermodynamic and Magnetic Properties of the System Ca$_3$Co$_{2-x}$Zn$_x$O$_6$*  ALEXANDER MANTILLA (Presenter), JANI JESENOVEC, BENJAMIN WHITE, Central Washington University —  The crystal structure of Ca$_3$Co$_2$O$_6$ is built from chains of Co$^{3+}$ ions that are separated by Ca ions. Magnetic moments associated with low-spin Co ions are located on trigonal prismatic sites within the spin chains. Ferromagnetic intrachain interactions are an order of magnitude stronger than antiferromagnetic interchain interactions, leading to a quasi-one-dimensional magnetic structure. In an effort to study its magnetic state, we substituted Zn$^{2+}$ for Co$^{3+}$ ions. Zinc ions occupy the trigonal prismatic (magnetic) sites and charge balance causes low spin Co$^{3+}$ ions occupying octrahedral sites to become low-spin Co$^{4+}$. Thus, Zn substitution dilutes moments on trigonal prismatic sites and induces them on octahedral sites. Samples of Ca$_3$Co$_{2-x}$Zn$_x$O$_6$ were synthesized via solid state reaction and phase purity was evaluated via x-ray diffraction. X-ray diffraction elucidated a solubility limit near $x = 0.1$. Heat capacity and magnetization were measured as a function of temperature and were used to construct a $T$ vs. $x$ phase diagram for Ca$_3$Co$_{2-x}$Zn$_x$O$_6$. In this poster, this phase diagram will be compared to the previously reported phase diagrams for Ca$_3$Co$_{2-x}R_x$O$_6$ with $R = $ Cu, Cr, Fe, Mn, Sc, and Ho.  

*Research supported by the Central Washington University Science Phase II Project and start-up funds.
C71.00080: Image Analysis and Model of Cytoskeletal Filament Density of C17.2 Cells
BENJAMIN HORINE (Presenter), Susquehanna Univ, SABRINA JEDLICKA, SWETHA CHANDRASEKAR, Lehigh University, MASSOOMA PIRBHAI, Susquehanna Univ — Single-Walled Carbon Nanotubes (SWCNTs) have great potential in the biomedical field as a way to deliver materials into the body. However, the long-term effects on the body are unknown, especially in regards to the cytoskeletal filaments. Many cellular functions such as differentiation, cell shape, and motility rely on the aid of filaments, such as actin and nestin. Recent studies have demonstrated that internal and external stimuli can affect these filaments thus affecting cellular behavior. In this project, neural stem cells, specifically C17.2 cells were used and the distribution of the cytoskeletal filaments were modeled. A data set was created through Filament Sensor, a program created by Benjamin Eltzner, and ImageJ, to quantitatively process and enhance images. This poster will look into the distribution of actin and nestin throughout the cell. Future work will look at how SWCNTs affect the distribution of these filaments.

C71.00081: Photo-reduction was used to reduce the oxygen content in Graphene Oxide and correlated to Young’s modulus measurements* ALEM TEKLU (Presenter), CAMERON GREEN, GEORGE RISER, NARAYANAN KUTHIRUMMAL, College of Charleston — Finding a cost-effective way to make graphene would be beneficial to our world. Mechanical properties of graphene oxide were studied using and AFM system. Specifically, Young’s modulus, stiffness, and hardness of graphene oxide samples were measured as a function of sample thickness. Results obtained for Young’s modulus ranged from 24 GPa to 277 GPa for samples of thicknesses 1.4 µm to 93 nm. Once the Young’s modulus values were obtained, photo-reduction was used to reduce oxygen content in graphene oxide samples using a 405 nm ultraviolet laser for 36 hours. Young’s modulus was reevaluated after photo reduction and its value increased from 24GPa to 44GPa for the 1.4 µm thick sample.

*The work was supported by Department of Physics & Astronomy and the School of Sciences and Math at the College of Charleston. The project was also supported by NSF/EPSCoR: SC EPSCoR/IDeA, Award no. OIA-1655740.

C71.00082: RF Antenna for Generation of Spin-Dependent Force on Cold Lithium Atoms* JIANYI CHEN (Presenter), ARIEL T SOMMER, Physics, Lehigh University — This study aims to design a small radio-frequency (RF) antenna that can generate magnetic fields with magnitude of 1 Gauss. This RF antenna is useful because the generated fields can magnify the hyperfine state of lithium atoms which are used to study the quantum atomic gas at low temperature. However, the function of the RF antenna is restricted when the diameter of the antenna is constrained in less than 1 inch. This restriction is the result of a high energy loss caused by signal reflection in the circuits if the antenna is directly connected with the power supply. In order to reduce the loss, an impedance matching configuration should be introduced between the antenna and the power supply. At the end of the experiment, a small RF antenna with impedance matching configuration that can generate a magnetic field with desired frequency and amplitude is designed.

*We acknowledge the support from Lehigh Physics Undergraduate Research Program (REU). We acknowledge the support from College of Arts and Sciences Research Grant, Lehigh University.
C71.00083: Investigation of a LCoS-SLM and Progressively More Difficult Applications of the SLM Including Optical Trapping* KADE TATKENHORST (Presenter), Department of Chemistry and Physics, Simpson College —
At the heart of all phase modulation applications is a Spatial Light Modulator (SLM). A Liquid Crystal on Silicon Spatial Light Modulator (LCoS-SLM) uses a voltage to phase retardation relationship that allows for easily programmable phase shifts. The programmable phase shifts are often programmed using phase masks. The LCoS-SLM is investigated and various applications of the SLM, including using the SLM as a “Projector”, to generate Bessel Beams, to generate a Vortex Beam with Orbital Angular Momentum, and flat-top beams of various shapes are performed. All applications are performed using a similar optical set-up with various phase masks. Finally, a vortex beam is used to optically trap micron sized nanoparticles.

*This work was done under the REU at Rensselaer Polytechnic Institute and sponsored by the National Science Foundation (Grant #1560266).

C71.00084: Achieving Flat Gold Surfaces for the Organization of Organic Molecules* JACOB MARTIN (Presenter), JESSICA BICKEL, Cleveland State University — Organic electronics are interesting for use in electronic devices but suffer in competition with inorganics due to their lower conductivity. Crystallizing organic semiconductors can increase their conductivities and a possible crystallization method is self-assembly driven by the topography and chemistry of an atomic surface reconstruction. This work aims to develop an atomically smooth Au(111) surface, which has a herring bone reconstruction. Many methods are known for samples in UHV, however these methods do not work in atmosphere or a glove box, such as is used in our lab. This work expands upon that of Maver et al. using torch annealing, which allows the atoms to rearrange into a lower energy state. We anneal the sample at 710±10°C for two minutes, and then three minutes at 410±10°C. This yields larger and flatter terraces compared to the unannealed material. The unannealed gold had mounds with no flat areas and a max depth of 7.6 nm. The annealed Au(111) had flat terraces, 13-30 nm in size, with step heights in the order of .235 nm, which matches the interplanar spacing for Au(111). In the future, we will optimize this process to achieve large terraces by adjusting the temperatures and times used.

*This work was funded by the National Science Foundation, Award Number: 1659541
C71.00085: Immunofluorescent biomarkers for distinguishing cell phenotypes in zebrafish somitogenesis and autonomous cellular oscillators.*  YIYANG CHEN (Presenter), Nankai University, QIONG YANG, Department of Biophysics, University of Michigan, Ann Arbor — During zebrafish embryogenesis, coordinated genetic oscillations occur in a population of cells in the posterior-most tissues of the body axis, the tailbud and presomitic mesoderm (PSM), which will subdivide the embryonic body into morphological segments, called somites. It has been proved previously that single cells dispersed from tailbud will oscillate automatically. However, it remains unclear that which phenotype of the cells will present as autonomous oscillators. T-domain transcription factors Ntla and Tbx16 will both express in the period of somitogenesis but in different regions. Immunofluorescence experiments for both genes demonstrated the distribution of cells in different phenotypes in zebrafish embryo during somitogenesis. Comparison of immunofluorescence results for 5-somite stage embryos and high-somite stage embryos showed the change of PSM region. Combined with results for single-cell oscillation and statistical analysis, immunofluorescence for cell dispersals was able to tell the phenotypes of the oscillating cells.

*This work was supported by the Pilot Scheme of Talent Training in Basic Sciences (Boling Class of Physics, Nankai University), Ministry of Education. This work was supported by Yang Lab from the Department of Biophysics, University of Michigan.

C71.00086: Stabilization of Francium Materials Using Cluster Compounds*  DAVID NUNN (Presenter), AJIT HIRA, EDWARDINE FERNANDEZ, ARRICK GONZALES, TINO PACHECO, ALICIA FRESQUEZ, MARIO VALERIO, Northern New Mexico College — We present a Quantum Mechanical study of cluster compounds Fr\(_l\)X\(_m\)Y\(_n\) and Ra\(_l\)X\(_m\)Y\(_n\) (X, Y = other; 0 <= l, m, n <= 10). Half-life \(\lambda\) of the most stable isotope of francium (\(^{223}\text{Fr}\)) is 22 minutes, and only 20–30 g of the element exists naturally at any given time. The melting point, the boiling point, and density of Fr are uncertain. Isotopes of radium are radioactive, but the most stable isotope \(^{226}\text{Ra}\) has a half-life of 1600 yr. The stabilization of radium is known to have been experimentally achieved, using a solution in which an effluent and a metal chloride are mixed, then the previously obtained mixture reacted with a sulfate ion, to obtain effluent containing stabilized radium. The chloride can be a barium, strontium or lead chloride. We are looking to see if there are similar trends, in properties, for francium. So far, we have achieved a factor of 2.7 stabilization for some of the francium cluster compounds, compared to bare Fr in our calculations. There is the possibility of application of a stabilized Fr material as a catalyst promoter, or a remover of oxygen from vacuum tubes and light bulbs, or in atomic clocks, or in petroleum exploration, analogous to the practical uses of Cs.

*New Mexico AMP program, funded by the NSF, provided some financial support for this research.
C71.00087: Arduinos and the X-Ray Diffractometer* MIA MANZER (Presenter), KELLEY D SULLIVAN, Ithaca Coll — For Ithaca College's Senior Project, it is required that a student develop an idea for a project, as well as the budget, goals, proposal, and design of the project itself. This project discussed in this presentation is developing a connection between an Arduino and the X-Ray Diffractometer owned by Ithaca College. The goal is to have the diffractometer and Arduino communicate easily and allow for data to be taken during the experiment easily. We wanted to make sure that students would be able to take, as well as save, data in the simplest way possible.

*Ithaca College Department of Physics & Astronomy

C71.00088: Assessing iOLab-based Laboratories in Online Instruction* EMMA KOLLER (Presenter), LOUIS LEBLOND, Department of Physics, Pennsylvania State University — We implement an online introductory mechanical physics laboratory course that features the Interactive Online Lab (iOLab) device and a class structure that encourages student engagement and collaboration. The students in the online class achieved a learning gain of $g = 0.55$ on the FCI. The end of class survey showed that the students overwhelmingly (93%) valued the lab portion of the course. However, we can only infer their mastery of the lab learning objectives from lab related questions on exams and lab reports. We present an ongoing study that seeks to understand student attitudes towards the labs, and the processes students use to complete them. We observe student help-seeking strategies, the amount of time they spend performing the lab, and student motivation. Student attitudes towards online physics labs will be accessed through the use of in-person interviews and a pre and post Colorado Learning Attitudes About Science Survey for Experimental Physics (E-CLASS). The overall goal is to form a more detailed picture of how students complete online physics labs to improve the quality of online physics instruction.

*We would like to acknowledge the Tombros Fellowship and a Schreyer Teaching Grant at Penn State University.

C71.00089: The Effects of Heat Exposure Over Various Time Intervals on the Performance Characteristics of Monocrystalline Silicon Photo-voltaic Cells MADALYNNE FORSTER (Presenter), HUNTER DAVIS, NOAH COX, JUSTIN L SMOYER, PAUL V QUINN, Physical Sciences, Kutztown University of Pennsylvania — With the rise of awareness for climate change and environmental protection, research into alternative energy sources has becoming increasingly important. One of the most popular forms of renewable energy is solar power. Most commonly built solar panels utilize a collection silicon photovoltaic cells to generate electricity. Our research specifically looks into the efficiency characteristics of monocrystalline silicon photovoltaic cells after they are exposed to intense heat for a predetermined amount of time. The cells were heated at temperatures of 190°C, 200°C, and 210°C, for times ranging from 10 minutes to 110 minutes. An analysis of our data shows an average increase in fill fraction with time for all three temperatures. These results indicate a permanent overall increase in efficiency of the cells compared to baseline values. This outcome proves that we do not need to significantly change the process of production of the cells in order to increase the efficiency.
C71.00090: Optimization of CoFeB Electrodes for Magnetic Tunnel Junctions  

GILLIAN BOYCE (Presenter), Florida State Univ, SUYOGYA KARKI, JEAN ANNE INCORVIA, University of Texas at Austin — A magnetic tunnel junction (MTJ) is the current standard for converting magnetic information into electrical information. It is formed by sandwiching an insulating barrier between two ferromagnetic electrodes. An external magnetic field is then used to switch the electrodes between parallel and antiparallel magnetic alignment. The focus of this research is to optimize the switching between magnetic states through the optimization of electrode thicknesses, especially when non-conventional barrier materials are used. The goal is to decouple the two FM layer switching fields, which allows read-out of two resistance states of the device. The method used is three-fold: First, MTJ stacks are grown using sputter deposition. Next, vibrating sample magnetometry is used to test for switching of magnetic alignment. Finally, atomic force microscopy is used to test for interfacial roughness, which could cause the layers to couple and prohibit antiparallel alignment. I will discuss our work developing a method for minimizing the coupling between the FM electrodes by focusing on understanding the interfacial roughness.

*Funding was provided by the NSF Research Undergraduate Experience hosted by the Center for Dynamics and Control of Materials at the University of Texas at Austin

C71.00091: Predicting and Synthesizing Photocatalytic Semiconductor Materials  

XAVIER QUINTANA (Presenter), Physics, Pennsylvania State University, NATHAN D KEILBART, JULIAN FANGHANEL, ISMAILA DABO, The Pennsylvania State University —  

The photocatalytic generation of hydrogen fuel is a promising way to store and utilize solar energy and mitigate carbon dioxide emissions. Water-spitting photocatalysts use solar energy to convert water into molecular hydrogen and oxygen. Yet, many of the photoactive materials required for water splitting are costly or inefficient. To accelerate the discovery of photocatalytic materials, a high-throughput computational screening protocol was developed, coupled with experimental synthesis and characterization, to select photoactive materials that can efficiently split water. Several candidates from the list were synthesized and their bandgaps and ability to produce hydrogen were characterized. Many of the compounds exhibited desirable photocatalytic water-splitting properties. This screening provides a framework from which viable photocatalytic materials can be discovered.

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C71.00092: Effects of Nanoparticle Size and Density on the Critical Current and Creep in (Y,Gd)BCO Films: Comparisons to Strong Pinning Theory* SARAH JONES (Presenter), Physics, Colorado School of Mines, ROLAND WILLA, Karlsruhe Institute of Technology, MASASHI MIURA, Graduate School of Science & Technology, Seikei University, SERENA M ELEY, Physics, Colorado School of Mines — Incorporating nanoparticle inclusions into superconducting films is a well-established route for boosting current carrying capacity. (Y,Gd)Ba$_2$Cu$_3$O$_7$ films containing various nanoparticles have been shown to demonstrate inexplicably slow rates of thermally activated vortex motion (creep, S). Understanding the microscopic source of these slow rates is key to determining how to reduce S in superconductors. In this project, we report on the effects of different sizes and densities of nanoparticle inclusions on the critical current and creep in (Y,Gd)Ba$_2$Cu$_3$O$_7$ films. Samples in this study all contain a low density of R$_2$Cu$_2$O$_5$ (R = Y,Ba) inclusions (naturally occurring during growth), and each contain either no other nanoparticles, BaHfO$_3$, BaSnO$_3$, or BaZrO$_3$ nanoparticles. The data presented was collected from low temperature magnetization measurements in fields of 0.3 T up to 35 T using a VSM at the NHMFL and a local commercial SQUID.

*Funding for this project was provided by the Mines Undergraduate Research Fellowship. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation Cooperative Agreement No. DMR-1644779 and the state of Florida.

C71.00093: Design Parameters of Liquid Crystal Elastomer Multi-Laminates* KELSEY LYNCH (Presenter), JOSELLE MCCRACKEN, TIMOTHY J WHITE, Chemical and Biological Engineering, University of Colorado, Boulder — Liquid crystal polymer networks or elastomers (LCEs) can be surface aligned into complex orientations that produce cooperative deformation and out-of-plane shape transformation.[1] When subject to thermal stimuli, thermotropic LCE films actuate and display significant weight lifting capabilities that scale with thickness.[2] Here, we investigate parameters that affect the mechanical output of LCE actuators including thickness, composition, disclination type, and geometrical packing. Specifically, we develop an LCE composition amenable to photoalignment processing that acts below 70°C. The mechanical response of this material (stroke and force displacement) are contrasted to canonical LCE material systems. The actuation output of the LCE is increased by lamination.[3] A multi-laminate LCE material actuator over 1mm in thickness is demonstrated, capable of lifting large objects (>1 lb).


* DARPA-SHRIMP
**C71.00094: Solid State NMR Physics Laboratory**

ROSA CARDENAS (Presenter), Univ of the Incarnate Word — We report on the progress of the newly developed physics laboratory at the University of the Incarnate Word (UIW). This laboratory is the first physics research laboratory at this institution. It includes a new solid state NMR experimental setup. The experimental setup is comprised of a 400 MHz variable temperature, cryogen free, superconducting magnet manufactured by Cryogenic. It also includes a Tecmag Redstone NMR Spectrometer. This spectrometer is very flexible and therefore many different samples may be analyzed. Field calibration was conducted by using Nuclear Magnetic Resonance (NMR) with liquid D2O. This allowed for successfully tracking the Te NMR signal of an iron-chalcogenide FeTeSe sample. The superconducting transition of different purity iron-chalcogenide FeTeSe samples will be analyzed in detail.

*Department of Defense HBCU/MI Equipment Grant

**C71.00095: Simulation of Efficient Perovskite Solar Cells**

MADISON J GUERRERO (Presenter), HONGKUN CAI, PROF WEINING WANG, Seton Hall University — While Perovskite popularity has skyrocketed since the efficiency reached 22% in 2018, there is still ample research to be done as to what characteristics and parameters affect the solar cell. In order to obtain a greater understanding of the mechanics of how a perovskite cell becomes more efficient, this project focuses on the simulation program wvAMPS and how parameters alter main characteristics such as Voc (open circuit voltage) and Jsc (short circuit current). The perovskite solar cells were obtained from National Renewable Energy Laboratory. The structure of the solar cell is Ag(120nm)orAu(100nm)/spiro-OMeTAD(180-200nm)/perovskite(550nm)/mesoporous-TiO_2(200nm)/compact-TiO_2(40-60nm)/FTO/glass. The measured solar cell parameters are: Voc = 1.06V, Jsc = 16.53 mA/cm^2, Fill Factor = 63.5% and Efficiency = 11.2%.

The simulation attempted to parallel the measured Perovskite solar cell. With given parameters, we were able to simulate a solar cell with a Voc = 0.93V, Jsc = 21.27 mA/cm^2, Fill Factor = 85.5% and Efficiency = 16.9%, which are very close to the measured parameters. We also varied the layer thickness to check how the device performance can be improved. These results will help determine how to optimize device structures for Perovskite solar cells.

*Clair Booth Luce
C71.00096: An Algorithm to Optimize the Search for Electromagnetic Counterparts to Gravitational Wave Events* PRIYADARSHINI RAJKUMAR (Presenter), ALESSANDRA CORSI, Texas Tech Univ, CHRIS COPPERWHEAT, DANIEL PERLEY, Astrophysics Research Institute, Liverpool John Moores University, — Our understanding of gravitational wave (GW) events is greatly enhanced by identifying and studying their electromagnetic (EM) counterparts. For nearby GW events with a small localization uncertainty, an effective strategy is to search for new transient sources in previously catalogued galaxies, whose properties are consistent with the GW data. Even with a limited field of view, it is plausible to discover the EM counterparts using an efficient observational strategy. But because many galaxies must be observed and the EM counterparts are faint and fade rapidly, a reliable automatic procedure is crucial to schedule observations efficiently. To meet these challenges, we designed an algorithm in Python that uses a catalogue of nearby galaxies and the three-dimensional GW localization map to create a prioritized list of galaxies based on GW error-map probability, observability, and absolute magnitude. We tested our algorithm with past GW events and, within a few minutes, obtained consistent results with previous observations. We conclude highlighting how this algorithm can more generally assist in formulating effective followup plans with various types of small field telescopes at a variety of wavelengths, including radio.

*NSF-funded and Caltech-led GROWTH program.

C71.00097: Machine learning for classifying the chiral phase transition in AdS/QCD* BEIXI HAO (Presenter), SEAN BARTZ, Indiana State University — AdS/QCD is a phenomenological application of the gauge/gravity duality to strongly-interacting nuclear matter, including the quark-gluon plasma (QGP). This work uses machine learning to classify the order of the chiral phase transition between ordinary nuclear matter and the QGP. Our machine learning method is a supervised-learning synthesis of four standard classification algorithms: classification and regression trees (CART), k-Nearest Neighbors (kNN), Support Vector Machines (SVM) with a linear kernel, and Random Forest (RF). It is trained on a subset of data with known behavior, and tested on the remaining data, with a 100% success rate. We also discuss the application of this machine learning method to the development of an AdS/QCD model featuring a critical point in the QCD phase diagram, which aligns with the current experimental program at Brookhaven National Laboratory.

*The authors wish to thank the Indiana State University SURE program for its support.

C71.00098: EARLY CAREER —
C71.00099: Development of a zinc manganese dioxide flow battery*  DAVID REYES-RAMIREZ
(Presenter), Mechanical Engineering, California State University Los Angeles — With larger penetrations of renewable energy on our electrical grid, there is a need for large-scale energy storage devices. A redox flow battery is an electrochemical device with great promise as a large-scale energy storage technology given the scalability of the technology and that power and energy output are decoupled. This study aims to incorporate the strengths of flow batteries with the abundance and relatively high safety of manganese dioxide batteries. However, manganese dioxide batteries historically suffer from poor reversibility. To improve reversibility, the effects of different electrolyte additives, as well as the synthesis of manganese nano-rods, were investigated. These solutions were then incorporated into a prototype flow battery to address the need for a safe and reliable energy storage device.

*Partnership for Research and Education in Materials

C71.00100: Achieving an efficient control of antiferromagnetic order in artificial layered iridates  LIN HAO (Presenter), University of Tennessee, Knoxville, DEREK J MEYERS, Brookhaven National Laboratory, JUNYI YANG, HIDEMARO SUWA, CRISTIAN BATISTA, University of Tennessee, Knoxville, MARK DEAN, Brookhaven National Laboratory, JIAN LIU, University of Tennessee, Knoxville — Antiferromagnetic (AFM) materials started to gain traction owing the advantages of reliability, ultrafast dynamics, etc. in spintronic applications. In our recent work, we investigated AFM order in layered iridates, which is a newly established Mott system similar to cuprates but features a strong spin-orbit coupling. By building the spin-orbit Mott insulators as SrIrO$_3$/$\text{SrTiO}_3$ superlattices, we gained controllability in the strength and sign of interlayer exchange interaction. This enables one to reach the 2D limit of a magnet, where the ordering temperature is only governed by magnetic anisotropy. The 2D antiferromagnet preserves a hidden SU(2) symmetry, which was first proposed in cuprates but never experimentally realized. Specifically, we unveiled that Dzyaloshinskii-Moriya interaction in the square-lattice magnet does not contribute to the spin anisotropy. The extremely strong 2D critical fluctuations enable us to achieve giant AFM responses to sub-tesla magnetic fields. The observed field-induced logarithmic increase of the AFM ordering demonstrates a new pathway for designing efficient AFM spintronics. These results were recently published on Phys. Rev. Lett. [119,027204, (2017)] and Nat. phys. [14, 806--810 (2018)].
C71.00101: Multimodal x-ray and electron microscopy of an Allende meteorite sample*
CHEN-TING LIAO (Presenter), JILA, University of Colorado, Boulder, YUAN HUNG LO, JIHAN ZHOU, ARJUN RANA, University of California, Los Angeles, CHARLES BEVIS, GUAN GUI, JILA, University of Colorado, Boulder, BJOERN ENDERS, Advanced Light Source, Lawrence Berkeley National Laboratory, KEVIN CANNON, University of Central Florida, DAVID A SHAPIRO, Advanced Light Source, Lawrence Berkeley National Laboratory, HENRY KAPTEYN, JILA, University of Colorado, Boulder, ROGER WIRTH FALCONE, Advanced Light Source, Lawrence Berkeley National Laboratory, CHRIS BENNETT, University of Central Florida, JIANWEI MIAO, University of California, Los Angeles, MARGARET MURNANE, JILA, University of Colorado, Boulder — Correlative multimodal microscopy that combines complementary nanoscale imaging techniques is essential for extracting comprehensive chemical, structural, and functional information of heterogeneous complex samples. Advanced electron microscopy provides atomic-scale spatial resolution with quantitative elemental composition, while x-ray microscopy can achieve high-resolution imaging of bulk materials with chemical, magnetic, electronic, and bond orientation contrast. In our recent work (Science Advances 5, eaax3009, 2019), we combine x-ray ptychography and scanning transmission x-ray spectromicroscopy with 3D energy-dispersive spectroscopy and electron tomography to perform structural and chemical mapping of an Allende meteorite sample as a model system. We use textural and quantitative elemental information to infer its mineral composition and discuss potential processes that occurred. This multimodal x-ray and electron microscopy of the same sample overcomes the limitations of individual imaging modalities and opens up a route to future multiscale microscopies of complex functional materials and biological systems.

*We gratefully acknowledge support for this work by STROBE: A National Science Foundation Science & Technology Center, under Grant No. DMR 1548924.

C71.00102: Rationale Design of Polymeric Materials for Biological and Energy Applications using Multiscale Simulation Methods*
VAIDYANATHAN SETHURAMAN (Presenter), DAVID CLARK MORSE, KEVIN D DORFMAN, University of Minnesota — Two broad areas are investigated in this poster: (i) *Self-assembly of Methylcellulose in Solution:* We employ coarse-grained molecular dynamics simulations to show that the current theories of stacked toroid model for fibril formation is valid only at certain polymer concentrations. Rather, we showed the existence of a nucleation mechanism and the importance of conformational fluctuations for systems containing randomly coiled chains. We also show how the conformational and structural characteristics change with grafting the backbone with flexible polymers; (ii) *Polyelectrolyte Complexation:* We utilize implicit solvent coarse-grained molecular dynamics to probe the influence of charge sequence along the polymer backbone, on their adsorption efficacy onto grafted polyelectrolytes. Our work show that adsorption is strongest when both the grafted and the free polyelectrolyte in the solution possess a block charge sequence architecture and is weakest when both the grafted and the free polyelectrolyte possess an alternating architecture. We then showed that the sequence dependence on adsorption efficacy is enthalpic in nature and not entropic. We also show the effect of influence of charge sequence on polydisperse polyelectrolytes.

*MRSEC, Award No. DMR-1420013.
C71.00103: Proximity effects in two-dimensional transition-metal dichalcogenide materials for quantum information science*

CHRISTOPHER LANE (Presenter), JIAN-XIN ZHU, Los Alamos National Laboratory — Significant strides have been made towards the storage and processing of quantum information. However, scalable robust material platforms are scarce. The two-dimensional (2D) transition-metal dichalcogenides provide a possible path forward due to their valley degrees of freedom, which may be probed by circularly polarized light. Unfortunately, these levels are commonly degenerate in energy. Therefore, to create a viable platform for valley-based qubits, it is crucial to break time reversal symmetry in a controllable manner, allowing for direct manipulation. Using state-of-the-art \textit{ab initio} techniques, we demonstrate that controllable valley splitting can be achieved through a magnetic exchange proximity effect generated by a ferromagnetic 2D material substrate. Furthermore, by introducing vacancies into the transition-metal dichalcogenide layer, long-lived two-level impurity states may be stabilized. This approach reveals a new path towards the rational design of new complex multilayer systems for direct application in quantum information technologies and spin-optoelectronic devices.

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C71.00104: Simultaneous Study of Structure and Correlation-Driven Transitions via X-ray Standing Waves*

MATTHEW J. WAHILA (Presenter), GALO J. PAEZ, CHRISTOPHER SINGH, Physics, Applied Physics, and Astronomy, Binghamton University, NICHOLAS F QUACKENBUSH, National Institute of Standards and Technology, HANJONG PAIK, PARADIM, Cornell University, DARRELL SCHLOM, Materials Science and Engineering, Cornell University, TIEN-LIN LEE, Diamond Light Source, WEI-CHENG LEE, LOUIS F. J. PIPER, Physics, Applied Physics, and Astronomy, Binghamton University — The possibility of decoupling electronic phenomena from those of the lattice has been a hot topic when discussing correlated metal-insulator transition materials such as VO$_2$, NbO$_2$, or V$_2$O$_3$.[1] A mainly electronic transition could enable ultra-fast switching, thin film electronics, with little risk of the inevitable physical degradation associated with bulk structural transitions. However, the roles of structural (Peierls) and electron correlation (Mott) effects in driving these transitions continue to be debated in the literature.[2] Using x-ray standing waves (XSW) and high quality epitaxial thin films, we have now concurrently investigated both the structural and electronic transition within some of these correlated materials using a single technique, directly measuring their simultaneity or lack thereof for the first time. We discuss these results and their wider implications.


*This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0024.
Due to its position at the boundary between the light and heavy actinides, Pu has exotic physical properties that are complex and challenging to model. The difficulties in obtaining a full theoretical understanding for this elemental solid stem from the transitional characteristics of Pu-5f orbital electrons and understanding the role of the fluctuating magnetism in the electronic structure. Focusing on the δ-phase of elemental Pu, we perform a careful comparison of Fermi surface topology calculations using DFT and DFT+U methods. The de Haas-van Alphen (dHvA) frequencies at the Fermi surface and band masses are calculated in both magnetic and nonmagnetic states. We also analyze the effective mass enhancement due to 5f-electron correlation effects with DMFT as compared to the Gutzwiller approximation (GA). The comparison study will be helpful for future experiments to validate theoretical modeling.

*LANL LDRD program project 20180025DR
**C71.00106: van der Waals photothermoelectric effect in atomic layer heterojunctions**

YUNQIU (KELLY) LUO (Presenter), Laboratory of Atomic and Solid State Physics, Cornell University, TONG ZHOU, Physics, University at Buffalo, State University of New York, MAHESH R NEUPANE, Sensors and Electron Devices Directorate, U.S. Army Research Laboratory, ALEX MATOS ABAIGUE, Physics and Astronomy, Wayne State University, RYAN BAILEY-CRANDELL, MICHAEL J NEWBURGER, IGOR LYALIN, Physics, Ohio State University, IGOR ZUTIC, Physics, University at Buffalo, State University of New York, ROLAND KAWAKAMI, Physics, Ohio State University — Two-dimensional (2D) van der Waals (vdW) heterostructures provide exceptional opportunities for new physics and devices due to their unprecedented ability to tune the electronic, optical, magnetic and spintronic properties by atomic layer stacking and electrostatic gating. Harnessing this versatility requires a fundamental understanding of light-matter interactions and establishing new functionalities for photon-charge and photon-spin conversions. Here, we report the first observation of a highly-tunable vDW photothermoelectric effect in dual-gated MoS$_2$/graphene junctions with a striking multiple-polarity switching of photocurrent as a function of junction bias and carrier density. In stark contrast to photovoltaic effects arising from excitonic absorption in MoS$_2$, the vDW photothermoelectric effect originates from photoexcitation of hot electrons in graphene and thermoelectric transport across the vdw junction. Systematic studies of photoconductance as a function of photon energy and intensity reveal vdw photothermoelectric effect as the dominant mechanism for photocurrent generation at room temperature, as opposed to excitonic absorption. These findings provide an important step for understanding and control of vdw-interface devices.

*NSF MRSEC DMR-1420451

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**C71.00107: New Approaches and Observations in Scaled Contacts for 2D FETs**

ZHIHUI CHENG (Presenter), NIST & Duke University & Purdue University, HATTAN ABUZAID, Electrical and Computer Engineering, Duke University, YIFEI YU, Materials Science and Engineering, North Carolina State University, SHREYA SINGH, Electrical and Computer Engineering, Duke University, LINYOU CAO, Materials Science and Engineering, North Carolina State University, CURT RICHTER, Physical Measurement Laboratory, National Institute of Standards and Technology, AARON FRANKLIN, Electrical and Computer Engineering, Duke University — Atomically thin 2D crystals are promising channel materials for extremely scaled field-effect transistors (FETs). For devices at the scaled regime, both channel and contact length must be scaled, with channel length being the distance from source to drain contacts and contact length being the length of the source/drain covering the 2D semiconductor channel. Contacting 2D materials at these scaled contact lengths (< 30 nm) has rarely been pursued or studied in depth. Moreover, the device community has not yet determined how contacts can be scaled without causing significant degradation in device performance; i.e., how long is the transfer length, below which current crowding effects appear? Here, we demonstrate new measurement approaches and results for determining the transfer length of MoS$_2$ FETs by physically scaling the contact length. We found that, contrary to previous reports, top contacts can be scaled to ~20 nm without obvious degradation in transistor performance. Our data from measurements of over 100 devices with different contact lengths statistically imply that contact resistance variation increases in the scaled contact regime. Our work illustrates the impact of current crowding in scaled contacts and the ultimate scalability of metal-2D contact interfaces.
C71.00108: Investigation into form factors for mechanical-resonance-based methods of information storage*  
CHRISTOPHER HAKODA (Presenter), CRISTIAN PANTEA, VAMSHI KRISHNA CHILLARA, Los Alamos National Laboratory — Non-traditional information storage has become increasingly ubiquitous as a means of providing interactive, environment-specific information. With this in mind, we have investigated potential form-factors for a PZT-based information storage method that has visibly indistinguishable features for improved security. By manipulating the poling of PZT transducers, we developed a frequency-dependent, embedded array of transducers which, when excited at the relevant frequencies, reveal an engineered velocity profile. This velocity profile is then measured using a scanning laser Doppler vibrometer and decoded. Since this storage method is capable of storing frequency-dependent information, it can also store multiple layers of information that can be easily separated by applying a fast-Fourier transform. These multiple layers can be used for storing additional information or further hiding the encoded data. Two potential form factors are simulated and discussed in this proceedings, one has a flat profile while the other has a cylindrical profile.

*We acknowledge the support of Laboratory Directed Research and Development Early Career Research program under the grant LDRD20190568ECR.

C71.00109: Spontaneous thermal Hall conductance in superconductors with broken time-reversal symmetry*  
FIRAT YILMAZ (Presenter), SUNGKIT YIP, Academia Sinica — The thermal Hall conductivities (THCs), $\kappa_{ij}$ s have extensively been studied in recent condensed matter experiments. THC can spontaneously become non-zero for a time-reversal symmetry (TRS) broken system, and have a contribution from topologically protected edge states. In this talk, we focus on an additional bulk effect, the impurity pair breaking mechanism (IPM) in superconductors (SCs). Previously, the THCs were calculated for the chiral p-wave[1-2] SCs for point impurities. Motivated by d-wave TRS broken SCs; URu$\text{Si}_2$, SrPtAs including Sr$_2$RuO$_4$ which is recently suggested to be also possibly, we calculate THCs at finite temperatures and for finite size impurities using the non-equilibrium quasiclassical Green's functions.

We find that the IPM is dominant in $\kappa_{xy}$ at finite temperatures when compared to the topological contribution except at very low temperatures. There are two experimental signatures of IPM: 1. a non-monotonic temperature dependence, 2. sign change as a function of temperature depending on the scattering process.


*F.Y. and S.K.Y. acknowledge the Ministry of Science and Technology of Taiwan with grant number 107-2112-M001-035-MY3.
C71.00110: Do Levinthals arguments lead to a paradox for Si$_{20}$H$_{20}$?*  
DEB DE (Presenter),  
BASTIAN SCHAEFER, STEFAN A C GOEDECKER, University of Basel — Levinthal argued that the folding of a protein should require a time longer than the age of the universe. However, since it is experimentally well established that proteins do fold on a quite short time scale, these arguments are known as the Levinthal paradox. The paradox is resolved by folding funnel hypothesis. Here we will present a system whose global minimum is not embedded in a large funnel. The global minimum is virtually not accessible on a reasonable time scale. The potential energy surface of Si$_{20}$H$_{20}$ is considered for this study. The dodecahedron cage of Si$_{20}$H$_{20}$ is the theoretically established ground state. However it has never been observed experimentally. Based on an extensive exploration of possible reaction pathways of Si$_{20}$H$_{20}$ we show that there exists a huge number of intermediate structures that consist mainly of collapsed cages. Among all these reaction pathways that lead into the ground state, the system has to go through energetically flat regions before it reaches the Si$_{20}$H$_{20}$ ground state. This implies that there is no clear driving force towards this ground state that would give rise to a short directional reaction pathway that would lead rapidly into the ground state.

*This work was done within the NCCR MARVEL.

C71.00111: Understanding the acoustic emission from gas bubble dynamics: a signature of CO$_2$ leakage*  
HUNG DOAN (Presenter), Los Alamos National Laboratory — The identification and characterization of CO$_2$ leakage signatures in water and other fluids are of interest in the geophysical study of geysers and aquifers. As several DOE programs are investigating the feasibility of operationally injecting CO$_2$ into the subsurface, detecting and characterizing the signatures associated with the interaction of CO$_2$ with water shows important implications for monitoring large scale Carbon storage. This project proposes the development of a laboratory-scale test bench to carry out experimental studies of the acoustic emission emanating from gas bubble dynamics in a bi-phasic (water and gas mixture) fluid system. Different air bubble sizes, varying from 1 cm to 10 cm, are injected from the bottom of a water bath. As the bubbles migrate to the top, the vibrational response of those bubbles is captured by an acoustic pressure sensor placed within the fluid. The interaction is expected to be dependent on the size of the bubble, which can be characterized using the recorded acoustic signal. The result provides a non-invasive technique for characterizing the air bubble-size in the water/gas system and enables us to develop a framework for determining signatures pertaining to the presence of CO$_2$ in water.

*The project is funded by Los Alamos National Lab.
C71.00112: Experimental Demonstration of a Superconducting 0-π Qubit* ANDRAS GYENIS (Presenter), Princeton University — Encoding a qubit in logical quantum states with wavefunctions characterized by disjoint support and robust energies can offer simultaneous protection against relaxation and pure dephasing. Using a two-dimensional circuit-quantum-electrodynamics architecture, we experimentally realize a superconducting 0-π qubit, which hosts protected states suitable for quantum-information processing. Our multi-tone spectroscopy measurements reveal the energy level structure of the system, which can be precisely described by a simple two-mode Hamiltonian. The parity symmetry of the qubit results in charge-insensitive levels connecting the protected states, allowing for logical operations. The measured relaxation (1.6 ms) and dephasing times (25 μs) demonstrate that our implementation of the 0-π circuit not only broadens the family of superconducting qubits but also represents a promising candidate for the building block of a fault-tolerant quantum computer.

*Work was supported by Army Research Office Grant No. W911NF-1910016, NSERC and the Canada First Research Excellence Fund.

C71.00113: Long-lived Floquet phases in interacting three-dimensional topological semimetals via bicircular laser fields THAIS VICTA TREVISAN (Presenter), Ames Lab, ROBERT-JAN SLAGER, Harvard, PETER ORTH, Iowa State University — The use of carefully tailored light fields to manipulate quantum states of matter is an important technique in condensed matter physics. By coupling to the electronic degrees of freedom, they can induce electronic phases that were otherwise absent, for example, by selectively breaking a certain symmetry. One important example is the breaking of time-reversal symmetry by circulary polarized light, which can lead to a photo-induced Hall effect or the splitting of a three-dimensional Dirac node into Weyl nodes. Interestingly, it was recently showed that bicircular laser fields can also break spatial symmetries such as inversion or rotation symmetries, thereby inducing a charge (or spin) density wave order. Importantly, the density wave order can persist even after the light field is turned off, leading to a long-lived light-induced phase. This idea was recently explored in graphene, where it was shown to lead to a long-lived Floquet charge-density wave phase due to a dynamic synchronization transition. Here, we report our findings on coupling bicircular laser light to three-dimensional materials in order to induce spin and/or charge density wave phases. We specifically discuss the effects on topological phases of matter in Dirac and Weyl semimetals.

C71.00114: Band engineering for quantum simulation with superconducting circuits* CHRISTIE CHIU (Presenter), ANDREW HOUCK, Princeton University — Quantum simulation has been implemented on a variety of experimental platforms such as neutral atoms, ions, quantum dots, and superconducting circuits, each offering unique features. Superconducting circuits can and have been used to realize artificial photonic materials in a wide range of lattice geometries and graph connectivities, due to the flexibility of on-chip fabrication. In addition, photon-photon interactions are possible using nonlinearities such as superconducting qubits, leveraging the vast toolkit developed for quantum computation. Here I report on recent progress towards engineering flat bands for studies of strongly correlated many-body physics.

*This research was supported by the Princeton Materials Science Postdoctoral Fellowship and the ARO MURI program.
**C71.00115: Using Machine Learning to Classify Phase Behavior of Oil/Water/Surfactant Systems**  SHIYAN WANG (Presenter), NATHAN SCHULTHEISS, SANGTAE KIM, Purdue Univ — According to BP Statistical Review of World Energy in 2019, total oil production from the US in 2018 was about 15 million barrels per day (MBPD). Thanks to the booming shale oil production, United States has become the world’s top oil producer. In fact, estimates show that up to two thirds of conventional crude oil in mature fields remains unproduced due to the physics of fluid flow. The techniques of chemical enhanced oil recovery could overcome the physical force holding hydrocarbons, and turn these accumulations into oil reserve, which would enhance the US energy security and maintain economic growth. For the oil/water/surfactant system, the goal is to form a microemulsion phase achieving the lowest interfacial tension, which increases the capillary number and dramatically recovers the remaining oil fraction within the pore. Therefore, it is critically important to understand the phase behavior for the oil/water/surfactant systems. In collaboration with Pioneer Oil Company, our current effort is to optimize the selection of surfactants and the constituents of the surfactant blend, which turns to be a high dimensional problem. In addition to the conventional analysis, we employ machine learning techniques to solve the system as a multinomial classification problem.

**C71.00116: Resonant Raman Spectroscopy of the Chiral Antiferromagnet CoNb3S6**  NORA HASSAN (Presenter), THUC MAI, AMBER MCCREARY, National Institute of Standards and Technology, NIRMAL GHIMIRE, George Mason University, ANGELA HIGHT WALKER, National Institute of Standards and Technology — We report here the first full Raman characterization of the chiral antiferromagnet CoNb3S6; i.e. cobalt-doped NbS2. CoNb3S6 exhibits a large c-axis anomalous Hall effect (AHE) not entirely attributable to the small intrinsic ferromagnetic component (Co) along the c-axis [1]. This interesting behavior suggests that the enhancement in AHE may be because of a combination of magnetic field in the presence of the near-Fermi energy Weyl nodes as predicted by theory [2]. Neutron scattering experiments of CoNb3S6 [3] showed incommensurate peaks; however, it was not clear whether the peaks are due to a spin spiral or a spin density wave. Magneto-Raman spectroscopy represents an optimal method to differentiate these structures. Wavelength- and polarized-dependent Raman spectra collected at room temperature from CoNb3S6 flakes are analyzed. Experiments of temperature- and magnetic field-dependent Raman spectroscopy to seek magnon (spin wave) signatures detected no change in the spectral weight at the Neel temperature implying absence of spin density waves suggesting that the magnetic structure is helical.

References
(3) Private communication N. Ghimire
C71.00117: Physics-based models and simulations of cancer drug response in solid tumors
AMINUR RAHMAN (Presenter), Texas Tech Univ, SOUPARNO GHOSH, University of Nebraska - Lincoln, ERDI KARA, EUGENIO AULISA, Texas Tech Univ — Over the past few decades, cancer related deaths have fallen significantly as noted by the National Cancer Institute. However, assessing cancer treatments is still predominantly a trial and error process. This approach may result in delays to administer the correct treatment, the use of more invasive procedures than necessary, or an increase in toxicity due to superfluous treatments. Although these procedures may end up saving the patient, the treatment may also have an adverse effect on their quality of life. Reliable mechanistic models of drug response can potentially be used to aid oncologists and doctors in deciding on an optimal treatment strategy for the patient. We develop a modeling framework for tumor ablation, and present coupled transport - population models of varying complexity. First, we present a radially symmetric drug diffusion and binary cell death model, which produces a theoretical dose for optimal efficacy to toxicity ratios. Further, we investigate inhomogeneous - anisotropic drug diffusion, and develop an algorithm to locate the optimal injection points. Finally, we derive stochastic tumor population models that can be coupled to transport models in our framework. Importantly, the mechanistic models outperform data-driven models in statistical tests.

C71.00118: A Patterning Approach to Untangling Critical Interface Phenomena with In-Situ Resonant Scattering
ISVAR CORDOVA (Presenter), MSD, Lawrence Berkeley National Lab, GUILLAUME FREYCHET, NSLS-II, Brookhaven National Lab, ROMAIN GENEAUX, UC Berkeley, CHENG WANG, ALS, Lawrence Berkeley National Lab — Resonant soft x-ray scattering (RSoXS) is a powerful spatiochemical mesoscale characterization tool that is often overlooked across the field of interfacial science. Herein, we present a simple, yet highly sensitive, patterning approach for interface characterization that takes advantage of the physical processes intrinsic to small angle resonant X-ray scattering in order to selectively probe and enhance signals from interfacial regions of a vast array of material systems. Using several case studies, we show how patterns with simple nanoscale features can be used to 1) decouple the bulk from the interface scattering signal, 2) extract interfacial morphology with sub-nm precision, and 3) collect site-specific x-ray absorption spectra (XAS).

First, as an operando demonstration, we leverage a custom in-situ cell compatible with many synchrotron X-ray beamlines and use it conduct an operando study of Ni/Ni(OH)2 core/shell electrode undergoing electrochemical cycling under aqueous conditions. Next, we apply the technique to study the femtosecond dynamics of a 1.5 nm SiO2 surface with a broadband XUV table-top source. Finally, we introduce the potential of this technique to study material interfaces under conditions critical to the future of the next generation of electronics.
C71.00119: Tuning block copolymer rheology and structure via low strength magnetic fields* KARTHIKA SURESH (Presenter), MICHELLE CALABRESE, Chemical Engineering and Materials Science, University of Minnesota — The control of block polymer (BCP) structural ordering is of significant scientific interest because of their wide applications including nanotemplates, drug delivery and biomineralization. BCP properties have been controlled using various external fields including electric, magnetic, and shear fields, and via plasticizing additives, interfacial effects, and thermal methods. To control ordering in BCPs using magnetic fields, previous studies had used field strengths (≥5T), liquid crystalline mesogens, high magnetic susceptibility anisotropy groups or combinations therein. Here, we show anomalous behavior upon application of low strength magnetic fields (≥0.1 T) in coil-coil BCPs. Magneto-shear rheology shows up to a six order increase in modulus upon the field application. This magnetic response is a function of temperature, concentration, field strength, ionic content and shear strain. A minimum molecular weight and block length are required for this liquid to gel transition via low strength magnetic field. In situ small angle scattering (SAXS and SANS) and imaging techniques showed field-induced orientation in the BCPs and this orientation direction can be tuned by changing the direction of field lines.

*Seed grant, UMN MRSEC

C71.00120: PHYSICS EDUCATION —

C71.00121: Can Fermi energy be estimated experimentally? CHETAN KOTABAGE (Presenter), Department of Physics, KLS Gogte Institute of Technology, ASHUTOSH ABHYANKAR, Department of Materials Engineering, Defence Institute of Advanced Technology — Fermions, particles with half integral spin, follow Fermi-Dirac distribution. For free electron gas at absolute zero, Fermi energy is the energy of highest occupied level by electron. For \( n \), which is density of free electrons, Fermi energy can be estimated by \( E_F = \frac{\hbar^2}{8m} \left( \frac{3\pi^2 n}{2} \right)^{2/3} \) [1]. Theoretical calculation of Fermi energy of a metal involves estimation of density of electrons utilizing number of valence electrons. Experimentally, Fermi energy can be estimated by measurement of density of electrons in Hall effect measurement at room temperature. The measurement at room temperature serves as a good approximation because of very less difference between electron distribution at 0K and 300K.

[1] Modern Physics, K. Krane Wiley
Unscientific determination of Fermi energy by heating and/or cooling a copper wire, C. Kotabage, A. C. Abhyankar, Resonance- Journal of Science Education, 24 (12), 1439-1443.
C71.00122: Two Content Pathways in Presenting Electromagnetism in Introductory Algebra-Based Physics Textbooks  
LIANG ZENG (Presenter), Department of Physics and Astronomy, The University of Texas-Rio Grande Valley, YI ZENG, Center for the Core Curriculum, Nanchang Institute of Technology, GUANG ZENG, Department of Educational Leadership, Texas A&M University-Corpus Christi — Vector cross products play a fundamental role in determining the directions of electromagnetism in introductory physics courses. After examining thirteen introductory algebra-based physics textbooks, we found authors adopt the following two content pathways in presenting the electromagnetic phenomena: Over 90% of the textbooks follow pathway one which presents only algebraic formulas and mnemonic techniques for right- and left-hand rules. Scarcely few follow pathway two, which presents vector cross products as a mathematical model and reinforces this model by presenting the specific cross product formula for each electromagnetic phenomenon. Physics instructors teaching college physics courses similarly present electromagnetism using these two content pathways. In light of Bloom’s taxonomy of educational objectives and constructivist learning theory, we recommend the second pathway.

C71.00123: Using Group Exams to Address Persistent Intuitively Appealing but Incorrect Student Reasoning*  
ALISTAIR MCINERNY (Presenter), LIUDMILA KRYJEVSKAIA, Physics, North Dakota State University — Many students tend to provide intuitively appealing (but incorrect) responses to some physics questions despite demonstrating (on similar questions) the formal knowledge necessary to reason correctly. While these inconsistencies are typically persistent even in active learning environments, we believe that adding a group component to the exam may engage students sufficiently to resolve these instances of inconsistent reasoning. In our study, students were given opportunities to revisit their answers to questions known to elicit strong intuitively appealing (but incorrect) responses in a collaborative group component of an exam immediately following a traditional individual component. Students discussed their responses with group members but were required to submit their own answers and reasoning. On this poster, we examine the effectiveness of a collaborative group exam approach in addressing and resolving inconsistencies in student reasoning and will compare the effectiveness of this approach to a more traditional peer instruction technique.

*This material is based upon work supported by the National Science Foundation under Grants Nos. DUE-1821390, DUE-1821123, DUE-1821400, DUE-1821511, DUE-1821561, DUE-1431940, DUE-1431541, DUE-1431857, DUE-1432052, and DUE-1432765.

C71.00124: Incorporating realistic aspects of experimentation into senior physics labs  
KIRSTIN PURDY DREW (Presenter), Pennsylvania State Univ — Here we present design changes to the senior physics lab course at Penn State, which were implemented in order to increase student engagement with modeling, experiment design, and the writing process in our lab curriculum. The goal of these changes was to restructure the course to emphasize planning, prediction, and assessment of experimental data during an experimental process, in mimicry of the scientific research process, while still providing students with exposure to a breadth of experiments and experimental techniques which are historically a required part of the course. Both structural and content changes made in the course will be presented along with initial assessment of changes in student perceptions and critical thinking skills.
C71.00126: Machine Learning Towards Optical Spectrum Estimation Using Nanomaterial Thin Films*  
DAVOUD HEJAZI (Presenter), SHUANGJUN LIU, AMIRREZA FARNOOSH, SARAH OSTADABBAS, SWASTIK KAR, Northeastern University — Some of the major challenges in optical spectrum estimation include the necessity to create an array of thousands of identical photodetectors, or intricate mechanical systems that make the estimation system bulky and expensive. Using the spectral transmittance of an array of 11 solution-processed nanomaterial thin film filters fabricated from two layered semiconducting materials, Molybdenum-Disulfide and Tungsten-Disulfide, we have estimated the wavelength of any incoming light in a wide spectrum range. By applying machine learning techniques we have used the variations in spectral transmittance of nanomaterials as the alternative method for optical spectrum estimation. We have studied the efficacy of various machine learning algorithms including k-nearest neighbors, artificial neural networks, support vector machines, and Bayesian statistics in spectrum estimation problem and identified the key advantages and limitations of each algorithm for real-time applications such as accuracy and speed. Furthermore, we have modeled the temporal drift of filters' spectral transmittance over a period of one year and showed that it is possible to overcome the drift-induced inaccuracies over time using a modeled drift function.

*NSF ECCS 1351424  
NEU Provost's Tier 1 Interdisciplinary seed grant

C71.00127: Improve the synaptic performance of resistive switching devices through interface engineering*  
YU SHI (Presenter), RABIUL ISLAM, GUOXING MIAO, Electrical and Computer Engineering, University of Waterloo — Transition metal based resistive switching devices (like HfO\textsubscript{2}, TiO\textsubscript{2}) has been shown to be a good candidate for neuromorphic computing for its bio-inspired synaptic properties, however, the non-linear conductance change synaptic behaviour prohibits further improvement due to poor accuracy of neural network training. Here, we provide a way to eliminate the intrinsic non-linearity through electrode-oxide interface engineering, including oxygen profile control and oxide heterostructure stacking, which can improve the neural network training accuracy and shorten the training time.

*Transformative Quantum Technologies (TQT)
C71.00128: High Thermoelectric Performance in Hexagonal 2D PdTe$_2$ Monolayer at Room Temperature

BRAHIM MARFOUA, JISANG HONG (Presenter), Pukyong National Univ — Motivated by the recent fabrication of hexagonal PdTe$_2$ monolayer, we investigated the thermoelectric properties of the hexagonal and pentagonal PdTe$_2$ structures using two approaches. The pentagonal monolayer has not been synthesized yet. The hexagonal layer had an indirect bandgap of 0.17 eV while the pentagonal structure had an indirect bandgap of 1.18 eV. By applying the semi-empirical Wiedemann–Franz law to calculate the electronic thermal conductivity, we found that both hexagonal and pentagonal structures had very high ZT more than 3. However, the Wiedemann–Franz law underestimated the electronic thermal conductivity and this resulted in high ZT. Thus, we employed the Boltzmann transport equation for the electronic thermal conductivity. At high temperature ( > 500 K), the pentagonal PdTe$_2$ structure showed a better thermoelectric performance than the hexagonal structure. However, both structures displayed the same ZT of 0.8 at 300 K. We propose that the hexagonal PdTe$_2$ can be a potential high performance thermoelectric material at room temperature.

*This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) (2019RA21B5B01069807).

C71.00129: Textile Thermoelectric Generator Based on Carbon Nanotubes

FARIBA ISLAM, NABILA FAIRUZ, AHMED ZUBAIR (Presenter), Electrical and Electronic Engineering, Bangladesh University of Engineering and Technology — Smart textile based on seamless device integration into clothing will dominate the wearable technology field in the near future. Carbon nanotubes (CNTs) are a favorable candidate for use in these flexible and wearable electronic devices due to tunability of their electrical and thermal properties, mechanical strength, and lightweight. The wearable devices demand wearable micro-sources of energy. Here, we propose a textile thermoelectric generator based on CNT that can utilize waste heat to generate power. The generator is fiber-structured to make it easily woven into clothing. We simulated a ~5 cm long fiber structured generator with p-n junctions at every 3 mm interval based on CNTs. To model CNTs, experimental data were used in our simulation. This generator generates a thermoelectric voltage of ~55 μV for just a 1 K temperature difference. The thermoelectric figure of merit, ZT for this CNT based device was smaller than previously reported materials. However, it is possible to fabricate CNT based devices with large ZT by proper doping and utilizing the Van Hove singularities in the density of states of CNTs.
C71.00130: Structural Phase Transition of Multilayer VSe$_2$  

XIONG WANG (Presenter), DIAN LI, XIAODONG CUI, Physics, The University of Hong Kong, CHUANHONG JIN, Materials Science and Engineering, Zhejiang University — Vanadium diselenide (VSe$_2$), a member of the transition metal dichalcogenides (TMDs) family, is emerging as a promising two-dimensional (2D) candidate for the electronic and spintronic device with exotic properties including charge density wave and ferromagnetism. The bulk crystal VSe$_2$ exists in a crystallographic form of 1T phase with metallic behavior. In this paper, we report a structural phase transition of multilayer VSe$_2$ from 1T to 2H, which occurs at about 650 K, accompanying a metal-insulator transition. The phase transition is verified by Raman spectra, as different polymorphs have different Raman signals related to different characteristic vibration modes. The electrical characteristics are also studied on VSe$_2$ nanoflakes, as the phase transition occurs along with the metal-semiconductor transition, which is consistent with the electronic band structure calculation. The results of in-situ selected area electron diffraction (SAED) is are accord with our simulated diffraction patterns, which is strong evidence of the structural phase transition. Moreover, we observe that the 2H phase is more thermodynamically stable than the 1T phase at the multilayer level.

C71.00131: Investigating the metal to insulator transition in crystalline NbO$_2$ for neuromorphic computing applications*  

GALO PAEZ FAJARDO (Presenter), MATTHEW J. WAHILA, JATINKUMAR RANA, Department of Physics, Binghamton University, BROOKS TELLEKAMP, National Renewable Energy Laboratory, WILLIAM A. DOOLITTLE, School of Electrical and Computer Engineering, Georgia Institute of Technology, LOUIS F. J. PIPER, Department of Physics, Binghamton University — The metal-insulator transition (MIT) of NbO$_2$ is promising for technological applications where a self-regulated resistivity is needed like in neuromorphic computing. Though the Mott nature (electron correlation) of the MIT of NbO$_2$ arises purely by comparison to VO$_2$, the actual transition mechanism in NbO$_x$-based memristors remains unclear mainly due to the degree of participation of multi-phases of niobium oxides, likely induced after electroforming. By investigating phase-pure, crystalline NbO$_2$, we avoid the uncertainty created in electro-formed NbO$_x$-based devices. Using surface sensitive techniques like LEED, HAXPES, and LEEM on NbO$_2$(440)/Al$_2$O$_3$(006) thin films, we show that the phase transition does not extend to the film surface. XPS of the crystalline NbO$_2$ reveals a second-order Peierls transition in the bulk, in agreement with DFT results, indicating electron correlation effects do not play a significant role. In addition, the observed temperature dependence of the Nb-Nb dimer distance which controls the NbO$_2$ resistivity suggests that the switching of future phase-pure NbO$_2$ memristors could be controlled by resistive heating in an analog rather than digital fashion.

*This material is supported by the Air Force Office of Scientific Research under Award No. FA9550-18-1-0024.
**C71.00132: Magnetically driven carbon nanotubes for a highly efficient mechanical single cell damage.** VICTORIA GABRIELE (Presenter), KRZYSZTOF KEMPA, MICHAEL NAUGHTON, THOMAS SEYFRIED, Boston College — Magnetized carbon nanotubes have previously been demonstrated as excellent candidates for the nanospearing transfection technique. In the presence of the moderate, spacially varying magnetic field, these magnetic nanorods exert motion, capable of piercing cell membranes, and allowing for highly efficient drug delivery. Here we study the possibility of enhancing this nanospearing technique, by varying magnetic strength and its time-space patterns, in order to inflict a highly efficient and selective, single cell mechanical damage.

**C71.00133: Quasiparticle and Optical Properties of Bulk and Monolayer Zirconium Disulfide**

GABE LOPEZ-CANDEALES (Presenter), GREIS JULIETH CRUZ REYES, ZHAO TANG, PEIHONG ZHANG, Physics, University at Buffalo — Zirconium disulfide (ZrS2) is a member of layered transition metal dichalcogenide (TMD) family that has rich and versatile chemical and physical properties. Despite much recent renewed interest in ZrS2, especially in few-layer ZrS2 systems, an accurate and systematic understanding of the quasiparticle and optical of ZrS2 from monolayer to bulk phase is still lacking. In this work, we present a fully converged GW+BSE study of the quasiparticle and optical properties of monolayer and bulk ZrS2, aiming at illustrating the subtle interplay between structural and electronic properties and the importance of the convergence issues in 2D many-body perturbation calculations.

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**C71.00134: Ab-Initio Computations of Electronic and Related Properties of cubic Magnesium Silicide (Mg$_2$Si)**

DIOUM ALLÉ, Department of Physics, Cheick Anta Diop University (UCAD), Dakar, Senegal, BLAISE AYIRIZIA, YURIY MALOZOVSKY (Presenter), DIOLA BAGAYOKO, Department of Mathematics and Physics, Southern University and A&M College — We have performed *ab-initio*, self-consistent calculations of electronic, transport, and bulk properties of cubic magnesium silicide (Mg$_2$Si). Our computations employed the local density approximation (LDA) potential of Ceperley and Alder and the linear combination of atomic orbital (LCAO) formalism. We followed the BZW-EF method to reach the ground state of the materials, verifiable, without using over-complete basis sets. For a room temperature lattice constant, our calculated, indirect band gap, from $\Gamma$ to X, is 0.86 eV. We discuss the total and partial densities of states, electron and hole effective masses, and the bulk modulus.

*This work was funded in part by the Department of Physics de l’UCAD and l’UCAD, the National Science Foundation [NSF Award HRD-1002541], the US Department of Energy – National Nuclear Security Administration (NNSA) (Award Nos. DE-NA0001861 and DE- NA0002630), LaSPACE, and LONI-SUBR.
**C71.00135: Ab-initio Calculations of Electronic Properties of Tin Selenide (SnSe)**

YURIY MALOZOVSKY (Presenter), SHAIBU MATHIAS, DIOLA BAGAYOKO, Southern Univ & A&M Coll — We present results from *ab-initio*, self-consistent density functional theory (DFT) calculations of electronic properties of tin selenide (SnSe) in the *orthorhombic B16* crystal structure. We utilized a local density approximation (LDA) potential and the linear combination of atomic orbital (LCAO) formalism. Our calculations performed a generalized minimization of the energy to reach the ground state, as required by the second DFT theorem. This process ensures the full, physical content of our findings that include electronic energy bands, total and partial densities of states, and electron and hole effective masses.

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**C71.00136: Calculations of third order nonlinear susceptibilities focused in two photon absorption on semiconductors.**

ALAN BERNAL (Presenter), Centro de Investigaciones en Optica, BRANDON FUREY, MICHAEL C DOWNER, University of Texas at Austin, BERNARDO MENDOZA SANTOYO, Centro de Investigaciones en Optica — We presented the calculation of nonlinear third order susceptibility focused on Two-photon absorption phenomena (TPA) on bulk crystal semiconductors. Our calculation considers the longitudinal gauge approximation to the interaction field, the non-local part of the crystal potential and the scissor operator as correction to LDA energies calculations.

**C71.00137: Observation of B 1s trion and A 2s trion in 2d limit**

TENGFEI YAN (Presenter), KE XIAO, XIAODONG CUI, department of physics, the university of Hong Kong — The distinct excitonic effect in two-dimensional (2d) layered material attracts lot of attentions in recent years. The largely reduced screening effect in 2d materials allows tightly bonding exciton. With gate tunable photoluminescence spectrum, we observe B 1s trion and A 2s trion in h-BN capsuled MoSe$_2$. The two states show much larger valley polarization compared with their low energy counterparts A 1s exciton and trion.

**C71.00138: Excited carrier relaxation in GaAs by mid-IR pump-probe spectroscopy**

ROISUL GALIB (Presenter), Mechanical and Aerospace Engineering, University of Virginia, JOHN A TOMKO, Materials Science and Engineering, University of Virginia, DAVID OLSON, ASHUTOSH K GIRI, JOHN T GASKINS, PATRICK HOPKINS, Mechanical and Aerospace Engineering, University of Virginia — Ultrafast laser spectroscopy is a versatile technique that is commonly used to both understand and manipulate carrier scattering mechanisms in semiconductors. We report the observation of excited carrier relaxation times in GaAs using optical pump mid IR probe spectroscopy. We find a sharp change in relaxation times occurs at the intervalley transitions of GaAs. Our results also show the relaxation times becomes faster with increasing photoexcitation fluence. These results provide direct evidence that excited carrier decay at greatly different rates based on their energy relative to the conduction band minimum. These findings provide additional insight into the energy-dependent nature and rate of phonon emission during electronic relaxation.
**C71.00139: Temperature dependent vibrational modes of TNT and CL-20 cocrystal in terahertz regime**  
ABDUR RAHMAN (Presenter), Physics & Technology, Edinboro University, TOWFIQ AHMED, ABUL AZAD, DAVID MOORE, Los Alamos National Laboratory — We employed terahertz time domain spectroscopy (THz-TDS), a non-invasive technique, in the range of 0.30 THz to 2.50 THz to measure the effective dielectric properties of a 1:1 molar ratio cocrystal of TNT and CL-20 in the temperature range 150K to 400K. We observed two distinguished absorption peaks at 0.80 THz and 1.3 THz at or below room temperature. The absorption peaks disappear at higher temperatures. We extracted the dielectric constants of the cocrystal using effective medium theories.

*Los Alamos National Laboratory’s LDRD program.*

**C71.00140: Point-of-care ultrahigh sensitivity magnetic lateral flow assay**  
MOHAMMAD KHODADADI (Presenter), Materials Science & Engineering, University of Houston, JOÃO TRABUCO, Chemical & Biomolecular Eng, University of Houston, LONG CHANG, Electrical & computer Engineering, University of Houston, KATERINA KOURENTZI, RICHARD WILLSON, Chemical & Biomolecular Eng, University of Houston, DMITRI LITVINOV, Electrical & computer Engineering, University of Houston — Today, many highly quantitative biomarker detection tools for medical diagnostics are readily available in state-of-the-art centralized clinical laboratories. However, there remains a critical need for inexpensive, versatile, and high-sensitivity diagnostic platforms which can bring the performance to the point of care (POC) or doctor’s office. Our team has developed an ultrasensitive point of care biosensor based on the miniaturized inductive detector of magnetic reporter nanoparticles ($10^{10}$ emu detection limit) in a test line of a lateral flow assay (like a pregnancy test). This technology represents a new general biosensor platform that can be broadly useful in various areas of molecular diagnostics, therapy monitoring, biomarker detection, and biomedical research. The biosensor prototype performance was evaluated using a standard hCG model system with well established LFA immunochemistry based on readily available, well-characterized, and inexpensive antibodies. The first target after proof of concept is to make a biosensing platform for detecting the recurrence of prostate cancer.

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Cancer Prevention and Research Institute of Texas (CPRIT)*

**C71.00141: WITHDRAWN ABSTRACT**
C71.00142: Obstacles to Undergraduate Research in Thin Film Semi-Conductor Characterization: The Creation of Inexpensive Hall Measurement Apparatus

OLUWASEKEMI ODUMOSU (Presenter), Ithaca Coll — The goal of my project was to grow and characterize thin semiconducting ZnO films grown on PET plastic via pulsed laser deposition (PLD) with a KrF laser. To characterize the electrical properties of these films, I had to create an automated Hall Measurement apparatus, as I did not have access to industrial equipment due to its unfeasible cost. The apparatus required a few components: I started by creating a Labview program to interface with an ArduinoMega, which operates a 16-switch relay. This relay was then connected to a nano-voltmeter, current source, and my sample film (which would be in a uniform magnetic field for some measurements). Labview would then compile the data into a .csv file, which my Python code would interpret and record measurements for the sheet resistance, bulk resistivity, semiconductor type, sheet carrier density, bulk carrier density, and hall mobility. The apparatus functions correctly, but improvements need to be made to get consistent data.

*Dana Internship Program at Ithaca College
Summer Scholars Program, School of Humanities and Sciences, Ithaca College

C71.00143: Thermoelectric effect in suspended Bi$_2$Se$_3$ grown by molecular beam epitaxy on GaAs(111)A

DONGUK KIM (Presenter), CHANUK YANG, JOON SUE LEE, YUN DANIEL PARK, Physics & Astronomy, Seoul National University — Bi$_2$Se$_3$ is well known as an efficient thermoelectric (TE) material. We report growth optimization of Bi$_2$Se$_3$ thin films and thermoelectric study of suspended Bi$_2$Se$_3$ beam structures. The Bi$_2$Se$_3$ thin films were grown on GaAs(111)A substrates by molecular beam epitaxy (MBE) and confirmed by (00n) series peaks of x-ray diffraction (XRD) that the material was grown along the c-axis of GaAs(111)A. Optimizing the desorption process of GaAs(111)A surface and growth conditions of GaAs buffer layers leads to low RMS roughness and less-defective structural aspect. Using the optimized Bi$_2$Se$_3$ films, we realize the suspended beam structures with minimal heat dissipation to GaAs substrate. The beam structures are fabricated by selective wet etching, and on the two membranes, platinum heaters and voltage channels are patterned to measure the thermoelectric effect, the conversion of temperature difference to electric voltage. Nanomachining technique enables to calculate the dimensionless figure of merit (ZT) of Bi$_2$Se$_3$ with minimal environmental factors.

*This work was supported by National Research Foundation of Korea (2017R1E1A1A01074650).
C71.00144: High quality Tantalum pentoxide thin film growth and its application for low loss nonlinear waveguide* JIA-WEI LIU (Presenter), CHAO-HONG LIN, TE-KENG WANG, FU-YAN YAN, ZI-DE XIE, Department of Photonics, National Sun Yat-sen University, MIN-HSIUNG SHIH, Research Center for Applied Sciences, Academia Sinica, CHAO-KUEI LEE, Department of Photonics, National Sun Yat-sen University — Tantalum pentoxide ($\text{Ta}_2\text{O}_5$) of a large bandgap material has shown its potential for Si photonics due to its low absorption loss coefficient in visible to infrared regions, high Kerr coefficients, and nonlinear absorption (TPA/FCA) free. Development of large scale high optical quality thin film for integrated photonics is therefore desired. In this work, by using e-gun evaporation, large scale $\text{Ta}_2\text{O}_5$ thin film growth was performed. Beside the measurement of x-ray and Ramen pattern for identifying the structure, the AFM and SEM results all show the grown thin film with high quality. In addition, a low-loss and high-Q $\text{Ta}_2\text{O}_5$ based micro-ring resonator was fabricated and characterized. The propagating loss of 0.3 dB/cm was obtained and unloaded quality as high as 300000 was accordingly estimated. This is, in our knowledge, the largest unloaded quality for $\text{Ta}_2\text{O}_5$ waveguide. This all show that electron beam thermal evaporation (E-gun) grown $\text{Ta}_2\text{O}_5$ film is with great potential for photonic integrated circuit.

*MOST108-2218-E-110-011-

C71.00145: WITHDRAWN ABSTRACT
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C71.00146: Dry surface cleaning of twisted bilayer graphene and angle dependent oxidation by UV irradiation. JIN HONG KIM (Presenter), MOHD MUSAIB HAIDARI, JIN SIK CHOI, KonKuk Univ — Since production of single layer graphene (SLG) by mechanical exfoliation, it has been focal to many researches thanks to its extraordinary electrical conductivity and surface to volume ratio. these characteristics of graphene have benefit for apply gas sensor devices. Recently, twisted bilayer graphene (tBLG) attracted much attention of its extra ordinary physical properties, especially for its twist angle opto-electrical dependant characteristic. specifically, the magic angle (~1.1°) which shows super conducting characteristics. Moreover, tBLG shows higher mobility and conductivity than SLG. However, stacking two layers of single crystalline SLG has been reported to show side effect of introducing interlayer impurities during transfer process. Furthermore, Impurities of graphene surface, such as PMMA residues, degrade electrical conductivity and mobility. Here we report a CVD synthesis of clean interlayer tBLG to containing various twist angles. Top layer of tBLG was cleaned and oxidized by angle dependency under UV irradiation at ambient condition and characterized by Raman and electrical properties. We suggest that UV cleaning is the most effective method for surface cleaning of graphene. Also, we expect a correlation between oxidation rate and twist angle.
C71.00147: High transmittance Er doped ZnO thin films as electrodes for organic light-emitting diodes  SHI YINGLI (Presenter), CHI-CHUNG LING, The University of Hong Kong — Transparent conducting oxides (TCO) have attracted great attention since the first demonstration in 1907 by Baedeker. TCO thin films with high transparency and electrical conductivity have been widely used in optoelectronic devices, such as thin-film transistors, perovskite solar cells and light emitting diodes (LEDs). Er doped ZnO films exhibit higher optical transparency (~95 %) than other reported metal elements doped ZnO TCO thin films. The effect of Er doping concentration on photoelectric properties of ErZO thin films was investigated in the range of 0-2.0 wt.%. The Er impurity substitutes the Zn site and Er\textsubscript{Zn} serves as charge donor in the ZnO crystal structure, thus resulting in the improvement of \textit{n}-type conductivity as compared with intrinsic ZnO thin films. The optimized ErZO thin films present the low resistivity of $3.4 \times 10^{-4} \ \Omega/$cm, high carrier concentration of $5.9 \times 10^{20} \ /$cm$^3$ and high visible optical transmittance (~93%) when the Er content is 1.0 wt.%. The ErZO thin films were used as transparent anodes to fabricate organic light-emitting diodes (OLEDs). Impressively, with the ErZO as anode, the current efficiency of the OLEDs device can reach as high as 86.5 cd/A, which was increased by 14% when compared with the reference OLEDs device (76.0 cd/A) using ITO as anode.

C71.00148: Thermally induced metal-to-insulator transition in NbO\textsubscript{2} thin films*  TOYANATH JOSHI (Presenter), ELI CIRINO, SOPHIE MORLEY, DAVID LEDERMAN, Department of Physics, University of California, Santa Cruz — Modification of the carrier dynamics in correlated oxide systems via epitaxial strain is a promising pathway for the practical realization of energy-efficient electronic devices. Here we present on the thermally induced metal-to-insulator transition (MIT) of epitaxial NbO\textsubscript{2} films grown on Al\textsubscript{2}O\textsubscript{3} substrates and the modulation of the MIT temperature via epitaxial strain from the substrate. The metal-insulator transition temperature increased from 910 K to 1066 K with increasing strain. An ultrathin 3.9 nm film consisting of a single strained layer with minimal structural defects yielded a bulk-like sharp transition. The substrate-induced strain offers a new degree of freedom to improve device functionality of MIT materials.

*This work is supported by the University of California Multicampus Research Programs and Initiatives Grant (MRP – 17-454963).
C71.00149: Synthesis and characterization of new multinary chalcogenides*  
MASOUD MARDANI (Presenter), National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA.; Department of Physics, Florida State University, Tallahassee, FL, USA., KAYA WEI, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA., THEO SIEGRIST, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA.; Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, — Multinary chalcogenides have drawn a lot of attention due to their interesting properties. We report on newly synthesized quaternary and quintenary chalcogenide family materials. The thermal, electrical, and magnetic properties of the new materials will be discussed in detail as well as their potential technological applications. Structural results will be presented and structure-property relationships will be discussed.

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C71.00150: Structural Design and Manufacturing of Three-Dimensional Porous Superstructures with Additive and Subtractive Electrochemistry for Flexible Self-Powered Electronics and Electromechanical Devices*  
WEIGU LI, DONGLEI (EMMA) FAN (Presenter), University of Texas at Austin — The recent search for advanced materials with desired properties for the next-generation flexible energy and electronics has been focused on the unique class of three-dimensional (3D) porous superstructures made of 2D materials, such as graphene, graphite, and molybdenum disulfide.

In this work, we report an innovative and rational approach to create 3D metallic foams with tunable multi-level porosity by using a process consisting of an additive electrodeposition and subtractive electroetching. The resulted metallic foams can readily serve as catalytic templates for the growth of 3D hierarchically porous thin graphite. The 3D graphite is freestanding after selective etching of the metallic template. They provide enhanced mechanical properties and electrochemical performances when applied as supercapacitor electrode supports. They can be readily integrated with our wearable GF/polymer strain sensors developed recently and nanomotor manipulation systems into self-powered sensing and electromechanical devices, respectively.

*The research is supported by the National Science Foundation and Welch Foundation.
C71.00151: In-situ Raman investigation of Laser-Induced Graphene using Machine
Learning*  VIVEK JAIN (Presenter), ALEX TYRRELL, HUD WAHAB, LARS KOTTHOFF, PATRICK A
JOHNSON, Univ of Wyoming — High-quality graphene was laser-induced from precursors graphene
oxide and commercial polyimide. Laser annealing is a promising method to create graphene-
based devices including sensors, biomedical equipment and thin-film transistors. A Bayesian
optimization-based machine-learning strategy was used to predict optimal process parameters.
We custom-built our system to allow simultaneous laser patterning processing and in-situ Raman
spectroscopy characterizations. The Raman G/D ratio is a good indication of the quality of the
laser-induced graphene. Rapid and significant improvements in the G/D ratios were seen with the
machine-learning predicted process parameters. This experimental setup has enormous
potential in Autonomous Research Systems for new materials discovery and can be scaled up for
advanced-manufacturing patterned graphene-based electronics.

*School of Energy Resources, University of Wyoming
College of Engineering & Applied Sciences, University of Wyoming

C71.00152: Optical phenomena of irradiation induced molybdenum disulfide*  KORY BURNS
(Presenter), ANNE MARIE ZHAO HUI TAN, University of Florida, ADAM GABRIEL, LIN SHOA, Nuclear
Engineering, Texas Agricultural and Mechanical University, RICHARD HENNIG, ASSEL AITKALIYEVA,
University of Florida — Irradiation introduces damage cascades, destroys the periodicity of the
lattice, and pushes the material away from equilibrium. In this contribution, we utilize heavy ion
and gamma irradiations to alter the optical properties of two-dimensional (2D) materials such as
MoS$_2$. Irradiation offers a pathway to introduce desired defect densities to any given material,
and, in case of low-dimensional materials, can be used to control physical properties. Defects
introduced using irradiation were characterized using transmission electron microscopy (TEM)
and photoluminescence (PL) measurements. We primarily focus our attention on the behavior of
valley excitons, as they dominate the optical response of the material even when the system is in
equilibrium and reveal the emergence of dark excitonic states in the K-valley. With this work, we
offer insight into how increased defect density can potentially engineer magnetism in 2D MoS$_2$.


*U.S. Department of Energy, Office of Science, Basic Energy Sciences, Award #DE-SC0019014
“Establishing defect-property relationships for 2D-nanomaterials”.
C71.00153: Non-Destructive Thickness Mapping of Wafer-Scale Hexagonal Boron Nitride Down to a Monolayer
ANDREA CROVETTO (Presenter), PATRICK WHELAN, DTU Physics, Technical University of Denmark, RUIZHI WANG, Department of Engineering, University of Cambridge, MIRIAM GALBIATI, DTU Physics, Technical University of Denmark, STEPHAN HOFMANN, Department of Engineering, University of Cambridge, LUCA CAMILLI, DTU Physics, Technical University of Denmark — Characterization of the thickness and continuity of wide band gap 2D materials with monolayer sensitivity over large areas has proven to be very challenging. A prime example is 2D hexagonal boron nitride (hBN). Optical contrast methods suffer from the lack of visible absorption in the material; Raman spectral signatures are weak and often not conclusive; and electrical measurements are not possible due to a high electrical resistivity. In this contribution, we will demonstrate an experimental method based on the ellipsometry technique, which makes it possible to map the thickness and continuity of large-area hBN monolayers and bilayers transferred to Si/SiO$_2$ substrates. The method has sub-monolayer thickness sensitivity, is relatively fast, non-destructive, and can be easily automated. The hBN thicknesses measured in this study have been confirmed by Raman spectroscopy, x-ray photoemission spectroscopy, and by a series of ellipsometry control experiments. We will present a workflow of our experimental procedure, so that other researchers can extend this characterization method to other 2D materials and hopefully accelerate their development.

C71.00154: Raman Enhancement effect using hexagonal Boron Nitride with a substrate*
JESSICA LEMOS (Presenter), ANDREJ DE CARVALHO GADELHA, CRISTIANO FANTINI LEITE, Physics, Universidade Federal de Minas Gerais, ELIEL GOMES DA SILVA NETO, Physics, Universidade Federal Fluminense — The Raman enhancement effect is a phenomenon for fundamental studies of both light-matter and matter-matter interactions and applications. Among the several Raman enhancement techniques, the surface-enhanced Raman scattering (SERS) has been the most studied. There are two different mechanisms for SERS effect, the first one is the electromagnetic mechanism when is the local electromagnetic fields around the metallic structures can be amplified. The second is the chemical mechanism which is lower understood, and its magnitude is smaller than the electromagnetic effect. The substrate surface is very important to control the necessary enhancement to make the technique as valuable as it has become. In this work, we study hexagonal boron nitride (hBN) a two-dimensional layered material with a substrate for a type of SERS, an insulator whose gap is approximately 5eV.

*Capes, CNPq and INCT(nanocarbono)
C71.00155: Dual comb spectroscopy for measuring the group velocity dispersion of optical fiber realized by fast locking of the beat note with a piezoelectric module*  
RYOSUKE TABUCHI (Presenter), Keio Univ, KANA ALYSSA SUMIHARA, Keio Univ / AIST, SHO OKUBO, AIST, MAKOTO OKANO, Keio Univ, HAJIME INABA, AIST, SHINICHI WATANABE, Keio Univ — Dual-comb spectroscopy (DCS) emerged a decade ago as a powerful tool for gas spectroscopy and metrology. DCS is based on two optical frequency combs (OFCs) with slightly different repetition rates. Using DCS, one can simultaneously obtain amplitude and phase of the light, resulting in the direct determination of complex refractive index. Thus, DCS promises for investigating the solid state materials. Here, we demonstrate an application of measuring the group velocity dispersion (GVD) of single-mode fiber (SMF) by using DCS. We constructed two Er-fiber-based OFCs and achieved the fast locking of the beat note by using PZT module based on Ref. [1]. The beat note was phase locked with the servo bandwidth of over 100 kHz and the integrated phase noise as 0.21 rad and we realized the DCS system. By using this system, we obtained a wavelength-dependent GVD of SMF and the GVD as -22.0 ps^2/km at 1550 nm with the standard deviation of 0.02 ps^2/km. It agrees well with the nominal value of the GVD. Thus, we conclude that our DCS works as a brilliant tool for solid state physics. 
Reference 

*Research Grant of Keio Leading-edge Laboratory of Science & Technology JSPS KAKENHI Grant Number JP18H02040.

C71.00156: Heavy Mediator at Quantum Dot/Graphene Heterojunction for Efficient Charge Carrier Transfer to Enhance the Performance of the Optoelectronic Devices*  
RAPTI GHOSH (Presenter), Academia Sinica — The two-dimensional mediator with heavy effective mass possesses a large density of states that can be inserted at the two-dimensional heterostructure interface. In general, the 2D heterostructure interfaces suffer from enhanced depletion region which deteriorates the charge carrier transfer efficiency and hence the device performance. The insertion of the mediator reduces the depletion region and form type–II band alignment which speeds up the carrier dissociation efficiency and hence eventually enhances the carrier transfer phenomena. 2D ReS_2 as a mediator has been employed at the heterojunction of graphene and perovskite quantum dots which results in enhancing photosensitivity (> 10^7 A/W). Moreover, the device can withstand 100% longitudinal strain making it ideal for the future wearable optoelectronic device industry^1.
Reference:

*Financial support: Higher Education Sprout Project by the Ministry of Education (107L9006) and the Ministry of Science and Technology in Taiwan (MOST 107-3017-F-002- 001).
C71.00157: Nonlinear Refractive Index Measurement of E-beam Evaporation Ta$_2$O$_5$ film*

TE-KENG WANG (Presenter), CHAO-HONG LIN, JIA-WEI LIU, FU-YAN YAN, HAN-TING HOU, Sun Yat-sen University, MIN-HSIUNG SHIH, Research Center for Applied Sciences, CHAO-KUEI LEE, Sun Yat-sen University — Tantalum pentoxide(Ta$_2$O$_5$) has been realized as a promising material for waveguide due to its great linear optical properties, such as high refractive index, large bandgap and so on. Recently, the nature of athermal property and high nonlinear refractive coefficient exhibit its potential for Si photonics application. In this work, using e-gun deposition growth Ta$_2$O$_5$ thin film, high quality micro-ring resonator was fabricated. The propagation loss as low as 0.3/cm was characterized from the transmission spectrum. Additionally, the nonlinear refractive coefficient (n$_2$) was investigated by using all optical modulation technique. The n$_2$ of 1.42 x 10$^{-14}$ cm$^2$/W was estimated. Compared to the conventional materials for Si photonics, such as Si$_3$N$_4$, SiO$_2$ and so on, the larger n$_2$ value reveal the value for application.

*MOST108-2218-E-110-011-

C71.00158: Investigation of the Resistive Switching Mechanism in Li$_x$NbO$_2$ Memristors*

SEBASTIAN HOWARD (Presenter), LOUIS F. J. PIPER, MATTHEW J. WAHILA, CHRISTOPHER SINGH, WEI-CHENG LEE, Binghamton University, TIMOTHY M. MCCORNE, WILLIAM A. DOOLITTLE, ALEX WEIDENBACH, Georgia Institute of Technology, GALO J. PAEZ, Binghampton University — A complete understanding of the origin of resistive switching in memristors is necessary for implementation into neuromorphic computing applications. However, the resistive switching of memristors is typically attributed to a complex combination of processes (e.g., redox reactions, ionic transport, phase changes, etc.) post an electroforming step, which limits tunability and scalability of the device. Li$_x$NbO$_2$ analog memristors circumvent the electroforming step and demonstrate a promising new mechanism wherein the diffusion of Li$^+$ ions enables precise control of the resistive states [1]. Here we utilize synchotron-based x-ray spectroscopy techniques to examine the electronic strucure of Li$_x$NbO$_2$ memristors. We employ x-ray absorption spectroscopy (XAS) across the active to observe variations in the Li content. Additionally, we investigate the origin of non-volatility by probing the buried interface at the metal contacts via hard x-ray photoelectron spectroscopy (HAXPES). This work opens a new avenue of methodology for illuminating resistive switching mechanisms in memristors from a fundamental perspective.


*This material is based on the work supported by the Air Force Office of Scientific Research under Award No. FA9550–18–1–0024.
C71.00159: Tunable Dirac points and zero-energy modes in periodic curved graphene superlattices* JIANLI LUAN, SHANGYANG LI, TIAXING MA (Presenter), Beijing Normal Univ, LIGANG WANG, Zhejiang University, HAI-QING LIN, Beijing Computational Science Research Center — We combined periodic ripples and electrostatic potentials to form curved graphene superlattices and studied the effects of space-dependent Fermi velocity induced from curvature on their electronic properties. With equal periods and symmetric potentials, the Dirac points do not move, but their locations shift under asymmetric potentials. This shift can be tuned by curvature and potentials. Tunable extra gaps in band structures can appear with unequal periods. The existence of new Dirac points is proposed, such that these new Dirac points can appear under smaller potentials with curvature, and their locations can be changed even under a fixed potential by adjusting the curvature. Our results suggest that curvature provides a new possible dimension to tune the electronic properties in graphene superlattices and a platform to more easily study physics near new Dirac points.

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C71.00160: On degradation and reliability testing GaN High-electron-mobility transistor (HEMT) PARVEEN KUMAR (Presenter), University of California, Merced — Gallium nitride (GaN) based high electron mobility transistors (HEMTs) have shown a lot of promise in high voltage, high power, and high radiation applications. However, the full realization of the III-nitride potential and large-scale adoption of this technology has been hindered by the existence of electrically active defects that manifest as deep levels in the energy bandgap. These deep levels can potentially act as charge trapping centers limiting device performance and long-term reliability. It is therefore imperative to monitor these traps in operational GaN HEMTs as close as possible to their real-world operational conditions. With that goal in mind, in this work, a suite of advanced thermal and optical-based trap spectroscopy methods and models are reported and expanded upon to directly probe and track traps in three-terminal operational of GaN HEMTs.
C71.00161: Stress/Strain Effects on Phonon Modes and Phonon Deformation Potentials in Monoclinic $\beta$-Ga$_2$O$_3$  
RAFAŁ KORLACKI (Presenter), MATHIAS SCHUBERT, University of Nebraska - Lincoln, ALYSSA MOCK, Naval Research Laboratory, SEAN KNIGHT, University of Nebraska - Lincoln, VANYA DARAKCHIEVA, Linköping University — Strain-induced shifts of phonon energies provide a powerful tool for modeling strain patterns in heterostructures and thin films. In the case $\beta$-Ga$_2$O$_3$, an emerging wide-bandgap semiconducting oxide, the low symmetry of its monoclinic structure is responsible for the high anisotropy and unusual ordering of phonon modes, while the effects of stress and strain on the phonon properties in general are not yet well understood. We present a rigorous, symmetry-based analysis on how the frequencies of optical phonon modes depend on the components of stress and strain tensors in monoclinic crystals, and we confront it with the results of density functional theory (DFT) calculations involving several distinct deformation scenarios, and the resulting shifts in phonon mode frequencies for $\beta$-Ga$_2$O$_3$. We derive sets of phonon deformation potential parameters for all phonon modes, including infrared-active ($A_u$ and $B_u$) and Raman-active ($A_g$ and $B_g$) modes. Additionally, we discuss how stress affects the order of phonon modes with $B_u$ symmetry.

C71.00162: Thermal and Magnetic Properties of Landau–Quantized Group VI Dichalcogenide Carriers in the Approach to the Degenerate Limit  
N J HORING (Presenter), Department of Physics, Stevens Institute of Technology, Hoboken, NJ 07030, USA, JAY D MANCINI, Department of Physical Sciences, Kingsborough College, CUNY, Brooklyn, New York 11235 — This work is concerned with determination of the thermal and magnetic behavior of the Group VI Dichalcogenides in a quantizing magnetic field. Our analysis treats the principal statistical thermodynamic functions (grand partition function and the ordinary partition function, as well as the grand potential, Helmholtz free energy and the entropy), providing the basis for calculation of the specific heat: Their dependencies on temperature and magnetic field strength are carefully examined, particularly in the degenerate regime and the approach to zero temperature. The joint dependence on magnetic field and temperature is also determined for the Dichalcogenide magnetic moment in the degenerate statistical regime, replete with de Haas–van Alphen oscillatory phenomenology and also above the zero–temperature limit.

C71.00163: Effect of electric potential fluctuations in Coulomb drag in double layer graphene systems  
RYAN A. BOGUCKI (Presenter), BEN HU, Department of Physics, Univ of Akron — We study theoretically the drag transresistivity in a graphene double layer system exhibiting electric potential fluctuations. The fluctuations are modelled as sinusoidal oscillations in the first layer, which induces a sinusoidal variation in the electron density in that layer, which in turn induces an electron density oscillation in the second layer. We calculate the drag resistivity as a function of average charge densities in each layer for various amplitudes of the electric potential fluctuations. Recent experiments have found that the drag transresistivity in graphene double layers systems exhibit a sign change when one layer is held at the charge neutrality point, and the average density of the electrons in the other layer is varied through the charge neutrality point. Our simple model is able to qualitatively reproduce these experimental results. We discuss extensions of the model which characterize more realistically the electric potential fluctuations that are caused by the presence of charge density impurities near the graphene layers.
**C71.00164: Thermal expansion coefficients of high thermal conducting BAs and BP materials**  
SHENG LI (Presenter), University of Texas at Dallas, KEITH TADDEI, Oak Ridge National Laboratory, XIQU WANG, University of Houston, HANLIN WU, University of Texas at Dallas, JOERG C. NEUEFEIND, Oak Ridge National Laboratory, DAVIS ZACKARIA, XIAOYUAN LIU, University of Texas at Dallas, CLARINA RELOJ DELA CRUZ, Oak Ridge National Laboratory, BING LV, University of Texas at Dallas — Recently reported very high thermal conductivities in cubic boron arsenide (BAs) and boron phosphide (BP) crystals could potentially provide a revolutionary solution in the thermal management of high power density devices. To fully facilitate such an application, the compatible coefficient of thermal expansion (CTE) between the heat spreader and the device substrate, in order to minimize the thermal stress, needs to be considered. Here, we report our experimental CTE studies of BAs and BP in the temperature range from 100 K to 1150 K, through a combination of X-ray single crystal diffraction and neutron powder diffraction. We demonstrated that the room temperature CTEs, $3.6 \pm 0.15 \times 10^{-6}/K$ for BAs and $3.2 \pm 0.2 \times 10^{-6}/K$ for BP, are more compatible with most of the semiconductors including Si and GaAs, in comparison with diamond, and thus could be better candidates for the future heat spreader materials in power electronic devices.

**C71.00165: OUTREACH AND ENGAGING THE PUBLIC** —

**C71.00166: Dying Fundamental Physics and Rising Digital Era of Engineering**  
PRITAM MANDAL (Presenter), Durgapur Women's College — From a study based on personal teaching experiences and one-to-one and in-group interaction with a large number of students (9th to 12th Grade and UG levels), teachers, research scholars and lab-experts across India, we found that most of the students in the science stream no longer “view” Physics as a branch of science to study the nature, rather Physics for them is a giant toolbox to design more sophisticated devices and medicines for “social use”. To most of them, knowing physics means becoming smarter at handling electricity, electronic gadgets, computers, smart-phones and apps. Most of the science students were found not driven to learn physics as a way to understanding and relishing the hidden deeper beauty of nature; for them the new wonderland is the “on-line” world. Given the trend in students’ attitude towards physics in current time, theoretical physics might severely suffer in near future. In this talk, I discuss the issues we found and the possible course of action to better cement the foundation of tomorrow’s fundamental physics.

**C71.00167: WITHDRAWN ABSTRACT** —

**C71.00168: PUBLIC POLICY** —
Research Integrity, the Responsible Conduct of Research, and Plagiarism Analysis
AARON MANKA (Presenter), National Science Foundation — Among its duties, the National Science Foundation (NSF) Office of Inspector General (OIG) is responsible for helping ensure the integrity of research programs at NSF. We investigate allegations of research misconduct (plagiarism, falsification, and fabrication) in NSF proposals and awards. We also handle allegations conflict of interests and violations of the confidentiality of NSF’s merit review to ensure the integrity of that process. We completed a review of how grantees implemented NSF’s requirement to provide responsible conduct of research training to undergraduate students, graduate students, and postdoctoral researchers. We have analyzed our plagiarism cases of the past decade to accumulate data and potentially identify institutional strategies for preventing and reducing plagiarism. We are also reviewing grants for characteristics of serial spending. I will briefly discuss these topics and present our results.

ENERGY RESEARCH AND APPLICATIONS —

Perovskite Electronic Ratchet for Energy Harvesting
JI HAO (Presenter), HAIPENG LU, JEFFREY L BLACKBURN, ANDREW FERGUSON, National Renewable Energy Laboratory — Hybrid organic-inorganic perovskite semiconductors (HOIS) have demonstrated great potential as absorbers in thin-film solar cells, but recently there is emerging research demonstrating their application as the electronic materials in transistors, diode, and optoelectronic devices due to their unique mixed ionic-electronic properties. Here we demonstrate a novel energy harvesting application based on both ionic and electronic transport in HOIS — Perovskite electronic ratchets. The electronic ratchet is a new type of energy harvesting device that can convert (rectify) a non-directional electrical signal into stable direct current through an asymmetric potential distribution across the device (i.e., the device acts as a charge pump). Here we demonstrate the first lead-halide perovskite electronic ratchet by manipulating the ion distribution within a transistor channel to realize an asymmetric potential distribution in the perovskite device. This asymmetric potential distribution allows the perovskite ratchet device to convert both electronic noise and unbiased, periodic alternating potentials into stable direct current. Such devices have the potential for providing low-voltage power in remote and portable applications.
**C71.00172: Ferrofluid-Based Generator Harvesting Waste Heat and Ambient Vibration**

XUEWEI ZHANG (Presenter), Texas A&M University, Kingsville — Ferrofluid is a stable colloidal suspension of permanently magnetized nanoparticles, in which Brownian motion keeps the nanoparticles from settling under gravity, and a surfactant is placed around each particle to provide short-range steric repulsion between particles to prevent particle agglomeration. Since magnetic field device has no limitations analogous to electrical breakdown in its electric field counterpart, ferrofluids have become an excellent choice for micro/nanoelectromechanical systems technology. On the other hand, ferrofluids have applications in the cooling of electronic devices, which has led to several designs of power generators using waste heat. In this work, we study a new version of ferrofluid generators harvesting both heat and vibration energy. A theoretical model based on fundamental physics principles is developed to evaluate the system's energy conversion efficiency (the ratio of generated power and the heat input). Further, we discuss the dependence of the output power on various design parameters (including the scale of the system) and methods to enhance the performance of the ferrofluid generator for potential aerospace applications.

**C71.00173: Thermoelectric properties of As-based 1111-Zintl compounds La\(_{1-x}\)Sr\(_x\)(Zn,Cd)AsO**

YUSUKE KIMURA (Presenter), National Institute of Advanced Industrial Science and Technology, Tokyo University of Science, KUNIHIRO KIHOU, HIROTAKA NISHIATE, National Institute of Advanced Industrial Science and Technology, HIDETOMO USUI, Shimane University, YUTO TOKUNAGA, Osaka University, TSUTOMU IIDA, Tokyo University of Science, KAZUHIKO KUROKI, Osaka University, CHUL-HO LEE, National Institute of Advanced Industrial Science and Technology, Tokyo University of Science — 1111-system with the ZrCuSiAs-type structure has attracted great attention not only as the high-Tc superconductors but the high-performance thermoelectric compounds. The highest ZT in 1111-system was found in BiCuSeO with the value of ZT to be 1.4 at 923 K [1], demonstrating the high potential of the 1111-system as thermoelectric compounds. Previously, we found that LaFeAsO\(_{1-y}\) exhibits large power factor with values of PF = 4.1 mW/mK\(^2\) at T = 75 K [2], demonstrating that As-based 1111-system can also be a candidate.

In this study, we focused on LaZnAsO and LaCdAsO (space group: P4 / nmm) compounds. Hole carriers were induced by Sr doping. Polycrystalline samples were synthesized by the solid reaction method. High dense samples were obtained by hot-press. As results, peak of the power factor of LaZnAsO was shift to high temperature comparing with LaFeAsO\(_{1-y}\), achieving the value of 0.118 mW/mK\(^2\) at T=747 K. Details of sample preparation as well as thermoelectric properties will be discussed in the conference.

C71.00174: Understanding pressure-driven thermoelectric properties of PdP$_2$ and PdAs$_2$ nanowires via band engineering

PRABAL BHUYAN (Presenter), Department of Physics, Gujarat University, Ahmedabad, India, YOGESH SONVANE, Department of Applied Physics, Sardar Vallabhbhai National Institute of Technology, Surat, India, P. N. GAJJAR, Department of Physics, Gujarat University, Ahmedabad, India, RAJEEV AHUJA, Ångströmlaboratoriet, Department of Physics, Uppsala University, Uppsala, Sweden, SANJEEV K. GUPTA, Department of Physics, St. Xavier's College, Ahmedabad, India — In the race of searching for alternative clean and sustainable energy sources, thermoelectric materials have shown potential hope by converting low-grade waste heat into electricity. The efficiency of thermoelectric devices is characterized by power factor or ZT. Therefore, enhancing ZT in nanowires for the thermoelectric application is highly desired. In recent work, we propose semi-metallic nanowire with asymmetry density of states near the Fermi energy as an alternative class of thermoelectric materials. We have considered the pentagonal structure of PdP$_2$ and PdAs$_2$ nanowires (NWs) and confirmed its dynamical stability by the phonon dispersion study. The PdX$_2$ structure shows the transition from semiconducting to semi-metallic behaviour at a compressive strain of 8% within sustainable pressure of 0.2~0.3GPa. The semi-metallic behaviour with the asymmetric density of states near the Fermi energy boosts Seebeck co-efficient value and therefore, ZT$_e$ value is enhanced for both the nanowires. Our study stimulates both nanowire synthetization feasibility and thermoelectric applications for the conversion of waste heat into electricity.

*We would like to thank Science and Engineering Research Board (SERB), India for providing high computing system (Grant no.: YSS/2015/001269).
C71.00175: Optimized Efficiency of a stochastically driven quantum dot Heat Engine*

MULUGETA BEKELE (Presenter), Addis Ababa Univ — We take a stochastically driven single level quantum dot embedded between two metallic leads at different temperatures which works as a heat engine. We analytically study the optimized efficiency that lies between the maximum efficiency and minimum efficiencies. The minimum efficiency either takes the efficiency value at maximum power or the lowest possible value which is zero. We study the optimized efficiency of a quantum dot heat engine according to the optimization criteria, to find their corresponding optimized quantities in an external magnetic field (stochastic driving force). Accordingly, we found 1) efficiency-wise optimized efficiency is better than efficiency at maximum power; 2) power-wise, the optimized power is smaller than its value at maximum power by 35% and 3) period-wise, is performs the task in a cycle twice that of the period at maximum power. We study the overall performance of the heat engine by introducing a figure of merit that takes into account the contribution of each of the above quantities as a function of Carnot efficiency. Based on the proposed figure of merit, the model shows that the 1st optimization criteria is 3 times better than the 2nd optimization criteria as a function of $\eta_C$.

*ISP Uppsala University, Uppsala, Sweden for the financial support.

C71.00176: Thermoelectric Properties of Solvothermal Grown Bismuth Telluride-Carbon Nanomaterials Composites

DANIEL CHOI (Presenter), National Research Council, KARIMA PERRY, CCDC Army Research Laboratory, PATRICK TAYLOR, CCDC Adlphi Laboratory Center, EVGENIYA LOCK, United States Naval Research Laboratory, SHASHI P KARNA, CCDC Army Research Laboratory — Current state of the art portable power source faces problems such as low-life, high production cost and weight penalty. As such, thermoelectric (TE) power generation and cooling have been considered as an alternative as low-cost, more efficient, environmentally responsible approach. One of more promising TE material of interest are alloys based on bismuth telluride ($\text{Bi}_2\text{Te}_3$) and thus much efforts have been made to improve TE properties by (1) reducing the materials’ dimension to nanoscale, and (2) incorporating other nanostructures such as graphene, to enhance electrical properties and thermal conductivity. This geometry offers a natural architecture for thermoelectric devices due to reduced thermal transport and enhanced electronic tunneling at the nanomaterial interfaces. Building upon this mechanism, we present thermoelectric properties of $\text{Bi}_2\text{Te}_3$ compositied with various carbon nanostructures. Our TE materials are synthesized via solvothermal method resulting in uniformly dispersed nanoplates interfaced with 1D and 2D carbon nanostructures. Our results not only show change in thermoelectric properties of $\text{Bi}_2\text{Te}_3$ upon incorporation of carbon nanostructures, but provide characterization of Bi2Te3-nanomaterial interface for development of next-gen, low power, portable power source.
C71.00177: Defects and band positions in the p-type transparent conductor CuI  ANDREA CROVETTO (Presenter), SERGIU LEVCENKO, HANNES HEMPEL, MARIN RUSU, THOMAS UNOLD, Helmholtz-Zentrum Berlin — While high-performance n-type transparent conductive materials (TCMs) have existed for decades, heavy p-type doping of wide band-gap materials has proven much more challenging. The simple cubic compound CuI was recently rediscovered for this application and is currently the p-type TCM with the highest figure of merit. However, the native defects responsible for p-type conductivity in CuI, as well as compensating defects limiting the maximum achievable doping levels, have not yet been identified experimentally. Furthermore, there is disagreement in the literature on the work function and absolute band positions of CuI relative to vacuum. In this experimental study, we employ temperature- and intensity-dependent photoluminescence to draw new conclusions on the defect landscape of CuI. We then employ a combined photoemission spectroscopy-Kelvin probe system to show that the measured band positions depend critically on surface phenomena. Finally, we demonstrate that terahertz spectroscopy is an ideal tool for characterizing the electrical properties of CuI reliably and non-destructively.

C71.00178: Computational Screening and Designing High-performance Solid Sorbents for CO₂ Capture Technology  YUHUA DUAN (Presenter), Natl Energy Technology Lab — CO₂ is one of the major combustion products which once released into the air can contribute to global climate change. Solid sorbents have been reported to be promising candidates for CO₂ sorbents due to their high CO₂ absorption capacities. With ab initio thermodynamic calculations, we proposed a theoretical screening methodology to identify the most promising CO₂ sorbent candidates from vast array of possible solid materials. The advantage of this method is that it identifies the thermodynamic properties of the CO₂ capture reaction as a function of temperature and pressure without any experimental input beyond crystallographic structural information of the solid phases involved. According to the requirements imposed by the pre- and post- combustion technologies and based on our calculated thermodynamic properties for the CO₂ capture reactions by the solids of interest, we were able to identify only those solid materials for which lower capture energy costs are expected at the desired pressure and temperature conditions. In addition, through investigating several mixed sorbent materials, we demonstrate that by mixing/doping different types of solids it’s possible for a sorbent to shift its turnover temperature to the range of practical operating conditions.
C71.00179: Improved optoelectronic properties in CdSe\textsubscript{x}Te\textsubscript{1-x} through controlled composition and short-range order* BISHAL DUMRE (Presenter), NATHAN J SZYMANSKI, VIJAYA ADHIKARI, INDIRAS KHATRI, Department of Physics and Astronomy, The University of Toledo, DANIEL GALL, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, SANJAY V. KHARE, Department of Physics and Astronomy, The University of Toledo — We employ first principles methods based on density functional theory and beyond to study CdSe\textsubscript{x}Te\textsubscript{1-x} alloys in the zincblende and wurtzite structures. From the cluster expansion formalism, we provide phase diagram showing consolute temperature of 325 K where zincblende-to-wurtzite phase boundary is found for Se concentrations of \( x = 0.5-0.6 \) owing to increasing ionic character of the Cd-anion bonds. Disordered CdSe\textsubscript{x}Te\textsubscript{1-x} configurations are modeled using special quasirandom structures, for which optoelectronic properties are computed with the hybrid HSE06 functional. Downward bowing in the band gap and effective hole mass of the zincblende structure is highlighted for its potential benefits in photovoltaics through increased net photocurrent. Absorption coefficient and reflectivity are also reported, showing promising results in zincblende CdSe\textsubscript{x}Te\textsubscript{1-x} as indicated by substantial optical absorption throughout all Se concentrations. Lastly, we identify the presence of short-range order in CdSe\textsubscript{x}Te\textsubscript{1-x} characterized by clustering among like atoms in order to minimize strain. The degree of clustering, which may be tuned by temperature, also controls the magnitude of the band gap.

*National Science Foundation, Air Force Research Laboratory and Ohio Supercomputer Center

C71.00180: A Multidimensional Approach to Structural Transformation Through Functionalization of Tellurene* GRACIE CHANEY (Presenter), DANIEL WINES, FATIH ERSAN, JARON KROPP, CAN ATACA, Univ of Maryland-Baltimore County — Two dimensional (2D) Tellurene (Te) structures have recently been synthesized, and have been shown to possess high mobility and stability. Using density functional theory (DFT) and molecular dynamics (MD), we investigated the stability and electronic structure of 2D, and phase sheets, and their hydrogen, oxygen, and fluorine functionalized counterparts. Our calculations show that bare - and -Te sheets are stable and have band gaps of 0.44 eV and 1.02 eV respectively. We see that H, O and F destabilize -Te; F and H cause -Te layers to separate into functionalized atomic chains; and O causes -Te to totally transform into a Te\textsubscript{3}O\textsubscript{2}-like structure. Also, we studied the coverage effects of different concentrations of H and O on and \( \beta \)-Te and found that the full coverage case results in the highest binding energy and stability for both adatoms. Finally, we examined the stability and binding nature of functionalized \( \beta \)-Te on a GaSe substrate. We noted that having O and H impurities not only enhances the stability of Te layer, but also results in a strong binding energy on GaSe substrate. Our results indicate that Tellurene monolayers and functionalized counterparts are suitable for future optoelectronic devices and as metallic contacts in nanoscale junctions.

*NSF DMR-1726213
C71.00181: Investigation of Au(111)/Li$_3$PO$_4$ Interface Structures using Neural Network Potential

KOJI SHIMIZU (Presenter), WEI LIU, Department of Materials Engineering, The University of Tokyo, WENWEN LI, YASUNOBU ANDO, National Institute of Advanced Industrial Science and Technology, EMI MINAMITANI, Institute for Molecular Science, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo — Recently, the construction of interatomic potentials using first-principles calculation data and machine-learning technique has been widely tried because of higher reliability and low computational costs. In the present study, we have tried to construct the four-element neural network potential (NNP) [1,2] to investigate the Au(111)/Li$_3$PO$_4$ interface system, where the understanding of the interface structures and Li-ion distribution near the interface is of significance for the development of all-solid state Li-ion batteries and novel memory devices [3]. Using the constructed NNP, we then performed structure optimization with a large interface model of Au(111)/Li$_3$PO$_4$. In the meeting, we will discuss the calculated interface structures and the Li defect formation energies.


*This work was supported in part by CREST-JST, JSPS KAKENHI (15H03561), MI$^2$I project of the Support Program for Starting Up Innovation Hub from JST.

C71.00182: Strong interplay between Na- and O-related defects in Cu-based chalcogenides

KOSTIANTYN SOPIHA (Presenter), Ångström Solar Center, Division of Solid State Electronics, Uppsala University, SIGBJØRN GRINI, Department of Physics/Centre for Materials Science and Nanotechnology, University of Oslo, CHARLOTTE PLATZER-BJÖRKMAN, Ångström Solar Center, Division of Solid State Electronics, Uppsala University, LASSE VINES, CLAS PERSSON, Department of Physics/Centre for Materials Science and Nanotechnology, University of Oslo — Recent advances in thin-film photovoltaics became possible by controlling the incorporation of impurities. The most notable among them are alkalis in-diffusing from soda-lime glass and oxygen incorporating from various sources during the baseline processing. Herein, we investigate the interaction between Na and O in co-sputtered Cu$_2$ZnSnS$_4$(CZTS) by combining theoretical and experimental techniques. First, using secondary ion mass spectrometry (SIMS), we demonstrate that Na and O distributions in the absorber are correlated. Then, employing first-principles methods, we show that the correlation is driven by a strong ionic Na-O bonding that triggers the formation of NaO and Na$_2$O complexes. The remarkably high binding energies for these complexes are proven to cause Na-O clustering at all temperatures of the baseline processing. Hence, the overall character of the impurity profiles is explained through O immobilizing Na by forming the defect complexes and leading to the Na accumulation near the CZTS surface. This defect interplay paves the way for a more accurate impurity control needed for fabricating high-performance devices.


*This work is supported by SSF #RMA15-0030 and RCN #243642.
Energetic and vibrational properties of carbon monoxide adsorption on platinum nanoparticles under applied voltage*  

CIERRA CHANDLER (Presenter), ISMAILA DABO, Material Science and Engineering, Pennsylvania State University — Carbon monoxide poisoning is a significant limitation to the performance of platinum-based transition metals. Manipulating the size of the catalytic particles could help inhibit carbon monoxide adsorption and increase the life cycle of the catalyst. This study models the energetic and vibrational properties of carbon monoxide on platinum nanoparticles under applied voltage using the self-consistent continuum solvation (SCCS) model. We determine adsorption patterns as the function of nanoparticle size and site coordination. It is found that the local surface charge strongly affects carbon monoxide adsorption particularly along the (111) and (001) facets of the nanoparticle. These results could prove useful in optimizing electrocatalytic systems such as proton exchange membrane (PEM) fuel cells where trace amounts of carbon monoxide in the hydrogen fuel can poison the nanostructured platinum electrodes and decrease the durability of the fuel cell.

*The authors acknowledge financial support from the U.S. Department of Energy, Office of Science,Basic Energy Sciences, CPIMS Program, under Award No. DE-SC0018646.

Evanescent field polarization for giant chiroptical modulation from achiral gold half-rings: Theoretical insight from simulations  

LUCA BURSI (Presenter), Department of Physics and Astronomy, Rice University, LAUREN A. MCCARTHY, KYLE W. SMITH, Department of Chemistry, Rice University, ALESSANDRO ALABASTRI, Department of ECE, Rice University, PETER J. NORDLANDER, Department of Physics and Astronomy, Rice University, STEPHAN LINK, Department of Chemistry, Rice University — Metal nanoantennas have been under intense investigation due to their strong light−matter interactions and significant polarization sensitivities determined by their nanostructure. For applications seeking to realize on-chip polarization-discriminating nanoantennas, efficient energy conversion from surface waves to far-field radiation is desirable. However, the response of individual nanoantennas to the particular polarization states achievable in surface waves, such as evanescent fields, has not yet been thoroughly studied. Here, we report the giant modulation of the visible light scattering predicted from gold half-ring, pinwheel, and other nanoantennas excited through total internal reflection of left- and right-handed circularly polarized light, by exploiting the distinct polarization properties of surface evanescent waves [ACS Nano, 12, 11657 (2018)]. This result provides a fundamentally different mechanism for chiroptical responses requiring a phase delay between transverse and longitudinal electric field oscillations, not found in free-space light. Specifically, we focus on the insight provided by theory, and in particular by the electromagnetic simulations, performed with COMSOL Multiphysics software, of the systems of interest and aspects of their chiroptical response.

WITHDRAWN ABSTRACT
C71.00186: Free Energy Landscape of Sodium Solvation into Graphite  ALI KACHMAR
(Presenter), QEERI, Hamad Bin Khalifa University, WILLIAM ANDREW GODDARD, Division of Chemistry and Chemical Engineering, Caltech — Sodium Ion Batteries (SIBs) are the most cost-effective alternative to current generation lithium ion batteries (LIBs), $^{[1,2]}$ but Na is known to deliver very low energy capacity for sodium intercalation compared to Lithium. We report here first principles moleculars dynamics aided by metadynamics $^{[3]}$ to obtain the free energy landscape including changes in the electronic coupling as a sodium ion in Dimethyl sulfoxide solvent intercalates into graphite, the first step in understanding how the local environment affects the free energy of solvation. We analyze the free energy landscape for all the possible sodium solvation scenarios, while quantifying their free energy barriers. Our simulations indicate that solvent plays an important role in stabilizing the sodium intercalation into graphite through shielding of the sodium while modulating the interaction of the solvent with the graphite sheets $^{[4]}$.

References

3. CP2K version 2.6.2 (Development Version), CP2K is freely available from http://www.cp2k.org

C71.00187: Catalytic growth of N-doped Multi-Layer Graphene/Carbon Composites for Supercapacitor Applications*  AYUSH BHARDWAJ (Presenter), ALEXANDER RIBBE, JAMES J WATKINS, Univ of Mass - Amherst — Multi-layer graphene (MLG) composites are excellent candidates for supercapacitor applications, but current approaches to device fabrication and the cost to produce graphene poses challenges for commercialization. Here, we use iron nitrate nonahydrate as a catalyst for the growth of graphene, melamine formaldehyde resin as a solid carbon source, and Pluronic F127 surfactant as a sacrificial porogen to enhance porosity and surface area. The MLG composites are produced via thermal carbonization. The resulting composites exhibit high surface area (2200 m$^2$/g) and significant nitrogen doping (4-5%), yielding specific capacitance values as high as 300 F/g at 0.5 A/g. The role of temperature and coordination between functional group of the carbon precursor & metal source has been investigated to understand MLG formation.

*We acknowledge The Center for Hierarchical Manufacturing (CHM) and NSF for the support.
C71.00188: Determination of the Enthalpy of Adsorption of Hydrogen in Activated Carbon at Room Temperature*  ERNEST KNIGHT (Presenter), ANDREW K GILLESPIE, MATTHEW JOHNSON PROSNIEWSKI, DAVID STALLA, ELMAR DOHNKE, TYLER RASH, PETER PFEIFER, CARLOS WEXLER, Univ of Missouri - Columbia — A very important quantity for adsorption performance is the enthalpy of adsorption $\Delta H$. The determination of $\Delta H$ for weakly adsorbing gases (e.g., $H_2$) in carbonaceous porous materials is difficult, normally requiring measuring adsorption isotherms at two cryogenic temperatures and calculation of $\Delta H$ using Clausius-Clapeyron's (CC) equation. Here we demonstrate a calculation of $\Delta H$ based on ca. room temperature isotherms at 273K, 296K. CC requires absolute isotherms; however, excess adsorption is measured; conversion between these requires the adsorbed film volume. We show that the film volume can be estimated by fitting the excess adsorption with an Ono-Kondo model and the auxiliary use of a fixed point corresponding to the saturation film density (estimated 100±20 g/L) which seems to be remarkably sample- and temperature-independent, i.e., an adsorbate property. We find that for high-quality porous carbons the film volumes are ~40%, ~12% of the total pore volume at 77K, 296K, respectively. Using these, we calculate $\Delta H = 8.3±0.4$ kJ/mol at room temperature, an excellent agreement with the low-coverage cryogenic determination. The methodology proposed facilitates reliable calculations of the $\Delta H$ at room temperatures for weakly-adsorbing gases.

*DOE-EERE DE-FG36-08G018142

C71.00189: Thermal conductivity of hydrogen sorbent materials for onboard storage applications  NOEMI LEICK (Presenter), ROBERT BELL, National Renewable Energy Laboratory, TROY ALLEN SEMELSBERGER, Los Alamos National Laboratory, BRANDON BARNETT, JEFFREY R LONG, Lawrence Berkeley National Laboratory, PHILIP ANTHONY PARILLA, National Renewable Energy Laboratory, THOMAS GENNETT, Colorado School of Mines, Chemistry, National Renewable Energy Laboratory — Measuring the thermal conductivity (TC) of $H_2$-physisorption storage materials under system conditions are critical in designing the most practical onboard $H_2$ storage vessels. Furthermore, knowing the TC helps understanding how the heat associated with the sorption/desorption of $H_2$ is distributed throughout the storage material. In this work, we will show that the thermal properties of the powder materials can differ significantly from those of the bulk materials as heat transfer within a powder mainly occurs via: a) conduction through the solid particles and the gas within the interstices; and b) convection through the gas. To this end, we measured the TC on pellets of MOF-5 and powder Cu-MFU-4I with our state-of-the-art TC apparatus. We studied the behavior under He and $H_2$ pressures ranging from 0.03 - 80 bar, at temperatures ranging from 40 K - 380 K, and for different degrees of powder compaction. We will discuss that we measure an effective thermal conductivity that depends on the TC of the powder particles, on the powder compaction, the TC of the surrounding gas, the number of binding sites occupied, and the possible expansion or contraction of sorbents during the gas sorption/desorption which in turn all depend on temperature and pressure.
C71.00190: Thermal and Spectroscopic (IR, NMR) Studies of Ammonia Borane-Polyethylene Oxide Hydrogen Storage Composites: Effect of Catalyst*  
OZGE GUNAYDIN-SEN (Presenter), KRISHNA KHAREL, EMILY INGRAM, CAITLYN CLARK, Lamar University, RIQIANG FU, National High Magnetic Field Laboratory — Ammonia Borane (NH₃BH₃, AB) has been a potential candidate for chemical hydrogen storage due to its high hydrogen content (19.6 wt%). A downfall to the applicability of AB is its slow dehydrogenation kinetics and production of unwanted byproducts/gases. Studies show that introduction of a polymer, such as polyvinylpyrrolidone and polyacrylamide, can improve the performance of AB and decrease the release of harmful byproducts. Furthermore, catalytic additions such as, magnesium chloride (MgCl₂) and calcium chloride (CaCl₂), have proven to lower the activation energy (Eₐ), improve kinetics, and lower the hydrogen release temperature. This study explores thermal and vibrational analysis of pristine AB blended with polyethylene oxide (PEO) and individual additions of MgCl₂ and CaCl₂ as catalysts. Dehydrogenation kinetics were studied using a differential scanning calorimeter and the data was then compared with AB, bulk composites and analyzed. The results with CaCl₂ catalyst and high PEO content exhibited the most improved properties (i.e. lower Eₐ). In addition, evidence of the interactions between AB:PEO:Catalyst were given by Fourier-transform infrared and nuclear magnetic resonance spectroscopy.

*Welch Foundation (V-0004) and OUR Grant - Lamar University

C71.00191: The Impacts of Synthesis Routes and Phase-Purity on Water-Splitting Behavior in the Barium-Cerium-Manganese System  
DAN PLATTENBERGER (Presenter), ROBERT BELL, SARAH SHULDA, NICHOLAS STRANGE, PHILIP ANTHONY PARILLA, National Renewable Energy Laboratory, ANTHONY MCDANIEL, Sandia National Laboratory, MICHAEL TONEY, Stanford Linear Accelerator Laboratory, DAVID S GINLEY, National Renewable Energy Laboratory — Solar thermochemical hydrogen production (STCH) is a promising technology for solar fuels with high theoretical solar-thermal water-splitting efficiency. However, many candidate STCH oxides are complex ternary oxides, and they have the potential for secondary phase formation during synthesis and subsequent redox cycling. During synthesis, pervasive refractory impurity phases can occur, which impede the ability to develop a basic understanding of the STCH potential and complicate structural refinement of chemical expansion during isothermal reduction/oxidation. This work focuses on high phase-purity synthetic routes for known water-splitting oxides; in particular, BaCe₀.₂₅Mn₀.₇₅O₃ (BCM). These are approached by synthesizing both bulk ceramic and thin films, which are analyzed via in-operando synchrotron-based X-ray diffraction (XRD) to provide the highest quality structural refinements on BCM and other complex STCH oxides to date. The relationship between chemical shift and oxygen vacancy concentration is determined using a combination of flow-cell measurements and in-operando XRD during isothermal reduction and oxidation. In addition, key data for training computational simulations of vacancy formation and the effect of vacancies on structures is presented.
C71.00192: Frustrated Lewis Pairs with Applications in Hydrogen Storage  GLORY RUSSELL-PARKS (Presenter), BRIAN TREWYN, Colorado School of Mines, THOMAS GENNETT, National Renewable Energy Laboratory — Due to the abundance and large gravimetric energy density, hydrogen has been considered a potential source of energy.\(^1\) Major challenges with utilizing hydrogen for energy include efficient and safe storage and transportation of it. Frustrated Lewis pairs (FLPs) have recently proven their importance in hydrogen storage.\(^2\) In contrast to commonly known Lewis acid-base pairs, functionalizing the acid and base with bulky groups prevents them from binding to their counterpart causing them to be “frustrated”.\(^3\) The acid and base are held together by weak intermolecular forces without neutralization, which allows small molecules such as hydrogen to weakly bond to the Lewis acid and base in a heterolytic mechanism. FLPs as catalysts have unique characteristics including a wide range of compatible donors and acceptors.\(^2\) These attributes may assist with lowering the sorption temperature and pressure, reducing the activation energy barrier and potentially allowing for hydrogenation and dehydrogenation to occur. This work focuses on the novel synthesis and characterization of an FLP system.


C71.00193: Improving Cyclability of Metal Borohydrides for Hydrogen Storage via Non-Metallic Borohydride Additives.  ROBERT BELL (Presenter), NICHOLAS STRANGE, NOEMI LEICK, National Renewable Energy Laboratory & Colorado School of Mines, MICHAEL TONEY, SLAC Linear Accelerator Laboratory, THOMAS AUTREY, Pacific Northwest National Laboratory, THOMAS GENNETT, National Renewable Energy Laboratory & Colorado School of Mines — The theoretical ~15 wt% hydrogen content of magnesium borohydride is inaccessible for cyclical desorption/hydrogenation cycles at reasonable temperatures (<300°C) and pressures (<350 bar). However, a variety of additive compounds lower the Mg(BH\(_4\))\(_2\) hydrogen evolution temperature, changing the end state when hydrogen is released, and lowering the melting point of the system. These additives have included other metal borohydrides, metal hydrides, and organics (ether/glyme). Despite many of these additives lowering the liquidus temperature, desirable due to better mixing and higher theoretical kinetics in the melt, these systems often resulted in undesirable matrices upon re-cooling and cease to thermally cycle as expected. This work investigated an alternative family of additives, non-metallic borohydrides; a broad class of low melting point borohydrides. The temperature and hydrogen-evolution dependent phase diagram of these magnesium borohydride and non-metallic borohydride systems was investigated via calorimetry and in-situ diffraction analysis. Results of heat flow and temperature programmed desorption measurements demonstrate the improved thermal cyclability of these systems. The effect of non-metallic cation size on the behavior of these systems will be discussed in detail.
**C71.00194: Tailoring cations in a perovskite cathode for proton-conducting solid oxide fuel cells with high performance**  
MARCO FRONZI (Presenter), ICRE, Xi’an Jiaotong University, XI XU, LEI BI, Quingdao University, ENRICO TRAVERSA, University of Electronic Science and Technology of China — A rational design of a high-performance cathode for proton-conducting solid oxide fuel cells (SOFCs) is proposed in this study with the aim of improving the hydration properties of conventional perovskite cathode materials, thus leading to the development of new materials with enhanced proton migration. Herein, potassium is used to dope traditional Ba$_{0.5}$Sr$_{0.5}$Co$_{0.8}$Fe$_{0.2}$O$_{3-δ}$ (BSCF), which is demonstrated to be a beneficial way for improving hydration, both experimentally and theoretically. The theoretical study was needed to overcome practical limits that hindered direct hydrogen mobility measurements. The novel material Ba$_{0.4}$K$_{0.1}$Sr$_{0.5}$Co$_{0.8}$Fe$_{0.2}$O$_3$ d (BKSCF) shows a lower overall proton migration energy compared with that of the sample without K, suggesting that K-doping enhances proton conduction, which shows an improved performance by extending the catalytic sites to the whole cathode area. As a result, a fuel cell built with the novel BKSCF cathode shows an encouraging fuel cell performance of 441 and 1275 mW cm$^{-2}$ at 600 and 700 °C, respectively, which is significantly higher than that of the cell using the pristine BSCF cathode. This study provides a new and rational way to design a perovskite cathode for proton-conducting SOFCs with high performance.

**C71.00195: Solid-state NMR Studies of Non-Fullerene Acceptor-Based Organic Photovoltaic Active Layers**  
YAO WU, WEIGUO HU, THOMAS RUSSELL (Presenter), Univ of Mass - Amherst — The efficiency of organic photovoltaics has undergone remarkable increases in power conversion efficiencies (PCEs) recently achieving values in excess of 17% due, primarily, to the advent of non-fullerene acceptors (NFAs). To further increase PCEs, understanding and manipulating the morphology over broad range of length scales is necessary. The similarity in the chemical composition of the donors and NFAs limit current methods based on electron densities or refractive indices in discerning details of the morphology. To fill this gap we have used solid-state NMR (ssNMR) where donor and acceptor nuclei have distinct relaxation times that can be used to characterize the crystallinity, crystal size and state of mixing. Here, we present results on several donors and NFA combination where characteristics of the morphology were obtained. Donor and NFA blend film and their pristine films were studied by ssNMR. For PTB7:ITIC, the crystalline forms of ITIC show sensitive dependence on processing conditions. Furthermore, $T_1$ and $T_1ρ$ relaxation times were used to elucidate the phase separation behavior. For PM6:Y6, spin diffusion experiments based on the contrast between the $T_1ρ$ relaxation times of PM6 and Y6 are able to detect phase separation at a length scale of <15 nm.

*We thank ONR.*
C71.00196: Single-junction and Tandem Cu$_2$BaSnS$_4$ Solar Cells with a TaS$_2$ hole contact

ANDREA CROVETTO (Presenter), RASMUS NIELSEN, DTU Physics, Technical University of Denmark, ALIREZA HAJJAFARASSAR, OLE HANSEN, DTU Nanolab, Technical University of Denmark, BRIAN SEGER, IB CHORKENDORFF, PETER VESBORG, DTU Physics, Technical University of Denmark — Solar cells based on the wide band-gap Cu$_2$BaSnS$_4$ (CBTS) absorber have achieved open circuit voltages up to 1.1 V over a short development period, making CBTS an attractive material for tandem photovoltaic and photoelectrochemical cells. In this work, we explore an alternative CBTS growth route based on sulfurization of reactively sputtered oxide precursors, and we propose TaS$_2$ as an alternative back contact material. Compared to direct deposition of CBTS films from ceramic targets, reactive sputtering of oxide precursors can ultimately achieve a higher throughput and a lower cost, with the additional advantage that sulfur contamination of vacuum systems is avoided. The TaS$_2$ compound is selected as a prospective hole-selective contact due to its high work function and its metallic conductivity, which could prevent the losses associated with carrier transport across the semiconducting MoS$_2$ layer. By comparing CBTS solar cells with Mo and TaS$_2$ back contacts, the latter shows a significantly lower series resistance, resulting in a 10% relative efficiency improvement. Finally, we fabricate a proof-of-concept monolithic CBTS/Si tandem cell using a thin Ti(O,N) interlayer intended both as a diffusion barrier and as a recombination layer between the two subcells.

C71.00197: INSTRUMENTATION AND MEASUREMENT SCIENCE —

C71.00198: Development of a Surface Forces Apparatus Featuring Ultrafast Non-resonant Imaging for Measuring Contact Electrification* MATTHEW LIPPY (Presenter), ALEXANDER W BATALLER, North Carolina State University — The charging of surfaces via physical contact, known as contact electrification, is an off-equilibrium phenomenon that spans many lengthscales and can exhibit extreme energy focusing by conversion of diffuse mechanical energy into high energy x-rays. Due to the challenges of performing in-situ measurements of charge separation from buried interfaces, the fundamental mechanisms of contact electrification are still unknown. To make experimental advances in this field, we have developed a new multimodal platform that combines the angstrom precision of a surface forces apparatus with the interfacial access provided by a nonlinear optical measurement, i.e., second harmonic generation. Details of the instrument's design and operation will be presented, which will include preliminary experimental results that tests how contact electrification is affected by monolayer-levels of surface absorbents.

*This project was supported by the Julian Schwinger Foundation through grant JSF-18-09-01000.
C71.00199: Revealing signatures of topologically protected surface states with STM  AN-PING LI (Presenter), Oak Ridge National Lab — Owing to their bulk band topology, 3D topological insulators possess a massless Dirac dispersion with spin–momentum locking at the surface. The onset of a spontaneous magnetization or a broken time-reversal symmetry leads to the formation of an exchange gap in the Dirac band dispersion. In this work, we will present two salient examples to show that STM spectroscopy can be used to detect these signatures of topological surface states. The first is to measure spin–momentum-locked conduction on topological insulator Bi$_2$Te$_2$Se. A multi-probe STM with spin-polarized tips allows us to perform in situ transport measurement to differentiate surface conductance from the bulk and spin-up chemical potential from the spin-down. As a result, a spin-momentum-locked current is revealed which shows ultra-high mobility and polarization. The second is to detect topologically nontrivial magnetic states in MnBi$_2$Te$_4$. Quasi-particle interference patterns are used to probe local dispersions of both surface and bulk electronic structures. The theoretically predicted gaped surface states are evaluated with high spatial resolution. It is expected that tuning of the Fermi level in the exchange gap will result in the emergence of a quantum anomalous Hall effect.

C71.00200: Neutron Scattering at Missouri: Current Status and Future Prospects* HELMUT KAISER (Presenter), THOMAS HEITMANN, JOSEPH SCHAEPERKOETTER, PAUL MICELI, Research Reactor-MURR; Physics & Astronomy, Univ of Missouri, Columbia — The University of Missouri has been operating a nuclear research reactor for more than 50 years and thus has a long history in neutron scattering research. Currently, we have four neutron scattering instruments in service: a triple-axis spectrometer (TRIAX), an unpolarized neutron reflectometer (GANS), and two double-axis diffractometers (2XC and PSD). We will give an overview of the performance of the instruments and of the ongoing research projects. The PSD powder diffractometer has recently been upgraded with new electronics and software and with an expansion from 5 to 15 linear position sensitive He-3 detector tubes. We will illustrate the vast improvement of signal-to-background ratio and highlight ongoing research projects. Future plans to expand our suite of neutron instruments include a thermal neutron beam imaging station. We present a conceptual design and Monte Carlo calculations. The science case concerning Plant Imaging and Tomography will be discussed.

*Supported by NSF Grant No. DGE-1060091 and MURR
C71.00201: A robust software interface for a green astro-comb: remote control and automation* WILLA DWORSCHACK (Presenter), Physics and Astronomy, Lawrence University, AAKASH RAVI, Physics and Astronomy, Harvard University, DAVID PHILLIPS, Physics and Astronomy, Harvard | Smithsonian Center for Astrophysics, RONALD WALSWORDTH, Physics and Astronomy, Harvard University — Using the Doppler effect to search for exoplanets is a powerful technique. State-of-the-art spectrographs such as HARPS-N at the Italian National Telescope are the workhorse tools in such searches. Though their stability is excellent, it isn't sufficient to detect Earth-like planets around Sun-like stars due to the extremely small Doppler shifts associated with such systems (~100 kHz shifts of optical transitions). A visible wavelength, broadband 16 GHz laser frequency comb (astro-comb) can precisely calibrate spectra to resolve these Doppler shifts, but operation of this instrument requires maintenance and laser expertise. Here, we report on the successful development and implementation of a LabVIEW program that remotely operates an astro-comb and has automation features, relieving the need for on-site scientists at the Italian National Telescope on the Canary Islands and making this tool accessible to a larger community of researchers.

*Clare Boothe Luce Foundation and the Harvard Origins of Life Initiative.

C71.00202: The Structure of Degassed Water-Enabled Oil-in-Water Microemulsions* KYLE WILLIAMS (Presenter), JOSE L BANUELOS, Physical Science, University of Texas at El Paso — Most anticancer agents are hydrophobic and their use on patients often requires an oil & drug delivery vehicle. The drug delivery vehicle tends to be the primary cause of side effects in patients. Growing evidence suggests that it may be possible to mix oil in water at higher concentrations if dissolved gases are removed from water. Understanding the structure of oil/water microemulsions could shed light on mechanisms of mixing. This project uses small-angle x-ray scattering, dynamic light scattering, and turbidity measurements to assess the structure of hydrophobic molecules mixed with degassed water. Results of nanostructure as a function of alkane molecule chain length and concentration will be presented. These results will be compared to the same measurements of biocompatible fatty acids. Determining the properties that enable their miscibility with an aqueous environment will be helpful for future drug delivery.

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C71.00203: Increasing the Nanoparticle Size Detection Sensitivity of Dynamic Light Scattering using Wavelength Dependent Excitation*  
DANIEL GUZMAN (Presenter), HRISTO V IVANOV, BRYAN M AUGSTEIN, JEFFREY SIMPSON, Physics, Towson University — We report on the development of homebuilt Dynamic Light Scattering (DLS) instrumentation to measure the size of monodisperse (MD), spherical nanoparticles (NPs) of gold. HeNe and Ar-ion lasers constitute the excitation sources for the scattering experiment, while an avalanche photodiode detects the scattered light, and an autocorrelation card analyzes the resulting signal to provide a measurement of the translational diffusion coefficient, which allows for the determination of NP diameter. We characterized our instrumentation using commercially-produced gold NPs with diameters ranging from 10nm to 200nm in aqueous solution. The strong wavelength \( \lambda \) dependence of the scattered light intensity \( (1/\lambda^4) \) provides increased sensitivity for smaller excitation wavelengths. We present DLS measurements on gold NPs using excitation from both a HeNe laser \( (\lambda = 632.8\text{nm}) \) and a tunable Argon laser \( (457\text{nm} < \lambda < 515\text{nm}) \). The increased scattering from the shorter wavelengths should increase our sensitivity to smaller particles.

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C71.00204: Application of edge detection techniques to ARPES data*  
LUIS PERSAUD (Presenter), CHRISTOPHER SIMS, GYANENDRA DHAKAL, FIROZA KABIR, MD MOFAZZEL HOSEN, YANGYANG LIU, SABIN REGMI, KLAUSS DIMITRI, MADHAB NEUPANE, Univ of Central Florida — Edge detection and similar image analysis techniques are commonly used in computer vision but have not been fully realized for the purpose of ARPES data analysis. Without applying any Image analysis, the interpretation of ARPES data is left to the eyes of researchers and can be tricky and unreliable due to many sources of noise and distortion from the experimental processes, as a result, some of the finer, defining, details required to classify a material can be missed. By applying edge detection techniques, we are able to highlight key features such as distinct, clustered bands and other fine details that may otherwise have been obscured by noise and other experimental artefacts. Here we show the implementations of various image processing techniques applied to ARPES data and how they not only aid the interpretation of results, but can also be looked upon as stepping stones for better data processing techniques and potential automation of the classification of quantum materials through ARPES.

*This project is supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0415 and the National Science Foundation (NSF) CAREER award DMR-1847962.
Constructing New Patterns for Structured Illumination Microscopy

CHI MING KAN (Presenter), The University of Hong Kong — Ernst Abbe derived his famous formula of diffraction limit in 1873. The implication of this formula is that resolution of light microscopy is limited, which is in the magnitude of half of the wavelength of the light used in microscope. With the advancement in information theory and fluorescence techniques, going beyond theoretical limit stated by Abbe became possible. These methods are known as ‘super-resolution microscopy’ and one of them is structured illumination microscopy (SIM).

The basic idea of SIM is similar to that of Moiré pattern. By overlapping two finely spaced patterns, a slowly varying pattern of large fringes can be observed, in analogous to sound beats. By constructing a known finely spaced pattern, and illuminate it onto an unknown finely spaced pattern, fine details of unknown pattern can be reconstructed from the overlapped pattern observed with computer algorithms. Our group would like to explore and design new interference light patterns by manipulating optics and investigate whether a better lateral and axial resolution could be achieved.

Focused Ion Beam Pt for Cryogenic Resistive Thermometry

PORTIA ALLEN (Presenter), KIRSTEN BLAGG, MEENAKSHI SINGH, Colorado School of Mines — Local temperature measurements at cryogenic temperatures are important for studying thermal effects, both classical and quantum, in nanoscale devices. Resistive thermometry is a relatively simple way to obtain these measurements. However, most metals’ electron transport saturates at low temperatures, leading to constant resistances and making them ineffective for cryogenic thermometry. An exploration of Pt thermometers, deposited using a focused ion beam (FIB) system, reveals that they are very effective for low temperature thermometry. This is believed to be because of the carbon contamination of the Pt. A detailed analysis of the dependence of composition of the contaminants on deposition parameters and its effect on thermometer performance is presented here. Through this research, it is clear that FIB Pt offers a tunable, sensitive, template-free thermometer for nanoscale, cryogenic thermometry.

*We would like to acknowledge NSF DMR 1807583.

Medical Physics

Aggregation Dynamics of Blood Platelets

SURESH AHUJA (Presenter), xerox corporation — Platelet aggregation at sites of vascular injury is necessary for hemostasis and arterial thrombosis and occurs via platelet–platelet adhesion, tethering and rolling on the injured endothelium, a critical initial step in blood clot formation. In straight vessels, the presence of erythrocytes, red blood cells (RBCs) is known to push platelets toward walls, which may affect platelet aggregation and thrombus formation. Blood Cells for required optimizing coagulation. Model predictions on platelet to platelet collisions and of platelets to the capillary wall showed that platelet size, platelet Young’s modulus and shear rate are most significant variables controlling capillary aggregation and thrombus. Results are compared with available experimental results.
C71.00209: A Novel Energy-Resolved X-Ray Semiconductor Detector  TENGFEI YAN (Presenter), XIAODONG CUI, department of physics, the university of Hong Kong, CHUNLEI YANG, Chinese academy of sciences, Shen Zhen Institutes of Advanced Technology — The hyperspectral X-ray imaging has long been sought in various fields from material analysis to medical diagnosis. Here we propose a new semiconductor detector structure to realize energy-resolved imaging at potentially low cost. The device is designed based on the strong energy-dependent absorption of X-ray in solids. Namely, depending on the energy, X-ray photons experience dramatically different attenuation. An array or matrix of semiconductor cells is used to map the X-ray intensity along its trajectory. With known X-ray attenuation coefficient, the X-ray spectrum could be extracted from a Laplace like transform or a supervised machine learning. We conceptually demonstrated an energy-resolved X-ray detection with a regular silicon camera.

C71.00210: Improved Sensitivity of a Single-Sided Magnetic Particle Imaging Scanner*  JASON PAGAN (Presenter), AMANUEL NEGASH, Physics Dept, Univ of Mass - Boston, JUEHAO LIN, Engineering Dept, Univ of Mass - Boston, ALEXEY TONYUSHKIN, Physics Dept, Univ of Mass - Boston — Magnetic Particle Imagining (MPI) is the new frontier of medical imaging, capable of imaging the distribution of superparamagnetic nanoparticles (SPIOs) in an expeditious and sensitive manner. For instance, the accumulation of SPIOs in tumor tissue, serving as tumor markers, presents the MPI device as a practical means of imaging for in vivo cancer imaging. The single-sided design is beneficial for this application allowing imaging of larger subjects. In our design of a scanner we utilize a field-free line (FFL) geometry of the magnetic field zero, which has a potential advantage of an increased sensitivity over the traditional approach with field-free point (FFP). Our prototype device uses a single primary coil to generate a magnetic excitation field. The SPIOs response to the excitation is detected by a planar receive coil on the surface of the device. Due to a single-sided geometry, differentiating a small signal on a strong excitation background becomes a challenging task and further impinges the potential sensitivity gain, thus a new planar gradiometer coil configuration was developed. Results from the numerical simulations and experimental data imply the improved sensitivity of the device over the single coil design.

*This work supported by NIH under Award 1R15EB028535-01.
C71.00211: Retrospective quantitative harmonization in PET using deconvolution and optimal filtering

MAURO NAMÍAS, Medical Physics, Fundación Centro Diagnóstico Nuclear, DANIEL HUFF (Presenter), AMY J WEISSMAN, TYLER J BRADSHAW, ROBERT JERAJ, Medical Physics, University of Wisconsin - Madison — The reliability of longitudinal quantitative PET image analysis suffers if scans are acquired on different PET scanners. Here, we describe a post-reconstruction harmonization method that can be implemented to enable quantitative PET analysis across scanners.

First, images are unfiltered by Wiener deconvolution. Then, the differences in contrast recovery coefficients (CRC) from NEMA phantom scans are minimized by finding isotropic 3D Gaussian filters for each scanner/reconstruction setting combination with a downhill-simplex optimizer. After optimal filters are established, PET images to be harmonized are unfiltered using Wiener deconvolution, and then re-filtered with the determined optimal settings.

We demonstrate that the method minimizes differences in CRC values for a set of 7 heterogeneous reconstruction protocols acquired on 3 different PET/CT scanners. We apply our method retrospectively to 18F-FDG PET/CT scans of a cohort of metastatic melanoma patients to show that performing harmonization has a significant impact in assigning lesion response as measured by change in PET SUV metrics.

In conclusion, the described method for harmonization enables accurate quantitative PET image analysis for retrospective datasets, and has clinical impact in response assessment settings.

C71.00212: WITHDRAWN ABSTRACT

C71.00213: Magnetic Resonance Imaging Thermography with Uniform Gd Microstructures

JASON NOBLES (Presenter), KEVIN SMILEY, SARA GOLDMAN, JOHN STROUD, University of Colorado, Colorado Springs, KARL STUPIC, National Institute of Standards and Technology, ZBIGNIEWS J CELINSKI, JANUSZ HANKIEWICZ, University of Colorado, Colorado Springs — Magnetic resonance imaging is an important technique in imaging living tissue and composite structures. Many medical procedures now use MRI as a critical component including MRI guided thermal ablation therapy used to treat cancer. Such procedures require real-time, spatially and thermally accurate temperature maps.

We demonstrate an MRI temperature contrast agent consisting of uniform gadolinium microstructures dispersed within a media. We report on the performance of 6 micron wide, disk-shaped Gd microstructures passivated by a layer of chromium. A SQUID magnetometer was used to determine the mass magnetization of these disks. The temperature dependence of the mass magnetization was then correlated to the nuclear magnetic resonance linewidth broadening of water protons in the presence of Gd disks. We used this correlation to demonstrate the MRI image brightness of the Gd microstructures suspended in a tissue-mimicking phantom can be related to the temperature of the sample indicating these Gd disks are a good candidate for use as an MRI temperature contrast agent.
**C71.00214: Simple physical modeling for comparing respirator breathing resistance standards**  
DANA ROTTACH (Presenter), SUSAN XU, CAITLIN MCCLAIN, WILLIAM KING, NIOSH-CDC — Air purifying respirators are designed to reduce the number of hazardous particles respired by wearers. One barrier to respirator use is their inherent increase in breathing difficulty. The National Institute for Occupational Safety and Health (NIOSH) evaluates respirators using Standard Test Procedures (STP) for various factors, including measuring the breathing resistance as the pressure drop across the filter at a certain relatively high flow rate. The International Standards Organization (ISO) has a competing standard based on a 'Work of Breathing' (WOB) concept, which considers Pressure-Volume (PV) work for a series of sinusoidal simulated breaths with frequencies and magnitudes reflecting a variety of occupational scenarios, from resting to intense physical exertion. We compare the WOB and NIOSH breathing resistance limits using a simple linear model, which reflects the most common type of particulate filtering respirators. We find that the NIOSH result is more stringent than the ISO standard for most of the ISO work rates, Resting, W1, W2, and W4, but is less stringent for the moderately high W3 work rate. The effect of the non-linear flow characteristics associated with exhalation valves will be discussed along with the results of a less rigorous treatment.

**C71.00215: Deflector Cavity Design for Rapid 2-D Proton Beam Scanning**  
EMMA SNIVELY (Presenter), XUEYING LU, EMILIO NANNI, ZENGHAI LI, VALERY DOLGASHEV, GORDON BOWDEN, ANN V. SY, SAMI TANTAWI, SLAC - Natl Accelerator Lab — We investigate the design of a 2.856 GHz deflecting cavity to provide rapid 2-D beam scanning for hadron therapy. We consider geometries for both conventional TM$_{11}$ modes and TE$_{11}$-like modes. Designs are optimized for the case of sub-relativistic protons with 150 MeV kinetic energy using simulations in HFSS to characterize the full 3-D field profile. We discuss the challenge of maximizing the transverse shunt impedance while mitigating variations in the transverse voltage as a function of distance from the nominal beam axis. These changes in the effective transverse kick can lead to significant beam profile aberrations for non-relativistic particles.

*This research has been supported by the U.S. Department of Energy (DOE) under Contract No. DE-C02-76SF00515.*
C71.00216: Comparative Pharmacokinetics, Biodistribution and Dosimetry of $^{212}$Pb labeled Antibody vs Peptide vs Small Molecule  
NADER MOSHIRI (Presenter), Florida Atlantic University, GEORGE SGOUROS, Radiology, Johns Hopkins School of Medicine, THEODORA LEVENTOURI, Florida Atlantic University — We study the impact of carrier molecules in biodistribution and absorbed dose in normal tissue and tumors using $^{212}$Pb radionuclide. $^{212}$Pb ($T_{1/2} = 10.64$ hrs) decays to $^{212}$Bi ($T_{1/2} = 60.6$ mins) via β emission then finally stable $^{208}$Pb via α and γ decays. The effective $T_{1/2}$ could vary a lot depending on the carrier molecule. In this study, rats and mice data of $^{131}$I, $^{166}$Ho, $^{153}$Sm and $^{177}$Lu labeled DOTATATE, $^{111}$In and $^{212}$Pb labelled trastuzumab and $^{188}$Re-HEDP were utilized and fitted via SAAM II software. To calculate absorbed doses, the AUC of each organ was multiplied by the S values provided in MIRD scheme. RBE value of 5 was used to take into account the biological effect of the doses.

The highest level of radioactivity indicating the amount of absorbed dose was detected in bladder, pancreas, intestines, bone and kidneys for DOTATATE, while it was cleared out of the blood within a few hours post injection. In contrast to the peptide carrier, the antibody carrier, remained in the blood significantly longer with increased uptake in the liver after 78 hrs while decreasing everywhere else steadily. For the small molecule carrier HEDP, the main concentration was found in bone followed by kidney, thyroid, stomach, liver and blood. Quantitative analysis of effective doses is in progress.

C71.00217: Rotation- and reflection-encompassing multispectral nonlocal means denoising filter for magnetic resonance imaging*  
MUSTAPHA BOUHRARA, NIKKITA KHATTAR, RICHARD SPENCER (Presenter), National Institutes of Health - NIH — Image denoising is used extensively in medical image processing. Compared to other advanced filters, nonlocal means (NLM) shows excellent performance while being straightforward to implement. NLM takes advantage of structural redundancy in images by comparing local neighborhoods (local patches) around voxels throughout the whole image. The index voxel is then restored based on a weighted average of all voxels, with the weighting dependent on the degree of similarity. We have extended this by exploiting multispectral (MS) similarity in related images, obtained with a sequence of imaging parameters (1). In addition, we have developed an adaptive user-independent method to define similar voxels (2). The filter exhibits excellent edge preservation and noise reduction in magnetic resonance (MR) images and has been applied to improve parameter determination (3, 4). Here, we introduce a rotation- and reflection-encompassing implementation of our filter, motivated by the fact that patches may be similar only upon rotation. Our results demonstrate the improved performance as compared to our original implementation. This filter has wide applicability in imaging.

1. IEEE TMI 2017;36:181-93
2. MRI 2019;55:133-9
3. JNM 2018;309:121-131
4. JON 2018;28:640-649

*IRP, National Institute on Aging, NIH.

C71.00218: QUANTUM INFORMATION —
C71.00219: Deterministic single photon subtraction for engineering exotic non-classical states of light*  SUPRATIK SARKAR (Presenter), JINJIN DU, MICHAL BAJCSY, Institute for Quantum Computing, University of Waterloo — We present an analytical and numerical simulation study of deterministic single photon subtraction using Single Photon Raman Interaction (SPRINT) [1] in a three level Λ-type quantum emitter coupled with a chiral waveguide or cavity. This process of deterministic single photon subtraction is fundamentally different from the usual probabilistic single photon subtraction, which is inherently just the application of the annihilation operator on the incoming light field. Unlike probabilistic single photon subtraction, the photon subtraction probability relying on SPRINT is independent of the number of photons in the input field. We investigate the effects of the repeated application of the deterministic subtraction operator on photonic fields and the resulting changes in phase space statistics that lead to exotic non-classical states of light, such as states with negative Wigner functions and squeezed states. We also discuss the prospects of experimental implementation of this approach.


*This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund.

C71.00220: Using Trapped Ion Chains for Realization of Quantum Error Correction  DAIWEI ZHU (Presenter), LAIRD EGAN, MICHAEL L GOLDMAN, MARKO CETINA, CRYSTAL NOEL, ANDREW REISINGER, DEBOPRIYO BISWAS, CHRISTOPHER ROY MONROE, Joint Quantum Institute, University of Maryland —

We are constructing a quantum processor based on a register of up to 32 trapped 171Yb+ ions, with high connectivity provided by high-fidelity entangling gates. Our goals are to implement an error-corrected logical qubit and to perform a range of quantum algorithms with a system size and gate depth that move beyond what has previously been demonstrated. Here, we report on the current status of our first-generation integrated system, including gate fidelity, hardware performance, and automatic control. We also present the progress toward implementing fault-tolerant logical qubits.
**C71.00221: Exploration of the Circularly Polarized Attosecond Pulse Generation Mechanisms by Polarization Gating**  CHON-TENG BELMIRO CHU (Presenter), Physics, Natl Taiwan Univ, XIAO-MIN TONG, Materials Science, Univ of Tsukuba, SHIH-I CHU, Physics, Natl Taiwan Univ — We perform a fully ab initio investigation of the generation of circularly polarized attosecond pulse of atomic H driven by polarization gating. The time-dependent Schrödinger equation is solved accurately and efficiently by means of the time-dependent generalized pseudospectral method. We investigate the physical mechanism of this process by solving the time-dependent Schrödinger equation in the integral form. In this way, the contribution of the wave function from different time segment to the induced dipole can be analyzed. The dynamic behavior during this process can be unveiled by the Bohmian trajectories of the dominant part of the wave function.

*This work was partially supported by National Taiwan University, the Ministry of Science and Technology and Ministry of Education of Taiwan.

**C71.00222: High resolution AC magnetometry NMR spectrometer development using diamond nitrogen-vacancy centers**  ZHIPAN WANG (Presenter), WILLIAM CASEY, NICHOLAS CURRO, University of California, Davis — Nitrogen-vacancy (NV) quantum defects in diamond are sensitive detectors of magnetic fields. Due to their atomic size and optical readout capability, they have been used for magnetic resonance spectroscopy of exceptionally low volume samples on diamond surfaces. Here we present our approaches to develop and construct a simple, low-cost NV-detected NMR spectrometer. The underlying theory and preliminary experimental data will be presented.

*The work was supported by the United States Department of Energy, Office of Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division for Grant DE-FG0205ER15693

**C71.00223: Microwave to Optical Transducer with Single Emitters**  VINODH RAJ RAJAGOPAL MUTHU (Presenter), WENFANG LI, JINJIN DU, RUBAYET AL MARUF, PRITAM PRIYADARSI, MICHAL BAJCSY, University of Waterloo — In this project, we aim to develop a quantum interface between microwave and optical photons. This is an essential component in realizing a hybrid quantum network where information needs to be interfaced between superconducting microwave circuits, which provide quantum information processing, and optical photons, which are suitable for long-distance communication. Our work investigates the potential of micro-fabricated devices with integrated optical and microwave cavities that use individual three-level solid-state emitters, such as NV centres, for the efficient conversion between the microwave and optical regimes. We present analytical and numerical simulation results that explore the required characteristics of the microwave and optical cavities to achieve high conversion efficiency between the microwave and optical regimes.

*This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund.*
**C71.00224: Growth and characterization of Si/SiGe heterostructures towards scalable qubit architecture**

CEDRIC CORLEY (Presenter), Materials Research, IHP – Leibniz-Institut für innovative Mikroelektronik, YUJI YAMAMOTO, MARKUS ANDREAS SCHUBERT, FLORIAN BÄRWOLF, Technology, IHP – Leibniz-Institut für innovative Mikroelektronik, MARVIN ZÖLLNER, Materials Research, IHP – Leibniz-Institut für innovative Mikroelektronik, INGA SEIDLER, MALTE NEUL, LARS SCHREIBER, JARA-FIT Institute for Quantum Information, RWTH Aachen University, GIOVANNI CAPELLINI, WOLFGANG MATTHIAS KLESSE, Materials Research, IHP – Leibniz-Institut für innovative Mikroelektronik — Strained Si/SiGe Quantum Well (QW) structures are a promising material system for the realization of spin qubits based on spatially confined electrons. A major advantage for Si-based structures is their compatibility with mature Si-CMOS technology, providing high scalability. In this study we show a first step towards determining the relationship between the material properties (e.g. interface roughness and defect density) and qubit performance of these structures. In order to discuss the influence of the material properties of the QW, tensile strained Si QW embedded in Si$_{0.7}$Ge$_{0.3}$ layers with different types of SiGe buffer layers are fabricated on 200 mm Si substrates. The material properties are characterized by various methods (X-Ray Diffraction, Secondary Ion Mass Spectrometry, Scanning Transmission Electron Microscopy).

*The "SiGeQuant (High-definition crystalline Silicon-Germanium structures for Quantum Circuits)" project is supported by the Leibniz-Gemeinschaft (Senatsausschuss Wettbewerb, SAW) under the project number K124/2018.*

**C71.00225: WITHDRAWN ABSTRACT**

**C71.00226: Electric manipulation of a valley qubit in a silicon quantum dot**

PEIHAO HUANG (Presenter), Institute of Quantum Science and Engineering, Southern University of Science and Technology — In a silicon quantum dot, the valley states can be encoded as a qubit for quantum information processing. Here, we study theoretically the electric manipulation of valley qubit in a silicon quantum dot. The valley qubit frequency and electric manipulation speed are studied as a function of the location of interface steps and the applied electric field. We find that the applied electric field or the interface state can enhance the electric manipulation of the valley qubit. We further study the combined effect of QD confinement and interface steps on the electric manipulation of valley qubit. We will discuss the consequence of the results on the valley qubit based quantum information processing.
C71.00227: A Platform for Light-Hole Qubits in Group IV Semiconductors  PATRICK DEL VECCHIO, ANIS ATTIAOUI, SIMONE ASSALI (Presenter), OUSSAMA MOUTANABBIR, Ecole Polytechnique de Montreal — Si-compatible quantum devices have been exploiting either tensile strained Si or compressively strained Ge QWs, which are the only group IV systems that can currently be routinely obtained using SiGe as growth template and barrier layers. For quantum information, the former has been used as the building block for electron spin qubits, whereas the latter has been explored in new schemes for hole spin qubits. Herein, we present a third low-dimension system consisting of highly tensile strained Ge QW integrated on an optically active platform and discuss its basic properties experimentally and theoretically. The growth of tensile strained Ge QW is achieved using direct bandgap GeSn as barrier layers grown on silicon wafers. This heterostructure yields high tensile strain in Ge QW and band structure corresponding to a sizable LH-HH splitting exceeding 100 meV. Unlike compressively strained Ge, the top of the valence band is occupied by LH in tensile strained Ge. We also found a high LH g-factor anisotropy in Ge/GeSn QW, with g = 21.8 for in-plane B-field and g = 0.69 for perpendicular-to-plane field. These properties lay the groundwork to implement LH spin qubits with potentially easier manipulation due to the combined effects of the large Rashba-type SOI, and the spin ½ of LH.

C71.00228: Observation and stabilization of photonic Fock states in a hot radio-frequency resonator*  MARIO GELY (Presenter), MARIOS KOUNALAKIS, CHRISTIAN DICKEL, JACOB DALLE, RÉMY VATRÉ, Delft University of Technology, BRIAN BAKER, Department of Physics and Astronomy, Northwestern University, MARK JENKINS, GARY STEELE, Delft University of Technology — Detecting and manipulating single-photons at MHz frequencies presents a challenge as, even at cryogenic temperatures, thermal fluctuations are significant. In our work [1], we use a GHz superconducting qubit to directly observe the quantization of a MHz radio-frequency electromagnetic field. Using the qubit, we achieve quantum control over thermal photons, cooling to the ground-state and stabilizing photonic Fock states. Releasing the resonator from our control, we directly observe its re-thermalization dynamics with the bath with nanosecond resolution. Extending circuit QED to a new regime, we enable the exploration of thermodynamics at the quantum scale and allow interfacing quantum circuits with MHz systems such as spins or mechanical oscillators. The tool used to design such a circuit, QuCAT [2], the "quantum circuit analyzer tool in Python" will also be featured in this poster.


*European Research Council under the European Union's H2020 program [grant numbers 681476-QOM3D, 732894-HOT, 828826-Quromorphic, 785219 - GrapheneCore2], the Dutch Foundation for Scientific Research (NWO) through the Casimir Research School, the Army Research Office through Grant No. W911NF-15-1-0421.
C71.00229: Single-Photon Dispersive Readout of a Qubit with a Photodetector: Theory Beyond the Rotating-Wave Approximation* ANDRII SOKOLOV (Presenter), Universität des Saarlandes, Institute of Physics of the National Academy of Sciences of Ukraine, EUGENE V STOLYAROV, Institute of Physics of the Ukrainian Academy of Sciences — We propose to use a single-photon pulse and a photodetector for the dispersive readout of a qubit. The scheme avoids the shot noise errors. However, another source of errors makes it challenging to perform a single-photon readout. To boost its performance, we propose to detune the qubit and the resonator further than usual, while coupling them stronger. The Bloch-Siegert shift then should be taken into account. It is shown how it can improve the readout. We provide simple analytical estimates for the readout contrast. Results of more complicated calculations that take the qubit relaxation into account are also presented. A contrast more than 75% can be achieved in 1μs for ideal detector and photon source.

*Work of A.S. was partly supported by a DAAD scholarship (2016).

C71.00230: Study on the cavity photon induced dephasing of a transmon qubit in circuit QED due to the measurement microwave leakage JISOO CHOI, Korea Research Inst of Standards and Science (KRISS), Korea University, GAHYUN CHOI (Presenter), Korea Research Inst of Standards and Science (KRISS), GWANYEOL PARK, Korea Research Inst of Standards and Science (KRISS), Korea University, JINSU SON, Korea Research Inst of Standards and Science (KRISS), KWAN-WOO LEE, SOON-GUL LEE, Korea University, WOON SONG, Korea Research Inst of Standards and Science (KRISS), YONUK CHONG, Korea Research Inst of Standards and Science (KRISS), University of Science and Technology (UST) — Qubit coherence is one of key features in quantum computing. In circuit QED architecture, it is known that the cavity photon induces dephasing of the qubit even in the dispersive regime [1, 2]. In this study, we studied in detail the dephasing of a 3D transmon qubit generated by the measurement microwave tone. First, we observed that the intense measurement microwave tone decreases the dephasing time. In order to avoid the dephasing, we controlled the mixer leakage by applying dc-offset voltage. We observed clear dependence of the measurement microwave leakage and dephasing, so that we can optimize our measurement setup to achieve maximum T_{2*}. This calibration method is one of the standard features in our measurement system to preserve the qubit coherence.


C71.00231: Enhancement in the cross-resonance gate performance XUEXIN XU (Presenter), MOHAMMAD ANSARI, Forschungszentrum Juelich — We theoretically model an experiment on a superconducting circuit made of a capacitively shunted flux qubit (CSFQ) and a transmon both capacitively coupled to a bus resonator in dispersive regime. We apply external driving microwave pulses over all energy levels and consider the transitions they impose effectively within the computational subspace. More specifically we apply entirely microwave two-qubit gate, the so called cross-resonance, on CSFQ at sweet spot and away from it. Interestingly the two-qubit fidelity is largely enhanced at certain external flux away from the sweet spot. This enhancement takes place as the result of suppressed leakage out of computational subspace.
C71.00232: Spectrum and Coherence of the Current-Mirror Circuit* DANIEL WEISS
(Presenter), CHEONG YIU LI, Northwestern University, DAVID FERGUSON, Northrop Grumman - Mission Systems, JENS KOCH, Northwestern University — The current-mirror circuit [1] exhibits a robust ground-state degeneracy and wave functions with disjoint support for appropriate circuit parameters. In this protected regime, Cooper-pair excitons form the relevant low-energy excitations. Based on a full circuit analysis of the current-mirror device, we introduce an effective model that systematically captures the relevant low-energy degrees of freedom, and is amenable to diagonalization using Density Matrix Renormalization Group (DMRG) methods. We find excellent agreement between DMRG and exact diagonalization, and can push DMRG simulations to much larger circuit sizes than feasible for exact diagonalization. We discuss the spectral properties of the current-mirror circuit, and predict coherence times exceeding 1 ms in parameter regimes believed to be within reach of experiments.


*This research was supported by the Army Research Office under contract W911NF-17-C-0024.

C71.00233: Qubit fast reset with QubiC* GANG HUANG (Presenter), YILUN XU, Lawrence Berkeley National Laboratory, RAVI KAUSHIK NAIK, BRADLEY MITCHELL, Physics, University of California, Berkeley, DAVID SANTIAGO, Lawrence Berkeley National Laboratory, IRFAN SIDDIQI, Physics, University of California, Berkeley — Fast reset is a basic qubit control feedback loop where the hardware latency is critical. We develop the fast reset logic on the QubiC system by implementing the qubit status classification and the feedback loop in the FPGA firmware. The experiment setup and initial testing results are presented here.

*This work was supported by the Department of Energy under Contract No. DE-AC02-05CH11231.

C71.00234: Exploring 3D architectures and superconducting interconnects using highly conformal ALD and CVD: a BEOL-compatible process for superconducting MgB$_2$ DAVID J MANDIA, DEVIKA CHOUDHURY, Argonne National Laboratory, NEIL T ANDERSON, GREGORY S GIROLAMI, University of Illinois at Urbana-Champaign, JEFFREY W ELAM, ALI NASSIRI, ANGEL YANGUAS-GIL (Presenter), Argonne National Laboratory — The ability to fabricate 3D architectures and superconducting interconnects can be an enabling technology towards the scale up of quantum computing architectures. One of the key challenges is that physical vapor deposition methods, such as evaporation or sputtering, struggle to coat or infiltrate high aspect ratio structures, being traditionally limited to aspect ratios of 10:1 or lower. In this work we explore how to take advantage of the high conformality of ALD and some CVD processes to overcome this limitation. In particular, we have developed a BEOL-compatible, diborane-free process that is capable of growing superconducting magnesium diboride at low temperatures. This process has allowed us to demonstrate critical temperatures exceeding 20K in films that are just a few nm thick, and the formation of stable interfaces with oxide materials. Together with existing ALD processes for superconducting nitrides, we believe that this process can help us explore new device configuration, including the design of architectures with vertical junctions, or the development of superconducting interposers for advanced packaging applications.
C71.00235: Impact of noise reduction in measurement of a super conducting flux qubit at 4.2 K
DAISUKE SAIDA (Presenter), AIST, NARI WATASE, MDR Inc., TAKEHITO KAMIMURA, SHINGO
SOBUKAWA, HIROHITO WATANABE, NF Corporation, YUKI YAMANASHI, Yokohama National University
— A flux state of a super conducting flux qubit is evaluated at 4.2 K prior to measurement of
quantum state at mK. At the 4.2 K measurement, a customized rod, where a sample is attached,
is inserted in the Dewar vessel filled in the liquid helium. An elimination of artifact from an
experimental system is crucial. In order to prevent signal quality deterioration by environmental
noise, countermeasures have been taken by strengthening the electrostatic shield and
introducing the twisted pair wiring. Low noise voltage source (LP6016) for bias current control of
SQUID is also effective in suppressing signal fluctuation from SQUID. As a result, noise density at
50 Hz and 150 Hz in the measurement became 1/300 and 1/500 compared to the previous
experiment, respectively. We evaluated the flux state in the super conducting flux qubit through
an observation of signal in a readout-SQUID. This sample was fabricated by AIST Nb standard
process 2, where $J_c$ was 25 μA/μm$^2$. On a flux dependence of threshold current ($I_{th}$) in the
readout-SQUID, standard deviations ($\sigma$) of $I_{th}$ was 0.16. This indicates that we can control an
operating point of the readout-SQUID in an accuracy of the measurement with an order less than
1 μA. Further, $\sigma << 1$ was evaluated when we observed flux conditions in the qubit.

C71.00236: Search by Lackadaisical Quantum Walk with Nonhomogeneous Weights*
MASON RHODES (Presenter), TOM WONG, Creighton University — The lackadaisical quantum walk, a
quantum walk with weighted self-loops, speeds up dispersion on a line and improves spatial
search on the complete graph and periodic square lattice. In these investigations, each self-loop
had the same weight, due to each graph's vertex-transitivity. In this paper, we propose
lackadaisical quantum walks with self-loops of different weight. We investigate spatial search on
the complete bipartite graph, which can be irregular with partitions of size $N_1$ and $N_2$, which
naturally leads to self-loops having different weights $l_1$ and $l_2$, respectively. We prove that if the $k$
marked vertices are confined to one partite set, then with the typical initial uniform state over the
vertices, the success probability is improved from its non-lackadaisical value when $l_1 = kN_2/2N_1$
and $N_2 > (3-2\sqrt{2})N_1$, regardless of $l_2$. When the initial state is stationary under the quantum walk,
however, the success probability is improved when $l_1 = kN_2/2N_1$ without a constraint on the ratio
of $N_1$ and $N_2$. Next, when marked vertices lie in both partite sets, then for either initial state, there
are many configurations for which the self-loops yield no improvement in quantum search, no
matter what weights they take.

*This work was supported by T.W.'s startup funds from Creighton University.
C71.00237: Trimming Grover's Quantum Search Algorithm*  GRANT EBERLE (Presenter), GONZALO ORDONEZ, Butler University — Grover's quantum algorithm is a complicated search algorithm made to run on a quantum computer. The algorithm allows users to search a database for a word in a significantly shorter time than a conventional computer. Past experiments have attempted to run iterations of the algorithm on a quantum computer and failed because of the complexity. My research modifies and simplifies the theory of Grover's algorithm by utilizing results from previous work that studied the diffusion of wave functions across a hypercube. I have directly applied this diffusion process to an edited and simplified version of Grover's algorithm based on the premise of simplifying the connections and paths between q-bits represented on a hypercube. The algorithm I have created has been run and tested on the open-source quantum computer simulations provided by IBM on their IBM Q website. My results display a trimmed and practical version of Grover's quantum search algorithm.

*Funding was provided by the Butler University CHASE scholars program and the Butler University Department of Physics and Astronomy.

C71.00238: Quantum simulations and force sensing experiments with 2D arrays of 100's of ions*  ELENA JORDAN (Presenter), MATTHEW AFFOLTER, KEVIN A. GILMORE, National Institute of Standards and Technology Boulder, ATHREYA SHANKAR, University of Colorado, Boulder, ARGHAVAN SAFAVI-NAINI, ROBERT J. LEWIS-SWAN, JILA, NIST, and University of Colorado Boulder, MURRAY J HOLLAND, University of Colorado, Boulder, ANA MARIA REY, JILA, NIST, and University of Colorado Boulder, JOHN JACOB BOLLINGER, National Institute of Standards and Technology Boulder — We perform quantum simulations and quantum sensing with two-dimensional arrays of >100 trapped ions in a Penning trap [1, 2]. In our quantum sensing experiments, we measure small displacements of the ion crystal. Electric fields excite center-of-mass (COM) motion of the crystal. By measuring the motion-induced spin precession we can determine the amplitude of the COM motion and the strength of the exciting field [2]. Improvements in the phase stability of our coupling lasers enabled phase coherent detection protocols, resulting in a single measurement sensitivity of 50 pm for the COM motion that was far off-resonant with the trap axial frequency. 50 pm is about a factor 40 below the size of the ground state wavefunction. Further, we show results of electromagnetically induced transparency (EIT) cooling for the drumhead motion of the single-plane arrays [3, 4]. We present results that show simultaneous cooling of all the drumhead modes to close to the ground state of motion.


*We gratefully acknowledge NIST, Leopoldina (German Academy of Sciences), NSF, and DOE.

C71.00239: WITHDRAWN ABSTRACT —
C71.00240: QAOA Algorithms for Traveling Salesman Problem Revisited

CHANGYUAN LIU (Presenter), BigCompute — The traveling salesman problem is a traditionally NP-hard problem. Earlier quantum algorithm encodes the qubits based on vertices, while we encode the qubits based on edges, with a resources requirement halved. With edge encoding scheme, QAOA algorithm is demoed with small cases, on a classical enumlator, with the optimal solutions successfully found. The algorithm has polynomial complexity in terms of the number of quantum operations.

*N/A - Self supported

C71.00241: Implementation of excited state energy and its analytical derivatives for photochemical reaction simulations on NISQ devices

YOHEI IBE (Presenter), TAKAHIRO YAMAMOTO, YUYA O. NAKAGAWA, QunaSys Inc., KOSUKE MITARAI, Graduate School of Engineering Science, Osaka University, TENNIN YAN, QunaSys Inc., GAO QI, TAKAO KOBAYASHI, Mitsubishi Chemical Corp. — A primitive but still powerful form of quantum computers called Noisy Intermediate-Scale Quantum (NISQ) devices is about to be utilized for the real-world problems. NISQ devices have a few hundreds to thousands of qubits under highly precise control although they are not fault-tolerant.

A quantum chemistry calculation is one of the most promising applications of NISQ devices in the near future, and Variational Quantum Eigensolver (VQE) is the most featured algorithm to take advantage of NISQ devices in quantum chemistry. Recently, numerous algorithms based on the VQE are proposed for solving problems that are hard for classical computers, such as calculations of electronic excited states of large molecular systems.

However, VQE-type algorithms are in general based on the variational principle, which makes it difficult to predict their performances when applied to actual molecular systems due to their heuristic nature.

In this study, using the high-speed simulator Qulacs, we implement VQE-type algorithms to calculate several physical properties (analytical energy derivatives and oscillator strengths) required for photochemical reaction simulations and create their unified benchmark of various proposed methods for small molecules compared with results from the classical computation.
C71.00242: The Quantum Alternating Operator Ansatz on Max-k Vertex Cover  JEREMY COOK (Presenter), STEPHAN EIDENBENZ, ANDREAS BÄRTSCHI, Theoretical Division, Los Alamos National Laboratory — We study the performance of the Quantum Alternating Operator Ansatz (a generalization of the QAOA for problems with hard constraints) on the problem of Max-k Vertex Cover due to its modest complexity, while still being more complex than the well studied problems of Max-Cut and Max-E3LIN2. Our approach includes (i) a performance comparison between easy-to-prepare classical states and Dicke states, (ii) a performance comparison between two XY-Hamiltonian mixing operators: the ring mixer and the complete graph mixer, (iii) an analysis of the distribution of solutions via Monte Carlo sampling, and (iv) the exploration of efficient angle selection strategies. Our results are: (i) Dicke states improve performance compared to easy-to-prepare classical states, (ii) an upper bound on the simulation of the complete graph mixer, (iii) the complete graph mixer improves performance relative to the ring mixer, (iv) the standard deviation on the distribution of solutions decreases exponentially in p (the number of rounds in the algorithm), requiring an exponential number of random samples find a better solution in the next round, and (iv) a correlation of angle parameters which exhibit high quality solutions that behave similarly to a discretized version of the Quantum Adiabatic Algorithm.

C71.00243: Optimizer-aware Circuit Design for Error Unfolding in Variational Quantum Eigensolver  WIM LAVRIJSEN, MIROSLAV URBANEK, MEKENA L METCALF, JULIANE MÜLLER, BENJAMIN NACHMAN, DIANA CHAMAKI, COSTIN IANCU (Presenter), WIBE A DE JONG, Lawrence Berkeley National Laboratory — Quantum hardware suffers from errors and any measured output is thus a convolution of the intended result and some error distribution. The Variational Quantum Eigensolver has a classical optimizer step that takes the output from the quantum chip to determine the input parameters for the next iteration. Errors can prevent the optimizer from making progress; and if they are too large, make it impossible to calculate, let alone find, the global minimum. If the error distribution were known, it could be unfolded, but this is generally not the case, especially if the errors do not commute with the whole circuit. Exploiting ideas from randomized compilation, we introduce twirl gates into the circuit, generating logically equivalent circuits with the same number of gates and same output, but with different error behavior. The physical processes do not change, thus error rates remain the same as well. Using a Markov chain as error model, we apply a maximum likelihood fit to find those rates that produce migration matrices for unfolding consistent with all observed distributions. This results in improved output estimates of the quantum computer, and better defined uncertainties as input to the classical optimizer leading to faster convergence and a more robustly defined global minimum.
C71.00244: Benchmarking Noise Extrapolation with OpenPulse*  EUGEN DUMITRESCU (Presenter), RAPHAEL POOSER, Oak Ridge National Lab, JOHN GARMON, Virginia Tech — In order to augment digital qubit metrics, such as gate fidelity, we discuss analog error mitigability, i.e. the ability to accurately distill precise observable estimates, as a hybrid quantum-classical computing benchmarking task. Specifically, we characterize single-qubit error rates on IBM's Poughkeepsie superconducting quantum hardware, incorporate control mediated noise dependence into a generalized rescaling protocol, and analyze how noise characteristics influence Richardson extrapolation-based error mitigation. Our results identify regions in the space of Hamiltonian control fields and circuit-depth which are most amenable to reliable noise extrapolation, as well as shedding light on how low-level hardware characterization can be used as a predictive tool for uncertainty quantification in error mitigated NISQ computations.

*This work was performed with DOE ASCR funding under the Quantum Testbed Pathfinder program, FWP number ERKJ332.

C71.00245: Modeling Quantum Devices and the Reconstruction of Physics in Practical Systems*  HANG REN (Presenter), Nankai University, YING LI, Graduate School of China Academy of Engineering Physics — Modeling quantum devices is to find a model according to quantum theory that can explain the result of experiments in a quantum device. We find that usually we cannot correctly identify the model describing the actual physics of the device regardless of the experimental effort given a limited set of operations. According to sufficient conditions that we find, correctly reconstructing the model requires either a particular set of pure states and projective measurements or a set of evolution operators that can generate all unitary operators.

*This work was supported by National Natural Science Foundation of China (Grant No. 11875050) and NSAF (Grant No. U1730449).
YICHEN ZHANG (Presenter), Beijing University of Posts and Telecommunications, ZIYANG CHEN, Peking University, BINJIE CHU, CHAO ZHOU, XIANGYU WANG, YIJIA ZHAO, YIFAN XU, CHAO XU, HONGJIE WANG, ZIYONG ZHENG, YUNDI HUANG, CHUNCHAO XU, XIAOXIONG ZHANG, TAO SHEN, GE HUANG, YUNWU ZHENG, ZHAOXUAN FEI, WEINAN HUANG, MENG LIN ZHU, LUYU HUANG, BIN LUO, SONG YU, Beijing University of Posts and Telecommunications, HONG GUO, Peking University — Continuous-variable quantum key distribution (QKD) is a very attractive method for the physical layer protection of information transmission by secure distribution of private keys, as it uses standard telecom components that operate at room temperature and it has higher secret key rates (bits per channel use) over metropolitan areas. The longest distance of continuous-variable QKD field tests has reached 50 km, which is enough to support the construction of metropolitan networks. Here, we report the long-term performance of three nodes continuous-variable QKD network in Qingdao, which is the first continuous-variable QKD application demonstration with clear application scenarios over a long period of time through existing commercial optical fiber links. The average secret key rate achieves higher than 12.00 kbps over 71.03 km optical fiber line. The system has been running for 28 days stably with a reliable performance, which paves the way to deploy continuous-variable QKD in metropolitan settings.

*This work was supported by National Natural Science Foundation of China under Grants 61531003.

YICHEN ZHANG (Presenter), Beijing University of Posts and Telecommunications, ZIYANG CHEN, Peking University, CHRISTIAN WEEDBROOK, Xanadu, BIN LUO, SONG YU, Beijing University of Posts and Telecommunications, HONG GUO, Peking University — The continuous-variable quantum key distribution with entanglement in the middle, a semi-device-independent protocol, places the source in the untrusted third party between Alice and Bob, and thus has the advantage of high levels of security with the purpose of eliminating the assumptions about the source device. However, previous works considered the collective-attack analysis, which inevitably assumes that the states of the source has an identical and independently distributed (i.i.d) structure, and limits the application of the protocol. To solve this problem, we modify the original protocol by exploiting an energy test to monitor the potential high energy attacks an adversary may use. Our analysis removes the assumptions of the light source and the modified protocol can therefore be called source-device-independent protocol. Moreover, we analyze the security of the continuous-variable source-device-independent quantum key distribution protocol with a homodyne-homodyne structure against general coherent attacks by adapting a state-independent entropic uncertainty relation. The simulation results indicate that, in the universal composable security framework, the protocol can still achieve high key rates against coherent attacks under the condition of achievable block lengths.
**C71.00248: Resource-Adaptable Quantum Algorithms for Scalable Simulation of the Schwinger Model**
ALEXANDER SHAW (Presenter), Oak Ridge National Lab, NATALIE M KLCO, University of Washington, PAVEL LOUGOVSKI, Oak Ridge National Lab, JESSE STRYKER, NATHAN WIEBE, University of Washington — The Schwinger model (quantum electrodynamics in 1+1 dimensions) is a testbed for the study of field theories underpinning the Standard Model. Quantum computers are anticipated to enable unprecedented simulations of field theories. In this work, we give scalable and explicit digital algorithms to simulate the Schwinger model using fault-tolerant quantum computation. We upper bound a relevant metric of computational complexity, the number of T-gates, in terms of the simulation parameters, confirming that the time evolution can be simulated efficiently. Additionally, we give circuits that could be used in a nearer-term (NISQ) implementation of our simulation algorithms.

**C71.00249: Space-Time Mixing of Quantum Computing in an Entangled Atomic Chain and Time Crystals**
ANDREW VAN HORN (Presenter), CHENG-HSIAO WU, Missouri Univ of Sci & Tech — Experimentally observed space-time crystals are modeled here as a 1-D 4-State Cellular Automata (CA) under a specific set of “cyclic” state-transition rules, three of which are analyzed here. The generations of these specific CA rule sets have been previously shown to model the properties of the recently described space-time crystals due to the underlying mathematical model present in these rules. The rules are shown here to display three space-time symmetry rotations in the time crystals generated. Hence, the rotational symmetry property of the computational states of these CA generations is of physical significance to the rules governing space and time in a space-time crystal. The time-crystal generations are mapped onto the surface of a space-time sphere, where the non-Euclidean geometry allows for the interchangeability between space and time in producing space-time crystals.

**C71.00250: Employing Variational Principles to Define the Effective Hamiltonian of a Periodically Driven Qubit**
DANIEL ZEUCH (Presenter), DAVID PETER DIVINCENZO, Peter Grünberg Institut, Forschungszentrum Julich — The trajectory of a linearly driven qubit in the rotating frame can be determined using the effective Hamiltonian introduced in [1], which improves on the rotating wave approximation. By its definition, this Hamiltonian (i) is analytic in time and, (ii), yields an effective driven-qubit trajectory that coincides with the exact trajectory at equally-spaced points in time. In general, these effective trajectories are significantly smoother than the exact ones. The effective Hamiltonian is determined by an infinite sum whose convergence, however, is not always guaranteed [1]. As the requirements (i) and (ii) are fulfilled by a continuum of Hamiltonians, here we hypothesize that the effective Hamiltonian additionally satisfies, (iii), a variational principle that is motivated by the smoothed trajectories mentioned above. Our variational principles state that the integral of a certain function of the Hamiltonian, e.g., its positive eigenvalue, over the full pulse duration is minimized by the effective Hamiltonian of [1]. To find evidence for or against our hypotheses, we carry out variational calculations aimed at numerically minimizing the corresponding integrals.

C71.00251: Entangled Excitons via Spontaneous Downconversion  ARIEL SHLOSBERG (Presenter), University of Colorado, Boulder, MARK T. LUSK, Colorado School of Mines — A class of centrosymmetric molecules support excitons with a well-defined quasi-angular momentum. Cofacial arrangements of these molecules can be engineered so that quantum cutting produces a pair of excitons with angular momenta that are maximally entangled. The Bell state constituents can subsequently travel in opposite directions down molecular chains as ballistic wave packets. This is a direct excitonic analog to the entangled polarization states produced by the spontaneous parametric downconversion of light. As in optical settings, the ability to produce Bell states should enable foundational experiments and technologies based on non-local excitonic quantum correlation. The idea is elucidated with a combination of quantum electrodynamics theory and numerical simulation.

C71.00252: Practical route to entanglement-enhanced communication over noisy bosonic channels*  HAOWEI SHI, James C. Wyant College of Optical Sciences, University of Arizona, ZHESHEN ZHANG, Materials Science and Engineering, University of Arizona, QUNTAO ZHUANG (Presenter), Electrical & Computer Engineering, University of Arizona — Entanglement can offer substantial advantages in quantum information processing, but loss and noise hinder its applications in practical scenarios. Although it has been well known for decades that the classical communication capacity over lossy and noisy bosonic channels can be significantly enhanced by entanglement, no practical encoding and decoding schemes are available to realize any entanglement-enabled advantage. Here, we report structured encoding and decoding schemes for such an entanglement-assisted communication scenario. Specifically, we show that phase encoding on the entangled two-mode squeezed vacuum state saturates the entanglement-assisted classical communication capacity and overcomes the fundamental limit of covert communication without entanglement assistance. We then construct receivers for optimum hypothesis testing protocols under discrete phase modulation and for optimum noisy phase estimation protocols under continuous phase modulation. Our results pave the way for entanglement-assisted communication and sensing in the radiofrequency and microwave spectral ranges.

*Army Research Office and was accomplished under Grant Number W911NF19-1-0418
E. CARL-LUDWIG SIEGEL (Presenter), FUZZYICS — QC has been alive and well since WWII in artificial neural-network(ANN) artificial-intelligence(AI), vs computing-quanta since quantum-theory, if not Newcomb(1881)-Poincare(1911)-Weyl(1916)-...-Benford(1938)[benfordonline.net] digits log-law inverse[Antonoff/Siegel(2002)]: digits=bosons. What does QC mean? In ANN AI, not counting Turing(1936 machine plagarism of Lenz-Ising model(1911) of localized magnetism, starting with Rosen(SRI). In the 1980s Charles Rosen(Machine-Intelligence), Jacob Goldman(Xerox PARC), Irwin Wunderman(HP), Vesco Marinov and Adolph Smith(Exxon Enterprises/AI) and Edward Siegel realized that ubiquitous standard sigmoid on-site switching-function \( N/[1+\exp(-E/T)] \) Fermi-Dirac quantum-statistics trapping the ANN in non-optimal local-minima necessitating time and memory costly Boltzmann-machine followed by simulated-annealing to eliminate the +1 converting Fermi-Dirac quantum-statistics into Maxwell-Boltzmann classical-statistics. They realized this time and memory costly crutch could be eliminated by reversing sigmoid-function to \( N/[\exp(-E/T)-1] \) Bose-Einstein quantum-statistics["Eureka!"] and then taking the limit as \( N \) approaches infinity. Bose-Einstein condensation (BEC) ["Shazam!"] blindingly quick ANN AI QC (N)-BEC-machine.

KA WA YIP (Presenter), MOSTAFA KHEZRI, DANIEL A LIDAR, Univ of Southern California — We devise a quantum feedback error correction method to reverse the effect of thermal excitations in quantum annealing. Conditioned on the output signal \( I(t) \) from continuous measurement records, feedback is applied to an adiabatically evolving system in the hopes of increasing the ground state population at the end of the anneal. We propose an experimental setting for such continuous measurement and feedback in the case of superconducting flux qubits. We simulate the error correction performance of a system weakly coupled to a thermal bath based on methods like quantum trajectories and quantum bayesian updates. We also derive a feedback master equation for markovian feedback (feedback delay \( \tau \to 0 \)) and further give the timescale condition for feedback Markovianity. Realistic feedbacks are also subjected to non-negligible feedback delay, detector efficiency, and restrictions on the form of the feedback Hamiltonian due to experimental challenges. We therefore study the effectiveness of feedback correction under such limitations and explore how the optimized feedback delay time depends on the annealing schedule and limitations in other experimental parameters.

*Work supported by IARPA and ARO under Contract No. W911NF-17-C-0050.
C71.00255: Constructing parsimonious control functions using B-splines with carrier waves* N. ANDERS PETERSSON (Presenter), Lawrence Livermore Natl Lab, FORTINO GARCIA, Applied Mathematics, University of Colorado, Boulder, JONATHAN L DUBOIS, Lawrence Livermore Natl Lab — We consider the optimal control problem for realizing logical gates in closed quantum systems, where the evolution of the state vector is governed by the time-dependent Schroedinger equation. The number of parameters in the control functions is made independent of the number of time steps by expanding them in terms of B-spline basis functions, with and without carrier waves. We use an interior point gradient-based technique from the IPOPT package to minimize the gate infidelity subject to amplitude constraints on the control functions. The symplectic Stromer-Verlet scheme is used to integrate a real-valued formulation of Schroedinger’s equation in time and the gradient of the gate infidelity is obtained by solving the corresponding adjoint equation. This allows all components of the gradient to be calculated at the cost of solving 3 Schroedinger systems, independently of the number of parameters in the control functions. The method is applied to Hamiltonians that model the dynamics of several coupled super-conducting qubits. We find that including judiciously chosen frequencies in the carrier waves of the basis functions can significantly reduce the number of parameters and lead to smoother control functions.


C71.00256: Learning Quantum Error Models* WILLIAM MOSES (Presenter), Massachusetts Institute of Technology MIT, COSTIN IANCU, WIBE A DE JONG, Lawrence Berkeley National Laboratory — In this abstract we propose a methodology for learning quantum error models from experimental data. This information is useful for characterizing the effectiveness of hardware, predicting how well a circuit should run in practice, and synthesizing corrected circuits that attempt to perform better by taking the error model into account.

We learn the error model by taking each gate in the original circuit and replacing it with a parameterized probability distribution over potential gates. For example, we could replace a Pauli X gate with a distribution having probability p of performing a random unitary and probability 1-p of performing the Pauli X. We then perform bayesian inference to deduce the most likely error model that gave us the desired error.

We test our methodology on experimental data, and evaluate the learned error models in its predictive power.

*William S. Moses was supported in part by a DOE Computational Sciences Graduate Fellowship DE-SC0019323, NSF Grant 1533644 and 1533644, LANL grant 531711, and IBM grant W1771646. Work at LBNL was supported by the DOE Office of Advanced Scientific Computing Research (ASCR) under contract DE-AC02-05CH11231 through the Quantum Algorithms Team.
C71.00257: An information entropy interpretation of photon absorption by dielectric media*  
SUNG WOOK HAN (Presenter), Department of Physics, Jeonbuk National University, 
PUREVDORJ MUNKHBAATAR, Institute of Photonics and Information Technology, Jeonbuk National University, KIM MYUNG-WHUN, Department of Physics, Jeonbuk National University — We measured photon absorption in dielectric media and proposed the photon-version Beer–Lambert’s law to quantify the absorption. We used a Hong–Ou–Mandel interferometer and 810 nm twin-photons. We found that the depth ratio of the null point in the interference patterns of the interferometer agreed with the classical transmittance of the samples. We established a statistical model of the photon absorption process and proposed an information entropy interpretation to understand the meaning of the Beer–Lambert law. Comparisons of the results of the photon absorption experiments with classical experiments demonstrate the validity of our model and interpretation.

*We acknowledge the support of the National Research Foundation of Korea (grant number: 2016R1D1A1B03934648).

C71.00258: Simulating broken PT-symmetric Hamiltonian systems by weak measurement*  
MINYI HUANG, School of Mathematical Sciences, Zhejiang University, RAY-KUANG LEE (Presenter), Natl Tsing Hua Univ, LIJIAN ZHANG, College of Engineering and Applied Sciences, Nanjing University, SHAO-MING FEI, School of Mathematical Sciences, Capital Normal University, JUNDE WU, School of Mathematical Sciences, Zhejiang University — By embedding a PT-symmetric (pseudo-Hermitian) system into a large Hermitian one, we disclose the relations between PT-symmetric quantum theory and weak measurement theory. We show that the weak measurement can give rise to the inner product structure of PT-symmetric systems, with the pre-selected state and its post-selected state resident in the dilated conventional system. Typically in quantum information theory, by projecting out the irrelevant degrees and projecting onto the subspace, even local broken PT-symmetric Hamiltonian systems can be effectively simulated by this weak measurement paradigm.

*National Natural Science Foundation of China (11171301, 11571307, 11690032, 61490711, 61877054 and 11675113), National Key R&D Program of China under Grant No. 2018 YFA0306202, Beijing Municipal Commission of Education (KZ201810028042), and Ministry of Science and Technology of Taiwan (105-2628-M-007-003-MY4).
C71.00259: Knowledge is the Foundation of the Functioning of the Physical World in QM: Everything Goes Through the Wave Function, Including Null Measurements, Expansion of On the Nature of the Change in the Wave Function in A Measurement in Quantum Mechanics [arxiv, 1995]  DOUGLAS SNYDER (Presenter), None — Nothing in quantum mechanics (qm) occurs without the involvement of the wave function (wf); the wf is non-physical. When a measurement is made of 1 quantity, a new wf accompanies the measurement wherein another quantity of the particle is uncertain due to the wf, eg, position requiring many superposed waves and momentum requiring only 1 wave. Many situations showing the indispensability of the wf are discussed. What prevents knowledge based on the wf from being acknowledged as the foundation of the physical world is the assumed unavoidable physical interaction (pi) between the measuring instrument and the physical entity measured in the change in the wf in a measurement. This is explored in part through Feynman's jolt of a photon on an electron in his 2 slit experiment with a light source between the 2 slits. The origin of this assumed unavoidable pi appears to be Bohr's description of complementarity. The source for Bohr appears the psychologist W. James who did not include this pi in his complementarity. Without this pi, the central role of the wave function and knowledge derived from it is clearly seen in quantum mechanics. With null measurements (no pi), the problem that appears to originate with Bohr cannot be avoided. It should not have been avoided in 1995.

C71.00261: How Knowledge Leads to the Demise of Schrodinger's Cat Through a Null Measurement (A Quantum Mechanical Measurement in Which There is No Physical Interaction Between the Measuring Instrument and the Entity Measured)  
DOUGLAS SNYDER (Presenter), None — The Schrodinger cat experiment (SCE) is presented. An alteration follows where the LACK of radioactive decay (rd) leads to the demise of the cat instead of the ACT of rd. The lack of rd is a negative (null) measurement (nm) (where there is NO physical interaction between the radioactive material and the Geiger counter). The nm is non-trivial because all knowledge about the radioactive material (rm) is derived from its associated wave function (wf) which itself has no physical existence. The wf is how we make probabilistic predictions regarding systems in quantum mechanics. Before the box in the SCE is opened, the wf for the rm is: psi_rm = 1/√2 [psi_rm does not decay + psi_rm does decay] which leads to the possibility of interference before the cat is observed. As Schrodinger wrote: “The psi_function of the entire system [including rm and cat] would express this by having in it the living and the dead cat (pardon the expression) mixed or smeared out in equal parts.” The wf is the foundation for knowledge since the probabilities are derived from the wf and the wf contains all the information concerning a system. This alteration of the SCE emphasizes that the lack of rd in the original SCE is also a nm that leads to the continued life of the cat.

C71.00262: A quantum mechanical interpretation of gravitational redshift of photon*  
DONALD CHANG (Presenter), Hong Kong University of Science and Technology — It was observed that electro-magnetic waves can undergo a frequency shift in a gravitational field. This effect is important for satellite communication and astrophysical measurements. Previously, this redshift phenomenon was interpreted exclusively as a relativistic effect. Recently we found this effect can also be explained based on a quantum mechanical consideration. We propose that, due to the quantum nature of the photon, its effective mass is not zero. In a gravitational field, the total energy of the photon includes both its quantum energy and its gravitational energy. Then, the condition of energy conservation will require a frequency shift when the photon travels between two points with different gravitational potentials. This result suggests that the gravitational redshift effect of a photon is essentially a quantum phenomenon. This new understanding has a strong implication; it suggests that some of the previous experimental tests of general relativity need to be re-interpreted.

*This work was supported by the Macro-science project of HKUST.

C71.00263: From Hopf fiberation to duality-entanglement relation  
YUSEF MALEKI (Presenter), Texas A&M Univ — We show that the entanglement-duality relation [Optica 5, 942 (2018)] can indeed be obtained, in its most generic form, from Hopf fiberation and stereographic geometry. We demonstrate that this relation is a natural consequence of the stereographic geometry, providing the first geometric approach to the notion of complementarity problem. We show that this geometry is duality-entanglement sensitive. This means that, it is sensitive to the wave nature, particle nature and entanglement nature of a single qubit.
C71.00264: Programming multi-level quantum gates in disordered computing reservoirs via machine learning and TensorFlow* GIULIA MARCUCCI, DAVIDE PIERANGELI, Univ of Rome La Sapienza, PEPIJN PINKSE, University of Twente, MEHUL MALIK, Herriott Watt University, CLAUDIO CONTI (Presenter), Univ of Rome La Sapienza — Novel machine learning computational tools open new perspectives for quantum information systems. Here we adopt the open-source programming library TensorFlow to design multi-level quantum gates including a computing reservoir represented by a random unitary matrix. In optics, the reservoir is a disordered medium or a multi-modal fiber. We show that trainable operators at the input and the readout enable one to realize multi-level gates. We study various qudit gates, including the scaling properties of the algorithms with the size of the reservoir. Despite an initial low slope learning stage, TensorFlow turns out to be an extremely versatile resource for designing gates with complex media, including different models that use spatial light modulators with quantized modulation levels.[1]


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C71.00265: Quantum Boosting SRINIVASAN ARUNACHALAM, Physics, Massachusetts Institute of Technology, REEVU MAITY (Presenter), Physics, University of Oxford — Boosting is one of the most famous classical machine learning techniques (in theory and practice) that can construct a strong machine learning algorithm given access to a weak learning algorithm. It is natural to consider boosting in the quantum setting for the following reason: suppose we implement a quantum machine learning (QML) algorithm on a NISQ device, then the guarantees of the QML algorithm could be much worse than it was designed for, due to the noise in the quantum system. This motivates the question whether we can "boost" the performance of a weak QML algorithm (implemented on a NISQ machine) to a *strong* QML algorithm?

Classically the time complexity for boosting the performance of a weak learner for a concept class C is characterized by the VC dimension of C. Here, we ask if quantum techniques can provide an improvement over the well-known AdaBoost algorithm introduced by Freund and Schapire '93 (for which they were awarded the Godel prize in 2003). In this work, we introduce the first quantum boosting algorithm which is provably faster than classical Adaboost with time complexity that scales quadratically in the VC dimension of C.
**C71.00266: Layerwise learning for quantum neural networks**  
ANDREA SKOLIK, Ludwig Maximilian University of Munich, JARROD MCCLEAN, MASOUD MOHSENI (Presenter), Google Research, PATRICk VAN DER SMAGT, Machine Learning Research Lab, Volkswagen Group, MARTIN LEIB, Data Lab, Volkswagen Group — We introduce a layerwise learning strategy for parameterized quantum circuits. The circuit depth is incrementally grown during optimization, starting with a shallow circuit and adding depth until the required loss is attained. By training only varying subsets of the circuit’s parameters, we keep a fixed number of training parameters while increasing circuit depth until it is sufficient to represent the data. We then show that this approach avoids the problem of saddle points, or barren plateaus, of the error surface to a large extent due to the low depth of circuits, low number of parameters, and larger magnitude of gradients compared to training the full circuit. These properties make our algorithm ideal for execution on noisy intermediate-scale quantum (NISQ) devices. We demonstrate our approach on an image-classification task on handwritten digits, and show that the number of trained parameters can be decreased substantially while keeping gradient magnitudes larger than those of quantum circuits of the same size trained on a fixed architecture.

*This project has received funding from the European Unions Horizon 2020 research and innovation programme under the Grant Agreement No. 828826.*

**C71.00267: Magnetic and electrical field detection using NV-based AFM**  
WENTIAN ZHENG (Presenter), Peking Univ — We develop a homemade NV-based scanning microscopy to detect both magnetic and electrical field induced by tips we used. As for the magnetic field, the Ni tip is required to provide magnetic field and field gradient on the surface of diamond membrane. The ODMR shift is observed during the Ni tip moving around a NV center, and we observe isomagnetic circle by ODMR mapping which shrinks to about 20nm indicating the actual location of the NV center.

Besides, the sensor we made allow us to apply bias voltage between metal tip and diamond. And the electrical field can be also measured by ODMR and Pulsed ODMR shift. Our results show the electrical field up to 100V/um which maybe controls the charge state of the NV center.
C71.00268: Time resolved diamond magnetic microscopy of single transition metal magnetic nanoparticles* ABDELGHANI LARAOUI (Presenter), Department of Mechanical & Materials Engineering, University of Nebraska - Lincoln, VICTOR ACOSTA, Department of Physics & Astronomy, University of New Mexico — Understanding the magnetic properties of small transition metal magnetic nanoparticles (TMMNPs) can help in exploiting their useful properties such as high surface-to-volume ratio and tailorable surface chemistry for applications in catalysis, biosensing, and ultra-high-density magnetic recording. At size below 10 nm, surface effects play a major role in determining their magnetic properties. Symmetry breaking of the crystal structure at the particle surface, dangling bonds, and surface strain can alter their properties. Accurate measurements of magnetic properties of single TMMNPs would therefore shed light on their critical properties. However, measuring these properties of such small particles at ambient conditions presents a great challenge due to the lack of sensitivity of current nonperturbative magnetic imaging techniques. Here we show recent measurements using magnetic microscopy based on nitrogen vacancy centers in diamond to measure the static and dynamic magnetic properties of individual 2-10 nm TMMNP (CoPt and FePt). Histograms of critical parameters such as magnetic anisotropy, saturation magnetization, and magnetic relaxation are extracted and correlated with morphology data taken by AFM, SEM, and TEM.

*We acknowledge support from NSF-DMR award #1809800

C71.00269: Phase estimation in a multimode nonlienar interferometer.* NARAYAN BHUSAL (Presenter), JONATHAN P DOWLING, Louisiana State University, Baton Rouge — Simultaneous estimation of multiple phase shifts is very important in quantum metrology as it has implications for the single-shot quantum imaging. Multiparameter estimation has been already demonstrated in linear optics even though its performance is greatly limited by computational difficulty associated with matrix permanent. Here, we propose a scheme that uses nonlinear optical parametric amplification (OPA) to estimate multiple simultaneous phase shifts. The performance of our scheme is compared with the SNL and the Heisenberg limit (HL). We choose homodyne as the measurement strategy in our scheme. As photon loss is the biggest experimental limitation, we also investigate the effect of photon loss in the phase sensitivity.

*NB would like to thank Army Research Office (ARO) for the support.
C71.00270: Rare Earth Quantum Information Science Decoherence Times and Hosts  
GAVIN NOP (Presenter), JONATHAN SMITH, Iowa State University — We present a brief review of the current state of Quantum Information Science (QIS), with a focus on Quantum Information Processing (QIP) and the challenges posed by short decoherence times. Rare earth based systems have the potential to resolve many of the issues faced in QIS. Due to their 4f orbitals, rare earth atoms, when implanted into an appropriate host, demonstrate relatively high coherence times. We cover benefits and challenges regarding QIP, specifically quantum processing and optical quantum memory. We emphasize important results in recent experiments regarding rare earth-based quantum computers, and compare these results to the current state of the art in qubit design. Specifically, we perform electronic structure calculations for a rare earth ion-doped wide band gap crystal and control quantum states offered by the doped ion. G.N. is grateful for an assistantship in the US DOE Office of Science, Science Undergraduate Laboratory Internship program.

C71.00271: WITHDRAWN ABSTRACT  —

C71.00272: Experimental demonstration of the validity of the quantum heat-exchange fluctuation relation in an NMR setup.*  
SOHAM PAL (Presenter), T.S. MAHESH, BIJAY AGARWALLA, IISER Pune — We experimentally explore the validity of the Jarzynski and Wójcik quantum heat-exchange fluctuation relation by implementing an interferometric technique in liquid-state nuclear magnetic resonance setup and study the heat-exchange statistics between two coupled spin-1/2 quantum systems. We experimentally emulate two models—(i) the XY-coupling model, containing an energy conserving interaction between the qubits, and (ii) the XX-coupling model—and analyze the regimes of validity and violation of the fluctuation symmetry when the composite system is prepared in an uncorrelated initial state with individual spins prepared in local Gibbs thermal states at different temperatures. We further extend our analysis for heat exchange by incorporating correlation in the initial state. We support our experimental findings by providing exact analytical results. Our experimental approach is general and can be systematically extended to study heat statistics for more complex out-of-equilibrium many-body quantum systems.

*The authors acknowledge the startup funding, IISER Pune, the IndiaMax Planck mobility grant, Department of Science and Technology, India (Grant No. DST/SJF/PSA-03/2012-13) and the Council of Scientific and Industrial Research, India (Grant No. CSIR- 03(1345)/16/EMR-II).
C71.00273: Collective enhancements in charging quantum batteries via a quantum heat engine

KOBUKE ITO (Presenter), Graduate School of Engineering Science, Osaka University, GENTARO WATANABE, Department of Physics and Zhejiang Institute of Modern Physics, Zhejiang University — As a model of so-called quantum battery, a quantum system as an energy storage, we study the charging of many two-level systems via a quantum heat engine. Especially, we focus on the collective effects in the charging. We show that the collective charging outperforms in the amount of the stored energy, its fluctuation, and the charging speed in comparison to the individual one. In the collective charging, symmetry of the interaction between the engine and the battery causes emergent bosonic quantum statistics, which result in a collective high probability excitation.

*This work is supported by the Zhejiang Provincial Natural Science Foundation Key Project (Grant No. LZ19A050001), by NSF of China (Grant No. 11674283), by the Fundamental Research Funds for the Central Universities (2017QNA3005, 2018QNA3004), by the Zhejiang University 100 Plan, and by the Junior 1000 Talents Plan of China. J. I. is also supported by MEXT Quantum Leap Flagship Program (MEXT Q-LEAP) (Grant No. JPMXS0118067394).

C71.00274: Controlling quantum dot level spacing: moving beyond the constant interaction model

ZACHARY PARROTT (Presenter), JACKSON KUKLIN, BRADLEY LLOYD, MEGAN SMITH, MEENAKSHI SINGH, Physics, Colorado School of Mines — Proposed large scale implementation of gate defined semiconductor quantum dots requires effective means to tune each dot to desired tunnel coupling, capacitive coupling to gates, and coupling to sources of decoherence such as the phonon bath. These parameters are currently understood within the context of the constant interaction model that predicts a periodic level spacing based on a constant capacitance of each dot to the relevant gates. Yet, the actual capacitance of the dot is not a constant and depends on parameters including the electron number, voltage of the associated gates, and size of the dot, leading to a nonlinear level spacing. We show how taking these parameters into consideration enables greater control of each quantum dot. We also present a means to change the dot level spacing, thereby changing the coupling to the phonon bath, while maintaining desired tunnel coupling in a framework similar to virtual gating for cross capacitance. The results are relevant to minimizing decoherence in quantum dot qubits.

C71.00275: Auto-tuned quantum dots in silicon as a candidate platform for scalable quantum computing and quantum neuromorphic devices

BRADLEY LLOYD (Presenter), MEGAN SMITH, ZHEXUAN GONG, MEENAKSHI SINGH, Colorado School of Mines — Spin qubits in gate defined quantum dots in silicon present a robust architecture for quantum information processing due to long coherence times, tune-ability, and scalability. However, the fabrication of such qubits leads to strong device variability, making it challenging to scale up the number of qubits for quantum computing applications. To address this challenge, we present our new device design and an automation protocol development to tune individual qubits. This automation protocol works to counteract device variability, resulting in greater scalability and versatility for the device. From this versatility we will explore the potential of using these auto-tuned quantum dots as quantum neuromorphic devices by engineering a non-Markovian bath for one or more qubits.
Controllable interaction between superconducting qubits is desirable for scalability architectures and quantum simulation applications. We experimentally demonstrate a simple-design tunable coupler, achieving a continuous tunability and almost zero coupling strength. Based on the tunable interaction between two qubits via the coupler, we first construct two-qubit iSWAP and control-Z (CZ) gate by applying standard rectangular pulses. We then propose a new 'Dynamic-Total-Closing' (DTC) technology to implement the CZ gate, which adopts a graded flux pulse for the qubit to approach the avoided crossing slowly, meanwhile dynamically closing the qubit-qubit coupling with a special pulse shape during the approaching process (fidelity up to 98.4%). Furthermore, we also try iSWAP gate by parametrically oscillating coupler at the qubit-qubit detuning and cross-resonance gate by tuning coupler frequency to explore the influence of ZZ interaction.

C71.00277: WITHDRAWN ABSTRACT —

C71.00278: THz Sommerfeld Wave Propagation on Superconducting Niobium Wire for Millimeter-Wave Interconnects* BHARAT KUCHHAL (Presenter), Stanford Univ, EMMA SNIVELY, SLAC National Accelerator Laboratory, KEVIN MULTANI, HUBERT STOKOWSKI, AMIR SAFAVI-NAEINI, Stanford Univ, PAUL B. WELANDER, EMILIO NANNI, SLAC National Accelerator Laboratory — Although there has been a stupendous development of superconducting microwave circuits, scalability and transmission of quantum information remain important issues. One approach involves the transduction of quantum information from microwave to millimeter-wave frequencies prior to transmission. For efficient transmission of THz waves, the development of millimeter-wave interconnects is a vital challenge. In this pursuit, we propose to transmit Sommerfeld waves in the THz regime on the surface of a single superconducting Niobium wire connected between a pair of horn antennas and W-band (75 – 110GHz) waveguides. The Sommerfeld mode on single conductors in the THz frequency range have demonstrated very low losses with room temperature conductors. Compared to the room temperature, our calculations show an increase in conductivity of superconducting Niobium by two orders of magnitude, which indicates significantly lower losses are possible for links at a few Kelvin.

*Work supported by the U.S. Department of Energy under contract number DE-AC02-76SF00515.
**C71.00279: Disorder-free localization in the Kitaev Honeycomb Model**

ADRIAN CHAPMAN, Physics, University of Sydney, SAYONEE RAY (Presenter), Physics, University of New Mexico — We study operator propagation and scrambling in the two-dimensional Kitaev honeycomb model. An exact solution for this model allows us to calculate the infinite-temperature out-of-time-ordered correlator for Pauli observables, where we find that the infinite-temperature average over gauge sectors manifests as a disorder average for this quantity. This induces a localization effect for observables in the bond algebra of the Hamiltonian, while observables outside of the algebra completely scramble. We interpret our result in terms of the diffusion of Pauli strings, whose endpoints are localized yet whose interiors propagate freely. We further find that, in the ground state gauge sector of the model, operators do not localize. We further extend our analysis to the finite temperature regime using Monte Carlo Metropolis-Hastings methods.

*NSF FRHTP grant, Centre for Engineered quantum systems

**C71.00280: DATA SCIENCE**

**C71.00281: Combinatorial fabrication and spectroscopic analysis of Fe-Co-Cr ternary alloy thin film**

TADASHI NISHIO (Presenter), MASahiRO YAMAMOTO, Sci Univ of Tokyo, TAKUO OHKOCII, SPring-8, MASATO KOTSUGI, Sci Univ of Tokyo — The development of a high-throughput experiment is an important issue in materials informatics, especially for materials discovery. Recently, combinatorial deposition and high-throughput analysis are rapidly progressed [1]. However, the combination of material fabrication and property analysis still leaves much room for development. Particularly, a question is raised about whether comprehensive phase diagram mapping is the optimum solution for materials discovery. Here, we focus on exploring the phase transition for the materials discovery and combined the combinatorial wedged thin film deposition, the synchrotron-based micro-spectroscopic characterization, and the statistical analysis of experimental bigdata. X-ray absorption spectrum and magnetic circular dichroism (MCD) information were recorded by photoelectron emission microscopy. We obtained chemical components and magnetic contrast in each pixel of the image and analysed the histogram of MCD contrast as a variation of the chemical composition of Fe-Co-Cr. We fitted MCD histogram by Landau theory to discuss the ferromagnetic phase transition.

Normal mode analysis of a relaxation process with Bayesian inference ITSUSHI SAKATA (Presenter), YOSHINO NAGANO, YASUHIKO IGARASHI, SHIN MURATA, Univ of Tokyo, KOHJI MIZOGUCHI, Osaka Prefecture University, ICHIRO AKAI, Kumamoto University, MASATO OKADA, Univ of Tokyo — Relaxation processes provide many insights into atomic/molecular structures and the kinetics and mechanisms of chemical reactions. For the analysis, the extraction of modes that are specific to the phenomenon of interest is unavoidable.

In this study, to construct a data-driven technique for relaxation processes, we propose a framework to systematically extract normal modes from the viewpoint of model selection with Bayesian inference. Our approach consists of a well-known method called sparsity-promoting dynamic mode decomposition, which decomposes a mixture of damped oscillations, and the Bayesian model selection framework. We numerically verify the performance of our proposed method by using coherent phonon signals of a bismuth crystal and virtual data as typical examples of relaxation processes. Our method succeeds in extracting the normal modes even from experimental data with significant trends. Moreover, the selected set of modes is robust to observation noise, and our method can estimate the level of observation noise. From these observations, our method is applicable to normal mode analysis, especially for data with significant trends, which broadens the applicability of the data-driven approach in analyzing relaxation phenomena in material science.

Predicting Ionic Liquids Properties with Machine-Learning ZAFER ACAR (Presenter), MICHAEL MUNJE, PHU NGUYEN, Computer Science, California State University, Northridge, KAHCHUN LAU, Physics and Astronomy, California State University Northridge — Since the last decade, there has been a dramatic increase in the number of ionic liquids (ILs) synthesized, tested and utilized in various applications (e.g. energy storage, CO₂ capture, catalysis, lubricant additives, etc.). The intense interest has been due to the various novel properties that can be found in ionic liquids, such as tunable ionic conductivity, negligible vapor pressure, liquid phase within a wide temperature range, non-flammability at ambient condition, etc. Among these properties, the melting point (Tₘ) of ionic liquids (IL) are very important in various applications. However, the Tₘ can change considerably depending on the molecular structures of the anions and cations. In this study, we will explore the use of various machine learning methods to predict the melting points of various ILs that consists of several different cation and anion classes. In addition to melting point prediction, some of the related structures-properties studies of ILs will be discussed.

*This work is supported by Alfred P Sloan Foundation and CSUN Faculty start-up fund.
C71.00284: Interpretable modeling by linearly independent descriptor generation method

HITOSHI FUJII (Presenter), National Institute for Materials Science, TAMIO OGUCHI, Osaka University — For interpretable modeling, linear regression combining descriptor generation and selection operator, such as approach of Ghiringhelli[1] and Ouyan[2], is very effective. However, multicollinearity (MC) (and near multicollinearity) between descriptors that are problematic in linear regression analysis can reduce the quality of the descriptor selection. Therefore, we proposed the linearly independent descriptor generation (LIDG) method[3] that generates descriptors while removing MC. This approach can improve their approach.

In this presentation we will present some application examples.

References:

C71.00285: Artificial Intelligence to detect gravitational waves from a network of detectors

THILINA SHIHAN WEERATHUNGA (Presenter), Department of Physics and Astronomy, University of Texas Rio Grande Valley — The application of artificial intelligence in astronomical data analysis is becoming more popular among the scientific community. In our recent work [1,2], we have shown the effectiveness of Particle Swarm Optimization (PSO), a well-known algorithm in the field of swarm intelligence, in addressing signal detection and parameter estimation problem related to gravitational waves from compact binary coalescences (CBCs). The fully coherent network analysis of data from multiple gravitational wave (GW) detectors is computationally expensive since it is associated with a high dimensional numerical optimization problem. In our previous work, we showed using a non-spinning 2.0 post-Newtonian order waveform and four gravitational wave detectors (two LIGO detectors, Virgo and Kagra) that PSO can achieve the same performance as a grid search with less than 200,000 templates for a component mass range of 1.0 to 10.0 solar masses at a network signal to noise ratio of 9. Currently, we are increasing the dimensionality of the optimization problem by adding spin parameters to the waveform and exploring the effectiveness of the algorithm.

C71.00286: Machine learning to predict microbial community traits driving carbon fixation*
JARON THOMPSON (Presenter), Colorado State University — Microbial communities are ubiquitous influencers of macroscopic environments, yet overwhelming complexity makes it difficult to decipher functional relationships between specific microbes and ecosystem properties. Integrating advances in DNA sequencing technology with computational approaches like machine learning (ML) could address this problem. In [Thompson et al, PLoS One, 2019], we applied neural networks, random forest models, and indicator species analyses to correlate microbiome data (16S rRNA gene profiles) with dissolved organic carbon (DOC) content after 44 days of plant litter decomposition. We analyzed 300+ soil microcosms, including 1709 total bacterial operational taxonomic units (OTUs), and performed multiple-model feature reduction. We are now leveraging Bayesian network structure learning to infer mechanistic interactions between microbial species abundance and DOC. After training a Bayesian network model using pine litter data, we predict DOC results of independent oak litter experiments and demonstrate that relationships between microbial species abundance and DOC are conserved across litter types.

*This research was supported by grant F255LANL2018 from the U.S. DOE/BER, Genomic Science program and under award R35GM124747 from NIH/NIGMS.

C71.00287: ParaMonte: A high-performance parallel library for Monte Carlo optimization, sampling, and integration  FATEMEH BAGHERI (Presenter), AMIR SHAHMORADI, University of Texas at Arlington — At the foundation of predictive science lies the scientific methodology, which involves multiple steps of observational data collection, developing testable hypotheses, and making predictions. Once a scientific theory is developed, it can be cast into a mathematical model whose parameters have to be fit via observational data. This leads to the formulation of a mathematical objective function for the problem at hand, which has to be then optimized to find the best-fit parameters of the model or sampled to quantify the uncertainties associated with the parameters, or integrated to assess the performance of the model. Toward this goal, a highly customizable, user-friendly high-performance parallel Monte Carlo optimizer, sampler, and integrator library is presented here which, can be used on a variety of platforms with single to many-core processors, with interfaces to popular programming languages including Python, and Fortran/C/C++. In particular, we discuss the parallel implementation of a variant of Markov Chain Monte Carlo known as Delayed Rejection Adaptive Metropolis (DRAM) and its scalability.

C71.00288: COMPUTATIONAL PHYSICS —
Building a DLS Device to Measure In Situ Glycine Cluster Formation

HANNAH FEJZIC (Presenter), California State University, San Bernardino, BRUCE ALLEN GARETZ, OMAR GOWAYED, Chemical Engineering, New York University — Laser trapping nucleation uses optical tweezers focused at the air-solution interface to grow crystals. Research has shown that focusing a continuous wave (CW) laser at the glass-solution interface of a solution of glycine in deuterium oxide, does not lead to nucleation, but to laser-induced phase separation (LIPS) droplet formation. The LIPS droplet is about double the concentration of the initial solution, past the metastable zone. This droplet is believed to be made up of large, liquid-like clusters of glycine that are organized in a size gradient with larger clusters in the center of the solution. Minutes after the LIPS droplet relaxes over a few minutes, clusters in the LIPS droplet spontaneously organize into a critical nucleus. Microscopic demixing of the solution is believed to leads to the observed polymorph-selectivity for LIPS droplet-grown crystals. To better understand the LIPS droplet, a dynamic light scattering (DLS) device will be constructed to observe the LIPS droplet in situ. By measuring the hydrodynamic radius of the glycine particles in situ, one can better understand this crystal growth mechanism.

This work was supported by the MRSEC Program of the National Science Foundation under Award Number DMR-1420073.

First-principles calculations study of electronic structure, optoelectronic, vibrational analysis, linear and nonlinear optical properties of 4,5-dibromo-2,7 dinitrofluorescien

JEAN BAPTISTE FANKAM FANKAM (Presenter), Department of Physics, University of Yaounde I — Theoretetical inverstigation on 4,5-dibromo-2,7 dinitrofluorescien at the RHF level and different DFT with the cc-pVDZ basis set with the help of Gaussian 09 suit of program software. We have firstly modeled and optimized the geometry of the structure and further, we have computed the frequencies' analysis to understand the thermodynamic, optoelectronic, linear and nonlinear optical properties. As far as this analysis is concerned, we have also been able to come out successful with a well calculated chemical reactivity and stability of the molecule through frontier molecular orbitals defined by the higher occupied and lower unoccupied molecular orbitals (EHOMO and ELUMO). Our results insinuate that this molecule has a potential application in linear and nonlinear optical materials, and optoelectronic devices due to his large hyperpolarizability and can be a promising compound for optical limiting applications. Presently, no experimental and theoretical values in literature were determined for the above properties are available, we are hopeful that our final results will provide important information for further studies of this compound in NLO materials and optoelectronic devices.

No finding
C71.00291: Computational Synthesis of 2D Materials: A High-Throughput Approach to Materials Design* TARA BOLAND (Presenter), ARUNIMA SINGH, Arizona State Univ — The emergence of two dimensional materials opened up many potential avenues for novel device applications such as nanoelectronics, topological insulators, field effect transistors, microwave and terahertz photonics and many more. To date there are over 1,000 theoretically predicted 2D materials. Only 55 2D materials have been experimentally synthesized. Computational methods such as density functional theory can be used to determine the suitable substrates to synthesize 2D materials. Using various 2D materials databases and van der Waals corrected density functional theory we investigate the suitability of 12 substrates to stabilize 2D growth. For materials which meet the criteria for suitable substrate-assisted synthesis methods such as chemical vapor deposition or mechanical exfoliation, the density of states is computed to characterize the electronic properties of these materials for device applications.

*The authors would like to acknowledge Research Computing at Arizona State University and XSEDE for providing HPC resources and storage that has contributed to the research results to be reported.

C71.00292: Predicting the properties of ultrathin magnetic $H_xCrS_2$ from first principles and machine learning* DANIEL WINES (Presenter), JARON KROPP, CAN ATACA, Univ of Maryland-Baltimore County — An air stable $H_xCrS_2$ layered material has been synthesized by soft chemical methods, which can be exfoliated down to ultrathin layers, providing a promising path for the synthesis of two-dimensional (2D) magnets\(^1\). Although a reliable synthesis method has been developed, the atomic structure is still unknown. Variables such as Cr vacancies and H impurities must be determined in order to understand the properties of this material for device applications. We used a combination of density functional theory (DFT), molecular dynamics (MD) and cluster expansion formalism to study the energetics as a function of Cr vacancies and H impurities. From here, we studied the stability, electronic and magnetic properties of these $H_xCrS_2$ structures and examined the effect of layering on these properties. In order to extend our calculations to a wider range of structures, we trained a machine learning algorithm with our DFT and MD calculated data to predict the properties of other $H_xCrS_2$ based materials outside our training set.

\(^1\)X. Song et. al, J. Am. Chem. Soc. 141, 15634 (2019)

*NSF DMR-1726213
C71.00293: Novel Solid-State Electrolytes for Li Ion Batteries by Computational Design and High-throughput Ab Initio Calculation  WONSEOK JEONG (Presenter), Seoul National University, YOUNGHO KANG, Korea Institute of Materials Science, SEUNGWU HAN, Seoul National University — Solid-state electrolytes (SSEs) can alleviate many of the issues of Li-ion batteries arising from the utilization of the organic liquid electrolytes. Up to date, several SSEs have been proposed from previous experiments or computational screening from publicly available materials databases, however, none of those SSEs are fully satisfactory. In this work, we take one step further; instead of simply exploring a pre-existing materials database, we try to design new materials with aliovalent substitution of cations. This aliovalent substitution is known to facilitate kinetics of Li diffusion. We first screen potential host materials for generating new SSEs by aliovalent substitution, considering fundamental properties such as the presence of transition metals, thermodynamic stability, and band gap. Afterward, we crudely examine the potential energy surface (PES) around the Li ion at interstitial sites. The materials with the most smooth PES are then chosen for the possible candidate for the host material. Finally, we choose some materials from the candidate list and demonstrate that indeed they become a Li ion conductor after aliovalent doping. Starting from 42,337 structures, we find a number of SSEs with predicted Li ionic conductivity comparable to the state-of-the-art \( \text{Li}_{10}\text{GeP}_2\text{S}_{12} \).

C71.00294: COMPUTATIONAL STUDY OF THE INTERACTION OF A WATER MOLECULE WITH 2D-HBN(TWO-DIMENSIONAL HEXAGONAL BORON NITRIDE) AND WITH TI-2D-HBN  GREGORIO RUIZ-CHAVARRIA (Presenter), UNIVERSIDAD AUTONOMA CHAPINGO — After graphene synthesis in 2004 many two dimensional systems has been studied, since the possible applications of these are many. In this work I made a computational study of the interaction of a water molecule with two dimensional hexagonal boron nitride(2D-HBN). First the stability of the 2D-HBN is obtained using Density Functional Theory, Atomic Pseudopotentials,Born-Oppenheimer approximation and molecular dynamics. Next I cause this system to interact with a water molecule. In a second moment, I made a computational study the stability of the system 2D-HBN, but adding a Titanium atom, the system Ti-2D-HBN. Again I provoke the interaction between a water molecule and the Ti-2D-HBN system. I show the results of my calculations, and these are compared with other computational and experimental results.
C71.00295: Real-space Moiré potential, lattice corrugation, and band gap variation in a MoTe$_2$/MoS$_2$ heterobilayer*  WENTONG GENG, National Institute for Materials Science, VEI WENG, Department of Applied Physics, Xi’an University of Technology, TAKAHISA OHNO, JUN NARA (Presenter), National Institute for Materials Science — To have a first-principles description of the Moiré pattern in a transition metal dichalcogenide heterobilayer, we have carried out DFT calculations, taking full accounts of both atomic registry in and the lattice corrugation out of the atomic layers, on a MoTe$_2$/MoS$_2$ system which has a moderate size of superlattice larger than an exciton yet not large enough to justify a continuum model treatment. We find that the local potential in the midplane of the bilayer can serve as an excellent illustration of the Moiré pattern in the van der Waals heterostructure. In the Mo atomic planes, the array of local potential planar maximum (LPPM), rather than the local potential itself, makes the Moiré pattern more obvious. Significant lattice corrugation is found in both MoTe$_2$ (0.30Å) and MoS$_2$ (0.77Å) layers. The interlayer Moiré potential, defined as the LPPM difference between the Mo atomic planes, has a depth of 0.20 eV and changes in direct correlation to the band gap variation in the Moiré cell, which has an amplitude of 0.04 eV. Wrinkling of the MoTe$_2$/MoS$_2$ bilayer enhances the spatial variation of the local band gap by 5 meV; by contrast, its influence on the global band gap is within 1 meV.

*This work was supported by Innovative Science and Technology Initiative for Security, ATLA, Japan.

C71.00296: Simultaneous Prediction of the Magnetic and Crystal Structure of Materials*  PHIL HASNIP (Presenter), ED HIGGINS, MATT I. J. PROBERT, University of York — The coupling between magnetic properties and crystal structure in many magnetic materials means that it is essential to take a holistic approach to predicting their structure. We present for the first time a genetic algorithm that performs a simultaneous global optimisation of both magnetic structure and crystal structure, and illustrate its utility in a range of systems including a complex interface structure between a half-metallic Heusler alloy and a semiconductor substrate.

*Funding from EPSRC grant EP/R025770/1 and a DTA scheme is acknowledged with gratitude. Computing resources on ARCHER were provided by UKCP under EPSRC grant EP/P022561/1.
C71.00297: Minimization studies of elemental carbon using LCBOP semi-empirical potential. PHILIP CHROSTOSKI (Presenter), CHATHURI SILVA, PHILIP FRAUNDORF, University of Missouri - St. Louis — Elemental carbon is interesting to study thanks to its material properties and structural diversity, which ranges from nanotubes through graphite to diamond. In our study of slow-cooled carbon droplets condensed in cool-star atmospheres, computational study with semi-empirical potentials is complementary to experiment and \textit{ab initio} work. We've used the long-range carbon bond-order potential to relax, via conjugate gradient, 1.8 g/cc liquid-like carbon tiled-cube and isolated-cluster systems with 13, 20 and 100 atoms, as well as tetrahedral nanodiamond clusters of 17, 22 and 29 atoms. Tiled-cube simulation nearest neighbor histograms show a bond defining gap between 1.7-2.0 Å. Coordination statistics then show a high percentage of sp and sp2 coordination. Ring sizes of 5 - 7 atoms form more prominently than others, with 5 and 6 atom rings especially abundant. Isolated cluster relaxations show a high amount of sp chains forming, and less ring formation than the tiled-cube simulations. We also see a volume increase for the isolated clusters, unlike comparable density functional theory (DFT) simulations. Our isolated diamond-cluster relaxations saw less surface reconstruction than with DFT.

C71.00298: Line integral approach for fiber-fiber interactions implemented in LAMMPS ANIRBAN PAL (Presenter), West Texas State Univ — Fiber networks are currently modelled using discrete bead-spring type molecular models or cylindrical discrete-element (DEM) models. Bead-spring models often suffer from issues arising from artificial friction originating at the bead-bead contacts, and DEM-type models suffer from high computational demands. Thus, there is a need for better models. Here, the cohesive interaction energy between straight fibers is expressed as a double integral. This double integral can be converted into a single integral that has two terms in its integrand: $g(r)$, which depends on the relative geometrical positioning of the fibers, and $V(r)$, which reflects the interaction energy. Although $V(r)$ is readily available in analytical form, $(can be of the lennard-jones type)$, $g(r)$, which is essentially a distance distribution function of point-pairs located across 2 fibers, requires computation. The method to compute $g(r)$ involves elliptic integrals and is computationally demonstrated in this work. An implementation of the resulting fiber-fiber interaction is demonstrated in LAMMPS, a popular molecular dynamics package, and its computational and scientific performance is evaluated.

C71.00299: First Principles Evaluations of the Spin-Orbit Couplings in Crystals* KENSUKE KURITA (Presenter), TAKASHI KORETSUME, Tohoku University — The spin-orbit coupling (SOC) plays a crucial role in many spin-related phenomena such as anomalous Hall effect and spin Hall effect. However, the strength of the SOC in solids and its relation to the isolated limit have not been well understood. Here, we quantify the atomic SOC in solids by constructing the tight-binding Hamiltonian from the Wannier functions obtained by the first-principles calculation. By calculating the atomic SOC in monatomic crystals and binary compounds systematically, we find that the strength of the atomic SOC is not the atom-specific property but depends much on the crystal structure and chemical composition. We show that its crystal dependence is well explained by the spread of the Wannier function.

*This work is supported by JSPS KAKENHI Grant Number JP18K03442 and JP19H00650 and the WISE Program for AI Electronics, Tohoku University.
C71.00300: Time-evolution of a Schrödinger electron driven by a localized oscillating potential

LIUBOV ZHEMCHUZHNA (Presenter), GODFREY GUMBS, Hunter college, M. LAWRENCE GLASSER, Clarkson University, ANDRII IUROV, Medgar Evers college, DANHONG HUANG, Air Force Research Lab — We have obtained a semi-analytical solution of the Schrödinger equation for a massive particle in the presence of a harmonic time-dependent \( \sim \cos (\omega t) \) single-point \( \sim \delta(x) \) potential. We present a detailed analysis for determining the dependence of the wave function on the amplitude and frequency of the oscillatory potential, and the chosen initial conditions for the particle wave function. We have considered separately when either the potential is negative and leads to a bound state or is positive thus yielding scattering. Our derived results could be interpreted as being related to the dynamics of an electronic Floquet state subjected to a localized laser-induced dressing field.

C71.00301: Theory of phonon glass behaviour in host-guest thermoelectrics with avoided crossing

BINGYU CUI (Presenter), Univ of Cambridge, MATTEO BAGGIOLI, Universidad Autonoma de Madrid, ALESSIO ZACCONE, University of Milan — An analytical model is developed to describe the phonon dispersion relations of thermoelectrics with the presence of heavy guest atoms (rattlers). The model also accounts for anharmonic effects in phonon damping. The spectrum of low energy states contains acoustic-like and (soft) optical-like modes, which display the typical avoided crossing, and which can be derived analytically by considering the dynamical coupling between host lattice and guest rattlers. Inclusion of anharmonic damping in the model allows us, for the first time, to compute the vibrational density of states (VDOS) and the specific heat, unveiling the anomalous boson peak (BP) relating to the glassy behaviour of phonons in the otherwise crystalline material. We discuss the dynamics of the BP as a function of the strength of the interaction between the soft modes and the anharmonic lattice, and of the energy gap between the two avoided-crossing branches. Moreover, we find a robust linear correlation between the BP frequency and the energy of the soft optical-like modes.

*M.B. acknowledges the support of the Spanish MINECOs Centro de Excelencia Severo Ochoa Programme under grant SEV-2012-0249.
B.C acknowledges financial supports of Cambridge-CSC scholarship,
C71.00302: Giant effect of spin-lattice coupling on the thermal transport in two-dimensional ferromagnetic CrI₃  GUANGZHAO QIN (Presenter), University of South Carolina, ZHENZHEN QIN, Zhengzhou Univ, HUIMIN WANG, Nanjing University, MING HU, University of South Carolina — Recently, two-dimensional monolayer chromium triiodide (CrI₃) with intrinsic magnetism was discovered, which shows promising applications in many technologies from sensing to data storage where thermal transport play a key role. So far the effect of spin-lattice coupling on the thermal transport properties has not been explored yet. In this talk, I would like to present the giant effect of spin-lattice coupling on the thermal conductivity of monolayer CrI₃. The thermal conductivity is more than two orders of magnitude enhanced by the spin-lattice coupling. The effect is found to be especially stronger for the acoustic phonon modes, which dominates thermal transport with spin-lattice coupling. Deep analysis shows that the reason lies in the weakened phonon anharmonicity by spin-lattice coupling. The bond angle and atomic position are changed due to the spin-lattice coupling, making the structure more stiff and more symmetric, which lead to the weaker phonon anharmonicity, and thus the enhanced thermal conductivity. This study uncovers the giant effect of spin-lattice coupling on the thermal transport, which would deepen our understanding on thermal transport and shed light on future research of thermal transport in magnetic materials.

C71.00303: Resonantly enhanced polariton wave mixing and Floquet parametric instability  SHO SUGIURA (Presenter), MIKHAIL LUKIN, EUGENE DEMLER, Harvard University, DANIEL PODOLSKY, Technion — Recent experiments by Cartella et al. [1] demonstrated terahertz optical amplification in SiC insulator following a strong mid-IR pump that resonantly excited the SiC stretching mode. Motivated by these experiments we study the problem of light reflection from a slab of insulating material with a strongly excited polariton mode. We introduce a new theoretical approach for analyzing this system using the Floquet formalism, in which polariton oscillations provide periodic time modulation. We present an analytic solution of the Fresnel light reflection problem. We demonstrate discontinuous dependence of the reflection coefficient on the incoming photon frequency, which we attribute to the existence of unstable polariton modes. We interpret these instabilities as resonantly enhanced polariton parametric wave mixing. Our results provide a simple physical interpretation of light amplification observed in recent experiments by Cartella et al. [1]. Moreover, we argue that Floquet parametric instability could already be present in these experiments. Our approach utilizing the Floquet formalism is applicable to a broad class of systems.  

C71.00304: Response at finite temperature  OLLE HELLMAN (Presenter), Linkoping University — We present recent developments using the temperature dependent effective potential technique (TDEP) to model strongly non-harmonic materials. The method employs model Hamiltonians that explicitly depend on temperature. I will present applications pertaining to thermal conductivity, inelastic neutron spectra and phase stabilities. In addition, we investigate the cross-terms between anharmonicity and non-adiabatic electron-phonon coupling and its influence on transport properties.
C71.00305: Deep Spectral Coarse Graining: Learning Simple, Dynamically Consistent Protein Models*  
NICHOLAS CHARRON (Presenter), FELIKS NÜSKE, JIANG WANG, LORENZO BONINSEGNA, ANKIT PATEL, CECILIA CLEMENTI, Rice Univ — Coarse grain models of proteins offer promising gains in both computational efficiency for molecular simulations and the development of simple physical interpretations. Recent efforts have focused on formulating the development of coarse grained force fields as a supervised learning problem, taking advantage of deep learning techniques for handling highly non-linear multibody effects produced by imposing coarse grained representations. In this work, we present a deep learning method that utilizes spectral information from simulation data to preserve essential dynamics of the original system. Following a Koopman-motivated approach, we optimize the dynamical consistency between fine grain and coarse grain systems by forming a cost from the dynamical generator eigenequation. Through this method, we can recover coarse grain empirical free energy landscapes that preserve essential dynamical information from the fine grain system.

*This work was funded by NSF grants: CHE-1265929, CHE-1738990, PHY-1427654, Welch Foundation grant C-1570m and NLM training grant 5T15LM007093-27. The researchers acknowledge the support of the Rice Center for Theoretical Biological Physics and the Gulf Coast Consortia.

C71.00306: Crystalin Protine Structure Prediction Algorithm  
DANAE STEPHENS (Presenter), Brigham Young Univ - Provo — The accurate prediction of protine structures is a continuously ongoing process, with the traditional method being a two step process of creating restraints and constructing a basic structure from that. Recent advancements in Machine Learning and Neural Networks have provided new avenues to increase accuracy for these predicted protein structures. By utilizing a Neural Network to estimate molecular distances, and running basic torsion angle predictions, enables us to more accurately fold proteins and create accurate protein structure predictions for use. Hopefully this neural network will allow further research and utilization of proteins that we are currently unable to crystalize and study by traditional means.
C71.00307: Constructing the Neural Network Potential With the Energies of the Atom and Its Derivatives  
JISU JUNG (Presenter), WONSEOK JEONG, SEUNGWU HAN, Seoul Natl Univ — 
Neural Network Potentials (NNPs) are highly anticipated as a possible breakthrough to overcome the trade-off between accuracy and speed in atomistic simulations. NNP learns the potential energy surface from the reference first principle calculations. The most widely used first principle calculation is based on the density functional theory (DFT) with the plane-wave basis, which does not provide atomic energy. Thus it is not possible to directly train the NNP to learn target atomic energy from plane-wave DFT. To overcome this limitation Behler and Parrinello designed high-dimensional NNP such that it represents the atomic energy as the sum of total energy. However, the mapping of atomic energy from the total energy is not unique, and if not carefully considered, there could be a loss of information leading to errors. We call this ad-hoc mapping problem. In contrast, because a pseudo-atomic localized basis can define atomic energy by its decomposition formalism, it enables NNP to avoid the above problem. In this presentation, we demonstrate the advantages of training NNPs directly from atomic energy and its derivatives, free from the high dimensional structure.


C71.00308: Grain boundary structures of elemental metals using machine learning potential  
TAKAYUKI NISHIYAMA (Presenter), ATSUTO SEKO, ISAO TANAKA, Kyoto Univ — 
Global optimization algorithms, such as multi-start local optimizations and Bayesian optimization, have been useful to determine the microscopic structure and its grain boundary energy for a given macroscopic grain boundary model. Together with the global optimization algorithms, the density functional theory calculation and interatomic potentials have been employed to estimate the grain boundary energy. However, the former is computationally demanding, and the latter often lacks the predictive power for a variety of grain boundary structures. Recently, several machine-learning potentials have been proposed, which are expected to enable computing the grain boundary energy accurately with less computational costs. In this study, we investigate symmetric tilt grain boundary structures and their grain boundary energy surfaces in elemental metals using a combination of global optimization algorithms and linearized machine learning potentials [1]. We compare the grain boundary structures and grain boundary energy surfaces obtained from machine learning potentials and embedded atom method potentials to examine the accuracy and stability of our procedure.

**C71.00309: Machine Learning-Aided Development of Empirical Force-Fields for Glasses**

MATHIEU BAUCHY (Presenter), University of California, Los Angeles — The development of reliable, yet computationally efficient interatomic forcefields is key to facilitate the modeling of glasses. However, the parametrization of novel forcefields is challenging as the high number of parameters renders traditional optimization methods inefficient or subject to bias. Here, we present a new parameterization method based on machine learning, which combines \textit{ab initio} molecular dynamics simulations, Gaussian Process Regression, and Bayesian optimization. By taking the examples of silicate and chalcogenide glasses, we show that our method yields new interatomic forcefields that offer an unprecedented agreement with \textit{ab initio} simulations. This method offers a new route to efficiently parametrize new interatomic forcefields for disordered solids in a non-biased fashion.

*This work was supported by the National Science Foundation under Grants No. 1762292, 1826420, and 1928538.

**C71.00310: A theoretical study on crystallization of chalcogenides via neural network potential**

DONGHEON LEE (Presenter), KYEONGPUNG LEE, DONGSUN YOO, WONSEOK JEONG, KYUHYUN LEE, SEUNGWU HAN, Seoul Natl Univ — Phase-change materials (PCM) have attracted wide interests in fields such as data storage and neuromorphic computing. Ge-Sb-Te alloys are a representative PCM, which show large contrast of optical and electrical properties between crystalline and amorphous phases. Atomic scale modeling of PCM has relied on ab-initio molecular dynamics (AIMD), but its large computational costs have limited simulation size and time. Neural network potential (NNP) can deal with more than thousands of atoms upto microseconds, while accurate potential energy surface can be obtained by learning the data of density functional theory (DFT).

In this work, we suggest the accurate and effective training scheme to develop reliable NNP for chalcogenides (e.g. GeTe and Ge$_2$Sb$_2$Te$_5$). It seems that NNP trained in the conventional way moderately predicts the basic properties but rapidly crystallizes an amorphous phase without any incubation time. We then propose a simple descriptor to diagnose it and an active learning scheme to manage it. Dependence of crystallization kinetics upon temperature and density is investigated using about 4000-atom cells. It shows that incubation and crystallization time is dependent on temperature and pressure, qualitatively consistent with experiments.
C71.00311: Direct prediction of quantum accurate forces for multicomponent systems

SUBODH TIWARI (Presenter), Univ of Southern California, PANKAJ RAJAK, Argonne National Lab, KEN-ICHI NOMURA, AIICHIRO NAKANO, Univ of Southern California, FUYUKI SHIMOJO, Department of Physics, Kumamoto University, RAJIV KALIA, PRIYA VASHISHTA, Univ of Southern California — Phase-change materials (PCM) are routinely exploited in optical data storage, flexible devices and neuromorphic computing due to the extreme electro-optical contrast between crystalline and amorphous states. However, high-quality force-field models for molecular-dynamics (MD) simulations of PCM are not available, while quantum molecular dynamics simulation is limited by the small size of system. We have developed neural-network (NN) force fields for GeTe and Ge$_2$Sb$_2$Te$_5$, which are trained using atomic forces computed by density functional theory. Radial and angular feature vectors are designed and trained, which feature permutational and translational invariance and rotational covariance of forces. The accuracy of the NN force fields is validated by performing MD simulation involving up to 100,000 atoms and computing multiple structural and dynamical properties.

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C71.00312: IFF-R Models to Accurately Simulate Stress-Strain and Failure Porpherties of Carbon Allotropes and Polymer Composites

JORDAN WINETROUT (Presenter), KRISHAN KANHAIYA, University of Colorado, Boulder, RAVINDRA PANDEY, GREGORY M. ODEGARD, Michigan Technological University, HENDRIK HEINZ, University of Colorado, Boulder — Stress induced mechanical failure of polymeric materials is a result of the breakage of covalent bonds. The occurrence of bond breakage and formation is only observed during reactions. This study focuses on the novel bond-breaking capabilities of the Interface Forcefield (IFF-R). Traditional IFF models simulated systems using harmonic potentials. The IFF-R model incorporates Morse potentials; thereby, eliminating the restoring force experienced by bonded atoms stretched at large distances. This enables accurate predictions of mechanical responses in a variety of periodic systems. This study shows moduli and strength predictions of a single-walled carbon nanotube, poly(acrylonitrile) crystal, cellulose β crystal, and steel FCC lattice to be comparable to experimental values. Mechanical property predictions using IFF-R models are realized magnitudes faster than reactive forcefield (ReaxFF).

*NSF
C71.00313: Enhanced Optical Properties of Single-Walled Carbon Nanotubes (via SP$^3$-Hybridization Defects) from Many-Body Perturbation Theory Based on Density Functional Theory Calculations  BRADEN WEIGHT (Presenter), ANDREI KRYJEVSKI, Department of Physics, North Dakota State University — The optical consequences of functionalized carbon nanotubes (CNTs) (via a pair of SP$^3$-hybridized functional groups attached to a carbon ring) have been explored in great depth due to their promise of superior electronic properties for tunable emission in infrared energies. These studies have relied on time-dependent density functional theory (TD-DFT) calculations to model the excited states of these particles, but very little work has been completed on multiple exciton generation (MEG) processes within these systems. Here we employ a novel method based in non-equilibrium, finite-temperature, many-body perturbation theory (MBPT) calculations that utilize output from density functional theory (DFT) to accurately model excited states of these systems. We solve the Boltzmann transport equation (BE), including phonon absorption/emission and biexciton formation/recombination terms [1,2]. With this approach we compute an array of CNTs of varying chirality and functionalization scheme. We see that SP$^3$-defect functionalization of pristine CNTs that had high-energy biexciton MEG thresholds ($E \approx 2.4E_g$) can be reduced to $2E_g$, which drastically increases their value as efficient multiple exciton sources.


C71.00314: Quasi-Diabatic Scheme for Non-adiabatic On-the-fly Simulations*  WANGHUAI ZHOU, ARKAJIT MANDAL, PENGFEI HUO (Presenter), University of Rochester — We use the quasi-diabatic (QD) propagation scheme to perform on-the-fly non-adiabatic simulations of the photodynamics of ethylene. The QD scheme enables a seamless interface between accurate diabatic-based quantum dynamics approaches and adiabatic electronic structure calculations, explicitly avoiding any efforts to construct global diabatic states or reformulate the diabatic dynamics approach to the adiabatic representation. Using diabatic dynamics methods, the QD propagation scheme enables direct non-adiabatic simulation with complete active space self-consistent field on-the-fly electronic structure calculations. The population dynamics obtained from both approaches are in a close agreement with the quantum wavepacket based method and outperform the widely used trajectory surface hopping approach. Further analysis of the ethylene photo-deactivation pathways demonstrates the correct predictions of competing processes of non-radiative relaxation mechanism through various conical intersections. This work provides the foundation of using accurate diabatic dynamics approaches and on-the-fly adiabatic electronic structure information to perform ab-initio non-adiabatic simulation.

*This work was supported by the National Science Foundation CAREER Award under Grant No. CHE-1845747

C71.00315: Abstract Withdrawn  —
C71.00316: Dielectric Screening by 2D Substrates KEIAN NOORI (Presenter), NICHOLAS CHENG, FENGYUAN XUAN, SU YING QUEK, Natl Univ of Singapore — While electronic screening within 2D materials has been studied extensively, the question of how 2D substrates screen charge perturbations or electronic excitations adjacent to them still remains.

In this work, we use first principles calculations to study the fully non-local dielectric screening properties of 2D material substrates. Our calculations give results in good qualitative agreement with those from electrostatic force microscopy (EFM) and Kelvin probe force microscopy (KPFM) experiments, indicating that the experimentally observed thickness-dependent screening effects and reduced charge potential fluctuations are intrinsic to 2D materials.

2D material substrates can also dramatically change the HOMO-LUMO gaps of small molecule adsorbates. We suggest an easy and reliable method to predict the HOMO- LUMO gaps of small physisorbed molecules on 2D and 3D substrates, using only the band gap of the substrate and the gas phase gap of the molecule.

C71.00317: Universal metric for plasmonicity of excitations at the nanoscale LUCA BURSI (Presenter), RUNMIN ZHANG, Department of Physics and Astronomy, Rice University, KYLE D. CHAPKIN, NAOMI J. HALAS, Department of Chemistry, Rice University, PETER J. NORDLANDER, Department of Physics and Astronomy, Rice University — A promising trend in plasmonics involves shrinking the size of plasmon-supporting structures down to a few nanometers, thus enabling control over light–matter interaction at extreme-subwavelength scales. In this limit, quantum mechanical effects, such as nonlocal screening and size quantization, strongly affect the plasmonic response, rendering it substantially different from classical predictions. For very small clusters and molecules, collective plasmonic modes are hard to distinguish from other excitations, such as single-electrons ones. Using rigorous quantum mechanical computational techniques for a wide variety of physical systems, we describe how the plasmonic character of a nanostructure’s optical resonance can be quantified. We define a universal metric, the generalized plasmonicity index (GPI), which can be straightforwardly implemented in any computational electronic-structure or classical electromagnetic approach to discriminate plasmons from single-particle excitations and photonic modes [ACS Nano, 11, 7321 (2017); PNAS, 115, 9134 (2018)]. The GPI metric deepens our fundamental understanding of what is a plasmon down to the molecular limit of plasmon-supporting nanostructures and provides a rigorous foundation for further development in molecular plasmonics.
**C71.00318: Particle-in-cell simulation of plasmons**  
WEN JUN DING, Institute of High Performance Computing A*STAR, JEREMY LIM (Presenter), Science and Math cluster, Singapore University of Technology and Design, DO THI BICH HUE, National University of Singapore, XIONG XIAO, Institute of High Performance Computing A*STAR, MICHEL BOSMAN, National University of Singapore, LAY KEE ANG, Science and Math cluster, Singapore University of Technology and Design, LIN WU, Institute of High Performance Computing A*STAR — Plasmons are collective oscillations of the free electron gas density in conducting media such as metals. In many cases of interest, plasmons are typically characterized by solving the Maxwell equations, where the electromagnetic response can be described by the bulk permittivity. Motivated by the physical similarity of plasmas and oscillating conduction electrons, we present a particle-in-cell-based method of simulating plasmons. By solving for the instantaneous particle position and momentum, which are connected to the electromagnetic fields through current, we demonstrate the capability of this novel approach in elucidating information on the formation of the plasmons. Specifically, we demonstrate plasmon formation in gold nanorods through laser irradiation and single-electron excitation. Lastly we investigate the non-local effects of ultra-small nanoparticles approaching quantum limit.

**C71.00319: Heat transport between two critical one-dimensional systems**  
SONJA FISCHER (Presenter), LARS FRITZ, DIRK SCHURICHT, Univ of Utrecht — Heat transport can reveal information about interacting many-body systems beyond other transport probes. In particular, in one dimension it has been shown that the energy current is directly proportional to the central charge, thus revealing information about the degrees of freedom of critical systems. In this work, we explicitly verify this result in two cases for translationally invariant systems based on explicit microscopic calculations. More importantly, we generalise the result to non-translation invariant setups and use this to study a composite system of two subsystems possessing different central charges. We find a bottleneck effect meaning the smaller central charge limits the energy transport.

**C71.00320: Thermal conductivity prediction from basic properties using a developed artificial neural network**  
GUANGZHAO QIN (Presenter), University of South Carolina, HUIMIN WANG, Nanjing University, ZHENZHEN QIN, Zhengzhou Univ, MING HU, University of South Carolina — High-throughput screening and material informatics have shown a great power in material discovery including Li-battery materials, alloys, photocatalysts, and nanowires. In this talk, we will present the accurate thermal conductivity prediction from machine learning technique using a developed artificial neural network (ANN). With 231 datasets of the basic properties describing materials calculated from first-principles and the corresponding thermal conductivity from experimental measurements as training data, the constructed ANN is well trained by iterating to reduce the loss function. The trained ANN model for thermal transport successfully captures the general correlation between basic properties and thermal conductivity for different types of materials, which is predictive spanning 4 orders of magnitude of the thermal conductivity. The developed ANN model in our work for fast and accurately predicting thermal conductivity provides a powerful tool for the large-scale thermal material screening with targeted thermal transport property.
C71.00321: Exploring structure and magnetism of collapsed lanthanides

EVGENY PLEKHANOV (Presenter), CEDRIC WEBER, Physics, Kings College London — By using DFT within VASP [1] and DFT+DMFT within CASTEP codes [2], we study the collapsed phases of Tb, Gd, Dy, Sm, Nd and Y at extreme pressure up to 240GPa.

In Tb, Gd, Dy we show that the collapsed phases have a 16-atom orthorhombic structure (oF16) not previously seen in the elements, whereas in Nd we show that it has an eight-atom orthorhombic structure (oF8) previously reported in several actinide elements. oF16 and oF8 are members of a new family of layered elemental structures, the discovery of which reveals that the high-pressure structural systematics of the lanthanides, actinides, and group-III elements (Sc and Y) are much more related than previously imagined. Our electronic structure calculations of Tb, combined with quantum many-body corrections, confirm previous and recent experimental observations by using synchrotron x-ray diffraction (see the Ref.[3] and the references therein), and predict that the collapsed orthorhombic phase is a ferromagnet, nearly degenerate with an antiferromagnetic state between 60 and 80 GPa. We also discuss in detail the magnetic properties of the lanthanides studied.


C71.00322: DFT studies of graphene in carbon droplets condensed in stellar atmospheres

CHATHURI SILVA (Presenter), PHILIP FRAUNDORF, ERIC MAJZOUB, PHILIP CHROSTOSKI, University of Missouri - St. Louis — Elemental carbon at low (ambient) pressure sublimates to vapor near 4000K, but liquid carbon is reported after laser ablation. Some meteoritic carbon particles, formed in red giant atmospheres, show a “graphene-core”/graphite-rim structure likely from super-cooled carbon droplets that nucleated graphene sheets on randomly-oriented 5-member rings. Similar core-rim particles form by slow cooling of carbon vapor in the lab (HAL-02238804). Our computations target growth of carbon rings & graphene sheets at the experimental 1.8 g/cc density estimate, by relaxing random liquid-like configurations of 13/20-atom clusters in a supercell. Inter-atom distances characteristic of covalent vs. metallic interactions (with a gap in 1.7-2 Å range) allow us to identify covalent “bonds” with small separation. Local energy minima at T = 0K show sp² & sp coordination numbers, as in the literature. Ring sizes vary from triangle to heptagon, but pentagons are more abundant than hexagons, also consistent with previous reports. Work remains to see if pent-loops can nucleate the growth of faceted pentacones, as suggested by HRTEM imaging. Unlayered graphene sheets in a frozen matrix may be an effective diffusion barrier.

C71.00323: Abstract Withdrawn
C71.00324: Dark Matter and Baryons (Surplus Quarks) Generated by Nonequilibrium Confinement of Quarks*  LEIF MATSSON (Presenter), Department of Physics, University of Gothenburg — The emergence of baryons (surplus quarks) at Big Bang, required a nonequilibrium binding and superconductor-like condensation of quark-antiquark pairs before the electroweak (EW) symmetry breakdown. (Similar for leptons). As will be further shown, the formerly unknown dimensionless coupling to the Ginsburg-Landau like potential and the scale parameter in the EW theory then become microscopic functions of the massive quark and antiquark fields, thus defining the matter-antimatter asymmetry and the dark matter content in the Universe at correct orders of magnitude. The number of free parameters in the Standard Model has thereby been reduced.

Key words: Baryogenesis; Quark Confinement; Matter-Antimatter Asymmetry, Dark Matter; Black Holes.

Earlier publications on this matter:

*No external funding

C71.00325: Effect of Surface Defects on Field-Induced Hot-Carrier Chemistry in Dielectric Polymers*  SUBODH TIWARI (Presenter), THOMAS LINKER, Univ of Southern California, HIROYUKI KUMAZOE, FUYUKI SHIMOJO, Department of Physics, Kumamoto University, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Univ of Southern California — Performance of dielectric polymers under high electric field is limited by the electrical breakdown, which is commonly understood as an avalanche of processes such as carrier multiplication and defect generation. We model the hot-carriers transport in dielectric polymer, polyethylene, with excited-state quantum molecular dynamics simulations in presence of electric field, which reveal multiple microscopic processes induced by hot electrons and holes under an electric field. The key chemical damage occurs due to localization of holes at the surface of slab which weaken carbon-carbon bonds on the surface. Introducing surface defects alter the valence-band maximum (VBM) state in polyethylene leading to bond breaking at lower field. Further, we have isolated C-C bond lengths and VBM localization as a proxy for dielectric breakdown. Such proxies allow us to perform one simulation to understand the effect of defect rather than scanning the complete electric field range. Such quantitative and qualitative information can be incorporated into first principles-informed, predictive modeling of dielectric breakdown.

*This work was supported by the Office of Naval Research through a Multi-University Research Initiative (MURI) grant N00014-17-1-2656.
C71.00326: Simulation of the effect of electric field on the performance of ion separation and water desalination using a graphene-carbon nanotube membrane  
SAMANEH RIKHTEHGARAN (Presenter), LUC T WILLE, Florida Atlantic University — Using molecular dynamics (MD) simulations, a graphene-carbon nanotube membrane is exposed to external electric field with intensities $E = 0.1, 1, 10, \text{ and } 100 \text{ mV/Å}$ in order to separate $\text{Na}^+$ and $\text{Cl}^-$ ions from a salt water solution to produce fresh water. The results show that by increasing the strength of the applied electric field, the ion separation will be increased to 100% for $E = 100 \text{ mV/Å}$. It is found that the ion separation efficiency of this filter is already greater than 90% for $E = 10 \text{ mV/Å}$. Based on the results of this study, it is suggested that the graphene-carbon nanotube membrane can be used as a device of water desalination under the application of electric field.

C71.00327: Effects of surface transition and adsorption on ionic liquid capacitors  
HUIKUAN CHAO (Presenter), ZHEN-GANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology — Room temperature Ionic liquids (RTILs) are a type of synthesized electrolytes possessing superb electrochemical stability and low vapor pressure compared with conventional aqueous-based electrolytes, which offers significantly enlarged electrochemical window and ease of maintenance for capacitors. Experiments measuring capacitance in concentrated RTILs often found hysteresis indicating that an underlying phase transition might exist. Current theories explaining the hysteresis in terms of phase transition either assume RTIL mixtures with neutral solvents or omit ion-ion correlations in RTILs. In this study, a variant of an existing RTIL model [1] is established for solvent-free RTIL capacitors incorporating both ion-ion correlations and nonelectrostatic interactions. We first use the model to explore the spontaneous charge separation in the capacitors and find that this transition is a common feature for realistic choices of the model parameters for most RTILs. Next, we investigate the effects of preferential ion adsorption on this charge separation transition. The results show that preferential ion adsorption can be a useful design parameter for optimizing the energy storage of the capacitors.


C71.00328: Disintegration of Surfactant Micelles at Metal-Water Interfaces Promotes their Strong Adsorption*  
SUMIT SHARMA (Presenter), HIMANSHU SINGH, Ohio Univ — We have studied adsorption behavior of surfactant micelles at metal-water interfaces via fully atomistic simulations. We show that micelles experience a free energy barrier to adsorption. Near the metal surface, surfactant molecules in the micelles slowly rearrange leading to complete disintegration of the micelles. Disintegration of the micelles results in much stronger adsorption. After the disintegration, surfactant molecules adsorb by lying flat on the metal surface. By simulating adsorption of micelles treated as rigid bodies, we show that when the micelles remain intact, they have a weak tendency to adsorb.

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C71.00329: Targeted Synthesis Conditions of Layered Bismuth Oxychalcogenides Via Electrochemical Phase Diagrams* LAUREN WALTERS (Presenter), CHI ZHANG, JAMES RONDINELLI, Northwestern University — We investigated how density functional theory calculations of electrochemical stability can guide the experimental hydrothermal synthesis of bismuth oxychalcogenides. The target phases, which are layered thermoelectrics and exhibit electronic anisotropy, represent exciting materials for catalysis, photoluminescence, and energy applications. We coupled experimental synthesis with DFT-calculated multielement Pourbaix diagrams to identify target pH and potential synthesis regions that ultimately proved successful. We further investigated numerous degrees of freedom present in the reaction, such as mass ratio of reactants, temperature, and concentration of ions, to qualitatively understand how changes in the chemistry of the oxychalcogenides alter phase stability. Last we discuss how these materials can be driven towards target phase production.

*The authors were supported by the ONR MURI “Understanding Atomic Scale Structure in Four Dimensions to Design and Control Corrosion Resistant Alloys” under Grant No. N00014-16-1-2280 and the National Science Foundation’s MRSEC program (DMR-1720139) at the Materials Research Center of Northwestern University.

C71.00330: Resolution of the identity approximation applied to PNOF family of correlation calculations JUAN FELIPE HUAN LEW YEE (Presenter), National Autonomous University of Mexico, MARIO PIRIS, Donostia International Physics Center, JORGE M. DEL CAMPO RAMÍREZ, National Autonomous University of Mexico — PNOFi (i = 1-7) family of functionals deal with electronic structure correlation calculations by means of the reduced electron density matrix approach (1-RDM). The major advantage of a 1-RDM formulation is that the unknown functional only needs to incorporate electron correlation. PNOFi family of functionals provide an efficient way of including dynamic and static correlation as compared to wave function methods. However, a transformation from atomic orbital integrals to molecular orbital integrals has to be performed in order to computate the Coulomb and Exchange matrices in molecular orbital representation J_{OM} and K_{OM} respectively, which involves an overall fifth power time scaling factor. Resolution of the identity (RI) approximation reduces the scaling factor of both, J_{OM} and K_{OM} matrices, and lowers the global scaling to fourth power. As a consequence, less memory is required to perform PNOFi calculations with an overall speed up in the calculation. RI is applied directly in the evaluation of J_{OM} and K_{OM} matrices, thus, improvement would be valid for all PNOFi family, however, the PNOF5 functional has been used in this work. Impact of RI on the convergence, and the obtained error in the correlation energy is analyzed for selected large size systems.
C71.00331: Coherent states, Gram matrix, and Hofstadter butterfly with flat band
YOUJIANG XU (Presenter), HAN PU, Rice Univ — A method to construct flat band model is exhibited. If a Gram matrix built upon a set of vectors is regarded as a Hamiltonian of certain physical system, then we can control the ground state degeneracy by modifying the vectors. If the vectors are chosen to be certain subsets of coherent states, the resulting Hamiltonians describe single-particle lattice models with a gauge field. The massive degeneracy of the lowest band in these models is a universal property independent from the shape of lattice, which is controlled by the completeness of the subsets of coherent states. The excitation spectra show Hofstadter-butterfly-like patterns which vary when the lattice changes. The models also feature ground state wave functions in universal form, which is like Landau lowest levels, but the dynamics differs. Experimental realization of the models is promising.

C71.00332: Computational simulation of patterns in a reaction-diffusion model
MONICA VELASCO (Presenter), CESAR MINOLLI, JOHN PRIAS, Physical Sciences Doctoral Program, Interdisciplinary Institute of Sciences, University of Quindío — Recent studies in reaction-diffusion models has been oriented to produce patterns for studying polycrystalline materials as graphene oxide and among others, here in show optimized algorithm for obtaining patterns of a reaction-diffusion equation. The optimization of algorithm were carried out by using fortran code and the respective visualization was employing the Visit software. The results suggest that is possible to obtain theoretical patterns of reaction-diffusion equation as expected, which could be comparable with the experimental patterns of high resolution transmission electron microscopy (HR-TEM) in graphite oxide samples.

C71.00333: Finite-Temperature Correlation Functions Using the Quantum Minimally Entangled Typical Thermal States Algorithm
SHI-NING SUN (Presenter), ADRIAN TAN, Caltech, MARIO MOTTA, IBM, FERNANDO BRANDÃO, GARNET CHAN, AUSTIN MINNICH, Caltech — Finite-temperature correlation functions provide fundamental information about the excitations and response properties of quantum many-body systems. Recently, the quantum minimally entangled typical thermal states (QMETTS) algorithm was introduced for calculating thermal averages of certain observables on near-term quantum devices. However, due to the computational cost of the quantum imaginary time evolution (QITE) subroutine underlying the QMETTS algorithm, the calculation of general thermal quantities with QMETTS remains challenging. Here, we report the calculation of finite-temperature correlation functions of quantum spin models with QMETTS. We describe how to reduce the cost of calculations by exploiting Hamiltonian symmetries and other constraints to eliminate qubits and reduce measurements. Our work advances efforts to study finite-temperature properties of quantum many-body systems on quantum computers.
C71.00334: Electrostatic screening, dynamics and structure of [BMIM+]\([\text{BF}_4^-]\) and [BMIM+]\([\text{PF}_6^-]\) with confinement*  
SUEHYUN PARK (Presenter), JESSE G. MCDANIEL, Georgia Inst of Tech — Ionic liquids are spotlighted as electrolytes for batteries and supercapacitors. Such applications have nanoconfined systems, where deviation of electrostatic screening, dynamics, and structure of ionic liquids from bulk properties is caused. Although electrostatic screening is a fundamental interaction for any charged particles, electrostatic screening condition for ionic liquids is not discovered yet in confined systems. To fully utilize ionic liquids in electronic devices, it should be fully revealed how confinement alters physical properties of ionic liquids. Here, we conducted molecular dynamics simulations of [BMIM+]\([\text{BF}_4^-]\) and [BMIM+]\([\text{PF}_6^-]\) between two graphene sheets with gap of 1.5 to 4.5 nm. Confined ionic liquids show slower dynamics by 2 orders of magnitude compared to bulk dynamics and have nonmonotonic behavior in dynamics. In addition to dynamics, we observed that capacitance is independent of confinement length. To explain this confinement effect, we computed electrostatic screening condition derived from Stillinger-Lovett sum rules. Furthermore, we investigated polarization effect on electrolytes and electrodes in confined system.

*Financial support from the U.S. Department of Energy, Basic Energy Sciences, through Grant No. DE-SC0020279

C71.00335: Finite-temperature auxiliary-field Quantum Monte Carlo study of dynamical correlation functions in correlated fermion systems*  
HAO SHI, YUAN-YAO HE (Presenter), SHIWEI ZHANG, Center for Computational Quantum Physics, Flatiron Institute — We compute dynamical (imaginary-time) correlation functions in correlated fermion systems using the finite-temperature auxiliary-field Quantum Monte Carlo method. The sign problem is eliminated by introducing constraints in auxiliary-field space. We carry out a systematic benchmark study of dynamical correlation functions in the two-dimensional repulsive Hubbard model, for various interaction strengths, density, and temperatures. At high temperatures, essentially exact results are obtained independent of the form of the constraint, similar to calculations of static quantities [1]. With decreasing temperature, we discuss how the constraint can be optimized to improve the accuracy of dynamical correlation functions. In the context of studying the pseudogap behavior, we apply the method to compute the self-energy and spectral functions in the Hubbard model. References:

*The Flatiron Institute is a division of the Simons Foundation.
**C71.00336: Low-energy physics in the critical phase of the bilinear-biquadratic spin-1 chain**

MORITZ BINDER (Presenter), THOMAS BARTHEL, Duke University — We use an efficient density matrix renormalization group (DMRG) algorithm to compute precise dynamic structure factors for the bilinear-biquadratic spin-1 chain with Hamiltonian \( H = \sum_i \left[ \cos \theta (S_i^* S_{i+1}) + \sin \theta (S_i^* S_{i+1})^2 \right] \). Here, we focus on explaining the physics in the extended critical phase \( (\pi/4 \leq \theta < \pi/2) \) of the model. The phase transition from the Haldane phase to the critical phase is marked by the SU(3)-symmetric ULS point \( (\theta = \pi/4) \), where the elementary excitations are spinons that can be obtained from the Bethe ansatz solution. As we move deeper into the critical phase, the spinon continua contract, and new striking features appear at higher energies. In the vicinity of the transition point from the critical to the ferromagnetic phase, a dispersion with a surprisingly simple functional form emerges, suggesting integrability of the model in the limit \( \theta \to \pi/2^- \).

*Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0019449.

**C71.00337: Entanglement decomposition for the simulation of quantum many-body dynamics**

THOMAS BARTHEL (Presenter), Duke University — Nonequilibrium dynamics in quantum matter are at the frontier of current research. Efficient and precise simulation techniques are needed to improve our understanding of equilibration and thermalization, dynamical phase transitions, decoherence effects, quantum transport etc. A major obstacle is the growth of entanglement with time which generally implies an increased complexity of the quantum state. For instance, the computation costs of simulations based on tensor network states generally grow rapidly in time, limiting the maximum reachable times. I will show how this problem can be addressed through entanglement decomposition. We can follow the dynamics, starting from an initial state, until the entanglement has grown to a point where our simulation resources are exhausted. We then decompose the current state into lower entangled components and continue by simulating the evolution of these components, decomposing them again when needed. I will demonstrate a specific entanglement decomposition scheme for matrix product state simulations and discuss its efficiency for the study of dynamics in quantum magnets.

*Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0019449.
C71.00338: Counter-diabatic Spin Squeezing  ZEYANG LI (Presenter), Massachusetts Institute of Technology, BORIS BRAVERMAN, University of Ottawa, ENRIQUE MENDEZ, VLADAN VULETIC, Massachusetts Institute of Technology — Spin squeezing states (SSS) are atomic entangled states that can be used to enhance the atomic precision measurements beyond the standard quantum limit. Existing implementations relying on unitary evolution are primarily based on one-axis twisting induced through coherent cavity feedback. By adding an auxiliary driving Rabi field, our work can generalize this one-axis twisting to an equivalent two-axis twisting, which features robustness against technical imperfections, as well as the potential to reach higher squeezing and therefore greater metrological gain. Moreover, by optimizing the time-varying auxiliary field, we obtain a fast preparation of SSS with high metrological gain, which we call as counter-diabatic spin squeezing.

C71.00339: Quantum Many-Body Effects in Optical Kerr Media  GIULIA MARCUCCI (Presenter), DAVIDE PIERANGELI, CLAUDIO CONTI, Physics Department, Sapienza University of Rome — Nonlinear quantum optics is emerging as one of the most important research directions in photonics. These include quantum solitons (QSs), and highly nonclassical supercontinuum generation (SCG). We need new strategies to design nonlinear optical devices operating at low photon numbers and theory to describe how they work.

Following Drummond et al. [1], we adopt a phase-space analysis to map the second quantized field theory of optical propagation in nonlinear dispersive media into a system of two coupled stochastic nonlinear Schrödinger equations (SNLSEs). This mapping allows numerical simulations of QSs, quantum dispersive shock waves (QDSWs) and quantum rogue waves (QRWs) generation by the nonlinear box problem [2] at low photon number.

As recently proved [3], quantum control furnishes new opportunities. By combining SNLSEs and CRAB optimization, we look for the best control function to limit effects as quantum spreading of QSs, to maximize the spectral generation of QDSWs, and to enhance the peak intensity of QRWs.

We believe that this approach unveils essential insights into the design of new quantum sources.

C71.00340: Bosonic entanglement crossover from groundstate scaling to volume laws*
Qiang Miao (Presenter), Thomas Barthel, Duke University — The crossover behavior of eigenstate entanglement entropies from an area law or log-area law for low energies and small subsystem sizes to volume laws for high energies and large subsystems can be described by scaling functions. We demonstrate this for two bosonic systems. The harmonic lattice model describes a system of coupled harmonic oscillators and is a lattice regularization for free scalar field theories. For dimensions \(d \geq 2\), the ground state of this model displays an entanglement area law, even at criticality, because excitation energies vanish only at a single point in momentum space. In contrast, Bose metals feature a finite Bose surface with zero excitation energy. One hence finds log-area laws for the groundstate entanglement. For both models, we sample excited states. The distributions of their entanglement entropies are sharply peaked around subsystem entropies of corresponding thermodynamic ensembles in accordance with the eigenstate thermalization hypothesis. In this way, we determine the scaling functions numerically. Eigenstates for quasi-free bosonic systems are not Gaussian. We resolve this problem by considering appropriate squeezed states instead, for which entanglement entropies can be evaluated efficiently.

*Research supported by DOE grant DE-SC0019449

C71.00341: A New Graphical Method for Designing Exactly Solvable Models
Masahiro Ogura (Presenter), Kyoto Univ — Exactly solvable lattice spin models have played important roles in physics. Since Onsager's work, some lattice spin models were exactly solved by treated as free fermion models (FFMs). For example, the one-dimensional XY model, the one-dimensional transverse field Ising model, and the Kitaev's two-dimensional honeycomb lattice model (KHL) can be solved in this way ([1],[2]). Based on these facts, in this talk we will present a new method to obtain a series of solvable models that include the Jordan-Wigner transformation and the Kitaev's method of the KHL as special cases [3]. For any given well-behaved graphs, we can construct FFMs corresponding to them. We can also design a set of operators from them. Therefore, we can create a lot of exactly solvable Hamiltonians. By this method we will introduce new solvable models, containing three-dimensional lattice models and spin systems corresponding to a fractal-like graph.

C71.00342: Application of the Recursive Projection Method to Electronic Structure Calculation*  SHOHAM SEN (Presenter), Carnegie Mellon University, YANG WANG, Pittsburgh Super Computing, Carnegie Mellon Univ, TIMOTHY BREITZMAN, Air Force Research Laboratory, KAUSHIK DAYAL, Carnegie Mellon University — In this work, we focus on the mixing scheme used during the Self-Consistent (SC) process of solving the Kohn-Sham (KS) equations. The two most common mixing schemes used in practice are the “Simple Mixing” and the “Modified Broyden Mixing”, the former is a fixed point method while the latter is a Quasi-Newton method. A characterization of the former method is that it takes less computation time per iteration but required a lot of iterations to converge; the latter gives quadratic convergence hence fewer iteration but takes more computational time per iteration. It can be shown that Simple Mixing converges if the eigen-values of the Jacobian lie within some ellipse. Thus even if only a few eigen-values lie outside the ellipse, Simple Mixing will not converge. We proposed the “Recursive Projection Method” (RPM) modified for electronic structure calculation, where we estimate the subspace spanned by the eigen-vectors whose eigen-values lie within the ellipse, call this the “stable-subspace”. We perform Simple Mixing on the stable-subspace and Modified Broyden on the complementary subspace. We expect that this method will improve convergence for systems of large size.

*We thank the DOD MURI Project for their Financial Support

C71.00343: The Energy Landscape Governs Brittleness and Ductility in Glasses*  LONGWEN TANG, MATHIEU BAUCHY (Presenter), University of California, Los Angeles — Based on their structure, non-crystalline phases can fail in a brittle or ductile fashion. However, the nature of the linkages between structure and propensity for ductility in disordered materials has remained elusive. Here, based on molecular dynamics simulations, we investigate the fracture of several disordered phases (metallic glass, glassy silica, colloidal gel, etc.) with varying degrees of disorder. We find that that, in general, structural disorder results in an increase in ductility. By applying the activation-relaxation technique (an accelerated sampling method to identify transition states), we show that the degree of plasticity is controlled by the topography of the energy landscape.

*This work was supported by the National Science Foundation under Grants No. 1762292 and 1826420.
C71.00344: Interface of Hydrated Perfluorosulfonic Acid Electrolyte with a Platinum Catalyst: Structural Analyses with Dissipative Particle Dynamics Simulations* NOBUO TAJIMA (Presenter), JUN NARA, MANA, National Institute for Materials Science, TAKU OZAWA, HIROYA NITTA, KOSUKE OHATA, Engineering Technology Division, JSOL Corporation, TAKAHISA OHNO, MANA, National Institute for Materials Science — Dissipative particle dynamics (DPD) simulations were performed to study structures of hydrated perfluorosulfonic acids (PFSA) in contact with platinum surfaces. Two types of interfacial systems were simulated, where PFSA molecules interact with a cube and a slab of platinum, respectively representing a small catalyst particle used in a regular fuel cell and a platinum substrate popularly used in a model system experiment. The calculated results suggest that the two systems form a shell structure and a layer structure, respectively, of PFSA components near the platinum surfaces. The water component covers the platinum surfaces popularly in both systems, of which the coverage depends on the hydration levels of PFSA. Detailed analyses revealed that the water component networks are quite different in the two systems, which are three-dimensionally connected in the systems with a platinum cube, while disrupted by hydrophobic components in the systems with a platinum slab.

*This work was partly supported by MEXT within the priority issue 6 of the FLAGSHIP2020 project (Project ID: hp160226, hp170253, hp180187, and hp190178). The calculations were primarily performed on NIMS super computer and K-computer.

C71.00345: Universal properties of creep flow in amorphous solids MARKO POPOVIC (Presenter), TOM.W.J. DE GEUS, École polytechnique fédérale de Lausanne, ALBERTO ROSSO, LPTMS, CNRS, Universite Paris-Sud, Universite Paris-Saclay, 69 91405 Orsay, France, MATTHIEU WYART, École polytechnique fédérale de Lausanne — Amorphous solids, such as atomic glasses, colloidal suspensions, granular matter or foams, begin to deform plastically when exposed to external stress $\Sigma$. Steady state deformation rate $\partial_t \varepsilon$ of these materials in absence of thermal fluctuations is usually described as $\partial_t \varepsilon \sim (\Sigma - \Sigma_c)^\beta$ for stresses above critical stress $\Sigma_c$ and vanishes below it, while in presence of thermal fluctuations flow persists below $\Sigma_c$, but is exponentially suppressed. The transient plastic deformation rate, called creep flow, is much less understood despite its importance in practical applications. Creep flow often displays a power-law decay in time $\partial_t \varepsilon \sim t^{-\mu}$ after which it can either arrest or eventually yield at fluidisation time $\tau_f$. In recent years various numerical values and/or laws have been suggested for the exponent $\mu$ and time $\tau_f$ in particular experimental or numerical studies. We propose that mechanism underlying creep flow is the same as that of the steady state flow, which allows us to predicts parameters $\mu$ and $\tau_f$ of creep flow in terms of the steady state flow parameters, both in athermal and thermally activated systems. We successfully tested all our predictions using different mesoscopic elasto-plastic models of amorphous solids and found them to be consistent with published experimental results.

C71.00346: SHOCK COMPRESSION OF CONDENSED MATTER —
C71.00347: Effect of structural collapse on electron density distribution and magnetic properties of ThCr$_2$Si$_2$-type pnictides* MICHAEL SHATRUK (Presenter), VINCENT YANNELLO, JUDITH K ROTH, Florida State Univ, ALEXANDER A YAROSLAVTSEV, European XFEL, ANDREI ROGALEV, European Synchrotron Radiation Facility, VASILE O GARLEA, Oak Ridge National Laboratory — The structural phase transitions in the ThCr$_2$Si$_2$-type materials involve a gradual or abrupt (first-order) collapse along the tetragonal c axis. Despite many examples of such transitions in the AT$_2$X$_2$ structures, the direct experimental assessment of changes in the electron density redistribution between the A and [T$_2$X$_2$] layers upon the formation and breaking of the X-X bonding interactions is largely lacking. Earlier studies have revealed fascinating pressure-induced transitions in EuCo$_2$Pn$_2$ (Pn = P, As) which are accompanied by the change in the Eu oxidation state and the transition from the localized (4f) magnetism to itinerant (3d) magnetism. In the present contribution, we demonstrate that the changes in the electron concentration in the [Co$_2$Pn$_2$] layer defy the formal electron-counting rules that are often used for Zintl-like phases. X-ray absorption measurements offer the direct insight into the changes in the Eu oxidation state and magnetism and the associated redistribution of the electron density in the [Co$_2$Pn$_2$] layer. Calculations of the band structure and analysis of chemical bonding have provided a satisfactory interpretation for the observed changes in the X-ray absorption spectra.

*This research was supported by the National Science Foundation (DMR-1905499).

C71.00348: Combining theoretical and experimental methods to study some zircon-type orthovanadates at high pressure.* ALFONSO MUNOZ-GONZALEZ (Presenter), PLACIDA RODRÍGUEZ-HERNANDEZ, IMN and Dept. de Fisica, Universidad de La Laguna, TOMAS MARQUEÑO, ENRICO BANDIELLO, DANIEL ERRANDONEA, Departamento de Física Aplicada, Universidad de Valencia — Many studies of zircon-type orthovanadates under high pressure have been performed. Some of these experiments using methanol-ethanol-water as pressure transmission medium report a zircon-to-monazite phase transition. In this work, we will focus on the study of the zircon-to-scheelite phase transition of some orthovanadates, combining high pressure experimental hydrostatic studies and ab initio simulations. Our approach provides information on the structural, electronic, dynamical, and elastic properties of these compounds. From our simulations, we found that around the transition pressure the zircon phase becomes dynamically unstable due to the softening of one B$_{1u}$ silent mode. Our study of the elastic constants and the analysis of the generalized mechanical stability criteria show a mechanical instability also appears near the transition pressure. We will also report on the new high pressure phase that appear after the zircon-to-scheelite transition.

*We thank the financial support from MINECO under projects MALTA Consolider Ingenio 2010 network (MAT2015-71070-REDC and RED2018-102612-T), MAT2016-75586-C4-1/3-P and by Generalitat Valenciana under grant Prometeo/2018/123 (EFIMAT). E. Bandiello thanks the Generalitat Valenciana for his postdoctoral contract (Vall+D, APOSTD2017).
C71.00349: New developments in large volume static compression with in situ synchrotron x-ray diffraction at High Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source*  ROSTISLAV HRUBIAK (Presenter), GUOYIN SHEN, CURTIS KENNEY-BENSON, CHANGYONG PARK, ARUN BOMMANAVAR, YU SHU, Argonne Natl Lab, ITARU OHIRA, Geophysical Laboratory, Carnegie Institution of Washington, YOSHIO KONO, Geodynamics Research Center, Ehime University — The integration of x-ray diffraction measurements with physical properties characterizations in a large volume cell provides a unique opportunity to investigate in-situ correlation between the atomic structure and the macroscopic properties of matter at high pressure (P) and high temperature (T) conditions. The beamline 16-BM-B capable of near comprehensive large-volume sample characterization at high P and high T conditions in a Paris-Edinburgh (PE) cell by using a multitude of in-situ x-ray-based techniques. An overview of the currently supported techniques that are available to users, with emphasis on new developments, is presented. Available techniques include: double-stage PE for amorphous structural measurements above 100 GPa, ultrasonic echo, fluid viscosity, high P-T synthesis, x-ray absorption density measurement, powder diffraction, phase contrast radiography, liquid (im)miscibility, and thermoelectric properties measurements.

*This work was performed at HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory (ANL). HPCAT operations are supported by DOE-NNSA's Office of Experimental Sciences. The APS is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by ANL under Contract No. DE-AC02-06CH11357.
C71.00350: Pressure induced phase transitions in topological crystalline insulator SnTe and its comparison with semiconducting SnSe: Raman and First-principles studies  SUKANYA PAL (Presenter), Indian Institute of Science - Dept of Physics, RAAGYA ARORA, Theoretical Sciences Unit, Jawaharlal Nehru Center for Advanced Scientific Research, SUBHAJIT ROYCHOWDHURY, New Chemistry Unit, Jawaharlal Nehru Center for Advanced Scientific Research, LUMINITA HARNAGEA, SAURABH KUMAR, Department of Physics, Indian Institute of Science Education and Research, SANDHYA SHENOY, Theoretical Sciences Unit, Jawaharlal Nehru Center for Advanced Scientific Research, D.V.S. MUTHU, Indian Institute of Science - Dept of Physics, KANISHKA BISWAS, New Chemistry Unit, Jawaharlal Nehru Center for Advanced Scientific Research, U.V. WAGHMARE, Theoretical Sciences Unit, Jawaharlal Nehru Center for Advanced Scientific Research, A K SOOD, Indian Institute of Science - Dept of Physics — We report Raman study of a topological crystalline insulator (TCI) SnTe and a normal semiconductor SnSe, as a function of pressure at room temperature along with first-principles density functional theory calculations. Under pressure, iso-structural transition is observed in SnTe as revealed by the anomalous softening of the strongest Raman mode up to 1.5 GPa. Further, SnTe undergoes structural transitions at ~ 5.8, ~ 12 and ~ 18.3 GPa. The 5.8 GPa transition is associated with a structural transition from ambient cubic (Fm-3m) to orthorhombic (Pnma) phase which is no longer a topological insulator. Above the transition pressure of 12 GPa another orthorhombic Pnma[GeS] phase is stabilized coexisting with Pnma phase. Above 18.3 GPa enthalpy calculations show a transition from orthorhombic Pnma to a more symmetric cubic (Pm-3m) structure. Our high-pressure study of SnSe on the other hand reveals that it undergoes two phase transitions: one from the orthorhombic (Pnma) structure to orthorhombic (Cmcm) structure at ~ 6.2 GPa and the other at ~ 12.9 GPa in which the Cmcm phase undergoes a semi-metal to metal transition. Density functional theory calculations capture the contrast in pressure dependent behaviour of topological crystalline insulator SnTe and a normal semiconductor SnSe.

C71.00351: WITHDRAWN ABSTRACT  —

C71.00352: Study of thermal properties of HMX in molten TNT.  NATALYA SUVOROVA (Presenter), DAVID M OSCHWALD, DENNIS K REMELIUS, LAURA SMILOWITZ, BRYAN HENSON, PAMELA BOWLAN, Los Alamos Natl Lab — Octol composed of 70 wt% of HMX and 30 wt% of TNT is one of the melt cast explosives that is widely used in many military applications, namely for shaped charges. Due to the presence of low melt TNT component octol exhibits complex thermal behavior. At the temperature above TNT melt, octol forms liquid-solid system that with further heating undergoes phase change and decomposition of its constituencies with release of thermal energy. In this presentation the thermal decomposition properties of octol were investigated via DSC/TG method and X-ray diffraction at various heating conditions. The thermal reactivity of heated octol was compared to other TNT- based melt cast compositions, such as Composition B and cyclotol.
C71.00353: Electrical and optical properties of tetragonal polymeric C60 under high pressure ZHONGYAN WU (Presenter), Department of Physics and HYU-HPSTAR-CIS High Pressure Research Center, Hanyang University, Seoul, 04763, South Korea, LIN WANG, Center for High Pressure Science & Technology Advanced Research, Shanghai 201203, China, ALEXANDER SOLDATOV, Department of Engineering Sciences & Mathematics, Lulea University of Technology, SE - 97187 Lulea, Sweden, JAEYONG KIM, Department of Physics and HYU-HPSTAR-CIS High Pressure Research Center, Hanyang University, Seoul, 04763, South Korea — C60 having unique icosahedral truncated structure is known to form polymer or dimer between fullerene cages under high pressure and temperature. In this work the electrical and optical properties of 2-dimensional tetragonal polymeric C60 were studied under high uniaxial pressure, p, to investigate the phase transformation. The electrical resistance value, R, decreased from $10^{10}$ to $5 \times 10^5$ Ω as a result of pressure cycling (with ramp pressure increase in each cycle) to a maximum pressure of 32 GPa by using a diamond anvil cell (DAC). A substantial drop in R after decompression (~$10^{10}$ Ω) was reached in a cycle with a ramp pressure of 22 GPa that we consider as a cross-over/phase transition p. A subsequent p-cycling to 32 GPa resulted in further (20 times!) drop in the R of the recovered sample and exhibited anomalies in R vs p behavior. The results of Raman measured after decompression showed that the ratio of the 2-dimensional T-phase to 1-dimensional O-phase decreased as increasing the cycling p. Raman-mapping of the recovered material showed Raman spectra inhomogeneities across the sample stemming from a non-hydrostatic pressure distribution in the DAC and the relationship between shear and normal stress.

C71.00354: Structural behavior of silicate liquids and glasses under extreme conditions by using synchrotron X-ray diffraction and Raman spectroscopy* YOUNG JAY RYU (Presenter), TONY YU, Center for Advanced Radiation Source, University of Chicago, FIONA BONNET, Geosciences, Universite Claude Bernard Lyon 1, VITALI PRAKAPENKA, SERGEY TKACHEV, Center for Advanced Radiation Source, University of Chicago, HEATHER WATSON, Physics and Astronomy, Union College, MARK L RIVERS, YANBIN WANG, Center for Advanced Radiation Source, University of Chicago — The behavior of silicate melts under high-pressure and high-temperature conditions is of primary interest in the field of geophysical, chemical, material science, and technological glass process industry, both for their fundamental properties and for their significant roles in thermal transport and chemical differentiation within Earth and other terrestrial planetary interiors. Recently, considerable progress has been achieved in understanding the structural differentiation of liquid and glass silicates by both theoretical predictions and various spectroscopic experiments, yet still many issues are puzzling and several challenges must be overcome to expand our understanding of silicate liquids and glasses. Here, we report spectroscopic properties of enstatite (MgSiO3), wollastonite (CaSiO3), diopside (CaMgSi2O6) and silica (SiO2). The local atomic structure of various silicates has been studied using synchrotron angle-dispersive X-ray diffraction combined with a multi-channel collimator. Atomic pair distribution functions (PDFs) were obtained from the X-ray data. Also, we have obtained the local vibrational modes by using Raman spectroscopy, providing additional structural information that cannot be obtained by X-ray diffraction.

*This project is supported by NSF EAR-1620548
C71.00355: Automated iterative forward analysis for pressure determination in dynamic compression experiments  
CONNOR KRILL, SUZANNE J ALI, Lawrence Livermore Natl Lab, JUNE WICKS, Johns Hopkins University, RAYMOND SMITH (Presenter), Lawrence Livermore Natl Lab — High powered laser compression experiments can provide insights into material behavior at solar and planetary cores - some of the most extreme conditions in the Universe. To fully understand material response at such extreme conditions, the pressure within the sample must be accurately determined. However, pressure cannot be measured directly. Experiments must measure the velocity of a sample and use knowledge of the equation of state to extract a pressure history. With new driver developments laser shot rate is increasing, going from once a day at NIF, to every few minutes at the Stanford Materials in Extreme Conditions (MEC) endstation and the near-term sub-Hz operation at the European X-ray Field Electron Laser (XFEL) facility in Hamburg. This increase creates a need for an automated process to convert experimentally measured velocities into pressure histories. The work reported here implements an automated iterative forward analysis using the HYADES hydrocode that can scale with the growth of modern laser facilities to accurately retrieve pressure histories from a broad range of experimental conditions. We discuss this work in the context of ramp compression of various materials on the OMEGA laser facility.

C71.00356: Liner Material Dependence on Penetration Ability of Metal Jet generated from Mini-Shaped Charge Devices against Iron Target  
FUMIKAZU SAITO (Presenter), Department of Applied Physics, National Defense Academy — New experimental data for the mass and density gradients of Cu and Zn metal jet using the original mass-estimation method are reported. The metal jets were generated by using shaped charges, which consist of conical Cu / Zn liners and PBX explosive charge. To compare the penetration ability of these two metal jets, Fe target-blocks were used as the target. At 3 CD (3 times charge diameter; ca. 100 mm from the shaped charge device), the breakup of Cu jet was observed, and the Cu metal segment at the jet tip was generated. On the other hand, the breakup of the Zn jet was not observed at 3 CD. The tip of the Zn jet exhibited a comet-like tail, which is unique compared to the morphology of the Cu leading jet. This result shows that the Zn jet tip reaches a state of liquid, and/or becomes a fine particle at the initial formation process. Against expectations, the penetration depth of the Zn jet against the Fe target placed at 5CD from the shaped charge device was higher than that of the Cu jet having a relatively large initial density. This result suggests that the penetration depth is more affected by the total mass of the metal jet and that the liner geometry to generate the jet mass effectively is differ depending on the material properties such as density and melting point.
HOSSAIN (Presenter), Univ of Delaware — Vacancy defects are ubiquitous in growing materials at the nanoscale. Yet their role in low-dimensional materials such as nanowires remains less understood. Here we report the observation of two mechanisms: elastic softening and stress localization that govern effective mechanical behavior of diamond and silicon carbide nanowires. They control different mechanical aspects of the nanowire at finite deformation. Elastic softening controls the effective mechanical properties such as stiffness in the linear regime of mechanical deformation, whereas stress-localization affects the effective toughness and strength of the nanowire. As a result, the condition for crack nucleation and the direction of crack growth are directly controlled by the stress-localization mediated by the higher-order elastic behavior of the lattice. With the increasing size of the defective regime, the nanowire shows softer effective elastic behavior that arises from the low-coordinated atoms forming the basis for the softening state of the defective regime. Results show that defect-size dependent effective stiffness is controlled by softening at the defective and surface regimes, whereas defect-size dependent toughness and strength are controlled by stiffening of the material by second-order elastic modulus.

MAURIZIO MATTESINI (Presenter), CAROLINA LÓPEZ-SÁNCHEZ, ELISA BUFORN PEIRÓ, AGUSTÍN UDÍAS VALLINA, Earth's Physics and Astrophysics, Univ Complutense — A key element to understand the mechanism of shallow-intermediate and very deep earthquakes is here provided by an accurate model description of the stress-strain curves of the subducting material, i.e. the metastable Olivine. Specifically, atomistic modeling was carried out through ab initio techniques for the Mg$_2$SiO$_4$ forsterite end-member at different pressure ranges. The achieved stress-strain relationships were finally compared to the Moment Rate Source-Time Functions (MRSTFs) and Fracture Energies values. We found that deep events have a common rupture pattern that differs substantially from that of shallow-intermediate earthquakes. This finding is in line with the different behavior observed in the stress-strain curves as a function of depth.

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C71.00359: X-Ray Absorption Spectroscopy Fingerprints for bcc and hcp Iron at Earth’s Core Conditions* MAURIZIO MATTESINI (Presenter), Department of Earth Physics and Astrophysics, University Complutense of Madrid, ANATOLY BELONOSHKO, Department of Physics, AlbaNova University Center, Royal Institute of Technology (KTH) — The shapes of Fe K-edge of X-ray absorption spectra (XAS) were theoretically computed at Core conditions by using a number of molecular dynamics snapshots from a previously equilibrated iron system at 360 GPa and 7000 K. Reference fingerprints for the different iron polymorphs, namely Fe-bcc and Fe-hcp, were thus obtained within the multi-scattering method and therefore proposed as specific spectroscopic fingerprints. It is shown that is possible to unfold the long-standing controversy about the structural complexity of iron at the Earth’s inner core conditions. Specifically, high pressure studies from static laser heated diamond anvil cell and dynamic compression can take advantage of the proposed spectroscopic fingerprints.

*This work has been partially supported by the Spanish Ministry of Economy and Competitiveness, Project CGL2017-86070-R.

C71.00360: Phase diagram of solid hydrogen SAM AZADI (Presenter), Physics, King’s College London — We present new results for the phase diagram of low-temperature high-pressure solid hydrogen, which are obtained using independent-particle and many-body wave function-based approaches. To discover the nature of phase III, density functional theory calculations within the meta-generalized gradient approximation by means of the strongly constrained and appropriately normed (SCAN) semilocal density functional are employed to investigate eleven molecular structures within wide pressure ranges of 100-500 GPa. The SCAN-DFT predicts two structures of C2/c and P6122 as the best candidates for phase III. We employ the diffusion Monte Carlo (DMC) method to verify the stability of competitive phases which requires an accurate description of exchange interaction. Our DMC results indicate that the optimised percentage of exact-exchange in many-body wave function equals to 40%. We name the corresponding exchange and correlation functional as PBE\textsubscript{1}. The PBE\textsubscript{1}-predicted phase diagram shows that the phase III of high-pressure solid hydrogen is polymorphic [1].

References:
Coarse-grain simulation study of the shear-band deformation mechanism in molecular crystals

SERGEI IZVEKOV (Presenter), PATRICK G. LAFOND, JOHN K. BRENNAN, JAMES P. LARENTZOS, US Army Rsch Lab - Aberdeen — Computationally inexpensive particle-based coarse-grained (CG) models are crucial for simulations of mesoscopically slow cooperative phenomena such as plastic deformations in solids. Molecular crystals possessing complex symmetry present an enormous practical challenge for coarse-graining at molecularly resolved scales, where the molecule is mapped into a CG particle and beyond. In this paper, we present the successful bottom-up coarse-graining of a molecular energetic crystal, cyclotrimethylene trinitramine in the alpha phase (α-RDX), using the force-matching based multiscale coarse-graining (a.k.a. MSCG/FM) approach. The new MSCG/FM model offers a potentially powerful free-energy tool to analyze the lattice instabilities that lead to plastic response. A specific application of this model involves a study of the molecular-level mechanisms of shear microband formation, which is observed in the atomistic simulations of α-RDX under both static and shock-wave uniaxial compressions. These were hypothesized to contribute to plasticity, and potential shock initiation in RDX-based explosives.


Atomistic Predictions for Reaction Mechanisms, Kinetics, and Detonation Properties of the Insensitive Explosive LLM-105

ALEJANDRO H STRACHAN, BRENDEN HAMILTON (Presenter), Purdue Univ, BRAD STEELE, MATTHEW P KROONBLAWD, I-FENG W KUO, Lawrence Livermore National Laboratory — Understanding the mechanical and chemical characteristics of insensitive high explosives (IHEs) is key for the design of new insensitive materials with improved response. We explore high temperature reaction kinetics and identify reaction mechanisms for the IHE LLM-105 through all-atom molecular dynamics performed at two levels of quantum chemical theory and with classical reactive potentials. Short timescale DFT-MD simulations are used to cross-validate density functional tight-binding (DFTB) predictions, which in turn are compared against multiple ReaxFF parametrizations. High-throughput DFTB simulations are coupled with the Hugoniotstat technique to simulate shock loading and to characterize the Hugoniot curves for both unreacted LLM-105 and its products. DFTB predictions for the CJ state and detonation properties are in good agreement with ReaxFF-LG. Effects of pressure on reaction products and pathways are identified and isothermal-isobaric simulations are used to study reactions at CJ conditions. Prepared by LLNL under Contract DE-AC52-07NA27344. Approved for unlimited release, LLNL-ABS-793765.
C71.00363: Development of low-adiabat drives for Rayleigh-Taylor strength experiments* 
TOM LOCKARD (Presenter), Lawrence Livermore Natl Lab, MATTHEW P HILL, Atomic Weapons Establishment, ANDREW KRYGIER, ALEX ZYLSTRA, Lawrence Livermore Natl Lab, PETER GRAHAM, Atomic Weapons Establishment, PHILIP POWELL, DAMIAN C SWIFT, SHON T. PRISBREY, HYE-SOOK PARK, JAMES M MCNANEY, Lawrence Livermore Natl Lab — We have used the expansion of a shocked reservoir assembly across a gap to induce ramp loading, and hence infer strength from the growth of ripples at an interface. For multi-megabar loading, the reservoir comprises a sandwich of several materials, and the resulting load history has a large amount of structure, including shocks. This structure leads to a degree of shock heating, and some uncertainty in the heating that actually occurs. We report on progress in studies to improve the reservoir drive by reducing the shock heating, including the performance of the models used for the components of the experiment in hydrodynamic simulations.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

C71.00364: LASER SCIENCE —

C71.00365: Electron cyclotron emission with a helical wavefront in millimeter-wave regime from an electron accelerated by a circularly polarized wave YUKI GOTO (Presenter), Department of Applied Energy, Nagoya University, SHIN KUBO, TORU II TSUJIMURA, National Institute for Fusion Science, National Institutes of Natural Sciences — In this study, we calculated an Electron Cyclotron Emission (ECE) with a helical wavefront in the millimeter-wave regime from an electron accelerated by a Circularly Polarized (CP) wave. Recently, it has been shown that radiation from a charged particle with spiral motion has a helical wavefront. Since an electron cyclotron motion is also a type of spiral motion, the ECE should also have a helical wavefront. In particular, we attempt to generate the high power coherent ECE with a helical wavefront from a multi-electron system. Because the radiation with helical wavefront from a single electron is low power, the superposition of the electric field is necessary to detect the radiation. For this reason, the CP wave plays an important role to control the electron' rotation motion. We have confirmed in the calculation that the rotation phase of the electrons is controlled by an externally applied CP electric field. It was also confirmed by calculation where the radiation from such the electron has a helical wavefront. We will show the details of the calculation results at the meeting.
C71.00366: Evolution from Periodic Oscillation to Chaos in Q-switched Vortex Lasers of a Unit Topological Charge  YUAN-YAO LIN (Presenter), CHAO-YI WU, Natl Sun Yat Sen Univ — Recently direct vortex lasing from azimuthal symmetry breaking resonator were demonstrated both in continuous wave [1] and in Q-switched [2] operations. Regarding to the investigation of laser dynamics we rebuild the Q-switched vortex laser system following the same configuration reported in REF [2]. Produced Q-switched laser emits annular intensity pattern and its positive unit topological charage is quantified by spiral phase pattern sensed using a interferometer. Clear transition from periodic oscillation of every 2 pulses, 4 pulses and 6 pulses to completely disorders in pulse sequences can be identified in delay maps using the pulse-to-pulse duration as an observable. This spatial-temporal dynamic can be explained by Tang-Statz-DeMars model that describes the coherent coupling and nonlinear interactions of the off-axis multiple pass resonance modes. Moreover pumping a KTP crystal by this Q-switched vortex laser at the wavelength of 1064 nm, second harmonic wave at 532 nm exhibits unconventional intensity distribution other than a vortex with doubling topological charges because of the interactions among the resonating off-axis modes in fundamental wave.


C71.00367: Discrete evolution on temporal separation and phase difference for bound solitons in an Yb mode-locked fiber laser* CECÍLIA CAMPOS (Presenter), LUCAS B. A. MÉLO, LÚCIO H. ACIOLI, MARCIO H. G. DE MIRANDA, Departamento de Física, Universidade Federal de Pernambuco — Multiple pulse regime is a common feature in passively mode-locked fiber lasers (MLFL). They could either be equally spaced, randomly distributed or arranged in a state of close interacting pulses. The later is often called bound solitons and presents strong modulation in the optical spectrum, which contains information about average relative phase, Δφ, and temporal separation between the pulses, τ. In this work, we study how increments in the total intracavity energy act on τ and Δφ for an Yb MLFL. For this, we continuously monitored the optical spectrum and the autocorrelation as the pump power was increased. We observed a discrete nature of τ, which is in agreement with previous works that observed its quantization for Er-doped fiber lasers [1] and predicted the quantization of binding energy between bound solitons [2]. Our work provides a systematic experimental study capable of capturing the jumps in τ, besides reporting a discrete behavior that is also present in Δφ.


*We acknowledge support from CNPq, CAPES and FACEPE.

C71.00368: ATOMIC, MOLECULAR, AND OPTICAL PHYSICS —
C71.00369: Using Light to Simulate the Quantum Mechanics of the Simple Pendulum*
ENRIQUE GALVEZ (Presenter), JAKE FREEDMAN, YINGSI QIN, FABIO J AUCCAPUCLLA, KRISTINA WITTLER, Colgate University — We present experiments with a type of non-diffracting optical beams that satisfy a form the 2-dimensional Helmholtz equation that is identical to the Schrödinger equation for the simple pendulum. This form is known as the Mathieu equation. As a result the optical beams are in spatial modes that are related to the quantum solutions of the pendulum. The light intensity in the far field is proportional to the probability of the pendulum bob as a function of the angular position. Depending on the parameters of the problem we can select either states that describe the pendulum swinging or rotating. This system also allows us to investigate an array of interesting quantum phenomena: stationary states with non-classical analogs, wavepacket revivals and even cat states.

*This work was funded by NSF grant PHY1506321

C71.00370: Effects of Spin-orbit-coupling-induced Resonance in Ultracold Bosonic Systems
YUNCHENG XIONG (Presenter), LAN YIN, Peking Univ — We calculate renormalized two-body interactions using T-matrix method, which is the sum of all orders of ladder diagrams in the bare basis. Apart from corrections to three types of diagonal interactions, there emerge many off-diagonal ones. We interpret the divergence of T-matrix as SOC-induced resonance, with the aid of which, the contrast of density modulation in stripe phase in Rb87 can be enhanced by ten times of its original value and wavelength enlarged by two times so that the stripe phase may be observed directly with conventional absorption image technique. Besides SOC-induced resonance, we also recalculate the critical value for Stripe-Plane wave transition which is shifted by a small value. Finally, we find the correction to the density profile when Raman coupling $\Omega>4E_r$.

C71.00371: Phonon Stability and Sound Velocity of Bose Mixture Droplet  
QI GU (Presenter), LAN YIN, School of Physics, Peking University — When the mean-field energy is as small as the quantum fluctuation, the self-energies under Bogoliubov approximation do not necessarily include all the contributions of the same order. For quantum droplets of a Bose mixture, the lower Bogoliubov mode is unstable at small momentum. Considering all the same order self-energies, the excitation spectrum is qualitatively different from the Bogoliubov mode. We develop Beliaev's method to calculate the elementary excitation and phonon velocity accurate to the order of gas parameter $(na^3)^{1/2}$ in the homogeneous droplet. We discuss quasi-particles' Beliaev damping and find that density phonons are almost undamped. The sound velocity is found to be positive, which determines the nonzero superfluid critical velocity of droplet. In experiments, our results can be tested by measuring sound speed, superfluid critical velocity or collective mode.
**C71.00372: Quench-produced solitons in a box-trapped Bose-Einstein condensate**

ELI HALPERIN (Presenter), MICHELLE WYNNE C SZE, JOHN CORSON, JOHN L BOHN, JILA — We describe a protocol to prepare solitons in a quasi-1d box-trapped Bose-Einstein condensate using only a quench of the isotropic s-wave scattering length. A quench to exactly four times the initial scattering length creates one soliton at each boundary of the box, which then propagate in a uniform background density and collide with one another. No nonsolotonic excitations are created during the quench. We investigate the robustness of this procedure to the scattering length ramp rate and a mismatch of the final scattering length.

*This material is based upon work supported by the National Science Foundation under Grants No. PHY 1125844 and No. PHY 1806971.

**C71.00373: Manipulation of cold chiral molecules using electronic and rotational spectroscopy**

ALICIA HERNANDEZ-CASTILLO (Presenter), JOHANNES BISCHOFF, JU HYEON LEE, MARCO DE PAS, HENRIK HAAK, GERARD MEIJER, SANDRA I EIBENBERGER, Molecular Physics, Fritz-Haber Institute — The two non-superimposable mirror images of a chiral molecule are referred to as enantiomers; that is, structures that cannot be transformed into each other by pure translation or rotation. Many molecules of biological interest have a stereogenic center that determines their functionality. However, most physical properties of enantiomers are identical, thus, chiral analysis remains a challenge, and there is a need for fast and reliable methods that can differentiate and/or separate enantiomers. Recently, the enantiomer-specific state transfer method\(^1\) was developed. This method provides the means to populate or depopulate a rotational state of an enantiomer. We have designed, built, and characterized a compact spectrometer capable of performing chirped-pulse Fourier transform microwave and electronic spectroscopy. By combining optical methods with microwave spectroscopy, we seek to maximize the state-specific enantiomeric enrichment. We also implement more sensitive detection schemes such that small population changes can be detected. Recent experimental results and details on the new spectrometer will be discussed.


**C71.00374: Photoassociation of Fermionic \(^{87}\)Sr via the \(^{1}S_0 - ^{1}P_1\) Transition**

JOSHUA HILL (Presenter), THOMAS CHARLES KILLIAN, Rice Univ — The fermionic isotope of strontium, \(^{87}\)Sr, is of interest for the development of optical frequency standards and the study of quantum many-body phenomena. In many of these experiments, \(^{87}\)Sr is confined in an optical lattice. Detecting the presence of doubly occupied lattice sites is a valuable tool for studies of atomic gases in optical lattices, and this is typically done with photoassociation, in which two ground-state atoms in a scattering state are photo-excited to a molecular state. No resonance frequencies have been reported for transitions to molecular states of any excited electronic potential for \(^{87}\)Sr. Here we present results for photoassociation of \(^{87}\)Sr atoms via the \(^{1}S_0 - ^{1}P_1\) transition at 461nm (\(\Gamma= (2\pi*30.5)\)s\(^{-1}\)), and measurements of optical lengths for select photoassociation spectra.

*National Science Foundation; PHY-1607665
C71.00375: **Cold polar molecules in superfluid helium nanodroplets: Electrostatic deflection of imidazole, its complexes and fragments**  
BENJAMIN KAMERIN (Presenter), JOHN W NIMAN, VITALY V KRESIN, Physics, University of Southern California — Helium nanodroplet isolation is a unique method for investigating molecules and molecular structures captured in an inert, superfluid matrix. In particular, it is a highly productive tool for the study of very cold polar molecules and their assemblies. We recently demonstrated that beams of nanodroplets doped with polar molecules can be interrogated by electrostatic deflection, leading to remarkably large deflections on the order of millimeters. Here we apply this method to the imidazole molecule, which is a five-membered polar ring which plays an important role in biological processes. We are able to differentiate polar complexes of imidazole by their dipole moments, and identify their fragmentation pathways.

*This work was supported by the NSF (CHE-1664601).

C71.00376: **Structures with local minima at low energies in above-threshold ionization electron spectra**  
DMITRY A. TELNOV, Dept. of Physics, St. Petersburg State University, Russia, SHIH-I CHU (Presenter), Center for Quantum Science and Engineering, and Center for Advanced Study in Theoretical Sciences, Dept. of Physics, National Taiwan University, Taiwan — We perform a theoretical and computational study of multiphoton above-threshold ionization (ATI) of several one-electron atomic (H and He\textsuperscript{+}) and diatomic (H\textsubscript{2}\textsuperscript{+} and HeH\textsubscript{2}\textsuperscript{+}) quantum systems. The driving laser fields are in the near- and mid-infrared frequency range and have moderate peak intensities corresponding to the Keldysh parameter slightly larger than unity. Our calculations reveal structures with local minima in the low-energy part of the ATI electron energy spectra if the targets are initially in the excited electronic states: 2s states for H and He\textsuperscript{+}, 1\sigma\textsubscript{u} state for H\textsubscript{2}\textsuperscript{+}, and 2\sigma state for HeH\textsubscript{2}\textsuperscript{+}. The effect is non-perturbative and depends on the frequency and intensity of the driving field. The structures in the ATI electron energy spectra have the same nature for all the systems under consideration. Although the ionization process is generally nonresonant, our analysis shows an important role of intermediate electronic energy levels between the initial state and the onset of the continuum. For the hydrogen atom initially in the 2s state, we identify the intermediate states with the principal quantum number n=3 as those responsible for shaping the structure with the local minimum in the low-energy part of the ATI electron energy spectrum.

*MOST and NTU (Taiwan)*
C71.00377: A relativistic single-particle potential for photoexcited electron orbitals of open-shell atoms  JAMES BOYLE (Presenter), Boyle, PLLC — A single-particle potential for the calculation of relativistic photoexcited electron orbitals is introduced. Based upon the earlier work of Qian et al. (Phys. Rev. A 33, 1751 (1986)) and Boyle (Phys. Rev. A 48, 2860 (1993)) for non-relativistic electron orbitals, this relativistic potential is defined to include exactly all of the first-order electron correlations that appear in the diagrammatic perturbation series of the dipole polarizability and that contain potential corrections in the intermediate state. Analytic relationships associated with initial state jj-couplings are also considered. For example, among other things, the ability to rewrite the defined relativistic potential for a final state as an average term plus a correction to the defined average is investigated and presented.

C71.00378: The Link between Artificial Neural Networks and Propagation in Random Media  GIULIA MARCUCCI (Presenter), DAVIDE PIERANGELI, CLAUDIO CONTI, Physics Department, Sapienza University of Rome — Random media (RM) with tailored optical properties are attractive for their many applications. Transmission channels (TCs) in RM can be effectively controlled, and their rich behavior is due to the multitude of interacting optical modes. We demonstrate that TCs in RM act as an untrained artificial neural network (ANN), as deep as the amount of perturbations. This lets us obtain a random optical machine (ROM), able to do computation by reservoir computing (RC).

TCs in RM can be modulated by tuning the transmission matrix (TM) through iterative algorithms that modify the input until a designed output is obtained. This approach treats RM as black boxes, i.e., it treats the TM as an ANN hidden layer of a reservoir computing (RC) strategy, a machine learning technique that left untrained the ANN internal part and optimizes weights only at input and readout.

By electromagnetic perturbation theory, we prove that weakly tampering the medium generates a new TM, given by the product between the previous TM and the perturbative one. We then design the ANN depth of our ROM by optimizing the amount of perturbations, moving from an extreme learning machine (unperturbed system) to untrained deep learning (many perturbations).

C71.00379: Infinite temperature adiabatic flows and quantum many-body scar states in a chaotic system  SHO SUGIURA (Presenter), Harvard University, PIETER W CLAEYS, Boston University, AN DYMARSKY, University of Kentucky, ANATOLI S POLKOVNIKOV, Boston University — Under any operation in many-body chaotic systems, quantum states usually experience dissipation. However, this dissipation can be drastically suppressed through the application of additional appropriate control fields, as is done in counterdiabatic driving. Here, we restrict control to few-body operations and draw flows of the optimal path for quantum control in a non-integrable Ising chain. We find that these flows are highly anisotropic; we can realize almost dissipationless driving in one direction while dissipation is hard to reduce in the perpendicular direction. This indicates that the choice of the path is crucial for quantum operations in many-body chaotic systems. Furthermore, states which are eigenstates of the counterdiabatic term are shown to exhibit small dissipation even without counterdiabatic fields, and are closely related to quantum many-body scar states and many-body dark states.
C71.00380: Atom-Light Interactions in Integrated Photonics: en Route to an Atomic Lab on a Photonic Chip*  HADISEH ALAEIAN (Presenter), ARTUR SKLJRAW, ROBERT LOEW, HARALD KUEBLER, TILMAN PFAU, University of Stuttgart — The integration of photonic structures with thermal atomic vapors on a chip provides efficient atom-light coupling on a miniaturized scale well beyond the diffraction limit hence, opening a new regime in the field of cavity quantum electrodynamics. In this talk, we present the results of our study on interactions of thermal Rb atoms with integrated SiN and Si Nano-devices. In the former case, the atoms are probed with a laser at the D$_2$ transition, whereas in latter the atoms are further excited to the 4D states with an additional excitation at telecom wavelength. Our studies on Si structures benefit from stronger mode confinement due to the large reflective index as well as a larger dipole moment. Moreover, we demonstrate novel measurements on the effects of Si surface potentials on Rb 4D states. Promising results on ring resonators pave the way towards further investigations of high-Q photonic crystal cavities in order to reach the strong coupling regime.

*IQST Young Investigator award and Baden Württemberg Foundation

C71.00381: An optical fiber simulator of three interacting atoms in one dimensional parabolic trap*  MIGUEL GARCIA-MARCH (Presenter), Univ Politecnica de Valencia, NATHAN L HARSHMAN, American University, THOMAS FOGARTY, OIST - Okinawa Institute of Science and technology, HEITOR DA SILVA, Federal University of Rio Grande do Norte, THOMAS BUSCH, OIST - Okinawa Institute of Science and technology, MACIEJ A LEWENSTEIN, ICFO - The Institute of Photonic Sciences, ALBERT FERRANDO, Universitat de Valencia — We introduce an optical fiber that simulates a system of three trapped ultracold and strongly interacting atoms in one-dimension. To simulate the contact interactions among the atoms, we consider a sharp and narrow jump in the refractive index. To this end, we consider here three thin metallic slabs. To simulate the parabolic trap we assume that the fiber has a graded refractive index profile. While the wave-nature of single quantum particles leads well-known analogies with classical optics, for interacting many-particle systems such analogs are not straightforward. We discuss: i) how by spatially modulating the incident field, one can select the atomic statistics, i.e., emulate a system of three bosons, fermions or two bosons or fermions plus a distinguishable particle; ii) how this system can produce classical non-separability resembling that found in the analogous atomic system.


The surface plasmon-polariton (SPP) waves guided by one-dimensional photonic crystals (1DPCs) are usually excited at the interface perpendicular to the direction of periodicity. In this work, we will present the formulation and the numerical results delineating the excitation of the SPP waves on the interface perpendicular to the direction of periodicity. Both the eigenvalue problem of finding and solving the dispersion equation and the problem of the excitation of the SPP waves will be discussed. The eigenvalue problem is solved using the rigorous coupled-wave approach. The results indicate the presence of the plasmonic bandgap that can help in designing the plasmonic optical filters.

References:

In present work, we resolve the unified equation of motion for a quantum system on the adiabatically changed Finsler manifold, suggested by Lipovka (2017), for the particular case of the hydrogen atom. The radial part for the equation of motion is obtained to model a hydrogen atom, where the electron and the nucleus rotate around a center of mass. By using this expression, the total energy of the system under consideration (charged particles and EM field) is obtained.

By expanding in series in the small parameter $\alpha = v/c$, the value of the anomalous magnetic moment of the electron is obtained. The value calculated by J. Swinger $= \alpha /2\pi=0.0011614$ is obtained as a particular case.
THOMAS VARBERG (Presenter), SAMUEL P GLEASON, DALIR H. P. KELLETT, PAUL P. REISCHMANN, Chemistry, Macalester Coll — We have recorded electronic spectra of tantalum hydride (TaH) over the region 605–665 nm. The spectra were recorded by laser excitation spectroscopy at Doppler-limited resolution using a continuous-wave ring dye laser. We have assigned and fitted a total of 12 different bands, which originate from one of three low-lying electronic states. Calculations by Mark Gordon’s group and previous experimental work in our group confirm that the Ω = 2 ground state is largely derived from a σ^2δπ, 3Φ_2 state. An Ω = 0^+ state, largely a mixture of ^3Σ− and ^3Π, lies only 76 cm⁻¹ above the Ω” = 2 ground state. By recording dispersed fluorescence, we found and characterized a total of six low-lying states of the molecule. The electronic states have been fitted by least-squares using a Hund’s case (c) Hamiltonian. We report term energies, vibrational frequencies, rotational and centrifugal distortion constants, and bond lengths for these states, which were found to be in good agreement with the computational results.

*This work has been supported by two grants from the National Science Foundation, CHE-1265741 and CHE-1565969.

KAYA MONDRY (Presenter), Engineering Physics Nuclear Engineering, University of Madison Wisconsin — Overall Objective
The goal of this project is to investigate the engineering physics phenomenon of critical heat flux (CHF) for surfaces of accident tolerant fuel (ATF) cladding materials that are being considered for implementation jointly by industry, utilities, and the Department of Energy (DOE). This effort involves testing at small scale in a pool boiling environment and testing at intermediate scale in flow boiling under prototypical conditions, along with associated analysis.

*Dr. Peng Xu – Westinghouse Electric Company
Dr. William Byers – Westinghouse Electric Company
Dr. Christian Deck – General Atomics
C71.00386: Floquet approach to the study of the dynamical Lamb effect* MIRKO AMICO (Presenter), ROMAN KEZERASHVILI, The Graduate Center, City University of New York — The dynamics of N qubits coupled to a harmonic oscillator with time-periodic coupling is investigated in the framework of Floquet theory. This system can be used to model nonadiabatic phenomena that require a periodic modulation of the parameters of the system. An example is the dynamical Lamb effect, the simultaneous excitation of the qubits and the harmonic oscillator out of the ground state due to the nonadiabatic change in boundary condition of the system. The time-dependent Schroedinger equation describing the system’s dynamics is solved within the Floquet formalism and two other equivalent methods that rely on a perturbative approach in the time- and Laplace-domain. Because of the periodicity of the problem analyzed, the Floquet formalism provides a framework where analytical and numerical results are closest to each other. Nonetheless, the time- or Laplace-domain perturbative approaches can be used in the presence of simple or complicated, respectively, aperiodic time-dependent terms in the Hamiltonian.

*This work is partially supported by the U.S. Department of Defense under Grant No. W911NF1810433.

C71.00387: Symmetric Rotating Wave Approximation for the Generalized Two-Mode Two-Photon System Coupled with a Bosonic Field DAVID WU (Presenter), Caltech — We study the analytically approximated eigenenergies of the two-mode two-photon quantum Rabi model coupled with a Bosonic field. By equipping the previously established generalized symmetric rotating wave approximation (G-SRWA) method used on single-mode spin-boson systems with a unitary squeezing operator and applying it onto the two-mode two-photon system, we obtain a more generalized and simplified closed-form expression for eigenenergies of the system compared to other expressions derived using the functional Bethe ansatz method. We further investigate the effectiveness of the squeezing operator by examining the eigenenergies of the generalized resonant and nonresonant case for the two-level two-photon system. The accuracy of the updated G-SRWA method in the ultra and deep-strong coupling regimes reveals interesting symmetries within the mathematical structure of the two-level two-photon systems.
C71.00388: Topological Control of Extreme Nonlinear Waves  GIULIA MARCUCCI (Presenter), DAVIDE PIERANGELI, Physics Department, Sapienza University of Rome, AHARON J. AGRANAT, Applied Physics Department, Hebrew University of Jerusalem, RAY-KUANG LEE, Institute of Photonics Technologies, National Tsing Hua University, EUGENIO DELRE, CLAUDIO CONTI, Physics Department, Sapienza University of Rome — Controlling nonlinear optical processes is a significant challenge in photonics. Shock waves, rogue waves and solitons are widespread, from optics to hydrodynamics. Intense research is dedicated to advanced techniques for tailoring extreme waves and finding the conditions to induce transitions between different waves.

We develop a new strategy to supervise, modify and tune a laser beam in third-order nonlinear materials, when light propagation is ruled by the nonlinear Schrödinger equation (NLSE). We denote our approach topological control (TC) [1]. TC is based on the one-to-one correspondence between the number of wave packet oscillating phases and the genus of toroidal surfaces associated with the NLSE solutions by the Riemann theta function.

We prove that our method is experimentally realizable in a photorefractive crystal [1]. Specifically, we use the parametric time-dependence of photorefractive nonlinearity to shape the asymptotic wave profile. We tailor propagation coefficients, as nonlinearity and dispersion, to observe all the phases in the nonlinear wave evolution of a rectangular-shaped beam, and to control transitions from shock to rogue waves.


C71.00389: Theory of High-Energy Electron Thermionic Emission from Graphene  LIEMAO CAO (Presenter), YUEYI CHEN, LAY KEE ANG, YEE SIN ANG, Singapore University of Technology and Design — Graphene thermionic electron emission across high barrier involves energetic electrons residing far away from the Dirac point. In this work, we construct a full-band model beyond the simple Dirac cone approximation for the thermionic injection of high-energy electrons in graphene [1]. We show that the thermionic emission model based on the Dirac cone approximation is valid only in the graphene/semiconductor Schottky interface operating near room temperature but breaks down in the cases involving high-energy electrons. We further reveal a critical potential barrier height beyond which the Dirac cone approximation crosses over from underestimation to overestimation. In the high-temperature thermionic emission regime, the Dirac cone approximation severely overestimates the electrical and heat current densities by more than 50% compared to the more accurate full-band model. Our findings reveal the fallacy of Dirac cone approximation in the thermionic injection of high-energy electrons in graphene. The full-band model developed here can be readily generalized to other 2D materials and shall provide an improved theoretical avenue for the accurate analysis, modeling and design of graphene-based thermionic energy devices.

C71.00390: Generation of optical vortices from a spatial light modulator, vortex phase plate, and mode converter*  TING-HUA LU (Presenter), TENG-DE HUANG, Department of Physics, National Taiwan Normal University — First introduced in 1992 by Prof. Allen et al., light with orbital angular momentum (OAM), also called the Laguerre-Gaussian mode, possesses an OAM of per photon. Its twisted phase wavefront is a manifestation of the azimuthal phase term in its wavefunction, while the phase singularities along the beam axis are defined as the optical vortices. The twisted light which possesses OAM can be generated by laser cavities, spiral phase plate, metalens, and spatial light modulator (SLM). In this work, we utilize a vortex phase plate, mode converter, and spatial light modulator to generate high-order vector vortex beams. The mode converter is used to transform the vortex beam with circular symmetry into rectangular symmetry and form the vortex array. This is a convenient and powerful method to produce and control the optical vortex array of the vector superposed optical field, which is composed of different orders of crossed Hermite-Gaussian bases with opposite helicity of circular polarization. The SLM provides an extra degree of freedom to increase and control the order of the bases in the vector superposed optical field, which can induce optical vortices of different sizes and quantities.

*MOST 108-2112-M-003-009

C71.00391: Multipole Excitation of C_{60} Molecules in a Semi-Classical Approach  KRISHNA LAMICHHANE (Presenter), Physics, Diablo Valley College Pleasant Hill, CA — This work investigated the collective dynamic response of the 240 delocalized valence electrons of the C_{60} molecules to external stimulations such as electromagnetic radiation or scattering of the charged particle, using local current approximation (LCA), which is a semiclassical approach based on general variational principle. Here the bulk of the valence electrons is treated as a semi-classical fluid that exhibits both the translational and compressional vibrations. The coupling of these two modes has been studied and the results are in good agreement with the experimental data from photoionization experiments on C_{60}. The same semi-classical approach has been applied to study the energies of higher angular momentum resonance.

C71.00392: Ab Initio Potentials for Low-Energy Positronium Scattering  JESSE KINDER (Presenter), Oregon Institute of Technology — This poster presents ab initio potentials for positronium-atom and positronium-molecule interactions. Two methods are used to calculate the potential energy: self-consistent solution of the Hartree-Fock equations and solution of the Kohn-Sham equations at the level of the local density approximation. The total energy is computed for a wide range of positronium-molecule separations, molecular orientations, and basis sets. Comparing the two methods illustrates the importance of both electron-electron and electron-positron correlations in obtaining realistic potentials.

Low-energy positronium scattering may soon become experimentally feasible in facilities such as the positronium beam line at the University College in London. This goal of this study is to provide a starting point for the theoretical analysis of positronium scattering at low energies from first principles, to complement existing studies based on semi-empirical potentials.
C71.00393: New Atomic Model from the spectra of Hydrogen, Helium, Beryllium, Boron, Carbon, and Deuterium and their ions  
JANEEN HUNT (Presenter), APS — A cohesive unifying theory of the atom does not currently exist in Quantum Physics. In this research, the atomic spectra are allowed to determine the model for the atom based upon the finding of patterns of the Balmer-Rydberg formula in the first 20 ions and neutral atoms of the periodic table. From this data, the model postulates a standing wave of varying energy antinodes originating from the particles in the nucleus of each atom which is able to predict the ionization energies of these atoms. The transitions of the electrons in atoms are defined by the energies of each antinode represented by the difference in energy between each spectral line. The spectral patterns for H, He-I, He-II, Li-I, Li-II, Li-III, Be-I, Be-II, Be-III, Be-IV, B-I, B-II, B-III, B-IV, B-V, C-I, C-II, C-III, C-IV, and Deuterium are charted and the ionization energies are calculated from the data including general inferences this model predicts about the unification of atomic forces, electron transitions, heat, and electromagnetism. This model predicts that the nucleus of every atom is held together by energy in the form of a standing wave originating from the nucleus and surrounding it. This is the Sollism Theory of the atom.

C71.00394: WITHDRAWN ABSTRACT —

C71.00395: Casimir Juggling  
CONNOR HAFEN (Presenter), DANIEL SHEEHAN, Univ of San Diego — Casimir forces can dominate system behavior at the nanoscale; increasingly, efforts are being made to control and exploit them [1-3]. Here we propose a simple method for contact-free, dynamic levitation, handling, and physical diagnosis of micron and sub-micron particles in vacuum using these forces. This ‘Casimir juggling’ should sidestep the negative effects of stiction and contact contamination. Analytic calculations and numerical modeling show particles can be levitated, transported and deposited with nanometer precision using kHz-MHz active-feedback Casimir probes. Standard laboratory techniques appear adequate to experimentally test this proposal.
C71.00396: Survey of Molecular Rotational Transitions for Millimeter-Wave Frequency Metrology.  MARK YEO (Presenter), ANTOINE ROLLAND, TOMOHIRO TETSUMOTO, Boulder Research Laboratory, IMRA America — User-defined, spectrally pure and tunable millimeter-wave oscillators, using emerging photonic technologies, enables the probing of pure rotational molecular transitions (from 30 GHz to 1 THz). This work promises to open new applications in frequency metrology, precision molecular spectroscopy, and trace gas sensing. Here we report a theoretical survey of a wide range of molecular candidates to compare their suitability for use in a rotational based clock. We will report calculations that lead to theoretical estimations of clock factors of interest such as line positions and strengths, and sensitivity to environmental perturbations. This work will provide an understanding of the utility of ultra-precise measurements of the rotational spectrum in blooming applications such as radio-astronomy and remote sensing, non-invasive sensing, wireless communications, and for THz frequency metrology.

C71.00397: WITHDRAWN ABSTRACT —

C71.00398: WITHDRAWN ABSTRACT —

C71.00399: Design of a viable radiation-balanced fiber laser or amplifier*  ARASH MAFI (Presenter), MOSTAFA PEYSOKHAN, ESMAEIL MOBINI, University of New Mexico — Recent advances in power scaling of fiber lasers are hindered by the transverse mode instability (TMI), which deteriorates the output beam quality. TMI is blamed on the overheating of the fibers. Anti-Stokes fluorescence (ASF) cooling of the rare-earth-doped gain material has been suggested as a potentially viable heat removal scheme. In this scheme, the fiber is pumped at a pump wavelength, which is longer than the mean fluorescence wavelength of the active ions. Therefore, the fluorescence removes some of the excess heat. It may be possible even to balance the ASF cooling against all other sources of heating and make a non-heating radiation-balanced laser (RBL). I will focus on the general scaling laws that govern the design of RBLs. I will show that the magnitude of the parasitic absorption plays an essential role in the feasibility of such designs, especially in a double-cladding setting, and the measures that need to be taken to achieve net heat-balancing in a viable RBL.


*AFOSR MURI: FA9550-16-1-0362
C71.00400: Uncovering the Role of Excited States of Dication in Controlling the Dissociative Double Ionization of Ethane  
GIHAN BASNAYAKE (Presenter), DUKE DEBRAH, WEN LI, Wayne State Univ — With the aid of newly developed coincidence detection imaging system, we demonstrate that the branching ratios of dissociative double ionization channels of ethane can be controlled by varying the ellipticity of the intense ultrashort laser pulses. The $\text{CH}_3^+$ formation channel and $\text{H}^+$ formation channel show a significant yield changes, producing the highest and lowest at ellipticity of 0.59 respectively. With the help of theoretical calculations, we attribute such a control to both angle dependent ionization and intensity dependent ionization to excited dication states.

C71.00401: High bandwidth, bidirectional microwave to telecom conversion using an electro-optic transducer operating at millikelvin temperatures*  
WILLIAM HEASE (Presenter), ALFREDO RUEDA, RISHABH SAHU, JOHANNES FINK, Institute of Science and Technology Austria — Long distance connectivity of superconducting qubits poses an interesting challenge because their fragile microwave quantum states need to be protected from thermal noise. A hybrid quantum network, which combines the advantages of microwave quantum information processing and the robustness of optical telecommunication, appears as the natural solution. In this context, coherent conversion between optical and microwave photons is the key ingredient. We present a triply resonant electro-optic modulator [1] as a bidirectional and low noise microwave to optics converter. Our system is based on a LiNbO3 whispering gallery mode resonator coupled to a superconducting 3D microwave cavity. Unlike electro-opto-mechanical systems, a low frequency mechanical mediator is not needed, allowing for a 10 MHz conversion bandwidth and low added conversion noise of less than 1 quanta for continuous wave optical pump powers up to 25 $\mu$W.


* Supported by European Research Council under grant agreement number 758053 (ERC StG QUNNECT), and by the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 754411.
C71.00402: Towards cavity quantum circuit electromechanics with millimiter-sized silicon nitride membranes
SARWAN PEITER, ADRIAN SANZ MORA (Presenter), GARY STEELE, Delft University of Technology — Due to their extremely high mechanical quality factors, silicon nitride membranes are commonplace in optomechanical experiments conducted with light fields. However, to strongly couple optical radiation to the vibratory motion of such membranes down in the quantum regime is still a sought-after target in these experiments. We use here an original assembly to couple instead microwave radiation to a vibrating membrane of submillimiter dimensions, obtaining interaction strengths approaching state of the art values achieved in the optical realm. The assembly is based on a mechanically adjustable pressing frame through spring screws, that holds a chip with an integrated lumped element resonator antenna facing another chip hosting the membrane. The membrane is coated with a layer of metal so that the two chips couple capacitively to form a resonant circuit, the capacitance of which, and thus its resonance frequency, is modulated by the membrane vibrations. Besides its potential to challenge the foundations of quantum mechanics at unconventional mass and length scales, our electromechanical device may be well suited to study nonlinear phenomena in the framework of classical mechanics such as the emergence of chaotic dynamics in the weak damping limit.

C71.00403: Acoustic modes of superfluid helium in a cross geometry
VAISAKH VADAKKUMBATT (Presenter), THOMAS CLARK, Univ of Alberta, SWATI SINGH, University of Delaware, JOHN DAVIS, Univ of Alberta — Superfluid helium is a low-loss optomechanical element, and an acoustic quality factor value up to $10^8$ has been realized experimentally in a macroscopic quantum system using a cylindrical microwave cavity [1]. It has been predicted that three orders higher quality factor may be attained with improvements to the experimental system. With these parameters, superfluid helium is a potential candidate for detecting continuous gravitational waves [2]. Here, we study the acoustic modes of superfluid helium inside a cross geometry using a re-entrant microwave cavity that provides improved detection of the acoustic modes. The cross shaped geometry is also predicted to be more sensitive than a cylinder for detection of gravitational waves.


*The University of Alberta; the Natural Sciences and Engineering Research Council, Canada (Grants No. RGPIN-04523-16, No. DAS-492947-16, and No. CREATE-495446-17); the Canada Foundation for Innovation; and National Science Foundation grant PHY-1912480.
C71.00404: Coherent coupling completes an unambiguous optomechanical classification framework*  
XIANG LI (Presenter), California Institute of Technology, MIKHAIL KOROBKO, Universität Hamburg, YIQIU MA, California Institute of Technology, ROMAN SCHNABEL, Universität Hamburg, YANBEI CHEN, California Institute of Technology — Cavity optomechanics studies the dynamics of systems in which optical and mechanical degrees of freedom are coupled, e.g., optical resonators with movable/deformable boundaries and/or shapes. A system's behavior depends crucially on the nature of optomechanical coupling. In addition to the previously well-known dispersive (when real parts of optical eigenfrequencies depend on mechanical displacement) and dissipative coupling (when imaginary parts of optical eigenfrequencies depend on mechanical displacement), we identify coherent coupling as a new type of coupling (when neither depend on mechanical displacement) and show that the three together fit into a general, unambiguous classification framework. We discuss in detail a ring cavity with a movable mirror inside, a system that has pure coherent coupling without any dispersive or dissipative coupling.

*The work of X.L., Y.M. and Y.C. are supported by the National Science Foundation through Grants PHY-1612816, PHY-1708212 and PHY-1708213, the Brinson Foundation, and the Simons Foundation (Award Number 568762). The work of M.K. and R.S. was supported by the Deutsche Forschungsgemeinschaft (DFG) (SCHN 757/6-1).

C71.00405: Two-tone optomechanical instability and its fundamental implications for backaction-evading measurements*  
ITAY SHOMRONI (Presenter), AMIR YOUSSEFI, NICK SAUERWEIN, LIU QIU, Ecole Polytechnique Federale de Lausanne, PAUL SEIDLER, IBM Research-Zurich, DANIEL MALZ, Max-Planck-Institut für Quantenoptik, ANDREAS NUNNENKAMP, Cavendish Laboratory, University of Cambridge, TOBIAS J. KIPPENBERG, Ecole Polytechnique Federale de Lausanne — We report a new type of optomechanical instability that arises in two-tone backaction-evading (BAE) measurements of mechanical motion, a protocol designed to overcome the standard quantum limit. We demonstrate the effect both in the optical and microwave domains using different optomechanical systems, and find excellent agreement with theory. In contrast to the well-known parametric instability that occurs in single-tone, blue-detuned pumping, and results from a two-mode squeezing interaction between the optical and mechanical modes, the two-tone instability results from single-mode squeezing of the mechanical mode due to small detuning errors in the two pump frequencies. The instability can occur even with balanced intracavity fields and for both signs of detuning errors. The required tuning accuracy increases with pump power, putting an intrinsic limit on the sensitivity of BAE measurements and on other two-tone schemes.

*SNSF grant agreement No. NCCR-QSIT: 51NF40-160591; ERC Advanced Grant QUENOCOBA under the EU Horizon 2020 program (grant agreement 742102); University Research Fellowship from the Royal Society; Winton Programme for the Physics of Sustainability; EU Horizon 2020 research and innovation program, grant agreement No. 732894 (FET Proactive HOT).
C71.00406: Ultraviolet resonator integrated in a hollow-core fiber for Xenon plasma lasing*

JEREMY FLANNERY (Presenter), SEMA KURU, SUPRATIK SARKAR, VINODH RAJ RAJAGOPAL MUTHU, MICHAL BAJCSY, University of Waterloo — We integrate a cavity in a large-diameter hollow-core optical fiber based on inhibited coupling as a step towards realization of a fiber-integrated gas laser in the ultraviolet (UV) region. This is accomplished by attaching highly reflective photonic crystal (PC) membranes onto the ends of a fiber segment to form a Fabry-Perot cavity. The PC membranes are fabricated using e-beam lithography and reactive ion etching, which are then mounted on the fiber face using a micromanipulator stage. The presence of the PC holes allow for injection loading of atomic species into the fiber-cavity. Specifically, Xenon gas can be introduced through the perforated membrane into the hollow-core of the fiber to act as a gain medium for UV lasing when exposed to RF discharge.

*This research was undertaken thanks in part to funding from Canada First Research Excellence Fund.

C71.00407: Numerical Modeling of Optomechanical Sensors for Dark Matter Detection*

RUSSELL STUMP (Presenter), JACK MANLEY, SWATI SINGH, Univ of Delaware — Ultralight scalar dark matter can be represented as an atomic strain that can drive the acoustic breathing modes of an elastic body. We propose various laboratory-scale mechanical resonators for measuring the acoustic excitations at frequencies ranging from kilohertz (kHz) to Gigahertz (GHz)[1]. These devices include bulk acoustic wave resonators, phononic crystals, superfluid helium detectors and suspended sapphire micropillars. We use numerical modeling techniques to characterize each device’s performance as a dark matter detector. These techniques can be applied to an arbitrary mechanical resonator to measure its viability as a sensor for these signals.

*National Science Foundation grant PHY-1912480
C71.00408: Observation of dynamical quantum phase transitions in spinor condensates with no correspondence in ground-state phase diagram*  HAOXIANG YANG (Presenter), TIAN TIAN, LIYUAN QIU, HAIYU LIANG, YANBIN YANG, YONG XU, LUMING DUAN, Tsinghua University — Dynamical quantum phase transitions are closely related to equilibrium quantum phase transitions for ground states. Here, we report an experimental observation of a dynamical quantum phase transition in a spinor condensate beyond this conventional wisdom. We observe that the quench dynamics exhibits a non-analytical change with respect to a control parameter in the absence of a corresponding phase transition for the ground state there. We make a connection between this singular point and a phase transition point for the highest energy level in a subspace with zero spin magnetization of a Hamiltonian. We further show the existence of dynamical phase transitions for finite magnetization corresponding to the phase transition of the highest energy level in the subspace with the same magnetization. Our results open a door for studying dynamical phase transitions beyond the conventional ground-state phase diagram and using them as a tool to probe the phase transitions at higher energy eigenlevels of many-body Hamiltonians.

*This work was supported by the Frontier Science Center for Quantum Information of the Ministry of Education of China, Tsinghua University Initiative Scientific Research Program, and the National key Research and Development Program of China (2016YFA0301902)

C71.00409: Hydrodynamics of shock waves in ultracold non-degenerate dipolar gases.*  REUBEN WANG (Presenter), ANDREW SYKES, JOHN L BOHN, JILA — The hydrodynamics of an ultracold, non-degenerate gas of harmonically trapped dipolar atoms is studied. We numerically simulate this system using direct simulation Monte Carlo methods in the regime where interactions are dominated by two-body collisions, as for instance can be achieved in ultracold gases of Dy or Er. We subject the gas to a short-pulse perturbation which is common in hydrodynamic studies of shock waves, emphasizing the anisotropies in hydrodynamic phenomena resulting from the anisotropic collision cross sections of the dipoles. This work extends observations of anisotropic rethermalization of a cold, dipolar gas previously seen in [1,2]. Here, shock wave hydrodynamics is studied in the less explored low-temperature regime, leading to a emergence of rich phenomena. This work was supported by the NSF.


*National Science Foundation.
C71.00410: Self-organization and stroboscopic dynamics of a driven Rydberg gas
KAI KLOCKE (Presenter), MICHAEL BUCHHOLD, Caltech — Motivated by recent experiments observing signatures of self-organized criticality (SOC) in driven Rydberg ensembles, we develop a Langevin description to explore how SOC can emerge from the microscopic interactions in experimental Rydberg setups. We demonstrate that drift and diffusion of atoms arising from an inhomogeneous trapping potential capture the stroboscopic evolution observed in experiments. The trap dynamics induces a continuous reorganization of the atoms, which pins the central density to a critical point and gives rise to scale invariant excitation avalanches. We further discuss how additional external driving can be used to extend and manipulate the SOC avalanche dynamics. This offers a detailed perspective on how avalanche dynamics can be controlled in driven Rydberg gases.

C71.00411: Photon blockade in the Tavis Cummings model
RAHUL TRIVEDI (Presenter), MARINA RADULASKI, KEVIN A FISCHER, SHANHUI FAN, JELENA VUCKOVIC, Electrical Engineering, Stanford University — We use the scattering matrix formalism to study single- and two-photon transport through the Tavis Cummings model as a function of the number of emitters coupling to the cavity mode. It is shown that for a resonant Tavis Cummings system, photon blockade at the output of the cavity mode worsens with the number of emitters while for a detuned Tavis Cummings system, photon blockade at the output of the cavity mode improves with the number of emitters. By explicitly calculating the two-photon scattering properties of this system in the thermodynamic limit of an infinite number of emitters, we show that the light emitted from Tavis Cummings system under excitation by a coherent drive transitions from bunching to anti-bunching as the emitters are detuned from the cavity mode. Finally, we analyze the impact of inhomogeneous broadening in the emitter frequencies on both resonant and detuned photon blockade through the Tavis Cumming system.

*We acknowledge financial support from the AFOSR MURI Center for Attojoule Optoelectronics Award No. FA9550-17-1-0002. Rahul Trivedi acknowledges support from Kailath Stanford Graduate Fellowship. Marin Radulaski acknowledges support from Nano- and Quantum Science and Engineering Postdoctoral Fellowship at Stanford University.
C71.00412: Point-coupling Hamiltonian for frequency-independent linear optical devices*
RAHUL TRIVEDI (Presenter), KEVIN A FISCHER, SATTWIK MISHRA, JELENA VUCKOVIC, Electrical Engineering, Stanford University — We present the point-coupling Hamiltonian as a model for frequency-independent linear optical devices acting on propagating optical modes described as continua of harmonic oscillators. We formally integrate the Heisenberg equations of motion for this Hamiltonian, calculate its quantum scattering matrix, and show that an application of the quantum scattering matrix on an input state is equivalent to applying the inverse of classical scattering matrix on the annihilation operators describing the optical modes. We show how to construct the point-coupling Hamiltonian corresponding to a general linear optical device described by a classical scattering matrix, and provide examples of Hamiltonians for some commonly used linear optical devices. Finally, in order to demonstrate the practical utility of the point-coupling Hamiltonian, we use it to rigorously formulate a matrix-product-state based simulation for time-delayed feedback systems wherein the feedback is provided by a linear optical device described by a scattering matrix as opposed to a hard boundary condition (e.g. a mirror with less than unity reflectivity).

*Rahul Trivedi acknowledges Kailath Graduate Fellowship

C71.00413: Efficient numerical integration of the adiabatic master equation*
HUMBERTO MUNOZ-BAUZA (Presenter), DANIEL A LIDAR, Univ of Southern California — The capability to simulate open quantum systems under the adiabatic condition is critical for verifying the behavior of quantum annealers. While adiabaticity is a useful condition for theoretical analysis, straightforward numerical implementations of the adiabatic master equation (AME) suffer from the need to integrate an adiabatic but highly oscillatory quantum state over a very long period of time. We show that the AME in the adiabatic frame can be split in a way that prevents large superoperator evaluations and is amenable to geometric integration methods for split time-dependent problems.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050
C71.00414: A perturbative view from the master equation: Electromagnetically induced transparency revisited

XIN WANG (Presenter), Beijing Computational Science Res Ctr — We show that by treating the weak probe field as a perturbation to the strong coupling fields in the atomic system and using the perturbative method in a master equation, the features of linear response of phenomena of electromagnetically induced transparency (EIT) can be uniformly demonstrated, regardless of the details of atomic energy level configuration. We compare our estimation with both typical and atypical EIT-observed configurations and find that our model indeed provides a description of the sharp transmission window in central area of typical EIT curve.

It can also be inferred hereby that for various systems other than atomic gas, as long as the description of the system’s dynamics comes down to the simplified form of master equation, the corresponding EIT analogs and EIT-like phenomena can also be explained in this way.

*NSFC No. 11847244, 11534002, 11447609

C71.00415: Vacancies effect on the BEC critical temperature of an ideal Bose gas within an imperfect crystal

MIGUEL A. SOLIS (Presenter), Theoretical Physics, Institute of Physics, Universidad Nacional Autónoma de México, EMILIO I GUERRERO, Postgraduate in Physical Sciences, Universidad Nacional Autónoma de México — After we have shown [1] that an ideal Bose gas in one, two or three-dimensional crystal with one structural vacancy presents Bose-Einstein condensation (BEC) at higher finite critical temperature than that when the crystal is perfect; here we report the BEC critical temperature as a function of the number of random vacancies. The particle energy spectrum is obtained using finite difference numerical method, which we use to calculate the critical temperature as the temperature at which the isobaric specific heat has its maximum [2]. When our finite system is taken to the thermodynamic limit, the critical temperature starts at the one vacancy value, it increases reaching a maximum when we have about 17 % of vacancies and then decays almost linearly to zero when the crystal has been removed.


*We thank partial support form grants CONACyT 221030 and DGAPA-PAPIIT IN110319
C71.00416: Quantum system chaos in a PT-symmetry breaking potential* CARLA QUISPE
FLORES (Presenter), Physics Department, Colorado School of Mines, INES DE VEGA, Department of
Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig Maximilian University of Munich,
RENAN CABRERA, Department of Chemistry, Princeton University, LINCOLN CARR, Physics Department,
Colorado School of Mines — We studied the dynamics of N bosons confined in a triple well potential
in phase space. The system is tackled by using the truncated Wigner approximation (TWA) and
exact diagonalization of Bose-Hubbard model including a perturbative PT-symmetry breaking
potential. We find a region in which the symmetry breaking develops smoothly with the control
parameters enabling to break many symmetries of the Hamiltonian and reduce energy
degeneracies. The model shows signatures of stationarity, chaos and mixing as a consequence of
the inter-particle interactions. Generation of entangled states and loss of purity is also observed
and monitored by the Meyer's measure of the impurity and the von Neumann entropy S. Finally,
the system chaotic behavior is conveniently tracked within the phase space by the growth rate of
the out-of-time ordered correlator.

*This work is supported by NSF

C71.00417: Continuous protection of a quantum state from inhomogeneous dephasing
RAN FINKELSTEIN (Presenter), OHR LAHAD, OMRI DAVIDSON, EILON POEM, OFER FIRSTENBERG,
Weizmann Institute of Science — Room-temperature atomic vapors are known for their simplicity
and their potential scaling-up in applications. In spite of these benefits, laser-cooled atoms have
evolved to be the prevalent systems for studying strong and coherent light-matter interactions,
as the latter are unhindered by Doppler broadening.
Here we present several methods to overcome the effective decrease of both atom-photon
cross-section [1] and coherence time in vapors, and in fact in any inhomogeneously broadened
atom-like system.
The mechanism we study can be understood as the counteraction of the inhomogeneous
dephasing of two coupled states, where one state has enhanced sensitivity to the source of
dephasing. A far-detuned dressing field admixes a fraction $\Omega^2/\Delta^2$ of this "sensor" state into the
"protected" state, yielding a velocity-insensitive state and effective line-narrowing in two-color
transitions [2]. Finally, we apply this method to extend the lifetime of collective excitations stored
in a thermal atomic vapor. This method is continuous, in contrast to pulsed echo-based
techniques.
Lett. 123 173203
21 103024
C71.00418: Combined spontaneous symmetry-breaking and symmetry-protected topological order from cluster charge interaction*  
CHEN PENG, Department of Physics, Renmin University of China, YUAN-YAO HE (Presenter), Center for Computational Quantum Physics, Flatiron Institute, RONG-QIANG HE, ZHONG-YI LU, Department of Physics, Renmin University of China — The study of symmetry-protected topological states in presence of electron correlations has recently aroused great interest as rich and exotic phenomena can emerge. Here, we report a concrete example by employing large-scale unbiased quantum Monte Carlo study of the Kane-Mele model with cluster charge interactions. The ground-state phase diagram for the model at half filling is established. Our simulation identifies the coexistence of a symmetry-protected topological order with a symmetry-breaking Kekule valence bond order and shows that the spontaneous symmetry-breaking is accompanied by an interaction-driven topological phase transition (TPT). This TPT features appearance of zeros of single-particle Green's function and gap closing in spin channel rather than single-particle excitation spectrum, and thus has no mean-field correspondence.

*This work was supported by the National Science Foundation of China (Grants No. 11874421 and No. 11774422). Computational resources were provided by the Physical Laboratory of High Performance Computing at Renmin University of China and National Supercomputer Center in Guangzhou with Tianhe-2 Supercomputer. The Flatiron Institute is a division of the Simons Foundation.

C71.00419: Quantum Monte Carlo Simulations of the Attractive SU(3) Hubbard Model on a Honeycomb Lattice*  
YU WANG (Presenter), HAN XU, School of Physics and Technology, Wuhan University, LEI WANG, Institute of Physics, Chinese Academy of Sciences — We perform the projector quantum Monte Carlo simulation of the half-filled attractive SU(3) Hubbard model on a honeycomb lattice, exploring the effects of SU(3) symmetry on the correlated attractive Dirac fermions. Our simulation indicates the absence of pairing order in the system and shows a quantum phase transition from the semimetal to charge density wave (CDW) at the critical point $U_c = -1.52(2)$. We demonstrate that this quantum phase transition belongs to the chiral Ising universality class according to the numerically determined critical exponents $\nu = 0.82(3)$ and $\eta = 0.58(4)$. With the increase of coupling strength, the trion formation is investigated, and the change in probability of the on-site trion occupancy infers the coexistence of on-site trionic and off-site trionic CDW states at half-filling.

*This work is supported by the National Natural Science Foundation of China under Grants No. 11874292, No. 11729402, and No. 11574238.
C71.00420: Signatures of Majorana-like Quasiparticles in Few-body Lattice Models* JARED BLAND (Presenter), BIRGIT KAUFMANN, CHRIS H GREENE, Purdue Univ — There is a strong interest in number conserving systems that exhibit Majorana fermions as quasiparticles. We utilize a number-conserving analog of the Kitaev wire model due to Iemini et al. in the small-lattice limit to examine signatures of topological properties in small systems. This interacting model exhibits several signatures of topological regime, such as identical entanglement spectra for the ground states in distinct parity sectors. Additionally, the Hamiltonian is akin to the BCS Hamiltonian, suggesting Bogoliubov rotations and approximations, allowing us to further examine this model in this regard. In this work, we demonstrate these signatures of different topological order in small lattice sizes to find evidence of isolated Majorana quasiparticles.

Refs:

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C71.00421: Effect of Core Size on Vortex Interactions in Light* JASMINE ANDERSEN (Presenter), ANDREW A. VOITIV, Univ of Denver, MARK T. LUSK, Colorado School of Mines, MARK SIEMENS, Univ of Denver — Optical vortices are characterized by a helical wavefront with integer winding, also referred to as the topological charge, around the center of the vortex. These vortices exhibit dynamic behavior when implanted in different locations of a Gaussian beam, and it is possible to observe vortex-vortex interactions as the beam propagates. In the case of an oppositely charged vortex pair separated symmetrically about the beam axis, the vortices begin with a downward motion in the transverse plane and then accelerate toward each other. When the beam propagates, these vortices will at some point annihilate each other, without reemergence on the other side of the collision. The exact dynamics depend on the shape and size of the core. For smaller cores, the diffraction of the core has an effect on the dynamics and the annihilation distance is farther along the propagation axis. I will present our theoretical and experimental results including the impact of charge and core size on the vortex trajectories. I will also discuss the role of the underlying phase and amplitude gradients at the location of a given vortex on its motion as the beam propagates.

*NSF
W.M. Keck Foundation
C71.00422: Finite Orbital Angular Momentum Pairing in Atomic Fermi Gases with Spin-Orbital-Angular-Momentum Coupling  
WANG LIANG-LIANG (Presenter), Westlake University — Fulde-Ferrell-Larkin-Ovchinnikov states represent superconducting states with finite momentum Cooper pairs and have become one of most sought-after exotic states of matter. The recent realization of a new type of spin-orbit coupling in ultracold atomic gases, namely the spin-orbital-angular-momentum coupling, provides a novel perspective to study Fulde-Ferrell-Larkin-Ovchinnikov states in orbital angular momentum space. In this letter, we demonstrate that the combined effects of spin-orbital-angular-momentum coupling and level detuning can induce an exotic Fulde-Ferrell-Larkin-Ovchinnikov phase, where Cooper pairs have finite center-of-mass angular momenta. This implies that vortex with high-vorticity can be generated without rotation or effective vector potential field. The orientation of the phase winding can be altered by adjusting the sign of level detuning.

C71.00423: Quantum Defects in Diamond: Identifying Nitrogen Isotopes of Nitrogen-Vacancy Centers*  
MORGAN CHAMBERLAIN (Presenter), Linfield College, SRIVATSA C VARDARAJ, ZEESHAWN KAZI, ELYSSA B ROEDER, KAI-MEI CAMILLA FU, University of Washington — Nitrogen-vacancy (NV) centers are point defects in diamond formed by one substitutional nitrogen atom and an adjacent vacancy. Low spectral diffusion is a necessary property for NV centers to be qubit candidates. To characterize differences between naturally formed and ion implanted NV centers, diamond samples were studied that contained both types. The ion implantation used $^{15}$N to be able to differentiate from the $^{14}$N naturally formed NV centers. This project focused on identifying the isotope of a single NV center, which is the first step toward understanding differences in their emissive properties. Code was developed to execute, and then automate, the three experiments necessary to identify the isotope of a single NV center: Continuous Wave Optically Detected Magnetic Resonance (CW ODMR), Rabi oscillations, and Pulsed ODMR. These experiments resolve the hyperfine interaction of the nuclear spin states. The code was implemented on a test sample, where it successfully identified the isotope of several NV centers. The next step in this project is to link the isotopes of NV centers to their emissive properties, with a goal of producing reliable qubits for quantum information processing circuits.

*Financial support from the National Science Foundation is gratefully acknowledged.
C71.00424: Dynamics of Inhalation  FELIX KRATZ (Presenter), JEAN-FRANCOIS LOUF, ANVITHA SUDHAKAR, NATHANAEI LJI, SUJIT DATTA, Department of Chemical and Biological Engineering, Princeton University — The process of inhalation relies on the complex interplay between muscular contraction in the thorax, elasto-capillary interactions in the individual airway branches, connectivity between different branches, and overall air flow into the lungs. Sophisticated pulmonary fluid dynamics models have been developed to elaborate the competition between capillarity, which tends to keep flexible branches closed, and elasticity, which favors opening, for single airway branches. However, a quantitative model combining the physiological opening process of flexible airway branches with the biomechanics and interconnected geometry of the lungs is still missing. To address this issue, we develop a statistical model of the lungs as a symmetrically-branched network of liquid-lined flexible cylinders coupled to a viscoelastic thoracic cavity. Each branch opens at a rate and a pressure that is determined by input biomechanical parameters, enabling us to test the influence of changes in the mechanical properties of lung tissues and secretions on inhalation dynamics. By summing the dynamics of all the individual branches, we quantify the evolution of overall lung pressure and volume during inhalation, and find good agreement with typical breathing curves obtained in the literature.

C71.00425: Charge Carrier Transport in Cuprous Oxide: A Puzzle  GARIMA AGGARWAL (Presenter), SANDEEP K. MAURYA, K. R. BALASUBRAMANIAM, Dept. of Energy Science and Eng, Indian Institute of Technology — Deciphering the carrier transport mechanism in Cu$_2$O has been elusive, as none of the classical scattering mechanisms seems to be operative. Towards this, we study electrical properties of Cu$_2$O, wherein samples are prepared via thermal oxidation (TO), pulsed laser deposition (PLD), and electrodeposition. These methods provide a large range of grain sizes (100nm to 5mm), type of grain boundaries (high & low angle), and intrinsic defect concentration (10$^{13}$ to 10$^{18}$ cm$^{-3}$). T dependent Hall measurement is used to study carrier concentration and hole mobility. We observe the presence of two acceptor levels; a normal and a split Cu vacancy for the first time experimentally. The mobility vs. T data exhibits a maximum at 200 K for polycrystalline samples, while, monotonically decreases for single crystal and textured PLD thin film in the entire T range of study (80 – 300 K). Grain boundary (GB) scattering mechanism explains the dependence of transport at T < 200 K for samples with high angle GB. We find that trap mediated scattering is dominant for single crystal and poly-crystal at T > 200 K. This suggests that instead of increasing grain size or doping, the neutralization of trap centres is the only possible way to increase the mobility and thereby, performance of Cu$_2$O based devices.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D01 DAMOP: Open Quantum Systems I  Igor Lesanovsky - Tag(s): Focus
2:30PM D01.00001: Discovering feedback strategies for open quantum systems via deep reinforcement learning [Invited] FLORIAN MARQUARDT (Presenter), Max Planck Institute for the Science of Light — Recent rapid advances in deep neural networks are helping to revolutionize science and technology. In this talk, I will describe how neural networks can discover from scratch feedback strategies to help control open quantum systems, by exploiting the toolbox of reinforcement learning. A few-qubit quantum memory can be protected against decoherence via quantum error correction strategies that have been autonomously constructed in this way. Additional illustrative examples from our recent research include reinforcement learning applied to systems from the domain of cavity quantum electrodynamics and to arrays of coupled modes.

3:06PM D01.00002: Integrability Meets Dissipation: Critical Dynamics of Open Driven Systems DANIEL PAZ (Presenter), MOHAMMAD MAGHREBI, Physics & Astronomy, Michigan State University — Driven quantum systems coupled to an environment are generally non-integrable and typically exhibit relaxational dynamics. We investigate the paradigmatic open Dicke model which describes collective light-matter interactions subject to dissipation. In a certain limit (at large detuning), this model is governed by an effective driven-dissipative Ising model in a transverse field, which is integrable in the absence of dissipation. In the limit of weak dissipation though, integrability is only weakly broken. We show that, in this regime, the system undergoes a dynamical crossover from relaxational dynamics to underdamped critical dynamics, each described by a distinct dynamical exponent. We identify these critical behaviors with the infinite-range classical (stochastic) and quantum (unitary) Ising models at finite temperature, respectively. These results are obtained through a non-equilibrium quantum-to-classical mapping in addition to an efficient numerical analysis that exploits the permutation symmetry.

3:18PM D01.00003: Dissipative generation of highly entangled states of light and matter* CATALIN-MIHAI HALATI (Presenter), AMENEH SHEIKHAN, PI, University of Bonn, HELMUT RITSCH, ITP, University of Innsbruck, CORINNA KOLLATH, PI, University of Bonn — We investigate the full quantum evolution of ultracold interacting bosonic atoms confined to a chain geometry and coupled to the field of an optical cavity. Extending the time-dependent matrix product state techniques to capture the global coupling to the cavity mode and the open nature of the cavity, we fully include the light-atom entanglement. We examine the long time behavior of the system beyond the mean-field elimination of the cavity field. We show that in the self-organized phase the steady state consists in a mixture of the mean-field predicted density wave states and coherent states with lower photon number, with a large entanglement between the atomic and photonic degrees of freedom. In the regime of large dissipation strengths we develop a variant of the many-body adiabatic elimination technique and obtain a highly entangled steady state with a fully mixed atomic sector. We observe numerically the crossover from the density wave state towards the fully mixed state.

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Deutsche Forschungsgemeinschaft: project number 277625399-TRR 185, project B3, and CRC 1238 project number 277146847 - projects C05, and Einzelantrag
3:30PM D01.00004: Boundary dissipation in Ising CFT  UMAR JAVED (Presenter), MICHAEL KOLODRUBETZ, University of Texas at Dallas — Boundary conformal field theory (CFT) is one of few exact analytical tools for the study of quantum non-equilibrium systems, yet so far has been primarily restricted to closed Hamiltonian systems. We study one of the simplest CFTs, namely the quantum critical Ising model with boundary dephasing along the direction of the most relevant boundary operator. Naïve scaling arguments suggest that such dissipation should be marginal. Numerically for large systems, we find that boundary spin in the presence of dissipation, with or without boundary field, depolarizes and reaches a nonequilibrium steady state (NESS). In the presence of RG-relevant boundary term, scaling functions appear unmodified, suggesting that the dissipation is marginally irrelevant in that case. In the absence of boundary field, we study modifications of the Zeno effect by Keldysh RG and numerical calculations of the two-time correlation function of the boundary spin. Finally, we comment on potential application to other CFTs

3:42PM D01.00005: On the nature of the non-equilibrium phase transition in the non-Markovian driven Dicke model  REX LUNDGREN (Presenter), ALEXEY V. GORSHKOV, Joint Quantum Institute, University of Maryland / National Institute of Standards and Technology, MOHAMMAD MAGHREBI, Department of Physics and Astronomy, Michigan State University — The Dicke model exhibits a phase transition to a superradiant phase with a macroscopic population of photons and is realized in multiple settings in open quantum systems. In this work, we study a variant of the Dicke model where the cavity mode is lossy due to the coupling to a Markovian environment while the atomic mode is coupled to a colored bath. We find a simple effective theory for this model allowing us to derive analytical expressions for various critical exponents, including those, such as the dynamical critical exponent, that have not been previously considered. We find excellent agreement with previous numerical results when the non-Markovian bath is at zero temperature; however, contrary to these studies, our low-frequency approach reveals that the same exponents govern the critical behavior when the colored bath is at finite temperature unless the chemical potential is zero. Furthermore, we show that the superradiant phase transition is classical in nature, while it is genuinely non-equilibrium. Finally, we consider finite-size effects at the phase transition and identify the finite-size scaling exponents, unlocking a rich behavior in both statics and dynamics of the photonic and atomic observables.
3:54PM D01.00006: Anomalous exceptional point and non-Markovian Purcell effect at threshold in 1-D open quantum systems*  
SAVANNAH GARMON (Presenter), Osaka Prefecture Univ, GONZALO ORDONEZ, Butler University, NAOMICHI HATANO, University of Tokyo — We show that when a quantum emitter is coupled near threshold to a generic 1-D continuum with a van Hove singularity in the density of states, a characteristic spectral configuration appears involving a bound state, a resonance state and an anti-resonance state, as well as several exceptional points (EPs). At one EP appearing below the threshold, the resonance and anti-resonance states coalesce while the bound state instead experiences an avoided crossing. Meanwhile, if one considers the limit in which the coupling $g$ vanishes, all three states converge on the continuum threshold itself. For small $g$ values the eigenvalue and norm of each of these states can be expanded in a Puiseux expansion in terms of powers of $g^{2/3}$, which suggests a third order EP occurs at the threshold. However, in the actual $g \to 0$ limit, only two discrete states in fact coalesce as the system can be reduced to a 2x2 Jordan block; the third state instead merges with the continuum. We further demonstrate the influence of the EP on non-Markovian dynamics characterizing the relaxation process of the quantum emitter in the vicinity of the threshold.

*This work is supported by JSPS KAKENHI Grant No. JP18K03466 and the Research Foundation for Opto-Science and Technology.

4:06PM D01.00007: Non-Markovian collective emission from macroscopically separated emitters  
KANUPRIYA SINHA (Presenter), Army research lab/Joint quantum institute, University of Maryland, PIERRE MEYSTRE, University of Arizona, PABLO SOLANO, MIT — We study the collective radiative decay of a system of two two-level emitters coupled to a one-dimensional waveguide in a regime where their separation is comparable to the coherence length of a spontaneously emitted photon. The electromagnetic field propagating in the cavity-like geometry formed by the emitters exerts a retarded backaction on the system leading to strongly non-Markovian dynamics. The collective spontaneous emission rate of the emitters exhibits an enhancement or inhibition beyond the usual Dicke super- and sub-radiance due to a self-consistent coherent timedelayed feedback.

4:18PM D01.00008: Analysis of matter-wave emission dynamics and polariton formation in a quantum-emitter array coupled to a band structure*  
ALFONSO LANUZA (Presenter), MICHAEL A STEWART, JOONHYUK KWON, YOUNGSHIN KIM, DOMINIK SCHNEBLE, State Univ of NY - Stony Brook — Recent progress on a spontaneous emitter for atomic matter waves [1] has enabled studies of exotic emission phenomena in bandgap materials. Here we present analytic solutions for the single excitation dynamics in a 1D sinusoidal lattice potential and a finite or infinite array of emitters. The calculated phenomenology ranges from non-Markovian decay into bound states for the case of one emitter, to the emergence of an additional band structure of polaritons for the case of infinite emitters.


*Supported by NSF PHY-1607633/1912546 and SUNY Ctr for QIS on LI.
4:30PM D01.00009: Generalized Theory of Pseudomodes for Exact Descriptions of Non-Markovian Quantum Processes  GRAEME PLEASANCE (Presenter), Univ of KwaZulu-Natal, BARRY M GARRAWAY, University of Sussex, FRANCESCO PETRUCCIONE, Univ of KwaZulu-Natal — In this talk we develop a general approach to analyzing the non-Markovian behavior of an open quantum system in a setting where the interaction is modelled by a generalized class of spectral density function. By introducing an auxiliary model in which the environment is replaced by a set of discrete bosonic modes exhibiting Markovian dissipative interactions, we prove the validity of the conditions allowing for a non-Markovian open system dynamics to be amended to a Markovian description, where the dynamics in the latter is governed by an exact master equation of Lindblad form. Initially we apply our result to obtain a generalization of the pseudomode method [1] in cases where the spectral density function has a Lorentzian structure. For many other types of spectral density function, we extend this result to show that an open system dynamics may be modelled physically using discrete modes which admit a non-Hermitian coupling to the system, and for such cases determine the equivalent master equation to no longer be of Lindblad form. For applications involving two discrete modes, we demonstrate how to convert between pathological and Lindblad forms of the master equation via [1].


4:42PM D01.00010: Stabilization of Fractional Quantum Hall States of Light: Effects of Fractionalization  PAVEL KURILOVICH (Presenter), JOSE LEBREUILLY, VLADISLAV KURILOVICH, STEVEN GIRVIN, Yale University — Recently, the possibility of realizing strongly-correlated states of matter with photons has started to become an experimental reality. In combination with artificial gauge fields this paves the way to simulation of fractional quantum Hall states with light. A major hindrance to such simulations is the inevitable dissipation of photons into the environment which creates holes in the correlated state. The leakage of light can be counteracted by a stabilization scheme in which lost particles are irreversibly refilled. We investigate the efficiency of such a scheme for the preparation of a photonic Laughlin state at half-filling. We explore the limitations imposed by the ability of holes in the Laughlin state to fractionalize into several spatially separated quasiholes. Quasiholes correspond to the absence of a fraction of a particle and thus cannot be refilled efficiently. We find that the fractionalization drastically restricts the steady-state fidelity of the Laughlin state and leads to a long relaxation time in the system.
Transport through a quantum critical system: A thermodynamically consistent approach*

CHRISTOPHER WÄCHTLER (Presenter), GERNOT SCHALLER, Institut of Theoretical Physics, Technical University Berlin — Quantum phase transitions are striking phenomena of many-body systems at low temperatures. The current experimental feasibilities enable us to bring such critical systems out of equilibrium in a controlled manner. Due to the vanishing energy gap above the ground state [1], appropriate methods have to be developed to study the dynamics and thermodynamical applications. We show for a class of critical systems connected to several non-Markovian heat baths that by combining the reaction coordinate mapping [2] and a polaron technique [3] it is possible to find analytic expressions of the reduced system dynamics in the vicinity of quantum critical points, which are consistent with the laws of thermodynamics. As an example we consider the Lipkin-Meshkov-Glick model in a transport setup, where the underlying phase transition manifests itself in the heat transfer statistics.


*We acknowledge financial support from Deutsche Forschungsgemeinschaft through project BR1528/8-2 and are thankful for stimulating discussions with A. Knorr, S. Restrepo, S. Böholing and especially V. M. Bastidas.

Deconstructing Effective Non-Hermitian Dynamics in Quadratic Bosonic Hamiltonians*

VINCENT FLYNN (Presenter), Dartmouth Coll, EMILIO COBANERA, SUNY Polytechnic Institute, LORENZA VIOLA, Dartmouth Coll — Unlike their fermionic counterparts, the dynamics of Hermitian, bosonic, quadratic Hamiltonians are governed by a generally non-Hermitian Bogoliubov de-Gennes Hamiltonian. This effective non-Hermiticity gives rise to two distinct dynamical phases: one with bounded evolution of observables in time, and one without. We elucidate the physical manifestations of the transitions between these two dynamical phases. We show how a generalized notion of $PT$ symmetry may be used to classify the mechanisms by which this transition can occur. By combining this understanding with tools from Krein stability theory, we derive an indicator of dynamical phase boundaries inspired by the notion of phase rigidity in non-Hermitian quantum systems. As an example, we fully characterize the dynamical phase diagram of a bosonic analogue to the Kitaev-Majorana chain under a wide class of boundary conditions, and further establish a connection between phase-dependent transport properties and the onset of instability. We discuss potential applications of our techniques to quadratic Lindblad dynamics.

*Research supported in part by US NSF through grant No. PHY-1620541.
Non-Hermitian Linear Response Theory  LEI PAN (Presenter), XIN CHEN, Institute for Advanced Study, Tsinghua University, YU CHEN, Capital Normal University, HUI ZHAI, Institute for Advanced Study, Tsinghua University — Linear response theory lies at the heart of quantum many-body physics because it builds up connections between the dynamical response to an external probe and correlation functions at equilibrium. Here we consider the dynamical response of a Hermitian system to a non-Hermitian probe, and we develop a non-Hermitian linear response theory that can also relate this dynamical response to equilibrium properties. As an application of our theory, we consider the real-time dynamics of momentum distribution induced by one-body and two-body dissipations. We find that, for many cases, the dynamics of momentum occupation and the width of momentum distribution obey the same universal function, governed by the single-particle spectral function. We also find that, for critical state with no well-defined quasi-particles, the dynamics are slower than normal state and our theory provides a model independent way to extract the critical exponent. We apply our results to analyze recent experiment on the Bose-Hubbard model and find surprising good agreement between theory and experiment. We also propose to further verify our theory by carrying out a similar experiment on a one-dimensional Luttinger liquid.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D02 DAMOP: Nonequilibrium dynamics in ultracold matter

Quantum Cherenkov Transition in Bose Polaron Systems  KUSHAL SEETHARAM (Presenter), Massachusetts Institute of Technology MIT, YULIA SHCHADILIOVA, Department of Physics, Harvard University, FABIAN GRUSDT, Department of Physics, Technical University Munich, MIKHAIL ZVONAREV, LPTMS, Universite Paris-Sud, EUGENE DEMLER, Department of Physics, Harvard University — We study the behavior of a finite-momentum impurity immersed in a weakly interacting Bose-Einstein condensate (BEC) of ultra-cold atoms near an interspecies Feshbach resonance. Using the time-dependent variational approach and a non-Gaussian transformation, we study both ground state properties and quench dynamics of the system after a sudden immersion of the impurity into the BEC. While in the subsonic regime dynamics corresponds to relaxation into the quasiparticle state, in the supersonic regime we observe rapid emission of Cherenkov phonons. This phenomenon manifests in several ways during real-time dynamics of the system and showcases a rich interplay between polaronic physics and Cherenkov physics. We see qualitatively different long-time behavior of average impurity speed and Loschmidt echo depending on the impurity-boson interaction strength. Aspects of the discussed dynamical behavior can be probed in experimental protocols.
2:42PM D02.00002: Tuning of Scattering Resonances by Time-Periodic Driving*  
CHRISTOPH DAUER (Presenter), AXEL PELSTER, SEBASTIAN EGGERT, Technical University of Kaiserslautern —  
Scattering by a short-range inter-particle potential with time-periodic modulation is investigated with Floquet theory without assuming any high frequency approximations. For a harmonic drive it turns out that strong resonances occur, which allow versatile tuning of the s-wave scattering length and the resonance width by adjusting frequency and driving amplitude. Our approach leads to a simple description of the effect in terms of a generalized Fano-Anderson model, which in turn identifies the physical origin and leads to an analytic quantitative description of the resonances. Results for general experimental situations of magnetic and optical driving using two coupled channels and including higher harmonics are discussed.

*Supported by the Deutsche Forschungsgemeinschaft (DFG) via SFB/TR185 "OSCAR"

2:54PM D02.00003: Quench dynamics of two-component dipolar Fermions in a Quasiperiodic potential*  
BRADRAJ PANDEY (Presenter), ELBIO DAGOTTO, University of Tennessee, Knoxville, SWAPAN K. PATI, TSU, jncasr —  
Motivated by the recent experiments in fermionic polar gases, we study the quenched dynamics of two-component dipolar fermions, in the presence and absence of a quasiperiodic potential. We investigate the localization of the charge and spin degree of freedom separately, by probing local and global dynamical observables [1]. To study non-equilibrium dynamics, we start with two different product states, doublons and a Neel state. We calculate the long time dynamics of the fermionic Hamiltonian using exact-diagonalization and matrix-product-state formalisms. In the case of doublons, we demonstrate the transition from delocalized to localized MBL phase. In the case of Neel state, by introducing strong enough disorder, we show that the localization of the spin degree of freedom is also possible along with the charge degree of freedom when on-site and long-range interaction couplings are equal in strength. Our predictions for localizations of both charge and spin degrees of freedom should be observed in experiments with fermionic dipolar atoms subject to a quasiperiodic potential.  

3:06PM D02.00004: Enabling ultrastrong-coupling phenomena with single-drive Jaynes--Cummings models  CARLOS SÁNCHEZ MUÑOZ, Oxford University, ANTON FRISK KOCKUM (Presenter), Chalmers Univ of Tech, ADAM MIRANOWICZ, Adam Mickiewicz University, FRANCO M NORI, RIKEN — We propose the effective simulation of light-matter ultrastrong-coupling phenomena with strong-coupling systems. Recent theory and experiments have shown that the single-atom quantum Rabi model can be simulated by the Jaynes-Cummings model with two additional classical drives. Here, we show that quantum nonlinear optical phenomena, relying on the counter-rotating terms of the quantum Rabi model, can be implemented by the Jaynes-Cummings and Tavis-Cummings models with only a single classical drive. We analyze three examples (one atom exciting two photons, frequency conversion, and one photon exciting two atoms) and show that they could be demonstrated with several currently available experimental quantum-optics systems, including superconducting circuits and trapped ions.

3:18PM D02.00005: Dynamics of the decay of dark solitons in superfluid Fermi gases* WOUT VAN ALPHEN (Presenter), Department of Physics, University of Antwerp, HIROMITSU TAKEUCHI, Department of Physics, Osaka City University, JACQUES TEMPERE, Department of Physics, University of Antwerp — Dark solitons are solitary matter waves which retain their shape while propagating at a constant velocity. They emerge in a wide variety of physical systems, including ultracold atomic gases. In superfluid Bose gases, dark solitons have been observed to decay into quantized vortices through the so-called snake instability mechanism. Recent experiments in superfluid Fermi gases have also interpreted soliton decay via this mechanism. However, using both numerical simulations and a perturbative analysis based on a low-energy effective field theory, we show that there is a qualitative difference between soliton decay in the BEC- and BCS-regimes of superfluid Fermi gases.

In the BEC-regime, the characteristic snaking deformations of the soliton plane are induced by fluctuations of the amplitude of the order parameter, while in the BCS-limit, fluctuations of the phase destroy the soliton core through the formation of local Josephson currents, without the occurrence of a snaking pattern. The difference between both mechanisms should be experimentally observable, providing an incentive to consider both past and future experiments from a new perspective.

*W. Van Alphen acknowledges financial support in the form of a PhD fellowship of the Research Foundation - Flanders (FWO).
3:30PM D02.00006: Operator complexity of adiabatic gauge potential  MOHIT PANDEY
(Presenter), Physics, Boston University, DRIES SELS, Physics, Harvard University, PIETER W. CLAEYS, ANATOLI S POLKOVNIKOV, DAVID K CAMPBELL, Physics, Boston University — Recently, there has been great interest in studying the growth rates of operator complexity and out-of-time-order correlators in many-body quantum systems. Here we characterize the complexity of the adiabatic gauge potential (AGP), which encodes the geometry of eigenstates when varying a control parameter in a Hamiltonian. For generic systems, the AGP is a highly non-local and entangled operator. We find that its Frobenius norm, which can be explicitly related to operator growth, shows remarkably different scaling with system size for integrable and non-integrable systems: polynomial versus exponential. Using the length of Pauli string operator as a measure of the AGP complexity, we compute operator weight distributions and the Shannon entropy to better understand the norm’s system size scaling.

3:42PM D02.00007: Transport in a bosonic superfluid point contact  SHUN UCHINO
(Presenter), Waseda Univ, JEAN-PHILIPPE BRANTUT, EPFL — We discuss heat and particle transport of a weakly interacting, low temperature Bose-Einstein condensate in a quantum point contact. We show that the presence of gapless phonon modes in the condensate yields a contact resistance at zero temperature and a corresponding nonzero DC conductance. As a consequence, we predict zero thermopower and Lorenz number at zero temperature, a breakdown of the bosonic Wiedemann-Franz law. The consequences on heat and particle transport measurements in bosonic two-terminal setups should be readily observable in existing experiments.

3:54PM D02.00008: Entanglement production by interaction quenches of quantum chaotic subsystems  JETHIN PULIKKOTTIL JACOB (Presenter), Washington State University Pullman, ARUL LAKSHMINARAYAN, Indian Institute of Technology Madras, SHASHI C. L. SRIVASTAVA, Variable Energy Cyclotron Centre Kolkata India, ARND BÄCKER, Technische Universität Dresden Germany, STEVEN TOMSOVIC, Washington State University Pullman — The entanglement production in bipartite quantum systems is studied for initially unentangled product eigenstates of the subsystems, which are assumed to be quantum chaotic [1]. Based on a perturbative computation of the Schmidt eigenvalues of the reduced density matrix, explicit expressions for the time-dependence of entanglement entropies, including the von Neumann entropy, are given. An appropriate re-scaling of time and the entropies by their saturation values leads a universal curve, independent of the interaction. The extension to the non-perturbative regime is performed using a recursively embedded perturbation theory to produce the full transition and the saturation values. The analytical results are found to be in good agreement with numerical results for random matrix computations and a dynamical system given by a pair of coupled kicked rotors.

**4:06PM D02.00009: The entanglement membrane in deterministic systems**  
TIANCI ZHOU  
(Presenter), Kavli Institute for Theoretical Physics, ADAM NAHUM, Physics, University of Oxford —  
In certain analytically-tractable quantum chaotic systems, the calculation of out-of-time-order correlation functions, entanglement entropies after a quench, and related dynamical observables, reduces to an effective statistical mechanics of an ‘entanglement membrane’ in spacetime. These tractable systems involve an average over random local unitaries defining the dynamical evolution. We show here how to make sense of this membrane in more realistic models, which do not involve an average over random unitaries. Our approach relies on introducing effective ‘pairing’ degrees of freedom in spacetime, inspired by the structure emerging in random unitary circuits. We also provide an efficient algorithm for determining the ‘line tension’ of the entanglement membrane in 1+1D models.

*TZ acknowledges the Gordon and Betty Moore Foundation for postdoctoral fellowship under Grant GBMF4304 and support from the National Science Foundation under Grant No. NSF PHY-1748958. AN acknowledges a Royal Society University Research Fellowship.*

**4:18PM D02.00010: Nonequilibrium dual-boson approach**  
FENG CHEN (Presenter), MICHAEL GALPERIN, University of California, San Diego, MIKHAIL KATSNELSON, Institute for Molecules and Materials, Radboud University Nijmegen —  
We develop nonequilibrium auxiliary quantum master equation dual boson method (aux-DB), and argue that it presents a convenient way to describe steady states of correlated impurity models (such as single molecule optoelectronic devices) where electron and energy transport should be taken into account. The aux-DB is shown to provide high accuracy with relatively low numerical cost. Theoretical analysis is followed by illustrative simulations within generic two-level junction model, where the new scheme is benchmarked against numerically exact results.

*we acknowledge support by the National Science Foundation (grant CHE-1565939).*
4:30PM D02.00011: Modeling Collective Emission in Cavities by Phase Space Trajectories

TAO LI (Presenter), HSING TA CHEN, ABRAHAM NITZAN, JOSEPH E SUBOTNIK, Chemistry, University of Pennsylvania — We model N electronic two-level systems (TLSs) coupled to a multimode cavity by sampling independent trajectories in Wiger phase space with a Meyer-Miller-Stock-Thoss (MMST) mapping Hamiltonian. We show that this approach can not only provide us an intuitive physical interpretation of quantum electrodynamics (i.e. sampling electronic and photonic zero-point energies in phase space represents radiative self-interaction and vacuum fluctuations respectively), but also correctly describe many intriguing collective emission phenomena, including spontaneous emission for an array of TLSs in the singly excited manifold, Dicke's superradiance and subradiance when all TLSs are excited, and even the quantum statistics for the delay time in superradiance. We also discuss possible further improvements of this approach.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0019397. The research of A.N. is supported by the Israel-U.S. Binational Science Foundation. This research also used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.

4:42PM D02.00012: The role of integrability in speeding up collective spin polarization.

TAMIRO VILLAZON (Presenter), Boston University, PIETER W CLAEYS, Trinity College, Cambridge, ANATOLI S POLKOVNIKOV, ANUSHYA CHANDRAN, Boston University — The central spin problem plays an important role in a variety of condensed matter systems, including quantum dots and nitrogen vacancy centers in diamond. We study an anisotropic central spin model with two classes of special eigenstates: bright and dark. We find these states to be robust against perturbations around two integrable points of the model. By driving of the central magnetic field, the structure of these eigenstates can be harnessed to access highly polarized many-body configurations. Using approximate shortcuts to adiabaticity, we develop a highly efficient and experimentally viable polarizing scheme.

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BU CMT Visitors program (Pieter Claeyts)
AFOSR FA9550-16-1-0334 (Anatoli Polkovnikov).
Sloan Foundation, Sloan Research Fellowships (Anushya Chandrnan).
4:54PM D02.00013: Quantum Weak Measurement Back-action Control On A Strongly Interacting BEC  
YUEHENG SHI (Presenter), Carleton College, STUART SZIGETI, Department of Quantum Science, Australian National University, ARJENDU KISHORE PATTANAYAK, Carleton College — The choice of weak measurement phase can affect the energy dynamics of a nonlinear quantum system. We report on progress towards controlling the measurement back-action on a strongly interacting Bose Einstein condensate (BEC) continuously monitored under phase-contrast imaging setup. We have derived the master equation using the fixed number state approximation. These have been reduced to a coupled set of differential equations of motions under Gaussian Approximation for the BEC. We use measurement phase dependent back-action in these equations for feed-back control. We discuss potential applications and experimental realizations.

5:06PM D02.00014: Unitary Subharmonic Response of Floquet Majorana Modes  
OLES SHTANKO (Presenter), University of Maryland, College Park, RAMIS MOVASSAGH, IBM Tj Watson Research Center — Detection and manipulation of Majorana fermions are essential for creating a topological quantum computer. To this end, we show that unpaired Majorana modes in Floquet systems can directly be visualized using the phenomenon of unitary subharmonic response. Namely, starting from highly non-equilibrium initial states, the unpaired Majorana modes exhibit boundary oscillations that have twice the driving period, are localized, and have up to exponentially long lifetimes with respect to the system’s parameters. While the lifetime is still limited in translationally invariant systems, we show how disorder can be engineered to stabilize the subharmonic response of Majorana modes. We also suggest a viable implementation in modern multiqubit systems, such as superconducting circuits and atomic systems.

5:18PM D02.00015: Real time dynamics of impurity and disorder scattering with interacting Fermion wave packets*  
SEBASTIAN EGGERT (Presenter), KEVIN JÄGERING, IMKE SCHNEIDER, BENJAMIN NAGLER, ARTUR WIDERA, University of Kaiserslautern, Germany — Recent advances for ultra-cold gases allow the controlled scattering by disorder and localized impurities using moving interacting Fermion wave packets in a trap after a quick displacement in position. We analyze the damping and scattering behavior from large scale numerical t-DMRG simulations in 1D as a function of interaction, displacement and disorder strength in a regime where a comparison with our experiments is possible. Attractive interactions make the wave-packets more susceptible for both single impurities and disorder scattering, which leads to a significant larger damping and quicker breakdown of the oscillations. Repulsive interactions have a much smaller effect, but overall a reduction of scattering can be observed. The corresponding experiments for 3D scattering show maximum stability and minimal damping near the unitary point.

*Supported by the Deutsche Forschungsgemeinschaft (DFG) via SFB/TR185 "OSCAR"

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D03 GSCCM: Materials in Extremes: Multiscale Models of Energetic Materials 107 - Mitchell Wood, Sandia National Laboratories - Tag(s): Focus
2:30PM D03.00001: Understanding the Role of Microstructure in Energetic Materials Using a Predictive Hierarchical Multiscale Simulation Approach* [Invited] JAMES P. LARENTZOS (Presenter), BRIAN C. BARNES, Weapons and Materials Reserach Directorate, US Army CCDC Army Research Laboratory, KENNETH W. LEITER, Computational and Information Sciences Directorate, US Army CCDC Army Reseach Laboratory, JOHN K. BRENNAN, SERGEI IZVEKOV, Weapons and Materials Reserach Directorate, US Army CCDC Army Research Laboratory, JAROSLAW KNAP, Computational and Information Sciences Directorate, US Army CCDC Army Reseach Laboratory, JOHN K. BRENNAN, SERGEI IZVEKOV, Weapons and Materials Reserach Directorate, US Army CCDC Army Research Laboratory — Composite energetic materials contain microstructural heterogeneities (i.e., crystal defects, voids, interfaces, etc.), where the community consensus is that this microstructure plays a critical role in the energetic material response. However, an understanding and characterization of its precise role for system design is lacking. This is due in part to the significant experimental challenges caused by the extreme conditions occurring at short time and length scales. Modeling and simulation are not hampered by these conditions; rather, limitations are due to the approximations made in the models and the available computational resources.

In this talk, new capabilities for investigating the role of microstructure in energetic material response through both explicit, large-scale and multiscale simulation approaches will be discussed. A hierarchical multiscale simulation approach that directly couples a coarse-grain particle level description of the chemistry and material heterogeneities (via dissipative particle dynamics simulation) to macroscale, finite element continuum simulations of an energetic material is established. The new methodology closes a gap in modeling capabilities for a key time and spatial regime in the multiscale material landscape (i.e., the mesoscale). The computational capabilities are demonstrated through at-scale comparisons of thermal cookoff and plate impact simulations with experiment to provide key insight into the role of microstructure on the response of the energetic material cyclotrimethylene trinitramine (RDX) to thermal and shock loading.

*This work was supported by the US Army CCDC Army Research Laboratory, the Office of Naval Research (BAA number 12-001), and a grant of computer time from the DOD High Performance Computing Modernization Program at the ARL, Navy, AFRL and ERDC DoD Supercomputing Resource Centers.
3:06PM D03.00002: Microstructure-informed, statistical approach for shock to detonation transition modelling in high explosives  
AHMED HAMED (Presenter), MARISOL KOSLOWSKI, Purdue Univ — Shock to detonation transition phenomenon (STDT) is a synergistic effect of different underlying mechanical, chemical, and thermal processes, where the racing between different modes of energy production and dissipation is the key factor. Accurate prediction of these far-from-thermodynamic-equilibrium phenomena dictates careful consideration of different entropic fluxes associated with various inelastic processes, along with their characteristic modes of transport. Hot-spot formation and initiation is the main paradigm to tackle STDT, which, in turn, is known to be heterogeneous in nature. Accordingly, mean-field approaches, which employ averaged-measures of microstructural properties, predict critical parameters for STDT regime that can deviate significantly from experiment. In the present study, we seek a statistical approach to represent the heterogeneity in the microstructure of polymer-bonded explosives, which better captures the sensitivity of hot-spot initiation to local variation in the microstructure. The reactive flow system of equations is solved in Lagrangian framework, within finite strain formalism. In addition, this thermo-mechanical-chemical model is supplemented by the Hugoniot equation of state for closure purposes and solved using finite-element technique.

3:18PM D03.00003: Mesoscale modeling of explosive mixtures containing TNT and HMX*  
H. KEO SPRINGER (Presenter), SORIN BASTEA, CRAIG M TARVER, Lawrence Livermore Natl Lab — Different energetic constituents can be combined to achieve desired explosive mixture properties. One example of an explosive mixture is Octol which is comprised of a less ideal constituent, TNT, and a more ideal constituent, HMX. Changes to HMX content in this mixture can alter its shock sensitivity and performance. However, the microscale reaction mechanisms underlying such changes are not well understood. In this study we perform mesoscale simulations to investigate different TNT-HMX mixtures. Simulations are performed with the multi-physics code, ALE3D. A coupled thermochemical code provides equation-of-state and chemical kinetic properties. Simulations are performed for TNT-HMX weight ratios of 25-75, 40-60, and 70-30 with 2 and 5% porosity. A range of shock pressures are considered. Non-reactive studies examining changes to the p-v response and temperature distribution will be discussed with comparisons to common mixture rules. Trends for the mixture reaction rate with varying HMX content and porosity will also be discussed. These studies are important for developing mixture reactive flow models when the constituents are mixed at length-scales below the reaction zone size.

*Work performed under auspices of U.S. DOE by LLNL under contract DE-AC52-07NA27344. LLNL-ABS-XXXXX.
Mesoscale Dynamic Damage Visualization and Simulation of Energetic Materials under Impact

JONATHAN DRAKE, WEINONG CHEN (Presenter), MARISOL KOSLOWSKI, Purdue Univ, KAMEL FEZZAA, APS, Argonne National Laboratory — Energetic materials may be subjected to impact. Under such loading conditions, local stress or strain concentrations may lead to the formation of hot spots and unintended reaction. To visualize the dynamic damage and reaction processes in polymer bonded energetic crystals under dynamic compressive loading, a high-speed X-ray phase contrast imaging setup was synchronized with a Kolsky bar and a light gas gun. Controlled compressive loading was applied on PBX specimens with a single or multiple energetic crystal particles and impact-induced, time-resolved damage and reaction processes were captured using the high-speed X-ray PCI. Numerical simulation models were built based on the experimental results and used to investigate the impact damage in PBX over a wider range of parameter variations.

*Office of Naval Research as this research is funded through the project award N00014-16-1-2557 to Purdue University.
AFOSR Award No. FA9550-16-1-0315 (Dr. Martin Schmidt, Program Officer).
Use of the Advanced Photon Source, an Office of Science User Facility operated for the US Department of Energy (DOE) Office of Science by Argonne National Laboratory was supported by the US DOE under contract No. DE-AC02-06CH11357.
Developing and validating thermomechanics models for explosives with experiments on commensurate scales [Invited]  

KYLE RAMOS (Presenter), FRANCIS L ADDESSIO, CLAUDINE ARMENTA, JOHN L. BARBER, CYNTHIA BOLME, MARC CAWKWELL, Los Alamos National Laboratory, LEORA DRESSELHAUS-COOPER, Lawrence Livermore National Laboratory, ARIANNA E GLEASON, SLAC National Accelerator Laboratory, ADAM GOLDER, ERNEST HARTLINE, BRIAN JENSEN, Los Alamos National Laboratory, HAEJA LEE, SLAC National Accelerator Laboratory, DARBY J LUSCHER, Los Alamos National Laboratory, CHRISTOPHER MEREDITH, Army Research Laboratory, PAULO A RIGG, Washington State University, RICHARD L SANDBERG, Los Alamos National Laboratory, MATTHEW H SEABERG, SLAC National Accelerator Laboratory, NICHOLAS SINCLAIR, Washington State University, GARY K WINDLER, Los Alamos National Laboratory — In both manufacturing and dynamic loading, the interplay between deviatoric stress, plastic strain, and heat generation at the mesoscale dictate the responses of plastic bonded explosives (PBX). In situ mesoscale insights are needed to quantify structure-property relationships, inform theory, and enable simulations. We have attempted such an effort and will present an overview of our progress so far.

Laser-driven shock, gas gun, and split-Hopkinson pressure bar experiments have been performed to span multiple orders of strain rate, using synchrotron and X-ray free electron laser radiation to measure time-resolved X-ray diffraction (XRD) and phase contrast imaging (PCI) in situ for single crystal and plastic bonded explosives. This range of strain rates enables investigation of coupling between crystal mechanics, thermal softening, and microstructure that governs explosive response.

Multiphase single crystal plasticity models have been developed. They consist of non-linear thermo-elasticity, Orowan expressions for slip rate using the Austin-McDowell model for dislocation velocity, and multiphase equations of state (EOS) imposing phase transitions through Gibbs free-energy. Constitutive equations were parameterized with density functional theory and atomistic calculations for EOS and elastic constants along with experimental measurements of anisotropic deformation mechanisms and rates. These models are capable of predicting anisotropy, grain size, and pressure dependent effects remarkably well.

Combining the new capabilities, mesoscale thermomechanics can be investigated from the average lattice response up to PBX microstructures. For the first time, XRD quantify average lattice response and allows for direct comparison of experiments and simulations through measured and computed diagnostics. Using the experimentally validated models, simulation can be compared to PCI of heterogeneous micorstructure effects such as void collapse and grain boundaries.
4:18PM D03.00006: Non-Schmid effect of pressure on plastic deformation in molecular crystal HMX

ANIRBAN PAL (Presenter), West Texas State Univ, CATALIN PICU, Mechanical Aerospace and Nuclear Engg., Rensselaer Polytechnic Inst — The energetic molecular crystal HMX is a key constituent in common plastic bonded explosives. Its plastic deformation under shock conditions is important in reaction initiation and detonation. Here, we study the effect of high pressure on dislocation slip using isothermal-isobaric atomistic simulations. We consider 2 slip planes, (011) and (101), that are reported to be most active under ambient conditions. For all slip systems considered, the effect of pressure is to increase the critical resolved shear stress for dislocation slip. Pressure may fully inhibit dislocation-based plasticity if the resolved shear stress is not increased in proportion. On the other hand, at sufficiently high shear stresses, the crystal loses shear stability. Therefore, in a broad range of shock conditions, plastic deformation takes place by a combination of dislocation glide in some slip systems and localization in some other systems, with dislocation activity being gradually inhibited as the shock pressure increases.

*This work was supported by the US Air Force Research Labs(AFRL/RWK).

4:30PM D03.00007: Atomistic mechanisms in the plasticity of energetic crystal HMX

MOHAMMAD KHAN (Presenter), ANIRBAN PAL, CATALIN PICU, Rensselaer Polytechnic Institute — The energetic molecular crystal cyclotetramethylene tetranitramine (HMX) is a key constituent in common plastic bonded explosives. Its plastic deformation under shock conditions is important in reaction initiation and detonation. In this work we identify, using atomistic simulations, the slip systems in b-HMX and compute the critical resolved shear stresses for dislocation motion. We also evaluate the mobility of dislocations in various slip systems and the likelihood of cross-slip. The implications of these results for the overall physical picture of plasticity in HMX are discussed.

M. Khan, R.C. Picu, J. Appl. Phys. 126 (2019) 155105

*Work supported by US AFRL/RWK through grant FA8651-16-1-0004.
4:42PM D03.00008: Anisotropic Thermal Conductivity and Elasticity of RDX Using Impulsive Stimulated Thermal Scattering*  JOHN LAZARZ (Presenter), SHAWN DAVID MCGRANE, ROMAIN PERRIOT, CYNTHIA BOLME, MARC CAWKWELL, KYLE RAMOS, Los Alamos National Laboratory — Anisotropy of single crystals plays an integral role in meso-scale behavior of materials. In energetic materials, the anisotropy of thermal conductivity and elasticity plays a key role in hot spot generation during dynamic loading, potentially leading to deflagration or detonation. Precise measurements are needed to validate predictive models of these materials during accident scenarios. Toward these goals, we are investigating single crystal orthorhombic 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) using impulsive stimulated thermal scattering (ISTS). Here we present results of the experimentally determined thermal diffusivity and its comparison with the anisotropic values predicted by atomistic simulations, as well as experimentally measured anisotropic acoustic velocities.

*LANL Laboratory Directed Research and Development project 20180100DR.

4:54PM D03.00009: Dynamic fracture and frictional temperature rise in HMX-Sylgard microstructures under impact and vibration  AKSHAY DANDEKAR (Presenter), MARISOL KOSLOWSKI, Purdue Univ — Polymer bonded explosives are sensitive to impact and vibrations and can form critical hot-spots under certain conditions leading to ignition. Thus, understanding the behavior of PBXs under mechanical loading is crucial to avoid accidents during manufacturing, handling, and transport of these materials. In this study, the response of HMX-Sylgard samples is numerically studied using a finite element approach that includes dynamic damage coupled with temperature evolution due to frictional heat. At impact velocities close to 100 m/s several cracks develop and grow. Consequently, critical hot spots are observed in agreement with PBX. The maximum frictional temperature rise is found at particle polymer interfaces. The effect of crystal orientation of the particles including plasticity and orientation and cleavage planes is analyzed under vibration and impact in 3D simulations.

5:06PM D03.00010: Temperature- and pressure-dependent lattice constants of CL-20 polymorphs from ab initio molecular dynamics simulations*  IGOR SCHWEIGERT (Presenter), BENJAMIN DATKO, United States Naval Research Laboratory — Hexanitrohexaazaisowurtizane (CL-20) is a high-density nitramine compound with several known polymorphs. We're interested in using density functional theory (DFT) to predict the thermodynamic stabilities of various polymorphs at elevated temperatures and pressures. This presentation will describe DFT-based molecular dynamics simulations of temperature- and pressure-dependent lattice constants for the epsilon and zeta polymorphs and compare the results to available experimental data.

*This work was supported by the Office of Naval Research (ONR), both directly (project N0001416WX0003, Dr. Chad Stoltz) and through the U.S. Naval Research Laboratory (NRL).
5:18PM D03.00011: Material Diffusion and Combustion Process Modeling Using a Stochastic Particle-Based Framework  
NIKOLAI PETSEV (Presenter), XIA MA, BRYAN HENSON, BRAD EDWIN CLEMENTS, Los Alamos National Laboratory — We describe a novel mesoscale particle-based computational strategy for modeling non-isothermal reaction-diffusion problems. Importantly, this simulation framework gives the foundation for investigating the deflagration-to-detonation transition (DDT) in combustion, where the material transitions from burning at a rapid subsonic pace (deflagration) to the emergence of a shockwave (detonation). The basis for this approach is "smoothed dissipative particle dynamics" (SDPD), a stochastic thermodynamically-consistent approach for solving the fluctuating hydrodynamic equations of Landau and Lifshitz. Presently our new approach incorporates heat and mass transfer driven by conduction and diffusion, exchange of heat and chemical species due to thermal fluctuations, and source terms arising from the chemical reaction. In future work, this will be coupled to the fluctuating momentum equation, or included in multiscale molecular-continuum simulations, opening the possibility for simulations studying DDT in energetic materials, in addition to a broad range of other applications involving chemical reactions and concurrent mass and heat transfer.

Monday, March 2, 2020 2:30 PM - 5:06 PM

Session D04 DCP DCOMP DBIO DSOFT: Water Dynamics in Different Environments: Experiment and Theory II. Ice

2:30PM D04.00001: Interfacial water: from atmospheric ice nucleation to nano-confinement [Invited]  
ANGELOS MICHAELIDES (Presenter), Univ Coll London — Recent work from our research group in which we are trying to understand the intimate molecular level details of water freezing will be discussed. A particular emphasis will be placed on the role the surfaces of foreign materials play in accelerating the nucleation process [1-3] and on the dynamical nature of the nucleation event.

References
**3:06PM D04.00002: Atomic imaging of edge structure and growth of a two-dimensional hexagonal ice**  
RUNZE MA (Presenter), DUANYUN CAO, International Center for Quantum Materials, Peking University, CHONGQIN ZHU, Department of Earth and Environmental Sciences, University of Pennsylvania, YE TIAN, JINBO PENG, JING GUO, International Center for Quantum Materials, Peking University, JI CHEN, XIN-ZHENG LI, School of Physics, Peking University, JOSEPH S FRANCISCO, Department of Earth and Environmental Sciences, University of Pennsylvania, XIAO CHENG ZENG, Department of Physics, University of Nebraska–Lincoln, LIMEI XU, ENGE WANG, YING JIANG, International Center for Quantum Materials, Peking University — The formation and growth of water ice layers on surfaces and of low-dimensional ice under confinement are common occurrences. While structured water adlayers and 2D ice have been imaged, capturing metastable or intermediate edge structures involved in their growth is extremely challenging due to their fragile and short-lived nature.

Here we show that noncontact atomic force microscopy with a CO-terminated tip allows real-space imaging of the edge structures of a 2D bilayer of hexagonal ice grown on an Au(111) surface. We find a new edge type that coexists with the zigzag edge commonly observed in 2D hexagonal crystals, and freeze samples during growth to identify intermediate structures.

When combined with MD simulations, these allow us to reconstruct growth processes that in the case of the zigzag edge involve addition of water molecules to the existing edge and a collective bridging mechanism. Armchair edge growth, in contrast, involves local seeding and edge reconstruction and thus is in stark contrast to conventional views of ice growth. The growth mechanism we have uncovered might also occur at the surface of bilayer hexagonal ice and might support a bilayer-on-bilayer ice growth to 3D ice transformation.

RICCARDO DETTORI (Presenter), Department of Chemistry, University of California, Davis, MICHELE CERIOTTI, Laboratory of Computational Science and Modeling, École Polytechnique Fédérale de Lausanne, JOHANNES HUNGER, Max Planck Institute for Polymer Research, LUCIANO COLOMBO, Dipartimento di Fisica, Università degli Studi di Cagliari, DAVIDE DONADIO, Department of Chemistry, University of California, Davis — We introduce a nonequilibrium molecular dynamics simulation approach, based on the generalized Langevin equation, to study vibrational energy relaxation in pump-probe spectroscopy. A colored noise thermostat is used to selectively excite a set of vibrational modes, leaving the other modes nearly unperturbed, to mimic the effect of a monochromatic laser pump. Infrared pump-probe spectroscopy provides detailed information about the dynamics of hydrogen-bonded liquids. Due to the dissipation of the absorbed pump pulse energy, thermal equilibration dynamics also contribute to the observed signal. Disentangling this contribution from the molecular response remains a challenge. By performing non-equilibrium molecular dynamics simulations of hydrogen-bonded liquids, we show that faster molecular vibrational relaxation and slower heat diffusion are decoupled and occur on different length scales. Transient structures of the hydrogen bonding network influence thermal relaxation by affecting thermal diffusivity over a length scale of several nanometers. Energy relaxation is probed by analyzing the evolution of the system after excitation in the microcanonical ensemble, thus providing direct information about the energy redistribution paths at the molecular level and their time scale.
3:30PM D04.00004: Complete Lattice Vibration Dispersion Curves (36 Branches) for the Frozen (T=0K) Bernal-Fowler Hexagonal Close Packed Crystalline Ice with Four Water Molecules in One Primitive Unit Cell Containing 8 Protons and 4 Oxygen Nuclei*  

BIN JIE (Presenter), Physics Department, Xiamen University, CINDY TIANHUI JIE, Massachusetts Institute of Technology, CHIH-TANG SAH, Physics Department, Xiamen University — In 1969, Faure computed the lowest 12 branches of dispersion curves of lattice vibrational modes for Ice Ih, assuming the water molecule H$_2$O in the crystalline ice as point mass (PM), in order to analyze the experimental infrared and Raman spectra of ice. In 1973, Bosi-Tubino-Zerbi removed the PM approximation of H$_2$O in the 1933 Bernal-Fowler Hexagonal Close Packed (HCP) Primitive Unit Cell (PUC) containing 4 H$_2$O (8 protons and 4 Oxygen nuclei) in order to account for the experimental spectra in the low vibrational frequency (LVF) range. During 1969-2019 (50 years) theoretical and experimental spectra of hexagonal Ice Ih are lacking in the high vibrational frequency (HVF) range. Our 2013 melted-ice model for pure liquid water, demonstrated the dominance of the HVF modes in accounting for the abnormally high mobilities of positive and negative ions in pure liquid water. This talk gives the computed 36 branches of dispersion curves of Ice Ih at 0K, using six prime force constants, four values of which from isolated water molecule, further proving the connection of water’s crystalline solid phase and single molecule gas phase, by our 2013 melted-ice lattice model for the liquid phase of water.

*TJ & BJ supported by CTSA.US, LLC, Florida, USA. BJ & CTS, partially supported by XMU.

3:42PM D04.00005: Probing interfacial water by H-sensitive and non-invasive scanning probe microscopy [Invited]  

YING JIANG (Presenter), Peking Univ — Water/solid interfaces are a central theme across an incredibly broad range of scientific and technological processes. Scanning probe microscopy (SPM) has been extensively applied to probe interfacial water in many interdisciplinary fields. However, there exist two longstanding limitations in the past two decades, which makes SPM fall short compared with conventional spectroscopic methods. First, H atoms of water molecule are very small and light, so it is very difficult to image them directly; Second, the water molecules are linked by weak H bonds, and it is highly possible to disturb the fragile water structure during the imaging process. In order to overcome these two grand challenges, we have developed a new-generation SPM based on a qPlus sensor, which is sensitive to H and non-invasive to water structure [1]. The key lies in probing the high-order electrostatic force between the quadrupole-like CO-terminated tip and the polar water molecules at large tip-water distances. In this talk, I will first discuss the application of this technique to determine the microscopic structure of metastable water clusters [1]. In addition, we have unraveled the detailed atomic structures of ion hydrates at interfaces and discover a magic-number effect on the transport of ion hydrates [2]. Finally, I will show the ability of visualizing the growth of a two-dimensional ice in real space with atomic resolution, by capturing various metastable and intermediate structures during the ice growth at the ice edges [3].


CHIH-TANG SAH (Presenter), Physics Department, Xiamen University, CINDY TIANHUI JIE, Massachusetts Institute of Technology, BIN JIE, Physics Department, Xiamen University — Our 2013 melted ice model extends the 1933 Bernal-Fowler Hexagonal Close Packed Ice crystal model to pure liquid water (0-100°C). The periodically-extended 2 trisector proton sites between 2 nearest neighbor oxygen nuclei, occupied or unoccupied by a proton, are the 2 physical spaces for the migrations of the 2 protonic fermion species, the protons and prohols. The physical space describes, in the statistically large sensible volume, the 2 protonic energy bands, for protons migrating among the unoccupied proton sites and prohols migrating among the occupied proton sites. The vibrational modes of the protons and oxygens give the 2 atomic phonon species: 12 oxygenic bosons in the low energy range and 24 protonic bosons in the high energy range. Electrical charge and inertia mass transports in pure liquid water, are carried by the protons, and dominated by the strong localized (local mode & self trap) interaction between the protonic fermions and protonic bosons, with noisy background from the oxygenic bosons. Our computed temperature variations (0–100°C) of the three parameters (the proton product and the two protonic mobilities) are in excellent agreement with the international handbook values.

*TJ & BJ supported by CTSA.US, LLC, Florida, USA. BJ & CTS, partially supported by XMU.

4:30PM D04.00007: Nanoindentation of Ice I\textsubscript{h} - Atomistic simulations

PEDRO ANTONIO SANTOS-FLÓREZ (Presenter), UNICAMP - Universidade Estadual de Campinas, CARLOS JAVIER RUESTES, UNCUYO - Universidad Nacional de Cuyo, MAURICE DE KONING, UNICAMP - Universidade Estadual de Campinas — Using molecular dynamics simulations we study the mechanical response of ice I\textsubscript{h} through nanoindentation tests perpendicular to the basal plane. Using a smooth spherical tip represented by a repulsive potential we explore the deformation mechanisms and hardness estimates for ice as described by the all-atom TIP4P/Ice potential and the coarse-grained mW models. We assess the sensitivity to the tip radius and the penetration rate both for low temperatures as well as for conditions close to the melting point, where the formation of a quasi-liquid layer (QLL) on the surface becomes relevant. We find that during plastic deformation the main mechanism for stress relief for the low temperatures is the amorphization of the crystalline ice bilayers. On the other hand, for high temperatures the plastic deformation occurs by bilayer-by-bilayer melting, consistent with previous literature. Considering the difference between the behaviors of the mW and TIP4P/Ice models, we observe that the latter also involves the nucleation and motion of dislocations. This is consistent with recent observations concerning uniaxial deformations and provides further indications that the absence of explicit protons in the mW model gives rise to excessive ductility.
**4:42PM D04.00008: Sum Frequency Generation Spectroscopy of Ice/Air and Water/Air Interfaces from Ab Initio Deep Potential Molecular Dynamics**

MARCOS ANDRADE (Presenter), LINFENG ZHANG, ANNABELLA SELLONI, ROBERTO CAR, Princeton University — The interfaces of liquid water and ice with air abound on Earth and impact non-negligibly atmospheric sciences. Directly probing the structure of interfacial water is challenging, and the surface-specificity of Sum Frequency Generation (SFG) spectroscopy has offered important insights on both structure and dynamics of interfacial water and ice. *Ab initio* molecular dynamics (AIMD) could, in principle, aid interpret the experimental observations since it accesses both molecular and electronic structure of interfacial water. However, AIMD stumbles on the slow convergence of the SFG spectrum with simulation time. We here overcome this difficulty using Deep Neural Networks (DNN) to represent the *ab initio* potential energy surface. DNNs were also used to obtain molecular dipole moment and polarizability of water in agreement with first-principles methods, which allows a proper computation of the SFG spectrum of water/air and ice/air interfaces relying only on the dipole approximation. Our method can be easily extended to other interfaces and should enable *ab initio* level simulations of SFG spectra for a wide variety of systems.

*This work was conducted within the Computational Chemical Center: Chemistry in Solution and at Interfaces funded by the DoE under Award DE-SC0019394.

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**4:54PM D04.00009: How crystals form: a theory of nucleation pathways**

JAMES LUTSKO (Presenter), Universite libre de Bruxelles — Classical Density Functional theory is combined with fluctuating hydrodynamics to describe nucleation in general and crystallization in particular. The nucleation pathway is characterized as the most likely path connecting the initial homogeneous solution to the critical cluster[1]. Classical Nucleation Theory can be recovered with additional approximations[2]. Results for a Lennard-Jones system[3] show a two-step path with the formation of a dense fluid-like droplet followed by the development of order within. During ordering, the system passes through a metastable, subcritical phase that could be identified as a nucleation precursor. The precursor is a sub-critical crystalline cluster stabilized by completed crystalline shells and a wetting layer.


*This work was supported by the European Space Agency (ESA) and the Belgian Federal Science Policy Office (BELSPO) in the framework of the PRODEX Programme (contract number ESA AO-2004-070).
**D04.00010: Surface and bulk contributions to sum-frequency vibrational spectroscopy of single crystalline ice**

XU XIAOFAN (Presenter), Fudan Univ, YUEN-RON SHEN, Physics Department, University of California, Berkeley, CHUANSHAN TIAN, Fudan Univ — We study the bulk and surface contributions to the sum-frequency vibrational spectroscopy (SFVS) of ice I_h(0001) interfaces in the bonded OH stretching band at 223K. Using phase-sensitive SFVS with selected polarization combination and beam geometry, a pure electric quadrupole SF spectrum from bulk ice was obtained. Based on analysis of selection rule, an electric quadrupole sub-band near 3120 cm\(^{-1}\) originated from the bulk was found to constitute large portion in the reflected SF spectrum of vapor/ice interface. Via modification of ice surface by absorption of a monolayer of ethanol, the SF vibrational spectrum was significantly reduced at ~3170 cm\(^{-1}\), suggesting the surface is also important in the ice SF spectrum. These results not only reveal the importance of bulk contribution in SFVS spectrum of ice, but pave the way for investigation of ice surface, e.g. surface premelting, in practical environments.

\(\text{*}(1)\) National Natural Science Foundation of China Grants (No.11874123)
\(\text{(2) National Key Research and Development Program of China (No. 2016YFA0300902).}\)

**Monday, March 2, 2020 2:30 PM - 5:30 PM**

**Session D05 DCP DAMOP DCMP DPOLY: Electronic-Vibrational Coupling in Light Harvesting I. Photosynthetic Light Harvesting**

111 - Jacob Krich, Univ of Ottawa - Tag(s): Focus
2:30PM D05.00001: Investigating the Energy Transfer Dynamics in the Baseplate of Green Photosynthetic Bacteria using 2D Electronic Spectroscopy* ALEXA RAE CAROLLO (Presenter), Department of Chemistry, University of Colorado Boulder, CARRIE GOODSON, Department of Biology, Washington University in St. Louis, ROBERT E. BLANKENSHIP, Department of Biology and Department of Chemistry, Washington University in St. Louis, NIELS-ULRIK FRIGAARD, Department of Biology, University of Copenhagen, DONATAS ZIGMANTAS, Department of Chemical Physics, Lund University — The structure of the baseplate, a pigment-protein complex that mediates energy transfer in green photosynthetic bacteria, is not fully understood. The baseplate cannot be isolated from the chlorosome light harvesting antenna, but their spectral signatures can be separated with femtosecond two-dimensional electronic spectroscopy (2DES)[1]. In this work, 2D spectra of the baseplate in a mutant of Chlorobaculum tepidum, which was previously found to contain dimeric pigments[2], will be compared to 2D spectra of Chloroflexus aurantiacus to characterize the pigment interactions and energy transfer pathways in both samples.

References

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2:42PM D05.00002: Probing quantum coherence in photosynthetic energy transfer in the presence of fluctuating environment with levitons and time-dependent nonequilibrium Green functions* PRIYANKA MONDAL (Presenter), BRANISLAV NIKOLIC, Univ of Delaware, ALEXANDER EISFELD, Max Planck Institute for the Physics of Complex Systems — The first few steps of photosynthesis in light harvesting complexes involve creation of exciton at chlorosome and its transport to reaction center, where the charge separation takes place. The transport of exciton from chlorosome to reaction center is highly efficient but the role of long-lived quantum coherence towards this efficiency is highly debatable. Here we present a prototype that uses a leviton voltage pulse to map a single exciton entering Fenna-Matthews-Olson pigment complex which is mapped as coupled quantum dots with attached leads, in presence of environmental fluctuation coming from molecular dynamics simulation. Our main result includes long-lived quantum beating in population dynamics and the dependency of quantum dephasing on exciton transport efficiency in fluctuating environment using time-dependent nonequilibrium Green functions approach.

*This work was supported by DOE Grant No. de-sc0016380. The supercomputing time was provided byXSEDE, which is supported by NSF Grant No. ACI-1053575.
Exploring electronic-vibrational coupling in chlorophylls and photosynthetic complexes by polarization-controlled 2D electronic spectroscopy* [Invited]

DONATAS ZIGMANTAS (Presenter), EGLE BUKARTE, ERLING THYRHAUG, Lund Univ/Lund Inst of Tech, DAVID PALECEK, University of Cambridge, ROEL TEMPELAAR, Columbia University, ANJA HAUFE, Goethe University Frankfurt, MARCELO ALCOCER, KAREL ZIDEK, Lund Univ/Lund Inst of Tech, THOMAS LA COUR JANSSEN, University of Groningen, DAVID BINA, The Institute of Plant Molecular Biology, JASPER KNOESTER, University of Groningen, CLAUDIA BUCHEL, Goethe University Frankfurt — Electronic-vibrational (vibronic) coupling has been suggested to play an important role in energy transfer and charge separation processes in photosynthesis. It is, however, highly elusive phenomenon to investigate. To this end we have employed polarization-controlled 2DES together with advanced Fourier analysis [1]. We use double-crossed polarization scheme, which extracts signals generated by excitation of coherences, involving transitions with different orientation of dipole moments. It allows for studying electronic and vibronically mixed coherences, and therefore enables to directly detect the presence of vibronic mixing (coupling).

In one study we investigated chlorophyll c molecule, where we found a clear evidence of mixing of the two lowest electronic states, Qx and Qy via vibronic coupling. Interestingly, we discovered at least two vibrational modes that are involved in the coupling. Since this type of coupling is expected to be rather general, vibronic mixing is expected in all chlorophyll-type molecules.

In another study we revisited coherence dynamics in the FMO complex at 77 K [2]. Applying the same experimental method and analysis techniques, and aided by theory, we find a very rich picture of the coherence signals. We determined that all long-lived coherences have clearly vibrational origin. While electronic coherences are also observed, they dephase on the ~100 fs time scale. Importantly, we further observe that specific vibrational coherences are excited via vibronically coupled excitonic transitions.

Finding ubiquitous vibronic coupling in photosynthetic pigments and complexes that contain them raises a question if its presence is the signature of smart Nature's design, or an unavoidable consequence of the photophysical properties of the porphyrin-type molecules.


*Swedish Research Council, Knut and Alice Wallenbergs Foundation, Crafoord Foundation.
3:30PM D05.00004: Matrix-product-state-based calculations of exciton-phonon dynamics for light-harvesting complexes*  R. KEVIN KESSING (Presenter), SALVATORE MANMANA, Institute for Theoretical Physics, Georg-August-Universität Göttingen, JIANSHU CAO, Department of Chemistry, Massachusetts Institute of Technology MIT — Excitonic systems with one to a few dozen sites are an important topic in contexts such as quantum optics, molecular spectroscopy or the dynamics of light-harvesting complexes. However, the dynamics are often strongly influenced by coupling to the external or internal vibrational modes, which presents a computationally much more challenging problem. We investigate the dynamics of excitonic oligomers with such non-perturbative coupling to a quantum bath using a symmetry-adapted state-of-the-art matrix-product-state (MPS) code[1] which has not been previously applied to this type of system. Using this accurate, unbiased method, we focus on studying spreading, coherence and entanglement behavior. The insights gained from these analyses help us better understand exciton dynamics in photosynthesis, e.g. in the purple bacteria light-harvesting complex LH2, which exhibits efficient energy transfer and a notable symmetric structure. [2]

2: Optimal fold symmetry of LH2 rings; L. Cleary, H. Chen et al.; PNAS 110 (21), 8537-8542 (May 2013); DOI: 10.1073/pnas.1218270110

*The German Academic Scholarship Foundation provides funding for RKK.

3:42PM D05.00005: Vibronic Structure and Coherence in the Bacterial Reaction Center* [Invited]  JENNIFER OGILVIE (Presenter), VERONICA POLICHT, Univ of Michigan - Ann Arbor — Much of our current understanding of photosynthetic charge separation has been derived from studies of the bacterial reaction center (BRC) from purple bacteria. We report two-dimensional electronic spectroscopy (2DES) experiments on the BRC that reveal previously hidden excitonic and vibronic structure. Through analysis of the coherent dynamics of the BRC and careful comparison with monomeric bacteriochlorophyll we report vibronic coherence and identify resonances between a number of key intramolecular pigment vibrations and electronic energy gaps in the BRC. Such resonances have been proposed to play a functional role in photosynthetic energy transfer and charge separation.

*The authors gratefully acknowledge support from the National Science Foundation (grant # PHY-0748470). J.P.O. acknowledges support from the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award #DE-SC0016384.
Organic solar cell materials are a cheaper option to traditional silicon but lack the efficiency for which silicon is famous. Quantum computers can outperform the greatest supercomputer, but the short-lived coherences lead to classical-like behavior. Light-harvesting systems (LHS) serve as an example to both applications. LHSs absorb sunlight and convert it into an electrochemical gradient with near unity quantum efficiency and maintain long coherence times. Probing the exciton dynamics of these systems, one of which is the Photosystem II reaction center (PSII RC), can elucidate how these systems are able to transport excitons with approximately 99% efficiency. This revelation could propel solar-cell and quantum-computing research forward at unprecedented levels.

To do this, we have employed a projection-free version of the Generalized Quantum Master Equation (GQME) whose memory kernel is calculated using approximate methods, such as the Mean-Field Approximation (MFA) and the Linearized Semiclassical Method (LSC). This approach, verified against a Spin-Boson model and the well-studied LHS Fenna-Matthews-Olson (FMO) complex, is more computationally efficient and yields a high level of accuracy compared to exact methods such as the Quasi-Adiabatic Propagator Path Integral (QuAPI).

The discovery that quantum coherence might enhance biological processes such as photosynthesis is not only of fundamental importance but also leads to hopes of developing bio-inspired ‘green’ quantum technologies that mimic nature. A key question is how the time scale of coherent processes in molecular systems compare to that of the driving light source — the sun. Across the community, the coherence time quoted for sunlight spans at least two orders of magnitude, ranging from 0.6 to >10 of femtoseconds. This difference can potentially be significant in deciding whether the induced light-matter coherence is long enough to affect macro system behaviour. Here we revisit the historic calculations of sunlight coherence starting with the blackbody spectrum and then proceed to provide values for the more realistic case of atmospherically filtered light. We corroborate these values with interferometric measurements of atmospherically filtered sunlight in the visible spectrum, the wavelength range most relevant for photosynthetic organisms on Earth. This is the first step in our development of a novel sunlight emulator utilizing a train of ultrafast laser pulses.

*BVR acknowledges support from the EPSRC Scottish Doctoral Training Centre in Condensed Matter Physics (UK Grant # EP/L015110/1).
4:42PM D05.00008: Quantum coherence in a photosynthetic dimer driven by incoherent sunlight* PEI-YUN YANG (Presenter), Beijing Computational Science Research Center, JIANSHU CAO, Massachusetts Institute of Technology MIT — In this work, we demonstrate noise-induced coherence in a model of a photosynthetic molecular dimer driven by an incoherent radiation field. Through perturbation theory associated with white noise approximation, the dynamics of the excitons is characterized by the dressed exciton states. The exciton coherence exhibits respectively quantum beats among the exciton states and quasistationary relaxation processes in two opposite parameter limits. We further examine the steady-state physics, where the exciton coherence can be classified into light-induced and trap-induced coherences that break detailed balance. At last, the steady-state population and energy fluxes in the dimer system are discussed.

*Pei-Yun Yang is supported by Beijing Computational Science Research Center

4:54PM D05.00009: Carotenoid-mediated light harvesting in plants Minjung Son, Gabriela Schlau-Cohen (Invited) GABRIELA SCHLAU-COHEN (Presenter), MINJUNG SON, Massachusetts Institute of Technology MIT — Plants absorb across the visible region of the solar spectrum followed by rapid and efficient collection of the photoenergy in lower-lying states. Previous experiments have been limited to the dynamics of the low-energy states, leaving the higher-energy states, including how they transfer energy downhill, unexplored. We describe ultrabroadband 2D electronic spectroscopy that enables us to map out the excited states and dynamics of the major antenna complex of plants across the visible region. By analyzing the vibrational wavepackets in the spectra, we identify a debated dark state on a single carotenoid, lutein 2, that mediates relaxation. This result reveals that the protein binding pocket controls the electronic structure of carotenoids, and therefore their function in photosynthesis.

Monday, March 2, 2020 2:30 PM - 5:18 PM

Session D07 DQI: NISQ: Quantum Chemistry and Quantum Simulation

2:30PM D07.00001: Demonstration of a large-scale quantum chemistry calculations using the Sycamore quantum processor NICHOLAS RUBIN (Presenter), JARROD MCCLEAN, ZHANG JIANG, MATTHEW HARRIGAN, Google Inc., TYLER TAKESHITA, Daimler Research, RYAN BABBUSH, Google Inc. — Variational simulation of quantum chemistry is a likely first application for noisy intermediate scale quantum (NISQ) computers in the post supremacy age. We simulate a chemistry model that is significantly larger than previous implementations on any quantum computing platform. The model is optimized through a variational outer loop and a new iterative method using an approximate Hessian. Upon application of an error mitigation scheme based on pure-state n-representability conditions our experiments run on Google's Sycamore quantum processor achieve chemical accuracy. The model provides an efficiently verifiable circuit that has a large degree of entanglement and is a circuit primitive for broader fermionic simulation.
2:42PM D07.00002: Energy gap calculation on near-term quantum hardware with robust phase estimation* ANTONIO RUSSO (Presenter), ANDREW BACZEWSKI, BENJAMIN C MORRISON, KENNETH RUDINGER, Sandia National Laboratories — Can alternative approaches to phase estimation yield better results for chemical simulation on NISQ hardware? Robust phase estimation (RPE) calculates the difference in phases between two eigenstates of a unitary, provided oracular access to that unitary and the relevant eigenstates. In contrast to conventional phase estimation, it does not require a controlled-U and is naturally resistant to state preparation and measurement errors.

We evaluate the suitability of RPE on near-term hardware. In particular, we calculate the energy landscapes of H_2 and H_3 on extant quantum hardware (pre-compiling to emulate hardware with significantly higher fidelities). Resource requirements for larger molecules are considered.

*Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in this presentation do not necessarily represent the views of the DOE or the U.S. Government.

2:54PM D07.00003: Quantum simulation of molecular vibronic spectra on a superconducting bosonic processor: Part I* JACOB CURTIS (Presenter), CHRISTOPHER WANG, BRIAN LESTER, YAXING ZHANG, YVONNE GAO, JESSICA FREEZE, VICTOR BATISTA, PATRICK HENRY VACCARO, Yale University, ISAAC CHUANG, Massachusetts Institute of Technology, LUIGI FRUNZIO, LIANG JIANG, STEVEN GIRVIN, ROBERT SCHOELKOPF, Yale University — A promising and practical application of quantum machines is the simulation of quantum chemistry. Recent proposals have introduced problems naturally suited for bosonic platforms, such as the simulation of Franck-Condon factors [Huh et. al, Nature Photonics 9 (2015)]. These simulations require a wide range of Gaussian operations and non-Gaussian resources, such as arbitrary state preparation and photon-number measurement. Here, we present a blueprint for realizing these capabilities in a superconducting architecture consisting of long-lifetime cavity modes coupled to transmon ancillae. Driven four-wave mixing processes implement bilinear interactions such as single-mode squeezing and beamsplitters, which, when combined with resonant displacements, generate a complete set of Gaussian operations. Furthermore, we present a novel single-shot measurement scheme that extracts the binary decomposition of the photon number in each cavity mode.

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NSF Center for Ultracold Atoms (ILC)
Packard Foundation (LJ)
Quantum simulation of molecular vibronic spectra on a superconducting bosonic processor: Part II

CHRISTOPHER WANG (Presenter), JACOB CURTIS, BRIAN LESTER, YAXING ZHANG, YVONNE GAO, JESSICA FREEZE, VICTOR BATISTA, PATRICK HENRY VACCARO, Yale University, ISAAC CHUANG, Massachusetts Institute of Technology, LUIGI FRUNZIO, LIANG JIANG, STEVEN GIRVIN, ROBERT SCHOELKOPF, Yale University — A promising and practical application of quantum hardware is the simulation of quantum chemistry. As one example, a programmable bosonic machine can be configured to obtain Franck-Condon (FC) factors associated with molecular vibronic spectra [1]. Implementing such an algorithm in the linear optical domain is experimentally challenging due to the imperfect initialization and detection of optical photons. In this talk, we present a superconducting bosonic processor that combines high fidelity non-Gaussian state preparation, a complete set of Gaussian operations, and a novel single-shot photon number resolving measurement scheme. We utilize this processor to extract FC factors for photoelectron processes in H₂O, O₃, NO₂, and SO₂, including those from vibrational excited states. We exemplify the efficiency of this approach by comparing the resources needed to perform our simulation with that of a qubit-based architecture.


*US ARO Grants (W911NF-18-1-0212, W911NF-16-1-0349)
NSF Grants CHE-1900160 (VSB), CHE-1464957 (PHV), and DMR-1609326 (SMG)
NSF Center for Ultracold Atoms (ILC)
Packard Foundation (LJ)

Quantum computation of magnon spectra

AKHIL FRANCIS (Presenter), North Carolina State University, JAMES FREERICKS, Georgetown University, ALEXANDER F KEMPER, North Carolina State University — We demonstrate quantum computation of two-point correlation functions for a Heisenberg spin chain. Using the IBM Q 20 Tokyo machine, we find that for two sites the correlation functions produce the exact results reliably. For four sites, results from the quantum computer are noisy due to read out errors and decoherence. Nevertheless, the correlation functions retain the correct spectral information. This is illustrated in the frequency domain by accurately extracting the magnon energies from peaks in the spectral function.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Grant No. DE-SC0019469. J. K. F. was also supported by the McDevitt bequest at Georgetown University.
3:30PM D07.00006: Improving chemistry calculations with virtual quantum subspace expansion*  MIROSLAV URBANEK (Presenter), WIBE A DE JONG, Computational Research Division, Lawrence Berkeley National Laboratory — Accurate calculations in quantum chemistry require the use of large basis sets which amounts to a large number of molecular spin-orbitals. Each spin-orbital is typically mapped to a separate qubit. Many qubits are therefore necessary to achieve a desired accuracy. However, noisy intermediate-scale quantum computers have only a small number of qubits which limits the reach of quantum computing algorithms in quantum chemistry. A promising approach to overcome this problem is to use a quantum computer to solve only the classically hard part and a classical computer to solve the rest. A recently proposed virtual quantum subspace expansion (VQSE) method achieves this by modeling only the active space, that captures essential quantum effects, on a quantum computer. We report experimental results obtained using the VQSE algorithm to model small molecules. This work explores practical viability of hybrid quantum-classical methods in quantum computing.

*This work was supported by the Office of Advanced Scientific Computing Research, Quantum Algorithms Team Program, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

3:42PM D07.00007: Accuracy of the effective Hamiltonian in the quantum simulation experiments*  EVGENY MOZGUNOV (Presenter), Viterbi school of engineering, University of Southern California — Superconducting qubits and cold atom systems can simulate a variety of quantum Hamiltonians by implementing the couplings directly, as opposed to Trotterization of the quantum evolution and gate-based simulation. In this approach, the effective Hamiltonian is often calibrated experimentally to match the desired properties. We develop a rigorous mathematical foundation for the calibration of the building blocks to obtain a target effective Hamiltonian. The building blocks we consider are both superconducting circuits and cold atoms. For both approaches we provide an error estimate: the difference in the norm between the obtained effective Hamiltonian and the target. Our approach extends to time-dependent Hamiltonians via a version of adiabatic theorem.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.
3:54PM D07.00008: Hybrid quantum-classical simulations of correlated materials within Gutzwiller variational approach*  YONGXIN YAO (Presenter), Ames Laboratory and Department of Physics and Astronomy, Iowa State University, NOAH BERTHUSEN, Department of Electrical and Computer Engineering, Iowa State University, FENG ZHANG, CAI-ZHUANG WANG, KAI-MING HO, PETER ORTH, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — We develop a hybrid quantum-classical simulation framework that leverages existing noisy intermediate-scale quantum (NISQ) computing technology to study ground-state properties of correlated electron materials. It combines classical Gutzwiller variational embedding theory with state-of-the-art quantum computing algorithms to solve the effective multi-orbital embedding problem. The theory amounts to finding a self-consistent solution of coupled eigenvalue equations. The effective quasi-particle Hamiltonian is diagonalized efficiently using classical computers, while the ground state of the Gutzwiller embedding Hamiltonian is obtained using variational quantum eigensolvers implemented on quantum computing devices. This is feasible on NISQ devices and takes advantage of relatively shallow quantum circuits for error mitigation. The approach is applied to the periodic Anderson model and Hubbard models. Various variational ansatz and quantum noise forms will be compared on their numerical convergence and calculation accuracy.

*This work was supported by US DOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. The research was performed at Ames Laboratory, which is operated for US DOE by Iowa State University under contract # DE-AC02-07CH11358.

4:06PM D07.00009: Improvements in quantum algorithms for quantum chemistry and condensed matter*  THOMAS O'BRIEN (Presenter), Lorentz Institute — The simulation of many-body systems in condensed matter and chemistry is a challenging task in which quantum computers promise to be of some use. While initial quantum algorithms for such purposes had costly requirements for coherence times or numbers of state preparations needed, a flurry of work in recent years has significantly reduced these costs and found new methods, opening the question whether quantum computers can become of use for this class of problems in the NISQ era. In this talk, I will overview a number of recently developed algorithms and algorithmic improvements, and some experimental implementations thereof, including methods for state preparation, error mitigation, partial state tomography, and derivative estimation on a quantum device.

*This research was funded by the Netherlands Organization for Scientific Research (NWO/OCW) under the NanoFront and StartImpuls programs, and by Shell Global Solutions BV.
4:18PM D07.00010: Quantum Chemistry as an application-inspired Benchmark on near-term quantum computers*  RAPHAEL POOSER (Presenter), TITUS MORRIS, ALEXANDER MCCASKEY, JACEK JAKOWSKI, TRAVIS HUMBLE, SHIRLEY MOORE, Oak Ridge National Lab — Near term quantum computing applications can inspire benchmarks and can serve as predictors for future machine performance as the hardware improves. We will present results from application-inspired benchmarks, including Quantum Chemistry. The quantum chemistry benchmark for noisy intermediate-scale quantum computers leverages the variational quantum eigensolver, active space reduction, a modified unitary coupled cluster ansatz, and reduced density purification as error mitigation. We demonstrate this benchmark on the 20 qubit IBM Tokyo and 16 qubit Rigetti Aspen processors via the simulation of alkali metal hydrides (NaH, KH, RbH), with accuracy of the ground state energy as the primary benchmark metric. We also show how to reduce the noise in post processing with specific error mitigation techniques. The adaptation of McWeeny purification of noisy density matrices dramatically improves accuracy of quantum computations, which, along with adjustable active space, significantly extends the range of accessible molecular systems. We demonstrate that for specific benchmark settings, the accuracy metric can reach chemical accuracy when computing over the cloud on certain quantum computers.

*This work was supported by the Quantum Testbed Pathfinder program under FWP ERKJ332.

4:30PM D07.00011: Quantum simulation of the dynamics of the Fermi-Hubbard model on Sycamore  ZHANG JIANG (Presenter), Google Inc - Santa Barbara — Studying strongly correlated systems is among the many applications of a quantum computer. Here, we report such an experiment on the dynamics of the Fermi-Hubbard model using Google’s Sycamore quantum chip. I will discuss the physics that we learned from the experiment as well as the compilation and error mitigation tools that make the experiment possible. I will also walk you through the tutorial that we develop for the Fermi-Hubbard experiment.
Experimental realization of a nonlinear 3-wave mixing gate for quantum simulation*  
ALESSANDRO CASTELLI (Presenter), YUAN SHI, ILON JOSEPH, VASILY GEYKO, FRANK R GRAZIANI, STEPHEN BERNARD LIBBY, JEFFREY PARKER, YANIV J. ROSEN, JONATHAN L. DUBOIS, Lawrence Livermore Natl Lab — The ability to simulate an arbitrary Hamiltonian on a quantum device is an important step towards achieving universal quantum computing. We present a simulation of nonlinear 3-wave processes on a single qudit of the LLNL Quantum Design and Integration Testbed (QuDIT) resulting from iterative application of a gate developed to emulate these interactions. We describe our experimental protocol for realizing this simulation on the first three levels of a qudit and present results of average state population as a function of time. This experiment consists of a transmon-style qudit that is capacitively coupled to a superconducting 3D microwave cavity field. The qudit is addressed by a single-input RF signal that has been numerically optimized to perform 3-wave mixing unitary gate operations with fidelity of over 99%. We find that the average population of the qudit states evolve in a manner that matches the theoretically predicted quantum numbers of each wave in the 3-wave mixing process over many gate iterations.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported in part by the Laboratory Directed Research and Development grant 19-FS-072.

Matrix product state simulations on a quantum computer  
MICHAEL FEIG (Presenter), HQS, Honeywell, ANDREW POTTER, University of Texas, Austin — Matrix product states (MPS) afford a compressed representation of many states that are relevant to physical systems. While many classical algorithms have been developed to compute the properties of physical systems using MPS as an ansatz, in many cases of practical interest these algorithms still require exponential resources (for example in the size of the system, or in the evolution time when out of equilibrium). We discuss near-term prospects for using small and non-error-corrected quantum computers to aid in MPS simulations.
5:06PM D07.00014: Quantum simulation of nonlinear three-wave interactions with engineered cubic couplings*  YUAN SHI (Presenter), ALESSANDRO ROBERTO CASTELLI, ILON JOSEPH, VASILY GEYKO, FRANK R GRAZIANI, STEPHEN BERNARD LIBBY, JEFFREY PARKER, YANIV J ROSEN, JONATHAN L DUBOIS, Lawrence Livermore National Laboratory — Quantum three-wave gates are building blocks for simulating lattice gauge theory, nonlinear optics, weak turbulence, and laser plasma interactions. Although the underlying cubic couplings are usually absent in the quantum hardware, we show that effective three-wave vertices can be generated using control pulse engineering. In particular, for a three-wave Hamiltonian whose conserved actions are positive, we show that its Hilbert space can be decomposed into a direct sum of $D$-dimensional subspaces. Within each subspace, the quantum states are readily mapped onto the memory of quantum computers, and the Hamiltonian matrix becomes tridiagonal. Such a Hamiltonian is realized on the LLNL Quantum Design and Integration Testbed (QuDIT), utilizing three levels of a qudit. The qudit is controlled by digitally synthesized microwave pulses, whose wave forms are optimized numerically. Less accurate but cheaper control pulses may also be generated by interpolation, when parameters of the Hamiltonian vary. The resultant three-wave gates are applied to simulate the temporal three-wave problem, and physically meaningful results are obtained despite noise in the quantum computer.

*This work was supported by DE-AC52-07NA27344, DOE FES AT1030200-WA-OP SCW-1680, LLNL-LDRD 19-FS-072 and 19-ERD-038.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D08 DQI: Quantum Control and Quantum Gates 104 - Gregory Quiroz, Johns Hopkins University

2:30PM D08.00001: Simulated Randomized Benchmarking of Dynamically Corrected Cross-Resonance Gate*  RALPH KENNETH COLMENAR (Presenter), JASON PAUL KESTNER, Univ of Maryland-Baltimore County — We theoretically simulate a cross-resonance (CR) gate implemented by pulse sequences proposed in Phys.Rev. Lett. 118, 150502 (2017). These sequences allow mitigation of systematic noise to first order, but their effectiveness is limited by one-qubit gate imperfections. To improve the feasibility of such sequences, we make use of the fact that arbitrary Z rotations can be implemented virtually and with negligible error. We illustrate this by simulating randomized benchmarking for a system of coupled transmons and show that it is possible, under certain conditions, to improve the CR gate fidelity in the presence of quasistatic noise.

*This work was supported by the National Science Foundation under Grant No. 1620740
2:42PM D08.00002: Experimental protection of qubit coherence up to relaxation times by using an image drive* SYLVAIN BERTAINA, Inst Mat Microelectronique et Nanosciences de Provence, UMR7334, CNRS, Aix-Marseille Universite, Marseille, France, HERVE VEZIN, Laboratoire de Spectrochimie Infrarouge et Raman, UMR8516, CNRS, Universite de Lille, Villeneuve d’Ascq, France, IRINEL CHIORESCU (Presenter), Dept of Physics and The National High Magnetic Field Laboratory, Florida State Univ — The protection of spin coherence is an essential task in order to manipulate, store and read quantum information. It has been proposed to dynamically decouple (DD) qubits from their surroundings by applying a series of distinct pulses\(^1\). For nitrogen vacancy centers, such protection was achieved by using concatenated DD up to the second order of dressing\(^2,3\). We go beyond their specific case and demonstrate a new pulse protocol in a number of materials with different spin Hamiltonians and environments. We demonstrate the regime T2~T1 for temperatures ~40K. The protocol uses two coherent microwave pulses: one drives the Rabi precession while a low-power, circularly polarized (image) pulse continuously sustains the spin motion. The initial phase of the image drive allows tuning the spin dynamics by altering the Floquet modes. The technical implementation is simple and can be generalized to any type of qubit, such as superconducting circuits or spin systems.


*Work supported by the CNRS infrastructure RENARD (award IR-RPE CNRS 3443). Partial support by the NSF Cooperative Agreement No. DMR-1644779 and the State of Florida is acknowledged.

2:54PM D08.00003: Complete quantum-state tomography with a local random field CHRISTIAN ARENZ (Presenter), Princeton University, RALF BETZHOLZ, JIANMING CAI, Huazhong University of Science and Technology — Single-qubit measurements are typically insufficient for inferring arbitrary quantum states of a multi-qubit system. We show that if the system can be fully controlled by driving a single qubit, then utilizing a local random pulse is almost always sufficient for complete quantum-state tomography. Experimental demonstrations of this principle are presented using a nitrogen-vacancy (NV) center in diamond coupled to a nuclear spin, which is not directly accessible. We report the reconstruction of a highly entangled state between the electron and nuclear spin with fidelity above 95%, by randomly driving and measuring the NV-center electron spin only.
3:06PM D08.00004: High sensitivity spectral characterization of local microwave fields using two-photon absorption processes of a transmon qudit*  

SPENCER TOMARKEN (Presenter), JONATHAN L DUBOIS, Lawrence Livermore Natl Lab — Optimal control methods for quantum information processing require precise knowledge of the local microwave amplitudes generated by control pulses arriving at the cryogenic stage of the quantum processor. We present a scheme for characterizing the spectral transfer function of a superconducting transmon qudit capacitively coupled to a 3D cavity resonator. We apply two simultaneous drive tones close to the transmon's 0-1 and 1-2 state transition frequencies while varying both the duration of the pulses as well as their relative detuning. Through measurement of the 0-, 1-, and 2-state occupations, we map out the 0 to 2 state two-photon absorption process. The relative occupation of the three lowest transmon levels provides a sensitive probe of the local microwave field over a large range of detuning. By comparing our measurement results to master equation simulations incorporating a spectral filter, we recover the amplitude-corrected transfer function over an approximately 200 MHz bandwidth.

*This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was partially supported by LDRD grant 19-ERD-013, ASC Beyond Moore's Law quantum effort, and DOE ASCR quantum testbed pathfinder program.

3:18PM D08.00005: Implementation of the XY interaction family by calibration of a single pulse*  

DEANNA ABRAMS (Presenter), NICOLAS DIDIER, BLAKE JOHNSON, MARCUS P DA SILVA, COLM RYAN, Rigetti Quantum Computing — Near-term applications of quantum information processors will rely on optimized circuit implementations to minimize gate depth and therefore mitigate the impact of errors in noisy intermediate-scale quantum (NISQ) computers. More expressive gate sets can significantly reduce the gate depth of generic circuits. Similarly, structured algorithms can benefit from a gate set that more directly matches the symmetries of the problem. The XY interaction generates a family of gates that provides expressiveness well tailored to quantum chemistry as well as to combinatorial optimization problems; while also offering reductions in circuit depth for more generic circuits. Here we implement the full family of XY entangling gates in a transmon-based superconducting qubit architecture using a composite pulse scheme that requires calibration of only a single gate and maintains constant gate time for all members of the family. This allows us to maintain a high fidelity implementation of the gate across all entangling angles. The average fidelity of gates sampled from this family ranges from 95.67 ± 0.60% to 99.01 ± 0.15%, with a median fidelity of 97.35 ± 0.17%, which approaches the coherence-limited gate fidelity of the qubit pair.

*This work was funded by Rigetti & Co Inc., dba Rigetti Computing.
3:30PM D08.00006: Selective number-dependent arbitrary Hamiltonian engineering for a cavity CHIAO-HSUAN WANG (Presenter), University of Chicago, JOSÉ LEBREUILLY, KYUNGJOO NOH, STEVEN GIRVIN, Yale University, LIANG JIANG, University of Chicago — Cavity resonators are promising resources for storing and processing quantum information. Here we investigate a scheme to engineer the Hamiltonian for a photonic cavity using an ancilla qubit. In the strong dispersive coupling limit and number-split regime, one can drive the qubit near selective photon-number-dependent transition frequencies to address the individual photon number states of the cavity. By choosing control driving detunings much larger than the driving strengths, we propose a general approach to engineering a selective number-dependent arbitrary Hamiltonian for the cavity. The engineered Hamiltonian admits various applications including canceling unwanted cavity Kerr effect, creating higher-order nonlinearities for quantum simulations, designing quantum gate operations resilient to noise, and even realizing quantum error correction. Our scheme can be implemented with a coupled microwave cavity and transmon qubit in superconducting circuits systems.

3:42PM D08.00007: Implementing robust Holonomic quantum gates using dynamical invariant YINGCHENG LI (Presenter), YIDUN WAN, Fudan Univ — Holonomic quantum computing operates quantum systems using berry's phase, or more generally, Aharanov-Anandan phase. It is proved that quantum gates implemented by using these geometric phases are more robust against certain errors. While Holonomic gates have been realized in many systems, extra degrees of freedom are usually required. In this work, we propose a general dynamical invariant for 1 qubit and 2 qubit that is restricted in logical space that enables holonomic quantum computing without inverse engineering. In particular, a Holonomic CNOT gate can be implemented with extremely high fidelity. Moreover, an investigation in the aspect of geometry shows the Hamiltonians used to control the system all have monopole-type gauge field in parameter space, which provides a hidden mathematical structure that contributes to extra robustness.

3:54PM D08.00008: Superconducting cavity QED: box modes for quantum control of qubits RAINA OLSEN (Presenter), MOHAMMADREZA REZAEE, Aurora Quantum Technologies, ELIAHU COHEN, Bar-Ilan University, EBRAHIM KARIMI, University of Ottawa — Circuit QED uses two types of superconducting cavities: one-dimensional superconducting resonators that contain charge excitations, and two or three-dimensional regions of space between superconducting mirrors that contain photons. This latter type of cavity does not necessarily need to be enclosed. Any superconducting circuit acts as a cavity for the surrounding photonic modes with wavelengths on the order of the circuit geometry. Normally these are referred to as box modes, and treated primarily as a source of dissipation (except when a box mode frequency happens to be close to qubit frequencies). However, quantum transduction methods show that a system can be designed so that energy flows between modes at very different frequencies. We treat the problem of a superconducting qubit in a THz cavity by quantizing Maxwell's equations, showing that the driven system is described by the linearized Hamiltonian of cavity optomechanical systems used for quantum transduction.
4:06PM D08.00009: Adiabatic Quantum Control of Dissipative State Preparation  EMERY DOUCET (Presenter), TRISTAN BROWN, ARCHANA KAMAL, Univ of Mass - Lowell — Dissipative protocols for state preparation provide the ability to produce complex entangled states which are inherently robust to decoherence. Protocols based on parametric interactions are particularly powerful in this regard, with the potential for much superior performance compared to resonant schemes while simultaneously providing a large degree of flexibility and control over the stabilized state [1]. In this talk I will describe a scheme for preparing Bell states which employs only parametric qubit-qubit and qubit-resonator couplings. Both the amplitudes and phases of these couplings are tunable in situ, providing a natural avenue to implement time-dependent control of the state preparation dynamics. I will present numerical and analytical results on the application of time-dependent parametric controls while ensuring that the evolution is adiabatic, such that the system remains in the instantaneous dark state of the dynamics. Such fast time-dependent control is within reach of current experimental capabilities, and can enable a large (>10x) reduction in state preparation times. [1] E. Doucet, F. Reiter, L. Ranzani, and A. Kamal, arXiv:1810.03631 (2018).

4:18PM D08.00010: Investigating the speed limit of two-qubit entangling gates with superconducting qubits*  JOEL HOWARD (Presenter), Colorado School of Mines, JUNLING LONG, Physics, CU Boulder, MUSTAFA BAL, RUICHEN ZHAO, National Institute of Standards and Technology - Boulder, TONGYU ZHAO, Physics, CU Boulder, DAVID PAPPAS, National Institute of Standards and Technology - Boulder, ZHEXUAN GONG, MEENAKSHI SINGH, Colorado School of Mines — Fast two-qubit entangling gates are essential for quantum computers with finite coherence times. Due to the limit of interaction strength among qubits, there exists a theoretical speed limit for a given two-qubit entangling gate. This speed limit has been explicitly found only for a two-qubit system and under the assumption of negligible single qubit gate time. We demonstrate such speed limit experimentally using two superconducting transmon qubits with an always-on capacitive coupling. Moreover, we investigate a modified speed limit when single qubit gate time is not negligible, as in any practical experimental setup. Finally, we discuss the generalization to multiple qubit systems where the coupling to additional qubits can significantly increase the speed limit of a two-qubit entangling gate, thus requiring the co-design of the quantum computer from both theorists and experimentalists for optimal gate performance.

*NSF Grant: 1839232

4:30PM D08.00011: High fidelity quantum gates for NV center defect registers based on dynamical decoupling sequences  WENZHENG DONG (Presenter), FERNANDO A CALDERON, SOPHIA ECONOMOU, Virginia Tech — The spinful nuclei surrounding a defect such as the NV center in diamond are promising qubits for a modest-size quantum register. Recent experimental advances demonstrated control of the nuclear spins through microwave manipulation of the NV spin via dynamical decoupling ‘CPMG’ sequences. Here we show that more complex dynamical decoupling sequences improve the nuclear spin operations, i.e., gate fidelity, applicability range, and nuclear spin selectivity. We numerically show the efficacy of our method on NV centers in diamond, but our results are general and applicable to other types of defects in solids.
4:42PM D08.00012: Time-optimal robust controls for Molmer-Sorensen gates in large ion chains
ANDRE CARVALHO (Presenter), CLAIRE EDMUNDS, HARRISON BALL, MICHAEL HUSH, MICHAEL BIERCUK, Q-CTRL — Performing high fidelity entangling operations in multi-qubit systems is an essential requirement for the scalability of quantum information processing. In trapped-ion architectures, these gates are achieved through external driving fields that excite shared oscillator modes: Molmer-Sorensen (MS) gates are a widely used example. In this talk, we present numerically optimized modulation protocols which enable the realization of pairwise MS interactions in long ion chains. We demonstrate how these protocols achieve efficient decoupling of the motional modes employed to effect the entangling operation and provide robustness against fluctuations in experimental parameters. We then demonstrate a routine for time-optimization of the gates on chains of up to 10 ions. The novel gates are not only more robust and faster than standard MS gates, but also more flexible in the choice of experimental parameters.

4:54PM D08.00013: Probing the quantum nature of electronic transport by sub-nanosecond time-resolved measurements
JEAN OLIVIER SIMONEAU (Presenter), CHRISTIAN LUPIEN, BERTRAND M REULET, Universite de Sherbrooke — Mesoscopic microwave measurements are usually carried out in the frequency domain. However, for some experiments involving large bandwidths (including frequency-resolved measurements) or short timescales (e.g. subcycle waveforms), the time domain can be a more suitable or convenient measurement framework.[1] In this talk, we present ultrafast time-domain measurements of the noise emitted by a tunnel junction under DC and AC excitation. The measurements are done at 32 GSa/s with an analog bandwidth of $\Delta f = 10$ GHz. We show that, at fixed time lag, the excess noise is an oscillating function of the bias voltage. It is thus possible to control noise correlations through the bias voltage. We also present recent advances in phase-resolved probing of the photoassisted noise.


*We acknowledge technical help of G. Laliberté. This work was supported by the Canada Excellence Research Chair program, the NSERC, the CFREF, the MDEIE, the FRQMT via the INTRIQ, the Université de Sherbrooke via the EPIQ and the Canada Foundation for Innovation
5:06PM D08.00014: Optimizing pulses with geometric parameters for dynamically-corrected single qubit gate  
XIUHAO DENG (Presenter), Shenzhen Institute of Quantum Science and Engineering, Southern University of Science and Technology — We used geometric parametrization to solve for the constraints of the control pulses to implement dynamically-corrected single qubit gate for superconducting qubits. We considered errors due to: I) crosstalk with other qubits; II) strong coupling to TLS defect; III) coupling to low frequency noisy background, and so on. The errors to be corrected are modeled in perturbative and non-perturbative regime respectively, resulting in different geometric parameters. The pulses obtained using geometric parametrization could corrected the errors and, furthermore, could be optimized in such parameter space with the number of parameters much less than discrete temporal parameter space associated with traditional quantum optimal control numerical approach such as GRAPE. Hence, our optimization approach performs much faster. We compare our optimized pulses with those generated with GRAPE, differential evolution, and other numerical approaches.

5:18PM D08.00015: Robust and optimal control for SC qubits, two-qubit gates, and circuits  
HARRISON BALL (Presenter), PER LIEBERMANN, ANDRÉ CARVALHO, HARRY SLATYER, VICKTOR PERUNICIC, RAJIB CHAKRAVORTY, MICHAEL HUSH, MICHAEL BIERCUK, Q-CTRL — Superconducting quantum computers manifest distinct error processes at different levels of system complexity: from leakage or dephasing in individual transmon qubits to errors in two-qubit gates arising from dephasing, imperfect control signals, and unwanted cross-couplings. Quantum control at the physical-layer provides a pathway to combating these errors in today's quantum hardware. In this talk we describe error modelling of dominant error channels in superconducting circuits relevant for parametrically-activated or cross-resonance gates. Advancing on previous work, we present optimal and robust controls that reduce sensitivity to both leakage and dephasing errors by orders of magnitude, as well as other optimized controls to reduce hardware errors at higher levels of system complexity.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D09 DQI: Quantum Thermodynamics 106 - Ruichao Ma, Purdue University -  
Tag(s): Focus
2:30PM D09.00001: Analyzing the efficacy and work extraction of a quantum Maxwell's demon*  
XINGRUI SONG (Presenter), Department of Physics, Washington University, St. Louis, MAHDI NAGHILOO, Electrical Engineering & Computer Science, Massachusetts Institute of Technology, KATER MURCH, Department of Physics, Washington University, St. Louis — In a quantum Maxwell's demon experiment, two major quantities are commonly investigated - the average work extraction \( \langle W \rangle \), and the efficacy \( \gamma \) which measures the violation of Jarzynski's equality when extracted information and feedback is not accounted for. Here, we carefully analyze the relation between these two quantities, and find that they are not maximized simultaneously, requiring different feedback protocols. Furthermore, we investigate Maxwell's demon protocols for higher dimensional Hilbert spaces finding even stronger violations of Jarzynski's equality. Our study further reveals the thermodynamic implications of the exponentially large state space available in quantum systems.

*This work was supported by the NSF grant No. PHY-1752844 (CAREER)

2:42PM D09.00002: Simulating a quantum heat engine on transmon qubits*  
NICHOLAS MATERISE (Presenter), ELIOT KAPIT, Colorado Sch of Mines — We devise a scheme to simulate a quantum heat engine using an array of flux-tunable transmon qubits. This device provides a one-to-one mapping to a fixed nearest-neighbor coupled, disordered Bose-Hubbard model, with precision control over transitions between the many body localized (MBL) phase and the thermal or superfluid phase [Nature 566, 51 (2019)]. Our approach expands on a previous MBL engine proposal [Phys.Rev.B 99, 024203 (2019)], where the adiabatic strokes involve transitions between the two nondegenerate ground states and first excited states of the MBL and thermal phases. We expect that this choice of energy levels reduces the likelihood of excursions to higher levels, especially in the case of the ground states, serving as a prototype for future investigations into studies of MBL as a thermodynamic resource.

*We acknowledge funding support from the National Physical Sciences Consortium graduate fellowship and NSF grant (PHY-1653820)
2:54PM D09.00003: Macroscopic Thermodynamic Reversibility in Quantum Many-Body Systems* PHILIPPE FAIST (Presenter), Freie Univ Berlin, TAKAHIRO SAGAWA, University of Tokyo, KOHTARO KATO, Caltech, HIROSHI NAGAOKA, University of Electro-Communications, Tokyo, FERNANDO BRANDÃO, Caltech — The resource theory of thermal operations, an established model for small-scale thermodynamics, provides an extension of equilibrium thermodynamics to nonequilibrium situations. On a translation-invariant lattice with local interactions, we show that ergodic states (i.e. states that have sharp statistics for any translation-invariant observable) can be reversibly converted to and from the thermal state with thermal operations and a small amount of coherence. This proves the emergence of an operationally well-justified thermodynamic potential for this class of states, which includes states that are not in equilibrium. As an intermediate result of independent interest, we show that the gap between the min- and max-relative entropies controls the amount of coherence that is present in the state and that if this gap is small, the state can be approximately reversibly converted to and from the thermal state with a small reference frame. Our results provide a strong link between the abstract resource theory of thermodynamics and more realistic physical systems that go beyond the i.i.d. setting.

*The authors are supported by JSPS KAKENHI, NSF, DOE, and SNSF.

3:06PM D09.00004: What is Quantum Thermodynamics? [Invited] SEBASTIAN DEFFNER (Presenter), Univ of Maryland-Baltimore County — We are the verge of a technological revolution. Over the last couple of years the first computational devices have become commercially available that promise to exploit so-called quantum supremacy. Even though the thermodynamic cost for processing classical information has been known since the 1960s, the thermodynamic description of quantum computers is still at its infancy. This is due to the fact that many notions of classical thermodynamics, such as work and heat, do not readily generalize to quantum systems. In this talk, we will outline a novel conceptual framework of an emerging theory, Quantum Thermodynamics, and illustrate its applicability, mindset, and questions with a few pedagogical examples.
3:42PM D09.00005: Entanglement transport and thermalization in an isolated quantum spin chain

SHUNJI TSUCHIYA (Presenter), RYOSUKE YOSHII, Department of Physics, Chuo Univ —
Entanglement transport is considered to be essential for understanding thermalization in an isolated quantum system. In this work, we study transport of entanglement entropy (EE) in the Ising model with the next-nearest-neighbor interaction as well as the transverse and longitudinal magnetic fields. We calculate EE in a spin chain which consists of a single spin at the edge (A) and the bulk part (B). We compare time-evolution of EE for two different initial settings: the one with entanglement between A and B and the other one without it. The propagation speed of EE can be estimated by the time at which the EEs starting from the two initial conditions show deviation. We find that EE propagates ballistically with a constant velocity and that the propagation speed is enhanced when thermalization occurs. We also calculate the propagation speed of EE from mutual information between A and a subsystem in B. The velocities calculated by the two different methods agree well. We will discuss the relation between propagation of EE and thermalization.

*S. T. was supported by Chuo University Grant for Special Research. This work was supported by KAKENHI Grant No. JP19K14616 and No. JP19K03691.

3:54PM D09.00006: Characterizing complexity of many-body quantum dynamics by higher-order eigenstate thermalization

KAZUYA KANEKO (Presenter), Univ of Tokyo, EIKI IYODA, Physics, Tokai University, TAKAHIRO SAGAWA, Univ of Tokyo — Characterizing quantum many-body chaos has attracted renewed attention in condensed matter physics, quantum information, and high-energy physics. There are two fundamental concepts regarding this problem. One is the eigenstate thermalization hypothesis (ETH) stating that individual energy eigenstates are thermal. The other is information scrambling, which is quantified by out-of-time-ordered correlators (OTOCs). We propose a higher-order generalization of the ETH, named by the $k$-ETH ($k=1, 2,...$), which provides a unified view on the above two concepts. The lowest order ETH (1-ETH) is the conventional ETH, and the second order ETH (2-ETH) is a sufficient condition of the decay of OTOCs at late times. Our basic idea is that chaotic dynamics share common properties with random unitary dynamics even at a higher level than conventional ergodicity. The $k$-ETH also implies a universal behavior of the $k$th-Renyi entanglement entropy of individual energy eigenstates. In particular, we show that the Page correction originates from the higher-order ETH. We numerically verified that the 2-ETH approximately holds for nonintegrable systems, but does not hold for integrable systems.

*This work is supported by JSPS KAKENHI Grant No. JP17J06875, No. JP16H02211, No. JP15K20944, and No. JP19H05796.
4:06PM D09.00007: Collective phenomena in quantum thermodynamics: from mitigation to amplification of the baths' action* CAMILLE LOMBARD LATUNE, ILYA SINAYSKIY, FRANCESCO PETRUCCIONE (Presenter), Univ of KwaZulu-Natal — An increasing number of papers in quantum thermodynamic have shown that collective effects can be beneficial for thermodynamic tasks. In order to understand better why and when such enhancements can happen, we analyse in details the energetic, entropic, and more generally thermodynamic consequences of collective coupling between an ensemble of identical systems (spin or atoms) and their bath.

We reach the conclusion [1] that collective coupling, through the coherences it intrinsically generates, effectively shield the ensemble from the bath's action, affecting dramatically the thermodynamic characteristic of the ensemble (energy, entropy, and free energy). Strikingly, in presence of two thermal baths, the combination of these mitigation effects can result in a great amplification of the baths' action. This is illustrated through a cyclic (Otto) thermal machine, resulting in a large output power enhancement. We also highlight that such enhancements are not systematic: depending on the value of the bath temperatures, the number of spins, and their dimension, either enhancement or degradation of performances can happen.


*South African Research Chair Initiative, National Research Foundation and NITheP.

4:18PM D09.00008: Thermalization of a qubit strongly interacting with a bosonic environment PATRICK ORMAN (Presenter), DEXTER GRANT MITCHELL, RYOICHI KAWAI, Physics, Univ of Alabama - Birmingham — When a quantum system is placed in a thermal environment, we assume that the system relaxes to the Gibbs state in which decoherence takes place in the system energy eigenbasis. However, when the coupling between system and environment is strong, the thermal state is not necessarily the Gibbs state, and the system density matrix does not have to be diagonal in the energy eigenbasis. The theory of einselection by Zurek suggests that decoherence takes place in the pointer basis rather than in the energy eigenbasis, which can be interpreted as continuous measurement by the environment. However, the actual matrix elements are not known. Based on the theory of environment-induced decoherence, we introduce a couple of propositions: (1) in the strong coupling limit, the Gibbs state is projected to the convex hull spanned by the pointer basis, which necessarily increases the system entropy, and (2) the transition from the Gibbs state to the pointer limit takes place along the projection line perpendicular to the convex hull. We justify these propositions by exact numerical simulation of a qubit interacting with an infinitely large bosonic environment through various coupling Hamiltonians.
Kinetics of many-body reservoir engineering

HUGO RIBEIRO (Presenter), FLORIAN MARQUARDT, Max Planck Inst for Sci Light — Quantum simulators based on superconducting circuits can be used to study many-body physics with microwave photons. In particular, lattice systems can be used to study the thermalization of an engineered condensed matter system to a cold reservoir. However, in stark contrast to naturally occurring condensed matter systems, most engineered quantum lattice systems do not have a well-defined chemical potential. Here, we show that it is possible to cool a reservoir engineered many-body system with a well-defined chemical potential if the coupling with the reservoir is a density-density type coupling. Specifically, we consider an array of single-mode microwave cavities with each site of the array coupled to a driven, lossy cavity. The lossy cavities will act as an engineered non-equilibrium bath that mediates transitions between the eigenstates of the array while simultaneously conserving the number of excitations. We show that the steady state of the system can be described via a modified Bose-Einstein distribution with a momentum-dependent temperature.

Topological effects in quantum thermodynamics

CHARLES STAFFORD (Presenter), Physics, University of Arizona, YIHENG XU, Physics, UC San Diego, FERDINAND EVERS, Physics, University of Regensburg — The thermodynamics of open quantum systems coupled to topological fields is analyzed. Both the Aharonov-Bohm effect for systems of charged particles and the Aharonov-Casher effect for systems of neutral spin-1/2 particles are considered, and a general definition for the flux of a physical observable is proposed. A proper treatment of the work done by the topological fields is necessary to ensure that the entropy of the system is a state function, and to avoid certain thermodynamic paradoxes. In particular, the flux of entropy in the system induced by the topological fields naively appears to diverge as the temperature approaches absolute zero, in violation of the 3rd law of thermodynamics.

This work was supported by the U.S. Department of Energy (DOE), Office of Science, under Award No. DE-SC0006699. F. Evers acknowledges support by the German Science Foundation.

Fluctuations in stored work bound the charging power of quantum batteries

LUIS GARCIA-PINTOS (Presenter), University of Maryland, College Park, ALIOSCIA HAMMA, ADOLFO DEL CAMPO, University of Massachusetts Boston — We investigate the connection between the charging power of a quantum battery and the fluctuations of the work stored in it. We show that in order to have a non-zero rate of change of the extractable work, the work fluctuations must be non-zero. This is presented in terms of an uncertainty relationship that bounds the speed of the charging process of any quantum system. Our findings also identify quantum coherence in the battery as a resource in the charging process, which we illustrate on a toy model of a heat engine.
Thermodynamics features of quantum memristors* LUCAS CÉLERI (Presenter), Universidade Federal de Goias, MIKEL SANZ, ENRIQUE SOLANO, University of Basque Country, GABRIEL LANDI, University of São Paulo — Quantum memristors are devices holding great promise as a platform for quantum computation, especially when considering neuromorphic quantum computation. These devices are characterized by their non-Markovian behaviour. Here we describe such devices as a kind of thermodynamic engine operated by a Maxwell demon, but, instead of work, the output of such engine is non-Markovianity (time correlations), that can be employed to power quantum computation, for instance. We are therefore able to provide a thermodynamic description of this device, thus paving the way for establishing the limits of its applicability for information processing.

*The funding agency CNPq, FAPEG, CAPES (Finance Code001) and support from Spanish MCIU/AEI/FEDER(PGC2018-095113-B-I00), Basque Government IT986-16, the projects QMiCS (820505) and OpenSuperQ (820363) of the EU Flagship on Quantum Technologies and the EU FET Open Grant Quromorphic and the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR) quantum algorithm teams program, under field work proposal number ERKJ333.

Heat Transfer in Mesoscopic Systems GABRIEL WEIDERPASS (Presenter), State University of Campinas, GUSTAVO MONTEIRO, The City College of New York, AMIR O. CALDEIRA, State University of Campinas — In this talk, we present an analytical solution for the heat flux along a harmonic chain connecting two identical reservoirs at different temperatures, in the stationary regime. In this model, the end points correspond to Brownian particles with different damping coefficients. This analytical expression for the heat conductance in mesoscopic chains allows for direct comparison with experiments and shed some light on the validity of the Fourier law in one-dimensional quantum systems.

Monday, March 2, 2020 2:30 PM - 4:54 PM

Session D10 GIMS: Scattering and Diffraction 108 - Zahir Islam, Argonne National Lab
2:30PM D10.00001: Developing Wide Angle Spherical Neutron Polarimetry at Oak Ridge National Laboratory

Nicolas Silva (Presenter), Oak Ridge Assoc Univ, Chenyang Jiang, Tianhao Wang, Oak Ridge National Laboratory, Jillian Ruff, Oak Ridge Assoc Univ, Masaaki Matsuda, Fankang Li, Barry Winn, Lisa Debeer-Schmitt, Oak Ridge National Laboratory, Roger Pynn, University of Indiana — Spherical Neutron Polarimetry (SNP) analyzes complex magnetic structures through distinguishing contributions from nuclear-magnetic interference and chiral structure in addition to nuclear magnetic scattering separation. This analysis is achieved through determining all components in the polarization transfer process. Wide-angle SNP is being realized at Oak Ridge National Laboratory (ORNL) for multiple beamlines including: the polarized triple-axis spectrometer (HB-1) and general-purpose small angle neutron scattering instrument (CG-2) at the High Flux Isotope Reactor (HFIR), as well as the hybrid spectrometer (HYSPEC) at the Spallation Neutron Source (SNS). The SNP device consists of three units: incoming/outgoing neutron polarization regions, sample environment and a zero-field chamber. The neutron polarization regions use high- superconducting YBCO films, magnetic guide fields, and mu-metal to achieve full control of neutron polarization. The sample environment is an orange cryostat with a customized tail piece placed into the zero-field chamber. The device has been fabricated and demonstration experiments were run at the University of Missouri Research Reactor (MURR) and at HYSPEC.

2:42PM D10.00002: Kilohertz-Rate MeV Ultrafast Electron Diffraction for Time-resolved Materials Studies

Khalid M Siddiqui (Presenter), Materials Sciences Division, Lawrence Berkeley National Laboratory, Daniel B Durham, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Fuhao Ji, Accelerator Technology and Applied Physics Division, Lawrence Berkeley National Laboratory, Andrew M Minor, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Robert A Kaindl, Materials Sciences Division, Lawrence Berkeley National Laboratory, Daniele Filippetto, Accelerator Technology and Applied Physics Division, Lawrence Berkeley National Laboratory — Ultrafast electron diffraction (UED) enables direct insight into structural dynamics of solids. Relativistic MeV-scale electron beams yield access to high-momentum scattering and preserve beam coherence, yet their application at high repetition rates for high-sensitivity UED has been limited. We discuss the High Repetition-rate Electron Scattering (HiRES) instrument at Berkeley Lab and its first applications to UED of metallic films and quantum materials. HiRES employs a state-of-the-art photoinjector with RF bunch compression to generate high-brightness, relativistic 0.75 MeV electron pulses with up to $10^5$-$10^6$ el./pulse and with highest achievable coherence length of 10 nm. The resulting high momentum range ($\pm 10$ Å$^{-1}$) yields access over multiple Brillouin zones. The sub-500 fs electron pulses are provided at 0.1-250 kHz repetition rate, and combined with optical pumping via a 1.03 µm fiber amplifier enable UED of cryogenically cooled materials. We will show examples of first experiments including transient Debye-Waller dynamics in ultrathin metals at kHz repetition rate as well as studies of charge density waves in 2D materials.

*Work at LBNL was supported by the DOE Office of Basic Energy Sciences.
2:54PM D10.00003: Directive steerable emission from an opened chaotic cavity controlled through a reconfigurable metasurface*  
SAMUEL METAIS (Presenter), JEAN-BAPTISTE GROS, Institut Langevin, GEOFFROY LEROSEY, Greenerwave — Chaotic reverberating cavities have been demonstrated to have a large number of exploitable degrees of freedom[1] that can be controlled with a reconfigurable metasurface [2]. Following previous work on the emission of opened electromagnetic cavity in the GHz regime[3], we demonstrate here that a reconfigurable metasurface in a small volume cavity, 4*6*0.5 λ^3, allows us to control the emission through a large opening (3.5*5.5λ^2). Measuring the transmission between a single source inside the cavity and an outside antenna, we show that a simple partitioning algorithm allows us to reach very high directivity, as well as a steering capacity over 120°. We compare those results with known limitations on the performances of antenna [4] and conclude on the performances of our device.


*The author acknowledges funding from Greenerwave, ESPCI Paris Incubator PC'up, 75005 Paris, France which produces the metasurfaces.

3:06PM D10.00004: Spatially-Resolved Layer, Interface and Dopant Profiling Using Tabletop Coherent EUV Beams  
YUKA ESASHI (Presenter), MICHAEL TANKSALVALA, CHRISTINA L. PORTER, BIN WANG, NICHOLAS W. JENKINS, ZHE ZHANG, MATTHEW N. JACOBS, University of Colorado, Boulder, GALEN P. MILEY, Northwestern University, NAOTO HORIZUCHI, imec, JIHAN ZHOU, University of California, Los Angeles, ROBERT M KARL, CHARLES BEVIS, PETER JOHNSEN, JOSHUA KNOBLOCH, University of Colorado, Boulder, SETH L. COUSIN, KMLabs, EMMA CATING, MICHAËL HEMMER, CHENTING LIAO, MICHAEL GERRITY, HENRY KAPTEYN, MARGARET MURNANE, University of Colorado, Boulder — Next-generation devices, nanomaterials, quantum and magnetic materials necessarily have increasingly complex layers, dopants and 3D structures. As a result, non-destructive techniques that can image through visibly opaque layers with sensitivity to layer and interfacial composition are critical for synthesizing and optimizing these systems. We present a tabletop complex-imaging reflectometer illuminated by coherent high harmonic extreme ultraviolet (EUV) beams. Unlike most reflectometers that transversely average quantities such as film thicknesses over the sample, our reflectometer can attain diffraction-limited spatial resolution with high sensitivity to material composition by using coherent diffractive imaging (CDI). Our complex imaging reflectometer uses grazing-incidence CDI to generate high-resolution, high-fidelity phase and amplitude images of a sample at many incidence angles. The phase images are extremely sensitive to composition, allowing us to extract a 3D map of the sample. We demonstrate the ability to very sensitively probe diffusion at buried interfaces, layer thickness and dopant profiles in a non-destructive and spatially resolved manner, distinguishing our technique from others such as SIMS, Auger sputtering, or electron imaging.
3:18PM D10.00005: 3D-ΔPDF Investigations of Structural Phase Transitions* RAYMOND OSBORN (Presenter), MATTHEW KROGSTAD, STEPHAN ROSENKRANZ, Materials Science Division, Argonne National Laboratory — By exploiting a new generation of fast area detectors with wide dynamic range optimized for high-energy x-rays, it is possible to measure single crystal total scattering, $S(Q)$, over large volumes of reciprocal space encompassing thousands of Brillouin zones in under 20 minutes. This allows detailed investigations of the temperature evolution of both weak Bragg peaks from modulations in the long-range crystal structure and diffuse scattering from short-range fluctuations in the atomic order. $S(Q)$ can be transformed into real space to generate “difference” pair-distribution-functions (3D-ΔPDF), a powerful way of eliminating the average crystal structure to reveal subtle structural modifications and determine the correlation length of atomic fluctuations above and below $T_c$, all without detailed simulations.¹ I will show examples of 3D-ΔPDF applied to both long-range and frustrated short-range structural transitions in correlated electron systems and intercalation compounds.


*Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division

3:30PM D10.00006: Interferometric tracking of nanoparticle orientation with quantitative optical anisotropy imaging ZHIXING HE (Presenter), Physics, Virginia Tech, CHENGSHUAI LI, YIZHENG ZHU, Electrical and Computer Engineering, Virginia Tech, HANS ROBINSON, Physics, Virginia Tech — We introduce Quantitative Optical Anisotropy Imaging (QOAI), an interferometric spectral multiplexing technique that allows imaging and tracking of the orientation of individual nanoparticles at the microsecond timescale. In QOAI, incident light whose polarization is modulated in the spectral domain is scattered off particles and structures, interfered with a reference beam, and detected spectroscopically. The signal is directly proportional to anisotropies in the particle polarizability, and can therefore be used to extract both orientation and shape information about each individual particle, even at sizes well below the diffraction limit of conventional microscopy. We use this technique to categorize the aspect ratio of gold nanorods and to characterize their rotational diffusion near a solid interface. QOAI can be straightforwardly combined with existing particle tracking techniques so that position and orientation can be tracked simultaneously and can also be modified to provide quantitative measurements of the chirality of individual particles.

MAKOTO SCHREIBER (Presenter), MATTHIAS WOLF, Okinawa Inst of Sci & Tech — The atomic structure of amorphous materials has long been a mystery. Due to the lack of long-range periodical order, traditional techniques such as X-ray diffraction cannot be used to directly measure atomic coordinates. Through the analysis of pair-distribution functions, measurements of averaged structural features such as average bond lengths can be determined. By combining experimental data with simulations such as in reverse Monte-Carlo simulations, some models of 3D atomic structures can be determined. However it has not yet been possible to determine any local structure directly from experiment.

In this work, a type of image processing commonly applied in single particle cryo-electron microscopy is applied to a large set of nanobeam electron diffraction patterns. This produces a set of class-averaged patterns that represent dominant SRO structures within the material. This for the first time allows direct measurements on such structures and may eventually be extended to determine experimental 3D electron density distributions of SRO structure within amorphous materials.

*M.T.S. was supported by JSPS fellowship (DC1) 201820215 and Kakenhi Grant-in-aid for JSPS fellows 18J20132. M.W. is grateful for direct funding from OIST.


EMMA SNIVELY (Presenter), MOHAMED A. K. OTHMAN, MICHAEL E. KOZINA, BENJAMIN K OFORI-OKAI, STEPHEN P. WEATHERSBY, SUJI PARK, XIAOZHE SHEN, XIJIE WANG, MATTHIAS C. HOFFMANN, SLAC - Natl Accelerator Lab, RENKAI LI, Tsinghua University, EMILIO NANNI, SLAC - Natl Accelerator Lab — We discuss the results of a THz-driven electron bunch compression experiment in which interaction between a quasi-single-cycle THz pulse and a relativistic electron beam in a parallel plate waveguide produced a beam energy chirp for velocity bunching. Measurements at the SLAC MeV-UED facility show a simultaneous reduction in the bunch length and timing jitter by up to a factor of 3, improving the overall timing resolution for applications like ultrafast electron diffraction and other beam-based ultrafast measurements. This technique employs unique advantages of all-optical beam manipulation, including the inherent synchronization which allows the compensation of electron beam timing jitter and the high field gradient which enables efficient chirping of the electron beam in a sub-millimeter interaction region.

*This research has been supported by the U.S. Department of Energy (DOE) under Contract No. DE-C02-76SF00515. The SLAC MeV-UED program is supported in part by DOE Basic Energy Sciences (BES) Scientific User Facilities Division and SLAC UED/UEM program development: DE-AC02-05CH11231. M. K. and M. C. H. are supported by the DOE Office of Science, BES, award no. 2015-SLAC100238-Funding.
4:06PM D10.00009: Laboratory Based Hard X-ray Photoelectron Spectroscopy  SUSANNA ERIKSSON (Presenter), BRANDON GILES, Scienta Omicron — Hard X-ray photoelectron spectroscopy (HAXPES) is generally used to study core topics in condensed matter physics. However with a worldwide increase in the number of HAXPES focused endstations, many other interest groups now recognize its broad appeal.

In a HAXPES experiment 2-10 keV X-rays are used to excite photoelectrons to study the chemical environment and electronic structure of materials non-destructively. In contrast to standard XPS, HAXPES is more sensitive to what is beneath the surface. This makes it an ideal technique for studying structured samples that cannot be analyzed using traditional XPS. Bulk sensitivity means that realistic samples can be investigated without the need for surface preparation.

Unfortunately, there are very few existing HAXPES systems. Most are predominantly located at synchrotrons, as the photoionization cross sections at high energies is small and necessitates large X-ray intensities.

This work shows a new laboratory based HAXPES instrument capable of delivering monochromated 9.25 keV X-rays in a focused 30x45 μm² X-ray spot with energy resolution <0.5 eV. Systematic reference measurements demonstrate the system’s capability. Application based results from various fields, including measurements of energy related materials, are also presented.

4:18PM D10.00010: Probing bulk electronic structure with a laboratory-based hard x-ray angle-resolved photoemission spectrometer*  JOSEPH D GRASSI (Presenter), Temple Univ, ARIAN ARAB, Paul Scherrer Institute, JAY PAUDEL, RAJ K SAH, WEIBING YANG, RAVINI U CHANDRASENA, Temple Univ, KEISUKE KOBAYASHI, Japan Atomic Energy Agency, ALEXANDER GRAY, Temple Univ — Hard x-ray angle-resolved photoemission (HARPES) employing multi-keV x-rays as the excitation source has recently emerged as a powerful tool for the direct measurement of momentum-resolved bulk electronic structure [1-3]. To date, comprehensive HARPES spectroscopic studies have only been feasible at large-scale national synchrotron facilities. Here, we describe a newly completed laboratory-based hard x-ray photoemission spectrometer system with HARPES capabilities. The system utilizes a high-flux (3E9 ph/s) high-resolution (<0.45 eV) monochromated Cr Kα x-ray source tuned to the intermediate hard/tender energy regime (5.4 keV), which enables bulk- and buried-layer/interface sensitivity (up to 10 nm deep) while still being sensitive to the valence-band states due to appreciable photo-ionization cross sections. We present a wide range of examples of angle-resolved investigations of solids, including core-level and valence-band spectroscopy, momentum-resolved band structure mapping, and element-sensitive x-ray photoelectron diffraction.


*A.X.G acknowledges support from the U.S. Army Research Office, under DURIP grant (W911NF-18-1-0251).
4:30PM D10.00011: Development of in-situ differential thermal analysis for crystal growth experiments*  
YURI JANSSEN (Presenter), JOSE NICASIO, KEMAR DUDLEY, BINGYING XIA, JACK SIMONSON, State Univ of NY - Farmingdale — Differential thermal analysis (DTA) can give valuable information on melting and freezing of mixtures that are used for flux or solution growth of single crystals for materials research, and increasing the success rate of crystal growth attempts. DTA is especially valuable as a tool for undergraduate research involving crystal growth, as it can quickly give a realistic and easy-to-understand picture at what is happening inside a growth crucible as it is hiding the cooling crystal-growth mixture from view. In the past, we have performed DTA in a dedicated instrument, with small crucibles containing exactly the same composition as the larger growth crucible in the larger growth furnace. Now we are performing in-situ DTA inside the growth furnace and on as-prepared growth samples, for different type growths and furnaces, quickly improving crystal growth performed by undergraduate students with limited time dedicated to lab, and, moreover, on very inexpensive equipment. Here, we will present results of these developments.

*This project was funded by contributions from the Office of the Provost, the CSTEP program, and the Physics Department at Farmingdale State College.

4:42PM D10.00012: Early stage of iron anodic oxidation measured by 25ms-resolution X-ray reflectometry  
HIROMASA FUJII (Presenter), Graduate School of Engineering Science, Osaka University, TAKASHI DOI, Research and Development, Nippon Steel Corporation, YUSUKE WAKABAYASHI, Graduate School of Science, Tohoku University — Anodic oxidation at metal/water interface is a general phenomenon that commonly takes place on many metals. Time evolution of the oxide thickness is proportional to log(t)[1]. However, early stage clearly deviates from log(t) and the mechanism has not been understood yet in spite of its fundamental importance[2]. To reveal the early-stage mechanism, precise structural basis is needed. Here we report 25ms-resolution X-ray reflectivity experiments[3] to investigate the early stage of anodic oxidation at Fe (100), (110) and (111) in pH 8.4 borate buffer solution as model materials. Experiments were performed at the BL13XU of SPring-8, Japan with a 25keV monochromatic X-ray. The film density in the early stage is lower than in the later stage by 13 %, which suggests that the film structure is a highly defective spinel oxide. Moreover, the growth rate in the early stage is found to be proportional to about $t^{-1.5}$ but in later stage is $t^{-1}$. The presumed mechanism based on the Point Defect Model[1] will be discussed in the presentation.


Monday, March 2, 2020 2:30 PM - 5:18 PM

Session D11 APS/SPS: Undergraduate Research IV 110 - Chrisy Xiyu Du, Harvard University - Tag(s): Undergrad Friendly
2:30PM D11.00001: High-pressure pretreatment of rice straw for optimizing the fermentable sugar yield  
PRATHAM GUPTA (Presenter), BAHIRU TSEGAYE, CHANDRAJIT BALOMAJUMDER, Indian Inst of Technology Roorkee —  
Rice straw has proved to be a prospective source of renewable energy owing to high polysaccharic content and abundant availability. On hydrolyzing rice straw, fermentable sugars could be produced. In this research, organosolv was used to pretreat rice straw in high-pressure autoclave reactor under multiple conditions for removal of lignin and release of trapped polysaccharides. Rice straw composition was evaluated in accordance with the rules of the National Renewable Energy Laboratory. The temperature ranged from 130, 140 and 150 degrees Centigrade and time varied as 20, 30 and 40 minutes. Temperature and time have significantly impacted the quantity of sugar and lignin. Sugar yield at 140 degrees Centigrade and 30 minutes was discovered to be maximum. In this condition of pretreatment, it was observed that nearly all hemicellulose was solubilized, about 75% of lignin was removed and over 80% of cellulose was released. Removal of lignin promotes the release of cellulose from the matrix of biomass. Overall, this research demonstrated the potential for a high-pressure reactor to effectively remove lignin, enhancing fermentable sugar output.

Reference:
National Renewable Energy Laboratory (NREL), Chemical analysis and testing laboratory analytical procedures. NREL, Golden, CO, USA

2:42PM D11.00002: NSF IRES: Exploring the Effect of Temperature on a Plant's Photocyle by Observing the Blue-Light Photoreceptor Protein Arabidopsis Cryochrome*  
MAROOTPONG POOAM, CNRS, Photobiology Research Group, Sorbonne University, NYKIERA DIXON, Chemistry, Xavier University, MICHAEL HILVERT (Presenter), Physics, Xavier University, PETER MISKO, KRISTY WATERS, Biology, Xavier University, STEPHEN MILLS, Chemistry, Xavier University, SORIA DRAHY, CNRS, Photobiology Research Group, Sorbonne University, DOROTHY ENGLE, Biology, Xavier University, JUSTIN LINK, Physics, Xavier University, MARGARET AHMAD, CNRS, Photobiology Research Group, Sorbonne University — Cryochrome is a blue-light photoreceptor protein involved in both plant and animal circadian rhythms. When illuminated by blue light, the flavin cofactor of cryochrome is photoreduced, thus yielding the active state of the protein. This photoreduction and subsequent reoxidation can be observed spectroscopically. However, the effect of temperature on the photoreduction has not been extensively studied. Here, using a UV-Vis spectrophotometer, we demonstrate the effects of temperature on the photoreduction and reoxidation of purified Arabidopsis cryochrome 1 (AtCry1) and cryochrome 2 (AtCry2) proteins. It was hypothesized that at higher temperature, an increase in the rate of photoreduction and reoxidation would occur. However, our experimental results demonstrated that when comparing the reactions at 15°C and 25°C, temperature had no effect on the photoreduction of the flavin, but the rate of reoxidation was increased at the higher temperature. These results suggest increased activation in AtCry1 and AtCry2 at lower temperatures.

*This material is based upon work supported by the National Science Foundation under Grant No. (NSF #1658640).
2:54PM D11.00003: Temperature Dependence in Stochastic and Deterministic Models of the Circadian Rhythm of Cyanobacteria  THOMAS BAER (Presenter), ORRIN SHINDELL, Physics and Astronomy, Trinity University — The chemical reactions that lead to circadian rhythms in organisms are deterministically described in the limit where the number of cells is large. However, for each individual cell these reactions are stochastic as the number of molecules involved in them is small. Here, the circadian rhythms of cyanobacteria are considered. Using mathematical models of biochemical oscillations, we analyze the characteristic behavior of the deterministic system near a non-equilibrium phase transition. The control parameter that drives the transition is the temperature, which must be high enough for any biochemical oscillations to occur. We analyze the same set of reactions near the transition temperature in the stochastic limit and discuss features that emerge in the probability distributions of oscillation amplitudes and frequencies. We also comment on the thermodynamic connection between the small and large scale descriptions.

3:06PM D11.00004: Nano-optical imaging of bacteria on 2D materials* LIANA SHPANI (Presenter), Clark University, SHARAD AMBARDAR, DMITRI VORONINE, University of South Florida — Bacteria cause hazards via biofouling and develop resistance to antibiotic treatments. However, due to their small size, spectroscopic imaging and analyzing bacteria using conventional optical microscopy is challenging. Moreover, atomically thin 2D materials, especially transition metal dichalcogenides, with their wide range of applications in optoelectronics, have also shown promising biological applications. In this work, we developed a novel nanoscale imaging approach to characterize bacteria-substrate interactions. Untreated and antibiotic-treated bacteria were deposited on the junction of monolayer MoS$_2$-WS$_2$ materials on top of a Si substrate. The optical characterization with 532 nm laser excitation provided far-field photoluminescence (PL) and near-field tip-enhanced photoluminescence (TEPL) measurements. When the bacteria were placed on the 2D materials, a higher PL signal was observed compared to the pure material. The enhancement and the red shift of the PL signal can be accounted as strain caused by the bacteria on the 2D materials. These observations show promising results to prompt further studies to analyze interactions of different bacteria with TMDs.

*This work was supported by the National Science Foundation (NSF) grant DMR-1852269.
3:18PM D11.00005: Human Gene Expression and the Protein-Protein Interaction Network: Identification of Potential Disease Module Association to Differential Gene Expression for Patient-to-Drug Matching  AYDIN WELLS (Presenter), Northeastern University, DEISY MORSELLI GYSI, Center for Complex Network Research, ALBERT L BARABASI, Northeastern University — The relationship between human gene expression (GE) and precision medicine applications is central in understanding how patients are affected by and how to better treat a disease. Even though it is of extreme importance, this knowledge is still absent from almost any disease analysis resulting in misdiagnosis and mistreatment based on symptomatic and physical observation criteria devoid of high throughput sequencing technologies. By detecting disease modules in the protein-protein interaction (PPI) network, along with the identification of patient differential GE sets (DGE), we can suggest effective individual treatment options. Here, we collect public RNA sequencing data for a diverse population and arrange unique GE patient profiles. DGEs are computed using machine learning techniques and are identified within the PPI network, where disease modules can be pinpointed. Those modules can be used for disease classification specific to expression levels and cohort phenotype. By elucidating these interactions using network approaches with an individual patient’s features, human diseases can be identified not by peripheral approaches, but by a personal genetic diagnosis; essentially redefining disease diagnostics from a “one size fits all” philosophy, to a “one size fits you” reality.

3:30PM D11.00006: Focused Ultrasound as a Replacement for Endodontic Therapy*  TALISI MEYER (Presenter), JENNIFER CANFIELD, MICHAEL JORDAN, JASON WHITE, Simmons College — Focused ultrasound has exhibited promising results as a therapeutic modality in its ability to minimize the invasiveness of a number of medical treatments that are physically and mentally traumatic to the patient. We propose the investigation of its use for non-invasive endodontic therapy (a.k.a. a “root canal”), with the ultimate goal of removing microbial infection from the root canal system of a contaminated tooth.

To avoid thermal damage to adjacent healthy tissues, we considered using the mechanical effects created by ultrasound, specifically that of cavitation. To generate proof-of-concept data, we designed, constructed, and tested a series of ultrasound transducers that delivered sufficiently low frequencies operating below 300 kHz and pressures below -30MPa to induce cavitation in degassed water with less than 3ppm. Our initial experiments have shown that sufficient ultrasound energy can be transmitted through intact ex vivo human teeth to elicit nonlinear streaming in the root canal of intact ex vivo human teeth. We have also demonstrated the use of equivalent parameters to kill bacteria. We will further determine and refine the optimal ultrasound parameters for eliciting bactericide in the intact tooth.

*SARP (Formally SCARP of Simmons University)
3:42PM D11.00007: Enhanced magnetic hyperthermia of copper ferrite nanoparticles for biomedical applications*  
ENYA SILVA (Presenter), J. ROBLES, SARATH WITANACHCHI, Department of Physics, University of South Florida, ANH-TUAN LE, Faculty of Materials Science and Engineering, Phenikaa University, MANH-HUONG PHAN, Department of Physics, University of South Florida — Magnetic hyperthermia is a promising cancer treatment that has minimal side effects compared to chemotherapy and radiation therapy. The heating efficiency of magnetic nanoparticles is central to the effectiveness of magnetic hyperthermia as a treatment and, while Copper is a well-known thermal conductor, little research has been done regarding its ability to increase the heating efficiency of magnetic nanoparticles. In this experiment, the heating efficiency of different samples of Copper Ferrite nanoparticles was quantified by dispersing the nanoparticles in a solution and measuring the solution's temperature change over time in an alternating magnetic field. This method is common in the study of magnetic hyperthermia because it best replicates the experiment's clinical applications. This experiment yielded a value of about 300 W/g for the heating efficiency of Copper Ferrite, which is significantly higher than the value of about 80 W/g obtained for Iron Oxide nanoparticles from previous experiments. These results suggest that Copper is a viable option for increasing the heating efficiency of magnetic nanoparticles and that Copper Ferrite nanoparticles are viable candidates for magnetic hyperthermia therapy.

*Work was supported by VISCOSTONE (VS-1253113200).

3:54PM D11.00008: Correlative photoluminescence and micro-Raman spectroscopy determining disorder from two-dimensional heterostructures to rare-earth minerals  
JOY J. MA (Presenter), TAO JIANG, JUN YAN, MOLLY A MAY, MARKUS B. RASCHKE, Physics, University of Colorado, Boulder — Atomic composition and structural arrangement determine the correlation of electronic and lattice degrees of freedom in solids. With combined photoluminescence (PL) and Raman spectroscopy, simultaneous insight into electronic properties and structural disorder can be gained. Here, we use micro-Raman imaging to study spatial heterogeneity in structural disorder in the rare-earth mineral gadolinite as determined from correlative peak position and spectral linewidth analysis. We find the disorder associated with spatial variability in light and heavy rare earth element content. We then use micro-PL to investigate the effect of a plasmonic nano-slit on the excitonic landscape in a two-dimensional heterostructure of transition metal dichalcogenides and identify plasmonic enhancement of both intralayer and interlayer exciton emission as well as strain-induced spectral variations. In summary, this work demonstrates the combination of micro-PL and micro-Raman imaging to understand electronic and structural properties and disorder in crystal materials.
4:06PM D11.00009: Electron emission from randomly-oriented and vertically-aligned carbon nanotubes synthesized directly on conducting surface* MATTHEW KURILICH (Presenter), Department of Physics and Astronomy, Middle Tennessee State University, ARUN THAPA, WENZHI LI, Department of Physics, Florida International University, SUMAN NEUPANE, Department of Physics and Astronomy, Middle Tennessee State University — Field emission properties of carbon nanotubes (CNTs) have been intensively studied for various applications. It is desirable to synthesize CNTs directly on conducting substrates to develop field emission displays capable of operating at low voltages and at room temperature. As compared to the randomly-oriented CNTs, vertically-aligned CNTs demonstrate improved field emission properties with greater electric field enhancement and lower turn-on/threshold electric fields. In this work, we compare the electron emission between randomly-oriented and vertically-aligned CNT emitters synthesized directly on stainless steel substrates. The surface morphology of these CNTs has been studied with electron microscopy and the defects are analyzed by the Raman spectroscopy. The vertical alignment of the CNT emitters benefits the emission process by reducing the screening effect and by streamlining the path of ejected electrons directly onto the anode.

*We would like to acknowledge the financial support from startup funds by the Middle Tennessee State University and the National Science Foundation (NSF) under Grant No. DMR-1506640.

4:18PM D11.00010: Tunable 3D Photonic Crystal Cavity for Coherent Coupling between Microwave Fields and Solid State Spins* ABHIJATMEDHI CHOTRATTANAPITUK (Presenter), HYEONGRAK CHOI, DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — We present a theory and experiment of a three dimensional (3D) photonic crystal (PhC) cavity for the control of microwave fields with ultra-low loss. The cavity consists of an engineered defect in a woodpile photonic crystal made of low-loss alumina rods. We measure a large complete bandgap of 13% of the center frequency and a cavity quality factor exceeding 22,000. The architecture allows for easy mechanical tuning of the cavity and waveguide. Our design has a variety of applications including the coherent coupling of microwave photons with electron and nuclear spins in solids.

*The authors acknowledge the support from the Defense Advanced Research Projects Agency (DARPA) DRINQS (HR001118S0024). A. Chotrattanapituk acknowledge the support from MIT RLE UROP.
4:30PM D11.00011: Viscosity of a Crowding Medium Obtained Through Optical Trapping*
JAMES HOWARD (Presenter), JAVIER E HASBUN, SUVRANTA TRIPATHY, Univ of West Georgia — The dynamic viscoelasticity a cellular medium is mainly due to the crowding of a large number of interacting and non-interacting proteins. Our research presents how the viscosity of a medium is altered in the presence of globular proteins. Using an optical trap paired with a 980 nm infrared laser and Nikon inverted microscope we have developed a synthetic approach to calculate the viscosity of a medium. The method involves comparison of Equipartition theorem and Passive power-spectrum technique to determine viscosity. This approach has enabled us to calculate the viscosity of several water and glycerol concentrations. The method has been extended to investigate the viscoelasticity of the medium with various concentrations of globular Polyethylene glycol proteins.

*Student Research Assistant Program, University of West-Georgia, GA, 30118

4:42PM D11.00012: Computation of Forces and Torques on Clusters of Micron-Sized Spheres in Optical Tweezers  WYATT VIGILANTE (Presenter), JEROME FUNG, Ithaca Coll — Optical tweezers are a focused laser beam that exerts forces and torques on micrometer-sized particles. Calculations of optical forces on non-spherical particles whose size is comparable to the wavelength of the trapping beam are challenging. Here, we use a $T$-matrix code to calculate how clusters of spheres scatter light. The resulting $T$-matrix is exported to a software package that calculates optical forces and torques. We present calculations of optical forces and torques on clusters of two and three spheres. We discuss how the forces and torques depend on the orientation, size, and refractive index of the clusters.

4:54PM D11.00013: Nano-Optical Imaging of CVD Grown Lateral Heterostructures  RANA KAMH (Presenter), SHARAD AMBARDAR, HANA HRIM, DMITRI VORONINE, Univ of South Florida — Transition Metal Dichalcogenides (TMDs) have attracted a lot of attention due to their properties such as direct band gap, photoluminescence, and applications in electronics. Several combinations of TMD monolayer heterostructures have been fabricated and studied for their unique optical and electrical properties. Here we explore CVD grown WSe$_2$-MoSe$_2$ heterostructures with the presence of telluride in order to observe the effects that arise from the integration of this material in CVD growth. We characterize the resulting material using techniques such as Kelvin Probe Force Microscopy (KPFM), Atomic Force Microscopy (AFM), and Tip Enhanced Photoluminescence (TEPL), revealing the optical properties and surface topographies of the 2D heterostructures after exposure to telluride during growth. We observe alloying and quenching of the near field PL in the 2D lateral heterostructures and propose reasons for these effects after the incorporated material. The integration of telluride to 2D materials can provide potential applications in optoelectronic devices.
5:06PM D11.00014: Computer generated holograms for optical trapping using a Spatial Light Modulator* ANTHONY HEWITT (Presenter), Department of Physics & Astronomy, University of Delaware, KOOK SIANG GAN, RAINER DUMKE, Division of Physics and Applied Physics, Nanyang Technological University, MICHAEL LIM, Department of Physics & Astronomy, Rowan University — The general experimental modeling of quantum behavior with a well-characterized and well-controlled quantum system is now a possibility using a Bose-Einstein condensate loaded into programmable optical potentials. Through the use of a spatial light modulator (SLM), these patterns can be dynamically modified in real time to further increase the scope of these modelling capabilities. Accurate focal-plane intensity patterns can be generated using an SLM with appropriate algorithms. We demonstrate that the Mixed Region Amplitude Freedom (MRAF) algorithm can generate a desired intensity ring in the focal plane of a lens. We plan to use the MRAF output as the initial guess for a second algorithm that uses Conjugate Gradient Minimization (CGM) to reduce convergence time and increase overall accuracy.

*The authors acknowledge support from NSF-IRES 1559410.

Monday, March 2, 2020 2:30 PM - 5:06 PM

Session D12 APS/SPS: Undergraduate Research V 112 - Ivy Jones, Marquette University

2:30PM D12.00001: Magnetohydrodynamic (MHD) Modeling of Kelvin-Helmholtz Instability and Associated Magnetosonic Wave Emission in Solar Coronal Mass Ejections (CMEs) SARA BUTLER (Presenter), HAVA TURKAKIN, Bucknell University — Interrupted telegraphy systems, regional power outages, and damaged satellites demonstrate a few of the consequences to earth technology by mechanisms that can be analyzed and prevented. The impact of solar wind on the earth and other objects in interplanetary space is relatively understudied, yet has far-reaching applications. Previous related studies have observed through close study of shear flow regions in the Solar-terrestrial environment, that Kelvin-Helmholtz Instability (KHI) and Magnetohydrodynamics (MHD) wave emissions along these boundaries may be a method by which energy is transported from flow. In order to gain a deeper understanding of the non-linear dynamics that distribute energy throughout the Solar Corona, we expand upon these previous studies to investigate the nonlinear evolution of KHI and MHD waves along the boundaries of coronal mass ejections (CMEs), large eruptions of the corona that have a significant effect on satellites, earth's power grids, and humans in space. We utilize different criteria for measuring efficiency, including 2-D/3-D magnetohydrodynamic modeling software. We also discuss in detail the implementation of this software in our analysis about the nature of MHD instabilities in astrophysical plasmas throughout the universe.
2:42PM D12.00002: Cradle-to-Grave Evolution and Explosiveness of the Magnetic Field from Bipolar Ephemeral Active Regions (BEARs) in Solar Coronal Holes*  CAROLINE NAGIB (Presenter), University of California, Los Angeles, NAVDEEP K. PANESAR, Lockheed Martin Solar and Astrophysics Laboratory, RONALD L. MOORE, ALPHONSE C. STERLING, NASA Marshall Space Flight Center — We report on the magnetic evolution of magnetic-explosion eruption production of each of seven BEARs observed in on-disk coronal holes in line-of-sight magnetograms and in coronal EUV images. One of these BEARs produced no eruptions. The other six BEARs display three kinds of magnetic-explosion eruptions: (1) blowout eruptions, (2) partially-confined eruptions, (3) confined eruptions. The seven BEARs are a subset of 60 random coronal-hole BEARs, with visually estimated emergence phases. In this work, we obtain a reliable determination of when the emergence phase ended by finding the time of the BEAR's maximum minority flux from a time plot. These plots show: (1) none of the seven BEARs had an inside eruption while the BEAR was emerging, and (2) for these seven BEARs, the visually-estimated emergence end time was never more than six hours before the measured time of maximum minority flux. Our findings support that a great majority of the explosive magnetic fields from BEARs in coronal holes are prepared and triggered to explode by magnetic flux cancellation, and that such flux cancellation seldom occurs inside an emerging BEAR.

*This work is supported by the NSF REU grant AGS – 1460767, support from NASA’s SDO/AIA contract (NNG04EA00C) to LMSAL, support by the NASA HGI program.

2:54PM D12.00003: Magnetic and Electronic Structure of CuTeO4  ZUBIA HASAN (Presenter), Johns Hopkins University, THAO TRAN, Clemson University, TYREL MCQUEEN, Johns Hopkins University — Cu2+ based materials have been extensively studied over the past decades due to their importance in high temperature superconductivity as well as their potential as quantum spin liquids. Recently,1 CuTeO4 has been proposed as a candidate material that combines a geometrically frustrated triangular lattice with potential high temperature superconductivity upon doping. To date, CuTeO4 has only been made as a secondary phase while making other Copper Tellurates, under extreme hydrothermal conditions over months 2. We developed a novel method of synthesizing CuTeO4 in single phase form, enabling us to characterize its physical properties by magnetization, heat capacity, and neutron diffraction. CuTeO4 was initially predicted to have a quasi-2D Neel ground state. Our magnetic susceptibility data shows no long range ordering with an upturn at T=50K and an intriguing hump around T=120K indicative of low dimensional antiferromagnetic interactions. Heat capacity data shows no magnetic transition at T=50K, an inconsistency that needs to be explored further. With the bulk characterization to date, CuTeO4 seems to be a prime candidate for low-dimensional magnetism.

3:06PM D12.00004: Properties of Magnetic High-Entropy Alloys*  
VALERIA ROSA ROCHA (Presenter), ABBY M NASH, JOHN-PAUL E. CESARE, TROY MESSINA, Berea College — Magnetic high-entropy alloys are a promise for many fields. From cryogenic to aircraft and spacecraft applications, the possibilities are varied but one thing is necessary: we must have a better understanding of the properties of these materials in order to put them to good uses. Korman et al. made predictions for the Curie Temperatures (Tc) of HEAs of the form Cr\textsubscript{x}CoFeNiQ\textsubscript{x} with Q being Pd, Cu, Ag, or Au. In our study, we focused on the Pd alloys varying both Cr and Pd in order to check the accuracy of the Tc predictions. Using the ’’Treasure Maps’’ provided by Korman et al. we chose combinations of Cr and Pd that were predicted to have a Tc near room temperature. Based on our work, we found the maps to be very reproducible with the procedure used, which is further explained in this presentation.

*Berea College Undergraduate Research and Creative Projects Program (BC-URCPP) Berea College Labor Program

3:18PM D12.00005: Magnetic Heat Capacity Characterization of Magnetite  
SILVIA SHERMAN (Presenter), STEPHEN A TSUI, California State University, San Marcos — We investigate the magnetic and thermal properties of magnetite using both vibrating sample magnetometry (VSM) and heat capacity measurement. Magnetite undergoes the Verwey transition, which is a structural phase transition near 120 K. The magnetization behavior vs. temperature differs between field cooled (FC) and zero field cooled (ZFC) measurements in the VSM, due to the preferential alignment of the magnetic spin moments with respect to applied magnetic field. The application of magnetic field also contributes to an enhancement in the heat capacity. In this study, we investigate the behavior of the heat capacity of different specimens of magnetite under these FC and ZFC conditions.

3:30PM D12.00006: H-T phase diagram of antiferromagnetic topological insulator MnBi\textsubscript{2}Te\textsubscript{4} under hydrostatic pressure to 2.5 GPa*  
RAKIN NUMAIR BATEN (Presenter), TIMOTHY A ELMSLIE, DERRICK VANGENNEP, JAMES J HAMLIN, Department of Physics, University of Florida, Gainesville, Florida 32611, USA — MnBi\textsubscript{2}Te\textsubscript{4} is a layered compound that is an intrinsic antiferromagnetic topological insulator. Metamagnetic transitions have been observed at 3.2 T and 7.8 T at ambient pressure. By compressing the unit cell with hydrostatic pressure and applying a magnetic field we can track these metamagnetic transitions and investigate the magnetic ordering. In this talk I will present transport data and temperature-field phase diagrams of MnBi\textsubscript{2}Te\textsubscript{4} single crystals up to 2.7 GPa and 9 T.

*This work was funded by the National Science Foundation CAREER award DMR-1453752. RNB partially supported by The Ronald E. McNair Post-Baccalaureate Achievement Program.
Modeling Hyperfine Coupling in Molecular Magnets

CONG HU (Presenter), Physics, Univ of Connecticut - Storrs, JIA CHEN, XIAOGUANG ZHANG, Physics, University of Florida — Nuclear or electron spins of magnetic molecules are promising qubit candidates. Electron spins are advantageous due to faster operational times, but they decohere faster due to stronger coupling to environment. This project investigates hyperfine couplings in four vanadyl complexes with long decoherence times as qubits by electron structure calculations. In all complexes, electron spins are localized on V$^{4+}$ ion. Using the analytic derivative method based on density functional theory, the Fermi-contact and spin-dipole interactions were calculated. Total hyperfine coupling to vanadium nuclear spin is compared to experiment; Using hybrid functional, good agreement can be achieved. Due to the localized nature of electron spins, the Fermi-contact interaction between an electron spin and hydrogen nuclear spin is only strong for the smallest complex. Hyperfine coupling to hydrogen nuclear spins as the main source of electron spin decoherence can be modeled by spin-dipole interactions.


* C.H. acknowledges support from NSF under grant DMR-1852138.

Mössbauer spectroscopy of iron oxide nanoparticles containing both magnetite and maghemite

JEREMY WINSETT (Presenter), SAEED KAMALI, SUMAN NEUPANE, Middle Tennessee State Univ — Iron oxide nanoparticles are available in two common phases, including magnetite (Fe$_3$O$_4$) and maghemite (Fe$_2$O$_3$). Upon exposure to oxygen atoms, the magnetite phase readily oxidizes into the maghemite phase with the partial conversion of ferrous ions into ferric ions. We report on the approach to determine the ratio of magnetite and maghemite in iron oxide nanoparticles synthesized by the hydrothermal process. The crystallinity of these nanoparticles has been investigated by X-ray diffraction studies and transmission electron microscopy observations. The hysteresis loops of the iron nanoparticles demonstrated the “S-shaped” pattern corresponding to superparamagnetic behavior. The Mössbauer spectrum of the sample is compared with the theoretically predicted model to determine the contributions from magnetite and maghemite. Such characterization is necessary for the synthesis of magnetic nanoparticles of uniform size with potential for biomedical applications.

*We would like to acknowledge the financial support from startup funds by the Middle Tennessee State University.
4:06PM D12.00009: Computational Modeling of Magnetorheological Elastomers* TONG DANG (Presenter), ANDY T CLARK, Department of Physics, Bryn Mawr College, JIAJIA LI, Department of Physics, Fudan University, DAVID MARCHFIELD, KRISTEN S. BUCHANAN, Department of Physics, Colorado State University, XUEMEI CHENG, Department of Physics, Bryn Mawr College — Ultra-soft polydimethylsiloxane (PDMS) based magnetorheological elastomers (MREs) are composite materials of polymeric matrix with embedded micro- or nano- sized ferromagnetic particles. They are promising candidates for dynamic cell culture substrata due to their magnetic field dependent mechanical properties. In this work, we have used a two-step, multi-scale approach to model the complex magnetic reversal behavior of MREs. Micro-magnetic simulations were performed using MuMax3 to obtain a detailed description of the magnetic reversal process of individual Fe particles. The micromagnetic modeling results are then used as input parameters for a particle interaction model that includes dipolar interactions and elastic deformations. This model was used to study the magneto-mechanical interactions between a large collection of particles and their surrounding elastomer matrix, which provides insight into the complex magneto-mechanical interactions of MREs.

*This work is supported by the Center for Engineering MechanoBiology (CEMB), an NSF Science and Technology Center, under grant agreement CMMI: 15-48571.
Work at Colorado State University is supported by NSF (DMR # 1709525)

4:18PM D12.00010: CsPbBr$_3$ Perovskite Quantum Dots as Single Photon Sources* GEORGIA NELSON (Presenter), Department of Physics, Bryn Mawr College, GIORGIO ADAMO, CESARE SOCI, Division of Physics and Applied Physics, Nanyang Technological University, MICHAEL LIM, Department of Physics & Astronomy, Rowan University — Cesium Lead Bromide (CsPbBr$_3$) Perovskites Quantum Dots (PQDs) are zero-dimensional semiconducting particles with tunable optical properties. We are interested in PQDs as possible single photon sources with applications in quantum computing and quantum cryptography. We have successfully fabricated CsPbBr$_3$ PQDs and measured their photoluminescence intensity as a function of wavelength. As temperature is varied from 77K to 293K, the central wavelength undergoes a blue-shift. The fabricated CsPbBr$_3$ PQDs are stable at 77K and 293K. Diluting the solution used in fabrication should allow us to create samples of individual, spatially-resolved quantum dots, which can then be verified with $g^{(2)}$ measurements.

*The authors acknowledge support from NSF-IRES 1559410.
4:30PM D12.00011: Quantum entangled breathers in Goldilocks quantum cellular automata

HALEY COLE (Presenter), MATTHEW JONES, Colorado Sch of Mines, LOGAN HILLBERRY, Physics, University of Texas Austin, MINA FASIHI, LINCOLN CARR, Colorado Sch of Mines — We conducted robustness studies of quantum entangled breathers (QEBs) to evaluate their stability. QEBs are an emergent dynamical structure appearing in a continuous time generalization of Goldilocks quantum cellular automata. This system is a qubit spin chain on which sites evolve according to a local unitary operator if and only if 2 or 3 sites in a 5 site neighborhood are spin-up. The QEB is a quantum entangled generalization of a discrete breather or excited bright soliton on a lattice, a famous and robust classical solution to nonlinear wave equations. We consider four sources of noise: uniform and non-uniform spatial noise in the state; uniform spectral noise in the state; perturbations to the closed system Hamiltonian; and open quantum system evolution including T\(_1\) and T\(_2\) decoherence processes. We find that QEBs present a robust signal of quantum complexity in a simple system that can be studied on a wide variety of quantum simulators.

*Funded by NSF.

4:42PM D12.00012: Synthesis and Characterization of Quantum Dots Based on Transition Metal Dichalcogenides

PEDRO JUAN RODRÍGUEZ FERNÁNDEZ (Presenter), Physics Department, University of Puerto Rico, Mayaguez, NALAKA A KAPURUGE, HUMBERTO GUTIERREZ, Physics Department, University of South Florida — Atomically transition metal dichalcogenides (TMDs) have attracted a significant attention due to their novel and promising physical properties. However, Quantum Dots (QDs) based on TMDs have been less studied. QDs present size-dependent optical and electronic properties due to quantum confinement of electrons and phonons. Consequently, they have potential applications in medicine, renewable energy, and electronics, among others. In this presentation we will describe a simple synthetic approach to produce TMD-based QDs as well as the study of their physical properties. The synthesis involves mechanical rupture of large TMD flakes using a high power ultrasonic horn, bath sonication and/or thermal reflux. Subsequently, QDs of different sizes are selected by centrifugation. The effect of different parameters such as ultrasonic power, time, solvent type and centrifugation conditions on the final size distribution were studied. The morphology of the TMD fragments was studies by scanning electron microscopy and atomic force microscopy. The optical response of the as-prepared materials was evaluated using optical absorption spectroscopy, photoluminescence and Raman spectroscopies.

*This work was supported by the National Science Foundation (NSF) grants DMR-1852269 and DMR-1557434
4:54PM D12.00013: Single Hole Based Magneto-Impedance Biosensor for Particle Detection*

BAYLEE SENATOR (Presenter), Department of Physics and Engineering, West Virginia Wesleyan College, VALEY ORTIZ JIMENEZ, MANH-HUONG PHAN, Department of Physics, University of South Florida — GMI (giant magneto-impedance) sensors have been used for biomedical applications that require maximum sensor detection sensitivity for accurate magnetic field detection. To create better biosensors, Fe$_3$O$_4$ nanoparticles are applied to holes drilled into a ribbon-based GMI biosensor which should increase the sensor detection sensitivity. A focused ion beam is used to drill various sized holes – 3, 4, 5, 7, and 10 μm diameters – into soft ferromagnetic Metglas® 2714A ribbons. The sensor sensitivity of these samples is measured as-cast, with holes, and with iron oxide nanoparticles at frequencies between 50 and 175 MHz. The addition of iron oxide nanoparticles has shown to increase the sensor sensitivity of the samples while the GMI ratio decreases. In conclusion, the sensor detection sensitivity of ribbon-based GMI biosensors improves when the iron oxide nanoparticles are applied and measured between 110 and 150 MHz, therefore, creating biosensors with greater detection sensitivity. The maximum sensitivity measured for the ribbon as-cast was 60 %/Oe, this increased to 105 %/Oe when the iron oxide nanoparticles were applied.

*This work was supported by the National Science Foundation (NSF-DMR) under Grant No. 1852269.

Monday, March 2, 2020 2:30 PM - 5:06 PM

Session D15 DFD DSOFT: Thin Films, Surface Flows, and Interfaces I

210/212

2:30PM D15.00001: Physical Limits of Marangoni-driven Patterning*  STEVEN STANLEY (Presenter), ROGER T BONNECAZE, University of Texas at Austin — Marangoni-driven patterning is a novel technique that harnesses photochemically-applied surface tension gradients to pattern thin polymer films. When heated, the polymer flows away from regions of lower surface tension and into regions of higher surface tension, thereby generating hill-and-valley patterns. This new technique offers potential advantages over traditional patterning methods in creating functional coatings and flexible electronics at the roll-to-roll scale. To understand the full scope of applications this new patterning method could serve, it is necessary to understand the fundamental limits of pattern aspect ratio and pattern periodicity, both key metrics in evaluating pattern quality. Here, we present a model for Marangoni-driven patterning and perform a nonlinear analysis to determine the physical limits of pattern aspect ratio and feature pitch for an equal line-space system.

*This work is supported by a grant from the National Science Foundation under Cooperative Agreement No. EEC-1160494.
ABHEETI GOYAL (Presenter), Fluids and Flows Group, Theory of Polymers and Soft Matter Group, Dept. of Applied Physics, Eindhoven University of Technology, PAUL VAN DER SCHOOT, Theory of Polymers and Soft Matter Group, Dept. of Applied Physics, Eindhoven University of Technology, FEDERICO TOSCHI, Fluids and Flows Group, Dept. of Applied Physics. Dept. of Mathematics and Computer Science, Eindhoven University of Technology — Understanding the phase separation dynamics in thin films is crucial for the performance of many optoelectronic and photovoltaic device because their functioning relies on a well-defined morphology. The morphology forms in the fluid stages of the production process, and to control and improve the performance of thin-film composites it is vital to predict it quantitatively. Typically, the dynamics of fluid-fluid demixing is modeled using relaxational phase field-type theories that ignore the role of hydrodynamics. We study the impact of hydrodynamics on the demixing of binary fluid mixtures in contact with a wetting substrate by comparing lattice Boltzmann simulations with a diffusion-dominated phase field theory. Special focus is on the impact of a short-range surface interaction that favours one of the two fluids, particularly important in the context of photovoltaics. We find that incorporating hydrodynamics is crucial to quantitatively predict the relevant length scales both in the early and late stages of demixing. Indeed, we find that hydrodynamic processes suppress any dependence of the associated growth exponents on the strength of the substrate interaction predicted by phase field theory. We attribute this to flow-induced transport that significantly speeds up coarsening.

ANDERS JOHANSSON (Presenter), HENRIK A SVEINSSON, Department of Physics, University of Oslo, KJETIL THØGERSEN, Department of Geosciences, University of Oslo, ANDERS HAFREAGER, Department of Physics, University of Oslo, EINAT AHARONOV, Institute of Earth Sciences, Hebrew University of Jerusalem, ANDERS MALTHE-SØRENSSEN, Department of Physics, University of Oslo — Geophysical processes are traditionally studied at the continuum level, but large scale molecular simulations now allow detailed studies of the underlying nanoscale mechanisms responsible for large scale behavior. An outstanding question in geoscience is the dynamics of water in thin water films in geological materials under high pressure. In this work, we demonstrate that molecular dynamics simulations provide new insights on creep in water-wetted silicates. We have performed nonequilibrium molecular dynamics simulations of the creep process in a pair of opposing quartz asperities under constant load. The results are compared with a microphysics-based model for thermally activated creep. The thermal activation energy and the time evolution of the system height agree with theory when there is a vacuum between the asperities. Replacing the vacuum with water drastically alters these results by introducing chemical effects which dominate the creep process. Pressure solution of silica and the formation of an amorphous gel at the asperity interface are found to greatly increase the creep rate.

*Notur grant NN9272K
3:06PM D15.00004: Nonlinear Interface Equation For Capillary Driven Flow in 3D Open Curved Trajectories* NICHOLAS WHITE (Presenter), SANDRA TROIAN, Applied Physics, Caltech — Capillary driven flow of wetting liquids in open V-grooves and interior corners is known to be an especially robust and rapid means of fluid transport in gravity free environments and in small scale systems where gravity plays a negligible role. Nowadays, such flows are routinely used for propellant management in space based systems, lab-on-a-chip devices and high performance chip with micro heat pipes. The low-order inertia-free model developed by Romero and Yost (1996) and Weislogel (1996) first elucidated the flow behavior of an incompressible Newtonian liquid in a straight V-groove whose length far exceeds the film thickness. Here we present an extension of this classic work to flow in 3D open and curved channels in which the trajectory radius of curvature is larger than the film thickness. Despite the complexity of trajectories allowed by this model, a first-order perturbation analysis of the governing conservation equation yields a surprisingly simple form of the nonlinear equation governing the behavior of the moving interface. This thin film equation can now be used to design deterministic flow trajectories for ultracompact microfluidic systems featuring arbitrarily curved 3D channel flows.

*Sponsored by a 2017 NASA Space Technology Research Fellowship (NCW).

3:18PM D15.00005: Theory of the two-dimensional paraelectric structural transformation of ferroelectric group-IV monochalcogenide monolayers* SALVADOR BARRAZA-LOPEZ (Presenter), JOHN VILLANOVA, PRADEEP KUMAR, Univ of Arkansas-Fayetteville — After the initial description of a thermally-driven two-dimensional structural transformation in group-IV monochalcogenide monolayers [1] and its subsequent experimental demonstration [2], an additional publication claimed that the transformation can be determined via a Landau model based on an unidirectional optical phonon mode going soft [3]. In this presentation, we disclose a quadratic dispersion of softening modes and analyze molecular dynamics data to understand the atomistic motions underlying the ferroelectric to paraelectric transformation in these atomically thin membranes. We are then able to characterize a hierarchy of critical temperatures Tc that are dependent on structural constraints. Additional dependencies of Tc on the assumptions used to set interatomic forces are discussed as well [4].

References:

*This work has been funded by an Early Career award from the DOE (DE-SC0016139). Calculations were performed at Cori at NERSC (DE-AC02-05CH11231).
3:30PM D15.00006: Evolution of elastic moduli through a two-dimensional structural transformation* ALEJANDRO PACHECO-SANJUAN, Departamento de Ingenieria Mecanica, Universidad Tecnica Federico Santa Maria, TYLER BISHOP (Presenter), ERIN FARMER, PRADEEP KUMAR, SALVADOR BARRAZA-LOPEZ, Univ of Arkansas-Fayetteville — We use an analytical elastic energy landscape describing SnO monolayers to estimate the softening of elastic moduli through a mechanical instability occurring at finite temperature. Although not strictly applicable due to a quantum paraelastic phase in this material [1], this exercise is relevant as it establishes a conceptual procedure to estimate such moduli straight from a two-dimensional elastic energy landscape. As additional support for the existence of a quantum paraelastic phase, we use a qualitative WKB analysis [2] to estimate escape times from an energy well on the landscape. These results continue to establish a case for the usefulness of soft matter concepts in 2D materials and of the potential lurking of quantum effects in soft matter [3].


*This work was funded by FONDECYT in Chile (1171600), the National Science Foundation (DMR-1610126), and the DOE (Early Career Award DE-SC0016139, Contract No. DE-AC02-06CH11357). Part of this work was performed at the Center for Nanoscale Materials at Argonne National Laboratory.

3:42PM D15.00007: Laser-induced strong Marangoni effect in deformation and manipulation of ferrofluid FENG LIN (Presenter), Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, TALARI VISHAL, Department of Mechanical Engineering, University of Houston, JUNYI ZHAO, Department of Electrical and Systems Engineering, Washington University in St. Louis, JOHN SCHAIBLEY, Department of Physics, University of Arizona, DONG LIU, Department of Mechanical Engineering, University of Houston, ZHIMING WANG, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, JIMING BAO, Department of Electrical and Computer Engineering, University of Houston — Optical manipulation of fluid or droplet has long been investigated for applications in microfluidics. The light-induced thermocapillary effect is one of the strategies in optical control of liquid. We demonstrate the laser-induced deformation of ferrofluid surfaces with ultra-violet to infra-red lasers. The surface deformation reaches the bottom and breaks the liquid, achieving the highest liquid rupture thickness for over 1000 μm. The deformation process and rupture are related to strong Marangoni effect, high laser absorption and low viscosity of ferrofluid. As applications of the laser-controlled ferrofluid, we show that a ferrofluid droplet in the capillary can be easily moved horizontally and vertically by the illumination of a laser beam. We also demonstrate that letters and patterns can be written on the black surface of ferrofluid thin film with a laser beam even with a common laser pointer. Laser manipulation of ferrofluid also makes it a controlling vehicle for varieties of liquid or droplets.
3:54PM D15.00008: Long-time evolution of interfacial structure in dewetting* MENGFEI HE (Presenter), SIDNEY ROBERT NAGEL, University of Chicago — When a solid plate is withdrawn from a partially wetting liquid, a liquid layer dewets the moving substrate. High-speed imaging reveals alternating thin and thick regions in the entrained layer in the transverse direction at steady state. To quantify the absolute thickness of these steady-state structures precisely, I have developed an interferometric technique taking advantage of a varying angle of incidence. This method allows us to measure the absolute thickness as well as the local slope of the thin film. A new technique of likelihood maximization is applied to detect interference fringes. The result shows that the thicknesses of both regions of the film scale with the capillary number, Ca. In addition, a new region is observed during onset which differs from the behavior predicted by previous models.

*The work was primarily supported by the University of Chicago MRSEC, funded by the National Science Foundation under Grant No. DMR-1420709 and by NSF Grant No. DMR-1404841.

4:06PM D15.00009: Flows at Molecular Scales: Probing and Manipulating Ultra-Thin Supported Liquid Films CECILE CLAVAUD (Presenter), LAURENCE TALINI, CHRISTIAN FRÉTIGNY, ESPCI Paris — A hydrodynamical description of a liquid down to molecular levels has to take into account the effects specific to these very small scales. At molecular distances from a solid wall, phenomena such as slip or confinement-induced molecular layering have been observed with liquids in both experiments and numerical simulations. The ability to predict those effects is crucial in many fields involving flows at small scales close to a solid, such as nanofluidics or flows in mesoporous media. However, a unifying picture of the different reported features is still lacking, partly because their manifestations critically depend on the chemical nature of both the liquid and the solid medium.

We have developed a fully non invasive optical technique [Phys. Rev. Lett., 114, 227801 (2015)] in order to characterize the dynamics of a liquid by measuring the spontaneous thermal fluctuations of its free surface. Liquid films lying on solid substrates are formed with a thickness down to 5 nm using a Marangoni (surface tension gradient induced) flow. Using this technique, we evidence disjoining pressure effects, and are able to probe flow properties of ultra-thin liquid films.
4:18PM D15.00010: Towards nanoscale confinement in TEM liquid cells*  KYLE SENDGIKOSKI (Presenter), University of Maryland, College Park, ALOKIK KANWAL, JAMES ALEXANDER LIDDLE, Physical Measurement Laboratory, National Institute of Standards and Technology, JOHN CUMINGS, University of Maryland, College Park — Liquid confinement below micrometer thicknesses is of interest to several scientific disciplines and is inherently challenging to study experimentally. More extreme confinement at the single-digit nanometer scale is possible through the use of self-assembled nanostructures such as carbon nanotubes. Bridging the gap between micro- and nanoscale liquid confinement has been achieved with two-piece liquid cells within a transmission electron microscope (TEM), but irreproducibility and difficulties maintaining uniform liquid layer thickness makes high spatial and spectroscopic resolution challenging. We report on improvements made to a monolithic, in-situ TEM liquid cell\(^1\) with sub 40nm liquid thickness that overcomes the common challenges encountered with two-piece TEM liquid cells.


*This work is supported as a part of the Center for Enhanced Nanofluidic Transport (CENT), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0019112.

4:30PM D15.00011: Chemical Vapor Deposition Growth of Nickel Sulfide for optoelectronic device applications  NIDHI . (Presenter), TASHI NAUTIYAL, Physics, Indian Inst of Technology Roorkee, SAMARESH DAS, C.A.R.E., IIT Delhi — Nickel Sulfide (Ni\(_2\)S\(_2\)), a Transition Metal Di-chalcogenide (TMDC) has become an interesting material for the scientific community owing to its intrinsically small bandgap within the mid-infrared range [1] and superior charge transport properties. Experimentally, it is challenging to characterize the quality of NiS\(_2\). Although it offers a great opportunity for nanoelectronic devices. However, very few efforts have been given for the growth of NiS\(_2\) thin film for device applications. To date, NiS\(_2\) has been grown by the solution process and hydrothermal method and used for energy storage device applications. Here, we grow the NiS\(_2\) thin film on SiO\(_2\)/Si substrate by the chemical vapor deposition (CVD) technique. Several spectroscopic studies reveal the high-quality crystalline nature of CVD grown NiS\(_2\) film. We also fabricated the field-effect device at the nickel sulfide platform with thickness up to few nanometers (~23 nm). The performance of the fabricated device is characterized at room temperature. Nickel Sulfide field-effect device shows the drain current up ~10\(^{-6}\) A with drain voltage from -2 to +2 V.

References

Colloidal particle migration in combined Poiseuille and electrokinetic flows away from or towards the microchannel walls has recently been shown to be due to the particle slip velocity with respect to the fluid. The particle migration was attributed to an electrophoretic lift-like force, analogous to the inertial lift forces in sedimentation flows. The migration of colloidal particles towards the walls for dilute colloidal particle suspensions with diameters < 1 micron led to the assembly of distinct colloidal bands within microchannels (100 – 300 microns wide x 34 microns deep x 4cm long). Band formation requires opposing Poiseuille and electrokinetic flows. Band formation also requires a minimum applied potential threshold at a given shear rate. Band formation is a function of particle size and volume fraction, particle and channel wall zeta potential, electrolyte concentration, and the minimum electric field thresholds change non-monotonically for particle mixtures. Here, we discuss the effect of manipulating particle properties and fluid inertia over broad parametric ranges to elucidate robustness of particle migration to and away from walls, and the formation of particle bands.

Lattice Boltzmann Method for Designing cellular solids for effective acoustic noise cancellation

Acoustic technology based on Passive Noise Cancellation (PNC) has emerged as an excellent noise reduction strategy for both small and large environments. In general, PNC primarily focuses on designing specialty cellular materials, that can effectively attenuate unwanted sounds by virtue of its intrinsic morphology. Here, we design sound-absorbing materials and establish that by tailoring their morphological features, we can achieve acoustic noise cancellation, effectively. Our approach harnesses Lattice Boltzmann Method (LBM) to simulate sound propagation in two-phase cellular viscoelastic materials and our simulation results are in good agreement with the analytical calculations. In particular, using LBM, we designed various morphologies for cellular viscoelastic solids and demonstrate that the higher frequency waves attenuate faster compared to lower frequency waves. Further, we extend our approach for designing indoor acoustics and use reverberation time to quantify PNC for these systems. Our findings can be used not only to design miniaturized noise-canceling acoustic gadgets but also to design specific sound-absorbing materials for large indoor systems.

The authors thank IIT Gandhinagar for funding and support.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D16 DQI: Fluxonium and Novel Superconducting Qubits II
2:30PM D16.00001: Tunable Current Mirror Qubits: Experimental Status* JAMES WENNER (Presenter), MOE S KHALIL, Northrop Grumman Corporation, DANIEL WEISS, JENS KOCH, Northwestern University, DAVID FERGUSON, Northrop Grumman Corporation — In the last few years significant progress has been made in the development of tunable current-mirror qubits. This novel qubit type is projected to exhibit high coherence due to its insensitivity to environmental noise. However, as a consequence of their noise immunity, tunable current-mirror qubits are also insensitive to control signals, requiring novel control approaches. This talk reviews the successful demonstration of current-mirror test structures that share the same ‘Mobius’ capacitance connectivity as current-mirror qubits. The collective modes of these test structures exhibit a mode frequency parity effect such that even modes are much higher in frequency than odd modes—an indicator that such circuits can generate a parity valve effect—strong double-vortex hopping relative to single-vortex hopping—a key requirement for generating noise insensitivity. This talk also describes design optimizations of current-mirror qubits, and gives a status report on coherence tests, including tests that utilize adiabatic protection sweeps.

*This research was supported by the Army Research Office under contract W911NF-17-C-0024.

2:42PM D16.00002: Phase-shift flux qubit with a ferromagnetic π junction* TARO YAMASHITA (Presenter), Department of Electronics, Nagoya Univ, KUN ZUO, YOSHIRO URADE, Center for Emergent Matter Science (CEMS), RIKEN, WEI QIU, HIROTAKA TERAI, Advanced ICT Research Institute, National Institute of Information and Communications Technology, AKIRA FUJIMAKI, Department of Electronics, Nagoya Univ, YASUNOBU NAKAMURA, Research Center for Advanced Science and Technology, The University of Tokyo — A flux qubit with high anharmonicity is an attractive choice for large-scale superconducting quantum circuits. However, one of the biggest challenges is the necessity of an external flux bias corresponding to half flux quantum to achieve flux-insensitive point with the longest coherence time for each flux qubit. In light of this, we developed phase-shift flux qubits by integrating a ferromagnetic π junction in the qubit loop providing spontaneous π phase shift, enabling flux-bias-free operations [1]. The developed qubit consists of a superconducting loop with three Al/AlO$_x$/Al junctions and an NbN/CuNi/NbN π junction [2] on an Si substrate. The qubit is shunted to a large capacitor and is capacitively coupled to a coplanar waveguide resonator made of NbN/TiN. Our results indicate that the phase-shift qubits are indeed at their flux-insensitive point without any external flux, with a relatively long coherence. In this talk, we will discuss the NbN-Al hybrid fabrication process and the results of the spectroscopy and time-domain measurements.


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2:54PM D16.00003: Electrically-tunable phase-slip qubits  AHMED KENAWY (Presenter), Katholieke Univ Leuven, WIM MAGNUS, University of Antwerp, BART SOREE, imec — The simplest form of a flux qubit is constructed by interrupting a superconducting loop (e.g., a ring) with an insulating barrier, thus forming a Josephson junction. The tunneling of Cooper pairs across the insulating barrier allows for a coherent coupling of two macroscopic flux states with oppositely circulating currents. In a similar manner, one can interrupt the superconducting loop with a nanowire over which superconducting vortices are coherently exchanged, a mechanism referred to as quantum phase slips (QPSs), giving rise to phase-slip qubits. Here, we investigate the possibility of using a voltage-biased superconducting ring to realize a phase-slip qubit. Using time-dependent Ginzburg-Landau equations, we show that the bias voltage modulates the free energy barrier between subsequent flux states of the ring. For a small but non-zero barrier, we calculate the rate of QPSs as a function of bias voltage, and investigate the possibility of realizing electrically-tunable phase-slip qubits.

3:06PM D16.00004: Influence of charge fluctuations on Josephson phase-slip qubits*  CYRUS F. HIRJIBEHEDIN (Presenter), STEVEN WEBER, GABRIEL ORR SAMACH, DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, DANNA ROSENBERG, KYLE SERNIAK, JONILYN YODER, WILLIAM OLIVER, ANDREW JAMES KERMAN, MIT Lincoln Laboratory — The Josephson phase-slip qubit (JPSQ) [1] is a superconducting circuit designed to emulate a quantum S=1/2, with a vector dipole moment that is nearly independent of applied effective field, even near zero. This property should enable the realization of full quantum vector spin interactions, including non-Stoquastic interactions that are of interest for quantum annealing and Hamiltonian quantum computing. We characterize the influence of charge fluctuations on the JPSQ, examining both discrete quasiparticle tunneling as well as drifts and jumps in the background charge offset. In addition, we describe methods for mitigating the influence of these effects to enhance operational robustness.


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3:18PM D16.00005: Bifluxon: Fluxon-Parity-Protected Superconducting Qubit*  

KONSTANTIN KALASHNIKOV (Presenter), Rutgers University, New Brunswick, WEN TING HSIEH, Engineering Department, University of Massachusetts Boston, Boston, MA, WENYUAN ZHANG, WEN-SEN LU, PLAMEN KAMENOV, Rutgers University, New Brunswick, AGUSTIN DI PAOLO, ALEXANDRE BLAIS, Institut Quantique and Departement de Physique, Universite de Sherbrooke, Sherbrooke, Canada, MICHAEL GERSHENSON, Rutgers University, New Brunswick, MATTHEW T BELL, Engineering Department, University of Massachusetts Boston, Boston, MA — We have developed and characterized a symmetry-protected superconducting qubit that offers simultaneous exponential suppression of energy decay from both the charge and flux noise, and dephasing from flux noise [1]. The qubit is implemented as a superconducting loop formed by a Cooper-pair box (CPB) and a superinductor. Provided the offset charge on the CPB island is an odd number of electrons, the qubit potential corresponds to that of a cos (φ/2) Josephson element, preserving the parity of fluxons in the loop via Aharonov-Casher interference. Importantly, the protection can be turned on and off by controlling the CPB charge. In the protected state, the logical-state wavefunctions reside in disjoint regions of phase space, thereby ensuring protection against energy decay. By turning the protection on, we observed a ten-fold increase of the decay time, up to 100 μs. We will discuss strategies for mitigation of the charge noise effects by designing small arrays of cos (φ/2) elements.


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3:30PM D16.00006: Blochnium: A flux-tunable qubit with flux-insensitive coherence times  

RAY MENCIA (Presenter), IVAN PECHENEHKSIIY, LONG NGUYEN, YEN-HSIANG LIN, VLADIMIR MANUCHARYAN, University of Maryland, College Park — We introduce a flux-insensitive superconducting artificial atom nicknamed “blochnium", which is dual to a transmon. A blochnium circuit consists of a small-area Josephson junction shunted by a hyperinductance -- a micro-Henry range linear inductance whose impedance reaches above 160 kΩ. Using innovative circuit design and fabrication tricks, we significantly reduced the parasitic capacitance previously associated with such large inductances. The flux dispersion of the qubit transition is reduced to about 100 MHz while transitions to non-computational states can be tuned in the usual few-GHz range. Such a unique spectrum eliminates flux-noise induced dephasing during flux-controlled logical gates on coupled blochnium qubits, which in theory allows for gate fidelities better than 0.999.

3:42PM D16.00007: Novel Qubit Designs [Invited]  

LEV IOFFE (Presenter), University of Wisconsin — Lev ioffe has pioneered the field of topologically protected superconducting qubits, including the development of the rhombus qubit. This is a growing area within the superconducting community.
Rabi Oscillations in a Superconducting Nanowire Circuit

YANNICK SCHÖN (Presenter), JAN NICOLAS VOSS, MICHA WILDERMUTH, ANDRE SCHNEIDER, SEBASTIAN T. SKACEL, Karlsruhe Institute of Technology, MARTIN WEIDES, University of Glasgow, JARED H. COLE, Royal Melbourne Institute of Technology, HANNE ROTZINGER, ALEXEY V. USTINOV, Karlsruhe Institute of Technology — At feature sizes of nanometer scale, superconducting wires made from a material with high normal state resistance show a pronounced nonlinear microwave response. Disordered oxidized (granular) aluminum is a new material for superconducting quantum circuits, featuring not only a very high kinetic inductance but also microwave resonators with high quality factors [1,2]. Microscopically, it can be described as a disordered network of nano-scale aluminum grains, coupled via the Josephson effect [3].

We investigate the circuit quantum electrodynamics of superconducting nanowire oscillators. The sample circuit consists of a capacitively shunted nanowire with a width of about 20 nm and a varying length up to 350 nm, capacitively coupled to an on-chip resonator. By applying microwave pulses we observe Rabi oscillations, measure coherence times and the anharmonicity of the circuit. Despite the very compact design, simple top-down fabrication and high degree of disorder in the granular aluminum material, we observe lifetimes in the microsecond range. [4]


Ultrastrong coupling to parasitic modes in superconducting circuits with hyperinductors

IVAN PECHENEZHSKIY (Presenter), RAY MENCIA, ROMAN KUZMIN, LONG NGUYEN, YEN-HSIANG LIN, VLADIMIR MANUCHARYAN, University of Maryland, College Park — Parasitic modes are inevitable in any real-world circuit. The hope of any practical circuit design is that these modes are sufficiently above the frequency band of interest and do not participate in the low-frequency dynamics of the circuit. A notorious example is a large-value inductor. As the value of the inductance increases with the inductor length, so does the parasitic capacitance. Even in the simplest qubit circuit, in which a Josephson junction is shunted by a hyperinductor, the distributed nature of parasitic capacitance leads to multiple parasitic modes that couple ultrastrongly to the qubit. This ultrastrong coupling of the parasitic modes prevents a perturbation theory treatment of the qubit excitation spectra, while a complete quantum description of the underlying qubit circuit is computationally prohibitive. Progress can be made using an effective multi-mode Hamiltonian that fully reproduces the experimental data both below and above the lowest parasitic modes. This method allows the extraction of the bare qubit circuit parameters that are not renormalized by the presence of parasitic modes.
4:42PM D16.00010: Relaxation and decoherence of 2D fluxonium*  KARTHIK SRIKANTH BHARADWAJ (Presenter), FARSHAD FOROUGHI, Univ. Grenoble Alpes and Institut Néel, CNRS, 38000 Grenoble, France, ETIENNE DUMUR, Institute for Molecular Engineering, University of Chicago, Chicago IL 60637, USA, LUCA PLANAT, ARPIT RANADIVE, CÉCILE NAUD, OLIVIER BUISSON, NICOLAS ROCH, WIEBKE HASCH-GUICHARD, Univ. Grenoble Alpes and Institut Néel, CNRS, 38000 Grenoble, France — High anharmonicity and wide frequency tunability of the Fluxonium qubit make it an indispensable candidate for emerging quantum computers. Moreover fluxonium qubit in a 3D cavity or environment, when biased at sweet spot, shows very high relaxation time well above 1ms with a potential to achieve higher magnitude [1]. However, 2D and on-chip qubits are more favorable to scale up. The transition from 3D to 2D is not trivial as the coupling to the unwanted degrees of freedom increases a lot. In this work we coupled the fluxonium qubit to on-chip lumped element and distributed resonators. We have studied effect of different qubit parameters on the coherence times T1 and T2.


*This work is supported by the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No. 754303

4:54PM D16.00011: A Rotary Echo Flux Qubit*  ALEXANDER K SIROTA (Presenter), DAVID FERGUSON, Northrop Grumman - Mission Systems, DAVID I SCHUSTER, University of Chicago, RYAN J EPSTEIN, Northrop Grumman - Mission Systems — Flux qubits can have long T1 decay times due to nearly disjoint support of their flux basis wavefunctions. However the coupling of flux noise to circulating currents can lead to short dephasing times. This talk describes a qubit that utilizes a rotary echo control technique to maintain long T1 times yet also generating insensitivity to flux noise below a cutoff frequency. As the majority of the flux noise is low frequency in nature, this generates a qubit design capable of achieving high coherence.

*This research was supported by the Army Research Office under contract W911NF-17-C-0024.

5:06PM D16.00012: Characterization and control of topologically protected charge-parity qubits: Part 1*  KENNETH DODGE (Presenter), YEBIN LIU, MICHAEL SENATORE, Syracuse University, FNU NAVEEN, SHAOJIANG ZHU, ABIGAIL J SHEARROW, ANDREY KLOTS, LARA FAORO, LEV B IOFFE, ROBERT F MCDERMOTT, Physics, University of Wisconsin - Madison, BRITTON L PLOURDE, Syracuse University — Superconducting qubits with topological protection against local noise hold the promise of significantly enhanced coherence times and higher gate fidelities than is possible with conventional qubits. We are developing one such protected design — the hybrid charge-parity qubit — that combines arrays of compact, high inductances and conventional Josephson junctions with individual flux control for tuning each plaquette to a regime with a pi-periodic Josephson energy. With this scheme, concatenating multiple pi-periodic elements further enhances the degree of protection. Here, we will describe our experimental characterization of one- and two-plaquette devices through spectroscopy and time-domain measurements.

*Supported by the U.S. Government under Grant W911NF-18-1-0106
Decoherence poses a major impediment to the implementation of large-scale quantum processing with superconducting qubits. There have been tremendous improvements in superconducting qubit coherence times over the past two decades, with current state-of-the-art coherence levels approaching the threshold for fault-tolerant quantum computing. Nevertheless, for scalability, high-fidelity qubit control and qubits protected from sources of noise at the hardware level are needed. We implement qubit protection with pi-periodic superconducting elements made from flux-biased plaquettes of kinetic inductors and Josephson junctions that allow only double Cooper pair tunneling. The amount of protection from noise in such plaquette-based qubits can be further increased by concatenating plaquettes. We describe the design and characterization of a plaquette-based qubit with an embedded SQUID switch.

*Supported by the U.S. Government under Grant W911NF-18-1-0106

Monday, March 2, 2020 2:30 PM - 5:18 PM

Session D17 DQI: Focus Entanglement in Quantum Dot Arrays 203 - Patrick Harvey-Collard, Delft University of Technology - Tag(s): Focus
JOHN NICHOL (Presenter), University of Rochester — Among the different experimental platforms for quantum information processing, individual electron spins in semiconductor quantum dots stand out for their long coherence times and potential for scalable fabrication. The past years have witnessed substantial progress in the capabilities of spin qubits. However, coupling between distant electron spins, which is required for quantum error correction, presents a challenge, and this goal remains the focus of intense research. Quantum teleportation is a canonical method to transmit qubit states, but it has not previously been implemented in quantum-dot spin qubits. Here, we present a conditional quantum teleportation protocol for electron spin qubits in semiconductor quantum dots. We demonstrate this method, which relies on a recently-developed technique to distribute entangled states of spin qubits, through conditional teleportation of spin eigenstates, entanglement swapping, and gate teleportation. This method is a promising addition to the quantum-dot spin-qubit toolbox, and it will alleviate many of the challenges associated with long-distance coupling between spins and open the door to scalable spin-based quantum information processing.

*This work was sponsored the Defense Advanced Research Projects Agency under Grant No. D18AC00025 and the Army Research Office under Grant Nos. W911NF-16-1-0260 and W911NF-19-1-0167. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the Army Research Office or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein.

ELEANOR CRANE (Presenter), Electrical Engineering, University College London, ALEXANDER SCHUCKERT, Department of Physics and Institute for Advanced Study, Technical University Munich, NGUYEN HUY LE, Advanced Technology Institute, University of Surrey, ANDREW JAMES FISHER, Physics and Astronomy, University College London — Spin qubits of donors in silicon show some of the longest coherence times recorded and promise seamless integration of quantum computing into current semiconductor fabrication. However, current entangling gate implementations rely on knowledge of the exact value of the exchange interaction between donors, which decays as a highly oscillating exponential, making high fidelity entangling gates in multi-qubit fabricated devices a challenge. In this work, we show how this constraint can be released by using Rydberg blockade entangling gates between orbital excited states of donors, which are robust against variations in the interaction strength. We obtain these results by calculating induced dipole interactions of shallow and singly ionised deep donors using the finite element method and by simulating the entangling gate pulse sequence in the presence of decoherence with a Markovian Lindblad Master equation. Our study paves the way for near-term large scale quantum computations with donors in silicon by lowering the precision requirements on single donor placement.

*UK Engineering and Physical Sciences Research Council [COMPASSS/ADDRFSS,Grant No. EP/M009564/1].
International Max Planck Research School for Quantum Science and Technology (IMPRS-QST).
3:18PM D17.00003: Entanglement of encoded spin-qubits via curvature couplings to a superconducting cavity

RUSKO RUSKOV (Presenter), CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD 20740, U.S.A. — We propose entangling operation and preparation procedures based on curvature couplings of encoded spin qubits to a superconducting cavity, exploring the non-linear qubit response to a voltage variation. For two-qubit (n-qubit) entangling gate we explore acquired geometric phases via a time-modulated longitudinal \( \sigma_z \)-coupling, offering gate times of 10s of ns. No dipole moment is necessary: the qubit transverse \( \sigma_x \)-coupling to the resonator is zero at full sweet spot. This approach allows always-on, exchange-only qubits, for example, to stay on their `sweet spots" during gate operations, minimizing the charge noise and eliminating an always-on static longitudinal qubit-qubit coupling. We calculate gate errors due to the diffusion noise and damping of the resonator, the qubit charge dephasing, and a static spin-dependent resonator frequency shift (via a `dispersive-like" curvature coupling). Using spin-echo-like error suppression at optimal regimes, gate infidelities \( 10^{-2} \)-\( 10^{-3} \) can be achieved. For entangling preparation, one uses designated resonators to perform joint n-qubit quantum measurements with entangling times of 10s of ns, exploring both longitudinal and dispersive-like curvature couplings. The proposed schemes seem suitable for remote spin-to-spin entanglement.

3:30PM D17.00004: Far-detuned two-qubit operation of the quantum-dot hybrid qubit coupled to a microwave resonator

JOSE CARLOS ABADILLO-URIEL (Presenter), CAMERON KING, University of Wisconsin - Madison, SUSAN NAN COPPERSMITH, University of New South Wales, MARK G FRIESEN, University of Wisconsin - Madison — The quantum-dot hybrid qubit has a natural spin-charge hybridization that provides an electric dipole that can be used to perform EDSR or to couple the qubit to cavity photons. This electric-dipole moment is maximized in the charge-like regime, at small detuning, and it is reduced by going to the far-detuned regime. In this latter regime, the qubit behaves as a spin qubit, with good coherence properties, yet with a small dipolar moment.

In this work, we explore this far-detuned regime. The control parameters of the quantum-dot hybrid qubit can be adjusted to form a sweet spot in the far-detuned regime, increasing the qubit coherence times enough to allow operation with a small dipolar moment. At this sweet spot, the qubit can be strongly coupled to a superconducting resonator, allowing two-qubit gates to be performed. We find that the optimal operation of two-qubit gates, in terms of gate speed and experimental feasibility, is obtained by exploiting sideband transitions, achieving a 99% two-qubit gate fidelity in the best case.
3:42PM D17.00005: Coherent transport of spin by adiabatic passage in quantum dot arrays*

MICHAEL GULLANS (Presenter), JASON PETTA, Princeton University — The coherent transport of spin in arrays of quantum dots is important for distributing quantum information, or realizing more efficient spin-readout, across the array. A natural strategy to achieve charge transport in quantum dot arrays is known as coherent transport by adiabatic passage (CTAP). The simplicity of this method motivates the search for spin-based analogs of CTAP (spin-CTAP) that may allow robust spin transport. We develop the theoretical framework of spin-CTAP using the Heisenberg exchange interaction in a linear array of quantum dots. Applying an AC exchange modulation according to CTAP pulse sequences allows adiabatic spin-transfer across arbitrarily large arrays of dots. By choosing a staggered static exchange profile, we can ensure that only certain spin configurations realize the transfer protocol across the array, while other states are blocked from spin-CTAP. We show how to use this feature to generate arbitrarily large Greenberger-Horne-Zeilinger (GHZ) states in the system. Our transfer and entanglement generation protocols are immediately applicable to current experiments in quantum dot arrays.


3:54PM D17.00006: Robust two-qubit entangling gates using shaped pulses in silicon double quantum dots*

UTKAN GUNGORDU (Presenter), JASON PAUL KESTNER, Univ of Maryland-Baltimore County — Addressibility of spin qubits in a silicon double quantum dot setup in the (1,1) charge configuration relies on the difference between Zeeman splittings of electrons. When the difference is not sufficiently large, rotating wave approximation breaks down. We consider a device working in this regime, with always-on exchange coupling, and describe how a CZ gate and arbitrary one-qubit gates which are robust against charge noise can be implemented by smoothly pulsing the microwave source, while eliminating the crosstalk stroboscopically. We find that the correction required to compensate the most significant errors due to rotating-wave approximation, which is analogous to Bloch-Siegert shift in two-level systems, can be implemented by using virtual local gates.

*This research was sponsored by the Army Research Office (ARO), and was accomplished under Grant Number W911NF-17-1-0287.

4:06PM D17.00007: Democratizing Spin Qubits

CHARLES TAHAN (Presenter), Laboratory for Physical Sciences — I've been building Powerpoint-based quantum computers with electron spins in silicon for 19 years. Unfortunately, real-life-based quantum dot quantum computers are harder to implement. Fabrication, control, and materials challenges abound. The way to accelerate discovery is to make and measure more qubits. Here, I discuss separating the qubit realization and testing circuitry from the materials science and on-chip fabrication that will ultimately be necessary. This approach should allow us, in the shorter term, to characterize wafers non-invasively for their qubit-relevant properties, to make small qubit systems on various different materials with little extra cost, and even to test spin-qubit to superconducting cavity entanglement protocols where the best possible cavity quality is preserved. Such a testbed can advance the materials science of semiconductor quantum information devices and even enable small quantum computers.
4:18PM D17.00008: Fabrication and Measurement of Arrays of Few-Donor Quantum Dots

RICK SILVER (Presenter), XIQIAO WANG, RANJIT KASHID, ALBERT RIGOSI, JONATHAN WYRICK, FAN FEI, PRADEEP NAMBOODIRI, National Institute of Standards and Technology — NIST is using atomically precise fabrication to develop electronic devices for use in quantum information processing and quantum materials research. We are using hydrogen-based scanning probe lithography (STM) to enable deterministic placement of individual dopant atoms with atomically aligned contacts and gates to fabricate single and few atom transistors, as well as coupled few donor/quantum dot devices for spin and charge readout.

Here, we extend the STM-patterning method to fabricate coupled arrays of few atom clusters having multiple donors per dot, including a functional 3×3 quantum dot array device. Using the Si(100)2×1 surface reconstruction lattices as a natural atomic ruler, we designed the separation between a dot and its nearest neighbor dots or source/drain leads to span the regime from weakly coupled to strongly coupled ~ 5 to 8 nm separation. Low-temperature transport measurements are used to investigate the electron levels and energy spectra formed in individual dots versus energy spectra across the array of dots that result from the hybridization of quantum states. Combining electrical measurement results with simulations, we analyze the tunnel and capacitance couplings within this device to explore the rich physics in dot-arrays.

*Funded by a DOE grant.

4:30PM D17.00009: Realizing Discrete Time Crystals in Quantum Dot Spin Arrays with Magnetic Field Gradients

BIKUN LI (Presenter), JOHN VAN DYKE, ADA WARREN, SOPHIA E. ECONOMOU, EDWIN BARNES, Virginia Tech — A discrete time crystal is a non-equilibrium phase of matter that arises from a combination of interactions, disorder, and periodic driving. Previous work showed that it is possible to realize this phase in quantum dot spin arrays with nearest-neighbor exchange interactions if the number of pulses per period is substantially increased. Here, we show that the same result can be achieved using a magnetic field gradient instead of additional pulses, significantly reducing the demands on experimental capabilities. Numerical simulations of the return probability and mutual information confirm the time crystalline structure, which survives over a broad range of parameters and perturbations. In addition, we derive a stroboscopic effective Hamiltonian that provides further insight into the nature of this phase and the quantum state preservation properties it features.

*This work is supported by DARPA Grant No. D18AC00025.
4:42PM D17.00010: Exploring Many-body Localization in Quantum Dot Systems* BIKUN LI, JOHN VAN DYKE (Presenter), ADA WARREN, SOPHIA ECONOMOU, EDWIN BARNES, Physics, Virginia Tech — Recent experimental progress in the design and control of quantum dot arrays has opened new possibilities for studying one-dimensional spin chains within a highly tunable platform. We theoretically investigate the realization of many-body localized phases in a quantum dot system, the latter naturally yielding the nearest-neighbor Heisenberg model subject to a magnetic field gradient. We demonstrate how strong gradients take the Heisenberg model into an effective Ising Hamiltonian, and calculate various experimental and theoretical signatures of many-body localization in these systems. These include the quantum Fisher information and energy absorption, which are shown to agree with other metrics recently discussed in the literature. Our results indicate that gate-defined quantum dots provide a promising platform on which to explore many-body localization and related phenomena such as discrete time crystal phases in a controlled setting.

*This work is supported by DARPA Grant No. D18AC00025.

4:54PM D17.00011: Fine-tuning electron entanglement in two-dimensional artificial atoms DUNG N PHAM (Presenter), SATHWIK BHARADWAJ, Department of Physics, Worcester Polytechnic Institute, Worcester, MA, L RAMDAS RAM-MOHAN, Department of Physics, Electrical & Computer Engineering, and Mechanical Engineering, Worcester Polytechnic Institute, Worcester, MA — The spatial correlation of few electrons confined in semiconductor quantum dots is of great interest for realizing solid state quantum computing devices. Tunability of inter-electron interaction in quantum dots through geometrical manipulations, and external fields facilitates an enhanced level of control of their electronic properties. To this end, there have been several proposals to define deterministic teleportation protocols for quantum information processing using these artificial atoms. However, for all application purposes it is important to fabricate devices operating at resonant entanglement values. Here, we develop an action integral formalism in coordinate space for solving few-particle wavefunctions in arbitrary confinements. We obtain the spatial entanglement values for a wide range of two-dimensional quantum dots with varying potentials. Spectroscopy of two-electron entanglement reveals several novel phenomena such as entanglement resonances due to anti-crossings of excited states, and electron cluster formation. We further investigate the dependence of entanglement on external electric and magnetic fields and discuss the fine-tuning of electron correlation for useful quantum processes.
Operating four singlet-triplet qubits in a two-dimensional array of GaAs dots

FEDERICO FEDELE (Presenter), ANASUA CHATTERJEE, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark., SAEED FALLAHI, GEOFF C GARDNER, MICHAEL MANFRA, Department of Physics and Astronomy, Microsoft Quantum Purdue, Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, USA, FERDINAND KUEMMETH, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark. — Building small-scale spin-based quantum processors requires the ability to perform simultaneous, fast measurements in single- and two-dimensional qubit arrays, as well as overcome challenges like gate crosstalk, tuning in large parameter spaces, and pulse calibration. Here we present the simultaneous coherent manipulation and readout of a two-by-two singlet-triplet qubit array in GaAs, with a large multielectron dot coupler at the center. Using four independent charge-sensors read out via a frequency-multiplexed RF-reflectometry setup, we show coherent exchange oscillations, concurrently monitor the Overhauser field at the four sites of the array, and interlace different pulse operations. Finally, we establish a coherent exchange coupling between one qubit and the central multi-electron dot coupler, suggesting its use as a mechanism to provide on-demand connectivity within the array.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D18 GSNP: Flow of Dense Granular Materials and Suspension

205 - Jeremy Lechman, Sandia National Laboratories - Tag(s): Invited
Dense suspensions of hard particles in a simple liquid have become a model system in the soft condensed matter, granular materials, and rheology communities for the investigation of strongly non-Newtonian behaviors. A key aspect underlying the recent surge of activity has been the realization that, in addition to hydrodynamic interactions, frictional contact between particles can occur. In fact, friction forces were found to be essential in order to explain some of the most striking phenomena observed, such as an abrupt, essentially discontinuous onset of shear thickening, whereby the viscosity can jump up by over an order of magnitude as a critical shear rate is exceeded. So far, however, friction has typically been modelled as a parameter without considering its origin. Furthermore, a focus on the steady-state response has prevented most models from capturing transient phenomena, most notably the propagating jamming fronts associated with the transition from a shear-thickened to a solid-like, shear jammed state. Thus, there remain fundamental questions both at the nano-scale about the nature of the frictional interactions, and at the macro-scale about the relation between steady-state and transient dynamic phenomena.

This talk will discuss recent experiments and simulations that address these questions, focusing on the differences between discontinuous shear thickening (DST) and shear jamming (SJ). In particular, I will show how controlling the particles' shape, their surface chemistry, and the suspending solvent opens up new opportunities for designing the dynamic stress response of dense suspensions as they transform into a shear jammed state.

*In collaboration with Endao Han, Gray Jackson, Nicole James, Mike van der Naald, Abhi Singh, and Liang Zhao.
Work supported by ARO W911NF-16-1-0078, the Chicago MRSEC (NSF DMR-1420709), and CHiMaD.
3:06PM D18.00002: Investigating viscous to inertial transitions in granular suspensions with internal imaging* [Invited] ARSHAD KUDROLLI (Presenter), Clark University — We discuss experiments that probe the rheology of fluid-saturated granular beds coupled with the micromechanics of their flow using refractive index matching (RIM) techniques. These studies are fundamental to problems of erosion, sedimentation, and biolocomotion in such mediums. We will first discuss a sedimented bed which is sheared in a conical rheometer geometry which allows us to examine the system over prolonged periods under steady driving conditions. The shear experienced as a function of prescribed shear rate can be measured in this system along with the motion of the granular phase and the fluid phase. This allows us to determine the granular and fluid component of shear above and below the bed. We demonstrate that the appropriate control variable for the onset of bed motion with increasing shear is in fact the granular packing of the bed rather than the strength or the duration of the applied shear. Then, we show that the velocity profile of the suspended phase which develops between the clear fluid phase on top and a dense creeping granular bed below can be obtained from the applied strain rate and the Krieger-Dougherty model for the effective viscosity. We shall also discuss the drag and the unsteady flow of the medium resulting from the motion of a large solid intruder through the medium. The differences in the flow and drag encountered versus those observed in a viscous fluid and in dry granular media will be discussed going from the frictional to the inertial regime. We will highlight the difficulties encountered in interpreting the encountered rheology simply in terms of inertial and viscous numbers even in cases where the grains are weakly sedimenting.

*Supported by NSF Grant CBET-1805398 and DOE Grant DE-FG02-13ER16401.

3:42PM D18.00003: Continuum modeling of flow and size-segregation in dense granular materials* [Invited] DAVID HENANN (Presenter), DAREN LIU, SHIHONG LI, HARKIRAT SINGH, Brown University — Dense granular systems that consist of particles of disparate size segregate based on size during flow, resulting in complex, coupled segregation and flow fields. In this talk, we study size-segregation phenomenology using discrete-element method simulations of dense, bidisperse particles and propose a continuum model for coupled size-segregation and flow in dense, bidisperse granular systems. In our discrete simulations, we consider four flow configurations: (1) gravity-driven flow down a long vertical chute, (2) annular shear flow, (3) gravity-driven flow down a rough, inclined surface, and (4) planar shear flow in the presence of gravity - all while varying system parameters, such as the flow rate, flow configuration size, fraction of large/small grains, and grain-size ratio. Selected discrete simulation data inform continuum constitutive equations for the relative flux of large and small particles. The segregation model accounts for two driving forces - shear-strain-rate-gradients and pressure-gradients. When coupled with the nonlocal granular fluidity model - a nonlocal continuum model for dense granular flow - we show that both flow fields and segregation dynamics may be simultaneously captured using the coupled, continuum model - across all considered flow configurations, driving conditions, and mixture properties.

*This work was supported by funds from NSF-CBET-1552556.
Bedform dynamics: interaction, attraction and repulsion of dunes*

NATHALIE VRIEND (Presenter), KAROL A BACIK, Department of Applied Mathematics and Theoretical Physics, Univ of Cambridge, PAUL JARVIS, School of Earth and Environmental Sciences, University of Geneva — Bedforms are fascinating and captivating self-organising patterns; from wind-blown dunes on Earth and other planets to regular ripple patterns on riverbeds or coastal beaches. Loose sediment reorganizes when the aeolian (wind-driven) or aqueous (fluid-driven) forcing exceeds a critical value for mobilization of grains. The resulting sediment ripples can coarsen into larger-scale dunes. The migration speed of individual dunes depends inversely on their dimensions: the larger the dune, the slower it migrates.

Here, we present a unique, recirculating, laboratory experiment in which we create and trace aqueous dunes over long times. We examine the interaction between two dunes of different sizes, and present a phase space diagram with outcomes of the resulting interaction. Furthermore, we explore the feedback mechanism between a bedform and the flow providing the forcing, and identify a repulsion mechanism that ensures that bedforms do not coarsen without limit.

*NMV is supported by a Royal Society Dorothy Hodgkin Fellowship (DH120121). This research was partly funded by Royal Society Challenge Grant CH160065, an Isaac Newton Trust Early Career Grant RG 74916 and a PhD studentship from Schlumberger Research Cambridge Limited.
Granular materials are inherently heterogeneous, and it is therefore difficult to construct a continuum model that successfully spans all the way from creeping to well-developed flows. This deficiency has serious consequences for making predictions in geological and industrial flows, but also presents a very interesting challenge for physicists. Local rheologies, such as the $\mu(I)$ rheology, relate the local shear rate to the local stresses. However, they fail to describe creeping flows, non-trivial particle size scaling, and the influence of small vibrations on the flow. Recently, the development of nonlocal rheologies has made inroads into solving this problem by allowing the fluidity at any position in the flow to depend on a spatially-extended region. In my talk, I will describe several experiments on two-dimensional granular materials which bridge particle-scale, meso-scale, and continuum-scale approaches. We test the efficacy of local and nonlocal models for describing flows across various particle shapes, particle stiffness, packing fractions, shear rates, and geometries. Through a combination of photoelastic force measurements, boundary stress measurements, and particle-tracking, it is possible to both fully-characterize the flows and test the assumptions of nonlocal models. We find that a single set of material parameters is able to capture the rheology of a particular granular material under a variety of flow conditions. Our measurements confirm the prediction that there is a growing lengthscale at a finite yield stress ratio associated with a frictional yield criterion. Finally, we observe rearrangements of the force network extending into quasi-static regions of the flow where shear rates vanish, and propose connections between their dynamics and the mechanisms responsible for nonlocal behaviors.

*National Science Foundation, International Fine Particle Research Institute, James S. McDonnell Foundation

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D19 GMAG: Topological Spintronics using Chiral Antiferromagnets

2:30PM D19.00001: Physics of domains and domain walls in topological magnets* [Invited]
LEON BALENTS (Presenter), University of California, Santa Barbara — We will discuss the energetics and dynamics of domains and the boundaries between them in two examples of topological magnets: antiferromagnetic Weyl metals, as exemplified by Mn3Sn, and quantum anomalous Hall states as is observed in twisted bilayer graphene. The two cases will be distinctly contrasted and compared, and implications for experiments outlined.

*The work on Mn3Sn was supported by the NSF CMMT program under Grants No. DMR1818533, and that on QAHE by the DOE, Office of Science, Basic Energy Sciences under Award No. DE-FG02-08ER46524.
3:06PM D19.00002: Large magneto-optical Kerr effect in the non-collinear antiferromagnetic metal Mn₃Sn [invited]  TOMOYA HIGO (Presenter), ISSP, University of Tokyo, HUIYUAN MAN, Department of Physics and Astronomy, Johns Hopkins University, DANIEL B GOPMAN, National Institute of Standards and Technology, LIANG WU, Department of Physics and Astronomy, University of Pennsylvania, TAKASHI KORETUME, Department of Physics, Tohoku University, OLAF M VAN T ERVE, United States Naval Research Laboratory, YURY KABANOV, National Institute of Standards and Technology, DYLAN REES, Department of Physics, University of California, Berkeley, YUFAN LI, Department of Physics and Astronomy, Johns Hopkins University, MICHI-TO SUZUKI, Institute for Materials Research, Tohoku University, SHREYAS PATANKAR, Department of Physics, University of California, Berkeley, MUHAMMAD IKHLAS, ISSP, University of Tokyo, CHIA-LING CHIEN, Department of Physics and Astronomy, Johns Hopkins University, RYOTARO ARITA, RIKEN-CEMS, ROBERT D SHULL, National Institute of Standards and Technology, JOSEPH ORENSTEIN, Department of Physics, University of California, Berkeley, SATORU NAKATSUJI, Department of Physics, University of Tokyo — There has been a surge of interest in antiferromagnetic (AF) materials due to their favorable properties for device applications including a vanishingly small stray field, faster spin dynamics, and more abundance in nature compared to their ferromagnetic counterparts. In fact, motivated by these intriguing properties, several breakthroughs have been made: an anisotropic magnetoresistance (even-function response under time-reversal (TR)) for detecting collinear AF ordering [1]. Another breakthrough is an odd-function response under TR in the non-collinear antiferromagnetic metal Mn₃Sn such as an anomalous Hall effect (AHE) [2] and anomalous Nernst effect (ANE) [3] at zero magnetic field. Moreover, recent studies have revealed that Mn₃Sn is a TR symmetry breaking Weyl metal possessing a large and controllable Berry curvature in momentum space [4].

In this presentation, we will mainly talk about the magneto-optical properties of Mn₃Sn [5]. We found that despite a vanishingly small magnetization (~2 mμ₆/B/Mn), Mn₃Sn exhibits a large zero-field MOKE (~20 mdeg), comparable to that in ferromagnetic metals. Our first-principles calculation has clarified that the ferroic ordering of cluster magnetic octupoles in the AF state causes the MOKE even in its fully compensated AF state. This large MOKE further allows imaging of the octupole domains, which are strongly related to other TR-odd responses induced by the Berry curvature. We will also show that Mn₃Sn thin films exhibit the large time-reversal-odd response as well as the bulk Mn₃Sn [6]. These findings provide an important step for the further development of spintronics devices using AF materials.

Mn$_3$Sn exhibits a substantial anomalous Hall effect (AHE) at room temperature, the magnitude of which reaches almost the same order of magnitude as in ferromagnetic metals irrespective of a small spontaneous magnetization of about 1 mT [1]. This large AHE originates from a significantly enhanced Berry curvature associated with the formation of Weyl points near Fermi energy [2]. A detailed comparison between angle-resolved photoemission spectroscopy measurements and density functional theory calculations revealed significant bandwidth renormalization and damping effects due to the strong correlation among Mn 3d electrons. Magnetotransport measurements provide strong evidence for the chiral anomaly of Weyl fermions[3]. All the above characteristic electronic properties of Mn$_3$Sn imply that the spin Hall effect could also take place in the Mn$_3$Sn.

Our SHE experiments showed that the non-collinear antiferromagnet Mn$_3$Sn has richer spin Hall properties than non-magnetic materials, that is, the SHE has an unusual sign change when its triangularly ordered moments switch orientation. Our observations demonstrate that a novel type of contribution to the SHE (magnetic SHE) and the inverse SHE (MISHE) can be dominant in some magnetic materials, including antiferromagnets. We attribute this magnetic mechanism in Mn$_3$Sn to the momentum-dependent spin splitting produced by the non-collinear magnetic order [4]. This discovery further expands the horizons of antiferromagnet spintronics and motivates a universal outlook on spin-charge coupling mechanisms in spintronics.


*This work was supported by a Grant-in-Aid for Scientific Research on Innovative Area, “Nano Spin Conversion Science” (Grant No. 26103002) and CREST(JPMJCR15Q5).
Mn₃Ge* [Invited] JONATHAN GAUDET (Presenter), YOUZHE CHEN, SAYAK DASGUPTA, GUY G MARCUS, Johns Hopkins University, JIAO LIN, Neutron Scattering Division, Oak Ridge National Laboratory, YANG ZHAO, WANGCHUN CHEN, NIST Center for Neutron Research, National Institute of Standards and Technology, MATTHEW STONE, Neutron Scattering Division, Oak Ridge National Laboratory, MUHAMMAD IKHLAS, TAISHI CHEN, TAKAHIRO TOMITA, Institute for Solid State Physics, Univ of Tokyo-Kashiwanoha, OLEG TCHERNYSHYOV, Johns Hopkins University, SATORU NAKATSUJI, Institute for Solid State Physics, Univ of Tokyo-Kashiwanoha, COLLIN LESLIE BROHOLM, Johns Hopkins University — The kagome hexagonal compound Mn₃Ge is a room temperature non-collinear antiferromagnet with anomalous transport properties associated with electronic Weyl nodes near the chemical potential. The coupling of its electronic transports with magnetic order presents important technological opportunities for which, I will describe our experimental efforts to understand the magnetism of Mn₃Ge through neutron scattering techniques. Using polarized neutron diffraction, we show the magnetic order is a k=0 co-planar anti-chiral state with weak ferromagnetism described by a Γ₉ irreducible representation with magnetization remarkably aligned perpendicular to an applied field. Using time-of-flight neutron spectroscopy, we find three collective excitations above distinct Γ-point anisotropy gaps. These can be modeled as the normal modes of an anti-chiral triangular spin plaquette where an out-of-plane mode anti-crosses an optical phonon near 15-18 meV. Away from the zone center, magnetic excitations form a broad maximum near 75 meV with a half-width at half maximum of 25(5) meV indicative of itinerant magnetism. We develop a field theory of spin waves, which accurately describes the long wavelength magnetic properties, and use it to determine an effective low energy spin hamitonian for Mn₃Ge.

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331. JG acknowledges support from the NSERC Postdoctoral Fellowship Program. CB and YC were supported by the Gordon and Betty Moore Foundation under GBM-4532.
Despite the significant academic interest in them and their richness in nature, antiferromagnets have always been overshadowed by ferromagnets in real-life applications based on magnetism or spintronics. This is primarily due to the fact that antiferromagnet order parameters, in contrast to the ferromagnetic magnetization, are only weakly coupled to magnetic fields, and are hence difficult, in conventional view, to be manipulated. In this talk I will discuss a number of recent theoretical and experimental developments that counter this conventional wisdom, in a class of antiferromagnets that have stable noncollinear magnetic order. I will first explain a theory for the recent experimental discovery of time-reversal-symmetry-breaking counterparts of the conventional SHE and ISHE in the noncollinear antiferromagnet Mn3Sn, which we name as the magnetic spin Hall effect (MSHE) and the magnetic inverse spin Hall effect (MISHE), respectively. Then I will discuss the concept of spin density polarization, and how to use it to describe spin-Hall effects in a magnetic insulator as bulk effects, without using the spin current language. The talk will end with an exploration on the nontrivial orbital coupling between chiral antiferromagnets and external magnetic fields.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D20 DBIO GSNP: Physics of Social Interactions 301 - Orit Peleg, University of Colorado, Boulder - Tag(s): Focus, Undergrad Friendly
2:30PM D20.00001: Collective Behavior in Growth-Driven Systems* [Invited] YASMINE MEROZ (Presenter), Tel Aviv University — A variety of biological systems are not motile, but sessile in nature, relying on growth as the main driver of their movement. Groups of such growing organisms can form complex structures, such as the functional architecture of growing axons, or the adaptive structure of plant root systems. These processes are not yet understood, however the decentralized growth dynamics bear similarities to the collective behavior observed in groups of motile organisms, such as flocks of birds or schools of fish. Equivalent growth mechanisms make these systems amenable to a theoretical framework inspired by tropic responses of plants, where growth is considered implicitly as the driver of the observed bending towards a stimulus. Here we set the stage for the study of emergent growth-driven structures by developing a model for interacting growth-driven organs. Particularly, we analytically and numerically investigate the 2D dynamics of pairs of organs interacting via allotropism, i.e. each organ senses signals emitted at the tip of their neighbor and responds accordingly. In the case of local sensing we find a rich state space.

*This work was performed in part at the Aspen Center for Physics, which is supported by National Science Foundation Grant PHY-1607611. Research was partially supported by the Israel Science Foundation Grant (1981/14), and by the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 824074 (GrowBot).

3:06PM D20.00002: Collective Aggregation via Directed Pheromone Signaling in Honeybee Swarms DIEU MY NGUYEN, MICHAEL IUZZOLINO, AARON MANKEL, ORIT PELEG (Presenter), University of Colorado, Boulder — While pheromones are a prevalent volatile communication signal in nature, the range and noise tolerance of information exchange is limited by the spatiotemporal decay of these signals. Using honeybees as a model organism, we study the communication network of honeybee swarms that locate their queen by tracking her pheromones. Specifically, how can honeybees that are far away from the queen locate her? Our results suggest that bees who locate her pheromones, stop at a certain distance from her, raise their abdomens and fan their wings, driving airflow across the Nasonov gland, which disperses pheromones to the rest of the swarm. We show that bees arrange in a specific spatial distribution with a characteristic distance between individuals and a characteristic direction in which individuals broadcast the signal. This dynamic structure recruits new broadcasting bees over time as the pheromones traveled a distance which is orders of magnitude the size of an individual. We connect our experimental results to an agent based model of volatile communication network, and characterize the advantage of this directional communication strategy vs. an axisymmetric one.
3:18PM D20.00003: Social context alters behavioral interactions in bumblebees  GRACE MCKENZIE-SMITH (Presenter), YAN WANG, JEAN CHO, TALMO PEREIRA, SARAH KOCHER, JOSHUA SHAEVITZ, Princeton University — Bumblebees are eusocial insects that rely on successful cooperation to carry out collective tasks which keep the colony running smoothly. Individual bumblebees must be able to correctly interpret and respond to social cues within a busy hive in order to properly fulfill their role. In this study, we investigate how social context alters behavioral interactions among bumblebee (*Bombus impatiens*) workers by probing the behavior of differently aged bees either alone or paired with another bee. We track the posture of bees over time using a deep learning algorithm and quantify variation in social behavior by clustering the dynamics of individual body parts in addition to relative positioning, bee-to-bee antennation, and locomotion. We find a number of interesting differences between bees of different ages and castes, including variation in the responsiveness of individual bees to novel social partners.

3:30PM D20.00004: Brownian motion of fire ants hinders raft formation  HUNGTANG KO (Presenter), DAVID HU, Georgia Inst of Tech — When flooded, fire ants aggregate and form rafts to avoid drowning. Finding neighbors and attaching to them is a critical first step for raft formation. In this study, we observe individual fire ants perform random walk on the water surface. We characterize this exploratory behavior by measuring the orientational and translational diffusivity. Brownian motion of fire ants can be considered as thermal fluctuations which in turn inhibit the assembly of small rafts. Our results suggest that this repulsive mechanism is balanced by the attractive surface tension effect in the formations of larger rafts.

3:42PM D20.00005: Behavioral plasticity in jackdaw flocks  NICHOLAS OUELLETTE (Presenter), Stanford Univ, HANGJIAN LING, University of Massachusetts, Dartmouth, GUILLAM E MCIVOR, JOSEPH WESTLEY, University of Exeter, KASPER VAN DER VAART, Stanford Univ, RICHARD T VAUGHAN, Simon Fraser University, ALEX THORNTON, University of Exeter — Bird flocks are a classic example of collective behavior, where the cohesive motion of the flock as a whole is presumed to arise purely from local interactions. Flocking models tend to assume that every individual is an identical agent that plays by the same rules, and these rules are usually assumed to be immutable. In reality, however, interactions may be influenced by many factors, such as external stimuli and social relationships. I will present evidence from field studies of jackdaws, a highly social corvid species, that indeed flocks of this single species display different interaction rules in different ecological contexts. During the roosting season, large flocks spontaneously form in the evening as the birds return to their roosts. In these transit flocks, individual jackdaws interact topologically with a fixed number of their neighbors. Jackdaws also gather together in mobbing flocks to drive away predators, and such flocks can be induced experimentally using a model predator and playbacks of scolding and recruitment calls. In these mobbing flocks, jackdaws interact metrically over a fixed physical distance. This change in interaction type leads to a clear ordering phase transition as a function of group density in mobbing flocks that is absent in transit flocks.
3:54PM D20.00006: Shared behavioral mechanisms underlie *C. elegans* aggregation and swarming* SERENA DING (Presenter), Imperial College London, LINUS SCHUMACHER, University of Edinburgh, AVELINO JAVER, University of Oxford, ROBERT G ENDRES, ANDRE BROWN, Imperial College London — In complex biological systems, simple individual-level behavioral rules can give rise to emergent group-level behavior. While collective behavior has been well studied in cells and larger organisms, the mesoscopic scale is less understood, as it is unclear which sensory inputs and physical processes matter a priori. Here, we investigate collective feeding in the roundworm *C. elegans* at this intermediate scale, using quantitative phenotyping and agent-based modeling to identify behavioral rules underlying both aggregation and swarming—a dynamic phenotype only observed at longer timescales. Using fluorescence multi-worm tracking, we quantify aggregation in terms of individual dynamics and population-level statistics. Then we use agent-based simulations and approximate Bayesian inference to identify three key behavioral rules for aggregation: cluster-edge reversals, a density-dependent switch between crawling speeds, and taxis towards neighboring worms. Our simulations suggest that swarming is simply driven by local food depletion but otherwise employs the same behavioral mechanisms as the initial aggregation. We further expand our work by examining swarming at very high densities.

*BBSRC grant to AEXB and RGE (BB/N00065X/1); MRC grant to AEXB (MC-A658-5TY30).

4:06PM D20.00007: Predicting residential segregation using statistical physics approaches* YUCHAO CHEN (Presenter), Physics, Cornell University, YUNUS A KINKHABWALA, Applied and Engineering Physics, Cornell University, MALLORY GASPARD, Center for Applied Mathematics, Cornell University, MATTHEW HALL, Policy Analysis and Management, Cornell University, TOMAS ALBERTO ARIAS, ITAI COHEN, Physics, Cornell University — We introduce a statistical physics based method to predict racial residential segregation in human populations. Such predictions are increasingly important for informing policy decisions as human populations become more diverse and mobile. Here, we demonstrate how to make such predictions by extending a novel statistical physics approach called Density-Functional Fluctuation Theory (DFFT) to multi-component time-dependent systems. This technique uses observations of fluctuations in the local density of neighborhood racial composition to extract functions that separately quantify social and spatial preferences/constraints to predict demographic changes. As a demonstration, we simulate a population distribution using a Schelling-type segregation model, and use DFFT to predict both steady-state probability distributions and migration events after changes in the environment, social interactions, or number of individuals. Should these results extend to actual human populations, DFFT could be applied to demographic data to quantify segregation between different groups of people and predict how such populations will respond to proposed demographic changes.

*The work was supported by ARO W911NF-18-1-0032 and W911NF-16-1-0433. Y.K. was supported by DGE-1650441.
4:18PM D20.00008: Leader cells in collective chemotaxis: optimality and trade-offs
AUSTIN HOPKINS, BRIAN CAMLEY (Presenter), Johns Hopkins University — Clusters of cells can work together in order to follow a signal gradient, chemotaxing even when single cells do not. This behavior is robust over many cell types and many signals. Cells in different regions of migrating streams show different gene expression, suggesting cells specialize to leader and follower roles in collective chemotaxis. We use a simple mathematical model to find when specialization would be advantageous. In our model, leader cells sense the gradient with an accuracy that depends on the kinetics of ligand-receptor binding while follower cells attempt to follow the cluster's direction with a finite error. Intuitively, specialization into leaders and followers should be optimal when a few cells have much more information than the rest of the cluster, such as in the presence of a sharp transition from one chemical concentration to another. We do find this - but also find that high levels of specialization can be optimal in the opposite limit of a very shallow gradient. There is also an important tradeoff: clusters have to choose between speed in following a gradient and ability to reorient quickly.

*We acknowledge an IDIES Seed Grant and computational resources from the Maryland Advanced Research Computing Center.

4:30PM D20.00009: One fish, two fish, win fish, lose fish: Imaging and analyzing the fighting behavior of zebrafish in 3D
LIAM O'SHAUGHNESSY (Presenter), Vrije Univ (Free Univ), TATSUO IZAWA, Biological Physics Theory Unit, OIST Graduate University, ICHIRO MASAI, Developmental Neurobiology Unit, OIST Graduate University, JOSHUA SHAEVITZ, Physics and the Lewis-Sigler Institute, Princeton University, GREG STEPHENS, Vrije Univ (Free Univ) — Social interactions represent some of the most intriguing aspects of animal behavior, yet principled methods for quantifying the joint actions of two individuals are lacking. We detail a novel effort to measure and model social behavior in the 3D swimming dynamics of the adult zebrafish, Danio rerio. We describe a custom tracking apparatus consisting of multiple fast cameras, a large imaging volume, and a transparent interior cage to avoid reflection artifacts. We leverage advances in convolutional neural networks to develop 3D markerless bodypoint tracking of interacting fish, while maintaining organism identity. We focus on small groups, below any obvious collective limit, yet with a rich repertoire of interacting behaviors. Specifically, we examine stereotyped male-male fighting behaviors and analyze the dynamics using short segments of bodypoint configurations to identify ethological motifs directly from tracked data. We quantify longer-time dynamics as transitions between motifs, and we repeat our analysis in mutant fish with known social deficits.

*Project supported from the Human Frontier Science Program and OIST Graduate University. JWS was supported in part by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030).
4:42PM D20.00010: A Foraging Approach to Analyzing Infant and Caregiver Vocal Behavior
RITWIKA VALLOMPARAMBATH PANIKKASSERYSU (Presenter), GINA M. PRETZER, SARA MENDOZA, CHRISTOPHER SHERIDDE, CHRISTOPHER T. KELLO, AJAY GOPINATHAN, University of California, Merced, ANNE S. WARLAUMONT, University of California, Los Angeles — Previous research on infant vocal development suggests that human infants and adult caregivers search for sounds that have social value. We hypothesized that this could be a foraging process in a high-dimensional acoustic space where the resources are adapting to the forager's behavior. We studied day-long recordings of vocalizations in a naturalistic setting over the infants’ first year. We examined inter-vocalization time intervals and distance steps in an acoustic space defined by mean pitch and mean amplitude. Infant inter-vocalization intervals were shorter immediately following a vocal response from an adult. Adult intervals were shorter following an infant response and adult inter-vocalization pitch differences were smaller following the receipt of a vocal response from the infant. These findings are consistent with the hypothesis that infants forage vocally for social input. Increasing infant age was associated with changes in adult and infant inter-vocalization step sizes. The study represents a novel application of foraging theory to characterize infant-caregiver vocal interactions by assessing vocal exploration in terms of patterns of movement in acoustic space, which will allow this domain of behavior to be compared to other foraging behaviors.

4:54PM D20.00011: The Superorganism’s Circulatory System: Collective control of development through a socially exchanged fluid* [Invited] ADRIA C LEBOEUF (Presenter), Department of Biology, University of Fribourg — How can a distributed system like a social insect colony collectively decide how to allocate resources and mature over the long-term? Many but not all species of social insects engage in the social fluid exchange of trophallaxis. In species that perform ample trophallaxis, each individual within the colony is connected through the trophallactic network, including larvae. In carpenter ants, we’ve shown that components of trophallactic fluid can influence larval development, regulating the number of new adults produced. Furthermore, we find that some trophallactic fluid proteins have been co-opted from typical insect developmental pathways: as these proteins have become abundant in this social fluid, they show increasing signatures of adaptation such as repeated duplications and positive selection. Recent advances using long-term fluorescence imaging reveal how the content and timing of larval feeding through trophallaxis controls growth and developmental timing. Thus, in species that engage in this behavior, trophallaxis and trophallactic fluid present a means by which adults can regulate larval development according to the needs of the colony.

*This work was supported by grants from the Swiss National Science Foundation to Adria LeBoeuf and to Laurent Keller, the European Research Council to Richard Benton and to Laurent Keller, and the Swiss Friends of the Weizmann to Adria LeBoeuf and Ofer Feinerman.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D21 GERA: Probing and Manipulating Energy Related Materials 302
2:30PM D21.00001: Stanford R. Ovshinsky Sustainable Energy Fellowship award talk: 
**Structural Evolution of Nickel Thiophosphate Electrode Materials** [Invited] VICKY DOAN-NGUYEN (Presenter), Ohio State University — Transition metal phosphorus trichalcogenides have demonstrated to be promising electrodes in secondary Li-ion batteries with relatively high initial gravimetric capacity, and NiPS3 is in class of materials [1]. With C2/m symmetry, layers consist of edge-sharing Ni–S octahedra with a third of the Ni sites substituted with phosphorus dimers. NiPS3 has a theoretical capacity of 865 mAh/g corresponding to 6 mol of Li ions. The dual mechanisms of Li insertion/extraction and conversion are not well understood and is of interest due to the potential for high capacity relative to that of intercalation–based host materials. To better advance our understanding of the chemical and structural changes that contribute to capacity fade and irreversibly trapping Li ions, we employ the pair distribution functions technique and density functional theory to investigate the local structure evolution of the parent layered structure of NiPS3. The intercalation mechanism of Li ions shows decreased capacity fade within an operating voltage window of 1.0 V - 3.5 V vs. Li/Li+, depending on mass loading. [1] R. Brec, D. M. Schleich, G. Ouvrard, A. Louisy, and J. Rouxel, Inorg. Chem. 18, 1814 (1979).

*This work was supported in part by The Ohio State University Institute for Materials Research.

MICHAEL BERKOWITZ (Presenter), ALEXANDER MCLEOD, WILLIAM J ZHENG, LEO LO, DMITRI BASOV, Columbia Univ — Plasmonics is one of the most exciting and rapidly developing fields in the broad category of nanostructure engineering and plasmon polaritons offer a unique window into physics occurring at the nanoscale. As such, the ability to analytically predict and simulate both the dispersion and real-space propagation of plasmons in materials and fabricated nanostructures is of great interest to condensed matter physicists. There have recently been important strides in the field of simulating the aforementioned dispersion using the near-field response of materials [1] as well as the optical constants of the layers of layered heterostructures [2] to construct their P-polarized reflectivity and, consequently, the plasmonic dispersion relation. Here, we present a computationally efficient implementation of a generalized spectral method [3] for the simulation of the real-space propagation and interference of plasmons in the near-field for a material or heterostructure with a given set of optical constants and geometry.

References:  
3:18PM D21.00003: Identifying Local Variations in PV Material Properties via EBIC using In-Situ Light and Voltage Bias*  SEAN JONES (Presenter), Colorado School of Mines, HARVEY L GUTHREY, JOHN MOSELEY, NREL, BRIAN GORMAN, Colorado School of Mines — Understanding the relationship between microstructure and excess charge carrier collection is key to the improvement of photovoltaic devices. Electron Beam Induced Current (EBIC) is a technique which creates a high-resolution spatial map of this excess charge carrier collection; however, it can be difficult to interpret due to the complex local variations in structure and chemistry characteristic of thin film devices. In this work we exploit the response of a CdTe device to applied light and voltage bias during the EBIC measurement in order to extract parameters related to the cause of collection variations in the EBIC map, namely local doping density and built-in potential of the p-n junction. Our results indicate that these parameters can vary from grain to grain within the polycrystalline film and can strongly impact grain boundary recombination behavior as well as overall collection profiles. In addition to a discussion of the physics associated with this measurement, we also use our results as input to a PV device model to estimate the impact of local variation on device performance.

*This work was funded under U.S. Department of Energy (DOE) Contract No. DE-AC36-08GO28308.

3:30PM D21.00004: The improvement of carbon quantum dots on the manganese-nickel phosphide for electrocatalytic hydrogen evolution reaction*  WEIWU CHEN (Presenter), ZHAOJUN QIN, ZHIMING M WANG, HAI-ZHI SONG, University of Electronic Science and Technology of China, ZHIFENG REN, University of Houston — Transition-metal phosphides are good electrocatalysts for hydrogen evolution reaction due to their high catalytic efficiency and low cost. Carbon quantum dots (CQDs) deposited on top of the surface could make the phosphides even better for HER by increasing the number of active sites and reducing the charge transfer resistance. Here we adopt a simple method to synthesize CQDs-modified manganese-nickel phosphide (CQDs/Mn\textsubscript{x}Ni\textsubscript{5-x}P\textsubscript{4}) for efficient and stable HER activity using inexpensive raw materials. In 0.5 M H\textsubscript{2}SO\textsubscript{4}, CQDs/Mn\textsubscript{x}Ni\textsubscript{5-x}P\textsubscript{4} requires a low overpotential of only 31 mV to achieve a current density of 10 mA cm\textsuperscript{-2}, as well as having a low Tafel slope of 41.0 mV dec\textsuperscript{-1}, a large exchange current density of 1.753 mA cm\textsuperscript{-2}, and good stability, making it comparable with the best transition-metal-based catalyst available. Moreover, CQDs/Mn\textsubscript{x}Ni\textsubscript{5-x}P\textsubscript{4} also displays high activity and stability in alkaline solution, revealing that the ancillary role played by CQDs could be beneficial in both acidic and alkaline conditions. Based on our results, we believe that CQDs have great potential to be applied to other materials with various morphologies and structures for designing high-performance HER catalysts.

*The National Natural Science Foundation of China (Grant Nos. 51272038 and 51672037).
Monolayer MoS$_2$ on TiO$_2$ nanorods for enhanced electrocatalytic hydrogen evolution reaction

ANH DUC NGUYEN (Presenter), THI HUE PHAM, TRI KHOA NGUYEN, YOUNG HAN SHIN, YONG SOO KIM, Physics, Univ of Ulsan — The core-shell nanostructures of TMDCs and another semiconductor has been attracted much attention due to high surface-to-volume ratio and excellent electrocatalytic hydrogen evolution reaction (HER). Furthermore, number of TMDCs layer is an important factor that remarkably have an influence on the catalytic activity, therein monolayer (ML) is basically requirement. Herein, we have fabricated 2D@1D nanostructure; core of TiO$_2$ nanorods and shell of monolayer MoS$_2$. Firstly, TiO$_2$ NRs was grown on graphite foil by hydrothermal method. Then, TiO$_2$ was conformally covered by ML MoS$_2$ using metal organic chemical vapor deposition. A density functional theory was used to investigate the influence of TiO$_2$ on hydrogen Gibbs free energy ($\Delta G_H$) of basal plane MoS$_2$. When ML MoS$_2$ composite with TiO$_2$, the $\Delta G_H$ is closer to 0 eV, indicating that basal plane of ML-MoS$_2$ become more catalytically effective for HER. The onset overpotential of 190 mV and Tafel slope of 102 mV/dec were obtained for this kind of hetero-structural, which are much lower than that of nanoscale pristine MoS$_2$, in agreement with theoretical simulation result.

*This research was supported by National Research Foundation of Korea (NRF; 2017R1E1A1A01075350, 2019R1A6A1A11053838) through the funded by the Korean government.

Theoretical Study of Hydrogen storage with Ti doped B40 boron fullerene

PARAMITA HALDAR (Presenter), Birla Institute of Technology and Science — Hydrogen has been considered as one of the most promising energy carrier because of its abundance, cheap and environmental friendliness. It is necessary to develop high capacity hydrogen storage medium. Metal doping has been found to be an effective method to improve hydrogen adsorption ability. B40 fullerene has been considered as promising hydrogen storage material due to its large surface area. In this work hydrogen storage capacity with B40 fullerene doped with titanium (Ti) has been investigated by density functional theory. We have calculated the binding energies of Ti doped endohedrally and exohedrally at the hexagonal and heptagonal cavities. The binding energy calculation shows that the doping of Ti atoms outside the the hollow sites of the B40 structure is most stable. It is observed that the shape and stability of the B40 cage structure rapidly changes with increased number of doping atoms. HOMO-LUMO study predicts that the transport is mainly controlled by LUMO. 5 and 6 H$_2$ molecules are attached with Ti atoms on each hexagonal and heptagonal holes respectively. From the average hydrogen adsorption energies and nudged elastic band method study, it is observed that most of the interaction is physisorption with weak Vander Waals force interaction.
4:06PM D21.00007: Multi-technique characterization of atomic-layer-deposition-functionalized magnesium borohydride hydrogen storage materials  MARGARET FITZGERALD (Presenter), NOEMI LEICK, Colorado School of Mines, Golden, Colorado, KARL GROSS, H2Technology Consulting, LLC, Alamo, California, STEVEN CHRISTENSEN, National Renewable Energy Laboratory, Golden, Colorado, SVITLANA PYLYPENKO, Colorado School of Mines, Golden, Colorado — Hydrogen storage technologies are essential for the implementation of a cost-effective hydrogen economy. This talk focuses on novel, atomic layer deposition (ALD)-functionalized, magnesium borohydride (MBH) materials with the potential to store hydrogen at relatively low temperatures, moderate pressures, and energy densities greater than liquid or compressed hydrogen.¹ This ALD functionality shows improved hydrogen desorption from the neat MBH material, however the coating is not well understood. In order to better understand the mechanism of hydrogen adsorption and desorption with this coated MBH material, a thorough set of characterization techniques is needed, however the air- and beam- sensitivity of MBH materials present significant challenges. This talk defines these challenges and proposes potential solutions in order to conduct multi-scale, multi-technique characterization including ex-situ, identical location scanning transmission electron microscopy (STEM) and X-ray-spectroscopies. Combined with temperature programmed desorption (TPD), these studies reveal elusive interactions between the MBH materials and their coatings to further optimize the functionalization of MBH materials for hydrogen storage.


4:18PM D21.00008: Hydrogen permeation in V₇₅Fe₂₅ alloy investigated by in situ neutron diffraction* IN HWA CHO (Presenter), Dept. of Physics and Photon Science, Gwangju Institute of Science and Technology, YONG NAM CHOI, HEEJU LEE, Neutron Science Division, Korea Atomic Energy Research Institute, JAE-HYEOK SHIM, JIN-YOO SUH, Center for Energy Materials Research, Korea Institute of Science and Technology, HO JUN OH, SEONGHYUN HAN, DO YOUNG NOH, Dept. of Physics and Photon Science, Gwangju Institute of Science and Technology — in situ neutron diffraction measurements were carried out to investigate the hydrogen permeation path in V₇₅Fe₂₅ alloy. During heating under D₂, replacing H₂ to enhance neutron scattering length, the atmosphere at 3 bar, deuterium atoms began to permeate into V₇₅Fe₂₅ alloy at around 350 °C signified by the increased diffuse background signal. While the scattering feature of vanadium-iron solid solution in a BCC structure exhibits just a thermal expansion, a new Bragg peak corresponding to the α-V phase, in which deuterium atoms occupy tetrahedral interstitial sites of V randomly, appeared indicating that deuterium atoms are permeated to segregated vanadium clusters in V₇₅Fe₂₅ alloy. At room temperature, the hydrogen ordering in the vanadium clusters occurred, which is evidenced by a phase transition from α-V (cubic, solid solution) to β-V (monoclinic, hydride). Interestingly, we could conclude that additional hydrogen atoms occupy randomly octahedral sites surrounding ordered hydrogen atoms in the β-V of V₇₅Fe₂₅ alloy.

*This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean government (MSIP) (No. NRF-2015R1A5A1009962, No. 2017R1A6A3A11035944, No. 2012M2A2A6004262).
**4:30PM D21.00009: Extraordinary cycling stability of pristine nickel hexaaminobenzene MOF supercapacitors**

**FATIMA AMIR** (Presenter), **SEAN C WECHSLER**, Winthrop University —

Metal-organic frameworks (MOFs) are a newly emerging class of materials that have received enormous attention because of their unique features such as high surface area, rich microporosity, and tunable pores size. MOFs are very promising electrode materials for supercapacitors; however, the application of MOFs as supercapacitors electrodes has been hindered by their conventionally poor conductivity. To improve their conductivity, MOFs have been mixed with different conductive additives and binders. Very few pristine MOFs have been explored as electrodes materials for energy storage devices. Herein, we report for the first time the fabrication of pristine nickel hexaaminobenzene (Ni$_3$(HAB)$_2$) supercapacitors electrodes via electrophoretic deposition. The obtained MOF supercapacitor delivered an outstanding areal capacitance of 13.65 mF cm$^{-2}$ and an exceptional ultra-high cycling stability with a retention of about 81.2% after 50,000 cycles. Moreover, the Ni$_3$(HAB)$_2$ supercapacitors exhibited an excellent areal energy density of 920 μWh cm$^{-2}$ at an areal power density of 130 mW cm$^{-2}$.

*NSF-EPSCoR Award #OIA-1655740

**4:42PM D21.00010: Various Graphene-Based Composites For an Efficient and Durable Supercapacitor**

**DINESH SINGH** (Presenter), **LEONARDO VIVAS**, Department of Physics, University of Santiago Chile, **RAJESH KUMAR**, Department of Electrical and Electronic Information Engineering, Toyohashi University of Technology —

Recently invented graphene and its astounding properties, such as very high theoretical surface area, excellent thermal conductivity, superior mechanical properties, and ultra-high electron mobility have led it to explore its widespread applications in electronics, optics, biomedicine, energy harvesting and storage. Electrochemical double layer capacitor also called as Supercapacitors have attracted a great attention due to its fast charging, instant power delivery and ability to sustain millions of charge-discharge cycles at higher current densities. Graphene, having very high surface area is the most suitable candidate for the efficient energy storage and low cost of production is another benefit for widespread commercialization. Here we present the variety of graphene-based structures/composites and their applications as a high-performance supercapacitor. Various metals and transition metal oxides (such as Au, TiO$_2$, cobalt oxides and Ni encapsulated CNT etc.) based composites with graphene are synthesized by hydrothermal/microwave methods and their potential applications as a supercapacitor will be discussed and described.

*The support from the Millennium Institute for Research in Optics (MIRO) Chile is acknowledged.
**4:54PM D21.00011: High Performance Structural Electrochemical Double Layer Supercapacitors Using Graphene-Metal Nanoparticle-Polymer Composites**  
SHASHI P KARNA (Presenter), Weapons & Materials Research Directorate, APG, MD, 21005, CCDC Army Research Laboratory, ASHWINI K SRIVASTAVA, Department of Chemistry, Vidyanagari, Santacruz (E), Mumbai - 400098, India, University of Mumbai — Electrochemical double layer (ECDL) supercapacitors (SCs) offer a promising technology to address the ever-increasing demand on power and energy in modern technologies. Unlike batteries, which have high energy density, but low power densities, the SCs can provide very high power density, but generally have low energy density. This can, however, be surmounted by using Gr which can act as a high mobility electrode as well as efficient charge collector from the electrochemical double layer formed near its surface. Additionally, use of Gr as electrode material puts little or no penalty on weight and can be easily integrated in structural platform. Taking advantage of such novel properties of Gr, we have begun to develop Gr-Metal/metal oxide nanoparticle (MNP)-polymer (Poly) composite – based electrochemical super-capacitors. The resulting SCs, where Gr-MNP-Poly composite serves as the electrodes, charged through a capacitive double-layer mechanism, exhibit considerably high power density as well as energy density, not achievable by batteries. Results on the electrochemical properties of ECDL SCs formed with the use of Gr-PdNP, Gr-porous CuO, and Gr-AgNP and conducting polymer composites will be presented.

**5:06PM D21.00012: Tracking the capacitive energy storage process in layered MXene across length scales**  
PAUL KENT (Presenter), QIANG GAO, WEIWEI SUN, Oak Ridge National Lab, POORANDOKHT ILANI-KASHKOULI, Georgia State University, ALEXANDER TSELEV, University of Aveiro, NADINE KABENGI, Georgia State University, MICHAEL NAGUIB, Tulane University, MOHAMED ALHABEB, Drexel University, WAN-YU TSAI, ARTHUR BADDORF, JINGSONG HUANG, STEPHEN JESSE, Oak Ridge National Lab, YURY GOGOTSI, Drexel University, NINA BALKE, Oak Ridge National Lab — Intercalation of ions in layered materials forms the basis of electrochemical energy storage and conversion and is especially attractive due to the typically ultra-fast intercalation kinetics. Enhancing the energy stored and power delivered by these materials relies strongly on improved understanding of the intercalation chemistry of cations including the intricate interplay of cations, water, and electrode interactions as well as the role of confinement. Here we report a highly integrated study between experimental and modeling approaches to investigate the intercalation processes for aqueous Li⁺, Na⁺, K⁺, Cs⁺, Mg²⁺ into Ti₃C₂ MXenes. Experiments include microcalorimetry, atomic force microscopy and cyclic voltammetry whose results are directly linked to the results of ab initio modeling. Our integrated analysis allows for a complete understanding of energy storage processes highlighting the importance of the dynamics of cations and positionings and their role in capacitive energy storage properties. Our findings will expedite the evolutions of various energy related functional devices driven by the design of higher-performing membranes and two-dimensional materials.
By using a photonic curing system (PulseForge 1300, NovaCentrix), we have instantaneously synthesized manganese oxide thin films. Characterizations are done by using Scanning Electron Microscopy, X-ray Diffraction, and Raman Spectroscopy. Electrochemical characterization, i.e., cyclic voltammetry, charge-discharge cycling, and electrochemical impedance spectroscopy (EIS) were carried out in three-electrode cell configuration (where Hg-HgO, Pt-wire, and our sample are reference, counter and working electrodes respectively) with 1 M KOH as the electrolyte. The presence of redox peaks in cyclic voltammetry curves confirms the pseudocapacitive behavior of the sample while identical CV curves even at higher scan rates further suggest excellent rate capability and ideal supercapacitor behavior. The galvanostatic charge-discharge measurements (GCD) performed at 0.2 mA current resulted in initial specific capacitance as high as 11 mF/cm² for 2-pulses irradiated electrode. After performing GCD measurements for 100000 cycles, we found that the electrode retains as high as 89%, which shows that as prepared electrode possesses excellent stability and long lifetime.

*This work was funded by Louisiana Board of Regents, Industrial Ties to Research Subprogram, Grant Number LEQSF(2017-20)-RD-B-04.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D22 DBIO: Physics of Proteins: Peptides and Small Proteins 303 -

Wouter Hoff, Oklahoma State University-Stillwater - Tag(s): Focus
HAO DONG (Presenter), Kuang Yaming Honors School, Nanjing University — Molecular self-assembly provides a chemical strategy for the synthesis of nanostructures by using the principles of nature, and peptides serve as the promising building block to construct adaptable molecular architectures. Recently, a series of hepta-peptides with alternative hydrophobic and hydrophilic residues were reported to form amyloid-like structures, which were capable of catalyzing acyl ester hydrolysis with remarkable efficiency. However, it remains elusive about the atomic structures of the fibrils: what is the origin of the sequence-dependent catalytic activity? How does the ester hydrolysis catalyzed by the fibril? In this work, the atomic structure of the aggregates was determined by using molecular modelling and further validated by solid-state NMR experiments, where the fibril with high activity adopts twisted parallel configuration within each layer, and the one with low activity is in flat antiparallel configuration [1]. The polymorphism originates from the interactions between different regions of the building block peptides, where the delicate balance between rigidity and flexibility plays an important role. We further show that the p-nitrophenylacetate (pNPA) hydrolysis reactions catalyzed by two different fibrils follow similar mechanism, and the difference in microenvironment at the active site between the natural enzyme and the present self-assembled fibrils should accounts for the different catalytic activities. The present work provides atomic understanding of the structure and function of self-assembled fibrils formed with short-peptides, and thus sheds new insight on designing aggregates with better functions.

References

*This work was supported by the National Natural Science Foundation of China (Grant Nos. 21503107, 21773115 and 21833002), the Natural Science Foundation of JiangSu Province (Grant No. SBK2015041570), and the "Jiangsu Specially-Appointed Professor" program.
3:06PM D22.00002: Representation of the Conformational Ensemble of Peptides in Coarse Grained Simulations*  MEHMET SAYAR (Presenter), Koc University — Proteins/peptides can adopt to different environments by altering their conformation. Novel experimental techniques have enabled a quantitative characterization of this structural heterogeneity. In molecular dynamics simulations capturing this conformational ensemble quantitatively remains a major challenge. Even in atomistic simulations one has to find the best force field for the molecule of interest. With coarse grained (CG) simulations, where the aim is to reduce the degrees of freedom to reach the relevant length and time scales, representation of the conformational ensemble becomes even more problematic. Here, we revisit a recent CG model from our group, which was designed and tested for representing the aggregation driven conformational change of LKa14 peptide. We demonstrate here, that the structure/physics based approach used in the original parameterization of our CG model, strongly depends on the reference system chosen and excluded volume interactions. The updated model can recover the whole conformational ensemble in a quantitative manner, while maintaining the aggregation driven conformational transformation feature. This balanced parametrization leads to a sequence transferable CG model.

*The authors thank TUBITAK for funding (grant no. 212T184).

3:18PM D22.00003: Polarization of Intrinsically Disordered Proteins in the Presence of Charged Biopolymers: the Case of Tau Protein  ISABEL RUFFIN (Presenter), Physics, Duke University, CHRISTIAN APONTE-RIVERA, Mechanical Engineering and Materials Science, Duke University, MICHAEL RUBINSTEIN, Mechanical Engineering and Materials Science, Chemistry, Biomedical Engineering, Physics, Duke University — Tau protein is an intrinsically disordered protein known to be associated with the progression of neurodegenerative diseases. In cells, tau interacts with charged macromolecules, including high charge density polyanions such as RNA and microtubules. Although attraction between tau protein and negatively charged biopolymers is thought to play an important role in cell function, the mechanisms leading to attraction between tau protein and negatively charged biopolymers remain poorly understood. We study tau protein conformations and polarization using molecular dynamics simulations. First, we study the electrostatically driven collapse of tau protein, and connect the resulting conformation to features of its charge sequence. We then study how the conformations of tau protein change in the presence of a constant electric field and in the presence of a negatively charged biopolymer. With the latter, we quantify polarization induced attraction of tau protein to biopolymers. The implications of conformational changes of tau protein as it interacts with polyanions inside the cell will be discussed.
3:30PM D22.00004: Strategic incorporation of fluorinated prolines can lead to faster folding and stable proteins  AJAY MURALIDHARAN (Presenter), JR SCHMIDT, ARUN YETHIRAJ, University of Wisconsin - Madison — A single atom substitution in a proline residue of ribonuclease A can lead to accelerated folding into its 3D structure with increased thermostability. It has been suggested that this can be caused by stereo-electronic effects due to fluorination of amino acids. In this work we use quantum chemistry and QM/MM methods coupled with accelerated sampling to study the static and dynamic properties of proline containing peptides in water, with a focus on the effect of fluorination on the free energy surface and conformational properties. We compare the free energy surfaces of plain vs fluorinated dipeptides along the amide dihedral and the proline ring pucker reaction coordinates to examine the effect of fluorination. Finally, we characterize the important interactions in the system: namely intramolecular H-bonding, n -> pi* and gauche interactions in the presence of explicit solvent. We find that the experimental data can be understood from the change in the dihedral potential surface due to electronic structure differences due to fluorination. The impact of this on the conformational properties of peptides and self-assembly in solution is discussed.

3:42PM D22.00005: Low Temperature Protein Refolding Suggested by Molecular Simulation*  DANIEL KOZUCH (Presenter), Chemical and Biological Engineering, Princeton University, FRANK H. STILLINGER, Chemistry, Princeton University, PABLO GASTON DEBENEDETTI, Chemical and Biological Engineering, Princeton University — The function of critical biological materials, such as proteins, is intrinsically tied to their structure, and this structure is in turn heavily dependent on the properties of the solvent, most commonly water. As water is known to exhibit anomalous properties, especially at supercooled temperatures, it is natural to ask how these properties might impact the thermodynamics of protein folding. To investigate this question, we use molecular simulation to explore the behavior of a model protein, Trp-cage, as low as 70 K below the freezing point of the solvent. Surprisingly, we find that while the expected cold denaturation of the protein is observed at moderate supercooling, further cooling to more than 55 K below the freezing point leads to cold refolding of the protein. Structural and hydrogen bonding analysis suggests that this refolding is driven by desolvation of the protein’s hydrophobic core, likely related to the pronounced decrease in density at this temperature. Beyond their intrinsic fundamental interest, these results have implications for cryo-microscopy and cryo-preservation, where biological materials are often transiently subjected to these extreme conditions.

*NSF - Award CHE1856704
NSF - Graduate Research Fellowship Grant No. DGE-1656466
van der Waals Forces in Biomolecular Systems: from Solvation to Long-range Interaction Mechanisms

MARTIN STOEHR (Presenter), Physics and Materials Science Research Unit, University of Luxembourg, MATTEO GORI, PHILIP KURIAN, Quantum Biology Laboratory, Howard University, Washington, DC, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, University of Luxembourg — One decisive characteristic of the biomolecular machinery is the access to a rich set of coordinated processes within a small energy window. Most of these processes involve collective conformational changes and occur in an aqueous environment. Conformational changes of (bio)molecules as well as their interaction with water are thereby largely governed by non-covalent van der Waals (vdW) dispersion interactions. By virtue of their intrinsically collective nature, vdW forces also represent a key influence on collective nuclear behavior. Our understanding of vdW interactions in large-scale (bio)molecular systems, however, is still rather limited [Chem. Soc. Rev. 2019, 48, 4118]. Here, we employ the Many-Body Dispersion framework to investigate the vdW interaction in biomolecular systems and its spatial and spectral aspects. In particular, we show the role of beyond-pairwise vdW forces for protein stability and highlight the delocalized character of the protein-water vdW interaction. We further examine intermolecular electronic behaviors and reveal a coexistence of strong delocalization with spatially-separated yet correlated, local domains. This, ultimately, forms the basis for a potential, efficient long-range interaction mechanism for coordinated processes in biomolecular systems.

The Assessment of MD Force Fields with Respect to Alanine Conformations in Aqueous Solutions

SHUTING ZHANG (Presenter), Physics, Drexel Univ, REINHARD SCHWEITZER-STENNER, Chemistry, Drexel Univ, BRIGITA URBANC, Physics, Drexel Univ — The ability to reproduce conformational ensembles of the central alanine residue in GAG and AAA obtained from experimentally-derived φ- and ψ-dependent J coupling constants and amide I’ profiles is examined for six molecular dynamics (MD) force fields (Amber ff14SB, Amber ff99SBnmr1, Amber ff03ws, OPLS-AA/L, OPLS-AA/M, and CHARMM36). Compared to the empirical Gaussian model, which is constructed to best fit the experimental data, MD-derived Ramachandran plots produce overly constricted polyproline II (pPII) basin, an overpopulated antiparallel β basin, and an underpopulated transitional β basin. Our results show that Amber ff14SB best reproduces the experimental J coupling constants and yields the highest pPII populations of the central alanine residue in GAG (55%) and AAA (63%), in a good agreement with the the Gaussian model (59% and 76%). The comparison between experimental and MD-derived results for GAG in water is extended to various water/ethanol mixtures in order to further evaluate Amber ff14SB, CHARMM36, and OPLS-AA/M. Amber ff14SB again outperforms CHARMM36 and OPLS-AA/M in reproducing experimental J coupling constants and amide I’ profiles.

*This material is based upon work supported by the National Science Foundation under Grant No. MCB-181765 and DMR-1707770.
4:18PM D22.00008: Developing an explicit solvent model for protein aggregation* JUTTA LUETTMER-STRATHMANN (Presenter), Physics and Chemistry, University of Akron — Protein aggregation is responsible for amyloid formation and implicated in many neurological diseases. Since protein aggregation is a slow process, intermediate resolution protein models with implicit solvent have been developed to extend the time scale accessible to computer simulations. These models have been improved over many years and have become a valuable tool to support and interpret experimental work on protein aggregation. However, explicit solvent models are required to describe such processes as thermophoresis, which has recently become a tool to study fibril formation. In this work, we start from an off-lattice, mesoscale protein model with implicit solvent to develop an explicit solvent model that reproduces the equilibrium conformational and aggregation properties of the original model. To this end, we choose a solvent that is compatible with the protein model and perform simulations where the interaction parameters are adjusted during the simulation to match the desired properties. Applying the approach to short peptides in water, we find that solvent-solvent interactions are essential.

*Research Center Juelich and the University of Halle (DFG - SFB TRR 102)

4:30PM D22.00009: A kinetic analysis of local fluctuations in ubiquitin by combining the LE4PD normal modes and Markov state modeling* ERIC BEYERLE (Presenter), MARINA GIUSEPPINA GUENZA, Univ of Oregon — Following the conformational selection hypothesis, accurately determining the location and magnitude of fluctuations along a protein’s primary sequence is important in describing its mechanism of binding, so methods describing precisely the fluctuation dynamics of proteins can help reveal their biological function. Here, we model the fluctuation dynamics and kinetics of the protein ubiquitin using a coarse-grained description of the protein's dynamics, the Langevin Equation for Protein Dynamics (LE4PD), which decomposes the dynamics of a protein into dynamical pathways that explore mode-dependent free-energy surfaces. Using as input to the theory statistics from a molecular dynamics simulation, we calculate the timescales of the slow LE4PD modes using Markov state models. The predicted timescales of these LE4PD modes can be elucidated using the committor function, and a version of the string method is used to extract real-space fluctuations of the protein from the mode representation. We find the dynamics predicted by the slow LE4PD modes correspond to motion in important binding regions of the protein. We also show that the fastest LE4PD modes correspond to localized, conserved fluctuations along the protein's primary sequence.

*NSF Grant No. CHE-1665466, NSF Grant No. ACI-154856
4:42PM D22.00010: Non-additive effects of denaturing and protective cosolvents on protein stability* PRITAM GANGULY (Presenter), JOAN-EMMA SHEA, University of California, Santa Barbara — The conformational stability of the Trpcage protein, in the presence of pure and mixed solutions of two denaturants, urea and guanidinium chloride (GdmCl), and one protective osmolyte, trimethylamine N-oxide (TMAO), are studied using enhanced-sampling all-atomistic molecular dynamics simulations. We find that the pure and the mixed solutions of urea and GdmCl denature Trpcage as a whole, but remarkably, the helical segment 1NLYIQWL7 of Trpcage is stabilized in mixed GdmCl-urea solutions. For this helical segment, we find that urea "over solvates" the peptide backbone by reorganizing water molecules from the peptide side chains to the peptide backbone and GdmCl strongly dehydrates the side chains. The effects of urea and GdmCl on the solvation structure of the peptide are non-additive and urea depletes Gdm+ from the surface of the peptide in mixed urea-GdmCl solutions. An intricate thermodynamic balance between these non-additive effects stabilizes the helix in mixed urea-GdmCl solutions. Interestingly, we find that the protective osmolyte TMAO also depletes Gdm+ from the peptide-surface in mixed TMAO-GdmCl solutions and the mixture of TMAO and GdmCl is less effective than GdmCl solutions in counteracting the urea-denaturation of the helix.

*NSF: TG-MCA05S027, MCB-1716956

4:54PM D22.00011: Short peptides assemble to produce enzyme-like catalysts.* [Invited] IVAN KORENDOVYCH (Presenter), Syracuse University — Design of a novel catalytic function in proteins and peptides, apart from its inherent practical value, is important for fundamental understanding of enzymatic activity. We will present applications of a minimalistic approach to design of artificial enzymes. We designed a series of short peptides that self-assemble into amyloid-like fibrils to act as Zn2+-dependent hydrolases. Zn2+ helps stabilize the fibril formation, while also acting as a cofactor to catalyze acyl ester hydrolysis and carbon dioxide hydration. These results indicate that amyloid fibrils are able to not only catalyze their own formation – they also can catalyze chemical reactions. Excitingly, the specific activities shown by these catalytic amyloids are on par with those shown by natural enzymes. Thus, amyloids might have served as intermediates in the evolution of modern-day enzymes. This work has implications for the design of self-assembling nanostructured catalysts including ones containing a variety of biological and non-biological metal ions.


*This work was supported by the NIH (grant GM119634), the Nappi Family, CRDF Global (grant OISE 18-63891-0), and the Alexander von Humboldt Foundation.

Monday, March 2, 2020 2:30 PM - 5:06 PM

Session D23 DBIO GSNP: Membranes and Channels 304 - Loren Hough, Univ of Colorado, Boulder
2:30PM D23.00001: Formation and Properties of Self-Assembled Nanoparticle-Supported Lipid Bilayer Probed Through Molecular Dynamics Simulations*  
HAOYUAN JING (Presenter), YANBIN WANG, PARTH RAKESH DESAI, Univ of Maryland-College Park, KUMARAN S. RAMAMURTHI, National Cancer Institute, National Institute of Health, SIDDHARTH DAS, Univ of Maryland-College Park  
— We have carried out coarse-grained molecular dynamics (MD) simulations to study the self-assembly procedure of a system of randomly placed lipid molecules, water beads, and a nanoparticle (NP). The self-assembly results in the formation of the NPSLBL, with the self-assembly mechanism being driven by events such as the formation of small lipid clusters, merging of the lipid clusters in the vicinity of the NP to form NP-embedded vesicle with a pore, and collapsing of that pore to eventually form the equilibrated NPSLBL system. Subsequently, we quantify the properties and the configurations of this NPSLBL system. We reveal that the equilibrated self-assembled NPSLBL system demonstrates a larger number of lipid molecules occupying the outer leaflet as compared to the inner leaflet. Secondly, the thickness of the water layer entrapped between the NP and the inner leaflet show similar values as that predicted by experiments. Finally, we reveal that the diffusivity of the lipid molecules in the outer leaflet is larger than that in the inner leaflet.

*Thanks UMD-NCI Graduate Partnership Program for fully supporting this work

2:42PM D23.00002: Leveraging the physics of a barbecue lighter to genetically transform living organisms  
GAURAV BYAGATHVALLI (Presenter), SOHAM SINHA, YAN ZHANG, MARK P. STYCZYNSKI, Georgia Inst of Tech, JANET STANDEVEN, Biotechnology, Lambert High School, SAAD BHAMLA, Georgia Inst of Tech  
— Electroporation is a powerful method for delivering small molecules (RNA, DNA, drugs) across cell membranes by application of an electric field with a specific voltage and time constant, with applications ranging from synthetic biology to drug delivery. Leveraging the piezoelectric mechanism found within a common barbeque lighter, we develop a low-cost electroporator that we call an ElectroPen. This ElectroPen device costs 23-cents, weighs 13g, utilizes a 3D-printed case, and can be applied to genetically transform \textit{E. coli} bacteria. In this talk, we will discuss both the physics of a lighter, as well as the synthetic biology protocol we have developed for electroporation using this frugal device. Using high-speed videos, we will discuss how the inner components of a lighter achieve extraordinary accelerations of 3000g force to ultimately deliver voltage pulses of up to 2,000 volts with a decay constant of 5ms. Finally, we will discuss applications of this low-cost device in broadening participation in synthetic biology in high school science laboratories.

2:54PM D23.00003: Listening to lipid membranes*  
KISUNG LEE (Presenter), Center for Soft and Living Matter, Institute for Basic Science, GURBAN CHOMMANOV, School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, STEVE GRANICK, Center for Soft and Living Matter, Institute for Basic Science  
— Fluctuations of giant unilamellar vesicle and cell membranes are detected with exceptional resolution. The motion of localized membrane (<1 μm cross-section) is resolved with 5 decades in both frequency (1 Hz - 100 kHz) and amplitude (0.01 nm - 100 nm). This allows to listen to surprises in underlying membrane mechanics.

*Korean Institute for Basic Science, project code IBS-R020-D1.
3:06PM D23.00004: Comparing microrheological methods for measuring lipid membrane viscosity* PHILIP JAHL (Presenter), RAGHUVEER PARTHASARATHY, Univ of Oregon — The fluidity of lipid membranes governs the motions of bound proteins and macromolecules. Despite this, measurements of the viscosity of a lipid bilayer remain challenging to perform and interpret. Two different microrheological methods for measuring bilayer viscosity have been developed in recent years, one involving tracking phase-separated domains in giant unilamellar vesicles, and the other involving tracking elliptical lipid-anchored tracer particles. The latter approach has so far been applied only to pore-spanning black lipid membranes. The membrane viscosity values obtained by these two methods differ by an order of magnitude, however, and it is unclear whether this indicates inaccuracy of one or both techniques, or whether it is due to the difference in membrane systems examined. To resolve this discrepancy, we applied both methods simultaneously to the same lipid vesicles, featuring both phase separated domains and bound elliptical beads. We show that when applied to identical systems these methods are in agreement. The elliptical tracer method is generally applicable to vesicles of arbitrary composition, and we use it to quantify the viscosity of bilayers composed of phosphatidylcholine lipids of different chain lengths.

*We acknowledge support from NSF award DMR-1507115

3:18PM D23.00005: Regulated ensembles and lipid membranes* MARTIN GIRARD (Presenter), TRISTAN BEREAU, Max Planck Institute for Polymer Research — Cellular membranes are composed of lipid bilayers, amphiphilic molecules with polar headgroups and hydrophobic tails. Their composition is highly complex, involving hundreds of different lipid types and the regulation mechanism is still the subject of intense research. A recent experiment [1] has shown that cholesterol concentration increases with temperature in zebrafishes, as well as the demixing temperature, two results which appear to be contradictory results since cholesterol promotes mixing. Here, we show that many aspects of the zebrafish experiments can be replicated if one assumes a chemical reaction network for regulation of acyl tails. Effectively, this would mean that acyl tail saturation is loosely regulated by cells and mainly directed by cholesterol fraction. This view also explains trends seen along the secretory pathway between cholesterol concentration and acyl tail saturation.


*Authors acknowledge support from the Deutsche Forschungsgemeinschaft (DPG) and Alexander von Humboldt Foundation
3:30PM D23.00006: Stable fabrication of a various-sized nanopore by controlled dielectric breakdown in a high-pH solution for the detection of various-sized molecules  ITARU YANAGI (Presenter), RENA AKAHORI, KENICHI TAKEDA, Hitachi Ltd — For nanopore sensing of various-sized molecules with high sensitivity, the size of the nanopore should be adjusted according to the size of each target molecule. For solid-state nanopores, a simple and inexpensive nanopore fabrication method utilizing dielectric breakdown of a membrane is widely used. This method is suitable for fabricating a small nanopore. However, it suffers two serious problems when attempting to fabricate a large nanopore: the generation of multiple nanopores and the non-opening failure of a nanopore. In this study, we found that nanopore fabrication by dielectric breakdown of a SiN membrane under high-pH conditions (pH ≥ 11.3) could overcome these two problems and enabled the formation of a single large nanopore up to 40 nm in diameter within one minute.

3:42PM D23.00007: Monte Carlo simulation of pH activated conformational changes of coarse-grained sodium-proton antiporters  MOJGAN ASADI (Presenter), ARIEH WARSHEL, Univ of Southern California — Sodium-proton antiporters are membrane proteins present throughout the eukaryotic and prokaryotic domains that have a critical role in balancing cell pH and cell volume. The *Escherichia coli* antiporter *NhaA* has pH-dependent behavior. There have been many studies regarding the function of this antiporter (Alhadeff and Warshel, PNAS (2015) 112 (40) 12378-12383), but the conformational energy landscape of this system at varying pH is not well-known. In this study, we map the energy landscape between two pH levels for two different conformations of the wild antiporter and a mutated variant using MD with coarse-graining. By Monte Carlo simulation on the energy landscape, we show that the mutated variant changes the stability of the antiporter without blocking the transport, in agreement with experimental results (Calinescu et. al. J. Biol. Chem. (2017) 292(19) 7932–7941).

3:54PM D23.00008: Multichannel Flow Cell for a Nanopore Array Sensor  HAI HUY NGUYEN PHAM (Presenter), ITARU YANAGI, KENICHI TAKEDA, Hitachi Ltd — Solid-state nanopore has been attracting remarkable research interest owing to its extensive potential in biological sensing applications, the robustness, and the possibility of a large-scale integration. A reliability and measurement time are two important criteria for practical uses of a nanopore sensor. An integration of nanopores into an array and simultaneous measurement are an effective approach to increase accuracy and to reduce measurement time. Recently, we have developed 4x4 SiN membrane arrays. However, the flow cell in this system had a bottle neck of exploiting all 16 membranes due to a real estate issue of flow paths. Another bottle neck was the generation of the air bubble that could cause the electrical conductance error. In this study, the mechanism of those issues is investigated. A novel 16-channel flow cell made by a 3D printer is introduced. In this flow cell, the flow paths are arranged in both parallel and orthogonal direction to the membrane surface; and the distance between the membrane surface and the flow path is adjusted to prevent the generation of the air bubble. Nanopores were successfully yielded in all 16 membranes by dielectric breakdown technique.
4:06PM D23.00009: Interaction of Graphene Oxide with Model Bio-membrane: Insights into the Structure of the Membrane  PRIYA MANDAL (Presenter), SAJAL KUMAR GHOSH, Shiv Nadar Univ — Graphene oxide (GO) holds a similar structure of graphene with a range of oxygen functionalities such as carboxyl groups on the edges and, the hydroxyl and epoxies on the basal plane. Presence of oxygen-containing functional groups increases its water dispersity and facilitate its applications in many bio-fields including cell imaging, drug-delivery and bio-sensing. As the cellular membrane is the first target of any foreign molecule. Hence, the mechanism of interaction of GO with this membrane is very crucial to understand for extending the future applications of graphene-based materials. In present work, the x-ray reflectivity (XRR) and grazing incidence small-angle x-ray scattering (GISAXS) techniques have been used to extract the structural details of the GO-membrane complex. XRR study from lipid multilayers has shown a distinct effect of added GO on the position and shape of Bragg peaks obtained from the smectic liquid crystalline phases. GISAXS has provided the in-plane organization of the lipid molecules in the presence of GO in the membrane. The electron density profile obtained from the XRR analysis and the lattice deformation detected by the GISAXS study has provided the detailed molecular organization of the complex.

4:18PM D23.00010: Detection of streptavidin-labeled DNA using solid-state nanopores for target sequence detection  RENA AKAHORI (Presenter), ITARU YANAGI, KENICHI TAKEDA, Hitachi Ltd — In recent years, the demand for rapid and on-site target gene detection has been increasing. For example, it is important for covering the increasing GMO (Genetically-modified-organisms) testings, and for preventing the spread of infectious diseases at an early stage. The conventional techniques for target DNA sequence detection are based on PCR and qPCR. Although these techniques are widespread, they are time-consuming and will not be able to cover all required testings. By comparison, solid-state nanopores have a potential to provide a rapid and portable testing device that is electronic and does not need optics. For realizing target sequence detection with solid-state nanopores, it is a promising approach to label the target sequence with a large molecule and enlarge a current-blockade value when DNA including the target sequence passed through a nanopore. In this study, the possibility of streptavidin (SA) as a labelled molecule was investigated. As a result, we found that the passages of SA-labelled and non-labelled DNA through a nanopore can be clearly distinguished.

4:30PM D23.00011: Moving while you're stuck; a mechanical model of binding facilitated transport in biological systems  KANGHYEON KOO, SHANKAR LALITHA SRIDHAR, NOEL ANTHONY CLARK, FRANCK J VERNEREY, LOREN HOUGH (Presenter), University of Colorado, Boulder — Binding is broadly understood in many biological processes as a mechanism to localize molecules. Binding is also used to dictate particle motion through some biopolymer filters including the nuclear pore complex, the extracellular matrix and mucus membranes. In these cases, flexible polymers transiently bind to transported molecules. Here we describe a mechanical model to probe how binding and thermal motion can enable transport. A particle experiences random forces during binding and unbinding events while being constrained by attached tethers. This model provides insight into the mechanisms and design rules involved in binding-mediated transport in both biological and synthetic polymeric systems.
Towards high-sensitivity phase cancellation microscopy*  
DOMINIKA LYZWA (Presenter), VIJAY SINGH, ZAHID YAQOOB, PETER SO, Biological Engineering, Massachusetts Institute of Technology — Label-free optical imaging techniques, such as light scattering and birefringence have long been used for detection of neural activity [1]. Wide-field interferometric microscopy has also been used for this purpose, most recently by Ling et al. [2]. Current interferometric systems are limited because of low phase measurement sensitivity of $10^{-3}$, while a sensitivity of $10^{-5}$ is necessary.

High sensitivity phase measurements will allow single-shot optical sensing of neural action potentials via imaging of optical path length changes. Here, we present a high phase sensitivity, phase cancellation interferometry system. We want to use a deformable mirror to generate a flat phase. A Wollaston prism is employed to split the beam into two orthogonally polarized beams with phase control. These beams are recombined for interferometric detection. A state-of-the-art 1.6M electron well-depth camera will be used for recordings. We report the analysis of our system’s sensitivity and compare it to theoretical predictions.


*DL is supported by a DFG postdoctoral fellowship.

Predicting optimal parameters for ion transport through nanopores and biological channels*  
WILLIAM GIBBY (Presenter), MIRASLAU BARABASH, DMITRY LUCHINSKY, PETER MCCLINTOCK, Department of Physics, Lancaster University — Understanding, predicting and optimising ionic transport properties of pores on an atomic scale remains a critical challenge to, nanotechnology and biophysics [1]. In general, pores are designed to fulfil two criteria: conduction of ions at a high rate; and the selectivity amongst ionic species. We have derived a statistical and linear response theory that calculates the occupancy and conductivity of nanopores for given parameters including: pore geometry and charge; type of competing ionic species; and bulk concentration [2]. We find resonant conduction under known conditions, resulting in the coexistence of resonance for one species and suppression for the other and can predict optimal parameters required to produce the desired function. Examples of applications to biological channels and nanopores will be discussed.


Monday, March 2, 2020 2:30 PM - 4:42 PM

Session D24 GSNP: Control of Noisy Nonlinear Dynamical Systems 401 -

Uwe Tauber, Virginia Tech - Tag(s): Focus
2:30PM D24.00001: Understanding the control process for non-equilibrium systems using scaling theory* [invited] PRIYANKA . (Presenter), UWE CLAUS TAUBER, MICHEL PLEIMLING, Department of Physics & Center for Soft Matter and Biological Physics, Virginia Tech — Control theory is a widely used tool in engineering to develop controlled, stable models of dynamical systems. The control of deterministic models has been extensively studied; however, studies on the control of non-equilibrium systems are less explored due to the presence of non-linearity and noise. I will focus on understanding the effect of both linear and non-linear control processes on the intrinsic dynamics as well as stationary properties of non-equilibrium systems. In particular, I will discuss the control of the following two systems: a) surface roughness in the KPZ growth process, and b) the dynamical states in a network model. In the KPZ growth process, control is achieved by manipulating a subset of Fourier modes, whereas, in the dynamical network, a metastable state is controlled using a closed feedback loop. In both cases, the control process limits the time and length scales within which the system behaves according to its intrinsic stochastic dynamics. These time and length scales show scaling behavior with the control parameter, and the associated scaling exponents are related to those of the unperturbed model.

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3:06PM D24.00002: Molecular machinery: quantifying the energetic cost of controlling nanoscale biological systems* STEVEN LARGE (Presenter), DAVID SIVAK, Simon Fraser Univ — At microscopic scales, biological systems must maintain a high degree of organization in order to properly function. Ultimately, this organization is achieved by the concerted efforts of a collection of nanoscale molecular machines: protein complexes that perform specific functions within the cell. Quantifying the flows of energy, information, and material through such systems is a central challenge in understanding their dynamics and in vivo operation. Currently, a number of important questions related to the function of molecular machines remain unanswered: what design principles produce efficient machines? What fundamental physical limitations are placed on these nonequilibrium systems? In this talk I will discuss our recent efforts to address some of these questions, making use of tools from nonequilibrium thermodynamics to quantify the energetic costs of driving strongly fluctuating systems. In particular, quantifying the dissipation associated with driving a fluctuating system between different states leads to conditions for efficient operation. Among other things, we find that there is an energetically optimal speed for systems to move at.

*This work is supported by the NSERC CRC program, a CGS 3 year Doctoral fellowship to SJL, and a Discovery Grant to DAS.
3:18PM D24.00003: Effects of structural and cellular heterogeneity on the control of nonlinear biological oscillator networks*  NARASIMHAN BALAKRISHNAN (Presenter), Chemical and Biological Engineering, Northwestern University, NEDA BAGHERI, University of Washington — Circadian rhythms are biological processes that have a period of roughly 24 hours. In most animals, these rhythms are orchestrated by a specialized network of neurons that possess a regulatory system involving oscillatory genes and proteins. The dynamics of these regulatory networks are highly nonlinear. In this work, we study the functional consequences of structural and cellular heterogeneity (extrinsic noise) on the control of these oscillator networks. Structural heterogeneity refers to variation in size, topology and edge weights within the network of oscillators. We present two optimal control problems, those of modifying the phase of the population of these oscillators in either minimal time, or using minimum effort. We find there is a sweet spot relating heterogeneity and average coupling strength for which the control cost is minimal, and a limit to which heterogeneity enables greater controllability. Insights relating to heterogeneity also suggest evolutionary advantages heterogeneous populations may carry over homogeneous ones. Our findings also may help provide guidelines for the design of synthetic oscillator networks, a field of growing interest.  

*This work was partially funded by the Northwestern University Biotechnology Cluster

3:30PM D24.00004: Corazon espinado: microelectrode closed-loop control in cardiac tissue  CONNER HERNDON (Presenter), FLAVIO H FENTON, Georgia Inst of Tech — Proper contraction of cardiac muscle relies on the coordinated propagation of transmembrane voltage, and disturbances of this propagation can result in deadly cardiac arrhythmias. One such disturbance strongly associated with the onset of fibrillation is a dynamical instability known as alternans, a beat-to-beat alternation in action potential duration (APD) arising from a period-doubling bifurcation. The restitution hypothesis claims that a return map in APD can describe and predict alternans, and decades of work have shown it can successfully reproduce many experimental observations. The restitution hypothesis likewise predicts a method for suppressing the onset of alternans which has been confirmed by some computational simulations; however, few experiments have addressed these predictions due to its difficult implementation. In this talk, I will discuss our development of a closed-loop control scheme to experimentally address predictions made by the restitution hypothesis via high resolution microelectrode recordings of transmembrane voltages in zebrafish, frog, and rabbit hearts. I will present our results which conclusively show the appearance of alternans in opposition to predictions made by theoretical models and provide an improved model that describes the dynamics.
Induction of spatio-temporal spiral defects in an inhomogeneous stochastic May-Leonard system*  

SHANNON SERRAO (Presenter), UWE CLAUS TAUBER, 
Department of Physics and Center for Soft Matter and Biological physics, Virginia Tech — We study the induction of spiral defects in an inhomogeneous two-dimensional Monte Carlo toroidal lattice simulation of the stochastic three-species May-Leonard model with asymmetric predation rates. In an isolated setting, strongly asymmetric predation rates cause fast extinction from coexistence of all three species to a single surviving population. However, when spatially coupled to a fully symmetric May-Leonard patch, the spiral patterns from this stable region induce transient plane wave fronts and ultimately quasi-stationary spiral patterns in the asymmetric region. We quantitatively analyze the initial injection of plane wave fronts from the symmetric region and the subsequent formation of spirals, and explore the conditions for the stabilization of the weaker ecosystem. To this end, we study characteristic correlation lengths and oscillation frequencies, the shape and size of the spirals induced in the asymmetric region in comparison to the isotropic spirals in the symmetric regime, and the effects of varying system size and individuals' mobility.

*Research was sponsored by the Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.

Extracting important parameters from dynamical systems models through coarse-graining*  

PRANAV KANTROO (Presenter), Computational Biology and Bioinformatics Program, Yale University, BENJAMIN B MACHTA, Department of Physics, Yale University — Known microscopic details often motivate models with large numbers of parameters. However, not all parameter combinations are relevant at large length-scales of observation. Some may affect coarse-grained system behavior sensitively, while others may have no discernible effect. Here we utilize the Fisher Information Metric formalism to identify which parameter combinations influence observables even for coarse-grained data. We first derive a general method for calculating this metric from a model whose data has been coarse-grained, and apply this to models coarse-grained by sparse-sampling observables in time. We make the resulting Fisher Information reparameterization invariant by transforming to a basis that measures how coarse-graining reduces observability. We then use this procedure to explicitly calculate the temporally coarse-grained Fisher Information Metric for several stochastic differential equation models. The expansion of the reparameterization invariant Fisher spectrum after coarse-graining separates relevant parameter combinations from irrelevant ones. We then draw concrete parallels between our formalism which uses coarse-graining of the Fisher Information, and the Renormalization Group framework.

*Partially supported by a Simons Investigator Award 624156
4:06PM D24.00007: NUMERICAL INVESTIGATION OF SIGNAL AMPLIFICATION VIA VIBRATIONAL RESONANCE IN A CHUA’S CIRCUIT. JOHN LAOYE, TAIWO OLAKUNLE ROY-LAYINDE (Presenter), KEHINDE ADAM OMOTESO, RASAKI KOLAWOLE ODUNAIKE, Olabisi Onabanjo Univ — In this paper, we numerically investigated the occurrence of Vibrational Resonance in a modified Chua’s oscillator with a smooth nonlinearity, described by a cubic polynomial. Response curves generated from the numerical simulation at the low frequency reveal that the system’s response amplitude could be controlled by modulating the conductance parameter of the Chua’s circuit, rather modulating the parameters of the fast periodic force. Modulating the frequency of the fast periodic force slightly reduces the response amplitude; shifts the peak point to a higher value of the amplitude of the fast periodic force by widening the resonance curves. Within certain parameter regime of the high frequency ($\Omega \geq 100 \omega$), the system’s response gets saturated, and further increase does not affect its amplitude.

4:18PM D24.00008: Resonance Coherence Optimization of Structure Formation in Nanofilms Undergoing Thermocapillary Instability YI HUA CHANG (Presenter), SANDRA TROIAN, Applied Physics, Caltech — External temporal modulation of time periodic phenomena is a well-known method for inducing resonant behavior in mechanical or electrical systems. While temporal modulation has been used as an effective control mechanism for decades, there have been far fewer studies of external spatial modulation to enforce pattern uniformity and growth in the presence of noise. One such example involves a liquid film undergoing a spinodal instability subject to an externally imposed wavenumber close to the stability threshold of the unforced homogeneous system, which has been shown to induce resonance leading to a bifurcation in equilibrium film shapes. In this talk, we examine a linear instability in molten nanofilms undergoing thermocapillary growth leading to structure formation resembling 3D microlens arrays. Noisy initial conditions, however, are found to generate non-uniform peak heights which accelerate at different rates and significantly compromise pattern fidelity. Using a combination of weakly nonlinear analysis and numerical simulations, we demonstrate the existence of a resonant regime with high spatial coherence leading to microarrays with uniform pitch and height. This regime should provide optimal conditions for fabrication of micro-optical arrays.

4:30PM D24.00009: An elementary renormalization-group approach to the Generalized Central Limit Theorem and Extreme Value Distributions ARIEL AMIR (Presenter), Harvard University — The Generalized Central Limit Theorem is a remarkable generalization of the Central Limit Theorem, showing that the sum of a large number of independent, identically-distributed (i.i.d) random variables with infinite variance may converge under appropriate scaling to a distribution belonging to a special family known as Levy stable distributions. Similarly, the maximum of i.i.d. variables may converge to a distribution belonging to one of three universality classes (Gumbel, Weibull and Frechet). I rederive these known results following a mathematically non-rigorous yet highly transparent renormalization-group-like approach that captures both of these universal results following a nearly identical procedure.

Monday, March 2, 2020 2:30 PM - 5:30 PM
2:30PM D25.00001: Recent Progress on 3D Chiral Mechanical Metamaterials* [Invited]
MARTIN WEGENER (Presenter), Karlsruhe Institute of Technology — We review our recent progress on three-dimensional (3D) microstructured chiral mechanical metamaterials. These architectures have been made by state-of-the-art 3D laser nanoprinting and lately also by rapid multi-focus multi-photon 3D laser nanoprinting. For the latter, the metamaterials contain more than one hundred thousand unit cells and more than three hundred billion voxels.
Concerning the static regime, we will present novel architectures that allow to bring the push-to-twist conversion effects previously reported by us to much larger absolute values at larger numbers of unit cells. Specifically, the twist/strain can be tailored to linearly increase up to a characteristic number of unit cells, beyond which the twist/strain asymptotically decays inversely with the number of unit cells (unpublished).
Regarding the dynamic regime, we will review our recently published results on acoustical activity, the elastic counterpart of optical activity. Moreover, we will also present unpublished result on a different unit-cell design, for which the observed rotation angles approach the fundamental limit of 90 degrees per unit cell.

*This research has been funded via the Excellence Cluster “3D Matter Made to Order” (EXC-2082 – 390761711).

3:06PM D25.00002: 3D Acoustic Zero Index Metamaterial* CHANGQING Xu, King Abdullah Univ of Sci & Tech (KAUST), GUANCONG MA, Physics Department, Hong Kong Baptist University, YUN LAI, Physics Department, Nanjing University, YING WU (Presenter), King Abdullah Univ of Sci & Tech (KAUST) — In this talk, I will report our design of a three-dimensional (3D) acoustic double-zero-index medium (DZIM) made of a cubic lattice of metal rods. Despite of several realizations of 2D DZIM in the past, achieving such a medium in 3D has remained an elusive challenge. Here, we show how a four-fold degenerate point with conical dispersion can be induced at the Brillouin zone center, such that the material becomes a 3D DZIM with the effective mass density and compressibility simultaneously acquiring near zero values. To demonstrate the features of the DZIM, we have fabricated an acoustic waveguide filled with 3D DZIM to form a “periscope” with two 90° turns and observed nearly perfect tunneling of a normally incident planar wave through the waveguide.

*King Abdullah University of Science and Technology OSR-2016-CRG5-2950 and BAS/1/1626-01-01; Hong Kong Baptist University through FRG2/17-18/056, RC-SGT2/18-19/SCI/006; HKRGC ECS2230718 and GRF 12300419; National Key R and D Program of China 2017YFA0303702; National Natural Science Foundation of China Grant No. 11802256, 61671314, 11974176, and 11634005;
3:18PM D25.00003: Micro-lattices for wide-band three-dimensional elastic wave attenuation  
NIKHIL GERARD (Presenter), MOURAD OUDICH, YUN JING, North Carolina State University — The past decade has witnessed the emergence of three-dimensional micro-lattices and state-of-the-art manufacturing techniques that have enabled their realization. The ability to fabricate bulk materials that are precisely architected at the microscopic scale is exhilarating to various scientific communities. This has thus greatly revived the yearning for futuristic multifunctional materials. From the perspective of mechanical wave propagation, this implies complete control over micro-structure that can be designed for exotic wave-based applications. In this work, we put forth new design strategies to engineer micro-lattices for desirable elastic wave bandgaps and discuss their experimental realization. The band gaps can be attributed to local resonance and Bragg mechanisms and can be precisely tuned via both unit cell geometry and the intrinsic material employed for its fabrication. Alongside being thin, lightweight and/or displaying a negative Poisson’s ratio, our micro-lattices are equipped with the capability of attenuating elastic waves in all directions over a wide frequency range and can facilitate novel elastic wave functional materials.

3:30PM D25.00004: Elastic Weyl Points and Surface Arc States in Three-Dimensional Mechanical Metamaterials*  
XIAOTIAN SHI (Presenter), RAJESH CHAUNSALI, University of Washington, FENG LI, South China University of Technology, JINKYU YANG, University of Washington — We investigate a novel Weyl mechanical metamaterial inspired by the discovery of Weyl semimetal. We propose a three-dimensional mechanical structure in analog to the AA-stacked graphene with chiral intralayer coupling, which carries Weyl points of topological charge ±1. We numerically confirm the existence of the elastic Fermi arc and the associated gapless topologically protected surface states. The full-scale numerical simulation on the hollow 3D mechanical structure demonstrates that the surface elastic waves are robust and directional, which can pass a corner or defect without reflections. The findings from our work can contribute to the novel ways of manipulating elastic energy in 3D structures for potential applications in vibration isolation, advanced sensing, and energy harvesting.

*X.S., R.C., and J.Y. acknowledge the support from U.S. National Science Foundation (Grants No. CAREER1553202 and No. EFRI-1741685).
Demonstration of the Majorana-like bound state in an elastic bolted plate  

CHUN-WEI CHEN (Presenter), Aeronautics and Astronautics, University of Washington, NATALIA LERA, Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, RAJESH CHAUNSALI, LAUM, CNRS, Le Mans Université, DANIEL TORRENT, GROC, Institut de Noves Tecnologies de la Imatge (INIT), Universitat Jaume I, JOSE VICENTE ALVAREZ, Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, PABLO SAN-JOSE, Materials Science Factory, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), JOHAN CHRISTENSEN, Department of Physics, Universidad Carlos III de Madrid, JINKYU YANG, Aeronautics and Astronautics, University of Washington — With the unveiling of the topological non-trivial phases, abundant demonstrations of the bulk-boundary correspondence in various domains of physics have been conducted in recent years. More recently, higher-order topological insulators are realized to reveal not only the boundary states but also the zero-dimensional corner states. In this work, another uniquely zero-dimensional non-propagating state, specifically a mechanical analog of the Majorana bound state, is shown numerically and experimentally in a mechanical system. We implement topological binding by creating a Kekulé distortion vortex on a two-dimensional thin plate with local resonators mounted in a honeycomb arrangement. It is renowned that Majorana bound states are protected by particle-hole (PH) symmetry. Similarly, to show our mechanical Majorana-like bound state is insensitive to certain type of disorder, we design a local perturbation to mimic the PH symmetry. We confirm that the Majorana-like bound state is indeed robust against the PH-symmetric perturbations and maintains pinned to Dirac frequency of the undistorted lattices. We anticipate that this finding will enrich the topological non-trivial phases in bosonic systems and broaden the applications of the energy localization or energy harvesting.

Tuning of 2D Phononic Band Structures via Buckling Instability  

TEJAS DETHE (Presenter), SIDDHARTH SARKAR, Princeton University, MATEVZ MARINCIC, University of Ljubljana, ANDREJ KOSMRLJ, Princeton University — Dispersion relation of propagating elastic waves through phononic crystals, which are periodic elastic structures, can be represented with band diagrams akin to the electronic band structures and band structures in photonic crystals. Of special interest in these diagrams are band gaps, which correspond to frequencies of waves that cannot be transmitted through the bulk of the phononic crystals. The location of band gaps depends on the material properties and on the geometry and symmetries of phononic structures. The symmetries of compressed elastic structures can be drastically altered via the buckling instability, and we are exploring how that affects the phononic band structures. First, we systematically investigated band diagrams for uncompressed 2D phononic structures that belong to different crystallographic groups. We employed recently developed tools for electronic systems, to analyze which band crossings are topologically protected/prohibited. We use this information to analyze how band structures are affected by the buckling instability, which causes a phononic structure to move from one crystallographic group to another. Such tuning of band structures with external load could then be used to engineer tunable sound filters as well as mechanical sensors.
4:06PM D25.00007: Robust gapless edge states and unconventional topological band properties in a two-dimensional elastic Kekulé phononic lattice* TING-WEI LIU (Presenter), FABIO SEMPERLOTTI, Purdue Univ — The existence of back-scattering-immune edge states in topological metamaterials has opened a new path for mechanical waveguide design. Recently, a “Brillouin-zone-folding” strategy was proposed to easily realize non-trivial topological properties in two-dimensional phononic systems. However, due to the intrinsic characteristics of phonons, the resulting edge states are generally gapped, indicating coupling between counter-propagating edge states. We report on the design of an elastic phononic structure that embeds a Kekulé distortion pattern to create the analogue of a quantum spin Hall system which, with proper tuning, can achieve fully decoupled and gapless edge states. Using \textit{ab initio} numerical calculations, we also discover unconventional characteristics of the phononic band structure including a six-lobe pseudospin texture and Berry curvature. We also find that the existence of edge-states does not depend exclusively on the topological invariants of the adjacent bulk lattices but also on the relative translation of the unit cell pattern, therefore it is possible to obtain edge states on an edge dislocation of one bulk lattice.

*The authors gratefully acknowledge the financial support of the National Science Foundation under grant MOMS #1761423.

4:18PM D25.00008: Valley Anisotropy and Valley Topological States in Elastic Metamaterials* SHUAIFENG LI (Presenter), Department of Aeronautics and Astronautics, University of Washington, INGI KIM, SATOSHI IWAMOTO, Institute of Industrial Science, The University of Tokyo, JIANFENG ZANG, School of Optical and Electronic Information and Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology, JINKYU YANG, Department of Aeronautics and Astronautics, University of Washington — Valley, as a new degree of freedom, has emerged as an efficient way in manipulating waves in electronics, photonics and phononics. We present the valley anisotropy by introducing asymmetrical metamaterials made of hard spiral and soft materials. We study the phononic band structure and valley pseudospin in these spiral elastic metamaterials. By numerical calculations, we show the deviated Berry curvature and valley Chern number. The adjustment of the geometrical parameters in the spirals allows an extreme tunability of the Berry curvature and valley Chern number, resulting in the topological transition. We exploit the adjustment of the geometrical parameters to demonstrate the formation of valley topological states unprecedented in conventional topological platforms. Lastly, we present the topologically protected transport of elastic waves in our anisotropic topological elastic metamaterials.

*S.L. and J.Y. are grateful for the support from NSF (CAREER1553202 and EFRI-1741685)
4:30PM D25.00009: Topological boundary modes in nonlinear mechanical lattices  DI ZHOU (Presenter), ZEB ROCKLIN, Georgia Inst of Tech — Mechanical lattices have been shown to possess interface modes lying in bulk band gaps. These boundary modes are protected by bulk topological invariants in which the geometric (Berry) phase is quantized by certain symmetries, the celebrated bulk-boundary correspondence. This relationship has been proved rigorously for linear mechanical systems, which can be mapped onto quantum systems, yet recent has demonstrated that the boundary modes extend into the nonlinear regime. In the present work, we investigate the topological protection of nonlinear normal modes. In particular, we consider a one-dimensional diatomic chain with spatial inversion symmetry, whose linear limit has a well-characterized topological invariant. By continuing the linear modes into the nonlinear regime via a mix of numerical and analytic methods, we characterize how nonlinear topological boundary modes emerge, paving the way to topological modes of strongly and inherently nonlinear systems.

4:42PM D25.00010: Programmable higher-order Euler buckling modes in hierarchical beams* MARIA-GABRIELLA TARANTINO, KOSTAS DANAS (Presenter), LMS, CNRS, Ecole Polytechnique — We present a numerical-aided experimental study on the buckling of hierarchical beams comprising multiple self-similar modules. Each module consists of multiple elemental beams and is arranged in series to form the hierarchical beam. We show, through a combination of experiments and computations, that these beams exhibit stable and realizable higher-order buckling modes. By contrast to the canonical Euler buckling problem, such modes emerge naturally in the proposed self-similar beams since they correspond to almost identical critical loads. By harnessing the imperfection sensitivity of the hierarchical structures, we 3D-print weakly imperfect polymer samples with a small geometric imperfection corresponding to the desired eigenmode. The ability to trigger higher-order buckling modes is found to depend on two main geometrical parameters which lead to scale coupling. Those are the slenderness of the macroscopic hierarchical beam and the slenderness of the lower-scale elemental beam. With increasing slenderness of the hierarchical beam, we observe a significant softening in the overall stress-strain response and patterns exhibiting curvature localization in the post-bifurcation regime.

*ERC Starting Grant Magneto
4:54PM D25.00011: Programmable metastructures featuring adaptable stiffness based on local bistability*  JANAV P. UDANI (Presenter), ANDRES F. ARRIETA, Purdue Univ — We present a novel class of programmable structures displaying large stiffness adaptability from local changes of shape. We connect a series of locally bistable semi-spherical shells (domes) within structural element geometries to create highly programmable properties. We demonstrate the property programmability by manufacturing and testing the dome patterned metasheets and beam-like metastructures, the properties of which are adapted by changing the local state of individual domes. We present bending and in-plane stiffness curves characterizing the global response as a function of the local unit cell states. Our results reveal extreme adaptability of properties ranging from high stiffness to high compliance as a result of the local changes of stable states. The properties of the metastructures depend on the local bistable state adopted by the domes and the global connectivity of the metastructures, thus departing from constraints imposed by specific constitute material choice for obtaining adaptability. We demonstrate the applicability of these metastructures in compliant/soft robotics particularly to enable stiffening without compromising on shape reconfiguration, all while using a simplified single input control to shift between stable states.

*AFOSR FA9550-17-1-0074

5:06PM D25.00012: Navigating the landscape of nonlinear mechanical metamaterials for advanced programmability  EDER MEDINA (Presenter), Harvard University, PATRICK FARRELL, Mathematical Institute, University of Oxford, KATIA BERTOLDI, CHRISTOPHER RYCROFT, Harvard University — We consider a flexible mechanical metamaterial comprising an elastomeric matrix with an embedded square array of circular holes. First, we use the deflated continuation technique of bifurcation analysis to explore its complex energy landscape, characterized by multiple bifurcations from which stable and unstable branches emanate. We then investigate how this landscape can be exploited for real-time programmability. We find that the response of the system can be constantly reprogrammed by locally manipulating it to move it from one stable branch to another and that small targeted imperfections can be harnessed to enhance such programmability.

5:18PM D25.00013: Space-time phononic crystals with anomalous topological edge states*  YUANCHEN DENG (Presenter), MOURAD OUDICH, Mechanical and Aerospace Engineering, North Carolina State University, MOLEI TAO, School of Mathematics, Georgia Institute of Technology, YUN JING, Mechanical and Aerospace Engineering, North Carolina State University — We introduce a one-dimensional topological phononic phase system with a dynamic modulation of its intrinsic properties that keep the topological feature of the system unchanged, while it leads to a multiplication of the edges-state into the continuum at the subwavelength regime. We use this feature to access the functionality of exciting the edge-state in the Bragg regime using harmonic deep subwavelength acoustic wave where the wavelength is about 55 times the whole topological system's length. This remarkable property introduces a promising alternative to achieve wave manipulation at the deep-subwavelength scale.

*M.Tao acknowledges the generous support from NSF DMS-1521667, DMS-1847802, and ECCS-1936776.
2:30PM D26.00001: Controlled neighbor exchanges drive intermittency and cell streaming in epithelial tissues  

AMIT DAS (Presenter), DAPENG BI, Northeastern University — Cell neighbor exchanges are integral to tissue rearrangements in biology, including development and repair. Often these processes occur via topological T1 transitions analogous to those in foams, grains and colloids. However, in contrast to non-living materials the T1 transitions in tissues are rate-limited and cannot occur instantaneously due to finite time required to remodel complex structure at cell-cell junctions. Here we introduce this important biological constraint in a vertex-based model as an intrinsic single-cell property and study how this rate-limiting process affects the mechanics and collective behavior of cells in a tissue. We report in the absence of this time constraint, the tissue undergoes a motility-driven glass transition characterized by a sharp increase in the intermittency of cell-cell rearrangements. Remarkably, this glass transition disappears as T1 transitions are temporally limited. As a unique consequence of limited rearrangements, we also find that the tissue develops dynamically heterogeneous pockets of fast and slow cells, in which the fast cells organize into long streams with leader-follower interactions, maintaining optimally stable cell-cell contacts. We compare our predictions with existing in-vivo experiments on Drosophila pupal development.
**2:42PM D26.00002: Mechanical Instabilities in Growing Biological Systems: Wrinkling and Branching** [Invited] ANDREJ KOSMRLJ (Presenter), Princeton University — Morphological shape transformations in biological systems often arise from patterned biochemical processes, which can produce mechanical forces either directly via molecular motors or indirectly via differential growth of connected tissues. The growth mismatch produces internal stresses, which can be released via shape transformations and mechanical instabilities. In this talk I will focus on mechanical instabilities that cause the wrinkling of Vibrio cholerae bacterial biofilms and branching in developing lungs. Biofilms grown on agar substrates form wrinkled patterns, which are radial in the outer region and zig-zag herringbone in the inner region. We demonstrate that the wavelength of wrinkles as well as their spatiotemporal pattern can be predicted by a chemo-mechanical model that takes into account the diffusion of nutrients and their uptake by bacteria, growth of the biofilm, mechanical deformation of the biofilm and the agar substrate, and the friction between them. In the second part I will discuss the branching morphogenesis of lungs. We investigate how patterned differential growth between the inner epithelium and the outer mesenchyme tissue as well as the spatial pattern of smooth muscles lead to formation of new branches and their subsequent development. Experiments and mathematical model suggest that the patterned formation of stiff smooth muscles is very important for the proper development of new branches. In the absence of smooth muscles, the wrinkling instability of growing epithelium on the soft mesenchyme produces several ectopic branches. However, when stiff smooth muscles are formed, they suppress the wrinkling instability and new branches are formed only between the gaps of smooth muscles.

*This work was supported by the NSF through the Princeton University Materials Research Science and Engineering Center DMR-1420541 and by the Eric and Wendy Schmidt Transformative Technology Fund.

**3:18PM D26.00003: Quasi-realistic modelling of expanding epithelial cell monolayer**
YOUYUAN DENG (Presenter), HERBERT LEVINE, Rice Univ — An expanding epithelial cell monolayer on a 2-dimensional substrate exhibits intriguing mechanical patterns. The distribution of mechanical quantities over space and time thereby hints a picture integrating cell-cell and cell-substrate interactions. We propose a quasi-realistic model for this phenomenon. Specifically, we model cells as active constituents that would maintain force-equilibrium at the end of each motile step. The model cells contract with a tension-dependent speed, and protrude after reaching the maximum allowed contraction. Cell-substrate and cell-cell elastic adhesion bonds form, break and relocate stochastically, so as to capture contact inhibition as well as other effects. We bring forward this bottom-up approach to reveal the essential mechanisms leading to the macroscopic patterns.
3:30PM D26.00004: Symmetry breaking and axis formation in Hydra* [Invited] EVA-MARIA COLLINS (Presenter), Swarthmore College — During animal development, a near-uniform collection of genetically identical cells self-organizes to form an organism with a well-defined anterior-posterior body axis. Axial patterning is the earliest and most fundamental event that gives rise to the complexities of a full animal. The freshwater polyp Hydra is an excellent model system to study axial patterning due to its simple anatomy and incredible regenerative abilities. Hydra can regenerate from small tissue pieces or from cell aggregates. The physicists Alfred Gierer and Hans Meinhardt recognized Hydra's self-organizing properties > 40 years ago. However, the physical mechanisms underlying cell sorting, symmetry breaking, and axis specification in Hydra remained elusive as existing studies failed to distinguish between different driving mechanisms. In my talk, I will present our recent work that answers some of these questions. Our results challenge key assumptions in existing mathematical models of Hydra regeneration and require that we re-examine the mechanisms driving axis specification and pattern formation.

*This work was funded by NSF grant CMMI-1463572, the Research Corporation for Science Advancement, and the Gordon and Betty Moore Foundation.

4:06PM D26.00005: Configurations and dynamics of membrane-bound elastic filaments* WILSON LOUGH (Presenter), University of Wisconsin - Madison — Changes in the curvature and topology of cell membranes are responsible for numerous biological processes. Many of these changes are driven by interactions with thin filament-like protein structures which form on the membrane surface. While there are a number of proposed mechanisms, how exactly the filament-membrane interactions produce changes in curvature remains an open question. The feasibility of proposed mechanisms can be investigated by modeling the filament as a thin elastic rod which is confined to the membrane surface. The interplay between the geometries of the surface and the filament give rise to complex distributions of force and torque which are believed to play a crucial role in reshaping the membrane. We discuss the mechanics of surface-bound filaments and present a collection of analytical and numerical results.

*NSF: DMS-1661900
4:18PM D26.00006: Bacteria sense and respond to the mechanics of the surface to which they attach* VERNITA GORDON (Presenter), LIYUN WANG, JACOB BLACUTT, University of Texas at Austin — The attachment of bacteria to a surface is often a key initial step in the development of biofilms, communities of bacteria that are significant contributors to disease, fouling, and damage to the built environment. Understanding how bacteria sense surface attachment and, in response, begin the process of biofilm initiation, should give rise to new avenues to biofilm prevention as well as advance basic science. Here, we examine the relationship between substrate stiffness, mechanical deformation of the bacterial cell, accumulation of bacteria on the surface, and dynamics of an intracellular signal that control biofilms development. 

*Pseudomonas aeruginosa*, a widely-used model organism for biofilm development and a common hospital-acquired pathogen. We find that when the chemistry of a gel substrate is held constant but the effective elasticity is increased, more bacteria accumulate and signaling activates earlier. The response to the substrate mechanics at times greater than one hour after attachment depends on different cellular structures than at earlier times. Thus, the bacterial mechanosensing leading to biofilm development is likely a multi-step process involving more than one sensory element.

*Cystic Fibrosis Foundation Gordon1710, NIH 1R01AI121500-01A1, NSF 727544

4:30PM D26.00007: Mechanical impacts of complex topology on epithelial cells* SUN-MIN YU (Presenter), BO LI, FRANCOIS AMBLARD, STEVE GRANICK, YOON-KYOUNG CHO, Institute of Basic Science, Center for soft and living matter — Although complex curvatures are general features of in-vivo tissues where the fundamental biological functions are performed in our bodies, no in-depth study on the impact of complex curvature has been provided yet. In the current study, we found that strong mechanical impacts of complex topology on the epithelial system. With a great advantage of a torus having positive, zero, negative Gaussian curvature in a single structure, we demonstrated that the cells on tori showed polarized architecture than that of a flat surface. In addition, the cells manipulate the cellular mechanical elements to gain physically stable conditions. The current study sheds light on the mechanical adaption of cells on complex topology by which the relevance can be expanded in the in-vivo biological processes such as tumorigenicity and morphogenesis, also can provide insights on the design of biomaterials, tissue engineering and organoid/organ-on-a-chips.

*This project was mainly supported by a grant from IBS-R020-D1 funded by the Korean Government.
4:42PM D26.00008: Three-dimensional Packing of Curved Epithelia: Biology and Topology meet Physics  PEDRO GÓMEZ-GÁLVEZ, PABLO VICENTE MUNUERA, Seville University, SAMIRA ANBARI, Lehigh Univ, LUIS M ESCUDERO, Seville University, JAVIER BUCETA FERNANDEZ (Presenter), Lehigh Univ — Building and shaping tissues and organs relies on the ability of epithelial cells to efficiently pack together. In this context, we recently produced a major breakthrough by showing that epithelial cells display a previously undescribed geometrical shape when tissues are subjected to bending (curvature): the scutoid [1]. This discovery has opened the door to a deeper understanding of morphogenesis. Yet, the consequences of this new paradigm in terms of the 3D cellular organization remains largely uncharacterized. Here we address this problem using a combination of experiments, mathematical analyses, computer simulations, and biophysical approaches. In that context we derive the "Flintstones' Law" [2]: the thickness and curvature of epithelial tubes are linked to the cellular connectivity of the tissue via energetic cues. This principle explains how the topological and physical constraints inherent to living matter contribute to build functional complex shapes and lead to the self-organization of tissues.


4:54PM D26.00009: Topological analysis of multicellular structures  DOMINIC SKINNER (Presenter), BOYA SONG, JÖRN DUNKEL, Massachusetts Institute of Technology MIT — Recent advances in microscopy techniques make it possible to study the growth, dynamics and response of complex biological systems at single-cell resolution, from bacterial biofilms to tissues. When seeking to understand the formation and mechanical properties of these multicellular materials, the local spatial arrangement of their discrete cellular building blocks is of principal importance. To compare the similarity of crystals, we can compare lattice vectors or motifs, but when there is no crystal structure it is less obvious how one can reliably distinguish two amorphous yet structurally different materials. In this talk we introduce a topological distance between materials that needs only the coordinates of the centroid of each discrete object, and is based on the local graph structure around each centroid. Using this distance we will differentiate and classify structures formed from various ellipsoid and sphere packings, as well as biological cell data.
5:06PM D26.00010: Tissue-Tissue Interactions at Boundaries of Colliding Monolayers*
MATTHEW HEINRICH (Presenter), DANIEL COHEN, ANDREJ KOSMRLJ, JAKE STRAIN, Princeton University — Classic ‘wound healing’ studies in epithelial monolayers use a wound or barrier removal to induce and study collective migration, focusing on the migration rather than the ultimate collision and tissue healing. Here, we address this by comprehensively studying epithelial tissue-tissue interactions in homotypic tissues from the initial outgrowth of multiple tissues through collision until a single, mature tissue is formed. We show the boundary between two non-mixing tissues is directly modulated by their size, shape, and density, and the boundary varies over time until the newly fused tissue stabilizes. In addition to characterizing interactions and boundary dynamics between colliding tissues, we predict the resulting fused tissue forms using a simple computational model assuming isotropic growth, which is used to systematically design the final resulting “mosaic” from many growing tissues. Finally, we show that unexpected boundary dynamics occur at the confluence of three or more tissues coming together that can lead to surprising planar extrusions where one tissue pushes out between converging neighboring tissues resulting in long, stretched regions of tissues.

*Work was supported by NIH grant R35 GM133574-01.

5:18PM D26.00011: Patterning Potential of Cell-cell signalling Molecules in Flowing Tissue
SUPRIYA BAJPAI (Presenter), Civil Department, IITB-Monash Research Academy, MANDAR M INAMDAR, Civil Department, Indian Institute of Technology, RANGANATHAN PRABHAKAR, Univ, Monash, RAGHUNATH CHELAKKOT, Department of Physics, Indian Institute of Technology Bombay — Cell motility and cell-cell signalling are expected to play important roles in determining the mechanics behind deformation and patterning in tissues. Modelling efforts have, thus far, treated these two processes separately. Experiments in recent years, however, suggest that both these processes could be tightly coupled.

Cell deformation depends on membrane and cytoskeletal elasticity, cell-cell adhesion and active forces. Cell-cell signalling occurs through signalling molecules. A large number of complex tissue behaviours are controlled by contact signalling. Such interactions can occur only between cells that are in physical contact, either directly at the junctions of adjacent cells or through cellular protrusions. It is as yet unclear how the spatial distribution these molecules or the kinetics of their interactions are influenced by the collective migration in tissues driven by cell motility.

We present a model which accounts for contact signalling between adjacent cells and between non-adjacent neighbours through long protrusions that occur along the direction of cell polarization. The spatial patterns that develop are observed to qualitatively depend on polarization of protrusions, cell motility and the relative strengths of adjacent and non-adjacent signalling interactions.

Monday, March 2, 2020 2:30 PM - 5:30 PM
2:30PM D27.00001: Development of a high-k gate stack for atomic-precision advanced manufacturing  
TZU-MING LU (Presenter), EVAN ANDERSON, DEANNA CAMPBELL, MICHAEL MARSHALL, PING LU, SCOTT W SCHMUCKER, LISA A TRACY, MITCHELL ROBISON, REZA ARGHAVANI, LEON N MAURER, ANDREW BACZEWSKI, DANIEL R WARD, SHASHANK MISRA, Sandia National Laboratories — Atomic-precision advanced manufacturing (APAM) is a process in which a scanning tunneling microscope is used to create atomically precise conducting channels in Si. Gating of APAM devices is typically achieved by patterning electrical gates in the same plane as the channel. Higher transconductance could be achieved by adopting a vertical metal-oxide-semiconductor gate stack. Here we report on the development of such a gate stack incorporating high-k dielectrics. The process flow is designed to be APAM compatible with an ultra-low thermal budget. We evaluate the quality of the gate stack using capacitance-voltage measurements. This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

2:42PM D27.00002: Phase Controlling in HfO$_2$ Bulk Single Crystal*  
XIANGHAN XU (Presenter), FEI-TING HUANG, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — Contingent upon the miniaturization of semiconductor circuits, high-dielectric hafnium oxide (HfO$_2$) serves an alternative to silicon oxide. Surprisingly, the continued scaling comes with unexpected ferroelectricity at nanoscale HfO$_2$ in both pure and doped forms. These unusual findings are attributed to polymorphic nature including monoclinic, tetragonal, and orthorhombic phases and phase transitions in thin films, which is a big challenge in bulk crystal growth. Here, we show that utilizing the state-of-the-art laser floating zone technique allows the stabilization of the metastable phases at room temperature and pressure. We investigate the evolution of structural phases with various thermal treatments and doping. A comprehensive study on the structural transition pathway using in-situ transmission electron microscope (TEM) will be discussed. Our results provide insights for an alternative route for phase controlling of HfO$_2$ and the comparisons with thin films.

*The work at Rutgers University was supported by the NSF under Grant No. DMR-1629059.
The effect of air-anneal on two-level tunneling systems of ion-beam sputtered amorphous SiO$_2$*  

XIAO LIU (Presenter), MATTHEW ABERNATHY, THOMAS METCALF, United States Naval Research Laboratory, MASSIMO GRANATA, LORENZO MERENI, ALEX AMATO, CHRISTOPHE MICHEL, Laboratoire des Matériaux Avancés, GIANPIETRO CAGNOLI, Institut Lumière Matière, Université de Lyon — Reducing mechanical loss, or internal friction, in amorphous dielectric coating materials is practically important in many present-day applications, such as mirror coatings of gravitational-wave detectors or dielectric insulating layer in superconducting quantum bits. It is known that mechanical loss is dominated by atomic tunneling through potential barriers of double-well potentials below ~10 K and by thermal activation over the same potential barrier landscape. It has been found that extended air anneal reduces near-room temperature mechanical loss of ion-beam sputtered amorphous SiO$_2$. We measured elastic properties of ion-beam sputtered amorphous SiO$_2$ from 0.3 K to room temperature that includes internal friction, shear modulus and the relative change of speed of sound, and found that internal friction increases slightly accompanied by a large drop of thermal activation peak at higher temperatures. We discuss possible mechanisms for our observations.

*Work supported by the Office of Naval Research

Demonstration of two-dimensional hole gases (2DHG) in strained GeSn quantum wells*  

CHIA-TSE TAI, CHENG-YU LIN (Presenter), CHIA-YOU LIU, TZ-MING WANG, Natl Taiwan Univ, CHARLES HARRIS, TZU-MING LU, Sandia National Laboratories, JIUN-YUN LI, Natl Taiwan Univ — In this work, capacitively induced two-dimensional hole gases in undoped Ge/GeSn heterostructures were demonstrated. Ge/GeSn heterostructures with Sn fractions of 6%, 9% and 11% were grown by chemical vapor deposition with surface roughness below 3 nm. Hall bar devices were fabricated and characterized at 4 K. Density saturation was observed and the highest mobility was $1.9 \times 10^4$ cm$^2$/Vs. The dominant scattering mechanism is likely background impurity scattering. Shubnikov-de Haas oscillations and the quantum Hall effect were observed at B > 1 T, indicating high-quality material growth of Ge/GeSn heterostructures. Effective masses were extracted by the temperature-dependent SdH oscillations.

*This work at NTU was supported by MOST (107-2112-M-002-014- and 108-2112-M-002-011-) and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy (DOE), Office of Basic Energy Sciences user facility. Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. DOE’s National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.
3:18PM D27.00005: High sensitivity neutron detectors based on hexagonal boron nitride epilayers*  
AVING MAITY (Presenter), SAMUEL GRENAUDIER, JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech Univ — Hexagonal boron nitride (h-BN) has emerged as a promising material for realizing high efficiency solid-state thermal neutron detectors. Here, we report the epitaxial growth of thick h-$^{10}$BN ($^{10}$B enriched) epilayers and demonstration of thermal neutron detectors with a record high detection efficiency. To increase the overall detection sensitivity, we have explored strategies in material growth and device processing to reduce the detector’s dark current, capacitance, and surface recombination field and realized h-$^{10}$BN detectors from 100 µm thick freestanding wafers with a detection area as large as 1 cm$^2$ and a detection efficiency as high as 59%. We discuss the detail design and implementation of horizontal h-$^{10}$BN detectors to overcome the detrimental effects associated with increased dark current, capacitance, and surface recombination with increasing detector size, through reduction in metal contact area of the detector and utilization of superior lateral transport properties of h-BN. This work lays the foundation for achieving highly sensitive large h-$^{10}$BN neutron detectors for practical applications.

*This research is supported by DOE ARPA-E (DE-AR000964). Drs. Jiang and Lin are grateful to the AT&T Foundation for the support of Ed Whitacre and Linda Whitacre endowed chairs.

3:30PM D27.00006: Defect effects on Electron Magneto-Transport in Quantum Wells*  
DANHONG HUANG (Presenter), Space Vehicles Directorate, Air Force Research Lab - Kirtland, ANDRII IUROV, Department of Physics, Medgar Evers College of City University of New York, FEI GAO, Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College of the City University of New York — The point-defect effects on the electron magneto-transport in a multiple quantum-well system are investigated by employing a many-body theory. By working within the ladder approximation, our theory takes into account the local-field vertex correction to a bare polarization function of electrons. Moreover, both intralayer and interlayer screening to defect-electron interactions are included within the random-phase approximation. Furthermore, by studying defect charging dynamics, both capture and relaxation times of a point defect, as well as captured density of electrons, are computed as functions of temperature, electron density and different types of point defects. Finally, numerically calculated defect effects on energy-relaxation and momentum-relaxation times of are presented and analyzed for various defect and electron densities and different temperatures as well.

*DH would like to acknowledge the financial supports from the Air Force Office of Scientific Research (AFOSR) and the Laboratory University Collaboration Initiative (LUCI) program.
3:42PM D27.00007: Atomistic Simulations of the Cold Source Field-Effect Transistor for Sub-60 mV/decade Switching*  
RAPHAËL PRENTKI (Presenter), Physics, McGill University, MOHAMMED HARB, NanoAcademic Technologies, HONG GUO, Physics, McGill University — Sub-60 mV/decade subthreshold swing (S) transistors have been the object of considerable research efforts due to their low power dissipations. The cold source field-effect transistor (CSFET) achieves low S by suppressing thermionic emission in the OFF-state through source density-of-states engineering. This device has thus far only been investigated by simulations based on effective mass, k.p, and ballistic approximations. We report the first simulations of CSFETs based on combining the nonequilibrium Green's functions (NEGF) formalism with the tight-binding (TB) method, thereby capturing the atomistic details of the devices under nonequilibrium conditions. Specifically, we consider gate-all-around Silicon nanowire CSFETs grown in [100], [110], and [111] with diameters ranging from a few Å to a few nm. We find that vacancies and surface roughness have little influence on the performance of the device, which maintains a low S even in the presence of elastic scattering. Finally, we present both n-type and p-type CSFETs, thus substantiating the compatibility of CSFETs with complementary metal–oxide–semiconductor (CMOS) technology.

*Supported by Fonds de Recherche du Québec - Nature et Technologies (FRQNT) and the Natural Sciences and Engineering Research Council (NSERC) of Canada.

3:54PM D27.00008: Looking Back to Look Forward: How scarcity affects electronics cost and drives material research*  
SAMANTHA REESE (Presenter), ALBERTA CARPENTER, ROBIN BURTON, National Renewable Energy Laboratory — Typically discussions of electronics focuses on high value semiconductor products. However, without commoditized components such as resistors and capacitors and materials such as printed circuit boards and solder, electronic devices are not possible. As Moore's Law enables the internet of things (IOT) and allows data to become even more ubiquitous, the consumer electronics market is projected to experience an annual growth rate of 11.6% reaching $528 billion in 2023. This means more components are needed. Case studies will be presented showing how electronics manufacturing volume effects the raw material cost. An analysis of materials needed for commoditized component manufacturing will be shown, it will identify raw materials that could either cause significant cost increases to or even interrupt the component supply chain. The information can then be utilized to direct research into substitution materials or to suggest process improvement opportunities.

*This work was authored by the National Renewable Energy Laboratory (NREL), operated by Alliance for Sustainable Energy LLC, for the U.S. Department of Energy (DOE) under contract no. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Advanced Manufacturing Office.
4:06PM D27.00009: Angular Characterization of Magneto Optical Kerr-Effect by Ellipticity Modulation in Ultrathin Samples  
FERNANDO RAMIRO-MANZANO (Presenter), JAUME MESEGUER-SÁNCHEZ, FERNANDO CANTOS-PRIETO, EFREN NAVARRO-MORATALLA, Crisol Lab. Institute of Molecular Science (ICMol), University of Valencia — Magnetism in 2D materials has become of paramount interest in the scientific community because of overcoming the limitations of the Mermin-Wagner theory, nevertheless, new puzzling questions have arisen. Establishing the thickness frontier between bulk ferromagnetism and few-layer antiferromagnetism or the determination of the spin model that the 2D magnets follow are some of the current unsolved questions. One of the most sensitive techniques for characterizing the magnetism is the polarization changes of ellipticity-modulated light when interacts with a magnetic material. This technique permits to characterize both the Kerr-rotation and magneto-circular dichroism with a sensitivity bellow 100 µrad. Here, we will show the peculiarities of the experiments and simulations of the angular response of Van der Waalls magnetic materials. In particular, the Fourier plane response is acquired and compared with the simulation of the magneto-optical behavior. The fit results could allow extracting important parameters such as the spin orientation.

4:18PM D27.00010: Designing and characterizing rare-earth upconverting nanoparticles as nanoNewton mechanical sensors.  
CLAIRE MCLELLAN (Presenter), STEFAN FISCHER, CHRIS SIEFE, JASON CASAR, DAYNE SWEARER, MASASHI FUKUHARA, Materials Science and Engineering, Stanford University, MIRIAM B. GOODMAN, Department of Molecular and Cellular Physiology, Stanford University, JENNIFER A. DIONNE, Materials Science and Engineering, Stanford University — Non-invasive nanoscale mechanical force sensors will enable the monitoring of nanoNewton-scale forces in biological and condensed matter systems. Due to their near-infrared excitation with visible emission and robust host lattices, rare-earth upconverting nanoparticles (UCNPs) are a promising technology for mechanical force sensing. When engineered correctly, UCNPs exhibit a ratiometric color response to applied pressure but maintaining brightness high enough to detect this ratiometric color change at the single-particle level remains an outstanding challenge in the field. To create bright and force responsive particles, we explore alkaline earth host lattices (CaLuF, SrLuF, BaLuF). All particles studied are sub-15nm in diameter, core-shell, and are doped with 30% Yb$^{3+}$ and 2.9% Er$^{3+}$. Ensemble measurements with a diamond anvil cell yield a red-to-green intensity ratio ($I_R/I_G$) pressure responses of 20 ± 1.2, 16.2 ± 0.5, 12.7 ± 0.8, and 40 ± 4% ($I_R/I_G$/GPa for CaLuF, SrLuF, BaLuF, and NaYF$_4$, the control sample, respectively. We find that SrLuF-based nanoparticles respond to mechanical pressures changes of 37 MPa or 27 nN of force. Using a custom confocal-AFM microscope, we explore the brightness of single UCNPs and are developing techniques to explore their force sensitivity.
4:30PM D27.00011: Porous Carbon Nanotube Ring Resonators for Gas Sensing Application
DAVID MCKENNA (Presenter), HENRY DAVIS, RJ CASS, RICHARD VANFLEET, ROBERT DAVIS, Brigham Young Univ - Provo — Using the carbon nanotube templated micro-fabrication (CNT-M) method we have formed and characterized porous micro-mechanical ring resonators for gas sensing applications. The tunable porosity of the CNT structures lends itself to high surface area to volume ratios. In the resonator, a high surface area to mass ratio coupled with a high quality factor (Q) can enable detection of gasses at very low concentrations. The gas concentration detection limit is proportional to the inverse of the Q of the resonator. Building on previous work with micro-cantilevers, here we present results of in-plane ring resonators designed to reduce clamping and thermoelastic losses. This in-plane mode has the added advantage of being less sensitive to manufacturing variations in the height of the resonator. We present our work characterizing the gas and time response of these resonators.

4:42PM D27.00012: Role of dimensionality on thermodynamic properties in layered sulfides* NATHAN KOOCHER (Presenter), JAMES RONDINELLI, Materials Science and Engineering, Northwestern University — Understanding thermal expansion of materials helps in assessing the capability, performance, and lifetime of materials operating in variable thermal conditions. Previously Ca$_3$Ti$_2$O$_7$ with the layered Ruddlesden-Popper (RP) structure (n=2 member of A$_{n+1}$B$_n$O$_{3n+1}$) was found to exhibit pressure-tunable negative thermal expansion (NTE) and a pressure-independent softening of the bulk modulus due to a quasi-two-dimensional vibration [Huang et al, Phys. Rev. Lett. 117, 115901 (2016)], whereas RP strontium titanates did not exhibit NTE [Huang et al, Chem. Mater. 30, 7100 (2018)]. Here, we evaluate structural, lattice dynamical, and thermodynamic properties of the barium zirconium sulfide family with layer thickness $n=1,2,$ and $\infty$ using the self-consistent quasi-harmonic approximation within density functional theory. We formulate layer thickness dependent models of the anharmonic lattice properties and discuss how they may be used for design of thermal expansion coefficients in other chemistries.

*This work was funded by the National Science Foundation through grant no. DMR-1720139.
4:54PM D27.00013: Elastic Constants of Boron Arsenide and Boron Phosphide Crystals
*SUSHANT MAHAT (Presenter), University of Illinois at Urbana-Champaign, SHENG LI, HANLIN WU, PAWAN KOIRALA, BING LV, University of Texas at Dallas, DAVID CAHILL, University of Illinois at Urbana-Champaign — We report experimental results for picosecond ultrasonics (PU) studies of boron arsenide and boron phosphide crystals with zinc blend structure. These materials have coefficients of thermal expansion similar to commonly used semiconductors like Si and GaAs, and the synthesis of BAs and BP single crystals with thermal conductivity as high as 1000 and 540 Wm⁻¹K⁻¹ respectively has made them into promising materials for thermal management applications. Using PU, we measure Brillouin scattering frequencies and calculate longitudinal and shear velocities along several directions of the BAs and BP single crystals. The crystal directions are determined using electron backscattering diffraction and associated Christoffel equations are used to solve for the elastic constants of the crystals. We report $C_{11}$, $C_{12}$, and $C_{44}$ values of 289.4, 113.5 and 159.0 GPa for BAs and 310, 87, and 160 GPa for BP, respectively. Furthermore, we also demonstrate the utility of PU in studying optical and acoustic attenuation in these crystals. The elastic constants and the attenuation measurements will help to predict thermal transport behavior in these materials.

*Office of Naval Research (ONR) MURI grant N00014-16-1-2436

5:06PM D27.00014: Microscopic model for contact electrification between solids and fluids
MORTEN WILLATZEN (Presenter), Chinese Academy of Sciences, LOK CHONG LEW YAN VOON, Physics Department, University of West Georgia, ZHONG LIN WANG, School of Materials Science and Engineering, Georgia Institute of Technology — Triboelectric charge transfer between materials is a well-known phenomenon since more than 2000 years that still causes dispute. Recent experimental evidence suggests electron transfer to be the main mechanism for contact electrification between dielectrics and metals, and the electron transfer is specified by the material bandstructures and Fermi levels [1]. We present a new microscopic formalism based on a tight-binding Hamiltonian to describe charge transfer between two materials. The model captures charge transfer dynamics on a femtosecond scale, reveals the influence of Coulomb interactions for charge transfer oscillations, and is able to predict charge transfer differences between materials whether structured or disordered solids and fluids. We demonstrate that charge transfer between fluids and solids is more effective than between two solids, that charge transfer between two similar materials is possible, and shed light on the differences between metal-dielectric and dielectric-dielectric contact electrification.

Due to their sizable bandgap and layer-dependent properties, the transition metal dichalcogenides (TMDs) are of interest for a variety of electronic and optoelectronic applications.\(^1\) While much research in the field of 2D materials has focused on the emergent properties as a result of confinement to two dimensions, further confinement into quasi-one-dimensional nanoribbons is expected to provide a further handle for tuning the electronic structure.\(^2,3\) In this work, we have employed a bottom-up gas-phase synthesis within carbon nanotubes to template the growth of TMD nanoribbons. By growing the materials within nanotubes we can create nanoribbons with variety of widths. The nanotubes also provide protection from degradation due to oxidation or solvents enabling the facile handling and study of air-sensitive materials.


**Monday, March 2, 2020 2:30 PM - 5:30 PM**

**Session D28 GMED FIAP: Metrology in Medical Imaging**

Invited
The standard paradigm in medical imaging uses sophisticated imaging systems that take advantage of a variety of phenomena that create image contrast, and those images are subjectively interpreted by highly trained clinicians. The trend toward measurement-driven medicine motivates an effort to convert imaging systems into measurement systems which provide quantitative imaging biomarkers. The mission of the Radiological Society of North America’s Quantitative Imaging Biomarker Alliance is to improve the value and practicality of quantitative imaging biomarkers by reducing variability across devices, sites, patients, and time. The core of the effort is the adoption of the principles of metrology into image analysis methods so confidence intervals can be claimed on imaging/measurement performance. Physicists’ contribution to this effort includes developing new imaging biomarkers, creating simulations of the physical interactions of image formation (in silico phantoms), and creating methods for objectively quantifying the technical performance of the system. Examples of objectively assessed parameters that are direct substitutes for subjectively assessed parameters, as well as other parameters that are not readily extracted from standard imaging methods, will be described. Methods for assessing their performance as quantitative imaging biomarkers will be described.

*Professor Hall is a Vice-Chair of the Quantitative Imaging Biomarker Alliance and is supported through a contract between The University of Wisconsin and the Radiological Society of North America. Some of the data shown was obtained under funding by NIH grants R01HD096361, R01HD072077, and R01CA140271.
3:06PM D28.00002: Importance of Statistical Metrology Framework for Quantitative Imaging Applications* [Invited] NANCY OBUCHOWSKI (Presenter), Quantitative Health Sciences, Cleveland Clinic Foundation — Quantitative imaging is being increasingly used to diagnose disease, predict patients’ outcomes, and monitor and adapt treatment. In clinical trials, quantitative imaging often serves as a non-invasive endpoint which can provide results earlier than traditional patient outcomes.

The precision and bias of quantitative imaging measurements drive their utility at the bedside and in clinical trials. Precision describes the closeness of replicate measurements, while bias describes how the measurements differ from the true value [1]. These technical performance characteristics are important in order to understand patients’ measurements, as well as to plan and analyze clinical trials [2].

In this presentation we examine several clinical trials using quantitative imaging. We discuss how the technical performance characteristics of the imaging biomarkers are used to determine sample size, identify eligible subjects, estimate treatment effect, and interpret measurements and change in measurements over time.


*Dr Obuchowski is a statistical consultant for the Quantitative Imaging Biomarker Alliance, through a contract between The Cleveland Clinic Foundation and RSNA.

3:42PM D28.00003: Quantitative Imaging Applications for Radiography and Computed Tomography [Invited] SAM ARMATO (Presenter), Department of Radiology, University of Chicago — Post-acquisition mathematical analysis of medical images can range from simple image processing to complex computer-aided diagnosis. The intent of such manipulation can range from the enhancement of aspects of the image for improved human visualization to artificial intelligence. The tools available for image analysis span the fields of mathematics, statistics, and computer science and incorporate biophysical aspects of the medical image acquisition system. The extraction of quantitative information (or “features”) from medical images and the use of this information to assist radiologists in their medical decision-making process (termed “radiomics”) has expanded medical imaging from a subjective art to much more of an objective science. Radiography, as the most common imaging modality, and computed tomography (CT), as the predominant tomographic imaging modality, both benefit from a vast array of quantitative techniques. Applications include volumetry of tumors and other abnormalities, assessment of response to therapy, patient prognosis, and evaluation of disease severity.
Due to its unique physical decay properties, positron emission tomography (PET) was developed, commercialized and marketed as a quantitative imaging technique. The first commercial scanners sold in the 1970s targeted the clinical research market, in particular for neurology and cardiology applications. The 1980s saw the rapid development of a new PET tracer called 18-F fludeoxyglucose (FDG), which is an effective tracer to quantitatively measure absolute glucose metabolism (e.g. umol of glucose/min/100 gm of tissue) non-invasively. It was soon shown that FDG PET filled an unmet clinical need for both the diagnosis and treatment of cancer patients, and the 1990s saw a rapid growth of clinical PET. PET innovations in the 2000s included whole body PET scans (e.g. moving the patient bed so patients can be scanned from head to toes), and the hybridization of PET scanners with CT and MR for better anatomical location. Today, 95% of all clinical PET scans are whole body FDG oncology scans. However, in order to make the scan time shorter and the analysis and reading faster, surrogate measures of absolute glucose metabolism were developed. The most popular surrogate is the standardized uptake value (SUV), and this talk will cover the pros and cons of using the SUV as a quantitative measure and initiatives driven by PET physicists and clinicians to make it a better universal and quantitative measure. The latest quantitative PET innovations from industry will also be presented, including making the measure of absolute glucose metabolism practical in the clinic – effectively bringing PET full circle and back to its commercial beginnings.

Magnetic Resonance Imaging (MRI) is able to interrogate a wide range of physical parameters. Some of these are intrinsic to magnetic resonance, such as relaxation times, while others are universal, such as diffusion coefficients, temperature, or magnetic susceptibility. This talk will provide an overview of important quantitative imaging biomarkers (QIBs) in MRI, highlighting their current and future applications, the challenges in measurement science and implementation, and the current status and progress of QIBs towards widespread clinical adoption.

The path from bench to bedside of QIBs involves researchers from many disciplines, and provides numerous opportunities for physics to inform approaches and improve the reliability of imaging. Bench scientists ensure that QIBs can be traced to primary standards, developing measurement infrastructure to establish ground truth values for reference materials and objects, known as phantoms. The Quantitative Imaging Biomarker Alliance (QIBA) is composed of stakeholders including equipment vendor and pharmaceutical representatives, statisticians, clinicians, technologists, and physicists. QIBA develops and promulgates standards-based documents known as Profiles that harmonize data acquisition and analysis, and which utilize reference standards, both physical and digital, to assess end users’ ability to conform to the Profile. The use of QIBA Profiles in clinical trials and clinical practice, backed by sound measurement science, can improve reproducibility of results, enhancing patient care and outcomes.
2:30PM D29.00001: Spatial-temporal organization of bacterial suspensions under confinement* [Invited] IGOR ARONSON (Presenter), Biomedical Engineering, Pennsylvania State University — Suspensions of motile bacteria or synthetic microswimmers, termed active matter, manifest a remarkable propensity for self-organization and formation of large-scale coherent structures. Most active matter research deals with almost homogeneous in space systems and little is known about the dynamics of active matter under strong confinement. We present experimental and theoretical studies on the expansion of highly concentrated bacterial droplets into an ambient bacteria-free fluid. The droplet is formed beneath a rapidly rotating solid macroscopic particle inserted in the suspension. We observed vigorous inability of the droplet reminiscent of a supernova explosion. The phenomenon is explained in terms of continuum first-principle theory based on the swim pressure concept. Furthermore, we investigated self-organization of a concentrated suspension of motile bacteria *Bacillus subtilis* constrained by two-dimensional (2D) periodic arrays of microscopic vertical pillars. We show that bacteria self-organize into a lattice of hydrodynamically bound vortices with a long-range antiferromagnetic order controlled by the pillars’ spacing. Our findings provide insights into the dynamics of active matter under extreme conditions and significantly expand the scope of experimental and analytic tools for the control and manipulation of active systems.

*NSF PHY-1707900

3:06PM D29.00002: Trapping of microswimmers in vortex flows* SIMON BERMAN (Presenter), KEVIN A MITCHELL, University of California, Merced — We theoretically investigate the trapping of rigid, ellipsoidal microswimmers in externally-driven two-dimensional vortex flows. Surprisingly, for swimmers that swim perpendicular to their elongation direction, we find that trapping depends non-monotonically on swimming speed. We identify certain stable periodic solutions of the swimmer equations of motion as the cause of trapping in individual vortices. A bifurcation analysis of these solutions explains the dependence of trapping on swimmer speed, shape, and swimming direction. We propose heteroclinic bifurcations between swimming fixed points as a general mechanism for the creation of stable swimmer trajectories.

*Supported by NSF grant CMMI-1825379.
3:18PM D29.00003: Sensorimotor processing and navigation in confined microswimmers
SAMUEL BENTLEY, VASILEIOS ANAGNOSTIDIS, FABRICE GIELEN, KIRSTY WAN (Presenter), University of Exeter — All living organisms are environmentally intelligent. This is the fundamental distinction between life, and other forms of matter. Even unicellular organisms are capable of complex behaviours, for they can sense as well as respond to changes in the environment. Here, we study spontaneous and constrained motor actions in algal microswimmers, using motility as a dynamic read-out of behaviour and physiology. Previous studies have focussed on locomotion transients over short timescales ranging from milliseconds to minutes. We present a novel microfluidic platform which allowed us for the first time to monitor and analyse algal cell motility over hours, and even developmental timescales. We focus on two species, a biflagellate which exhibits a form of run-and-tumble, and an octoflagellate which exhibits a tripartite behavioural repertoire termed run-stop-shock. Excitability and stochastic transitions in swimming gait are projected onto a low-dimensional state space. We reveal how flagellar mechanosensitivity mediates repetitive boundary interactions, and discuss the discovery of a light-dependent quiescent regime. Finally, we conduct pharmacological perturbations within these microenvironments, to shed new light on the physiological origins of excitable flagellar dynamics.

3:30PM D29.00004: Topographical guidance of highly-motile cells using cell-sized features
JOERI WONDERGEM (Presenter), KOEN K SCHAKENRAAD, Leiden University, PATRICK WITZEL, University of Würzburg, MARIA MYTILINIOU, Leiden University, DAVID HOLCMAN, École Normale Supérieure, DORIS HEINRICH, Leiden University — Cells navigate complex environments where they encounter a variety of physical cues. The extracellular topography is such a cue, as a substrate of anisotropically placed, sub-micron sized pillars, was recently shown to induce directed cell migration, a process named topotaxis. Here, we focused on a larger scale, and studied the influence of cell-sized obstacles on highly-motile, persistent cell migration. Using engineered topographies, reminiscent of pores cells squeeze though in vivo, and tracking cell migration, we explored the effects of spacing and obstacle geometry on cell motility. We show that cells undergo long-range topotaxis over large distances by anisotropically placed cell-sized obstacles. Furthermore, we performed active particle simulations, a minimal model for cell motility, to investigate the physics needed to reproduce key features of cell motion in different topographies. Finally, we show that long-range topographic guidance is conserved in chemical gradients, and moreover, the cues, topotaxis and chemotaxis, abide to linear summation, guiding the cell in the direction of both cues combined. Hence, topotaxis offers an independent way to steer cells, which can be exploited as a tool for in vitro applications, like lab on chip diagnosis and tissue engineering.
3:42PM D29.00005: Quenching active matter using light: Light mediated motility in swarming Serratia marcescens*  ARVIND GOPINATH (Presenter), JUNYI YANG, University of California, Merced, ALISON PATTESON, Department of Physics, Syracuse University, PAULO ARRATIA, Mechanical engineering, University of Pennsylvania — Understanding the connection between external stimuli such as light and emergent response manifested in multicellular, collective and long-range motility of cells and cell-like active systems remains a challenge. Swarming, a mode of bacterial surface migration is characterized by emergent flows, persistent structures and collaborative collective motility. Here we present the effects of light on the collective motility in a dense and far from equilibrium active system – swarms of the bacteria Serratia marcescens. Using a experimental light-based technique, we induce and generate localized condensed domains differing in motility. We then study immobilization and quenching of flow inside these domains and map the response to light in terms of the light intensity and duration of exposure. Together these parameters determine the reversibility of the response, domain size and extent of the mobility impaired region as well as its temporal evolution. Complementing our experimental results, we propose and analyze a minimal Brownian dynamics model to study the escape of bacteria from the exposed region before they are completely immobilized and trapped.

*Authors acknowledge funds from the UC Senate CORE grant and NSF CBET-1437482.

3:54PM D29.00006: Submerged micro-structures generate a soft boundary effect on active nematic flows*  DIMITRIUS KHALADJ (Presenter), AMANDA TAN, LINDA S. HIRST, University of California, Merced — Actively driven bundled microtubule networks have become a useful framework to study energy driven defects in structured fluids. Moreover, the implementation of soft boundaries instead of hard side walls can be a useful strategy to control defect flow and dynamics. We study the behavior of an active nematic microtubule system confined by submerged complex geometries. From our preliminary work, we have observed that submerged 3D structures can influence defect dynamics. We also demonstrate that the soft barrier generated by the submerged structures form stagnation points near the boundary reminiscent of those seen for hard boundaries. With the assistance of micro fabrication, we investigate the spontaneous flows of this novel system under confined conditions i.e. in proximity to the boundary of the submerged structures. For this investigation, we used cylindrical pillars and rectangular trenches. We are also interested to learn if the submerged surfaces will impact chaotic mixing dynamics.

*Acknowledgement of funding from the National Science Foundation: DMR-1808926, NSF-CREST: Center for Cellular, National Science Foundation MRI Award for confocal microscopy (DMR-1625733) and Biomolecular Machines at UC Merced (HRD-1547848) and from the Brandeis Biomaterials facility MRSEC-1420382.
4:06PM D29.00007: Lattices by design: exploring long-ranged interactions with gradient sensing droplets*  ANTON MOLINA (Presenter), MANU PRAKASH, SHAILABH KUMAR, Stanford Univ — Many body interactions are ubiquitous and occur across length scales, giving rise to a vast diversity of phenomena ranging from frustration to pattern formation with important implications for the design of new materials. However, their behavior can be challenging to predict since the number of relevant configurations scales exponentially with the number of particles. Two-component Marangoni-contracted droplets have been shown to interact via long-ranged vapor mediated attractions, resulting in a dynamic behavior that resembles chemotaxis and a capacity to self-organize. Meanwhile, hydrophobic barriers can create well-defined potential energy wells that are impassable to droplets but transparent to a vapor gradient landscape. Here, we develop exotic lattice systems that exploit the tools of photolithography to fabricate arbitrary patterns of hydrophobic boundaries, enabling us to experimentally manipulate the geometry in which long-ranged degrees of freedom interact. The macroscopic nature of this system provides real time access to microstate configurations, providing the opportunity for mechanistic insights and the development of control strategies in complex, interacting systems.

*AM is supported by the National Science Foundation Graduate Fellowship Research Fellowship Program

4:18PM D29.00008: Arresting Active Spinning Particle Coarsening in Passive Media via Actuation Protocols  JOSHUA STEIMEL (Presenter), Univ of the Pacific, RYAN TOLLEFSEN, Oregon State, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Active matter systems are unique in the rich non-equilibrium dynamical behavior that emerges such as flocking, lanning, swarming, and vortexting. Such emergent behavior has been previously observed in complex hybrid active-inactive systems with in-plane rotating magnetic particles; where active particle attraction is induced by the activity of the particles and the mechanical properties of the passive media. When continuously actuated these active particles will aggregate and coarsen. We present a novel approach which allows the control of coarsening behavior and resultant characteristic domain size via modulation of the activity actuation protocol. By tuning the frequency at which the rotational direction of the active spinning magnetic particles is changed, either clockwise or counter-clockwise, the system can exhibit microphase separation behavior distinct from the macrophase separation of active and passive particles. Changing the rotational direction is effectively equivalent to reversing the torque and unloading the stress in the system. This limits the ability of active particle clusters to attract, can arrest the coarsening behavior, and decrease the characteristic domain size. Thus, allowing control of the structure of these hybrid active-inactive systems.
4:30PM D29.00009: Flocking Transition in a Self-propelled Particle Model Using Experimental Motility Conditions*  JELANI LYLES, PAUL YANKA (Presenter), CHIH KUAN TUNG, North Carolina A&T State Univ, DANIEL SUSSMAN, Emory University, M. LISA MANNING, Syracuse University — Flocking transition has been studied using self-propelled particle models for decades. In these models, the initial angular distribution is random, the step-by-step angular fluctuation is either a bounded flat noise or a Gaussian noise, and the magnitude of the velocity of each moving particle is thought to be a constant. Experimental study of sperm flocking show that an aligned initial condition promotes sperm to form large flocks, angular fluctuation follows an exponential decay, and the velocity distribution follows a Gamma distribution. Our research has focused on using a computational model to understand the effects from those differences between experimental observation and the traditional model conditions. We found that aligned initial condition does help sperm to form larger flocks when the system is at the transition, but not much effect elsewhere. No major difference was seen between exponential and Gaussian angular noise. The Gamma velocity distribution was found to lower the density of the flocks. Our results provide evidence to rethink adapting the conclusion from active matter models to experimental systems.

*NSF HRD 1665004 and APS Bridge Program MSI Travel Grant

4:42PM D29.00010: Re-entrant self pumping in confined active fluids*  MINU VARGHESE (Presenter), ARVIND BASKARAN, MICHAEL HAGAN, APARNA BASKARAN, Brandeis Univ — Spontaneous flows in the form of swirls is ubiquitous in biological systems. Such active swirling/turbulent flows self organize into net pumping flows when confined appropriately. Studies on 2D systems suggest that self pumping results when the confinement length scale is smaller than the size of swirls that form spontaneously in the bulk. However, recent experiments have shown that when confined in 3D channels, the emergence of self pumping can be more sensitive to the aspect ratio of the channel than to the size of the channel itself. This is a phenomenon that is unique to 3D and to active fluids. In this talk, I will discuss the origin of this phenomenon using an active hydrodynamic theory.

*This project was funded by the Brandeis MRSEC, and supported by computational resources from XCEDE
4:54PM D29.00011: Tunable self-organization of swimming magnetic bacterial suspensions*
HIRAN WIJESINGHE (Presenter), CHRISTOPHER J PIERCE, ERIC MUMPER, BRIAN LOWER, STEVEN LOWER, RATNASINGHAM SOORYAKUMAR, Ohio State Univ - Columbus — When units of active matter are brought together, the properties of the new construct are not always equal to the sum of the properties of the components. Instead, at each level, new behavior and rules (i.e., emergent properties) appear. For instance, the emergence of spontaneous order in collections of disordered biological components, from suspensions of biofilaments to bird flocks, is widespread in nature. We present population-level self-organization in a flagellated magnetic bacterial suspension of *Magnetospirillum magneticum* (AMB-1) that is amenable to experimental control using programmable fields. A major hindrance to the understanding of the emergent properties in a typical biological system is its complexity due to competing inter-component interactions, biological and external constraints, non-equilibrium dynamics, as well as stochasticity. Detailed computational modeling of hydrodynamics and magneto-aerotaxis in these motile AMB-1 suspensions reveals the underlying mechanisms leading to their self-organization, by producing experimentally verifiable population-level dynamics. This approach can be generalized to other species and active matter systems in general.

*This material is based upon work supported by the National Science Foundation under grant ECCS 1710598.

5:06PM D29.00012: Dynamics of 2D Active Nematics Confined in an Annulus*
CHAITANYA JOSHI (Presenter), ZAHRA ZAREI, MICHAEL M NORTON, SETH FRADEN, APARNA BASKARAN, MICHAEL HAGAN, Brandeis University — Active nematics are a class of non-equilibrium systems with constituents that consume energy at the molecular level to generate motion. While the dynamics of a bulk 2D active nematic are turbulent, confinement can provide a systematic way of achieving control over the flow. An annulus confinement geometry is particularly interesting because it could generate self-driven circulating flows. Indeed, such states have been found in recent experiments. In this talk, we will discuss a theoretical and computational study of 2D active nematics confined to an annulus. By performing simulations and comparing results against experiments as a function of geometry, boundary conditions and activity, we identify the driving forces and factors that control net circulation. In addition, by comparing the spatiotemporal behaviors as a function of annulus geometry with those observed in a channel, we elucidate the effect of boundary curvature on emergent behaviors in an active nematic.

*This work is funded by the NSF MRSEC DMR-1420382 and DMR-1855914.
5:18PM D29.00013: Self-organization of bacterial active matter in space and time*  SONG LIU (Presenter), YILIN WU, Chinese Univ of Hong Kong — Simultaneous control of spatial and temporal organization of active matter is challenging and generally requires complex interactions. Here we found that tuning the rheological properties of bacterial active fluids enables large-scale spatial and temporal self-organization. Combining experiments with an active matter model, we explain the phenomenon in terms of the interplay between active forcing and viscoelastic stress relaxation. Our findings advance the understanding of bacterial behavior in complex fluids and demonstrate experimentally that rheological properties can be harnessed to control active matter flows.

*This work was supported by the National Natural Science Foundation of China (NSFC No. 21473152) and the Research Grants Council of Hong Kong SAR (RGC Ref. No. CUHK 409713). S.L. thanks the IBS Center for Soft and Living Matter (South Korea) for supporting the trip to the conference.

Monday, March 2, 2020 2:30 PM - 5:30 PM


2:30PM D30.00001: How do cells control the length of their flagella?  PRATHITHA KAR (Presenter), Harvard University, THOMAS FAI, LISHIBANYA MOHAPATRA, JANE KONDEV, Brandeis University, ARIEL AMIR, Harvard University — Cells assemble a number of filamentous structures which have a specific length. The question of how cells control the length has been studied extensively in model organism *Chlamydomonas reinhardtii* which has two flagella of the same length.

Past studies have shown that when one of the flagella is severed, its length increases over time while, remarkably, the other flagellum shortens. Upon reaching a common length, the two flagella grow together until reaching their steady state length. Although we know the molecular players involved in the process, the mechanism is not well understood.

Previously, several models have suggested length-control to occur via the length-dependent assembly of the flagella. Here, we show that within a wide class of models, length-control of multiple flagella can only occur if the disassembly (depolymerization) of the flagella is length-dependent. We provide concrete examples to show how such length-dependent-depolymerization can occur within simple biophysical models.
How cells regulate the size of filamentous structures, networks and organelles, despite continuous turnover in their component parts, is a longstanding question. Recent experiments suggest that size control of many intracellular structures and organelles is achieved through depletion of a limiting subunit pool in the cytoplasm. While the limiting pool mechanism ensures organelle size scaling with cell size, it does not provide a mechanism for sensing and regulating individual organelle size.

Here we present a physical theory for non-equilibrium self-assembly and size regulation of subcellular structures, based on negative feedback between structure size and growth rate. This model provides a mechanism for robust size regulation of multiple structures in the presence of stochasticity and competition for resources. Using this model we predict size regulation of multiple organelles, filaments, and networks, in quantitative agreement with available experimental data. We also demonstrate how competition for subunit resources between multiple networks can lead to spontaneous cell polarisation.

*Human Frontier Science Program (HFSP) and The Royal Society

Energy cost of protein gradient formation in cells  
ARNAB DATTA (Presenter), Brandeis Univ — Cells make protein gradients for various purposes, such as establishing position information in development or defining cell polarity in the process of cell division. Two classes of mechanisms for maintaining protein gradients in cells have been reported in the literature: i. those that combine protein diffusion and degradation, and ii. mechanisms that involve active transport of proteins by molecular motors. An example of the first mechanism is the Bicoid protein gradient in the Drosophila embryo, which provides positional information to the nuclei during development. A Smy1 gradient along actin cables in budding yeast cells regulates cable length and is formed by active transport of the proteins by myosin motors to the bud neck [1]. Establishing and maintaining these protein gradients require cells to expend energy. In this talk I examine different mechanisms of gradient formation in cells and estimate the energy costs associated with them. I also consider the scaling of the energy expenditure with cell size for the two different models of gradient formation, and discuss when one mechanism is energetically less costly than the other.

References:
First passage times in multi-protein self-assembly

BHAVYA MISHRA (Presenter), MARGARET JOHNSON, TC Jenkins Department of Biophysics, Johns Hopkins University — Self-assembly of proteins is essential for various cellular processes such as signalling, and clathrin-mediated endocytosis. In general, proteins diffuse in a 3D solution and recruit other proteins. But they can also localize to a 2D membrane surface via lipids. In a recent study, we quantified how localization of proteins to a 2D surface from 3D solution reduces their search space and proteins can exploit this dimensionality reduction to trigger self-assembly. Here we show how localization can in many cases accelerate the assembly process, despite significantly slower diffusion on the 2D surface. We formulate the self-assembly of protein binding pairs as first-passage problems and calculate the mean time to approach the thermodynamic equilibrium. We can theoretically approximate the role of localization in slowing or accelerating the overall assembly process and the regimes where diffusion becomes a limiting factor. We validate these predictions against numerical solutions using reaction-diffusion simulations. These results highlight the role of diffusion versus binding rates and concentration in controlling time-scales of assembly.

Quantifying kinetics of multi-protein self-assembly, remodeling, and disassembly

YIBEN FU, MARGARET JOHNSON (Presenter), Johns Hopkins University — In the cell, multi-protein assemblies cannot persist forever and must ultimately disassemble through active or spontaneous processes. Protein assemblies involved in virion formation and clathrin-coat formation also appear to undergo dynamic remodelling which is critical for successful function. We show here using reaction-diffusion simulations how the kinetics of these assembly and disassembly processes can be sensitively tuned by the binding kinetics and cooperative interactions of the coat components and the molecules linking them to the membrane. We determine regimes where assembled structures can spontaneously remodel or disassemble. For stable structures, we then predict how enzymatic reactions can be exploited to locally destabilize links to the membrane and drive remodelling and disassembly. Using our recently developed NERDSS software, these models generate space and time-dependent predictions that can be compared directly with experiment. Our generalized computational methods can directly simulate a broad range of assembly processes at the cell-scale, providing a natural companion to quantitative cell biology.

NIH MIRA, NSF CAREER
3:30PM D30.00006: Theoretical principles of viral shell assembly and self-organization*

[Invited] ROYA ZANDI (Presenter), University of California, Riverside — Spherical crystals are elementary models of geometric frustration in materials, with important realizations in a range of systems from viral shells and fullerenes to particle- and molecular-coated droplets. Using continuum elasticity theory, we study the structure and elastic energy of ground states of crystalline caps conforming to a spherical surface. We find that the ground states consist of positive disclination defects and that the ground states with icosahedral subgroup symmetries in caps arise across a range of curvatures, even far from the closure point of complete shells. Further, we use Monte Carlo simulations to investigate the kinetic pathway of formation of viral shells (capsids) and find that the key for the formation of perfect icosahedral capsids is in the strength of elastic energy compared to the protein-protein interactions and the chemical potential of free subunits.

*We acknowledge support from the NSF through Awards DMR-1719550

4:06PM D30.00007: Computational modeling to explain Hepatitis-B Virus capsid assembly, dimorphism, and disruption by antiviral drugs* FARZANEH MOHAJERANI (Presenter), BOTOND TYUKODI, Department of Physics, Brandeis University, CHRISTOPHER SCHLICKSUP, Department of Molecular and Cellular Biochemistry, Indiana University, JODI HADDEN, Department of Chemistry and Biochemistry, University of Delaware, ADAM ZLOTNICK, Department of Molecular and Cellular Biochemistry, Indiana University, MICHAEL HAGAN, Department of Physics, Brandeis University — Assembly of the outer protein shell (capsid) of a virus is an essential step in its lifecycle. Understanding the mechanisms underlying assembly and the factors that determine the final morphology will guide development of antiviral drugs that disrupt or redirect assembly processes. Hepatitis-B Virus (HBV) assembles from a single capsid protein, which adopts different conformations to form icosahedral capsids with different sizes containing 180 or 240 proteins, T=3 or T=4 respectively in the Caspar-Klug nomenclature. Despite intensive experimental and theoretical investigation, the assembly pathways and mechanisms that control HBV dimorphism remain unclear.

In this talk we will describe dynamical computer simulations of HBV assembly, using a model which is minimal and highly computationally tractable, but has parameters learned from atomistic simulation data of whole HBV capsids. The simulation results identify pathways leading to T=3 and T=4 capsid morphologies, and suggest key factors which control this dimorphism. We describe tests of the model against experimental data, and propose mechanisms of action for antiviral drugs that result in assembly of malformed shells in recent HBV experiments.

*Supported by Award Number R01GM108021 from NIGMS, NIH and Brandeis NSF MRSEC, DMR-1420382
4:18PM D30.00008: Thermodynamic and kinetic aspects of polymorphism in core controlled assembly of virus-like particles* ALIREZA RAMEZANI (Presenter), Physics and Astronomy, University of California: Riverside, ORFEAS AGIS KARACHALIOS, PAUL VAN DER SCHOOT, Physics and Astronomy, Institute for Theoretical Physics, Utrecht University, ROYA ZANDI, Physics and Astronomy, University of California: Riverside — Motivated by recent experiments we investigate the phenomenon of polymorphism in core- controlled self-assembly of virus-like particles, where identical nanoparticles are encapsulated in capsids with different sizes. Our goal is to understand how protein concentration, stoichiometry and preferred curvature of capsids influence the prevalence of one shell size over another one. Using the equilibrium statistical physics and classical nucleation theory, we study how kinetic traps modify the state diagrams. We find that the free energy penalty associated with the rim proteins that have fewer favorable contacts with other proteins plays an important role in determining the capsid size. We show that in and out of equilibrium phase diagrams differ significantly and that kinetics favors the co-existence of capsids with different sizes at large stoichiometric ratios and/or protein concentration.

*HFSP grant RGP0017/2012
National Science Foundation, DMR-171955

4:30PM D30.00009: RNA-mediated capsid nucleation of bacteriophage MS2 coat proteins confers RNA packaging selectivity TIMOTHY CHIANG (Presenter), REES F GARMANN, AARON GOLDFAIN, LANELL A. WILLIAMS, VINOTHAN MANOHARAN, Harvard University — Simple viruses, such as bacteriophage MS2, spontaneously assemble into a protein shell encapsulating a single molecule of genomic RNA. Infection of host cells by MS2 results in replication of the RNA and expression of viral coat proteins, which then package the cognate viral RNA with high selectivity despite the presence of competing host RNAs. How the MS2 coat proteins selectively self-assemble around their own RNA is poorly understood. Using interferometric scattering microscopy and quantitative gel electrophoresis, we show that the RNA-mediated nucleation-and-growth assembly pathway of MS2 coat proteins can drive preferential encapsidation of cognate RNA, and hence selective packaging.
4:42PM D30.00010: Role of C-Terminal "Arms" in the Assembly and Stability of SV40 Polymorphs*  CURT WALTMANN (Presenter), Materials Science and Engineering, Northwestern University, MONICA OLVERA DE LA CRUZ, Materials Science and Engineering, Chemistry, Northwestern University, ROI ASOR, URI RAVIV, Institute of Chemistry, The Hebrew University of Jerusalem — We study SV40 polymorphs by simulating the templated assembly process of VP1 pentamers. The simulations incorporate electrostatic effects and the connections formed between VP1 proteins by C-terminal flexible lateral units, termed here "arms". During assembly, VP1 pentamers connect to partial capsids before they bind to the template. The strength of these connections along with salt concentration can be manipulated leading to incomplete particles, T=1 particles, or aggregates of VP1 pentamers. In contrast to all other configurations, which are dynamic, the T=1 particles are static. The ability of VP1 pentamers to connect to other VP1 pentamers combined with the dynamic rearrangement of particles other than T=1 allows capsids to continue growing even when they are "pseudo-closed". The assembly mechanism described here is likely applicable to T=7 capsids.

*MOdlC and CW thank the support of the Sherman Fairchild Foundation. CW was supported in part by the Northwestern University Graduate School Cluster in Biotechnology, Systems, and Synthetic Biology, which is affiliated with the Biotechnology Training Program. UR and RA thank the ESRF synchrotron, ID02 beamline and the support of the NIH (Award Number R01GM108021). RA acknowledges support from the Kaye-Einstein fellowship foundation.

4:54PM D30.00011: Linking Capsomere Elasticity with Virus Capsid Size and Patterning* LAUREN NILSSON (Presenter), JCS KADUPITIYA, VIKRAM JADHAO, Intelligent Systems Engineering, Indiana University Bloomington — Self-limiting spontaneous assembly of proteins gives rise to many structures, including virus capsids. Often copies of a single type of protein are capable of assembling into an empty shell. Higher T-number viruses of this type, such as Hepatitis B virus (HBV), present an interesting challenge to model. Though these capsids exhibit a ubiquitous icosahedral symmetry, they can display distinct tiling patterns resulting from individual capsomeres in quasi-equivalent states. In order to model the assembly of these capsids, rigid-body models either use multiple monomeric subunits with different geometries or pre-formed pentamers and hexamers with fine-tuned interactions. We introduce SOUFFLE, a molecular dynamics simulation method with elastic capsomeres, to investigate capsid assembly. The method is used to study a model T1 system as well as nucleating tiling patterns associated with T3 and T4 HBV capsids. The assembly of full T3 and T4 capsids using pentamers and hexamers pre-formed with elastic capsomeres is also probed. Based on tiling-patterns and assembly diagrams, we propose that the heterogeneity of HBV capsids can be attributed to relatively low bending modulus of its capsomeres (10-15 kB T).

*This work is supported by the NSF through Awards 1720625 and DMR-1753182.
5:06PM D30.00012: Bulk light-scattering measurements of viral capsid self-assembly around RNA.*  LANELL A. WILLIAMS (Presenter), Physics, Harvard, TIMOTHY CHIANG, REES F GARMANN, Applied Physics, Harvard, VINOTHAN MANOHARAN, Physics, Applied Physics, Harvard — Self-assembly is a vital part of the RNA virus life cycle. The assembly of viral coat proteins around viral RNA occurs both in vivo and in vitro, suggesting that viral capsid assembly may be driven by minimization of free energy. To better understand this process, we modify the interactions between coat proteins and between the coat proteins and RNA of MS2 bacteriophage in vitro by varying the ionic strength and pH, and we study the assembly using dynamic and static light scattering. From dynamic light scattering we determine the assembly yield and the size distribution of assembled products. From static light scattering, we measure the kinetics of assembly in bulk. By comparing the results from these two different techniques to each other and to results from gel electrophoresis, we infer features of the assembly pathway.

*This work is supported by funding from the National Science Foundation Graduate Research Fellowship Program (NSF-GRFP).

5:18PM D30.00013: Membrane tubulation induced by chiral crescent-shaped proteins  HIROSHI NOGUCHI (Presenter), Institute for Solid State Physics, University of Tokyo — In living cells, structures of biomembranes are regulated by various proteins. We studied the protein assembly and membrane remodeling using coarse-grained meshless membrane simulations. We revealed how chirality of crescent-shaped protein rods changes their assembly and tubulation. The achiral rods deformed the membrane tube into an elliptical shape by stabilizing the edges of the ellipse. In contrast, the chiral rods formed a helical assembly that generated a cylindrical membrane tube with a constant radius in addition to the elliptical tube. This helical assembly could be further stabilized by the direct side-to-side attraction between the protein rods. The chirality also promotes the tubulation from a flat membrane. These results agree with experimental findings of the constant radius of membrane tubules induced by Bin/Amphiphysin/Rvs (BAR) superfamily proteins.

Monday, March 2, 2020 2:30 PM - 4:30 PM

Session D31 DSOFT GSNP DPOLY: Wetting and Adhesion of Soft Materials: Dynamics and Instability I  503 - Julien Chopin, ESPCI Paris - Tag(s): Focus
From dewetting to adhesion rupture - moving lines in dissipative, heterogeneous systems

ETIENNE BARTHEL (Presenter), MATTEO CICCOTTI, ESPCI Paris — Thirty five years ago, two theories for the pinning of elastic lines by heterogeneities have appeared almost simultaneously (Joanny & de Gennes, J. Chem. Phys. 81 (1984) 552; Rice, J. Appl. Mech 52 (1985) 571). Starting from these results, a large number of models and simulations have greatly advanced our understanding of complex line phenomena, and especially wetting hysteresis and fracture toughness of heterogeneous materials. However, these theories provide quasistatic pictures and they do not tell us much about what happens beyond the depinning threshold in the rather ubiquitous case where the response of the material itself is dissipative (e.g. viscous liquids or viscoelastic solids). In fact, even for homogeneous systems, evaluating the dissipation is still often a problematic question and the most simple cases - dewetting newtonian liquid or adhesion rupture for a linear viscoelastic solid - are far from being completely understood, especially when confrontation with experimental results is intended... Here we consider the dynamics of a front in a dissipative material moving on a heterogeneous surface at finite velocity. Based on recent numerical results for periodic substrates, we will first show how heterogeneities renormalize the dynamics of newtonian fluids near the dynamic wetting transition and actually obliterate some of the details of the wetting problem. We will then discuss the generalization to the case of dissipative soft solids.

Adhesion in Capillary Assembled Origami Structures

TIMOTHY J TWOHIG (Presenter), ANDREW CROLL, North Dakota State Univ — Adhesion plays an important and often overlooked role in capillary assembly driven thin-film origami systems. Strong adhesion to a substrate can completely inhibit capillary forces from assembling a structure, while weak film-film adhesion means a structure may not be stable in the assembled configuration. In this work, we experimentally study thin-film/substrate and thin-film/thin-film adhesive interactions in order to explore the interplay between capillary forces, thin-film elasticity, bending, and adhesion. We use elastocapillary scaling models to highlight how the basic underlying physics can provide guidelines for building stable thin-film origami structures.

Morphology of adhesive creases

MARTIN ESSINK (Presenter), ANUPAM PANDEY, Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, STEFAN KARPITSCHKA, MICHEL VAN LIMBECK, Max Planck Institute for Dynamics and Self-Organization, JACCO SNOEIJER, Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente — When a soft elastic material is compressed beyond a certain critical strain, the free surface turns unstable and forms a crease. This corresponds to a sharp fold of the surface onto itself, leading to intricate morphologies as observed for growing tissues and swelling gels. Self-adhesion within the folded region is known to affect nucleation and hysteresis, but a detailed description has remained elusive. Here we resolve the geometry and mechanics of adhesive creases, combining numerical simulations, analysis and experimental results — with specific attention to the singular edge of the self-contact. It turns out that adhesive creases exhibit a universal shape that arises from a balance of elastic and surface energies. From this we derive a scaling theory for the intricate bifurcation scenario, explaining the hysteretic nucleation of adhesive creases.
3:30PM D31.00004: Energy Approach to Understand Contact Mechanics on Rough Surfaces
SIDDHESH DALVI (Presenter), Univ of Akron, ABHIJEET GUJRATI, TEVIS D.B. JACOBS, Mechanical Engineering and Material Science, University of Pittsburgh, LARS PASTEWKA, Microsystems Engineering, University of Freiburg, ALI N DHINOJWALA, Univ of Akron — Understanding the deformation of elastic solids on rough surfaces is crucial for soft-hard contacts at different scales of applications such as biomedical adhesives, tire traction, soft robotics and even micro- or nano-electromechanical devices. It has been experimentally demonstrated that the apparent work of adhesion for a soft material brought in contact with rough surfaces is lower than the intrinsic work of adhesion. During separation, there is energy loss commonly attributed to viscoelastic dissipation, termed as adhesion hysteresis. Here, with experimentally controlled elastic modulus, roughness and surface chemistry, we demonstrate that the reduction in work of adhesion is equal to the energy required to achieve conformal contact. Further, the energy loss during contact and removal is equal to the product of the intrinsic work of adhesion and the true contact area. These findings provide a simple mechanism to quantitatively link the widely observed adhesion hysteresis to roughness rather than viscoelastic dissipation.

3:42PM D31.00005: Interfacial tension measurement of reconstructive interfaces
Hideaki YokoYama (Presenter), Masayuki Saito, Univ of Tokyo-Kashiwanoha — New fabrication method of polymer brushes, “dynamic polymer brush”, was developed recently. In the system where amphiphilic diblock copolymers are added to hydrophobic elastomer, they avoid the elastomer surface in air, but, upon contact with water, spontaneously segregate to the elastomer/water interface and form highly dense polymer brush to lower the interfacial tension. This system is one of many reconstructive surfaces, which change the interfacial structures upon contact with water and hence direct evaluation of interfacial tension is difficult with conventional contact angle measurement. To measure interfacial tension of reconstructive interface, we developed a novel method using elastomer thin films floating on water. Thin films on water was observed by Brewster imaging and their size change was analyzed using the force balance of surface tensions, interfacial tension and elastic force of thin film. The interfacial tension between water and reconstructive elastomer directly measured by this method drastically decreases down to zero due to the dense PEG brushes appeared at elastomer/water interface.
3:54PM D31.00006: Capillary instability of soft cylinders: Dynamical selection of nonlinear states  
MINKUSH KANSAL (Presenter), ANUPAM PANDEY, Univ of Twente, MIGUEL ANGEL HERRADA, Universidad de Sevilla, JENS G EGGERS, University of Bristol, JACCO SNOEIJER, Univ of Twente  
— Surface tension plays a key role for phenomena involving liquid interfaces. A prime example is the Rayleigh-Plateau instability, causing a liquid jet to break into droplets in order to minimise the surface energy. Remarkably, a similar capillary instability was observed in soft solids. Here we reveal the intricate morphologies that can be encountered during the capillary collapse of an elastic cylinder, from minimisation of capillary and elastic energy. Subsequently, we show the dynamical selection of the wavelength, which also dictates the final nonlinear state. It is found that near the onset of instability, the shapes resemble a “cylinders-on-a-string” configuration, while as the solid gets softer “beads-on-a-string” are observed — in analogy to the breakup of viscoelastic liquids. Our analysis explains recent experimental and numerical observations, and highlights how surface tension can dictate the mechanics of solids - provided that the solids are sufficiently soft.

4:06PM D31.00007: How Aqueous Salt Solutions Affect Hydrophobic Surfaces  
ADELE POYNOR (Presenter), CAYTON HORNBERGER, GRACE ROHALEY, JULIANA SEBOLT, Allegheny Coll  
— The study of how salty water meets a hydrophobic surface is important because in nature water is rarely pure. In order to study this phenomenon, we need smooth and homogenous surfaces; however, salt solutions can damage our surfaces. We study this damage for a variety of self-assembled monolayers (SAMs) in different aqueous salt solutions, using contact angle measurements, scanning electron microscopy, surface plasmon resonance.

4:18PM D31.00008: Determination of Interfacial Strain on Single-Layer Graphene Due to Ice Adhesion*  
SUBASH KATTEL (Presenter), JOSEPH R MURPHY, SAMUEL PASCO, JOHN ACKERMAN, VLADIMIR ALVARADO, WILLIAM RICE, Univ of Wyoming  
— Adhesion between two dissimilar media produces a strain that changes the bond character of both materials at the interface, like ice-material interface. To explore the interfacial adhesion properties of ice, researchers apply an external stress directly to ice while measuring strain until adhesive or cohesive failure. This destructive approach masks the intrinsic forces as well as complicated interfacial physics occurring at the ice-material interface. Here, we use Raman spectroscopy to non-perturbatively and contactlessly measure ice-induced strain. To isolate this interface, we probe the vibrational modes of single-layer graphene (SLG) from 20°C to -30°C with and without ice. Along with the well-known temperature-dependent Raman shift of SLG, a clear, ~2 cm⁻¹ change in the 2D-frequency (2650 cm⁻¹) developed upon ice formation. We found that at the same temperature, a decrease in the Raman shift emerged between supercooled water and ice, which corresponds to 0.013% strain in SLG solely due to ice. The localized nature of the Raman probe allows for spatial mapping of the ice-coated SLG surface, enabling precise correlation with surface roughness evaluation and theoretical models.

*We acknowledge support from NASA through Grant No. WY-80NSS17M0049 and UW School of Energy Resources.
D31.00009: Capillary imbibition in a square tube
TIAN YU, JIAJIA ZHOU (Presenter), MASAO DOI, BeiHang University — We study the wetting of a capillary with a square cross-section. When a square tube is brought in contact with bulk liquid, the liquid wets the corners of the tube and creates finger-like wetted regions. The wetting of the liquid then takes place with the growth of two parts, the bulk part where the cross-section is entirely filled with the liquid and the finger part where the cross-section of the tube is partially filled. In previous works, the growth of these two parts has been discussed separately. Here we conduct the analysis by explicitly accounting for the coupling of the two parts. We propose coupled equations for liquid imbibition in both parts and show that the lengths both increase in time following Lucas–Washburn’s law, but the coefficients are different from those obtained in the previous analysis that ignored the coupling.

*This work was supported by the National Natural Science Foundation of China (NSFC) through Grants No. 21504004 and 21774004.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D32 DPOLY DSOFT DBIO: Responsive Polymers, Soft Materials, and Hybrids I

2:30PM D32.00001: Silk-inspiration: hierarchy, assembly, and mechanics in polyurea-polypeptide hybrids
LASHANDA KORLEY (Presenter), DASEUL JANG, Univ of Delaware — Inspired by spider silk, we have designed a series of polymer-peptide polyurethane/ureas to explore the hierarchical arrangement critical to energy absorption and mechanical enhancement. We have developed chain-extended and non-chain extended peptide-polyurea hybrids with tunable secondary structure, modulating extensibility, toughness, and stiffness. The sheet-dominant hybrid materials were typically tougher and more elastic due to intermolecular H-bonding, while the helical-prevalent systems generally exhibited higher modulus. We have also explored the impact of a molecular design strategy that overlays a covalent and physically crosslinked architecture in these hybrids, demonstrating that physical constraints in the network hybrids influences hydrogen bonding and morphology. More recently, tailored physical associations within the soft and hard phases were engineered as a function of peptide content, leading to a rheological response dictated by block ordering and highlighting their potential as structural and injectable hydrogels. New efforts in silk composites that exhibit shape memory behavior, and 'green' pathways for silk-inspired materials are of current focus. These structural features have enabled new thrusts in injectable gels and responsive actuators.

*This work was supported by the National Science Foundation (NSF, DMR 1608441; NSF, OISE 1844463).
Ionic microgels are cross-linked polymeric networks that ionize and swell in a good solvent. The swelling behavior of the particles can be tuned by adjusting temperature, pH, and ionic strength, enabling applications to drug delivery and tissue engineering. Unlike spherical microgels, cylindrical microgels can swell in both radial and axial directions. Equilibrium swelling can be triggered by varying the balance between electrostatic and gel contributions to the osmotic pressure inside and outside of the particles [1, 2]. Within a cell model, we derive an exact statistical mechanical theorem for the electrostatic osmotic pressure of a cylindrical microgel to study the dependence of microion distribution and osmotic pressure on equilibrium size. To validate the theorem, we implemented Poisson-Boltzmann theory and molecular dynamics simulations. Combining our theorem with Flory-Rehner theory of polymer networks, we predict radial and axial equilibrium swelling ratios of cylindrical microgels as a function of salt concentration. Our results can help guide the design of smart, responsive particles.


*MOA acknowledges support of Shaqra University.

Soft materials are ideal for designing structures with useful properties. Especially, hydrogels have been extensively studied for their response to various external stimuli and reversibility. A gel under geometric confinements deforms anisotropically due to applied directional stresses, but otherwise it can be equilibrated and swollen by solvent homogeneously. In particular, wrinkling instability can be observed for line patterns of hydrogels bounded on a rigid substrate. Geometry and swelling ratio of the gel can decide a morphology – in the case of wrinkles, wavelength and amplitude - of the pattern. We controlled not only geometry factors of the micro patterns of hydrogel, but also the swelling ratio of the gel by varying the amount of Acrylamide (AAm) added during synthesis.

There has been much research on the effect of geometry on mechanical instability. However, in-depth studies on the material properties and constitutive law related to the swelling ratio of the gel have not been conducted. In this presentation, we propose modified nonlinear stress-strain relationship of our synthesized gels in scope of both continuum and molecular scales and compare it with our experimental results.
3:30PM D32.00004: Dynamics of 3D polymer gel with reversible linkers  SANTIDAN BISWAS (Presenter), VICTOR V YASHIN, ANNA BALAZS, Univ of Pittsburgh — We utilize the gel lattice-spring approach to develop the 3D computational model of polymer gels containing the temporary crosslinks. The polymer chains are assumed to incorporate the folded domains that encompass the reactive functional groups (cryptic sites). Under deformation, the domains unfold and expose the cryptic sites, which can then form labile bonds with the linker chains grafted to the network. Once the deformation is removed, the linkers detach from the cryptic sites, and unfolded domains go back to the folded configuration thus hiding the cryptic sites. The gel behavior under applied force is described by the equations of elasticity of the polymer network coupled to the chemical kinetics equations for the folding and binding transitions. The model equations take into account the effects of finite chain extensibility on the gel elasticity and mechanosensitive reaction rates. Elasticity of the transient network is introduced to the model through the Flory approach. We study the behavior of the system under uniaxial extension and compression, and determine the effect of temporary crosslinks on the bulk and shear moduli of the gel. We also compare the behavior of the gel with a similar gel not undergoing the transient binding of the linker chains.

3:42PM D32.00005: Phototunable Viscoelasticity in Hydrogels Through Thioester Exchange*  BENJAMIN CARBERRY (Presenter), VARSHA V RAO, KRISTI ANSETH, University of Colorado, Boulder — The extracellular matrix in which cells reside offers elastic and viscoelastic mechanical cues important for directing cell behavior. Recently, cellular responses to viscoelastic and elastic mechanical cues have been studied; however, questions remain as to how cells identify and transduce these cues differently, sparking a need for materials that can interrogate these properties separately. We present a cell culture substrate based on thioester exchange chemistry where viscoelasticity of the biophysical environment can be modulated in situ with light and the photoinitiated thiol-ene ‘click’ reaction. With this method, stress relaxation in thioester hydrogels with relaxation times ranging from 200,000-1,500,000s can be switched off in the presence of cells without change to the elastic modulus. NIH 3T3 fibroblasts cultured for 48 hr on viscoelastic substrates that transition to elastic substrates after 24 hr display cell morphology and YAP/TAZ expression similar to the elastic control. Phototunable viscoelastic thioester hydrogels provide a tunable materials system to investigate time-dependent cellular responses to viscoelasticity and should prove useful for understanding the dynamics of mechanoresponsive cellular pathways.

*NIH (DE016523)
**3:54PM D32.00006: Toughening mechanism of tough and self-healing physical hydrogels**
KUNPENG CUI (Presenter), JIAN PING GONG, Hokkaido University — Recently, we have developed a new class of tough and self-healing physical hydrogels composed of polyampholytes (PA). Those PA gels possess high toughness, stiffness, fatigue resistance and self-healing. However, the toughening mechanism of these gels is still unclear. In this work, we used real time small-angle X-ray scattering (SAXS) to study the toughening mechanism of PA hydrogels. We revealed that the high toughness of PA hydrogels is a synergistic effect due to multi-scale energy dissipation. We found that, this class of tough gels have a bicontinuous phase separation structure, consisting of a hard phase network and a soft phase network, of ~100 nm in scale. Upon loading, the microscopic deformation of phase structure is perfectly affine up to a quite large macroscopic uniaxial deformation range, followed by a wide nonaffine regime. In affine deformation regime, the breaking of ionic bonds dissipates energy, while in nonaffine deformation regime, hard phase rupture dissipate energy.


**4:06PM D32.00007: Anisotropic Hollow Microgels That Can Adapt Their Size, Shape, and Softness**
ANNE NICKEL (Presenter), ANDREA SCOTTI, RWTH - Aachen, JUDITH HOUSTON, European Spallation Source, JEROME CRASSOUS, RWTH - Aachen, JAN SKOV PEDERSEN, University of Aarhus, WALTER RICHTERING, RWTH - Aachen — We have recently shown how to create hollow, anisotropically shaped thermoresponsive microgels, polymeric networks with a solvent filled cavity that are swollen in a good solvent.[1] Sacrificial elliptical hematite silica particles were utilized as a template for the synthesis of a cross-linked N-isopropylacrylamide (NIPAm) shell. We characterized these microgels using a combination of light, X-ray, and neutron scattering. New form factor models, accounting for the cavity, the polymer distribution and the anisotropy, have been developed for fitting the scattering data. With such models, we demonstrated the existence of the cavity and simultaneously the anisotropic character of the microgels. Finally, the effect of temperature and shell thickness was investigated, showing that changes in size, softness, and aspect ratio are triggered. We believe that these hollow anisotropic microgels represent an attractive model system for fundamental physics (e.g. phase behavior or ordering phenomena) and a variety of applications especially in respect to their responsivity to temperature.


*Financial support from the SFB 985 “Functional Microgels and Microgel Systems” of Deutsche Forschungsgemeinschaft is greatly acknowledged.*
Ionic microgels are soft, permeable, colloidal particles made of crosslinked polymer networks that ionize and swell in a good solvent. Swelling of these particles is responsive to external stimuli and involves a balance of electrostatic and gel contributions to the single-particle osmotic pressure. The electrostatic contribution depends on the distributions of mobile microions and fixed charge on the polymer. Within the cell model, we derive the electrostatic contribution within Poisson-Boltzmann (PB) theory, by minimizing a free energy functional with respect to electrostatic potential, and extract the gel pressure from the pressure tensor. By varying the free energy with respect to microgel size, we also derive exact statistical mechanical relations for the electrostatic osmotic pressure for models of planar, cylindrical, and spherical microgels with fixed charge uniformly spread over their surface or volume. To validate these relations, we solve the PB equation and compute ion densities and osmotic pressures [1]. We show that microgel swelling depends on the electrostatic pressure profile inside the particle and discuss implications for interpreting experiments.


*MOA acknowledges support of Shaqra University.

Tuning Diblock Copolymer Morphologies by Stimuli-Responsive Supramolecular Interactions  

Xiangyu Zhang (Presenter), Jing Zong, Dong Meng, Mississippi State Univ — Ability to tune the microstructures formed by block copolymers via easy-to-use physical approaches offers additional handles to the materials for practical applications. One common approach is through adding homopolymers, which induces morphological changes due to preferential partitioning of homopolymers into specific micro-domains. Recently, supramolecular forces that are chemistry-specific and stimuli-responsive have been exploited to enable stimul

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4:54PM D32.00011: On the solvation of elastin-like polypeptides in aqueous mixtures  YANI ZHAO (Presenter), Max Planck Institute for Polymer Research, MANJESH KUMAR SINGH, Mechanical Engineering, Indian Institute of Technology Kanpur, KURT KREMER, ROBINSON CORTES HUERTO, Max Planck Institute for Polymer Research, DEBASHISH MUKHERJI, Stewart Blusson Quantum Matter Institute, University of British Columbia — The collapsed or expanded state of a polymer is determined by the quality of the solvents: a polymer collapses in a poor solvent, whereas in a good solvent it opens up. While this standard understanding is generally valid, there are examples when a polymer collapses even in a mixture of two good solvents. This phenomenon, commonly known as co-non-solvency, is usually associated with smart polymers. Recent experiments have shown that biopolymers, such as elastin-like polypeptides (ELP), show co-non-solvency in aqueous-ethanol mixtures. In this work, we compare conformational behavior of ELPs in aqueous-ethanol and -urea mixtures using explicit solvent generic simulations. These results may pave ways for operational understanding and advanced functional designing of biocompatible materials.


5:06PM D32.00012: Chemomechanical origin of directed gel locomotions driven by internal chemical pulses*  QINGYU GAO (Presenter), LIN REN, Chemistry, China Mining University, IRVING R EPSTEIN, Chemistry, Brandeis University — Our previous work reported the directed locomotion of self-oscillating polymer gels in asymmetric environments, such as retrograde and direct wave locomotion, reciprocal migration, photophobic and phototropic movement. We now ask whether directed locomotions and their transitions can be generated only from intrinsic chemical dynamics and its modulation. We examine this question by simulating the locomotion of a responsive polymer gel in a homogeneous environment. We find that autonomous directional locomotion emerges in the absence of asymmetric interaction with the environment, and that a transition between modes of gel locomotion can be induced by adjusting the spatially uniform intensity of illumination or certain kinetic and mechanical system parameters. We find that the internal wave dynamics and modulation of the system act as the impetus for signal-driven active locomotion in a manner similar to the way in which an animal's locomotion is generated via driving by nerve pulses.

*This work was supported by the National Natural Science Foundation of China (Grant No. 21573282 and 21972165), the Natural Science Foundation of Jiangsu Province (Grant No. BK20171186), and the U.S. National Science Foundation (Grant No. CHE-1856484).
Competition between Hydrophobic and Electrostatic Interactions determine pH-responsive Supramolecular Self-assembly

SAIKAT CHAKRABORTY (Presenter),
Institute of Physics, Johannes Gutenberg University Mainz, CHRISTIAN M. BERAC, POL BESENIUS,
Institute of Organic Chemistry, Johannes Gutenberg University Mainz, THOMAS SPECK, Institute of Physics,
Johannes Gutenberg University Mainz

We present results from a molecular dynamics simulations study, inspired by experiments on pH-regulated self-assembly into filaments. Experiments are performed in aqueous media, with 1:1 binary mixture of amphiphilic peptide monomers having oppositely charged side chains. In neutral conditions, the monomers self-assemble into alternating copolymers. In acidic and basic conditions, selective screening of Coulombic interactions occurs. This leads to formation of homopolymers. Building on our model for homopolymers in implicit solvent, we introduce charges to mimic the two monomers. Our simulations reveal that the consideration of pH-dependent hydrophobic interactions is essential to observe pH-switch in polymerization. Further, assembly kinetics is analyzed, comparing simulations to experimental data which are obtained from circular dichroism spectroscopy. We relate both to appropriate growth models. While the nucleation and elongation are key mechanisms in simulations, fragmentation is important in experimental kinetics.


Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D33 DPOLY: Morphology Characterization: Frontier of Scattering and Microscopy

Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) on Amphiphilic Block Polymer Solutions

ARTHI JAYARAMAN (Presenter), DANIEL J BELTRAN, MICHEL WESSELS, Department of Chemical and Biomolecular Engineering, University of Delaware

In this talk we will present a new computational method titled ‘Computational Reverse-Engineering Analysis for Scattering Experiments’ or CREASE to interpret the intensity profiles obtained from small angle neutron scattering done on amphiphilic polymer solutions. For a given input comprised of scattering intensity profiles and information about the amphiphilic polymers in solution, CREASE uses a genetic algorithm that outputs the structure of the self-assembled micelles (e.g., core and corona diameters, aggregation number) and then through molecular reconstruction simulations describes the conformations of the amphiphilic polymer chains in the micelle (e.g., blocks’ radii of gyration, chain radii of gyration, monomer concentration profiles). The primary strengths of CREASE are its ability to analyze scattering profiles without an off-the-shelf scattering model and its ability to provide chain and monomer level structural information that is otherwise difficult to obtain from scattering and microscopy alone.
2:42PM D33.00002: Feature Engineering for Small-Angle Scattering Model Selection  YUKE WANG, Physics, Mathematics, Computer Science, University of Kentucky, TYLER MARTIN (Presenter), National Institute of Standards and Technology — While many soft-matter characterization techniques can be unambiguously interpreted to yield information about chemical and material structure, small-angle neutron and X-ray scattering (SANS and SAXS) data must be interpreted via a library of physical and phenomenological models. Complicating this task is the unavoidable phase problem, which causes scattering patterns to be non-unique and makes model selection a non-trivial task. Here we present our efforts in developing shallow- and deep-classifiers which, given a scattering dataset, suggest applicable models to the user. In particular, we will focus on our efforts in feature vector engineering i.e., the optimization of input parameters in order to maximize classification efficiency. We show that simple data transformations greatly increase our classification efficiency over a naïve model, allowing us to achieve greater than 99 % top-3 accuracy in the model-selection task. More broadly, these optimized feature vectors will enhance machine learning models for tasks other than model selection (e.g., error detection, automated experimentation, on-the-fly analysis). The ultimate goal of this project is to formalize feature vector design for small-angle scattering, thereby enabling the creation of bespoke machine-learning models.

2:54PM D33.00003: Identification of Frank-Kasper Phases in Conformationally Asymmetric Linear Block Copolymer Self-assembly  SEUNGBAE JEON (Presenter), TAESUK JUN, SEONGJUN JO, Yonsei University, HYUNGJU AHN, Pohang Accelerator Laboratory, BYEONGDU LEE, Argonne National Laboratory, DU YEOL RYU, Yonsei University — The quasicrystalline phases which were originally observed in metal alloys have emerged with block copolymers (BCPs) self-assembly providing a new potential in soft materials. Theoretical and experimental studies have revealed that conformational asymmetry (ε) of the different blocks provides a key mechanism to stabilize the Frank-Kasper (FK) σ and A15 phases in BCPs self-assembly. In this work, polydimethylsiloxane-b-poly(2,2,2-trifluoroethyl acrylate)s (PDMS-b-PTFEAs) were designed using flexible silicon-containing blocks and rigid fluorine-containing blocks to produce linear BCPs with a high conformational asymmetry. Evaluated value of ε was 2.20 which is higher than other BCPs reported in the literatures. A series of PDMS-b-PTFEAs were synthesized to produce compositionally asymmetric, PDMS-rich phases ranging from \( f_{PDMS} = 0.746 \) to 0.869. Using small-angle X-ray scattering, the FK σ and C14 phases were observed at \( f_{PDMS} = 0.80 \) and 0.85, respectively. Based on the fact that the stability of σ phase increases by the value of ε, we speculate that the stability level of the C14 phase as well as σ phase is due to the relatively high ε of PDMS-b-PTFEAs.
Combining Advanced Experimental Methods to Characterization of Polymer Nanocomposites* [Invited] KAREN WINEY (Presenter), University of Pennsylvania — Each characterization method provides specific information about a polymer sample over a limited range of length and time scales. A comprehensive understanding of polymer morphology and dynamics is best developed by combining a set of characterization methods to capture a broader range of lengths and times. This talk will highlight examples from our studies of polymer nanocomposites that have combined methods to develop detailed and quantitative descriptions of these complex polymer systems. Specifically, the dynamics in polymer nanocomposites include segmental and chain-scale motion of the polymer, as well as diffusion of the nanoparticles. We apply ion beam methods (elastic recoil detection and Rutherford backscattering) and single particle tracking methods, as well as more accessible methods such as temperature-modulated DSC and broadband dielectric spectroscopy methods, to probe the molecular weight dependence of the polymer and nanoparticles are revealed for nanoparticles of various sizes and nanoparticle-polymer interactions. These vignettes will also serve to illustrate the capabilities of the individual methods and demonstrate the exceptional value of combining these advanced experimental methods.

*Department of Energy - BES; National Science Foundation - CBET

Deformation Mechanics during Drawing of Ultra-High Molecular Weight Polyethylene Fibers  CHRISTOPHER HENRY, GIUSEPPE PALMESE, NICOLAS ALVAREZ (Presenter), Drexel Univ — There has been extensive study of Ultra-high molecular weight polyethylene (UHMWPE) fibers owing to their remarkable tensile modulus and strength. It is understood that these properties are generated during the post drawing process. Questions remain however, regarding how the morphology of the polymer develops during processing, and how this leads to the observed properties. Basic information regarding strain rate, stress at failure, and the role of processing parameters is missing due to the difficulty of measurement with industrial processes. This information is critical to understanding the polymer response during drawing. In this study we use a modified extensional rheometer (VADER 1000) to perform the drawing process on a series of UHMWPE fibers spun at Drexel. We have shown previously that ASF crystalline structure is not limited to the isotropic states typically seen in literature. With the VADER 100, and this broad range of starting materials we can monitor true stress and strain throughout the draw, and discover the mechanical properties prior to, and at, the failure point. Small and wide-angle x-ray scattering is used investigate the crystalline morphology. With this information a fundamental understanding of the post-drawing will be developed.
3:54PM D33.00006: 3D Structure of Grain Boundaries in Tubular Network Block Copolymers

XUEYAN FENG (Presenter), AMANDA SUAREZ, DERRICK ONG, KAIQI YANG, HUA GUO, EDWIN THOMAS, Rice University — Multi-continuous microphases (such as double gyroid) have network structures with 3D interconnected, self supporting domains. The properties of the component in each domain are strongly expressed due to the geometrical continuity in all three dimensions. However, the occurrence of grain boundaries (GB), which interrupt the topological and geometrical order of the continuous ordered networks, will significantly affect their performance. Here, we examine GBs in a polystyrene-b-polydimethylsiloxane double gyroid system using high fidelity 3D reconstructions made by Slice and View scanning electron microscopy (SVSEM). Since large amounts of GB can be reconstructed, we employ machine learning to extract the shape/distribution of the GB. Also, two types of GBs are identified and described (grain-grain tilt and order-disorder-order boundaries). Different types of irregular nodes/topological loops/network connections within the GB region are identified. The local topological parameters, as well as curvature of the intermaterial dividing surface, node functionality distribution, strut length/orientation distribution and surface to volume ratio in the GB are analyzed and compared with the same set of morphological descriptors measured in the adjacent, ordered double gyroid grains.

4:06PM D33.00007: Local density and free volume inhomogeneities govern transport properties in reverse osmosis membranes

MICHAEL GEITNER (Presenter), TYLER CULP, Pennsylvania State University, JEFFREY D. WILBUR, STEVEN JONS, DuPont Water Solutions, MANISH KUMAR, The University of Texas at Austin, ENRIQUE D GOMEZ, Pennsylvania State University — Developing a mechanistic description of how microstructure affects membrane properties could lead to the development of next-generation materials for desalination. Quantification of the internal microstructure of fully-aromatic polyamide thin-films, which serve as the active layer in state-of-the-art desalination membranes, is a crucial component to developing such descriptions. Here, we studied a series of reverse osmosis membranes showing systematic increases in water permeance over currently available membrane materials without sacrificing water-salt selectivity. We quantified the internal morphology of the polyamide active layers via scanning transmission electron tomography, where 3D reconstructions were obtained and parameters, such as void fraction and surface area, were measured. Tomogram intensity analysis revealed the nanometer-scale density and free volume distributions, used in conjunction with the 3D polyamide models to model water transport properties in such materials. The combination of density and free volume distributions determined from electron tomography with water transport modeling has provided a robust approach towards the development of structure-property relationships in reverse osmosis membranes.
Three-Dimensional Imaging the Crystalline Structure of Polypeptoid Nanosheet with Atomic Resolution

XI JIANG (Presenter), Materials Sciences Division, Lawrence Berkeley National Laboratory, SUNTING XUAN, NAN LI, DAVID PRENDERGAST, RONALD ZUCKERMANN, Molecular Foundry, Lawrence Berkeley National Laboratory, NITASH BALSARA, The Department of Chemical & Biomolecular Engineering, University of California, Berkeley — Electron microscopy imaging of three-dimensional structures in soft materials with atomic resolution is challenging because soft materials are unstable under the electron beam, and techniques such as x-ray scattering or diffraction are not able to provide atomic resolution phase information in position space. The experiments were conducted on self-assembled crystalline polypeptoid nanosheets. Low-dose cryogenic electron microscopy micrographs were obtained from frozen hydrated crystalline nanosheets on the novel ultra-flat supporting grid at different tilting angles. A hybrid processing of crystallographic, tomography and single particle methods, developed for cryo-electron microscopy of biological macromolecules, was used to resolve the structure of crystals with atomic resolution in three dimensions. Our approach is robust and enable direct visualization of the arrangement of polypeptoid backbones and side chains in crystalline nanosheets. It also revealed the effect of side chain chemistry on the crystalline structure of polypeptoid nanosheets.

Funding for this work was provided by the Soft Matter Electron Microscopy Program (KC11BN), supported by the Office of Science, Office of Basic Energy Science, US Department of Energy, under Contract DE-AC02-05CH11231.

Pushing the resolution limits for imaging conjugated polymers in the transmission electron microscope

BROOKE KUEI (Presenter), ENRIQUE D GOMEZ, Pennsylvania State University — Transmission electron microscopy (TEM) of conjugated polymers has remained a challenge because resolution is limited by the electron dose the sample can handle. We have characterized beam damage in poly(3-hexylthiophene) (P3HT), poly(3-dodecylthiophene-2,5-diyl) (P3DDT), and poly[(5,6-difluoro-2,1,3-benzothiadiazol-4,7-diyl)-alt-(3,3’’-di(2-octyldodecyl)-2,2’:5’,2’’;5’,2’’-quaterthiophene-5,5’’-diyl)] (PffBT4T-2OD) via electron diffraction and electron energy-loss spectroscopy (EELS). Critical dose $D_C$ values were calculated from the decay of diffraction and low-loss EELS peaks as functions of dose rate, temperature, and beam size. At room temperature, $D_C$ first increases then decreases with increasing dose rate, whereas at cryogenic conditions this dose rate dependence is less pronounced and the overall $D_C$ increases; these results suggest that a significant mechanism for beam damage in conjugated polymers is diffusion of secondary free radicals. $D_C$ also increases with decreasing beam size. These new concepts in beam damage revealed strategies to push the resolution in the TEM, allowing us to image 3.6 Å π-π stacking in PffBT4T-2OD with 4D STEM, high-resolution TEM (HRTEM) at cryogenic conditions, and HRTEM at room temperature with antioxidants.

NSF DMR-1609417, DOE SCGSR, ALS.
**4:42PM D33.00010: Observation of Elongated Nano Domains in Organic Photovoltaic Active Layers with Electric Field Treatment using Cross-Sectional Scanning Tunneling Microscopy and Spectroscopy.**

RABINDRA DULAL (Presenter), Physics and Astronomy, Univ of Wyoming,

AKSHAY IYER, UMAR GHUMMAN, Department of Mechanical Engineering, Northwestern University,

JOYDEEP MUNSHI, Department of Mechanical Engineering & Mechanics, Lehigh University, AARON WANG, Physics and Astronomy, Univ of Wyoming, GANESH BALASUBRAMANIAN, Department of Mechanical Engineering & Mechanics, Lehigh University, WEI CHEN, Department of Mechanical Engineering, Northwestern University, TE-YU CHIEN, Physics and Astronomy, Univ of Wyoming — The effects of the electric-field-assisted annealing on the bulk heterojunction nano-morphology in the P3HT/PCBM active layer of the organic photovoltaic cells (OPVCs) are presented here. It was widely accepted that the electric field will facilitate the P3HT, the polar polymer, to be better crystallized hence enhance the charge mobility and improve the OPVC performance. However, the effects on the nano-morphology in the active layer treated with the electric field are not well understood. Here, by utilizing the cross-sectional scanning tunneling microscopy and spectroscopy (XSTM/S), it is revealed that the electric-field-assisted annealing will facilitate the P3HT-rich domains formed elongated shape with the orientation close to the direction of the external electric field which is beneficial to the OPVC charge collection. On the other hand, it was also observed that the electric-field-assisted annealed samples showed smaller energy gaps and smaller energy off-set between the molecular domains which might negatively impact the charge separation efficiency. The XRD and SAXS results indicate that the smaller energy gaps might be caused by the molecular intermixing. These results point out competing factors affecting the OPVC performance.

*This work is supported by NSF CMMI: 1662509

**4:54PM D33.00011: Directly Visualizing Conformations of Bottlebrush Polymers in Bulk Films using Super-Resolution Optical Microscopy**

JONATHAN CHAN (Presenter), AVRAM KORDON, ZHE QIANG, MUZHOU WANG, Northwestern University — Bottlebrush polymers have advantageous photonic and mechanical properties that are well suited for applications such as coatings, pigments, and super-soft materials. This architecture consists of a polymer backbone densely grafted by side chains, whose steric repulsions result in rigid, elongated conformations. While the single-chain conformations of these polymers have been studied experimentally for isolated chains on surfaces and within dilute solutions, few studies have probed their conformations in bulk environments. In this work, we directly visualize individual bottlebrush polymers in a bulk environment populated by other bottlebrushes, by mixing dilute quantities of fluorescently-labeled chains with unlabeled polymers and imaging through super-resolution optical microscopy (SROM). Using SROM, we resolved individual chains within thin films of bulk polymers and found the tangent correlation functions (TCFs) of the backbone. These TCFs were fit to a worm-like chain model, and values for the persistence length were extracted to quantify rigidity. Changes to these conformations were observed with variations to architectural parameters such as side chain length and grafting density.
5:06PM D33.00012: Kinetically Controlled Morphology in Copolymer-based Hydrogels Crosslinked by Crystalline Nanodomains Determines Efficacy of Ice Inhibition* PABLO SEPULVEDA-MEDINA (Presenter), Univ of Akron, CHAO WANG, Chemical and Biomolecular Engineering, University of Delaware, BRYAN VOGLT, Chemical Engineering, Pennsylvania State University — Confinement of water within physically crosslinked hydrogels can alter the physics associated with the water within the hydrogel. When water is confined between hydrophobic nanodomains that act as physical crosslinks, crystallization of water can be dramatically inhibited. In prior work, the inter-nanodomain spacing was controlled by changing the fraction of hydrophobic segments in the polymer, which leads to an inverse correlation between water content and confinement extent. However, water content and confinement effect have not been decoupled. Here, we decouple confinement and water content through kinetically controlled nanostructure in a hydrogel crosslinked by crystalline nanodomains based on 2-hydroxyethyl acrylate (HEA) and n-octadecyl acrylate (ODA). Zone annealing of the dry copolymer alters the structure of the crystalline ODA domains that effectively crosslink the hydrogel. Despite these changes in the ODA structure, the average hydrogel water content was not significantly altered. However, the unfrozen water inside the hydrogel varies from 60 to 99 wt%, determined from DSC and in-situ WAXS. The antifreeze efficacy is found to correlate directly with the structure where smaller spacing leads to higher unfrozen water fraction.

*Work founded by NSF grant CBET-1606685.

5:18PM D33.00013: Morphological Investigations of Anion-Conducting Polymer-Catalyst Interface* NORA BUGGY (Presenter), Chemical & Biological Engineering, Colorado School of Mines, YIFENG DU, Polymer Science and Engineering, University of Massachusetts Amherst, MEI-CHEN KUO, Chemical & Biological Engineering, Colorado School of Mines, BRYAN COUGHLIN, Polymer Science and Engineering, University of Massachusetts Amherst, ANDREW HERRING, Chemical & Biological Engineering, Colorado School of Mines — The heterogeneous microstructure of the electrode in polymer electrolyte-based electrochemical devices is not well understood. This is due in part to complex interactions between the ion-conducting polymer (ionomer), catalyst particles, and carbon. It is known that interactions at the polymer-catalyst interface induce restructuring that propagates through the bulk morphology of the material [1]. This is potentially to the detriment of species transport in the electrode, ultimately affecting device performance.

To simplify the system, model interfaces of polymer thin films on silver surfaces are studied. A set of tunable block copolymers, post-quaternized to produce anion-conducting polymers, are used to investigate how different parameters influence interfacial morphology. Their synthesis has been optimized to achieve a variety of block lengths and ratios, each with a unique set of characteristics (ionic conductivity, water uptake) and morphologies. Films have been investigated using GISAXS and AFM. An understanding of the ionomer morphology at the ionomer-catalyst interface will provide key insight toward rationally designing block copolymers for the electrode.


*Army Research Office W911NF-12-R-0012-04

Monday, March 2, 2020 2:30 PM - 5:30 PM
2:30PM D34.00001: Role of chain architecture and composition on dynamics and ionic solvation in polyether-based electrolytes*  PETER BENNINGTON (Presenter), DANIEL SHARON, MICHAEL WEBB, CHUTING DENG, JUAN DE PABLO, PAUL F NEALEY, SHRAYESH PATEL, University of Chicago — In recent years a great number of new polymer electrolytes have been developed towards improved performance and stability of energy storage devices. These new materials typically include polyether moieties to facilitate efficient ion transport. However, the presence of additional non-conducting groups influences the ability of polyethers to solvate ions and hopping between these solvation sites. We have examined a number of polyether-based electrolytes in linear, block, graft, and blend configurations to explore how chemical and physical interactions between different components affects ionic conductivity. Using a combination of impedance spectroscopy, vibrational spectroscopy, and atomistic simulations, we gain insight into the degree of ion conductivity, ionic interactions, and polymer dynamics of these materials. Both the polymer-polymer interaction strength and segmental mobility of non-solvating components show an effect on the overall conductivity and connectivity of ion solvation sites. These findings highlight the need for more complete models to account for various length scales of interaction in these nonuniform material systems.

*We gratefully acknowledge financial support from the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division

2:42PM D34.00002: Self Diffusion Dynamics and Viscoelasticity of Fluorescently Labeled Polymerized Ionic Liquids*  QIUJIE ZHAO (Presenter), CHRISTOPHER EVANS, University of Illinois at Urbana-Champaign — Scaling relationships for viscosity and diffusion coefficient as a function of degree of polymerization (N) are well-characterized in neutral polymers. We have synthesized fluorescently-labeled polymerized ionic liquids (f-PILs) with a broad range of molecular weights to understand these relationships in dry, ionic polymers with a charge on every repeat unit. Fluorescence recovery after photobleaching (FRAP) is used to measure polymer self-diffusion coefficients ($D$) using the post-bleached fluorescence images and fitting the intensity to a Gaussian profile over time. The zero-shear viscosity was measured via rheology. In the shortest f-PILs, the ionic interactions between imidazolium and bis(trifluoromethane sulfonamide) have little effect on extending the terminal regime. However, the terminal region did extend to lower frequencies as N increased. Interestingly, the wide-angle x-ray scattering shows an amorphous halo and anion-anion peak, but no longer range ionic aggregate peak which we assign as the origin of the rheologial behavior. Scaling relationships with molecular weight will be discussed.

*This work is supported by the National Science Foundation under Grant No. 1751291.
2:54PM D34.00003: First consideration of density scaling of the dynamic and thermodynamic properties in polymerized ionic liquid.*  MALGORZATA MUSIAL (Presenter), ZANETA WOJNAROWSKA, SHINIAN CHENG, Instytut of Physics, University of Silesia in Katowice, ADAM HOLT, CHARLES M. ROLAND, Chemistry Division, Naval Research Laboratory, ERIC DROCKENMULLER, Université de Lyon 1, MARIAN PALUCH, Instytut of Physics, University of Silesia in Katowice — The density scaling idea is a general feature of glass-forming materials, e.g., van der Waals liquids and polymer melts. According to this concept, the data of dynamic properties collected in isobars and isotherms collapse to a single curve when expressed versus $TV^γ$, where $T$ is temperature, $V$ is specific volume, and $γ$ is scaling exponent being a material constant independent of thermodynamic conditions. Herein, we test, for the first time, the scaling concept of dynamic and thermodynamic properties for polymerized ionic liquid (PIL). Since, various types of interactions can exist in ionic materials (balance between Coulomb interactions, van der Waals forces, and hydrogen bonds), and one of the ions is structurally constrained as part of the polymer skeleton, the validity of scaling concept is not obvious. We find experimentally that density scaling of ionic conductivity does not work. Additionally, concerning scaling of the entropy, a master curve can be obtained by taking the scaling exponent to be a linear function of total entropy.

*The authors are deeply grateful for the financial support by the National Science Centre within the framework of the Opus15 project (grant nr DEC- 2018/29/B/ST3/00889)

3:06PM D34.00004: WITHDRAWN ABSTRACT —

3:18PM D34.00005: Charging Neutral Polymer by Simple and Macro Ions in Solution
MANUELA FERREIRA (Presenter), BENXIN JING, YINGXI ELAINE ZHU, Wayne State Univ — It is recently reported that neutral polymers, such as poly(ethylene oxide) (PEO), could behave like weakly charged polyelectrolyte in highly polar solvents. We have examined the ion charging and resulting conformational structure of single PEO chains of varied molecular weight in water and mixed solvents by fluorescence correlation spectroscopy (FCS)-photon counting histogram (PCH) experiments. PCH results indicate that PEO becomes positively charged in LiCl-added solution, yet the measured electrical potential of PEO in LiCl solution decreases rapidly with the addition of multivalent polyoxometalate (POM) polyanion. The net charge of single PEO chains in solution shows strong dependence on the concentration ratio among Li+, POM, and monomer. FCS results show non-monotonic change of measured hydrodynamic size of single PEO chains in LiCl or LiCl-POM added solution with increasing ionic concentration, suggesting distinct ionic binding and screening effects. Further, the addition of a solvent with weak hydrogen-bond donor capabilities could further weaken the binding POM with PEO, but not so for the binding of Li+ cation with PEO. Therefore, the formation of PEO-Li+-POM complexes in different solvent mixture could lead to a facile process of PEO-based ionomers of tunable net charge.
3:30PM D34.00006: Addition of Zwitterions to Single-ion Conducting Ionomers*  WENWEN MEI (Presenter), AUGUST ROTHENBERGER, JOSH BOSTWICK, ROBERT HICKEY, RALPH H COLBY, Materials Science & Engineering, Pennsylvania State University — Applications of polymeric materials in energy-related areas are severely hampered by their limited conductivity at room temperature. The continuing pursuit of maximizing their room-temperature conductivity has driven novel design of polymeric systems. Ion aggregates are believed to be one of the major causes that stymies the ion conduction, due to the decreased mobile ion density and slowed segmental motion. Recently, much attention was drawn on additives that increase the dielectric constant due to its significant role in promoting conduction of small mobile ions such as lithium. Zwitterions are promising candidates for this purpose, owning to a large molecular dipole from covalently bonded cation and anion. Here, we studied a series of imidazolium-sulfonate zwitterions that are used as additives in single-ion conducting ionomers. Significant increases in both dielectric constant and ionic conductivity are reported. This work highlights the significance of zwitterion for promoting the conductivity, which benefits their further applications in a wide range of polymers.

*NSF#1807934

3:42PM D34.00007: Polymer Electrolytes Containing Solvate Ionic Liquid and Beyond* [Invited] MASAYOSHI WATANABE (Presenter), Yokohama Natl Univ — Certain molten solvates of Li salts can be regarded as solvate ionic liquids (SILs). A typical example is equimolar mixtures of glymes and Li[TFSA][TFSA]==[NTf2]). The amount (activity) of free glyme is a trace in [Li(glyme)][TFSA], and thereby can be regarded as solvate ionic liquids. Unlike conventional electrolytes, the solvation of Li⁺ by the glyme forms stable and discrete solvate ions ([Li(glyme)]⁺) in the SILs. Polymer electrolytes composed of ABA-triblock copolymers and [Li(glyme)][TFSA] SILs are proposed to simultaneously achieve high ionic conductivity, thermal stability, and a wide potential window. Intriguing points of the polymer electrolytes are decoupled ion transport from segmental motion of the matrix polymer and the persistence of solvate structure in the polymeric phase. Recently, we find that Li⁺ hopping conduction, which cannot be explained by conventional Stokes law, emerges in certain highly concentrated molten solvate electrolytes. Li⁺ diffuses faster than the solvent and anion, and thus the evolution of Li⁺ hopping conduction is confirmed, which leads to a higher Li⁺ transference number. Possible application of these new electrolytes will be discussed.

*This research was supported by JSPS KAKENHI (15H05758) and JST ALCA-SPRING project.
**4:18PM D34.00008: The Overlap Concentration in Strong Polyelectrolytes**

MARK STEVENS (Presenter), JON BOLLINGER, GARY GREST, Sandia National Laboratories, MICHAEL RUBINSTEIN, Physics, Duke University — Understanding strong polyelectrolytes in solution is a major challenge for theory. We have simulated a strong polyelectrolyte in a salt free solution for monomer numbers \( N = 10 \) to 1600. We calculated the overlap concentration \( c^* \) and find that \( c^* \) scales as \( N^{-2.5} \). Moreover, not until very large \( N \geq 800 \) does the end-to-end distance at \( c^* \) approach the infinite dilution limit. The chains at large \( N \) are fully stretched at \( c^* \), while at small \( N \) substantial stretching occurs below \( c^* \). For large \( N \) the chains are also rodlike in that the form factor at \( c^* \) is almost that of a straight line for lengths corresponding from a few bond lengths to the end-to-end distance.

*M. R. acknowledges financial support from National Science Foundation under Grant EFMA-1830957, the National Institutes of Health under Grant P01-HL108808. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525.

**4:30PM D34.00009: Salt Effect on Swelling of Polyelectrolyte Networks with Brush-like Strands**

MICHAEL JACOBS (Presenter), ZILU WANG, ANDREY DOBRYNIN, Polymer Science, University of Akron — We study effect of added salt, density of ionized groups and molecular architecture of the network strand on the swelling ability of networks with charged brush-like strands using a combination of the analytical calculations and coarse-grained molecular dynamics simulations. Analysis of the simulation results shows that in the salt-free case, when swelling of polyelectrolyte networks is controlled by a fine interplay between the osmotic pressure of counterions and nonlinear elasticity of the network strands, one can achieve a significant increase in the network swelling ratio by increasing the grafting density and degree of polymerization of the side chains. Addition of salt is manifested in the monotonic decrease of the network swelling ratio with increasing the salt concentration. At high salt concentrations, the electrostatic interactions between ionized groups are screened and swelling of the polyelectrolyte networks is similar to that of networks with neutral brush-like strands immersed in a good solvent. The computer simulation results are in a very good qualitative agreement with the developed theoretical model accounting for nonlinear elasticity of the network strands.

*The authors acknowledge funding from the National Science Foundation DMR-1921923.*
4:42PM D34.00010: Electrostatic Effects on Charged Block Copolymer Melts* YIHAO LIANG
(Presenter), BORAN MA, MONICA OLVERA DE LA CRUZ, Northwestern University — Electrostatic interactions can enrich the phase behaviors of charged block copolymer melts. However, due to limitations of simulation techniques and theoretic tools, the phase behavior of charged block copolymers remains elusive. In this talk we implement the event-chain Monte Carlo (ECMC) algorithm to describe charged block copolymer melts. ECMC is a new simulation technique which satisfies the maximum global balance and is good for systems with long relaxation time. Equipped with cell-veto method, ECMC can achieve O(N) time complexity for each cycle. Our work shows that ECMC is a promising approach to describe charged copolymer systems.

*ChiMAD

4:54PM D34.00011: Transference Numbers of Aqueous Polyelectrolyte Solutions TYLER LYTLE (Presenter), ARUN YETHIRAJ, University of Wisconsin - Madison — The demand for lithium-ion batteries with improved energy density and charging rates is growing, because of increasing use of consumer electronics and electrification of vehicles. However, lithium-ion batteries have several issues including long charging times. A potential route to circumvent this issue and increase the battery energy density is high transference number electrolytes. Lithium transference numbers using traditional liquid electrolytes are less than 0.5, which indicates the anion carries most of the current. In order to increase this transference number, it has been suggested to use polyelectrolyte solutions in which the polyanion mobility is less than the lithium ion mobility, but molecular-level understanding of counterion dynamics in polyelectrolyte solutions is underdeveloped. Our work uses molecular dynamics simulations of coarse-grained polymer models to elucidate how chain length, counterion size, and solution concentration affect the ion transference number in solution. These simulations show ion transference numbers depend non-monotonically on chain length, and smaller counterions have lower transference numbers. These simulation results can be used to guide experimental design of electrolytes with high lithium ion transference numbers.
5:06PM D34.00012: Hydration Phenomena in Sulfonated Poly(arylene ether sulfone) Membranes*  
CHENGYUAN WEN (Presenter), BRITANNIA VONDRASEK, JUDY RIFFLE, JACK LESKO, SHENGFENG CHENG, Virginia Tech — The hydration mechanism of ionic polysulfones remains poorly understood, which hinders their utility in water purification membranes. Differential scanning calorimetry (DSC), density measurements, and molecular dynamics simulations are combined to improve molecular-scale understanding of how water interacts with different parts of sulfonated polysulfones as water uptake is varied. The results reveal a threshold value of water uptake below which virtually all water molecules are located in the primary hydration shell of ions (Na$^+$ and SO$_3^-$) and polar groups (SO$_2$ and ether linkages). At higher water uptake, a significant fraction of the absorbed water molecules become more loosely associated with the polymer. This transition is indicated by the gradual appearance of a melting endotherm in DSC analysis, a maximum in measured density of the hydrated polymer, and appearance of water molecules with a bulk-like state in simulations. The simulation results further indicate that interactions between ions (Na$^+$ and SO$_3^-$) and polar groups, particularly SO$_2$, play an important role in the hydration behavior of sulfonated polysulfones.

*Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund (PRF #56103-DNI6), for support of this research.

5:18PM D34.00013: Dynamics at Internal Interfaces in Ionizable Polymer Blends*  
JAYME ALGER (Presenter), MANJULA SENANAYAKE, Department of Chemistry, Clemson University, Clemson, SC, United States,29634, GARY GREST, Sandia National Laboratories, Albuquerque, NM, United States,87123, DVORA PERAHIA, Department of Chemistry/Department of Physics, Clemson University, Clemson, SC, United States, 29634 — Ionizable polymers have found a large number of applications in the water-energy nexus, enabled by the segregation of the polymers into ionic and non-ionic domains. The morphology of the ionic domains varies as a function of numerous factors, among them are the number of ionic groups, their distribution and the topology of the polymers. To understand the segregation process, we probe the evolution and dynamics of internal interfaces formed by blends of polystyrene (PS) and polystyrene sulfonate (PSS) below their entanglement length using atomistic molecular dynamic simulations for temperatures above the glass transition temperature of either polymer. Melts of PS and PSS blends with varying sulfonation fractions with Na$^+$ and N(CH$_3$)$_4^+$ counterions were followed as a function of time. The development of the internal interface of the charged and the non-charged polymers will be discussed. We will compare blends of PS and PSS which can globally phase separate with diblock copolymers of PS and PSS which phase separate only locally.

*Supported in part by DOE Grant No. DE-SC007908

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D35 DPOLY DSOFT: Biopolymers, Polymer Bioconjugates, and Their Self-Assembled Phases 507 - Thomas Angelini, University of Florida - Tag(s): Focus
2:30PM D35.00001: Asymmetric Lipid/Polymer Vesicles  
YUTING HUANG (Presenter), Harvard University — Lipid vesicles are aqueous volumes surrounded by a bilayer of lipid molecules, which are amphiphilic molecules with their head groups facing water and tail groups facing oil. These vesicles are simple models for cell membranes and can be used for drug delivery. Similarly, block copolymers are amphiphilic molecules that form vesicles by themselves or with lipids. Like lipid vesicles, polymer vesicles can also be used for drug delivery and cell membrane mimicry. One interesting type of lipid/polymer vesicle is the asymmetric vesicle, in which its bilayer is composed of two dissimilar lipid monolayers or a lipid monolayer and a polymer monolayer. Importantly, all eukaryotic cell membranes exhibit this type of asymmetry and asymmetry is also proposed to enhance mechanical properties of the membrane. Here, we use microfluidics to fabricate mono disperse and highly controllable asymmetric vesicles, which unlike the conventional methods that often end up with highly poly disperse samples. To achieve this, asymmetric vesicles are produced using water/oil1/oil2/water emulsions in a glass capillary device, with different lipids/polymers immersed in two different volatile oil phases. In future, we envision asymmetric lipid/polymer vesicles could open a new door in the drug delivery field.

2:42PM D35.00002: Polyelectrolyte dynamical self-consistent field theory  
SYLVIA LUYBEN (Presenter), ROBERT WICKHAM, Univ of Guelph — Recent experiments that examine the reconstitution of proteins into artificial triblock copolymer membranes have implicated a charge-driven reconstitution mechanism. As a first step to model the dynamics of this mechanism, we incorporate electrostatic interactions into dynamical self-consistent field theory. We begin with microscopic Langevin equations for interacting polyelectrolytes, solvent, and counterions. These equations are recast as a dynamical functional integral over collective field variables. We then make a saddle-point approximation, leading to a coupled set of dynamical mean field equations which includes the Poisson equation governing the electrostatic potential. Our approach reduces the interacting many-chain problem to a single polyelectrolyte chain in a dynamical mean force field. This simplification enables us to probe a broad range of length- and time-scales. We simulate the dynamics of insertion of a charged triblock copolymer (a model protein) into an oppositely-charged, self-assembled, triblock copolymer membrane.

*We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC).
Dynamics of self-interacting bio-inspired polymers in shear flows

HELMAN AMAYA-ESPINOSA (Presenter), Vice-presidency of Research, University of the Andes, ALFREDO ALEXANDER-KATZ, Department of Materials Science & Engineering, Massachusetts Institute of Technology, CAMILO APONTE-SANTAMARÍA, Faculty of Engineering, University of the Andes — Biopolymers interact with each other, triggered by external stimuli, to carry out key biological functions. Blood clotting is a perfect example of that. Triggered by the shear of the flowing blood, the giant von Willebrand factor (VWF) adhesive protein establishes specific interactions with several partners, including with itself via specific protein-protein auto-inhibitory interactions. However, the impact of such self-interactions on the flow-induced non-equilibrium conformational dynamics of such polymers remained unclear. We tackled this question by implementing Brownian dynamics simulations at a coarse-grained resolution of VWF-like self-interacting biopolymers. In the absence of specific interactions, we recapitulated previous estimates of the critical shear-rate upon which the polymer underwent a globular-to-stretched conformation. Introduction of specifically interacting points within the polymer increased the critical shear-rate roughly by an order of magnitude. Accordingly, our data demonstrate that the state of self-interacting biopolymers, under shear flows, can be effectively tuned by increasing either the number or the strength of self-interacting units. This information is highly useful to understand how specific-molecular interactions modulate VWF assembly.

Computational prediction of molecular shape through the assembly of sequence-controlled polymers

DAVINDRA TULSI (Presenter), DAVID SIMMONS, Univ of South Florida — Nature employs molecular sequence to control macromolecular shape in order to realize exquisite control over biological nanostructures such as protein assemblies, membranes and DNA complexes. Over the last decade, significant strides have been made in synthesizing artificial sequence-controlled polymers, potentially paving the way for synthetic materials mimicking biological nanostructures. Further advances are hindered by the fact that the relationship between sequence and molecular shape remains poorly understood. Here we employ molecular dynamics simulations to probe the relationship between sequence and molecular shape in model synthetic polymers. Results point to a conformation diagram that provides fundamental physical insights towards design of molecular building blocks for hierarchical assembly.
Bottom-up Coarse-grained Molecular Simulations of Peptoids with Enhanced Sampling*  
MINGFEI ZHAO (Presenter), University of Chicago, JANANI SAMPATH, CHRISTOPHER J MUNDY, Pacific Northwest National Laboratory, JIM PFAENDTNER, University of Washington, ANDREW L FERGUSON, University of Chicago — Peptoids are a class of synthetic polymers that have similar biocompatibility but high stability compared to peptides. Peptoids can both self-assemble into highly ordered nanostructures and direct the organization of inorganic components. Computational modeling is promising in helping discover and design peptoid-based nanomaterials. Atomistic peptoid models have been developed but only consider small systems due to high computational costs. To reach the time and length scale of peptoid assembly, we develop a coarse-grained (CG) model reparametrized from all-atom (AA) simulations by fitting CG bonded interactions through iterative Boltzmann inversion and nonbonded interactions through potential of mean force matching. We use Parallel Bias metadynamics to obtain good sampling in the cis/trans isomerization. The proposed CG model demonstrates excellent agreement with AA distribution functions and opens a new avenue to the computational inverse design of peptoid-based nanomaterials.

*This material is based upon work supported by the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES), as part of the Energy Frontier Research Centers program: CSSAS--The Center for the Science of Synthesis Across Scales--under Award Number DE-SC0019288.

Solution Self-Assembly of Block Copolypeptoids with a Crystallizable Core-Forming Block  
NAISHENG JIANG (Presenter), University of Science and Technology Beijing, TIANYI YU, Louisiana State University, SHUO QIAN, Oak Ridge National Laboratory, IGOR KEVIN MKAM TSENGAM, VIJAY T JOHN, Tulane University, DONGHUI ZHANG, Louisiana State University — In this study, we investigate the solution self-assembly of coil-crystalline diblock copolypeptoids with one polypeptoid block having long n-alkyl side chains. Poly(N-methyl glycine)-b-poly(N-decyl glycine) (i.e. PNMG-b-PNDG) with lower volume fraction of the crystalline PNDG blocks were found to slowly self-assemble into one-dimensional long worm-like nanofibrils in methanol, which is induced by the crystallization of core-forming PNDG. Upon increasing volume fraction of PNDG, the final micellar morphology changed from worm-like nanofibrils to rigid short nanorods and then two-dimensional nanosheets. The molecular arrangement and self-assembly pathways of these anisotropic nanostructures were investigated by a combination of X-ray/neutron scattering and microscopic techniques to understand the underlying assembly mechanism. We believe the relationship between chemical composition, micellar morphology and self-assembly pathway provided here would not only benefit the rational design of polypeptoid-based nanostructures with tunable size, shape and morphology, but also shed lights on the crystallization-driven self-assembly of comb-shaped polymers bearing long aliphatic side chains in general.
3:42PM D35.00007: Transforming protein-polymer conjugate purification by tuning protein solubility* [Invited]  ALAN RUSSELL (Presenter), STEFANIE BAKER, Carnegie Mellon Univ, CORAY COLINA, University of Florida — Almost all commercial therapeutic and industrial proteins are purified by processes that include salting-out precipitation in ammonium sulfate. Protein-polymer conjugates are generally synthesized from already pure starting materials and the struggle to separate the conjugates from polymer, native protein, and from differently modified variants has vexed scientists for decades. Since ammonium sulfate precipitation is exclusively used as an initial step in crude protein purifications, it has had little relevance in the delicate purification of protein-polymer conjugates. We have discovered, however, that polymers grown from the surface of proteins have a transformational effect on the solubility of proteins in salt solutions. We generated a family of protein-polymer conjugates with a variety of polymers, grafting densities, and polymer lengths using surface-initiated atom transfer radical polymerization. Covalently attached polymers increased solubility of the conjugates in ammonium sulfate and completely prevented precipitation. Molecular dynamic simulations showed the impact was driven by an anti-polyelectrolyte effect. We then efficiently and simply purified mixtures of conjugates and native proteins.

*Defense Threat Reduction Agency: DTRA1-18-1-0028

4:18PM D35.00008: Characterization of Fiber Formation of Sugar-based Poly(D-glucose carbonate) Amphiphilic Block Copolymers in Solution* JEE YOUNG LEE (Presenter), Univ of Delaware, YUE SONG, KAREN L WOOLEY, Chemistry, Texas A&M University, DARRIN JOHN POCHAN, Univ of Delaware — Designing the new sugar-derived poly(D-glucose carbonate)s (PGC) is motivated by a need to develop sustainable materials in response to a long-term environmental impact of traditional petroleum-based polymers. Herein, the fiber assembly behavior of the PGC amphiphilic BCP with targeted block compositions, chain lengths and side chain chemistries are explored with kinetically controlled assembly pathways varying the solvent compositions. The kinetics of the fiber formation is characterized using cryogenic-TEM and SANS where we find the assembled fibers have a flat interface composed of fused disc subunits. The assembly behavior deviates from the traditional coil-based BCPs due to the inherent stiffness of the glucose backbone resulting a unique chain packing in response to a solvent quality change. To observe the relative chain behavior in the same assembly conditions, both hydrophilic and hydrophobic block equivalent homopolymers are studied using various scattering techniques to obtain polymer chain solution properties for a better understanding of the PGC block copolymer chains. These findings allow us to discover a robust fiber nanostructure that can be achieved by non-traditional polymers and their potential to be used in many engineering applications.

*NSF DMR 1629156
Computationally designed bundlemers for hybrid physical-covalent assembly of rigid polymers

NAIRITI SINHA (Presenter), Materials Science and Engineering, University of Delaware, GRETHE VESTERGAARD JENSEN, National Institute of Standards and Technology, DARRIN JOHN POCHAN, Materials Science and Engineering, University of Delaware — Peptide coiled coils present a diverse toolbox for constructing new polymers that display target nanostructures and properties. Computational prediction of coiled coil-forming peptides enables chain and material construction in which coiled coils, also known as ‘bundlemers’, are the modular building blocks. We use bundlemers that form robust antiparallel homotetramers to construct hybrid physical-covalent, supramolecular polymers. By end-functionalizing peptides with complimentary ‘click’ reactive groups, bundlemers are covalently linked to form polymers displaying desired length distributions and flexibility: a short organic linker between bundlemers yields absolutely rigid rods while a flexible linker yields semi-flexible fibers. Small-Angle Neutron Scattering (SANS) along with Transmission Electron Microscopy (TEM) have been used extensively to characterize the structure of the resulting polymers. Furthermore, recombinant expression of the peptides in *Escherichia Coli* was used to obtain deuterated bundlemer-forming peptides. This has facilitated contrast-matching experiments in SANS with which we have characterized the stability of bundlemers in solution and also investigated the alternating bundlemer assembly design of rigid rods.

Random Heteropolymer Self-Assembly into Protein-Like Nanoparticles

SHAYNA HILBURG (Presenter), Massachusetts Institute of Technology MIT, TING XU, University of California, Berkeley, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology MIT — Single-chain polymer nanoparticles are currently of great interest due to their potential applications, yet their properties have only recently started to be elucidated. Here, we study self-assembled single polymer nanoparticles to gain molecular insights into their structure and dynamics using molecular dynamics simulations. In particular, we study a four-component synthetic heteropolymer that has been experimentally investigated previously. Prior experimental findings showed favorable interactions with native proteins in non-native environments and during protein folding. Simulations of single chains demonstrate a rich energy landscape for these polymers, evident from the structure and dynamics of the molecules in solution. Specifically, spatial arrangement of amphiphilic monomers is characterized and shows many parallels to biological proteins. Multiple time scales are seen in system dynamics, showing a large impact of component chemistry and sterics. By bridging the gap between angstrom-scale NMR and bulk characterization, all-atom simulations provide valuable insight into potential mechanisms for these heteropolymer's behavior.

*This work was supported by the Defense Threat Reduction Agency contract HDTRA11910011.*
Both living cell cytoskeleton and their extracellular matrix are constituted mainly by biopolymer matrices. The physical properties of these matrices are known to significantly impact cell behavior, such as cell morphology, migration, and stem-cell differentiation. However, cells also constantly reorganize these intracellular and extracellular structures during physiological processes; this is thought to also change the mechanics of these biopolymer matrices, which may then have an immediate impact on cell behavior. In this talk, I will present our recent progress on characterizing the drastic local nonlinear matrix stiffening induced by contraction of individual living cells inside a 3D biopolymer matrix, through direct micromechanical measurement. Moreover, I will introduce a method, called Nonlinear Stress Inference Microscopy, with which we can determine the cell-induced local matrix stress from nonlinear microrheology measurements inside various types of extracellular matrix in 3D. In addition, I will also introduce our recent progress on characterizing the significant role of cytoskeletal intermediate filament in determining nonlinear mechanics, strength, toughness, and stretchability of the mammalian cytoskeleton.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D36 DMP: DMP Past Chair's Symposium: Tools That Explore Materials Physics 601/603 - Amanda Petford-Long, Argonne National Laboratory - Tag(s): Invited

In this talk, I will present our recent experimental results using the latest generation of monochromated aberration-corrected scanning and transmission electron microscopes (STEM). Four examples of how one can reveal the magnetic ordering and orbital ordering of materials with atomic size electron probes will be shown. We have also used the principle of detailed balance to morph the electron microscope in a primary thermometer and revealed the anharmonic behavior of materials at the nanoscale. Our efforts in studying the phonon dispersion of materials under the presence of different isotopic species will be also mentioned. Finally, current and future limitations in the experiments and requirements to reveal the magnetic moment (orbital and spin), charge ordering, crystal field splitting, spin-orbit-coupling, optical dichroism, and other physical phenomena associated with broken symmetries will be discussed.

*This research was supported by the Center for Nanophase Materials Sciences, which is a Department of Energy Office of Science User Facility, using instrumentation within ORNL’s Materials Characterization Core provided by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy, and sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy.
We have developed a powerful new method called ultrafast electron calorimetry that can uncover hidden phases in magnetic and charge density wave materials. By using time and angle-resolved photoemission spectroscopy to measure the dynamic electron temperature and full band structure as the laser excitation is varied, one can clearly identify when changes in state or couplings occur in a material. Recently we used this approach to coherently manipulate the structure, electron-phonon couplings, and state of the 2D charge density wave (CDW) material 1T-TaSe2. Instead of the two material phases normally accessible using temperature tuning (CDW and normal phases), ultrafast laser excitation expands the phase diagram to include at least two new phases: a new metastable CDW state, and an inverted CDW state. Moreover, the electron temperature, bandwidth, band gap and band shift are all modulated by the CDW breathing mode, and this modulation changes in phase as the material enters a new state. In addition to the ability to map the state of a material, we can use pulse sequences to coherently guide a material from one phase to another.

Zhang et al., http://arxiv.org/abs/1906.09545
Combining STM, AFM, and Magnetotransport Measurements for In-Operando Studies of Quantum Materials*

JOSEPH STROSCIO (Presenter), National Institute of Standards and Technology — Research in new quantum materials require multi-mode measurements spanning length scales, correlations of atomic scale variables with macroscopic functions, and with ultimate spectral resolution only obtainable at ultra-low temperatures. In this talk I describe a multi-mode instrument achieving μeV tunneling resolution with in-operando measurement capabilities of scanning tunneling microscopy (STM), atomic force microscopy (AFM), and magnetotransport inside a dilution refrigerator operating at 10 mK. I illustrate the capabilities of this new instrument in the study of quantum Hall edge states in graphene devices. The edge states, a set of alternating compressible and incompressible strips, are formed at the electrostatic pn junction boundary geometrically defining the Hall bar. To comprehensively characterize these microscopic objects, we apply all capabilities of the new instrument using modalities of AFM, STM, and magnetotransport measurements at mK temperatures. The Kelvin probe force microscopy (KPFM) mode of AFM detects the chemical potential transitions when Landau levels are being filled or emptied as a function of back gate potential and show the same fidelity for Landau level spectroscopy as STS measurements. In particular, symmetry breaking states can be resolved at filling factors ν = ±1 inside the N=0 Landau level manifold, showing the lifting of the graphene four-fold degeneracy due to spin and valley. With KPFM we can map the dispersion of the Landau levels across the quantum Hall edge boundary as a function of density and spatial position, including resolving the ν = ±1 edge modes. The microscopic properties of quantum Hall edge states can now be correlated with macroscopic magnetotransport measurements.


Capturing In Operando Electronic Structure of Microscopic 2D Materials*

ELI ROTENBERG (Presenter), Lawrence Berkeley National Laboratory — Angle Resolved Photoemission Spectroscopy (ARPES) is a premier technique for determining the electronic structure of correlated and topological materials. Recently, we and several other groups have adapted ARPES to submicron dimensions through the development of nano-scale scanning X-ray beams, creating so-called nanoARPES endstations at synchrotrons around the world. This exciting technique now enables the in operando measurement of electronic structure for materials in applied fields and currents, as well as the ability to probe the effect of screening and strain on many body physics in confined geometries. In this talk, I will present recent results in which nanoARPES is applied to 2D materials and heterostructures at length scales below 200 nm. These include few layer graphene and transition metal dichalcogenide / graphene heterostructures. Work done in collaboration with Professors T. Heinz (Stanford U.), J. Katoch (CMU), S Ulstrup, J. Miwa, and Ph. Hofmann (Aarhus U.).

*This research used resources of the Advanced Light Source, which is a DOE Office of Science User Facility under contract no. DE-AC02-05CH11231.
4:54PM D36.00005: Nanoscale quantum sensing of quantum materials through a single spin magnetometer [Invited] CHUNHUI DU (Presenter), University of California, San Diego — We introduce single spin magnetometry based on nitrogen-vacancy (NV) centers in diamond as a new measurement platform to locally probe the magnetic properties of quantum materials with a nanoscale spatial resolution. Utilizing this measurement platform, we have demonstrated control and local measurements of spin chemical potential in a magnetic insulator yttrium iron garnet (YIG) at the ambient condition, which opens up new possibilities for nanoscale imaging of spin-related phenomena. In addition, we investigate the temperature-dependent microwave response of an exfoliated high-$T_c$ superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ (BSCCO) flake, from which the superconducting phase transition and penetration depth can be obtained in a non-invasive fashion. Our results demonstrate the unique capability enabled by NV spin magnetometry in exploring the exotic local spin and charge behavior of emergent material systems.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D37 DFD: Transitional Flows & Chaotic Dynamics: In Honor of Bruno Eckhardt 605 - Alexander Morozov, Univ of Edinburgh - Tag(s): Invited

2:30PM D37.00001: What do we learn from the finite lifetime of turbulence?* [Invited] NIGEL GOLDENFELD (Presenter), University of Illinois at Urbana-Champaign — In a seminal paper published in 2006, Bruno Eckhardt and co-workers presented evidence to support the remarkable speculation that turbulence in shear flows --- specifically pipe flow --- has a finite lifetime at all Reynolds numbers, without the divergence that would be expected if the laminar and turbulent state were not analytically connected. I discuss these findings and their later extensions in terms of extreme value statistics and finite-size scaling, and show that the finite lifetime in pipe flow does not necessarily contradict the notion that there is a sharp laminar-turbulence transition in the universality class of directed percolation.

*This work was partially supported by a grant from the Simons Foundation (Grant number: 662985, NG) and by the National Science Foundation (Grant NSF-DMR-1044901).
3:06PM D37.00002: Is space time? A spatiotemporal tiling of turbulence [Invited]  PREDRAG CVITANOVIC (Presenter), MATTHEW N GUDORF, HAN LIANG, Georgia Inst of Tech — We address the long standing problem of how to describe, by means of discrete symbolic dynamics, the spatiotemporal chaos (or turbulence) in spatially extended, strongly nonlinear field theories.

One way to capture the essential features of turbulent motions is offered by coupled map lattice models, in which the spacetime is discretized, with the dynamics of small-scale spatial structures modeled by maps attached to lattice sites. The discretization that we study, the "spatiotemporal cat," has a remarkable feature that its every solution is uniquely encoded by a linear transformation from the corresponding finite alphabet symbol lattice. A spatiotemporal window into system dynamics is provided by a finite block of symbols, and the central question is to determine the likelihood of a given block's occurrence. As spatiotemporal states that share the same sub-blocks shadow each other exponentially well within the corresponding spatiotemporal windows, the dynamical zeta functions are now sums over spacetime tori, rather than time-periodic orbits.

In the spatiotemporal formulation of turbulence there is no evolution in time, there are only a repertoires of admissible spatiotemporal patterns. In other words: throw away your integrators, and look for guidance in clouds' repeating patterns.

3:42PM D37.00003: Deep learning to discover the dimension of an inertial manifold and predict dynamics on it [Invited]  MICHAEL GRAHAM (Presenter), University of Wisconsin - Madison — One of the senior author's last conversations with Bruno Eckhardt concerned the connection of machine learning tools and ideas to dynamical systems and turbulence. This talk concerns one such connection. Many flow geometries, including pipe, channel and boundary layer, have a continuous translation symmetry. As a model for such systems we consider the Kuramoto-Sivashinsky equation (KSE) in a periodic domain. We describe a method to map the dynamics onto a translationally invariant low-dimensional manifold and time-evolve them using neural networks (NN). Dimensionality reduction is achieved by phase-aligning the spatial structures at each time, then putting them into an undercomplete autoencoder that maps the original dynamics onto a lower-dimensional inertial manifold where the long-time dynamics live. We infer the dimension of the manifold by tracking the autoencoder error vs. dimension—this drops by orders of magnitude once the proper dimension is reached. The spatial structure and phase are then integrated forward in time using a NN. This approach significantly outperforms Principal Components Analysis.
4:18PM D37.00004: The onset of turbulence: from invariant solutions to a directed percolation phase transition [Invited]  BJOERN HOF (Presenter), Physics, IST Austria — Flows through pipes and channels exhibit an abrupt transition from ordered laminar to high dimensional turbulent flow. At the lowest Reynolds numbers where this transition can be observed the resulting flows are spatio temporally intermittent and are composed of patches of turbulence surrounded by laminar fluid. As will be shown, in direct numerical simulations individual turbulent patches (i.e. stripes and puffs) can be continued to much lower Reynolds numbers where they originate from spatially localized periodic orbit solutions. I will further discuss experimental studies of interacting turbulent patches and how the competition between the decay and the proliferation of turbulence gives rise to a phase transition to sustained turbulence.

4:54PM D37.00005: Nonlinear invariant solutions underlying spatio-temporal patterns in thermally driven shear flows * [Invited]  TOBIAS SCHNEIDER (Presenter), Ecole Polytechnique Federale de Lausanne — Driven wall-bounded fluid flows transitioning to turbulence are spatially extended chaotic dissipative non-equilibrium systems that support a large variety of self-organized patterns with regular spatial and temporal structure. In linearly stable parallel shear flows, patterns such as long-studied spontaneously emerging turbulent-laminar oblique stripes remain only partly understood. On the contrary, thermal convection in a fluid layer between two horizontal plates kept at different temperature, exhibits patterns that can often be described via a sequence of bifurcations off a base state undergoing a linear instability. If a Rayleigh-Bénard convection cell is inclined against gravity, buoyancy forces drive hot and cold fluid up and down the incline leading to a shear flow. In this so-called inclined layer convection (ILC) system, the competition of buoyancy and shear gives rise to a large variety of complex spatio-temporal flow patterns.

We study the dynamics of ILC using a fully nonlinear dynamical systems approach based on a state space analysis of the governing equations. Exploiting the computational power of highly parallelized numerical continuation tools based on matrix-free Newton methods (www.channelflow.ch), we compute a large set of invariant solutions of ILC and discuss their bifurcation structure. Specifically, equilibria, travelling waves, periodic orbits and heteroclinic orbits will be shown to form dynamical networks that support moderately complex dynamics at intermediate angles of inclination. At high inclination angles, where shear forces dominate, localized patches of weakly turbulent convection within a background of straight longitudinal convection rolls are observed. We present exact invariant solutions capturing both the dynamics and the spatial localization of these so-called transverse bursts.

*Supported by the Swiss National Science Foundation under grant no. 200021-160088

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D38 FHP: History of Materials Science 607 - Robert Crease, State Univ of NY - Stony Brook - Tag(s): Invited, Undergrad Friendly
2:30PM D38.00001: Overview of History of Materials Research [Invited] ARNE HESSENBRUCH (Presenter), Massachusetts Institute of Technology — How can one get a quick overview of the history of materials research in the last few decades? Maybe by examining session titles at the Materials Research Society meetings. What has changed, what has not?

3:06PM D38.00002: Bernadette Bensaude-Vincent Invited Talk [Invited] —

3:42PM D38.00003: From Hidden Utility to Heroic Machines [Invited] E. F. SPERO (Presenter), Materials Science and Engineering, Massachusetts Institute of Technology — How do scientists imagine (and possibly enable) futures through their practices of computation? How might particular tools and approaches transition from serving as hidden utilitarian elements to those that give rise to new subfields and styles of thought? This presentation takes a historical approach to the emergence of computation in macromolecular science, an interdiscipline focused on polymers that bridges physics, chemistry, and materials science and engineering. In this field today, there is a palpable enthusiasm for the power and speed of computation investing in the promise of big data to revolutionize what is possible within these disciplines. Employing tools of high-throughput simulation and new machine learning algorithms, scientists aim to close the gap between theory and experiment, and redefine what it means to create, designing new sustainable materials built with atomic precision. However, in the late 1950s when computation was yet a nascent tool, often used for verification of existing models (rather than one for creation) scientists studying the physical behavior of long chain molecules downplayed, mistrusted, or even openly disdained computational methods. Along with fellow panelists this presentation will open space for reflection on tools, methods, and imagination.

4:18PM D38.00004: Lynn W. Hobbs Invited Talk [Invited] —

4:54PM D38.00005: History of Materials Science Institutions [Invited] ROBERT CREASE (Presenter), State Univ of NY - Stony Brook — Materials science requires a diverse set of institutions to interact closely and flexibly in staging research events, and to allow different kinds of communities and facilities to intersect. These institutions, however, tend to drop out of the history of scientific research. This talk divides such institutions into five basic, though often overlapping, kinds: physical sites (laboratories), educational institutions, societies, funding agencies, and journals. The talk discusses the importance of these institutions and makes a brief survey of them.

Monday, March 2, 2020 2:30 PM - 5:06 PM

Session D39 DCOMP DMP DCP: First-principles modeling of excited-state phenomena in materials III: GW+BSE for Polaron and Optical Excitations 703 - Sahar Sharifzadeh, Boston Univ - Tag(s): Focus
2:30PM D39.00001: Polarons from first principles* [Invited]  FELICIANO GIUSTINO (Presenter), Physics, University of Texas at Austin — Polarons are among the most well-known quasiparticles in solid state physics, and are key to understanding fundamental concepts such as the electron mass enhancement in semiconductors and the formation of Cooper pairs in superconductors. Interest in polaron physics has been reignited by recent angle-resolved photoelectron spectroscopy studies, which revealed polaronic signatures in the band structures of several metal oxides and two-dimensional semiconductors. In this talk I will describe our recent work aimed at describing polarons and their spectroscopic signatures from first principles. In the first part of the talk I will outline a general many-body framework to compute and analyze polaron satellites in photoelectron spectra using the cumulant expansion approach [1,2]. I will discuss applications to titanium dioxide and europium oxide, and show that the calculations are able to reproduce very closely measured angle-resolved photoelectron spectra. In the second part of the talk I will address the question on how to compute the wavefunction of a polaron. I will describe a new approach to the polaron problem that overcomes some of the limitations of explicit supercell calculations [3]. This approach enables systematic calculations of wavefunctions and formation energies for both small and large polarons, and can be used to analyze the electron-phonon coupling mechanisms responsible for electron or hole self-trapping. I will illustrate these concepts using lithium fluoride and lithium oxide as examples, and I will discuss the connection with previous work on the polaron problem based on model Hamiltonians.


*Grant RL-2012-001 funded by the Leverhulme Trust; Grant DE-SC0020129 funded by the U.S. Department of Energy, Office of Science.

3:06PM D39.00002: Theory and First-Principle Calculation of Photoemission Spectra from Optically Excited States  TING CAO (Presenter), Department of Materials Science and Engineering, University of Washington and Geballe Laboratory for Advanced Materials, Stanford University, KESHAV M DANI, Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology Graduate University, TONY F HEINZ, Department of Applied Physics, Stanford University and SLAC National Accelerator Laboratory — The behaviors of optically excited states, such as excitons, not only give rise to a variety of fascinating phenomena in condensed matter, but also play vital roles in modern optoelectronics and energy harvesting. In this talk, I will present our recent development on the theory and first-principle methods in the study of the photoemission spectra of low-dimensional materials. By performing calculations based on many-body perturbation theories, we show that, in monolayer transition metal dichalcogenides, the excitons hold unique energy dispersions and spectra weights in photoemission, which unveil the fundamental physical properties of these excited states. We further connect our theoretical works to experimental results and explore their potential applications in other systems.

YU JIN (Presenter), Department of Chemistry, University of Chicago, MARCO GOVONI, Materials Science Division and Center for Molecular Engineering, Argonne National Laboratory, GIULIA GALLI, Pritzker School of Molecular Engineering, University of Chicago — In order to predict the opto-electronic properties of several classes of functional materials, an accurate description of absorption and photoluminescence processes is necessary. Building on our previous work on calculations of absorption spectra from first principles [1], we present a method to compute photoluminescence spectra based on the solution of the generalized quantum Liouville equation, including electron-phonon interaction [2]. We present results for the photoluminescence spectra of organic/inorganic perovskites and of optically controllable defects in semiconductors.


*This work was supported by the Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE), an EFRC funded by DOE/BES, and Midwest Integrated Center for Computational Materials (MICCoM) as part of the CMS Program funded by DOE/BES.

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**3:30PM D39.00004: Deep ultraviolet luminescence and charge-transfer excitons in atomically thin GaN quantum wells**

WONCHEOL LEE (Presenter), DYLAN BAYERL, NOCONA SANDERS, ZIHAO DENG, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — We investigate the electronic, excitonic, and optical properties of atomically thin GaN quantum wells embedded in AlN or AlGaN barriers using first-principles calculations based on density functional theory (DFT) and many-body perturbation theory. The strong quantum confinement results in deep ultraviolet luminescence. Also, the quasi-2D structural characteristic produces strongly bound excitons, which are even stable at room temperature. We also investigate the properties of pairs of atomically thin GaN wells, separated by polar AlN barriers. The perpendicular electrical polarization produces charge-transfer excitons, in which electrons and holes are spatially separated in the two different GaN wells. Compared to direct excitons, the reduced overlap of charge-transfer excitons enables exciton lifetime that are 3-4 orders of magnitude longer. By adjusting the separation distance between electrons and holes through variations of the well and barrier thickness we can control the exciton lifetime and the binding energy simultaneously.

*The work is supported by the University of Michigan College of Engineering Blue Sky Research Program. W.L. was partially supported by the Kwanjeong Educational Foundation Scholarship. Computational resources were provided by the DOE NERSC facility.
Analysis of diagonal $G$ and subspace $W$ approximations within fully self-consistent $GW$ calculations for bulk semiconducting systems*  

YASHPAL SINGH (Presenter), LIN-WANG WANG, Lawrence Berkeley National Laboratory — Fully self-consistent $GW$ (sc-$GW$) methods are now available to evaluate quasiparticle and spectral properties of various molecular and bulk systems. However, such techniques are computationally demanding and act as a bottleneck to include vertex function. In contrast, routinely used single-shot $G_0W_0$ approximation has an undesirable dependency on the choice of xc-functional. In this work, we consider AlAs, AlP, GaP, and ZnS as our prototype systems to perform sc-$GW$ calculations by expressing the full $G$ matrix using a plane-wave basis set. To reduce the computational cost, we present a framework within our sc-$GW$ scheme to consider diagonal $G$ and subspace $W$ approximations. We analyse our results obtained from the above techniques by comparing against our fully sc-$GW$ calculations and other similar approaches including experiments. The sub 2% difference in the values of the bandgap obtained from fully sc-$GW$ and subspace $W$ methods shows an encouraging direction to incorporate vertex function that could potentially improve overestimated sc-$GW$ bandgaps.

*This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231, as part of the Computational Materials Sciences Program.

Spin-wave dispersion of Cu$_2$MnAl, Ni$_2$MnSn, and Pd$_2$MnSn based on quasi-particle self-consistent $GW$ method*  

HARUKI OKUMURA (Presenter), KAZUNORI SATO, Osaka University, TAKAO KOTANI, Tottori University — We calculated the spin-wave dispersion and the stiffness constants of three metallic ferromagnetic Heusler alloys: Cu$_2$MnAl, Ni$_2$MnSn, and Pd$_2$MnSn. We determined the ground state by the quasi-particle self-consistent $GW$ (QSGW) method. In conjunction with the Wannier function, we obtain transverse dynamical spin susceptibility based on linear response method. It is found that the ground states within the QSGW are reasonably calculated to reproduce spin-wave dispersion around Gamma point. In Cu$_2$MnAl, the magnetic moment in QSGW agrees with the experiment, but stiffness constant is underestimated. In Ni$_2$MnSn, the QSGW overestimates the moment, as seen in the itinerant ferromagnetic case as FCC Ni; however, the stiffness in QSGW agrees with the experiment. In Pd$_2$MnSn, the QSGW reproduces the spin-wave throughout the Brillouin zone, and the stiffness is close to the experiments. This agreement is due to the reasonable exchange splitting of Mn 3d in accordance with the large screened Coulomb interaction in QSGW.

*This work was partly supported by JST CREST Grant number JPMJCR1812 and by JSPS KAKENHI Grant Number JP18H05212 and JP17K05499. This work was partly supported by MEXT of Japan.
4:06PM D39.00007: Self-consistent GW method for solids: efficient implementation*
ANDREY KUTEPOV (Presenter), Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — An efficient implementation of the self-consistent GW method in the FlapwMBPT code (https://www.bnl.gov/cmpmsd/flapwmbpt/) is presented. It features the evaluation of the polarizability and the self-energy which scales only linearly with respect to the system size. The total computational time scaling measurements show it to be between linear and quadratic up to 72 atoms in silicon supercells. Application to such materials as CoSbS (24 atoms), supercells of La2CuO4 (up to 56 atoms), and SmB6 (7 atoms) illustrate the potential of the approach in computational material science.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences as a part of the Computational Materials Science Program.

4:18PM D39.00008: Systematic QSGW calculations on the electronic structure of rare-earth nitrides*
KAZUNORI SATO (Presenter), Graduate School of Engineering, Osaka University, TAKAO KOTANI, Department of Applied Mathematics and Physics, Tottori University, KATSUHIRO SUZUKI, Graduate School of Engineering, Osaka University — Rare-earth (RE) based light emitting materials are distinguished for their narrow line width, small temperature dependence and insensitivity to the environment. These characteristic properties mostly come from localized nature of 4f-states. Therefore, for accurate prediction and design of RE related functional material, reasonable description of 4f-states is indispensable.

In this paper, we present systematic electronic structure calculations of RE nitrides by using quasi-particle self-consistent GW (QSGW) method. This method was implemented to ecalj package, and confirmed to give reasonable description of the electronic structure of several materials including f-electron systems [1, 2]. It is found that the present calculations reproduce previous LDA+U calculations [3] and calculated magnetic moments are reasonably described by the Hund's rule for most of the rare-earth nitrides. For example, SmN is calculated to be semi-metallic and predicted magnetic moments (S=2.50, L=4.96, J=2.46) are consistent to Hund's rule prediction.


*This work was partly supported by JST CREST (JPMJCR1812) and by JSPS KAKENHI (JP18H05212).
**4:30PM D39.00009: Jigsaw Puzzle Orbitals for Electronic Structure**

DIMITAR PASHOV, MARK SCHILFGAARDE (Presenter), Kings College London — We present the jigsaw-puzzle orbitals (JPOs), a recently developed basis set for solving the one-particle Schrödinger equation with an optimally constructed minimal basis set. We illustrate some of its advantages with QSGW bandstructure calculations. A significant improvement in self-energy interpolation is observed as well as physically intuitive dependency of the band gap on the projection range.

The better spatial localization of JPOs paves the way to efficient, real-space assembly of 1-particle matrices while simultaneously improving accuracy on wider energy window. The short-ranged functions both significantly less linearly interdependent and more accurate than traditional atom-centered basis functions.

*This work was supported by the Simons Many-Electron collaboration

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**4:42PM D39.00010: First-principles Studies of Tl activated Scintillator Phosphor Materials: Towards an understanding of the Scintillation mechanism**

ANDREW CANNING (Presenter), MAURO DEL BEN, Lawrence Berkeley National Laboratory, JAROSLAW GLODO, Radiation Monitoring Devices Inc. — Tl doped halide scintillator phosphors are amongst the most commonly used gamma ray detector materials for medical imaging, high energy physics and nuclear materials detection applications (e.g. CsI:Tl, NaI:Tl). Even so the complete scintillation process in these materials is still poorly understood. In particular in recent years there has been great interest in co-doping these materials to try and improve their detection performance. We have performed first-principles studies based on GGA, hybrid functionals and the GW/BSE method in tandem with experiments to understand the scintillation mechanism in these materials and how it could be improved by co-doping. In particular we have looked at the Tl exciton optical emission states and energy transfer mechanisms from the gamma ray to the Tl. Recently there has also been interest in new Tl bulk scintillators such as TLYC (Tl2LiYCl6) which we have also studied.

*This work was supported by the Director, Office of Advanced Scientific Computing Research, Office of Science of the U.S. Dept. of Energy and used resources of the National Energy Research Scientific Computing Center (NERSC). Work carried out at Lawrence Berkeley National Laboratory under contract DE-AC02-05CH11231.*
Excitation Pathways in Resonant Inelastic X-ray Scattering from Many-Body Perturbation Theory

CHRISTIAN VORWERK (Presenter), Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany, FRANCESCO SOTTILE, LSI, Ecole Polytechnique, CNRS, CEA, Institut Polytechnique de Paris, Palaiseau, France, CLAUDIA DRAXL, Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — Resonant inelastic x-ray scattering (RIXS) spectroscopy is a powerful tool to unravel the nature of elementary excitations in a wide range of crystalline materials. In the RIXS process, a core electron is excited through the absorption of an x-ray photon. Subsequently, a valence electron fills the core hole via the emission of a x-ray photon. The final many-body state contains an excited electron and a valence hole. Through resonant x-ray absorption and emission, RIXS offers an elemental and orbital selective probe of the electronic valence excitations. In this talk, we present a novel many-body approach to RIXS. We use explicit many-body excited states in the optical and x-ray region, as obtained from full diagonalization of the Bethe-Salpeter equation in an all-electron framework, to obtain an expression for the RIXS cross section. The RIXS cross section is expressed in terms of pathways between intermediate many-body states containing a core hole, and final many-body states containing a valence hole. We apply our in-depth analysis to the RIXS spectra of the flour K edge of LiF and carbon K edge of diamond. Our results show that the excitation pathways determine the spectral shape of the emission, and the importance of electron-hole correlation in the spectra.

Monday, March 2, 2020 2:30 PM - 5:18 PM

Session D40 DCOMP DMP DAMOP DCP: Building the Bridge to Exascale: Applications and Opportunities for Materials, Chemistry, and Biology III

705 - Jack Deslippe, Lawrence Berkeley National Laboratory - Tag(s): Focus
Preparing for exascale: additive manufacturing process modeling at the fidelity of the microstructure* [Invited] JAMES BELAK (Presenter), Lawrence Livermore Natl Lab — In FY17, the USDOE Exascale Computing Project (ECP) initiated projects to design and develop simulation codes to use exascale computing. This application development is organized around computational motifs. Here, we present an overview of the motifs of computational materials science, from the “particles” using by molecular dynamics to the “grids” using by phase-field models and the various solution algorithms such as FFTs. Examples will be taken from the co-design centers ExMatEx and CoPA, as well as the application development project ExaAM. This project includes an integration of all the computational components of the metal additive manufacturing (AM) process into a coupled exascale modeling environment, where each simulation component itself is an exascale simulation. What has emerged is that exascale computing will enable AM process modeling at the fidelity of the microstructure. Here we discuss what this means, in particular, tight coupling of Process-Structure-Property calculations. Macroscopic continuum codes (ALE3D, Truchas and OpenFOAM) are used to simulate melt-refreeze, within which mesoscopic codes (Phase-field and Cellular Automata) are used to simulate the development of material microstructure. This microstructure is then used by polycrystal plasticity codes (ExaConstit) to calculate local material properties. The project is driven by a series of demonstration problems that are amenable to experimental observation and validation. We present our coupled exascale simulation environment for additive manufacturing and its initial application to AM builds.

*Work performed with Tim Germann, John Turner, the ExaAM Team, and under the auspices of the U.S. Department of Energy by LLNL, LANL and ORNL under contracts DE-AC52-07NA27344, DE-AC52-06NA25396, DE-AC05-00OR22725, and supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.
3:06PM D40.00002: Enabling First Principles Multiscale-Multiphysics Simulations of Complex Thermo-Fluid Systems Through Exascale Computing* JOSEPH OEFELEIN (Presenter), KYLE SCHAU, Georgia Inst of Tech, RAMANAN SANKARAN, Oak Ridge National Laboratory — Understanding and controlling turbulence, aerothermodynamics, and propulsion processes in advanced thermo-fluid systems presents many challenges. A multitude of strongly coupled fluid dynamic, thermodynamic, transport, chemical, and heat transfer processes are intrinsically coupled and must be considered simultaneously in complex domains. These multiscale physics are not currently understood or modeled with sufficient accuracy. Without their inclusion, timely Research and Development of advanced systems will be significantly deficient. Exascale computing offers significant opportunities to treat these physics with unprecedented accuracy and speed. However, the foundational hybrid-CPU+GPU architectures present many challenges to exploit their full potential power. This presentation will highlight the inherent challenges associated with porting complex multiphysics solvers to these architectures and the approach taken to achieve optimal performance using the RAPTOR code framework developed by Oefelein et al. as an example application.

*This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

3:18PM D40.00003: Generating a Comprehensive Map of Cancer Morphology in Whole Slide Tissue Specimens* JOEL SALTZ (Presenter), RAJ GUPTA, DIMITRIS SAMARAS, LE HOU, HAN LE, SHAHIRA ABOUSAMRA, REBECCA BATISTE, TIANHAO ZHAO, JINGWEI ZHANG, CHAO CHEN, TAHSIN KURC, State Univ of NY - Stony Brook — Advanced imaging technologies can capture extremely high-resolution images of tissue specimens, and quantitative analyses of cancer morphology using these images have shown value in a variety of correlative and prognostic studies. Our work on Summit will generate a comprehensive multi-scale mapping of cancer morphology with a dataset of more than 10,000 whole slide tissue images from over 20 cancer types. The work will use a collection of deep learning analysis pipelines we have developed to study, quantify and characterize tissue structure in diseased and normal tissue specimens. These analysis pipelines generate distributions of nuclei and cells and patch-level maps of lymphocyte distributions and segmentations of tumor regions. The analysis results will provide a first-ever representations of lymphocyte maps, nuclear characterizations and characterizations of tumor regions on a dataset of this scale. We expect that studies supported by these rich datasets will enable the development of biomarkers to predict clinical outcome and a better epidemiological understanding of cancer subtypes and how constituent cells contribute to cancer invasion and expansion.

*U24CA180924, U24CA215109, UG3CA225021
3:30PM D40.00004: Operator Dynamics in Quantum Circuits with Subsystem Symmetry  
JASON IACONIS (Presenter), Physics, University of Colorado, Boulder, SAGAR VIJAY, Physics, Harvard University, RAHUL NANDKISHORE, Physics, University of Colorado, Boulder — Our understanding of quantum dynamics in many-body quantum systems has been revolutionized in recent years by the study of random quantum circuits. These models provide a tractable setting in which we can understand ideas such as thermalization, operator spreading and quantum chaos. Furthermore, it is known that a richer variety of phenomena can occur when such models are enriched with a set of symmetries. We will focus on a particularly exotic set of symmetries which act on lower dimensional sub-manifolds of our system, a situation which is relevant to the study of highly quantum ‘fracton’ phases of matter. I will discuss approaches we may take to simulate such quantum dynamics numerically in higher dimensional systems. In particular, we will see that a restricted class of automaton circuit dynamics can be efficiently simulated while retaining the essential attributes of generic quantum chaotic systems. This technique will allow us to understand the properties of circuits with subsystem symmetry and may provide a valuable new tool for future studies of chaotic quantum dynamics.

3:42PM D40.00005: Radiation-matter interaction in graphene molecules: implementation on Geant 4 and computational simulations  
CARLOS VIDAL (Presenter), JOHN PRIAS, HERNANDO ARIZA, Doctoral Program in Physical Sciences, Interdisciplinary Institute of Sciences, University of Quindio — The voxelized computational approximation of the graphene molecules for different amounts of carbon atoms was simulated, using computational programs with optimized Geant 4 type geometry. The computational simulation of radiation transport through matter with characteristic interactions in the Uv-Vis spectral range, were made for radiation sources, detectors and graphene molecules. The optimization of the theoretical Uv-Vis spectra obtained from Geant 4, was achieved through algorithms development on Matlab. A method for computational reconstruction of UV-Vis spectra was proposed. The results suggest that is possible observe the contributions of the conjugated pi and sigma bonds, in the UV-Vis characteristic spectra as expected. Also, it was found that the variation in the size of the graphene molecules, influence the height of the band associated with the sigma bond, in agreement with experiments broadly studied. As well as, the proposed methodology suggests Geant 4 as a potential tool to simulate radiation-matter interactions in graphene-based molecules.
3:54PM D40.00006: ExaTN - A Scalable Exascale Math Library for Hierarchical Tensor Network Representations and Simulations in Quantum Many-Body Theory and Beyond*

DMITRY LIAKH (Presenter), EUGEN DUMITRESCU, GONZALO ALVAREZ, TIFFANY MINTZ, ALEXANDER MCCASKEY, Oak Ridge National Lab — Tensor network theory has recently paved the path to efficient numerical simulations of two- and three-dimensional many-body Hamiltonians describing strongly correlated quantum particles, but it still requires efficient software infrastructure that scales well on leadership heterogeneous HPC systems. To address this need, we develop ExaTN: A scalable math library for processing hierarchical tensor representations. Our library enables the use of advanced hierarchical tensor network states capable of expressing local expectation values in strongly entangled quantum systems efficiently. ExaTN allows building arbitrarily complex tensor networks for which it exposes a set of high-level API functions which automate tensor optimization procedures. A highly modular design of ExaTN allows seamless switching of computational backends for the computer system of choice, from a laptop to a leadership GPU-accelerated HPC platform, like Summit. The internal task-based parallel runtime then assures a load-balanced execution of tensor processing workloads.

*This research was funded by the Oak Ridge National Laboratory LDRD project 9463 and used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

4:06PM D40.00007: Porting ITensor to Julia*

MATTHEW FISHMAN (Presenter), KATHARINE HYATT, MILES STOUDENMIRE, Simons Foundation — In this talk, we present iTensors.jl, a ground-up rewrite of the C++ ITensor library in Julia. ITensor is a leading software package for simulating quantum many-body systems with tensor networks. Julia is a relatively young just-in-time (JIT) compiled language that is particularly well suited for scientific computing. We will discuss the advantages and disadvantages of moving from C++ to Julia, including ease of development and performance. We will also discuss new designs for the Julia version that are in development or planned, such as a rewrite of the sparse tensor library optimized with multithreading, new tensor contraction backends, automatic fermion sign support, GPU support, and automatic differentiation for the automated optimization of tensor networks.

*This work is supported by the Simons Foundation.
4:18PM D40.00008: Breaking the entanglement barrier: Tensor network simulation of quantum transport  
MICHAEL ZWOLAK (Presenter), National Institute of Standards and Technology, MAREK M RAMS, Jagiellonian University — The recognition that large classes of quantum many-body systems have limited - or efficiently representable - entanglement in the ground and low-lying excited states led to dramatic advances in their numerical simulation via so-called tensor networks. However, global dynamics elevates many particles into excited states, and can lead to macroscopic entanglement (seen both experimentally and theoretically) and the failure of tensor networks. Here, we show that for quantum transport - one of the most important cases of this failure - the fundamental issue is the canonical basis in which the scenario is cast: When particles flow through an interface, they scatter, generating a "bit" of entanglement between spatial regions with each event. The frequency basis naturally captures that - in the long time limit and in the absence of an inelastic event - particles tend to flow from a state with one frequency to a state of identical frequency. Recognizing this natural structure yields a striking - exponential in some cases - increase in simulation efficiency, greatly extending the attainable spatial and time scales. The concepts here broaden the scope of tensor network simulation into hitherto inaccessible classes of non-equilibrium many-body problems [see arXiv:1904.12793].

4:30PM D40.00009: Accelerate Science on Perlmutter with NERSC*  
CHARLENE YANG (Presenter), JACK RICHARD DESLIPPE, Lawrence Berkeley National Laboratory — Towards exascale computing, the National Energy Research Scientific Computing (NERSC) Center has procured a ~100 PetaFLOP/s supercomputer called Perlmutter. This talk will give an overview of its architectural details and discuss what Perlmutter can offer to the scientific community especially to Material Science and Chemistry. These offerings not only include cutting-edge hardware and technology but also highly optimized software stack and expert user support. The NERSC Exascale Science Application Program (NESAP) provides resources such as hackathons with performance engineers, early access to hardware, and NERSC-funded PostDocs to select application teams, and lessons learned from these teams are then disseminated to the general community. NERSC also collaborates with vendors and other High Performance Computing (HPC) developers on math libraries, performance models and tools, compiler development and performance portability. With an emphasis on Material Science and Chemistry, we will pinpoint the opportunities that Perlmutter and NERSC can bring for exascale and beyond.

*This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.
4:42PM D40.00010: Central Moment Lattice Boltzmann Method with Fokker-Planck Guided Collision for Non-Equilibrium Flows*  WILLIAM TAYLOR SCHUPBACH (Presenter), KANNAN PREMNATH, FARZANEH HAJABDOLLAHI, University of Colorado, Denver — Central moments-based lattice Boltzmann method (LBM), a recent approach for flow simulations, is generally based on the relaxation of various central moments to their equilibria under collision. The latter is usually constructed either directly from the Maxwell distribution function or by exploiting its factorization property. We propose a central moment LBM from a different perspective, where its collision operator is constructed by matching the changes in different discrete central moments under collision to the changes in the corresponding continuous central moments as given by the Fokker-Planck (FP) collision model of the Boltzmann equation. The resulting formulation can be interpreted in terms of the relaxation of the various central moments to “equilibria” that depend only on the adjacent, lower order post-collision moments. We designate such newly constructed chain of equilibria as the Markovian central moment attractors and the relaxation rates are based on scaling the drift coefficient of the FP model by the order of the participating moment. We will demonstrate the accuracy and robustness of our new formulation for simulations of a variety of flows using the standard D2Q9 and D3Q27 lattices and also present a comparison against other collision models.

*NSF CBET-1705630

4:54PM D40.00011: Nonlocal Coulomb interaction and spin freezing crossover: A route to valence-skipping charge order  SIHEON RYEE (Presenter), Department of Physics, KAIST, P. SÉMON, Brookhaven National Laboratory, MYUNG JOON HAN, Department of Physics, KAIST, SANGKOOK CHOI, Brookhaven National Laboratory — Multiorbital systems away from global half-filling host intriguing physical properties promoted by Hund’s coupling. Despite increasing awareness of this regime dubbed Hund’s metal, effect of nonlocal interaction is still elusive. Here we study a three-orbital model with 1/3 filling (two electrons per site) including the intersite Coulomb interaction $V$. Using the $GW$ plus extended dynamical mean-field theory, the valence-skipping charge order transition is shown to be driven by $V$. Most interestingly, the instability to this transition is significantly enhanced in the spin-freezing crossover regime, thereby lowering the critical $V$ to the formation of charge order. This behavior is found to be closely related to the population profile of the atomic multiplet states in the spin-freezing regime. In this regime, maximum spin states are dominant in each total charge subspace with substantial amount of one- and three-electron occupations, which leads to almost equal population of one- and the maximum spin three-electron state. Our finding unveils another feature of the Hund’s metal, and has potential implications to the broad range of multiorbital systems as well as the recently discovered charge order in iron-pnictides.
5:06PM D40.00012: Improved methods for demonstrating that AKLT systems are gapped*  
NICHOLAS POMATA (Presenter), TZU-CHIEH WEI, State Univ of NY - Stony Brook — We examine recent advancements in proving the gaps of AKLT systems [1,2], in particular those proposed by Abdul-Rahman et al. [1], which we have later extended so that it can be applied numerically in more general settings. We discuss how this has been used in proving the AKLT gap on a variety of "decorated" lattices in 2D, where the number $n$ of decorating spin-1 sites on each edge of the original lattice is two or larger [3]. Furthermore, we investigate whether the gappedness can be established for several decorated lattices with $n=1$. We will further explore how the method may be used to demonstrate the existence of the AKLT gap on several uniform lattices without decoration.


*This work was supported by the National Science Foundation under Grants No. PHY 1620252 and No. PHY 1915165.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D41 GMAG DMP DCOMP: Emergent magnetism in correlated electron systems I  
707 - Chetan Dhital, Kennesaw State Univ - Tag(s): Focus

2:30PM D41.00001: Z2xZ2 magnetic domains and magnetic moment disproportionation in the spin-orbit Mott insulator Sr2IrO4 [Invited]  
BUMJOON KIM (Presenter), SUNWOOK PARK, HOON KIM, Physics, Pohang University of Science and Technology, J.-W. KIM, Advanced Photon Source, ALASKA SUBEDI, Centre national de la recherche scientifique — Sr2IrO4 is representative of the new class of materials dubbed “spin-orbit Mott insulators” which hosts a variety of unconventional magnetism that arise from spin-orbit entangled moments, or pseudospins. A prominent example is the possible realization of a Kitaev spin liquid when pseudospins are arranged in a honeycomb lattice. In this talk, I will discuss on a new aspect of pseudospins; they show propensity to spontaneously disproportionate and lead to rich magnetic structures where symmetrically equivalent sites are decorated with magnetic moments of different magnitudes. We start by showing that the observed Z2xZ2 domain structure cannot be explained by the known magnetic structure and necessarily requires mixing of two order parameters that belong to two different irreducible representations of the high symmetry phase, which in response to the magnetic moment disproportionation distorts to a low symmetry phase. We argue that this phenomenon may be found more generally in other systems with spin-orbit entangled magnetic moments and hence should be considered when solving for the magnetic structure.
Exploring magnetic frustration in a square-lattice metallic system: spin fluctuations in 15% Fe-doped CaCo$_2$As$_2$*

BENJAMIN UELAND (Presenter), Ames Laboratory, Ames, IA 50011, USA; BING LI, AASHISH SAPKOTA, Ames Laboratory, Ames, IA 50011, USA; Iowa State University, Ames, IA 50011, USA; SANGEETHA NEDIADATH SATHYANADHAN, Ames Laboratory, Ames, IA 50011, USA, DAVID C JOHNSTON, ALAN IRA GOLDMAN, Ames Laboratory, Ames, IA 50011, USA; Iowa State University, Ames, IA 50011, USA, TOBY G. PERRING, ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 OQX, UK, ANDREAS KREYSSIG, ROBERT MCQUEENEY, Ames Laboratory, Ames, IA 50011, USA; Iowa State University, Ames, IA 50011, USA — Magnetic frustration can arise in a square lattice of magnetic moments from competition between nearest-neighbor ($J_1$) and next-nearest-neighbor ($J_2$) exchange, with $\eta = J_1/2J_2$ governing the magnetic ground state. Remarkably, our inelastic neutron scattering (INS) measurements have shown that CaCo$_{1.86}$As$_2$ is a unique example of a metallic square-lattice system with nearly perfect frustration ($|\eta| \approx 1$) despite possessing A-type antiferromagnetic (AF) order below a Néel temperature of $T_N = 52$ K. Our recent neutron diffraction data on Ca(Co$_{1-x}$Fe$_x$)$_2$As$_2$ show that the A-type AF order is suppressed past $x = 0.12$, and here we give results from INS experiments made at $T = 6$ K on single-crystal samples of $x = 0.15$. Instead of the walls of magnetic fluctuations found for $x = 0$, we rather find ferromagnetic-like fluctuations emerging from zone centers that, depending on the energy, is quickly suppressed with increasing momentum transfer. We discuss our results in terms of the changing degree of frustration with increasing $x$.

*This research was supported by the U.S. DOE, BES, Division of Materials Sciences and Engineering under Contract No. DE-AC02-07CH11358. We gratefully acknowledge the Science and Technology Facilities Council (STFC) for access to neutron beamtime at ISIS.
3:18PM D41.00003: Nonreciprocal directional dichroism effect in Ni$_3$TeO$_6$ in the toroidal geometry

KIMAN PARK (Presenter), Chemistry, University of Tennessee, Knoxville, HEUNG-SIK KIM, Physics, Kangwon National University, MICHAEL YOKOSUK, Chemistry, University of Tennessee, Knoxville, JUNJIE YANG, Physics, Central Michigan University, JAEWOOK KIM, Physics, Rutgers University, MATEUSZ GORYCA, SCOTT CROOKER, National High magnetic Field Laboratory, Los Alamos, KRISTJAN HAULE, SANG-WOOK CHEONG, DAVID VANDERBILT, Physics, Rutgers University, JANICE LYNN MUSFELDT, Chemistry, University of Tennessee, Knoxville — We bring together high magnetic field techniques, optical spectroscopy, and first principles electronic structure calculations to reveal high-energy, broadband nonreciprocal directional dichroism in Ni$_3$TeO$_6$. We focus on the toroidal geometry where polarization is perpendicular to the chiral spin arrangement, and light is propagating orthogonal to both. We employ circularly polarized as well as unpolarized light to fully explore the symmetry properties and eigenstates of the system as well as potential for photonics applications. Due to the spectral range of our work, we demonstrate nonreciprocal effects in the Ni$^{2+}$ $d$-to-$d$ on-site excitations as well as the phonon side bands that appear on the leading edge of these structures. In addition to being a peculiar and fundamental light-matter interaction in low-symmetric crystals, nonreciprocal directional dichroism can support one-way transparency, optical rectifiers, and high fidelity holograms – just to name a few.

*Acknowledgement to the National Science Foundation Designing materials to Revolutionize and Engineer our Future (DMREF) program for the support (DMR-1629079 and DMR-1629059)

3:30PM D41.00004: Magnetic structure in square cupola compound Ba(TiO)Cu$_4$(PO$_4$)$_4$: $^{31}$P NMR Study

RAIVO STERN (Presenter), IVO HEINMAA, RIHO RÄSTA, Chemical Physics, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, KENTA KIMURA, TSUYOSHI KIMURA, Advanced Materials Science, University of Tokyo, Kashiwa, Japan — The magnetic structure of the antiferromagnetic square cupola compound Ba(TiO)Cu$_4$(PO$_4$)$_4$ single crystal is studied with $^{31}$P nuclear magnetic resonance techniques. The magnetic hyperfine shift $K$ shows a clear splitting at the Neel temperature $T_N = 9.5$ K, where the resonance splits into 2 lines when the external field is oriented along c-axis and into 4 lines when the field is along a-axis. In paramagnetic region $K(T)$ follows temperature dependence of the magnetic susceptibility $\chi(T)$. From $K$ vs $\chi$ plot we determined hyperfine field values $H_a^{hf} = 765$ mT/$\mu_B$ and $H_c^{hf} = 740$ mT/$\mu_B$ for magnetic field oriented along a- and c-axis, respectively. From the rotation of the single crystal in external magnetic field we determined 8 different orientations of K-tensor in paramagnetic region. In antiferromagnetic state at $T = 6$ K we found that the local field at phosphorus is mainly due to dipolar field of coppers. Here the rotation of single crystal shows 8 different orientations of the local field $B_{int} = 38 \pm 2$ mT. Experimental orientation of $B_{int}$ corresponds to the calculation of dipolar fields at phosphorus assuming magnetic quadrupolar configuration of magnetic moments $\Gamma_3(1)$.

*European Regional Development Fund (TK134)
Estonian Research Council (PRG4, IUT23-7)
JSPS KAKENHI (JP16K05449, JP19H01847)
3:42PM D41.00005: The Origin of Ising Magnetism in Ca$_3$Co$_2$O$_6$ Unveiled by Orbital Imaging

BRETT LEEDAHL (Presenter), MARTIN SUNDERMANN, ANDREA AMORESE, Max Planck Institute for Chemical Physics of Solids, ANDREA SEVERING, University of Cologne, HLYNUR GRETRARSSON, Deutsches Elektronen-Synchrotron (DESY), LUNYONG ZHANG, ALEXANDER KOMAREK, Max Planck Institute for Chemical Physics of Solids, ANTOINE MAIGNAN, Laboratoire CRISMAT, MAURITS HAVERKORT, Heidelberg University, LIU TJENG, Max Planck Institute for Chemical Physics of Solids —

One-dimensional CoO$_6$ chains in Ca$_3$Co$_2$O$_6$ arranged in a triangular lattice give rise to an Ising-like magnetism with an intriguing quantum tunneling staircase structure in its magnetization. To resolve the underlying local electronic configuration of the Co ions we applied $s$-core-level non-resonant inelastic x-ray scattering ($s$-NIXS), a new technique that is capable of imaging the shape of the 3$d$ orbitals in real space. The orbital shapes that we found established unequivocally that both Co sites (octahedral and trigonal prismatic) are in a 3+ valence state (i.e. 3$d^6$); the trigonal Co site has a high-spin configuration while the octahedral Co site is low spin. Interestingly, we directly ‘see’ that it is the complex $d_2$ orbital that is stabilized by the prismatic trigonal coordination, which naturally explains the Ising magnetism in the system. Utilizing this ability to image electron orbitals, and thus directly relating the orbital occupation with the local crystal structure—without the need for theoretical modeling—is essential for modeling magnetic properties. This is especially true in situations where one would like to make use of the delicate balance of competing interactions to stabilize a particular orbital state for a desired or optimized physical property.

3:54PM D41.00006: Finite, disordered chains of local and correlated moments in transition metal oxides*

JACK SIMONSON (Presenter), CRISTIAN FRANCO, State Univ of NY - Farmingdale, ALLISON WUSTROW, Colorado State University, ALICIA BACCARELLA, JAYLYN C UMANA, FRANCISCO BURGOS, State Univ of NY - Farmingdale, LUCIA STEINKE, University of Florida, ERIC DOORYHEE, Brookhaven National Laboratory, MEIGAN ARONSON, Stewart Blusson Quantum Matter Institute, JAMES NEILSON, Colorado State University — The structures of Bi$_2$CrAl$_3$O$_9$ and Li$_2$Mn$_2$(MoO$_4$)$_3$ are similar in that they both contain quasi-linear chains of octahedrally-coordinated atomic positions that are partially occupied by 3$d$ transition metals and partially occupied by a non-magnetic species. In the absence of long range occupancy ordering, this configuration gives rise to finite chains of moments with statistically varying lengths. We report the results of in situ diffraction experiments probing the synthetic pathways that yield high quality single crystals of these compounds. Ex situ UV/Vis diffuse reflectance spectroscopy measurements establish the magnitude of the charge gap and the local configuration of the magnetic species. Scaling of the magnetization at $T < 10$ K provides a probe to differentiate between independently fluctuating local moments and collective excitations along the chains.

*This work was supported as part of GENESIS: A Next Generation Synthesis Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award Number DE-SC0019212.
**4:06PM D41.00007: Complex magnetism and magnetic compensation in metal tellurate (Mn,Ni)$_3$TeO$_6$**

CHOONGJAE WON (Presenter), Center for Complex Phase Materials, Max Planck POSTECH/Korea Research Initiative, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University — The two of metal tellurate, Ni$_3$TeO$_6$ and Mn$_3$TeO$_6$, have rhombohedral lattice (Ni = R$3$, Mn = R-3), and they shows antiferromagnetic ordering with spin-induced ferroelectricity. However, we grown (Mn,Ni)$_3$TeO$_6$ single crystal, and found monoclinic structure, such as Co$_3$TeO$_6$. From magnetic susceptibility, and specific heat measurements, we discover ferrimagnetic transition and magnetic compensation state. These results significantly different from both end-member Ni$_3$TeO$_6$ and Mn$_3$TeO$_6$ and require further investigations of its magnetic structure.

*This work was supported by the National Research Foundation of Korea(NRF) funded by the Ministry of Science and ICT(No. 2016K1A4A4A01922028)*

**4:18PM D41.00008: High-energy nonreciprocal directional dichroism in a chiral magnet**

MICHAEL YOKOSUK, University of Tennessee, Knoxville, HEUNG-SIK KIM, Physics, Kangwon National University, KENDALL HUGHEY, University of Tennessee, Knoxville, JAEWOOK KIM, Rutgers University, ANDREAS V. STIER, Los Alamos National Laboratory, KENNETH O’NEAL, University of Tennessee, Knoxville, JUNJIE YANG, Central Michigan University, SCOTT CROOKER, Los Alamos National Laboratory, KRISTJAN HAULE, SANG-WOOK CHEONG, DAVID VANDERBILT, Rutgers University, JANICE LYNN MUSFELDT (Presenter), University of Tennessee, Knoxville — Nonreciprocal directional dichroism is an unusual light-matter interaction that gives rise to diode-like behavior in low symmetry materials. The chiral varieties are particularly scarce due to the requirements for strong spin-orbit coupling, broken time reversal symmetry, and a chiral axis. We bring together magneto-optical spectroscopy and first principles calculations to reveal high energy, broad band nonreciprocal directional dichroism in Ni$_3$TeO$_6$ with special focus on behavior in the metamagnetic phase above 52 T. In addition to demonstrating this effect in the magnetochiral configuration, we explore the transverse magnetochiral orientation in which applied field and light propagation are orthogonal to the chiral axis and by so doing, uncover an additional configuration with a nonreciprocal response in the visible part of the spectrum. In a significant conceptual advance, we use first principles methods to analyze how the Ni$^{2+}$ d-to-d on-site excitations develop magnetoelectric character and present a microscopic model that unlocks the door to theory-driven discovery of chiral magnets with nonreciprocal properties.
4:30PM D41.00009: Probing Spin-Excitations above the Ground State of 1T-TaS$_2$  
ITAI SILBER  
(Presenter), Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, ITAMAR KIMCHI, Department of Physics, University of Colorado, DAVID E GRAF, National High Magnetic Field Laboratory, AMIT KANIGEL, Department of Physics, Technion-Israel Institute of Technology, YORAM DAGAN, Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University — Spin-spin interactions can lead to exotic ground states with emergent excitations in frustrated quantum magnets. Such a system is the transition metal dichalcogenide 1T-TaS$_2$. While the material is electrically insulating and exhibits no magnetic ordering down to milikelvin temperatures, the specific heat has a linear fermionic-type contribution that suggests a large band-width. We analyse the low temperature specific heat data and torque magnetometry measurements to isolate the contribution of the spin excitations to the magnetization from the large background response. The magnetic torque is strongly anisotropic and has a singular response at low magnetic fields which we attribute to a continuous disassociation of singlet pairs. This picture is also supported by the perfect collapse of the specific heat data at various temperatures and magnetic fields onto a universal curve predicted for singlets with a random distribution of antiferromagnetic coupling strengths. We interpret our data in the framework of a quantum spin liquid ground state having a large bandwidth with minority spins forming an array of singlet pairs with a continuum of coupling constants. Finally, despite the presumed large spinon Fermi surface we could not observe quantum oscillations of the magnetization.

4:42PM D41.00010: Competition of itinerant magnetic states in SrCo$_2$As$_2$ from RPA spin susceptibility*  
ANA-MARIJA NEDIC (Presenter), Iowa State University, MORTEN HOLM CHRISTENSEN, University of Minnesota, YONGBIN LEE, Iowa State University, RAFAEL FERNANDES, University of Minnesota, ROBERT McQUEENEY, LIQIN KE, PETER ORTH, Iowa State University — The square-lattice layered 122-type cobalt pnictides ACo$_2$Pn$_2$ (A=Ca, Sr, Eu; Pn=As, P) are metals with fascinating magnetic properties reminiscent of local moment frustration. Among those, SrCo$_2$As$_2$ and CaCo$_2$As$_2$ stand out due to the competing nature of their in-plane magnetic fluctuations. While CaCo$_2$As$_2$ exhibits A-type antiferromagnetic order with ferromagnetically ordered Co planes, inelastic neutron scattering has revealed signs of extreme frustration towards stripe-like antiferromagnetism. SrCo$_2$As$_2$ does not order down to T=0.05 K, but shows an intricate competition between ferro- and stripe-like magnetic fluctuations instead. While some of these observations can be rationalized with $J_1$-$J_2$-type local moment models, several experimental facts cannot be reconciled within such a local moment picture such an approximate description. Here, we perform a fully itinerant analysis of the magnetic properties of these materials based on a tight-binding model obtained from DFT calculations for the bandstructure. We report our findings on the static transverse spin susceptibility for the resulting multiorbital Hubbard model within the random-phase approximation RPA approximation.

*Work at Ames Laboratory was supported by DOE, BES DMSE under Contract No. DE-AC02-07CH11358.
4:54PM D41.00011: Quantum-to-classical correspondence in two-dimensional Heisenberg models*  TAO WANG (Presenter), XIANGSHENG CAI, Univ of Mass - Amherst, KUN CHEN, Rutgers University, NIKOLAI PROKOF’EV, BORIS SVISTUNOV, Univ of Mass - Amherst — The quantum-to-classical correspondence (QCC) in spin models is a puzzling phenomenon where the static susceptibility of a quantum system agrees with its classical-system counterpart, at a different corresponding temperature, within the systematic error at a sub-percent level. We employ the bold diagrammatic Monte Carlo method to explore the universality of QCC by considering three different two-dimensional spin-1/2 Heisenberg models. In particular, we reveal the existence of QCC in two-parametric models.

*This work was supported by the Simons Collaboration on the Many Electron Problem, the National Science Foundation under the grant DMR-1720465, and the MURI Program "New Quantum Phases of Matter" from AFOSR.

5:06PM D41.00012: Theoretical Prediction of Bulk Rashba Effect in Pyroelectric Antiferromagnet BiCoO₃*  KUNIHIKO YAMAUCHI (Presenter), ISIR-SANKEN, Osaka University, PAOLO BARONE, SILVIA PICOZZI, CNR-SPIN — Rashba effect, a type of spin-momentum locking phenomena, commonly occurs at interfaces or surfaces, while it is nowadays well established that Rashba-like band splitting may also occur in non-centrosymmetric (chiral, polar or ferroelectric) bulk materials. Here we are taking a step further by considering a noncentrosymmetric antiferromagnetic oxide as a playground for bulk Rashba effect. In ferroelectric and antiferromagnetic systems, i.e., multiferroic systems, spin-flipping symmetry operations may exist (such as a mirror symmetry operation) which behave as time-reversal symmetry, thus enforcing two-fold degeneracy at specific high-symmetric points and allowing bulk Rashba effect to emerge. As a prototypical example, ab-initio DFT calculations of antiferromagnetic BiCoO₃ in the polar structure reveal that a large Rashba-like spin splitting occurs at the conduction band bottom, having a large weight from Bi-p orbital states [1]. In this presentation, we also show that the spin texture of such a multiferroic can be modulated by applying a magnetic field.


*This work was supported by JSPS Kakenhi (No.17H02916 and 18H04227) and JST-CREST (No. JPMJCR18T1).
WAYNE ZHENG (Presenter), Ohio State Univ - Columbus — On some one dimensional (1D) and 2D non-bipartite lattices, we study both free and Hubbard interacting lattice fermions when there are some magnetic fluxes threaded or appropriate gauge fields coupled. On one hand, we focus on finding out the optimal flux which minimizes the energy of fermions at specific fillings. For spin-1/2 fermions at half-filling on a ring lattice with an odd number of sites, the optimal flux is determined to be ±π/2. We prove this conclusion for Hubbard interacting fermions by means of a generalized reflection positivity technique. It can further lead to some applications towards 2D non-bipartite lattices such as triangle and Kagome. At half-filling, the optimal flux pattern on the triangular lattice can be ascertained to be [π/2, π/2]. We find that chirality emerges in these optimal flux states. On the other hand, we verify these conclusions and further study other fillings away from half with the numerical exact diagonalization (ED) method and find that, when it deviates from half-filling, Hubbard interactions can even alter the optimal flux patterns on these lattices.

*This work is supported by the National Science Foundation under award number DMR-1653769.
Magneto-Ionic Control of Heterostructures and Interfaces* [Invited] KAI LIU (Presenter), Georgetown University — Magneto-ionic approaches for modifying ion distributions in metal/oxide heterostructures offer exciting potentials to control material properties. Our recent studies show that such magneto-ionic effect, even though initiated at metal/oxide interfaces, can extend deep into the rest of the oxide films and drastically tailor their physical properties [1-4].

In antiferromagnetic systems, we have previously demonstrated a controllable positive exchange bias in GdFe/NiCoO [1], and that the oxygen migration can be reversibly driven by an electric field [2]. Recently, we have observed a strong exchange bias in Gd/NiCoO due to the magneto-ionic effect, above the Gd $T_C$. After electric biasing, up to 35% enhancement of the exchange bias is observed, which can be reset by field-cooling.

In studies of cuprates, we show a simple, scalable approach to tune superconductivity [4]. A thin Gd layer (up to 20 nm) deposited onto epitaxial YBCO films (100nm), is found to leach oxygen from deep within the YBCO and suppress the superconductivity. These effects arise from the combined impact of redox-driven electron doping and modification of the YBCO microstructure.

In ferromagnets chemisorbed with submonolayer oxygen, we have observed strong DMI induced by chemisorption at room temperature. The sign of this DMI and its surprisingly large magnitude are derived by examining the oxygen coverage dependent evolution of domain wall chirality. The large induced DMI has enabled direct writing of magnetic skyrmions.

Our findings demonstrate an effective solid-state ionic approach to control a wide variety of magnetic functionalities, opening up possibilities for electric gating.


*Supported by the NSF (DMR-1610060, ECCS-1611424, DMR-1905468, ECCS-1933527) and the nCORE SMART center through SRC/NIST.
### 3:06PM D42.00002: Tuning Electrochemical Response in Ion-Gel-Gated $\text{La}_{1-x}\text{Sr}_x\text{CoO}_{3-\delta}$ Films via Sr-doping and strain*

**Presenter**: Vipul Chaturvedi, William M. Postiglione, Chemical Engineering and Material Science, University of Minnesota, Biqiong Yu, School of Physics and Astronomy, University of Minnesota, Wojciech Tabis, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland, Sajna Hameed, Nikolaos Biniskos, School of Physics and Astronomy, University of Minnesota, Hua Zhou, Zhan Zhang, Advanced Photon Source, Argonne National Laboratory, Martin Greven, School of Physics and Astronomy, University of Minnesota, Chris Leighton, Chemical Engineering and Material Science, University of Minnesota.

Electrolyte gating has proven powerful for controlling electronic, magnetic, and optical properties of materials such as oxides. Understanding the true gating mechanisms (i.e., electrostatic vs. electrochemical), however, particularly in oxides, where O vacancy formation and diffusion is often facile, remains challenging. Here, we present a study of the Sr-doping and strain dependence of the ion-gel gate response of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_{3-\delta}$ (LSCO) films ($0 < x < 0.7$), using transport, magnetometry, and operando synchrotron X-ray diffraction. Consistent with prior work, small negative gate biases induce reversible electrostatic hole accumulation, whereas positive biases induce oxygen vacancies ($V_O$) [1,2]. The window of reversibility and bias threshold for $V_O$ formation are found to systematically decrease with $x$, consistent with higher electrochemical activity of Co$^{4+}$ than Co$^{3+}$; tensile strain similarly promotes electrochemical response. At sufficiently high $x$, a topotactic transformation to a brownmillerite phase occurs. These findings are placed in the context of prior literature and discussed in terms of $x$-dependent variations in $V_O$ formation enthalpy and diffusivity.

*Work supported by NSF MRSEC.

### 3:18PM D42.00003: Insight into the Electronic Phase Separation in Perovskite Manganites: The Role of Charge-Orbital Ordering in the Interface Region*

**Presenter**: Zhe Wang, Department of Physics, Fudan University, China, Ruqian Wu, Department of Physics and Astronomy, University of California, Irvine.

The electronic phase separation in perovskite manganites, with coexistence of ferromagnetic (FM) metallic and antiferromagnetic (AFM) insulating phase, provides possibilities for tuning their electronic and transport properties. However, the mechanisms that drive the electronic phase separation are still unclear. Using density functional theory calculations, we investigated the charge-orbital ordering (COO) in both the AFM and FM/AFM interface regions of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ (LSMO). We found that the interface region prefers a distinct COO phase compared with the AFM region, which facilitates the formation of FM/AFM domain boundaries. We further studied the thickness dependent COO phase transition in LSMO ultrathin film, and predicted its critical thickness of phase separation. The results are in well agreement with experiments. These findings suggest that the COO phase transition in the FM/AFM interface region plays a key role in the electronic phase separation. The influence of substrate strain and Sr doping level on the phase separation were also studied.

*Work was supported by DOE-BES Grant No. DE-FG02-05ER46237. ZW was supported by National Basic Research Program of China Grant No. 2015CB921403.
Engineering Magnetic Interactions in Complex Oxide Heterostructures

ALEXANDER MICHAEL KANE, MINGZHEN FENG, NOLAN AHLM, BINZHI LI, J. PAIGE BYERS, University of California, Davis, RAJESH V CHOPDEKAR, PADRAIC SHAFER, ALPHA T. N’DIAYE, Advanced Light Source, Lawrence Berkeley National Laboratory, NIGEL D. BROWNING, Imaging Centre at Liverpool, University of Liverpool, VALERIA LAUTER, Neutron Sciences Directorate, Oak Ridge National Laboratory, APRUVA MEHTA, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, ELKE ARENHOLZ, Cornell High Energy Synchrotron Source, Cornell University, YAYOI TAKAMURA (Presenter), University of California, Davis — Complex oxides possess a wide range of technologically relevant functional properties including ferromagnetism, ferroelectricity, and superconductivity. Furthermore, their interfaces exhibit unexpected functional properties not found in the constituent materials due to structural and chemical changes as well as electronic and magnetic interactions. These unique interfacial effects lead to fundamental differences compared to analogous metallic systems. For example, ferromagnetic (FM)/FM interfaces consisting of magnetically hard La$_{0.7}$Sr$_{0.3}$CoO$_3$ (LSCO) and soft La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) display exchange-spring behavior where the hard layer pins the moments of the soft layer, however, the hard/soft magnetic interface does not coincide with the chemical interface. Rather, an interfacial LSCO layer forms that is characterized by magnetically active Co$^{2+}$ ions which couple to the soft LSMO layer. The full characterization of the structural and magnetic properties of the LSCO/LSMO bilayers involves synchrotron-radiation and neutron-scattering based techniques as well as high resolution transmission electron microscopy. We find that the proportion of the Co$^{2+}$ ion-rich LSCO layer and magnitude of exchange bias shift depends sensitively on parameters such as individual layer thicknesses, epitaxial strain state, $BO_6$ octahedral tilt pattern of the underlying substrate, and stacking order of the layers. These results demonstrate how the competing interactions in complex oxides enable intriguing opportunities to tailor functional properties for new, versatile, and energy efficient spintronic devices.

We are grateful to the support by NSF (DMR 1745450), UC MRPI (No. MR-15-328528), and the DOE SCGSR program. This research utilized DOE user facilities including ALS at LBNL, SSRL at SLAC, SNS at ORNL, and EMSL at PNNL.

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2 B. Li, et al., *APL*, 109, 152401 (2016); A.M. Kane, Y. et al., *PRM* 3, 014413 (2019); J.P. Byers et al., *JAP*, 125, 082518 (2019).
4:06PM D42.00005: High temperature magnetism and charge ordering in multiferroic
(LuFeO$_3$)$_m$/((LuFe$_2$O$_4$)$_1$ $(m = 3, 7, 9)$ SHIYU FAN (Presenter), Physics and Astronomy, University of
Tennessee, Knoxville, HENA DAS, Laboratory for Materials and Structures, Tokyo Institute of Technology, Midori-ku, 4259 Nagatesuta, Yokohama, Kanagawa 226-8503, Japan, KEVIN ARTHUR SMITH, Chemistry, University of Tennessee, Knoxville, Tennessee, 37996, USA, ALEJANDRO R'EBOLA, JULIA MUNDY, School of
Applied and Engineering Physics, Cornell University, Ithaca, New York 14853, USA, CHARLES BROOKS, Kavli Institute at Cornell for Nanoscale Science, Ithaca, New York 14853, USA, MEGAN HOLTZ, School of
Applied and Engineering Physics, Cornell University, Ithaca, New York 14853, USA, RAMAMOORTHY RAMESH, Department of Materials Science and Engineering, University of California, Berkeley, California 94720, USA, DAVID ANTHONY MULLER, School of Applied and Engineering Physics, Cornell University, Ithaca, New York 14853, USA, DARRELL SCHLOM, Kavli Institute at Cornell for Nanoscale Science, Ithaca, New York 14853, USA, CRAIG J FENNIE, School of Applied and Engineering Physics, Cornell University, Ithaca, New York 14853, USA, STEPHEN A MCGILL, National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA, JANICE LYNN MUSFELDT, Chemistry, University of Tennessee, Knoxville, Tennessee, 37996, USA — We combined optical spectroscopy, magnetic circular dichroism, and first principles
calculations to uncover the microscopic origin of the high temperature magnetism in multiferroic
superlattices (LuFeO$_3$)$_m$/((LuFe$_2$O$_4$)$_1$, as well as the charge ordered state in the
$m = 3$ case.
Analysis of the dichroic spectra at characteristic energies reveals optical hysteresis loops of
different Fe centers. Comparison between coercivity vs temperature curves indicates the bulk
magnetization emanates mostly from the LuFe$_2$O$_4$ layer. Spectroscopic signature of the interface
demonstrates that the larger Lu distortion only selectively increases the local magnetization of
the Fe$^{2+}$ and Fe$^{3+}$ sites in the spin-up channel, which strengthens the exchange interaction,
increases the total magnetization in the LuFe$_2$O$_4$ layer and enhances $T_C$. Comparison between
the calculated and measured dichroic spectra affirms a non-polar charge ordered state in the $(3, 1)$ case. These findings provide a site specific technique to analyze the complex interactions in the
materials with multiple magnetic centers, and also broaden the possibilities in the hunt for novel
multiferroics with high $T_C$ and large magneto-electric coupling constant.

4:18PM D42.00006: Tunable Perpendicular Magnetic Anisotropy in Multiferroic Oxides
XUEZENG LU (Presenter), JAMES RONDINELLI, Department of Materials Science and Engineering,
Northwestern University — Here we present design rules to realize electric-field control of
perpendicular magnetic anisotropy (PMA) utilizing hybrid improper ferroelectricity by scaffolding
simple perovskite oxides into ultrashort period superlattices, (ABO$_3$)$_1$/((A'BO$_3$)$_1$, and in
multiferroic AA'BB'O$_6$ double perovskites. The study validates the strategy using first-principles
calculations and a single-ion-anisotropy model. We show a change of the magnetic anisotropy from the
in-plane to out-of-plane direction occurs in (BiFeO$_3$)$_1$/((LaFeO$_3$)$_1$ and a 50% decrease of
the magnetization along the out-of-plane direction occurs in LaYNiMnO$_6$ when a polar-to-
nonpolar phase transition is activated with strain. The origin of the PMA control is due to the
structural-tunable competitions among the $t_{2g}$ and $e_g$ orbital interactions on the magnetic ions
arising from relativistic spin-orbital interactions that are susceptible to changes in the oxygen
eohedral tilts with the transition. Our results allow us to search rapidly for other promising
multiferroics materials with voltage-controlled magnetic anisotropy for applications in low-energy
information storage and logic devices.
4:30PM D42.00007: Prediction of a Giant Magnetoelectric Cross-Caloric Effect Around a Tetracritical Point in Multiferroic SrMnO$_3$  ALEXANDER EDSTRÖM, CLAUDE EDERER (Presenter), Materials Theory, ETH Zurich — We study the magnetoelectric and electrocaloric response of strain-engineered, multiferroic SrMnO$_3$, using a phenomenological Landau theory with all parameters obtained from first-principles-based calculations. This allows to make realistic semi-quantitative and materials-specific predictions about the magnitude of the corresponding effects. We find that in the vicinity of a tetracritical point, where magnetic and ferroelectric phase boundaries intersect, an electric field has a huge effect on the antiferromagnetic order, corresponding to a magnetoelectric response several orders of magnitude larger than in conventional linear magnetoelectrics. Furthermore, the strong magnetoelectric coupling leads to a magnetic, cross-caloric contribution to the electrocaloric effect, which increases the overall caloric response by about 60%. This opens up new potential applications of antiferromagnetic multiferroics in the context of environmentally friendly solid state cooling technologies.

4:42PM D42.00008: Effects of Three-Dimensional Strain on LaCoO$_3$ Thin Films*  RONALDO RODRIGUEZ (Presenter), TOYANATH JOSHI, DAVID P BELANGER, DAVID LEDERMAN, Department of Physics, University of California, Santa Cruz — LaCoO$_3$ films grown on SrTiO$_3$ substrates are known to exhibit a net moment below T = 85 K while the same films grown on LaAlO$_3$ exhibit little to no moment [1]. The underlying mechanisms behind this net moment are poorly understood, but it is speculated that modulation of the Co-O-Co bond angle through epitaxial strain may play a key role. By growing LaCoO$_3$ films on SrTiO$_3$ substrates with a high angle (~ 7-9°) of miscut via pulsed laser deposition (PLD), we have been able to induce epitaxial strain along the in plane and out of plane film axes. In-situ reflection high energy electron diffraction (RHEED) detected layer-by-layer growth. Sample crystallinity and topography were measured using X-ray diffraction and atomic force microscopy, respectively. Magnetometry data were collected both parallel and perpendicular to the SrTiO$_3$ [100] surface, as well as parallel and perpendicular to 5 nm steps induced by the miscut of the substrate. In films of thickness ~3-10 nm grown on high angle miscut SrTiO$_3$ substrates, we measure a strong anisotropic magnetization in the plane where spins are realigned at low magnetic fields. Possible mechanisms will be discussed.


*This work was partially funded by the NSF REU program, grant #1659744.
Emergent antiferromagnetism in diamagnetically substituted pseudospin-1/2 iridate thin film  

JUNYI YANG (Presenter), LIN HAO, University of Tennessee, Knoxville, QI CUI, JIAQI LIN, Chinese Academy of Sciences, LUKAS HORAK, Charles University, JENIA KARAPETROVA, JONG WOO KIM, P. J. RYAN, Argonne National Lab, MARK DEAN, Brookhaven National Laboratory, JINGUANG CHENG, Chinese Academy of Sciences, JIAN LIU, University of Tennessee, Knoxville — Recent developments in 5d transition metal oxides have made it a fertile playground to explore exotic emergent phenomena due to the interplay among charge, orbital, spin degrees of freedom. A prominent example is the quasi-2D layered iridate systems where the electronic and antiferromagnetic states of the pseudospin-1/2 electrons are highly susceptible to changes in the structural degrees of freedom. In contrast, the 3D perovskite iridate SrIrO3 is a nonmagnetic semimetal, which is believed to be topologically protected. Recent study showed magnetic order emerges through chemical substitution with nonmagnetic ions, offering an intriguing planform to explore the cooperation between electronic correlation and strong spin orbit coupling beyond the 2D regime. However, bulk perovskite SrIrO3 only exists in polycrystalline form; thus, we have used epitaxial strain to stabilize nonmagnetic ion substituted SrIrO3 in single crystal quality thin film form. Combined with physical properties measurements and synchrotron-based x-ray diffraction and resonant x-ray magnetic scattering, we can resolve its G-type antiferromagnetic structure and further elucidate the structural modulation of its magnetic properties.

Weyl semimetal thin film Eu$_{1-x}$Sm$_x$TiO$_3$ on LSAT (001): field-polarized long-range order and interfacial ferromagnetism  

ZACH PORTER (Presenter), University of California, Santa Barbara, RYAN NEED, NIST Center for Neutron Research, KAVEH AHADI, University of California, Santa Barbara, YANG ZHAO, ZHIJUN XU, BRIAN JAMES KIRBY, JEFFREY LYNN, NIST Center for Neutron Research, SUSANNE STEMMER, STEPHEN WILSON, University of California, Santa Barbara — EuTiO$_3$ thin films have recently been reported to manifest complex magnetotransport phenomena upon carrier substitution, ranging from symmetry breaking anisotropic magnetoresistance to nonmonotonic anomalous Hall transport. Here we investigate the interplay between magnetism and transport behavior by studying the evolution of magnetic order in thin film samples of biaxially strained and electron-doped EuTiO$_3$ under an applied field. Neutron diffraction reveals that G-type antiferromagnetism is suppressed with the onset of in-plane field-polarized ferromagnetism for insulating, semimetallic, and metallic samples. However, polarized neutron reflectometry further reveals the onset of interfacial ferromagnetism at low fields far below the fully polarized state. The relationship between magnetic order and electron transport behavior associated with the Weyl semimetal phase in these films will be discussed.
Manipulating the magnetic ground state in complex oxides represents a main stream of research in condensed matter physics and materials science due to their fundamental importance. Here we report the emergence of an itinerant ferromagnetic state from a paramagnetic metallic CaRuO$_3$ through electrically induced protonation during ionic liquid gating. More importantly, this magnetic transition is accompanied with a structural expansion due to proton intercalation, and both which could be reversibly switched by external voltage. Despite the fact that the ruthenates remains metallic across the magnetic transition, we reveal that the ferromagnetic state is strongly correlated with a non-Fermi liquid toward Fermi liquid transition. The versatile magnetic state in protonated CaRuO$_3$ therefore strongly suggests that the electrically controllable protonation could sever as a novel pathway to manipulate the electronic and magnetic properties in complex oxides.

**Monday, March 2, 2020 2:30 PM - 5:18 PM**

**Session D43 DCOMP DMP: Electrons, Phonons, Electron Phonon Scattering, and Phononics I**

2:30PM D43.00001: **Gauge invariance of heat and charge transport coefficients** [Invited]  
STEFANO BARONI (Presenter), SISSA - Scuola Internazionale Superiore di Studi Avanzati, Trieste — Transport coefficients in extended systems have been recently demonstrated to be largely independent of the microscopic representation of the current density of the conserved quantity being transported (charge/mass/energy) [1]. This remarkable *gauge invariance* of transport coefficients has been leveraged to lay down a rigorous density-functional theory of heat transport [1], as well as a general approach to it, valid in the low-temperature regime, that nicely bridges the Boltzmann-Peierls kinetic model, that applies to crystals, and the Allen-Feldman one, that applies to glasses [2]. In the case of charge transport, a combination of gauge invariance and Thouless' quantisation of particle transport [3] allows one to express the electrical conductivity of an insulating fluid in terms of integer-valued, scalar, and time-independent atomic oxidation numbers, instead of real-valued, tensor and time-dependent Born charges [3]. In this talk I will review these concepts and report on some key applications of them to liquids and glasses.


*This work has been partially funded by the EU through the Max Center of Excellence for Supercomputing Applications (grants # 676598 and 824143).*
3:06PM D43.00002: Microscopic derivation of coarse-grained, energy-conserving generalized Langevin dynamics  SERGEI IZVEKOV (Presenter), Weapons and Materials Research Directorate, U.S. Army CCDC Army Research Laboratory — Properly simulating non-equilibrium phenomena such as thermal transport in condensed matter systems requires the conservation of system's internal energy. This precludes application of the coarse-grained (CG) generalized Langevin equation (GLE) dynamics. Attempts to address this issue have been pursued phenomenologically for dissipative particle dynamics (DPD, a Markovian variant of the CG GLE dynamics) by introducing an energy conserving extension of DPD (DPD-E). We present here a rigorous microscopic derivation of energy conserving variants of the CG GLE dynamics by extending the CG equations of motion to include the GLE for certain internal energy observables of the microscopic system. The derivation is performed using the Mori-Zwanzig projection operator method with the recently introduced interpretation of the Zwanzig projection operator.¹ Our extension of the GLE dynamics to quasi-equilibrium conditions (necessary to observe heat transport), are based on the generalized canonical ensemble approach and transport equation method. We derive closed microscopic expressions for conductive heat transfer coefficients. After employing the Markov approximation, we compare the equations of motion to the published DPD-E equations.

3:18PM D43.00003: Cavity Control of Nonlinear Phononics*  DOMINIK JURASCHEK (Presenter), TOMAS NEUMAN, JOHANNES FLICK, PRINEHA NARANG, Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University — Nonlinear interactions between phonon modes govern the behavior of vibrationally excited solids and molecules. We demonstrate here theoretically that optical cavities can be used to control the redistribution of energy from a highly-excited coherent infrared-active phonon state into the other vibrational degrees of freedom of the system. The hybridization of the infrared-active phonon mode and the fundamental mode of the cavity induces a polaritonic splitting that we use to tune the nonlinear interactions with other vibrational modes in and out of resonance. We show that not only can the efficiency of the redistribution of energy be enhanced or decreased, but also the underlying scattering mechanisms may be changed.

*D.M.J. acknowledges funding from the Swiss National Science Foundation under project ID 184259.
3:30PM D43.00004: A hydrodynamic description of the vibrational modes of ordered and disordered systems.* MATTEO BAGGIOLI (Presenter), Univ Autonoma de Madrid, ALESSIO ZACCONE, University of Milano — In ordinary crystals, Debye theory represents a very successful framework to characterize the dynamics of the vibrational excitations – the phonons, and to predict macroscopic quantities such as specific heat. Disordered systems and in general systems with dissipation provide a challenge to this description, which is manifested in several anomalous properties, e.g. the Boson Peak (BP) excess in the VDOS and the linear in temperature specific heat. Given the universality of these anomalies and their recent observation also in ordered single crystals with no disorder, a more general derivation (not necessarily relying on the presence of disorder) is needed. In this talk we provide such description using a hydrodynamic-effective field theory approach. We prove that a universal BP emerges naturally from the competition between propagation-elasticity and dissipation/diffusive damping. We also show a dependence of the BP in function of the material density which is in perfect agreement with the experimental data. Additionally, we show that the existence of hydrodynamic quasi-localized diffusive mode – the diffusons – can explain the linear in T specific heat in glasses and be therefore an alternative to the well-known TTLS theory.

*Mineco Severo Ochoa Fellowship, SEV-2012-0249

3:42PM D43.00005: Angular momentum radiation from current-carrying molecular junctions* ZUQUAN ZHANG (Presenter), Department of Physics, National University of Singapore, JING-TAO LÜ, School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, JIAN-SHENG WANG, Department of Physics, National University of Singapore — We study the radiation of angular momentum (AM) from current-carrying molecular junctions using the nonequilibrium Green's function method. The dependence of the the radiation on the molecular geometry is taken into account with a real-space tight-binding model coupled to the electromagnetic field. We study the relation between rotational symmetry of the molecule and the light radiation. We analyze the resonant effects when the applied bias crosses over the energy levels of the molecule. Our study maybe useful for generating radiation with AM from molecular junctions by simply applying an electrical bias.

*MOE tier 2, R-144-000-411-112
Ultrafast dynamics of hot carriers in bulk semiconductors and in accumulation layer: energy relaxation and screening effects.

JELENA SJAKSTE (Presenter), Laboratoire des Solides Irradiés, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris — The rapid development of the computational methods based on density functional theory, on the one hand, and of the time- energy- and momentum- resolved spectroscopy, on the other hand, allows today an unprecedentedly detailed insight into the processes governing hot electron relaxation dynamics, and into the role of the electron-phonon coupling. Recently, we have demonstrated, for the relaxation of hot carriers in GaAs, the existence of two distinct relaxation regimes, one related with the momentum, and the other with energy relaxation. In this work, we will present our new results, both experimental and theoretical, on hot electron relaxation in silicon. Numerous additional experiments were performed with respect to previous work, and a new interpretation of the measured relaxation times is provided [1]. Moreover, we will present our recent results on the hot electron relaxation in InSe. InSe is a quasi-2D material which was shown recently to have potential interest for optoelectronics [2]. In this work, we will discuss our new results on the relaxation and cooling dynamics in doped InSe.


Finite temperature full multiple scattering calculation of ultrafast x-ray absorption spectroscopy

TUN SHENG TAN (Presenter), JOHN REHR, JOSHUA KAS, University of Washington — Recent advances in ultrafast time-resolved (TR) x-ray absorption spectroscopy (XAS) have allowed us to probe the interaction between electronic temperature (T\text{e}) and lattice temperature (T\text{i}) on the femtosecond time-scale. We present a finite temperature multiple scattering Green's function calculations of XAS, which accounts for the finite T\text{e} of the system, to describe these extreme conditions. The effect of temperature on lattice can be included at different levels of approximation such as using correlated Debye (CD) model or dynamical matrix. We apply the method to TR-XANES of an Fe-MgO layered heterostructure [1] and a copper system [2]. We are able to qualitatively reproduce the experimental results with FEFF using CD model. We also obtain estimates of T\text{e} based on a shift in the edge and T\text{i} based on the size of the Debye-Waller factor.


*This work is supported by the Department of Energy Basic Energy Sciences program under Grant No. DE-FG02-97ER45623.
Variational Treatment Beyond the Mean-Field Approximation for the Half-Filled SSH model

STEPAN FOMICHEV (Presenter), MONA BERCIU, Stewart Blusson Quantum Matter Institute, University of British Columbia — The Su-Schrieffer-Heeger (SSH) model is a common approach to quantifying the effect of electron-phonon coupling on many-body behavior. Developed initially for polyacetylene chains, it assumes that the leading order effect of lattice motion is the modulation of the electronic tight-binding hopping amplitudes. While the SSH model successfully predicts Peierls distortion, the lattice is often treated semiclassically, as there is no known analytical solution for quantum phonons. Motivated by the successes of the momentum average approximation applied to a single Holstein polaron, and extensions to boson-modulated hopping and multiple phonon branches, we generalize the technique to a half-filled (one carrier per unit cell) one-dimensional SSH model. We begin by studying the SSH model in the Born-Oppenheimer approximation, and find that an expansion of the hopping amplitudes to second order in the atomic positions is needed for internal consistency. Using the Peierls distortion ansatz, we find that the acoustic and optical phonon branches emerge even at this mean-field level. We then systematically expand the variational space around this improved mean-field solution to study the nature of the ground state in the non-adiabatic limit.

Nanoscale Friction Control in Transition Metal Dichalcogenides

ANTONIO CAMMARATA (Presenter), TOMAS POLCAR, Department of Control Engineering, Czech Technical University in Prague — One of the main difficulties in understanding and predicting frictional response is the intrinsic complexity of highly non-equilibrium processes in any tribological contact.

To understand the physical nature of the microscopic mechanism of friction and design new tribologic materials, we conducted a systematic quantum mechanic investigation on prototipical Van der Waals MX₂ (M=Mo, W; X=S, Se, Te) Transition Metal Dichalcogenides. We combined structural and dynamic information from group theory and phonon calculations with electronic features using non-standard methods such us orbital polarization, bond covalency and cophonicity analyses. We propose a phonon-mode based method to identify possible sliding paths, to tune the corresponding sliding energy barriers and to characterize and control frictional/dissipation energy channels. We discuss how to extract information on the energetics of sliding from atomic force microscopy signals. We finally formulate guidelines on how to engineer intrinsic friction at the nanoscale in order to design novel materials with expected improved tribological properties.

The present outcomes can be promptly used to finely tune physical properties for the design of new materials with diverse applications beyond tribology.
4:42PM D43.00010: Electrical tuning of vibrational modes in transition metal dichalcogenides*

FLORIAN BELVISO (Presenter), Control engineering, Czech Technical University in Prague, TOMAS POLCAR, Engineering Materials, University of Southampton, ANTONIO CAMMARATA, Control engineering, Czech Technical University in Prague — Understanding frictional phenomena at nanoscale in layered materials is an important stage in order to control layer sliding, occurring in nanoelectromechanical devices.

To this aim, we studied the atomic scale tribological properties of transition metal dichalcogenides (TMDs) by using ab initio techniques.

We considered 6 prototypical MX$_2$ TMDs (M=Mo, W; X=S, Se, Te) with hexagonal P6$_3$/mmc symmetry, focusing on how some specific phonon modes contribute to the intrinsic friction. We described the exchange-correlation interaction energy within the DFT framework, including long range dispersion interactions in the Grimme formulation.

We identified and disentangled the electro-structural features that determine the intra- and inter-layer motions affecting the intrinsic friction by means of electro-structural descriptors such as orbital polarization, bond covalency and cophonicity.

We show how the phonon modes affecting the intrinsic friction can be adjusted by means of an external electrostatic field, the latter then acting as a knob to control intrinsic friction in layered materials.

The presented outcomes are a step forward in the development of TMD-based nanoelectromechanical systems.

*Funding from the European Union’s Horizon2020 research and innovation programme No. 721642: SOLUTION.
**4:54PM D43.00011: Effect of the presence of small molecule of contaminants on nanofriction in layered MX\textsubscript{2} Transition Metal Dichalcogenides: An ab initio investigation**

JAMIL MISSAOUI (Presenter), Control Engineering, FEL, Czech Technical University in Prague, Czech Republic, TOMAS POLCAR, Engineering Materials & nCATS, FEE, University of Southampton, United Kingdom, ANTONIO CAMMARATA, Control Engineering, FEL, Czech Technical University in Prague, Czech Republic — The control of friction at the nanoscale plays a central role in nanoengineered devices such as nano-electromechanical systems, the latter more and more based on multi-layered Transition Metal Dichalcogenides (TMDs). In the present work, we study the intrinsic friction in MX\textsubscript{2} (M = transition metal, X = chalcogen anion) TMDs in the presence of small molecules of contaminants from the atmosphere.

We perform quantum mechanic calculations on layered MX\textsubscript{2} TMDs-based systems with the hexagonal structure in the presence of contaminants between adjacent layers. We combine outcomes from phonon calculations together with the characterization of the electronic features using non-standard methods like orbital polarization, bond covalency and cophonicity, in order to study how the vibrational frequencies of pristine material are affected by the presence of contaminants. We show how changes in the phonon frequency are related to the nanoscale friction between adjacent layers. We finally present guidelines on how to engineer intrinsic friction in TMDs at the nanoscale.

*This work has been done with the support of the Czech Science Foundation Grant No. 17-24164Y

The study was supported by the project Novel nanostructures for engineering applications No. CZ.02.1.01/0.0/0.0/16_026/0008396.

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**5:06PM D43.00012: The Order of Longitudinal and Transverse Optical Phonon Modes in Monoclinic Oxides**

RAFAL KORLACKI (Presenter), MATHIAS SCHUBERT, University of Nebraska - Lincoln, ALYSSA MOCK, Naval Research Laboratory, SEAN KNIGHT, University of Nebraska - Lincoln, VANYA DARAKCHIEVA, Linköping University — In monoclinic crystals, as required by symmetry, the infrared-active phonon modes have their transition dipoles oriented parallel (A\textsubscript{u} modes) and perpendicular (B\textsubscript{u} modes) to the symmetry axis. In the absence of additional symmetry constrains, the B\textsubscript{u} modes are distributed within the monoclinic plane, the pairs of the transverse optical (TO) and longitudinal optical (LO) modes (TO-LO pairs) do not need to be parallel to each other, and this leads to the apparent violation of the TO-LO rule. The analysis of the limiting frequencies within the Born-Huang approach reveals that TO-LO pairs either belong to inner or outer phonon modes. Inner modes are nested within the outer modes. The directional limiting frequencies are bound to within outer mode frequency regions not occupied by inner mode pairs. Hence, an unusual phonon mode order can occur where both lower-frequency as well as upper-frequency limits for the directional modes can be both transverse and/or longitudinal modes. This behavior will be demonstrated in the results of first principles calculations of phonon modes for three different monoclinic crystals: β-Ga\textsubscript{2}O\textsubscript{3} (space group 12), CdWO\textsubscript{4} (space group 13), and Y\textsubscript{2}SiO\textsubscript{5} (space group 15), and compared with experimental results based on infrared spectroscopic ellipsometry.
2:30PM D44.00001: Relaxation Effects in the Electronic Structure of Twisted Bilayer Graphene: a Multi-Scale Approach*  NICOLAS LECONTE, SRIVANI JAVAJI (Presenter), JIAQI AN, JEIL JUNG, Physics, University of Seoul — We introduce a multi-scale approach to obtain accurate atomic and electronic structures for atomically relaxed twisted bilayer graphene. High-level exact exchange and random phase approximation (EXX+RPA) correlation data provides the foundation to parametrize systematically improved force fields for molecular dynamics simulations that allow relaxing twisted layered graphene systems containing millions of atoms making possible a fine sweeping of twist angles. These relaxed atomic positions are used as input for tight-binding band-structure calculations where the distance & angle-dependent interlayer hopping terms are extracted from ab-initio calculations & subsequent representation with Wannier orbitals. We benchmark our results against published force fields and widely used tight-binding models and discuss their impact in the spectrum around the flat band energies. We find that our relaxation scheme yields a magic angle of twisted bilayer graphene consistent with experiments between $1.0^\circ \sim 1.1^\circ$ using Fermi velocities $v_F=1.0 \sim 1.1 \times 10^6$ m/s. We present high-resolution spectral function calculations to compare with experimental ARPES.

*Acknowledges the grant NRF-2018R1C1B6004437 (for N.L), KRF-2016H1D3A1023826 (for N.L), NRF-2016R1A2B4010105 (for J.A) & SSTF-BAA1802-06 (for S. J. & J. J).


*NSF DMR-1830874 (C.A.), DOE DE-SC0007117 (I.V.B.)
2:54PM D44.00003: Real-Space Calculations of Dielectric Screening in Large Silicon Nanocrystals*  TIMOTHY LIAO (Presenter), KAI-HSIN LIOU, JAMES CHELIKOWSKY, University of Texas at Austin — The nature of dielectric screening in semiconductor nanocrystals (NCs) is an outstanding topic. We examine the screening of a point charge in hydrogen-terminated Si NCs. We consider NCs containing up to 5,400 atoms using pseudopotential-density-functional theory. We solve the Kohn-Sham equation in real-space using the PARSEC code. We compute the dielectric properties of a Si NC by replacing a Si nucleus at the center of the NC with a P nucleus while maintaining the electron number. We consider NCs of sufficient size to converge the dielectric properties to the bulk limit. We find the resulting screening functions are consistent with previous studies on smaller NCs. The ability to calculate dielectric properties of a large confined system allows us to consider charged defects in bulk Si in a straightforward manner without invoking a compensating background.

*Our work is supported by a subaward from the Center for Computational Study of Excited-State Phenomena in Energy Materials at LBNL, which is funded by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231, as part of the Computational Materials Sciences Program.

3:06PM D44.00004: Superconductivity in heavily boron-doped carbon materials*  YUKI SAKAI (Presenter), Oden Institute for Computational Engineering and Sciences, University of Texas at Austin, JAMES CHELIKOWSKY, Department of Physics, University of Texas at Austin, MARVIN L COHEN, Department of Physics, University of California at Berkeley — We investigate the superconducting properties of heavily boron-doped carbon materials composed of $sp^3$ hybridized atoms: cubic diamond, hexagonal diamond, and body centered tetragonal $C_4$ (bct $C_4$). We find that a high density of states (DOS) at the Fermi energy result in a high superconducting transition temperature ($T_c$) in all three materials. The high DOS is particularly realized when boron dopants are not placed at nearest neighbor sites. A $T_c$ above 60 K can be obtained for cubic diamond, although other allotropes can exhibit a $T_c$ of 40-50 K at 25 % boron-doping. We also discuss superconductivity in amorphous carbon.

*YS and JRC acknowledge DOE Grant No. DE-FG02-06ER46286. Computational resources are provided in part by NERSC and TACC. MLC acknowledges NSF Grant No. DMR-1508412 and Theory of Materials, LBNL, DoE Contract No. DE-AC02-05CH11231.
Discriminating functional groups, atomic species and molecular geometries in organic molecules using real-space simulations of non-contact atomic force microscopy*  

DINGXIN FAN (Presenter), YUKI SAKAI, JAMES CHELIKOWSKY, University of Texas at Austin — Noncontact atomic force microscopy (nc-AFM) with a CO functionalized probe tip is a powerful tool for molecular structure characterizations. In many organic molecules, the visualization of individual atoms is a real possibility, save for the complexity of interpreting the nc-AFM images. In order to gain a better understanding of such experimental images, we employ a real-space pseudopotential constructed within density functional theory code, PARSEC, to simulate nc-AFM images. We are able to discriminate functional groups (such as -C≡C-, -CH\textsubscript{2} and -C=O groups) and heteroatoms (such as O, N and S atoms) in organic molecules by mapping our simulated images to experimental images. Also, we find that nc-AFM is capable of directly visualizing the orientation of organic molecules at various adsorption sites on metal substrates. This can be very useful for characterizing large long-chain organic molecules in heavy oils and asphaltenes.

*This work is supported by the Welch Foundation under grant F-1837 and the U.S. Department of Energy under DOE/DE-FG02-06ER46286. Computational resources were provided by the National Energy Research Scientific Computing (NERSC) and the Texas Advanced Computing Center (TACC).

Time-dependent magnons from first principles  

NICOLAS TANCOGNE-DEJEAN, FLORIAN G EICH (Presenter), ANGEL RUBIO, Max Planck Inst Structure & Dynamics of Matter — We propose an efficient and not perturbative scheme to compute magnetic excitations for extended systems employing the framework of time-dependent density-functional theory. Within our approach we drive the system out of equilibrium using an ultra-short magnetic kick perpendicular to ground-state magnetization of the material. The dynamical properties of the system are obtained by propagating the time-dependent Kohn-Sham equations in real time and the analysis of the time-dependent magnetization reveals the transverse magnetic excitation spectrum of the magnet. We illustrate the performance of the method by computing the magnetization dynamics, obtained from a real-time propagation, for iron, cobalt and nickel and compare them to known results obtained using the linear-response formulation of time-dependent density-functional theory. Moreover, we point out that our time-dependent approach is not limited to the linear-response regime, and we present first results for non-linear magnetic excitations from first-principles in iron.
3:42PM D44.00007: A real-space pseudopotential method for magnetocrystalline anisotropy energies and the search for magnets without rare-earth metals*  

MASAHIRO SAKURAI (Presenter), JAMES CHELIKOWSKY, University of Texas at Austin — We present a real-space pseudopotential formalism for calculating magnetocrystalline anisotropy energies within relativistic density-functional theory (DFT). Our method is implemented in our real-space pseudopotential DFT code, PARSEC, which is designed to run efficiently on massively parallel computing platforms [1]. We show that our formalism works well for prototypical transition-metal compounds, such as YCo5 and Mn2Ga, yielding an accurate magnetization and a magnetocrystalline anisotropy constant consistent with other density-functional methods. We illustrate how our methods can be applied to the search for permanent magnets without rare-earth metals [2,3,4]. In particular, we identified several ZrCo5 and Fe–Ni–B compounds as possible candidate materials that can provide high magnetocrystalline anisotropy energies along with sufficient saturation magnetization.

References:

*This work is supported by the National Science Foundation (NSF), DMREF-1729202. HPC resources were provided by the Texas Advanced Computing Center (TACC) and the National Energy Research Scientific Computing Center (NERSC).
**3:54PM D44.00008: Ab initio calculations of electron and nuclear spin interactions in molecules and solids using a mixed pseudopotential-all electron approach**

KRISHNENDU GHOSH (Presenter), Mechanical Engineering, Univ of Michigan - Ann Arbor, HE MA, Chemistry, University of Chicago, VIKRAM GAVINI, Mechanical Engineering, Univ of Michigan - Ann Arbor, GIULIA GALLI, University of Chicago and Argonne National Laboratory — The interaction between electronic and nuclear spins in the presence of external magnetic fields can be described by a spin Hamiltonian (SH), with parameters obtained from first principles electronic structure calculations. We previously developed an approach [1] to compute these parameters, applicable to both molecules and solids, which is based on real space density functional theory (DFT) based all-electron calculations using finite elements. Here we improve the efficiency of our approach for the calculations of spin-defects in semiconductors by combining all-electron and pseudopotential calculations: for a small region around the defect we treat explicitly all the electrons, while the rest of the crystal is described using pseudopotential calculations. We present results for the nitrogen vacancy in diamond and for divacancies in silicon carbide, including hyperfine and zero-field splitting tensors, and we show that the results of the mixed approach are in an excellent agreement with those of all-electron calculations for the full crystals. Our strategy opens the way to accurate large-scale calculations of SH parameters for the prediction of spin defect qubits in complex systems.


*Supported by MICCoM and DoE-BES (DE-SC 0017380)

**4:06PM D44.00009: Nonlocal Density Embedding Theory**

WENHUI MI (Presenter), MICHELE PAVANELLO, Department of Chemistry & Department of Physics, Rutgers University, Newark — By invoking a divide-and-conquer strategy, density embedding methods dramatically reduce the computational cost of large-scale, *ab-initio* electronic structure simulations of molecules and materials. The central ingredient setting density embedding apart from Kohn-Sham DFT is the non-additive kinetic energy functional (NAKE). Currently employed NAKEs are at most semi-local (i.e., they only depend on the electron density and its gradient), and as a result of this approximation, only systems composed of weakly interacting subsystems can be successfully tackled. The limitation of semi-local NAKEs originate from the natural nonlocality of the underlying KEDF. Recently, we advance the state-of-the-art by introducing fully nonlocal NAKEs in density embedding simulations for the first time. Benchmark analysis based on the S22-5 set shows that nonlocal NAKEs considerably improve the computed interaction energies and electron density compared to commonly employed GGA NAKEs, especially when the inter-subsystem electron density overlap is high. Most importantly, we resolve the long standing problem of too attractive interaction energy curves typically resulting from the use of GGA NAKEs.

*This work supported by National Science Foundation under Grant No. CHE-1553993*
Modeling device-level semiconductors and their interfaces by orbital-free DFT

XUECHENG SHAO (Presenter), KAILI JIANG, MICHELE PAVANELLO, Chemistry / Physics, Rutgers University-Newark — Orbital-Free Density Functional Theory (OFDFT) is one of most promising methods for large-scale quantum mechanical simulations as it offers a good balance of accuracy and computational cost. Million atom simulations are nowadays achievable with OFDFT because the noninteracting kinetic energy functional is approximated by an explicit functional of the electron density removing the need to employ orbitals and diagonalizations. The commonplace belief is that because of the underlying approximations, OFDFT can only approach metallic systems. However, newly developed functionals allow the quantitative description of semiconductors and semiconducting quantum dots. We present an implementation of OFDFT entirely in Python providing some useful abstractions to deal with molecules and materials. The simulations are extremely computationally efficient, delivering converged electronic structures for million-atom system sizes realizing experimentally observed devices. We present calculations of work functions and Schottky barriers for an array of realistically sized systems that are still completely out of reach of commonly employed Kohn-Sham DFT methods.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D45 DCOMP DSOFT GSNP DPOLY: Understanding Glasses and Disordered Systems Through Computational Models III 706 - Pengfei Guan, Beijing Computational Science Res Ctr - Tag(s): Focus
The density of states of the vibrational modes (VDOS) plays a central role in determining macroscopic physical quantities of solids, such as specific heat, thermal conductivity and the critical temperature towards a superconducting phase. Also, the VDOS is directly linked to the elastic and viscoelastic moduli of the solid. For glasses, the VDOS at low frequency is not simply behaving quadratically in frequency as predicted long ago by Debye, but presents an excess of modes above some frequency where the quadratic Debye law breaks down. Upon normalizing the VDOS by the Debye law a peak is visible, known as the boson peak (BP). Consensus is emerging to explain the origin of the BP in terms of a (Ioffe-Regel type) crossover between ballistic phonon propagation and diffusive-like propagation dominated by randomness and scattering. The diffusive propagation shows up in a damping coefficient which is quadratic in the wavevector [1]. A theoretical description leads to the possibility of studying the VDOS in semi-analytical form as a function of physical parameters [2].

In glassy polymers, the BP has been shown to anti-correlate with the bending rigidity of the polymer chain [3,4], in spite of the BP occurring in a band of the VDOS spectrum dominated by Lennard-Jones type interactions [5]. This can be explained as due to redistribution of modes across the spectrum. The BP is shown to scale with the square root of the shear modulus [4], as predicted by theory [2]. The BP also controls the nonaffine contribution to the viscoelastic moduli [6] and thus is the central input to numerical predictions of mechanics [7], recently also at the atomistic level [8], thus leading to material design principles.

3:06PM D45.00002: Revealing the low-temperature fast relaxation peak in a model metallic glass  PENGFEI GUAN (Presenter), Beijing Computational Science Research Center — The relaxation dynamics and its underlying atomistic mechanism are one of the most important and challenging issues in metallic glasses. Here, we first report a pronounced low-temperature relaxation peak in a model metallic glass, which is located at a much lower temperature than the typical temperature for the conventional $\beta$ relaxation reported in prior works. Through extensive molecular dynamics simulations, we unravel its intrinsic link with reversible atomic motions, which bridges the vibrational modes and the structural rearrangements governing a normal $\beta$ relaxation process. Moreover, through the study of the local geometrical anisotropy, we reveal the microscopic mechanism of the fast relaxation process and clearly demonstrate that the fast relaxation dynamics is a trigger to a cascade of critical relaxation modes (such as $\beta$ and $\alpha$ relaxation). Our findings are of fundamental importance, and further our understanding of the heterogeneous dynamic response of metallic glasses and the dynamic origin of their physical properties.

3:18PM D45.00003: Accuracy of Classical Potentials for Polyethylene Structures Away from Equilibrium*  KEARA G FRAWLEY (Presenter), LIHUA CHEN, HUAN D TRAN, NARESH N THADHANI, RAMAMURTHY RAMPRASAD, Materials Science and Engineering, Georgia Institute of Technology — Realistic simulations of polymers require a large number of atoms due to the anisotropic nature of their morphology. Although density functional theory (DFT) is considered highly accurate, it is too computationally expensive to handle large systems. Classical potentials used for molecular dynamics studies are trained on experimental or quantum mechanical equilibrium structures, and their accuracy away from equilibrium is not well known. This work is a comparative study of two widely used classical potentials—Optimized Potentials for Liquid Simulations (OPLS) and the reactive force-field (ReaxFF)—with respect to DFT. Their performance for polyethylene (PE), a simple model polymer, is benchmarked by comparing the classical energies, forces, and stresses against DFT. Additionally, a pressure-temperature phase diagram for PE is computed using OPLS and ReaxFF. Although the classical potentials do not perfectly capture the DFT and experimental behavior, the results are close enough to justify their use when large system sizes are required. Consequently, these results will be used for shock simulations involving far from equilibrium structures.

*This work was supported by the Department of Defense through the National Defense Science and Engineering Graduate Fellowship.
3:30PM D45.00004: Disentangling glassy polymer dynamics: combining simulations and machine learning
ANNA LAPPALA (Presenter), Harvard University — Glass-forming liquids are an example of non-equilibrium systems: upon cooling, a glass undergoes a transition from a liquid into an amorphous solid without apparent long-range order. The problem of the glass transition combines the concepts of self-organization, collective and heterogenous dynamics and poses an unsolved fundamental problem in condensed matter physics. We investigate the role of connectivity and topology in the glass transition of polymers, combining coarse grained molecular dynamics simulations with machine learning. ML allows us to quantify the relation between local structural properties of polymers and their topology using clustering of correlated motions of polymer chain segments as an example descriptor to create a training set, leading to the development of a data-based model.

3:42PM D45.00005: Amorphous polymers in their glass transition regime: Comparison of local and macroscopic small non-linearities
AUDE BELGUISE (Presenter), FRANÇOIS LEQUEUX, SIMM, ESPCI Paris, SABINE CANTOURNET, Centre des Matériaux, Mines ParisTech, HÉLÈNE MONTES, SIMM, ESPCI Paris — The mechanical behavior of amorphous polymers in their glass transition regime is linked to dynamical heterogeneities at a nanometric scale. To describe them, we developed a finite elements method where a sample is described as a set of domains each characterized by its own relaxation time $\tau_i$. The relaxation times are randomly distributed over the domains. We showed that this approach quantitatively describes linear relaxation measured on glassy polymers.

In this work, we focus on the onset of non-linearities where non-linear relaxation is accelerated in comparison to the linear case. We describe the non-linearity effect as a decrease in local relaxation times due to stress i.e. $\tau_i$ becomes $\tau_i f(\sigma)$. In a homogeneous case, the local law accelerating relaxation ($f(\sigma)$) can be identified by comparing linear and non-linear macroscopic responses. However, we show that the local and macroscopic non-linear laws are different due to dynamical heterogeneities. Comparing experiments and simulations, the local non-linear law $f(\sigma)$ can be identified. We show that its shape would be as $\exp(\sigma^n)$ with $n$ larger than 1.

3:54PM D45.00006: Atomic-scale understanding of highly conducting polymer electrolyte
SUNGYEB JUNG (Presenter), Department of Physics, Pusan National University, YEONHWA SONG, U HYEOK CHOI, Department of Polymer Engineering, Pukyong National University, JAE HYUN PARK, Department of Aerospace and Software Engineering, Gyeongsang National University, JAEKWANG LEE, Department of Physics, Pusan National University — Electrolyte is one of the key and most important components determining the performance of lithium-ion batteries. Until now, solid polymer electrolytes have attracted considerable attention due to the rapid development of the need for more safety and powerful lithium ion batteries. Despite their high stabilities and endurance, extremely low conductivity has hindered their applications. Here, we find that novel poly acrylic acid polymer-based electrolyte exhibits at least two orders of magnitude higher ionic conductivity compared with conventional solid polymer electrolytes. By combining molecular dynamic simulations with temperature dependent conductivity measurements, underlying mechanism will be addressed at the atomic scale in detail.
4:06PM D45.00007: Effects of Coarse-Graining on Molecular Simulations of Mechanical Properties of Polymers  TING GE (Presenter), Department of Chemistry and Biochemistry, University of South Carolina, MARK ROBBINS, Department of Physics and Astronomy, Johns Hopkins University — Conventional coarse-graining methods for polymers are typically based on matching equilibrium thermodynamic properties in the melt state, such as the average structural correlations or forces. It is not clear whether the resulting coarse-grained potentials can be used to simulate non-equilibrium properties of melts at high rates or the mechanical properties of low-temperature crystals or glasses. As a case study, we simulate polystyrene using models with different levels of coarse-graining but the same structural correlations at thermal equilibrium. The elastic modulus, yield stress, and strain hardening of polystyrene in the glassy state show a steady decrease with increasing degree of coarse-graining. This reflects that the configurational average of fine-grained structure leads to a smoother coarse-grained potential with lower energy barriers between local configurations. We find that the stress-strain curves with different degrees of coarse-graining can be collapsed with a simple rescaling factor in some cases, but too much coarse-graining leads to qualitative changes of the curves. We develop a multi-scale method that uses properly selected coarse-grained models to accelerate the simulation of mechanical response while fine-grained models to capture the accurate stress value.

4:18PM D45.00008: Ubiquity of Entropy-Driven Local Organization  ANDREI A. KLISHIN (Presenter), Univ of Michigan - Ann Arbor, GREG VAN ANDERS, Physics, Engineering Physics, and Astronomy, Queen's University — Soft-matter and biological systems of crowded objects exhibit local organization into preferred motifs. Locally organized motifs in soft systems can, paradoxically, arise from a drive to maximize overall system entropy. The emergence of entropy-driven local order has been directly confirmed in model, synthetic colloidal systems, however similar patterns of organization occur in crowded biological systems ranging from the contents of a cell to collections of cells. In biological settings it is unclear whether entropy acts to promote or inhibit local organization. Answering this is difficult because entropic effects are intrinsically collective, complicating efforts to isolate them. Here, we employ minimal models that artificially restrict system entropy to show that entropy drives systems toward local organization, even when the model system entropy is below reasonable physical bounds. By establishing this bound, our results suggest that entropy drives local organization in all crowded soft and biological systems of rigid objects.
4:30PM D45.00009: Measuring configurational entropy of glasses using population annealing*  
CHRIS AMEY (Presenter), Physics, Univ of Mass - Amherst, JONATHAN LEE MACHTA, Physics, Univ of Mass - Amherst, Santa Fe Institute — In this talk we present two methods to calculate the vibrational ($S_{vib}$) and configurational ($S_c$) entropies of glassy fluids in the context of population annealing Monte Carlo. The first method for obtaining $S_{vib}$ integrates the pressure of individual configurations from the fluid phase to the glass phase, and the second method introduces a hard shell constraining potential to individual particles at fixed packing fraction in the glassy regime and integrates the entropy to the highly constrained, ideal gas limit. From population annealing, we also obtain the total entropy, $S_{tot}$, and from it the configurational entropy, $S_c = S_{tot} - S_{vib}$. We present numerical data for large-scale population annealing simulations of binary hard sphere fluids with 30, 60, and 100 particles. Our results show that the two methods agree and that for even modest-sized systems, finite-size effects appear to be small.

*NSF DMR-1507506

4:42PM D45.00010: Statistical structural and dynamic heterogeneity as signature of glass transition  
YUNJIANG WANG (Presenter), DONG HAN, Institute of Mechanics, Chinese Academy of Sciences — Glass transition is a ubiquitous phenomenon in nature yet it remains highly elusive. The puzzle is that there lacks intuitive rationalization for the dynamic arrest upon liquid-to-glass transition and a structural rationale is highly anticipated. Here I introduce two parameters based on the Shannon Information Entropy concept which can be served as intuitive signatures of glass transition. The first one is the Shannon entropy on structures, which characterize the diversity of atomic-level structures that undergoes a striking variation across the glass transition, and explains the change found in the excess configurational entropy. The other dynamic Shannon entropy is associated with the variation in the activation barriers to local structural excitations on the underlying potential energy landscape. It is also found to change dramatically at the glass-to-liquid transition and therefore can be treated as another signature of the glass transition. The two parameters can be evaluated based on the recent advanced atomistic simulations techniques, which moves a minor step towards the eventual understanding of physics of glass transition.
4:54PM D45.00011: RFOT theory explains fragile-to-strong crossover in Wigner glasses

HYUN WOO CHO (Presenter), MAURO LORENZO MUGNAI, Department of Chemistry, University of Texas at Austin, THEODORE KIRKPATRICK, Institute for Physical Science and Technology, and Department of Physics, University of Maryland, DAVE THIRUMALAI, Department of Chemistry, University of Texas at Austin — Colloidal suspension with various degrees of softness exhibits rich glass forming behavior, normally observed in molecular glasses. For over a decade, many experiments have shown that glass transition of colloidal suspensions can be either strong or fragile depending on the softness of potential, thus making them ideal testing ground for the structural glass transition (SGT) theories. However, it is still debated whether the softness alone is responsible for such a drastic change in fragility and if the glass transition of the soft colloid with the broad range of fragility can be described using a unified theory. We carried out Brownian dynamics simulations for a binary mixture of micron-sized charged colloidal suspensions and elucidate that they exhibit continuous transition from fragile to strong behavior due to the variation of the softness of potential that is achievable by changing the monovalent salt concentration. We found that the prediction of the random first order transition (RFOT) theory quantitatively describes the universal feature of the glass transitions of the charged colloids, such as growing length scales associated with heterogeneous dynamics. Our predictions are amenable to experimental tests.

5:06PM D45.00012: Cluster Dynamic Mean Field Theory of Glass Transition

CHEN LIU (Presenter), GIULIO BIROLI, Physics, Ecole Normale Superieure, DAVID REICHMAN, Columbia University, GRZEGORZ SZAMEL, Colorado State University — Recently, the infinite dimensional theory of the dynamics of super-cooled liquids was established in [1,2,3], and showed to be related to the mode coupling transition (MCT) theory [4]. One of the main mean field predictions is the existence of a sharp dynamical transition, akin to the MCT transition, at a temperature $T_d$, i.e. as the temperature approaches $T_d$ from above, the relaxation time diverges. However, in three dimensional glass-formers this transition is smeared out and a smooth crossover takes place. We extend the infinite dimensional analysis by developing a cluster dynamic mean field theory (CDMFT) where clusters of particles interact in a mean field way, while correlations involving several particles are taken into account inside clusters. This allows us to progressively take into account correlations between particles and activated dynamical processes. In this talk we will present CDMFT and present results for three dimensional super-cooled liquids.

5:18PM D45.00013: Understanding $T_A$ from dynamic heterogeneity in metallic glass-forming liquids  
NANNAN REN (Presenter), PENGFEI GUAN, LIJIN WANG, Beijing Computational Science Research Center, LINA HU, Shandong University — How to generally describe the structural relaxation upon cooling is still mysterious for metallic glass-forming liquids with various dynamic fragilities. Here a scaling collapse of the temperature dependence of structural relaxation time, $\tau_\alpha(T)$, is achieved by introducing the characteristic temperature $T^*(\alpha_{2,max})$ and characteristic time scale $\tau^*(\alpha_{2,max})$ with any identical dynamic heterogeneity $\alpha_{2,max}$ in 12 metallic glass-forming liquids, which is consistent with our previous reports[1]. The scaled master curve $\tau_\alpha/\tau^*(\alpha_{2,max}) \sim T^*(\alpha_{2,max})/T$ experiencing a crossover behavior from Arrhenius to non-Arrhenius implies that $T_A$ is one of $T^*(\alpha_{2,max})$. It is further confirmed by the almost constant $\alpha_{2,max}(T_A)$ for all the systems studied here and achieving a general description of relaxation time, together with $\tau_A$ (the structural relaxation time at $T_A$). Our findings provide a new insight of $T_A$ from the perspective of dynamic heterogeneity and shed light on the glass forming of metallic liquids.

References

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D46 GMAG DMP: Spin Liquids: Theory and Experiment 708 - Martin Mourigal, Georgia Inst of Tech - Tag(s): Focus
The search for the enigmatic quantum spin liquid (QSL) state has switched into high gear in recent years. Amazing experimental progress has resulted in several highly promising QSL materials such as ZnCu3(OH)6Cl2, YbMgGaO4, and NaYbO2, to list just a few. All of these quasi-two-dimensional materials are characterized by a broad continuum of spin excitations observed in neutron scattering experiments. Unfortunately, many, if not all, of these QSL candidates suffer from the presence of significant substitutional disorder which often tends to strongly broaden inelastic neutron spectra and thus calls into question the QSL interpretation of the experimental data. It is therefore incumbent upon the theoretical community to identify specific experimental signatures, more detailed than a “broad continuum” arguments, that evince the unique aspects of spin liquid states of magnetic matter.

In this talk, I focus on the prominent metal-like magnetic insulators – U(1) quantum spin liquids with spinon Fermi surface – excitations of which are represented by neutral spin-1/2 fermions (spinons) and emergent gauge fields. The gauge field mediates strong interactions between spinons. We argue that the full effect of this interaction becomes apparent when the spin liquid is partially magnetized by the Zeeman magnetic field. Under this condition, the spectrum of the spin liquid acquires a new transverse collective spin-1 mode, distinct from incoherent particle-hole excitations of the spinon continuum. Despite being located outside the spinon continuum, this novel collective excitation interacts with emergent gauge fluctuations which are responsible for partially damping it.

I will also discuss how this picture is modified by the spin-orbit interaction, and present a calculation of the ESR linewidth for one specific spin-orbit geometry.

*This research is supported by the NSF CMMT program under Grant No. DMR1928919.
Entangled Neutron Beams: A possible new avenue to exploring Quantum Materials

DAVID BAXTER (Presenter), Indiana Univ - Bloomington, COLLIN LESLIE BROHOLM, Physics, The Johns Hopkins University, ABU ASHIK M IRFAN, STEPHEN J KUHN, SHUFAN LU, GERARDO ORTIZ, ROGER PYNN, JIAZHOU SHEN, WILLIAM MICHAEL SNOW, Indiana Univ - Bloomington — We have recently demonstrated that the Larmor instrument at ISIS can be used to construct two and three-fold entangled states in a neutron beam [1]. Entanglement among the spin, energy, and trajectory degrees of freedom for neutrons was indicated by observing clear violations of both the Clauser-Horne-Shimony-Holt and Mermin contextuality inequalities in the same experimental setup. Moreover, the entanglement length associated with this experiment was 1 micron (as opposed to the cm length scales previously seen with neutron interferometer experiments [2]), and could be experimentally varied from several nm to several microns. We suggest that such a beam, with an experimentally controllable microscopic length scale, may represent a fundamentally new probe of correlated matter. Experiments are planned to demonstrate these methods to probe entanglement in quantum spin chains.


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Thermal conductivity of the quantum spin liquid candidate EtMe₃Sb[Pd(dmit)₂]₂: No evidence of mobile gapless excitations

NICOLAS DOIRONLEYRAUD (Presenter), PATRICK BOURGEOIS-HOPE, FRANCIS LALIBERTE, ETIENNE LEFRANCOIS, GAEL GRISONNANCHE, SAMUEL RENE DE COTRET, RYAN T GORDON, LOUIS TAILLEFER, Universite de Sherbrooke, HENGBO CUI, REIZO KATO, RIKEN, SHUNSUKE KITOU, HIROSHI SAWA, Nagoya University — The search for highly mobile gapless spin excitations in quantum spin liquids (QSL) is currently attracting considerable attention. We examined this specific issue via thermal conductivity measurements on one of the most promising QSL candidates, the organic insulator EtMe₃Sb[Pd(dmit)₂]₂ (dmit-131). We performed heat conduction experiments down to 0.07 K on a total of 8 high-quality single crystals of dmit-131. Contrary to previous reports, our body of data consistently and reproducibly shows the absence of a T-linear contribution to the thermal conductivity of dmit-131 at low temperatures, showing that no spin excitation contribute to the heat transport. Consequently, the spin excitations in dmit-131 are localized and not mobile. Our data further reveal a strongly suppressed phonon conductivity, evidence that the phonons are heavily scattered by those localized spin excitations. Comparison with published data on numerous spin-liquid materials shows, in fact, that this is a widespread phenomenon and that it should be considered in any future theory of QSLs.
3:30PM D46.00004: Evidence of Frozen Moments at Low T in κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Br*
TERESA LE (Presenter), ANDREJ PUSTOGOW, University of California, Los Angeles, JIERONG WANG, Physics, Nanjing University, AYSSA HENDERSON, Florida State University, JOHN A SCHLUETER, National Science Foundation, STUART BROWN, University of California, Los Angeles — Quantum Spin Liquids (QSLs) and the phenomena behind their manifestation continue to be a topic of debate in solid state physics. The charge transfer salt, κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Br or (κ-HgBr), has been proposed as a “quantum dipole liquid” [1], possibly exhibiting the necessary properties for QSL emergence. We examine the magnetic properties of κ-HgBr using 13C NMR Spectroscopy. 1/T$_1$ measurements show a first order transition at T$_{MI} = 90$ K, a possible crossover at T = 20 K, and a pronounced peak at 5 K characteristic of freezing moments. Analysis of the NMR spectra reveals an onset of broadening at T$_{MI}$ which becomes more pronounced at low T reaching a FWHM of approximately 1350 ppm at T = 2.5 K. The behavior and magnitude of the linewidth with respect to temperature is indicative of coupling to electron moments which are gradually freezing as temperature decreases and agrees with the 1/T$_1$ behavior.


*This work was supported by the National Science Foundation (DMR-1709304).

3:42PM D46.00005: Understanding Complex Magnetic Interactions Using Diffuse Neutron Scattering* JOSEPH PADDISON (Presenter), Oak Ridge National Lab — Many important magnetic materials have complex bond-dependent magnetic interactions, such as Kitaev and frustrated spin-liquid candidates [1,2]. Traditionally, spin Hamiltonians of such systems are determined by fitting to spin-wave spectra measured below the magnetic ordering temperature $T_N$. Unfortunately, this approach is often impractical in spin liquids, either because $T_N$ is unmeasurably low, or the ordering is poorly understood.

I discuss an alternative approach to parameterize the spin Hamiltonian that does not assume long-range magnetic order: fitting interaction models to diffuse magnetic neutron-scattering data measured above $T_N$. I demonstrate the sensitivity of this method for canonical models of bond-dependent interactions on triangular and honeycomb lattices. I discuss my results in the context of developments in reverse Monte Carlo refinement [3], pair distribution function analysis [4], and machine learning [5].


*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, and by Churchill College, University of Cambridge.
**3:54PM D46.00006: Effects of nuclear spins in the transverse-field Ising quantum magnet Ho$_3$Mg$_2$Sb$_3$O$_{14}$**  
MARTIN MOURIGAL (Presenter), ZHILING DUN, XIAOJIAN BAI, Georgia Inst of Tech, JOSEPH PADDISON, Oak Ridge National Laboratory, EMILY HOLLINGWORTH, University of California, Berkeley, FRANZ DEMMEL, SFTC, HAIDONG ZHOU, University of Tennessee  — Transverse Ising model is the simplest quantum model which can be realized in rare earth magnets with two-singlet crystal field ground state. Recent interests have been focused on non-Kramer ion based pyrochlore lattice where random transverse fields are introduced by lattice disorder. As all stable isotopes of all non-Kramers ion possess non-zero nuclear spins, the couplings between electronic and nuclear spins (hyperfine interactions) in these systems are usually nonnegligible, yet are little discussed so far. Here, we show that the tripod kagome magnet Ho$_3$Mg$_2$Sb$_3$O$_{14}$ offers us a new platform to study this effect because of a homogeneous transverse field brought in by the low symmetry of the lattice. Using neutron backscattering and specific heat measurements, we illustrate that nuclear spins dramatically alter the single-ion and collective behaviors of the system. Comparing to classical spin ice system such as Ho$_2$Sn$_2$O$_7$, our results highlight the crucial role played by hyperfine interactions in frustrated quantum magnets, and motivate further investigations of correlated nuclear spins.

*The work at Georgia Tech was sponsored by the Department of Energy under DE-SC-0018660.

**4:06PM D46.00007: Robust quantum spin liquid ground state in hydrogen-bonded organic Mott insulators**  
KENICHIRO HASHIMOTO (Presenter), Department of Advanced Materials Science, University of Tokyo, MASAAKI SHIMOZAWA, MINORU YAMASHITA, Institute for Solid State Physics, University of Tokyo, AKIRA UEDA, Department of Chemistry, Kumamoto University, HATSUMI MORI, Institute for Solid State Physics, University of Tokyo, TAKAHIKO SASAKI, Institute for Materials Research, Tohoku University  — κ-H$_3$(Cat-EDT-TTF)$_2$ is a hydrogen-bonded organic Mott insulator that provides a new class of quantum spin liquids (QSLs), where the strong coupling between the localized spins and the hydrogen atoms leads to a quantum paramagnetic and quantum paraelectric (QPE) state. Although this material has a 2D spin-1/2 triangular lattice, its anisotropy parameter $t'/t = 1.25$ is far from unity. This raises a question as to whether the geometric frustration of the triangular lattice is an important factor for realizing the QSL state in this system. Here, we investigate a series of κ-H$_3$(Cat-X)$_2$ (X = EDT-TTF, EDT-ST, EDT-d4-TTF, and EDSe-TTF), where the substitution of X affects the anisotropy of the triangular lattice as well as the hydrogen-bond dynamics. Our dielectric and thermal-transport measurements reveal that all the materials exhibit a QSL and QPE state in spite of the large $t'/t$ (for instance, $t'/t = 1.84$ for X = EDSe-TTF), indicating that the coupling between the π electrons and the hydrogen atoms plays an important role for stabilizing the QSL state. We also find that the QPE behavior is strongly enhanced in X = EDT-ST that is located near a regime where the hydrogen atoms are localized at low temperatures, suggesting the presence of a QCP related to the hydrogen-bond dynamics.
4:18PM D46.00008: Coherent spinon behaviour in quantum spin liquids at finite temperature  YUAN WAN (Presenter), Institute of Physics, Chinese Academy of Sciences, OLLIE HART, CLAUDIO CASTELNOVO, Theory of Condensed Matter group, Cavendish Laboratory, University of Cambridge — Realistic Hamiltonians for quantum spin liquids often exhibit a large separation of energy scales between their elementary excitations. At experimentally relevant temperatures, some excitations are in a low-temperature regime where they are sparse and hop coherently across the lattice, while others are thermally excited and behave as a dense, stochastic ensemble. We study the interplay of these quasiparticles in the case where it is driven solely by their nontrivial mutual statistics rather than by direct interaction energy terms. We consider toy models for Z2 quantum spin liquids, where the two species of excitation (dubbed spinons and visons) are mutual semions. The nontrivial statistical angle between the two species leads to interference effects that we study using a combination of numerical and analytical tools. In the limit of self-retracing paths, we are able to use a Bethe lattice approximation to construct exact analytical expressions for the time evolution of the site-resolved density profile of a spinon initially confined to a single site. We also highlight an intriguing feedback mechanism, akin to the Nagaoka effect, whereby the spinons become localised on patches of expelled incoherent visons, the typical diameter of which increases as temperature is reduced.

4:30PM D46.00009: Finite temperature dynamics of Coulomb spin liquids  SIDDHARDH MORAMPUDI (Presenter), CHRISTOPHER LAUMANN, Boston University, FRANK WILCZEK, Massachusetts Institute of Technology — Coulomb quantum spin liquids like quantum spin ice realize a phase of emergent quantum electrodynamics. However, the energy scales are very different resulting in features like a slow photon and a separation of scales between the spinon and photon. We compute the dynamics of spinons and photons at non-zero temperatures in multiple regimes realizable in neutron scattering and show characteristic changes as temperature is tuned across the different regimes.

4:42PM D46.00010: Schwinger boson approach to magnetically ordered quantum magnets  SHANG-SHUN ZHANG (Presenter), University of Tennessee, Knoxville, ESTEBAN GHIOLDI, Institute of Physics Rosario and National University of Rosario, YOSHITOMO KAMIYA, Shanghai Jiao Tong University, Shanghai, China, LUIS O. MANUEL, ADOLFO TRUMPER, Institute of Physics Rosario and National University of Rosario, CRISTIAN BATISTA, University of Tennessee, Knoxville — The quest for quantum spin liquids is producing a large number of magnetically ordered quantum magnets that exhibit anomalies in their dynamical spin structure factor. These anomalies include a strong renormalization of the single-magnon bands and a broad continuum of excitations, whose integrated spectral weight is larger than the weight of the single-magnon peaks. These observations call for novel approaches that can properly capture the effect of strong quantum fluctuations. By considering a Schwinger boson theory (large-$N$ approach) beyond the saddle-point approximation ($N = \infty$), we demonstrate that the inclusion of $1/N$ corrections is strictly necessary to remove unphysical modes (single-spinon poles) and to capture the true magnon modes, which emerge as two-spinon bound states (poles of the RPA propagator). Moreover, we show that for each Feynman diagram there is a counter-diagram that removes the unphysical single-spinon poles. The counter-diagrams are different for collinear and non-collinear orderings. Based on these results, we demonstrate that the large-$N$ approach can exactly reproduce the spin-wave theory in the large-$S$ limit.
4:54PM D46.00011: Theoretical proposal for novel experimental probe of fractionalized excitations in two-dimensional quantum spin liquids  WONJUNE CHOI (Presenter), Univ of Toronto, KI HOON LEE, Physics, Seoul National University, YONG-BAEK KIM, Univ of Toronto — Experimental smoking-gun signature for quantum spin liquids, highly entangled quantum paramagnets hosting fractionalized excitations called spinons, is a long-sought holy grail of modern condensed matter research. As spin excitations decay into a pair of fractionalized quasiparticles, conventional experimental probes do not have the resolving power for each individual fractionalized excitation. In fact, they only show a broad continuum for the pair of spinons. In this talk, we discuss a novel experimental protocol to identify the sharp coherent signals of each of the individual spinons to disambiguate quantum spin liquids from trivial paramagnets or magnon excitations.

5:06PM D46.00012: Effective theories for quantum spin clusters : State selection by singularity  SUBHANKAR KHATUA (Presenter), Institute of Mathematical Sciences, DIPTIMAN SEN, CHEP, Indian Institute of Science, GANESH RAMACHANDRAN, Institute of Mathematical Sciences — We state a general principle -- the low energy effective theory of a quantum spin cluster reduces to that of a quantum particle moving on the space of classical ground states. We demonstrate this mapping for a family of spin clusters where each pair of spins is connected by an XY antiferromagnetic bond. The simplest member of this family is a dimer-- it maps to a particle on a ring. The trimer, a cluster of three spin-S spins, is more complex -- it maps to a particle on two disjoint rings. Unlike the dimer and the trimer, the classical ground state space of the quadrumer, cluster of four spin-S spins, is non-manifold in nature -- consisting of three tori pairwise touching along lines. Particle moving on this space, successfully, captures the low energy spectrum of the quadrumer. The non-manifold structure leads to a remarkable effect -- the dynamics at low energies is not ergodic as the particle is localized around singular lines of the ground-state space. The low-energy spectrum consists of an extensive number of bound states around singularities. Physically, this manifests as an order-by-disorder like preference for collinear states. However, unlike order-by-disorder, this “order by singularity” gets better as we approach the classical limit.


5:18PM D46.00013: Density Matrix Renormalization Group Analysis of Quantum Spin Ice  MICHAEL FLYNN (Presenter), University of California, Davis, THOMAS BAKER, Universite de Sherbrooke, RAJIV RANJAN SINGH, University of California, Davis — One of the most studied systems in three dimensional many-body physics is a model of spins on the pyrochlore lattice dubbed quantum spin ice. The massive frustration of the model makes it a strong candidate for supporting a variety of exotic spin liquids with natural connections to lattice gauge theory. Here we initiate the use of the Density Matrix Renormalization Group (DMRG) to study the phase diagram of quantum spin ice, focusing on the transition from an XY antiferromagnet to a U(1) spin liquid. Using quasi-one-dimensional cylindrical cuts of the lattice, we compute the local spin properties of the phases and find that they converge remarkably quickly. With more effort, we extract the entanglement entropies and fit them to the Cardy-Calabrese scaling form to extract the central charge. Further discussions on detecting the photon of the U(1) spin liquid and more controversial aspects of the phase diagram may be included.
2:30PM D47.00001: Planar Hall driven torque in a FM/NM/FM system  
CHRISTOPHER SAFRANSKI (Presenter), IBM Tj Watson Research Center, JUN-WEN XU, ANDREW KENT, Center for Quantum Phenomena, Department of Physics, New York University, JONATHAN Z SUN, IBM Tj Watson Research Center — Electrical manipulation of magnetization is an intensely studied topic with goals of producing energy efficient nanodevices. The charge to spin current conversion in bilayers of magnetic and nonmagnetic materials is one area of investigation. Typically studied materials have been mostly limited to the generation of in-plane polarized spin currents. We investigate spin currents produced by the planar Hall effect in Co/Ni multilayers, which carry a polarization dictated by the FM magnetization direction. In a sample based on CoNi/Au/CoFeB, spin torque ferromagnetic resonance is used to measure the damping-like torque on the CoFeB layer. The response as a function of the applied field angle and current is consistent with the symmetry expected for a torques produced by the planar Hall effect. We find the strength of this effect to be comparable to that of the spin Hall effect. However, unlike the spin Hall effect, it can produce a partially out of plane spin polarization. Our results indicate that the planar Hall effect holds potential as a spin current source with a controllable polarization direction.
**2:42PM D47.00002: Exciton-phonon damping in the two and three-dimensional anisotropic XY model**

LEONARDO DOS SANTOS LIMA (Presenter), Centro federal de educacao tecnologica —
The effect of exciton-phonon interaction on spin transport properties and quantum information is analysed in the integer spin XY model with ion-single anisotropy in dimension \( d=2,3 \) in the square and cubic lattices and in the neighbourhood of a quantum critical point \( \Delta_c \) using the SU(3) Schwinger boson approach. For three dimensions, there is a quantum phase transition from the Néel phase to paramagnetic phase where recently, one has investigated the influence of this quantum phase transition on spin transport and obtained a strong influence of the line of separation among the phases on continuum spin conductivity.

**Keywords:**
spin transport, quantum entanglement, spin-phonon

**Bibliography**

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**2:54PM D47.00003: Probing Spin-wave Excitations in Layered Chromium Trihalides with Nitrogen-Vacancy Magnetometers in Diamond**

RUOLAN XUE (Presenter), Harvard University, MARK JEN-HAO KU, Harvard - Smithsonian Center for Astrophysics, DAHLIA KLEIN, DAVID MACNEILL, Massachusetts Institute of Technology, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, RONALD L WALSWORTH, Harvard - Smithsonian Center for Astrophysics, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology, AMIR YACOBY, Harvard University — Nitrogen-vacancy (NV) centers in diamond are highly sensitive, nano-scale magnetic sensors. NV magnetometry has demonstrated detection of spin-wave excitations in bulk magnets and has recently been used as a local probe to detect static magnetization in layered magnets. While monolayer and few-layer van Waals magnets have been discovered and their static properties investigated, spin-wave excitations in these materials remains unexplored. Understanding low-energy excitations in layered magnets is crucial to further elucidate dynamical properties of 2D spin systems and to explore applications of these materials. In this work, we report progress towards probing spin-wave excitations in chromium trihalides with NV magnetometry.
3:06PM D47.00004: Exceptional non-reciprocity in non-Hermitian spin dynamics  ALEXEY GALDA (Presenter), James Franck Institute, University of Chicago, VALERII VINOKUR, Materials Science Division, Argonne National Laboratory — We investigate topological structure of complex energy surfaces of non-equilibrium magnetic systems. We consider spin-transfer torque-driven single-spin model described by a non-Hermitian Hamiltonian. The spectrum of the Hamiltonian admits branch point singularities that appear as chiral exceptional points where both eigenvalues and eigenstates coalesce. The emergence of exceptional spectral points provides access to a wealth of topological effects unique to non-Hermitian spin systems, e.g. non-reciprocal spin dynamics. An implementation of an asymmetric spin-filter device based on this effect is proposed.

3:18PM D47.00005: Quantized ΔS=2 excitation spectra by confinement in an S=1 Ising spin chain under magnetic fields*  SEI-ICHIRO SUGA (Presenter), TAKAFUMI SUZUKI, Univ. of Hyogo — We calculate the dynamical spin-structure factor of the S = 1 Ising spin chain with negative single-ion anisotropy in transverse and longitudinal magnetic fields using the infinite time-evolving-block-decimation algorithm [1]. We show that when only a transverse magnetic field is applied, both the ΔS = 2 excitation continuum and one-magnon mode appear in the low-lying excitation. When a longitudinal magnetic field is further applied, the excitation continuum changes into quantized spectra. The quantized ΔS = 2 excitation spectra originate from the confinement of two domain walls, each of which carries ΔS = 1. The quantized excitation energies are explained by the zeros in the Airy function. [1] T. Suzuki and S. Suga, J. Phys. Soc. Jpn. 88, 053702 (2019).

*This work was supported by KAKENHI (Grant No. 19K03721).

3:30PM D47.00006: Spin dynamics in interacting ferromagnetic discs arranged on a Kagome lattice  MOJTABA TAGHIPOUR KAFFASH (Presenter), SERGI LENDINEZ, Univ of Delaware, WONBAE BANG, Northwestern University, AXEL HOFFMANN, Argonne National Laboratory, JOHN B. KETTERSON, Northwestern University, MATTHIAS BENJAMIN JUNGFLEISCH, Univ of Delaware — Artificial spin ice (ASI) consists of periodic arrays of nanomagnets in the shape of elongated elements where competing interactions between the elements lead to geometric frustration. Recently, non-Ising-like ASI have attracted great attention due to their exotic phase diagrams. One example is an array of ferromagnetic nanodiscs. Here, we report the experimental and theoretical characterization of angular-dependent spin dynamics in arrays of ferromagnetic nanodiscs arranged on a Kagome lattice. The arrangement consists of coupled discs that are 500 nm in diameter. The distance between the Kagome vertices is 76 nm. The magnetic field and microwave frequency dependence obtained by broadband ferromagnetic resonance reveals a rich spectrum of modes that is strongly affected by the microstate of the network. In the high-field range the magnetization is parallel to the applied field, while at low-fields vortices are formed. A comparison of the experimental data with micromagnetic simulations reveals that different subsections of the lattice predominantly contribute to the high-frequency response of the array. Furthermore, we find indications that nucleation and annihilation of vortex-like magnetization configurations in the low-field range affect the dynamics.
3:42PM D47.00007: Magnetization reversal driven by low dimensional chaos in a nanoscale ferromagnet* [Invited]  ERIC MONTOYA (Presenter), Department of Physics and Astronomy, University of California, Irvine, SALVATORE PERNA, Department of Electrical Engineering and Information Technology, University of Naples Federico II, YU-JIN CHEN, Department of Physics and Astronomy, University of California, Irvine, JORDAN A KATINE, Hitachi Global Storage Technologies, MASSIMILIANO D'AQUINO, Engineering Department, University of Naples "Parhenope", CLAUDIO SERPICO, Department of Electrical Engineering and Information Technology, University of Naples Federico II, ILYA KRIVOROTOV, Department of Physics and Astronomy, University of California, Irvine — Energy-efficient magnetization switching is an essential problem in the realization of practical nonvolatile magnetic storage [1] and magnetic neuromorphic computing [2]. In the past two decades, several efficient methods of magnetic switching were demonstrated including spin torque, magneto-electric, and microwave-assisted switching mechanisms. In this talk, we experimentally demonstrate that low dimensional magnetic chaos [3] induced by alternating spin torque can strongly increase the rate of thermally-activated magnetic switching of the free layer in a magnetic tunnel junction (MTJ)[4]. This mechanism exhibits a well-pronounced threshold character in spin torque amplitude and its efficiency increases with decreasing spin torque frequency. We present analytical and numerical calculations that quantitatively explain these experimental findings and reveal the crucial role played by low dimensional magnetic chaos near saddle equilibria in enhancement of the switching rate. This work shows that ac spin torque driven chaos can facilitate thermally-assisted switching of magnetization in a MTJ [5] and provides a new path towards improved energy efficiency of spin torque memory based on thermally stable MTJs. Furthermore, MTJs with superparamagnetic free layers are attractive for neuromorphic computing. Our results show that low dimensional can be used to tune the switching rate of such systems, and therefore, may lead to computing schemes that simultaneously harness stochasticity and deterministic chaos.


*National Science Foundation, Army Research Office, Defense Threat Reduction Agency
**4:18PM D47.00008: Effects of Low-Atomic-Number Dopants on Magnetic Relaxation in Epitaxial Fe Alloys**

DAVID SMITH (Presenter), YOUNGMIN LIM, MICHAEL CLAVEL, ZIJIAN JIANG, Virginia Tech, TIM HARTNETT, University of Virginia, MANTU HUDAIT, JEAN J HEREMANS, Virginia Tech, PRASANNA V BALACHANDRAN, University of Virginia, DWIGHT D VIEHLAND, SATORU EMORI, Virginia Tech — We investigate the dependence of magnetic relaxation on dopant concentration in epitaxial thin films of Fe$_{1-x}$V$_x$ and Fe$_{1-x}$Al$_x$ grown by magnetron sputtering. By substituting Fe with lighter elements, one can expect to observe a reduction in the Gilbert damping parameter due to reduced spin-orbit coupling. The magnetic properties of these alloys were determined using broadband ferromagnetic resonance. For low concentrations of V, we observe a reduction in magnetic relaxation (e.g., effective Gilbert damping), consistent with previous experimental [1] and theoretical [2] results. In contrast, introducing Al causes a monotonic increase in magnetic relaxation. We attribute these behaviors to a modification in the density of states at the Fermi level, as shown by our density functional theory calculations. Our results serve as an avenue for predicting how to reduce Gilbert damping for applications in energy-efficient spintronic devices.

References:


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**4:30PM D47.00009: Spin dynamics in La$_{0.67}$Sr$_{0.33}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-\delta}$ heterostructures**

JACOB WISSER (Presenter), Applied Physics, Stanford University, LAUREN RIDDIFORD, Stanford Univ, SATORU EMORI, Physics, Virginia Polytechnic Institute and State University, YURI SUZUKI, Stanford Univ — Spin polarization in superconductors has largely been studied via injection of spin-polarized electrical currents, with relatively little attention paid to spin currents generated via spin wave excitations. To this end, we have fabricated heterostructures of the cuprate superconductor yttrium barium copper oxide (YBCO) with the half-metallic ferromagnet lanthanum strontium manganite (LSMO) via pulsed laser deposition on (LaAlO$_3$)$_{0.3}$(Sr$_2$TaAlO$_6$)$_{0.7}$ (001) substrates. In this study, we fix the LSMO thickness at 30 nm and vary the YBCO thickness from 2-17 nm. We have verified that the YBCO superconducts with T$_c$ varying from 55-88 K depending on YBCO thickness (with a minimum thickness of 5 nm required for superconductivity). To characterize spin wave transport, we perform ferromagnetic resonance (FMR) as a function of temperature and YBCO thickness. We find that the resonance linewidth of bare LSMO increases with decreasing temperature, which is attributed to increased two-magnon scattering at lower temperatures. Additionally, with the addition of 17 nm of YBCO, we see a near doubling of the FMR linewidth at all temperatures, indicative of spin pumping into the YBCO and possibly the coexistence of spin polarization with superconductivity.
4:42PM D47.00010: Tuning the dynamic behavior of a bicomponent artificial spin ice*
SERGI LENDINEZ (Presenter), MOJTABA TAGHIPOUR KAFFASH, MATTHIAS BENJAMIN JUNGFLEISCH,
Department of Physics and Astronomy, Univ of Delaware — Artificial spin ices (ASI) are magnetic
metamaterials initially designed to mimic the frustrated behavior of crystalline spin ice systems
such as pyrochlore crystals. They show complex magnetic ordering and can exhibit exotic phase
diagrams. Unlike their crystalline counterparts, the ASI geometry can be designed and the state
of their constituent elements can be directly probed. Recent studies have focused on their
dynamics at high frequencies (GHz to tens of GHz), as they can be used as magnonic
metamaterials to modify the spin-wave properties by creating band gaps in the resonance
spectra. Previous works have shown that different geometries produce unique dynamic spectra.
Here, we performed angular-dependent broadband ferromagnetic resonance measurements on
a square ASI composed of different materials for each sublattice (NiFe and FeCo). Our
experiments show that the interaction between the sublattices results in unique spectra
attributed to the sublattices. By performing micromagnetic simulations, we identify the modes
observed in the experiment. Our results show that the interaction in the ASI can be tuned not
only by the geometry of the lattice, but also by the proper choice of the materials.

*This work was supported by the National Science Foundation under Grant No. 1833000.

4:54PM D47.00011: Ab-initio spin-lattice dynamics based on the tight-binding method*
SIMON STREIB (Presenter), Department of Physics and Astronomy, Uppsala University, DANNY THONIG,
School of Science and Technology, Örebro University, MANUEL PEREIRO, ANDERS BERGMAN, ERIK
SJÖQVIST, Department of Physics and Astronomy, Uppsala University, ANNA DELIN, Department of
Applied Physics, KTH Royal Institute of Technology, OLLE ERIKSSON, Department of Physics and
Astronomy, Uppsala University — Recent experiments on ultrafast demagnetization have shown
that the magnetization dynamics on ultrafast timescales involves both magnetic and lattice
degrees of freedom. We present a method for the quasi-classical simulation of coupled spin and
lattice dynamics in metallic magnets based on a tight-binding (TB) model. The TB parameters are
fitted to ab-initio data and take the structure dependence of the material into account. From the
TB model we calculate both magnetic and lattice forces for the integration of the equations of
motion. We use the CAHMD package [1], which implements the TB model and the atomistic spin-
lattice dynamics. Our approach opens the door for a better understanding of the transfer of
angular momentum between magnetization and lattice already on the electronic structure level.
We demonstrate the feasibility of our method by simulations of chains and clusters.

program package for atomistic magnetization dynamics simulations. (Danny Thonig,
danny.thonig@oru.se, 2013) (unpublished, available from https://cahmd.gitlab.io/cahmdweb/)

*This research is part of the project "Dynamic Phenomena of Magnetic Materials" funded by the
Knut and Alice Wallenberg Foundation.
D47.00012: Enhancement of damping factor in Fe/Bi$_2$Se$_3$ heterostructures via topological surface states modification

LI NA (Presenter), RUI SUN, YANG XU, YUNBIN SUN, WEI HE, XIANGQUN ZHANG, ZHAOHUA CHENG, State Key Lab. of Magnetism, Institute of Physics, Chinese Academy of Sciences — Owing to the spin-momentum-locked surface state of topological insulators (TIs), the spin dynamics in ferromagnetic materials (FM)/TI heterostructures is expected to be significantly different with that in FM/non-magnetic heavy metals. Previous studies suggested that TI can modulate the spin dynamics of FM layer, however, the temperature dependence of damping factors is controversial. Here, we report spin dynamics in Fe/Bi$_2$Se$_3$ heterostructures by changing thickness of Bi$_2$Se$_3$ with and without topological surface state (TSS). Compared with that in Fe/Bi$_2$Se$_3$(3QL), where Bi$_2$Se$_3$ containing only bulk state without TSS, a significant enhancement of damping factor was achieved in Fe/Bi$_2$Se$_3$(9QL) by TSS of Bi$_2$Se$_3$. On the basis of ab initio electronic structure calculations, we confirm that the enhancement of damping factor is originated from the strong band hybridizations of Fe and Bi$_2$Se$_3$(9QL) near the Fermi level. Furthermore, by inserting Cu layer between Fe and Bi$_2$Se$_3$, the contribution of spin pumping and magnetic proximity effect to the overall damping factor was separated. Our work not only reveals the mechanism of TSS-induced damping factor, but provides a new freedom to tailor the damping factor of FM/TI spintronic devices as well.

Monday, March 2, 2020 2:30 PM - 5:06 PM

Session D48 DCMP: Superconductivity: Transport Properties  Mile High
Ballroom 1A - Michael Osofsky, United States Naval Research Laboratory

2:30PM D48.00001: Analysis of thermal conductivity for pairing symmetry in high-\(T_c\) cuprate superconductors*

H.-T. KIM (Presenter), ETRI, MINGUEN CHOI, Dongguk U. — The pairing symmetry of high-\(T_c\) cuprate superconductors has been unsolved over 30 years. Most researchers have believed that the pairing symmetry is \(d_x^2-y^2\) (\(d\)) wave, nevertheless, several objections have been still suggested. Recently the objection was also disclosed [1]. We reanalyze the data of thermal conductivity, \(\kappa\), announced as experimental evidence of \(d\)-wave symmetry, which showed the presence of a finite value at nearest \(T=0\) K in a curve of \(\kappa/T\) vs \(T^2\) in thermal conductivity [2]. This is the metal characteristic coming from the nodes of the \(d\)-wave electronic structure of clover [2]. The characteristic of the curve of \(\kappa/T\) vs \(T^2\) increases a residual linear value of \(\kappa/T\) with going to \(T=0\) K, which does not describe the pairing symmetry characteristic of \(\kappa\). We redrew the curve of \(\kappa/T\) vs \(T^2\) to the curve of \(\kappa\) vs \(T\), deduced experimental data below 0.2 K unobservable by experiment through polynomial fitting, and discovered the behavior of the conductivity with nonlinear and no residual linear value. This is evidence denying \(d\)-wave symmetry, rather, supports s-wave symmetry. [1] arXiv:1710.07754. [2] M. Sutherland et al., Phys, Rev. B 67, 174520 (2003).

*This was supported by both the principal project (19ZB1320) in ETRI and a MS&ICT project (2017-0-00830) in 2019.
2:42PM D48.00002: DC Hall measurements in the strongly correlated Hubbard model*  
WEN WANG (Presenter), JIXUN DING, BRIAN MORITZ, Stanford University, EDWIN HUANG, University of Illinois at Urbana-Champaign, THOMAS DEVEREAUX, Stanford University — We investigate the DC Hall conductivity, an indicator of charge carrier properties, of the single-band Hubbard model in the zero field limit[1] using determinant quantum Monte Carlo (DQMC). Utilizing an effective expansion to lowest order, we observe a change of sign in the Hall coefficient as a function of temperature and interaction strength, which may signal a change in the topology of the Fermi surface. We relate the Hall coefficient to the frequency dependent resistivity, also obtained from DQMC following analytic continuation, to reveal the properties of charge carriers within the strange metal phase of the Hubbard model.


*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515.

2:54PM D48.00003: Hall Conductivity in the Hubbard Model from Determinant Quantum Monte Carlo*  
JIXUN DING (Presenter), WEN WANG, YONI SCHATTNER, BRIAN MORITZ, Stanford University, EDWIN HUANG, University of Illinois at Urbana-Champaign, THOMAS DEVEREAUX, Stanford University — We extend determinant quantum monte carlo (DQMC) to allow for the addition of a constant magnetic field to the usual Hubbard model hamiltonian. We calculate the frequency and field dependent electrical Hall conductance for the single-band Hubbard model on a two-dimensional square lattice as a function of doping and temperature. Limiting cases of our results are compared with both those from recent experiments and an alternative theoretical technique.

*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515.

3:06PM D48.00004: Resistance oscillations in the quantum metal phase of lithium intercalated TiSe$_2$  
MENGHAN LIAO (Presenter), HENG WANG, YUYING ZHU, MOHSIN RAFIQUE, XIANG XU, LEXIAN YANG, DING ZHANG, QIKUN XUE, Department of Physics, Tsinghua University — The nature of the metallic ground state, in the transition from a superconductor to an insulator at a temperature close to absolute zero, is still a mystery. In this work, we uncover quantum oscillations of this quantum metal or failed superconductor in a three-dimensional anisotropic superconductor—lithium intercalated TiSe$_2$. The quantum metallic state, hosting saturating resistance below the superconducting transition even after properly filtering of radio-frequency (RF) signals, depends sensitively on the lithium doping. Exactly in this metallic regime, we show that the resistance oscillates as a function of magnetic field with a period that changes gradually with temperature. We attribute this oscillation to flux effects imposed by the domains of a coexisting charge density wave (CDW). It suggests that a periodically perturbed superconductor, either by CDW or artificial patterning, may be key to realizing the quantum metal.
Transport properties of EuTiO$_{3-\delta}$ down to 50 mK

JIAMING HE (Presenter), JIANSHI ZHOU, Materials Science and Engineering program, Department of Mechanical Engineering, University of Texas at Austin — Tetravalent perovskite titanates garnered great attention due to its unique dielectric properties. Within the family, the electron-doped SrTiO$_3$ was found to be superconducting below 1 K; its superconducting transition temperature has a dome-shaped dependence with carrier concentration [1]. Low temperature transport properties of electron-doped SrTiO$_3$ can be described by Fermi liquid theory [2]. Cubic perovskite EuTiO$_3$ has identical Ti-O subarray as SrTiO$_3$. However, interaction between mobile electron spins and magnetic moments in Eu$^{3+}$ may dramatically change transport properties. So far, transport properties of EuTiO$_3$ at sub Kelvin temperatures have not been studied. We obtained high quality single crystal EuTiO$_3$ by floating zone method; oxygen deficiency is introduced by annealing the crystal at different temperatures. These samples are characterized by suite of measurements including resistivity, specific heat capacity, and Seebeck coefficient. The electron doping converts the crystal from semiconductor to metal. As revealed by the resistivity and the specific heat, EuTiO$_{3-\delta}$ exhibits filamentary superconductivity at 1.4 K.


This work was supported by National Science Foundation, DMR1729588.

Electronic phase diagram of Ta$_{1-x}$Mo$_x$S$_2$ and optimization of superconductivity in a charge density wave system

JOSE SALCEDO- PIMIENTA (Presenter), JUAN MENDOZA ARENAS, Departamento de Física, Universidad de Los Andes, JOSE GALVIS ECHEVERRY, Facultad de Ingeniería y Ciencias Básicas, Universidad Central, IAN FISHER, Geballe Laboratory for Advanced Materials, Stanford University, LUIS QUIROGA, FERNEY RODRIGUEZ, PAULA GIRALDO-GALLO, Departamento de Física, Universidad de Los Andes — Transition metal dichalcogenides are a family of quasi-2-dimensional quantum materials with a unique susceptibility to the variation of parameters such as pressure, chemical doping, disorder, etc. These materials have been extensively studied due to the wide variety of electronic ground states they can show. Of special interest are the compounds of this family that show charge density wave (CDW) ordering and superconductivity, since the exact mechanism for the stabilization and optimization of superconductivity in systems that show these two ground states is still an open question. In this talk we present experimental transport results in single crystals of the solid solution Ta$_{1-x}$Mo$_x$S$_2$. We observe a suppression of the CDW transition temperature with increasing Mo content, accompanied by a strong enhancement of the superconducting transition temperature. We discuss our results in the context of the evolution of the electronic and structural properties of this solid solution as we approach the MoS$_2$ compound, and their relationship to the possible existence of a CDW quantum critical point.

This project is funded by COLCIENCIAS (Grant No. 120480863414), and by Universidad de Los Andes. PGG thanks the support of the APS IRTA Program, and the L'oreal-UNESCO FWIS-Colombia program.
**3:42PM D48.00007: Thermoelectric Effects in Superconductor-Ferromagnetic Heterostructures**

KIRSTEN BLAGG (Presenter), PORTIA ALLEN, BRADLEY LLOYD, Colorado Sch of Mines, MICHAEL P LILLY, Sandia National Laboratories, MEENAKSHI SINGH, Colorado Sch of Mines — Superconductor-ferromagnetic (S-F) heterostructures have been predicted to show large thermoelectric effects at cryogenic temperatures with a figure of merit of ~1.8. Confirmation of these theoretical predictions requires S-F heterostructures, controlled temperature gradients, cryogenic thermometry, thermal conductivity measurements, and electrical transport measurements. To this end, we have developed an experimental platform for the measurements of thermal and electrical transport in nanoscale devices at cryogenic temperatures. S-F heterostructures have been fabricated using lithography, evaporation, and sputtering, providing precise control over interfaces, and a wide choice of materials and geometries. Heaters and resistive thermometers, patterned via focused ion beam assisted platinum deposition, have been calibrated and optimized for thermal transport measurements at cryogenic temperatures. Finally, the Seebeck coefficient of S-F heterostructures has been measured in the presence of a magnetic field. This measurement sets the stage for systematic examination of the effects of dimensionality, ferromagnet polarization, and interface quality.

*NSF grant DMR-1461275REU, Colorado School of Mines startup grant, and Center for Integrated Nanotechnologies user proposal 2016BU0023.

**3:54PM D48.00008: Thermal Transport as a Probe of the Hidden Rashba Effect in the High Temperature Superconductor YBa_2Cu_3O_{6+x}**

BILL ATKINSON (Presenter), Trent Univ, ARNO P KAMPF, University of Augsburg — The high temperature superconductor YBa_2Cu_3O_{6+x} is an example of a Rashba bilayer material. The crystal structure comprises a stack of CuO_2 bilayers, and while each bilayer is inversion symmetric, the individual CuO_2 planes within the bilayers are not. This leads to a so-called hidden spin polarization, in which each layer making up the bilayer has a Rashba coupling constant with opposite sign such that the net spin polarization vanishes. In this talk, I will discuss the origins of the effect in YBa_2Cu_3O_{6+x}, and show that the measurement of the transverse thermal conductivity in an in-plane magnetic field allows one to make a sensitive measurement of the Rashba coupling.

*This work is supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada.*
4:06PM D48.00009: Giant Edelstein effect in the surface states of non-centrosymmetric superconductors  
YUHEI IKEDA (Presenter), YOUICHI YANASE, Physical Society of Japan — It is an important topic in the modern field of spintronics to control magnetic moments by using local electric current. One of the representative methods is the Edelstein effect [1]. However, for practical applications, e.g. magnetic domain switching [2], it is widely known that quite a large amount of electric current density is needed. Therefore, Joule heating created by a dissipative current is the main obstacle for efficient control of magnetization.

In this study, we theoretically demonstrate that the edge state of a non-centrosymmetric superconductor is a good candidate for efficient magnetization control. By using tight-binding calculations, we have found that, in d-wave superconductors, the coefficient of the magneto-electric effect in the edge state is about eighty times larger than in the bulk state. We also have found that its topological winding number is the key factor of this giant Edelstein effect.


4:18PM D48.00010: Effect of Zeeman Splitting on Andreev Reflection in Quantum Hall--Superconductor Heterostructures*  
JOSEPH CUOZZO (Presenter), XIANG HU, STUART N THOMAS, ENRICO ROSSI, Physics, College of William & Mary — We study the effect of Zeeman splitting on Andreev processes and non-local transport in heterostructures formed by two-dimensional systems in the superconducting and integer quantum Hall regime. We obtain analytic expressions for the dependence of the Andreev reflection probabilities on the Zeeman splitting in the narrow-contact and long-contact limits using an low-energy effective edge-state Hamiltonian within the Bogoliubov de-Gennes formalism. We find that introducing a higher-order, spin-dependent contribution to the renormalized drift velocity in the effective model is important to obtain accurate results. We then correlate the scattering wave function's penetration into the superconducting region with the observed Andreev reflection probabilities.

*Work funded by ARO Grant No. W911NF-18-1-0290

4:30PM D48.00011: Manifestations of spin-orbit coupling in a cuprate superconductor  
ZACHARY RAINES (Presenter), Physics, Yale University, ANDREW A ALLOCCA, T.C.M. Group, Cavendish Laboratory, University of Cambridge, VICTOR GALITSKI, University of Maryland, College Park — Exciting new work on Bi2212 shows the presence of non-trivial spin-orbit coupling effects as seen in spin resolved ARPES data [Gotlieb et al., Science, 362, 1271-1275 (2018)]. Motivated by these observations we consider how the picture of spin-orbit coupling through local inversion symmetry breaking might be observed in cuprate superconductors.

Furthermore, we examine two spin-orbit driven effects, the spin-Hall effect and the Edelstein effect, focusing on the details of their realizations within both the normal and superconducting states.
A cyclic superconducting quantum refrigerator for adiabatic magnetization cooling*

SREENATH KIZHAKKUMPURATH MANIKANDAN (Presenter), University of Rochester, FRANCESCO GIAZOTTO, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, ANDREW N JORDAN, University of Rochester — We propose a solid-state refrigeration technique using adiabatic magnetization/demagnetization cycles of a superconductor, acting as the working substance. The gradual cooling down of a substrate (normal metal) in contact with the working substance is predicted, where the excess heat is given to a hot, large-gap superconductor. The selective cooling of the normal metal is due to an effective thermal switching mechanism owing to the asymmetry of heat transport between N/N versus N/S junctions. We predict cooling of a 0.3cm^3 block of Cu by almost two orders of magnitude starting from 200mK, and down to about 1mK starting from the base temperature of a dilution fridge (10mK). The cooling powers at 200mK and 10mK for a 1cmx1cm interface are 25 nW and 0.06 nW respectively, which scales with the area of the interface.

*Work by SKM and ANJ was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under Award No. DE-SC0017890. Work by FG was supported by the European Research Council under the European Union’s Seventh Framework Programme (FP7/2007-2013)/ERC Grant Agreement No. 615187-COMANCHE. This research was supported in part by the National Science Foundation under Grant No. NSF PHY-1748958 (KITP program QThermo18).

Parity dependent supercurrent amplitude and phase of InSb/Al hybridized island*

JIYIN WANG (Presenter), Delft University of Technology, CONSTANTIN SCHRADE, Massachusetts Institute of Technology, VUKAN LEVAJAC, DAVID VAN DRIEL, Delft University of Technology, SASA GAZIBEGOVIC, ROY OP HET VELD, Eindhoven University of Technology, KONGYI LI, Delft University of Technology, JOON SUE LEE, MIHIR PENDHARKAR, CONNOR DEMPSEY, CHRIS J PALMSTROM, University of California Santa Barbara, ERIK BAKKERS, Eindhoven University of Technology, LIANG FU, Massachusetts Institute of Technology, LEO P KOUWENHOVEN, JIE SHEN, Delft University of Technology — Semiconductor nanowires coupled with superconductors are a promising platform to construct Majorana zero modes as well as to build up topological fault-tolerant quantum computers. In semiconductor nanowire/superconductor hybridized island, charging energies are introduced and thus even/odd parity of two Majorana zero modes exhibit as a two-level quantum system, which could work as topological qubits. By embedding such hybridized islands into superconducting circuit, not only can trivial Andreev bound states and Majorana bound states be distinguished via the supercurrent phase of the island, but also topological-qubit readout and operation can be performed by supercurrent measurement. Here, we insert an InSb/Al hybridized island into NbTiN superconducting circuit forming a superconducting interference device (SQUID). In such a device, we find switching current of the InSb/Al island depends on its parity and the corresponding superconducting phase also show parity-dependent behaviours. In this way, the parity of bound state residing in hybridized island can be read out, which paves the way for parity read out of Majorana superconducting qubits.

*European Research Council (ERC), the Dutch Organization for Scientific Research (NWO), Microsoft Corporation Station Q.
Session D49 DCMP: Superconductivity in Ruthenates

2:30PM D49.00001: Effect of strain on critical temperature and Pauli-limit critical field of Sr2RuO4 with separable pairing interaction

YUE YU (Presenter), Stanford Univ, STUART BROWN, University of California, Los Angeles, SRINIVAS RAGHU, Stanford Univ — We study the critical temperature and Pauli-limit critical field of Sr2RuO4 as a function of uniaxial strain. A three-band tight-binding model is studied that includes effects of spin-orbit and Zeeman couplings and a separable pairing interaction. We compare with the experiment results obtained assuming pairing in various channels (d-wave, extended s-wave and p-wave). We will highlight the relationship of Tc with Hc2 for different pairing symmetries.

2:42PM D49.00002: Development of new phase in ruthenium oxides using molecular beam epitaxy method

MASAHITO SAKODA (Presenter), MIZUKI HIGASHIIZUMI, SATOSHI TANDA, Hokkaido University — The ruthenium oxides are known to have the layered structure and the anisotropic superconductivity. Especially, Ca2RuO4 shows remarkable property change applied by electrical field or pressure. We focus on Ca2RuO4 and its related compounds to research new phase in order to develop noble physical properties. We prepare the samples using a molecular beam epitaxy system. The substrates are LaAlO3, SrTiO3, CaF2, and YSZ. The growth temperature is 500-800 °C. We used O2, O*, O3 as the oxide source. We measured the X-ray diffraction, energy dispersive X-ray spectroscopy, temperature dependence of electrical resistivity. We have succeeded in fabrication of Ca2RuO4 films. The temperature dependence of electrical resistivity depends on \( \rho \sim \exp(1/T^{1/2}) \) which is consistent with the report by bulk samples. At the day, We will report the challenge to fabricate the Ca2RuO4 films which show metallic or superconductivity. We also fabricated CaRuO3 and CaRu(O,F)3 films. It is confirmed that the magnetic transition temperature is suppressed in the higher F-doped range.

*This work was supported by Takahashi Industrial and Economic Research Foundation, The Japan prize foundation, The Murata science foundation, and Yashima Environment Technology Foundation.
2:54PM D49.00003: Superconducting Sr$_2$RuO$_4$ thin film growth by controlling the structural defects  
JINKWON KIM (Presenter), Department of Physics and Astronomy, Seoul National University, JUNSIK MUN, Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, CARLA PALOMARES-GARCIA, Department of Materials Science and Metallurgy, University of Cambridge, JEONG RAE KIM, LINGFEI WANG, Department of Physics and Astronomy, Seoul National University, SEO HYOUNG CHANG, Department of Physics, Chung-Ang University, MIYOUNG KIM, Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, SUK BUM CHUNG, Department of Physics, University of Seoul, CHANGYOUNG KIM, Department of Physics and Astronomy, Seoul National University, JASON ROBINSON, Department of Materials Science and Metallurgy, University of Cambridge, YOSHITERU MAENO, Department of Physics, Kyoto University, TAE WON NOH, Department of Physics and Astronomy, Seoul National University — The layered perovskite superconductor Sr$_2$RuO$_4$ (bulk $T_c \sim 1.5$ K) has been studied extensively with its possible topological superconductivity and chiral gap function ($p_x \pm ip_y$) [1]. The superconducting Sr$_2$RuO$_4$ thin film has advantages not only for physical advances but also fruitful device application such as quantum computation [2]. However, superconducting Sr$_2$RuO$_4$ film growth has been limited since the superconductivity of Sr$_2$RuO$_4$ is extremely vulnerable to structural defects, especially out-of-phase boundaries (OPBs) [3]. In this presentation, we will present our Sr$_2$RuO$_4$ film growth focused on the suppression of OPBs. By optimizing substrates and growth condition, we achieved epitaxial Sr$_2$RuO$_4$ films with high crystallinity and smooth surfaces, confirmed by X-ray diffraction and atomic force microscopy and transmission electron microscopy. With reduced OPBs, Sr$_2$RuO$_4$ films exhibit superconductivity up to 0.8 K. Our work suggests a novel method to obtain superconducting Sr$_2$RuO$_4$ films enabling Josephson junction or spintronics device based on the Sr$_2$RuO$_4$.


3:06PM D49.00004: Mimicking superconductivity of Sr$_2$RuO$_4$ using SrRuO$_3$-SrTiO$_3$ superlattice  
BONGJAE KIM (Presenter), Physics, Kunsan National University, SERGII KHMELEVSKYI, Institute for Applied Physics, Vienna University of Technology, CESARE FRANCHINI, Faculty of Physics and Center for Computational Materials Science, University of Vienna, IGOR MAZIN, Naval Research Laboratory, KYOO KIM, Max Planck POSTECH/Korea Research Initiative — The putative chiral spin-triplet superconductivity in ruthenate is under intense controversy, where the various theoretical and experimental studies discuss the diverse alternative pairing symmetries. Currently, the investigation is solely focused on only one material, Sr$_2$RuO$_4$, and the field suffers from the lack of comparison target. Here, employing density functional theory-based analysis, we show that the heterostructure composed of SrRuO$_3$ and SrTiO$_3$ is inherent with all the key characteristics of Sr$_2$RuO$_4$, and eventually can host superconductivity. Furthermore, we show that the competing magnetic phases and associated frustration entangled with the superconducting state can be tuned by epitaxial strain engineering. This system offers an excellent platform for the study of superconductivity of the ruthenate system.
The unconventional superconductivity of Sr$_2$RuO$_4$ has been studied extensively due to the claim of unique $p$-wave pairing state, which is under recent scrutiny. One of the main difficulties of determining the pairing symmetry is the accurate estimation of relevant energy scales, which are competing. Small tuning of the microscopic parameters and the resulting evolution of pairing symmetry can offer more insight in the field, which is not easy from the experimental side due to the requirement of extremely clean sample and high-precision measurement. Here, based on the recent proposal of possible superconductivity in SrRuO$_3$-SrTiO$_3$ superlattice, we investigate the pairing symmetry of the system, which can be comparable target of Sr$_2$RuO$_4$. From a DFT calculation, we construct a tight-binding Hamiltonian and search for the pairing symmetry of the heterostructure by calculating the superconducting phase transition temperature. We also study the possibility of pairing transition by tuning the external parameters, which is attainable through epitaxial strain.
3:30PM D49.00006: Constraints on the superconducting order parameter in Sr$_2$RuO$_4$ from oxygen-17 nuclear magnetic resonance

*ANDREJ PUSTOGOW (Presenter), YONGKANG LUO, AARON CHRONISTER, YUE-SHUN SU, University of California, Los Angeles, DMITRY SOKOLOV, FABIAN JERZEMBECK, ANDREW P. MACKENZIE, CLIFFORD W. HICKS, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, NAOKI KIKUGAWA, National Institute for Materials Science, Tsukuba, Japan, SRINIVAS RAGHU, Stanford University, Stanford, ERIC BAUER, Los Alamos National Laboratory, Los Alamos, STUART BROWN, University of California, Los Angeles — The superconducting state of the quasi two-dimensional and strongly correlated perovskite Sr$_2$RuO$_4$ is considered to be a solid-state analogue to the superfluid $^3$He-A phase, with an odd-parity order parameter that breaks time-reversal symmetry. Recent experiments using in-plane uniaxial stress revealed a dramatic rise and peak of the transition temperature [1], related to a DOS enhancement [2]. Here we use $^{17}$O NMR spectroscopy to probe the nature of superconductivity in Sr$_2$RuO$_4$ and its evolution under uniaxial strain. A reduction of the Knight shift is observed below $T_c$ for all strain values, consistent with a drop in spin polarization in the superconducting state [3]. In unstrained samples, our results rule out a chiral $p$-wave order parameter. We discuss the issue of sample heating on a sub-millisecond time scale after the NMR pulse, which is particularly relevant to superconductors with a small transition temperature ($T_c \approx 1$ K).


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Reduced spin susceptibility in superconducting Sr$_2$RuO$_4$ measured by polarized neutron diffraction

ALEXANDER PETSCH (Presenter), MENGZE ZHU, Univ of Bristol, YOSHITERU MAENO, Kyoto University, ZHIQIANG MAO, Tulane University, MECHTHILD ENDERLE, Institut Laue-Langevin, STEPHEN HAYDEN, Univ of Bristol — Superconducting Sr$_2$RuO$_4$ has previously been considered as an analogue of superfluid $^3$He-A [1]. But the picture of odd-order parameter superconductivity with chiral triplet-pairing got recently challenged by the observation of a drop in the $^{17}$O-NMR Knight shift below the superconducting transition [2]. Herein, we present new data on the magnetic susceptibility in Sr$_2$RuO$_4$ collected by polarized neutron scattering. Consistent with the observations in NMR, a reduction below the superconducting transition is observed. In relation to previous work [3] we propose a complicated field dependence alongside large residual susceptibilities at zero temperature, arising from orbital and spin-orbit contributions. Our results support singlet-pairing with a complicated gap-symmetry or triplet-pairing with an in-plane $d$-vector, where time-reversal symmetry is still broken [4].


Understanding reduced NMR signals in Sr$_2$RuO$_4$

AUSTIN LINDQUIST (Presenter), HAE-YOUNG KEE, Univ of Toronto — The superconducting order parameter of Sr$_2$RuO$_4$ has been a topic of recent interest, as new NMR experiments are in contradiction with the previously proposed $p_x \pm ip_y$ triplet superconducting state [1]. The multi-orbital nature of the Fermi surface, in combination with the Hund's and spin-orbit coupling, allows various types of superconducting order parameters. We propose inter-orbital spin triplet pairing based on the Hund's and spin-orbit coupling [2], and study the NMR signals with and without uniaxial strain. These results are compared with recent NMR experiments, and future experiments which can test the validity of the proposed pairing symmetry are also discussed.

Muon spin relaxation studies of time-reversal symmetry breaking superconductivity in Sr$_2$RuO$_4$ along with the application of uniaxial stress and disorder*

SHREENANDA GHOSH (Presenter), VADIM GRINENKO, FELIX BRÜCKNER, RAJIB SARKAR, Institute for Solid State and Materials Physics, Technical University of Dresden, Germany, JEAN-CHRISTOPHE ORAIN, ARTEM NIKITIN, DEBARCHAN DAS, ZURAB GUGUCHIA, Laboratory forMuon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, JOONBUM PARK, MARK E BARTER, Max Planck Institute for Chemical Physics of Solids, NAOKI KIKUGAWA, National Institute for Material Science, Japan, JAKE BOBOWSKI, Department of Physics, Graduate School of Science, Kyoto University, Japan, DMITRY SOKOLOV, Max Planck Institute for Chemical Physics of Solids, TAKUTO MIYOSHI, YOSHITERU MAENO, Department of Physics, Graduate School of Science, Kyoto University, Japan, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, HUBERTUS LUETKENS, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, CLIFFORD W HICKS, Max Planck Institute for Chemical Physics of Solids, HANS-HENNING KLAUSS, Institute for Solid State and Materials Physics, Technical University of Dresden, Germany — After extensive research, the idea regarding the symmetry of the superconducting order parameter of Sr$_2$RuO$_4$ is still lacking a consensus. Recently, NMR experiments have ruled out the well-discussed $p_x \pm ip_y$ state [1]. Nevertheless, complex two-component order parameters are conventionally indicated by time-reversal-symmetry breaking (TRSB) superconductivity. In order to lift the degeneracy between such components, application of uniaxial stress is a plausible method [2]. One key prediction for Sr$_2$RuO$_4$, a splitting of the superconducting and TRSB transitions under uniaxial stress has not been observed so far. We report a large stress-induced splitting between the onset temperatures of superconductivity and TRSB transitions observed by muon spin relaxation (μSR) measurements under uniaxial stress. To perform these technically challenging experiments, a customized uniaxial pressure cell was developed, which will be presented. We also discuss the effect of disorder on the superconducting and TRSB states by μSR, concerning the chirality of the order parameter.


*The work is supported by DFG (GR 4667, GRK 1621, SFB 1143).
Spin-orbital coupling and spin-triplet pairing symmetry in Sr$_2$RuO$_4$  

WANG (Presenter), McMaster Univ, ZHIQIANG WANG, James Franck Institute, Chicago University, CATHERINE KALLIN, McMaster Univ — Spin-orbital coupling (SOC) plays a crucial role in determining the spin structure of an odd parity pseudospin-triplet Cooper pairing state. We discuss how SOC lifts the degeneracy among different p-wave pseudospin-triplet pairing states in a widely used microscopic model for Sr$_2$RuO$_4$ combining a Ginzburg-Landau free energy expansion, a symmetry analysis of the model, and numerical weak-coupling renormalization group, as well as random phase approximation, calculations. These analyses are also used to critically re-examine previous numerical results on the stability of chiral p-wave pairing. The symmetry analysis can serve as a guide for future studies, especially numerical calculations, on the pairing instability in Sr$_2$RuO$_4$ and can be useful for studying other multi-band spin-triplet superconductors where SOC plays an important role.

*This research is supported by the National Science and Engineering Research Council of Canada (NSERC).

Strontium Ruthenate's Superconducting Symmetries from First-Principles Calculations

OLIVIER GINGRAS (Presenter), MICHEL COTE, Universite de Montreal, REZA NOURAFKAN, ANDRE-MARIE TREMBLAY, Universite de Sherbrooke — The normal state of Sr$_2$RuO$_4$ is well understood but its superconducting state is still a subject of major debates [1]. From a first-principles correlated multiorbital calculation, we construct the spin and charge fluctuation pairing interactions. These interactions depend on the proximity to an instability and on the size of the screened Hund's coupling. We present the leading gap function symmetries obtained by solving the frequency-dependent linearized Eliashberg equation for the case where spin-orbit coupling is neglected [2]. Close to magnetic instabilities, we find spin-singlet d-wave pairing. Away, where charge fluctuations increase, we observe the emergence of two even-parity spin-triplet states: an odd in frequency s wave and two degenerate momentum-independent states that pair electrons on different orbitals and are odd in orbital indices. These exotic states are compared with experiments. Moreover, we discuss and present the effects of spin-orbit coupling and uniaxial strain on the system.


*NSERC, FRQNT, CIFAR, Calcul Québec, Calcul Canada, CFREF, Research Chair in the Theory of Quantum Materials.
4:42PM D49.00012: Effects of spin-orbit coupling on the superconducting pairing in Sr$_2$RuO$_4$

WEN HUANG (Presenter), Southern University of Science and Technology, YI ZHOU, Institute of physics, Chinese Academy of Sciences, HONG YAO, Institute for Advanced Study, Tsinghua University — In a superconductor with finite spin-orbit coupling (SOC), neither the orbital nor the spin angular momentum of a Cooper pair is good quantum number, but their sum is. We focus on two aspects of the SOC-influenced superconductivity in Sr$_2$RuO$_4$. In the first[1,2], we argue that the most frequently discussed p-wave state in the $E_u$ representation, which has Cooper pair angular momentum $|L_z,S_z\rangle = |\pm1,0\rangle$, must coexist with another pairing with $|L_z,S_z\rangle = |0,\pm1\rangle$. The two correspond respectively to the gap functions $(k_x,k_y)\hat{z}$ and $k_z(\hat{x},\hat{y})$ in the d-vector notation. If the latter dominates, the $E_u$ superconducting channel would favor a nematic rather than a chiral state. Moreover, in-plane uniaxial strains, which primarily perturb the orbital angular momentum $L_z$ of the Cooper pairs, split the components in the $|\pm1,0\rangle$ pairing linearly and those in the $|0,\pm1\rangle$ pairing quadratically. In the second[3], we show how SOC may inherently entangle spin-triplet and spin-singlet pairings in multi-orbital models of Sr$_2$RuO$_4$. Possible relevance to the recent experiments, such as the uniaxial strain and NMR Knight shift measurements, will be discussed. Refs: [1] Huang and Yao, PRL 121, 157002 (2018); [2] Huang, Zhou, and Yao, arXiv:1901.07041; [3] Huang, Zhou, and Yao, PRB 100, 134506 (2019).

4:54PM D49.00013: Emergence of high-temperature superconductivity in a Ca$_2$RuO$_4$ nanocrystals

HIROYOSHI NOBUKANE (Presenter), KOSEI YANAGIHARA, YUJI KUNISADA, YUNITO OGASAWARA, KAKERU ISONO, KAZUSHIGE NOMURA, KEITA TANAHASHI, TAKAHIRO NOMURA, TOMOHIRO AKIYAMA, SATOSHI TANDA, Hokkaido University — The search for high-temperature (high-$T_c$) superconductors is a fascinating topic in condensed matter physics. It is widely believed that high-$T_c$ superconductivity in cuprates emerges from doped Mott insulators. Recently, 4$d$ and 5$d$ transition metal oxides with a layer perovskite structure have attracted much attention because the possibility of the emergence of high-$T_c$ superconductivity has been recognized in several studies. Here we report the realization of high-temperature superconductivity in Ca$_2$RuO$_4$ nanofilm single crystals. We found that the induced bias current and the tuned film thickness cause a superconductor-insulator transition. We clarify two quantum critical phase transitions corresponding to the clean and dirty limits of the Harris criterion. Our results demonstrate the presence of two-dimensional high-temperature superconductivity in Ca$_2$RuO$_4$ nanofilm.
Possible 'symmetry-imposed' near-nodal superconducting pairing in Sr$_2$RuO$_4$

YU LI (Presenter), Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, WEN HUANG, Shenzhen Institute for Quantum Science and Engineering and Department of Physics, Southern University of Science and Technology — One key feature of the multi-orbital superconducting Sr$_2$RuO$_4$ is the presence of nodal or near-nodal quasiparticle excitations revealed in a wide variety of experiments. Typically, a nodal gap structure in a two-dimensional model would be inconsistent with the chiral or helical p-wave interpretations. However, we demonstrate that true gap nodes may emerge along certain high-symmetry directions on the quasi-one-dimensional Fermi surfaces, if the multi-orbital chiral or helical p-wave pairings acquire peculiar forms wherein the d$_{xz}$ and d$_{yz}$ orbitals develop k$_y$- and k$_x$-like pairings, respectively. Spin-orbit coupling $\eta$ induces a near-nodal gap of order ($\eta^2/W^2$)$\Delta_0$, where $\Delta_0$ is the gap amplitude and W roughly the bandwidth. Provided the aforementioned pairing is predominant, the near-nodal gap structure is robust upon the inclusion of other multi-orbital pairings that share the same symmetries. In light of the recent experimental progresses, our proposal suggests that two-dimensional p-wave pairings may still be viable candidate ground states for Sr$_2$RuO$_4$. A near-nodal helical p-wave order, for example, would also be consistent with the substantial drop in the NMR Knight shift under an in-plane magnetic field.

Monday, March 2, 2020 2:30 PM - 5:06 PM

Session D50 DCMP: Ferromagnetic Order and Instabilities Mile High Ballroom

2:30PM D50.00001: Time-stable remanence in Dzyaloshinskii-Moriya Interaction driven Weak ferromagnets NAMRATA PATTANAYAK (Presenter), Department of Physics, Indian Institute of Science Educaion and Research (IISER), Pune, India — We observe that a number of Dzyaloshinskii-Moriya Interaction (DMI) driven weak ferromagnets (WFMs) including α-Fe$_2$O$_3$, MnCO$_3$ and NiCO$_3$ exhibit two distinct time scale in the magnetization relaxation process as explored through SQUID magnetometry. One of the time scales of relaxation is short and, therefore, leads to a quick decay while the other is ultraslow leading to the observation of a time-stable remanence [1]. Furthermore, the time-stable remanence also varies with the strength of the magnetic field in a very unexpected way. We propose that these unique features of remanence explored in systems of different length scales covering bulk single-crystal to nanocrystallites can be taken as the footprint of weak ferromagnetism. We also find that this time-stable remanence which is intrinsic to WFMs can considerably be tunable by nano scaling as explored in the room temperature WFM α-Fe$_2$O$_3$ synthesized in various shapes, size, and morphologies. Corroborated by the synchrotron XRD measurements the study has provided us crucial insights to optimize the magnitude of time-stable remanence in α-Fe$_2$O$_3$ which has a prominent role in antiferromagnetic spintronics [2].

2:42PM D50.00002: Ferromagnetic kinetic exchange interaction  
NAOYA IWAHARA (Presenter), National University of Singapore, ZHISHUO HUANG, KU Leuven, AKSELI MANSIKKAMÄKI, University of Jyväskylä, VEACHESLAV VIERU, Maastricht University, DAN LIU, Northwestern Polytechnical University, LIVIU CHIBOTARU, KU Leuven — Anderson’s superexchange mechanism is indispensable for the description and prediction of the magnetic interactions in localized spin systems. Within the framework, weak ferromagnetism originates from Goodenough’s mechanism and potential exchange when strong antiferromagnetic kinetic exchange interaction is suppressed. However, Anderson’s model and also its modified version, Zaanen-Sawatzky’s model, fail to catch an important ferromagnetic contribution. Here, we report ferromagnetic kinetic exchange mechanism arising from overlapping of magnetic orbitals and their strong covalency with the bridging orbitals. Contrary to the conventional weak ferromagnetic exchange mechanisms, the present one can be larger than the antiferromagnetic kinetic exchange interaction, resulting in strong stabilization of ferromagnetic state. Based on first principles calculations, we demonstrate that the present mechanism is responsible for strong ferromagnetism in several existing materials with diamagnetic metal bridges: Fe$^{3+}$-Co$^{3+}$-Fe$^{3+}$ and Cu$^{2+}$-Cr$^{6+}$-Cu$^{2+}$ complexes, quasi-one-dimensional Cu chain, La$_4$Ba$_2$Cu$_2$O$_{10}$, and Co chain, Ca$_3$Co$_2$O$_6$.

2:54PM D50.00003: Small Moment, Itinerant Ferromagnetism Discovered in Single Crystalline La$_5$Co$_2$Ge$_3$* 
SCOTT SAUNDERS (Presenter), LI XIANG, Iowa State University, RUSTEM KHASANOV, Paul Scherrer Institut, TAI KONG, Princeton University, QISHENG LIN, SERGEY L. BUD’KO, PAUL C CANFIELD, Iowa State University — Single crystals of monoclinic La$_5$Co$_2$Ge$_3$ were grown using a self-flux method and were characterized by room-temperature powder X-ray diffraction, anisotropic temperature and field dependent magnetization, temperature dependent resistivity, specific heat, and muon spin resonance. La$_5$Co$_2$Ge$_3$ has a Curie temperature ($T_C$) of ~3.8 K, as well as a clear loss of spin disorder scattering in resistivity data and a sharp specific heat anomaly. The magnetism associated with La$_5$Co$_2$Ge$_3$ has $\mu_{\text{eff}} = 0.92$ $\mu_B$ per mol-Co, $\mu_{\text{sat}} = 0.11$ $\mu_B$ per mol-Co, and a change in the entropy at $T_C$ of ~0.05 R ln2 per mol-Co making it a rare, itinerant, low $T_C$ compound.

*This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358, the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4411, and the W.M. Keck Foundation.
LI XIANG (Presenter), SCOTT SAUNDERS, SERGEY L. BUD’KO, PAUL C CANFIELD, Iowa State University — A quantum phase transition is a phase transition that occurs at 0 K. For many second-order phase transitions, application of a magnetic field, doping or pressure can suppress the transition temperature and lead to a quantum critical point (QCP). However, avoided quantum criticality is often observed in intermetallic, ferromagnetic systems. The mechanism behind this phenomenon has been discussed intensively in recent years. Lately, we discovered a new ferromagnetic compound, La$_5$Co$_2$Ge$_3$, which has a Curie temperature $T_C \sim 3.8$ K. The physical properties under pressure and the pressure dependence of $T_c$ are studied up to $\sim 5$ GPa. We find that a ferromagnetic QCP is avoided by the appearance of a new, most likely magnetic, phase. Details of the $T$-$p$ phase diagram and the possible nature of the new phase will be discussed.

*This work was carried out at Iowa State University and supported by Ames Laboratory, US DOE, under Contract No. DE-AC02-07CH11358, by the Gordon and Betty Moore Foundation’s EPiQS Initiative and the W. M. Keck Foundation.

GOPI CHANDRA KAPHLE, Central Department of Physics, Kirtipur, Kathmandu, Nepal, Tribhuvan University, RAMESH DHAKAL (Presenter), SASHI NEPAL, RAM BABU RAY, Central Department of Physics, Tribhuvan University — Mn and Co based Heusler alloys found to exhibit interesting electronic and magnetic properties. We have investigated the effect of electronic and magnetic properties on Mn$_2$CoGa after doping Fe and Cr. Entire calculations were performed through plane wave pseudo-potential method using quantum espresso.

From the calculation it is observed that the band gap of Mn$_2$CoGa shifted (increases) on 25% doping of Fe (or Cr) to its pristine form due to the effect of which shifting the band gap on the right side and shows perfect half-metallicity character. The band gap is found to be 0.307 eV and 0.352 eV for Fe and Cr doping respectively which is also greater than the minority band gap in the pristine (0.113 eV). The decreasing rate of bandgap is more in case of Fe doping than Cr doping. This maybe due to exchange splitting and coulomb repulsion competition. At this case system follows the Slater Pauling’s rule and hence gives rise to integer magnetic moments. If percentage of doping increases non-integer value of total spin magnetic moment is observed indicating that half-metallicity were destroyed. Doping in higher degree drastically increases the Magnetic moments.

*Lumbini Engeening college, Bhalwari, Rupandehi, Nepal and CMPRC Butwal, Rupandehi, Nepal
3:30PM D50.00006: Small angle neutron scattering study of magnetic length scales in disordered ferromagnetic Ni-V alloys.* SHIVA BHATTARAI (Presenter), HIND ADAWI, JEAN GUY L LUSSSIER, ALMUT SCHROEDER, Kent State Univ - Kent, KATHRYN LYNN KRYCKA, National Institute of Standards and Technology — We used small angle neutron scattering (SANS) to reveal magnetic microstructures in a disordered ferromagnet (FM) close to quantum critical point (QCP) where long range order is suppressed with critical temperatures Tc approaching zero. First results of the alloy Ni-V with low Tc are presented on well characterized polycrystalline samples that demonstrated the quantum Griffiths phase signatures for “random” magnetic inhomogeneities [1]. SANS data were collected at NG7SANS, NIST. Full polarization analysis was effective to resolve weak magnetic scattering from dominating nuclear scattering. Angular dependent spin-flip scattering identified magnetic short-range clusters. Angular dependent non-spin-flip interference term recognized long-range magnetic domain contributions. The disordered FM Ni-V presents short-range correlations coexisting with long-range correlations at low temperatures well below Tc in the quantum Griffiths regime close to the QCP.


*This research is supported by ICAM and used resources at NIST provided by the Center of High-Resolution Neutron Scattering (through partnership of NIST and NSF)

3:42PM D50.00007: Unveiling electronic correlation and ferromagnetic superexchange mechanism in van der Waals crystal CrSiTe₃* JIAJIN ZHANG, XIAOCHAN CAI, ShanghaiTech University, LEXIAN YANG, Department of Physics, Tsinghua University, HONGTAO YUAN, Nanjing University, YULIN CHEN, Department of Physics, University of Oxford, SHILEI ZHANG, ZHONGKAI LIU (Presenter), GANG LI, ShanghaiTech University — The recent discovery of intrinsic ferromagnetic order in atomically thin van der Waals crystal CrXTe₃ (X=Si,Ge) stimulates intensive studies on the nature of low-dimensional magnetism. By combining advanced many-body calculations with angle-resolved photoemission spectroscopy we investigate CrSiTe₃ single crystals and unveil the pivotal role played by the strong electronic correlations at both high- and low-temperature regime. Above the Curie temperature (Tc), Coulomb repulsion (U) drives the system into a charge transfer insulating phase. In contrast, below Tc the crystal field arranges the Cr-3d orbitals such that the ferromagnetic super-exchange profits, giving rise to the bulk ferromagnetic ground state with which the electronic correlations compete. The excellent agreement between theory and experiment establishes CrSiTe₃ as a prototype low dimensional crystal with the cooperation and interplay of electronic correlation and ferromagnetism. Ref. [1] J. X. Zhang et al., Phys. Rev. Lett. 123, 047203 (2019)

*This work is supported by grant from the National Key R&D program of China and the National Natural Science Foundation of China.
3:54PM D50.00008: Existence of ferromagnetism in a two-dimensional two species bosonic Hubbard model with the presence of confinement  KALANI HETTIARACHCHILAGE (Presenter), Department of Physics, Seton Hall University, V. G. ROUSSEAU, KA-MING TAM, MARK JARRELL, JUANA MORENO, Department of Physics, Louisiana State University — With recent experimental advances on cold atoms in atomic traps, the realization of exotic magnetic phases in the presence of confinement is an area of renewed interest. We investigate a two-dimensional bosonic Hubbard model with two species in the presence of a harmonic trapping potential. In particular, we focus on the appearance of a novel high entropy ferromagnetic phase at finite doping and polarization. We find that in the presence of confinement, this ferromagnetic phase appears in both hard-core and soft-core bosonic models. In the hard-core limit, we observe phase separation where the heavy species is localized in the center of the trap, and it is surrounded by the light species. In the soft-core limit, we observe that the light species gets trapped in the center of the lattice, and it is surrounded by the heavy species. We link our results with experimental observables relevant for magnetic phases of trapped cold atoms.

4:06PM D50.00009: Z3 ferromagnet to Valence Bond Solid transition in 1d  BRENDEN ROBERTS (Presenter), SHENGHAN JIANG, OLEXEI I MOTRUNICH, Caltech — We continue recent efforts to discover examples of deconfined quantum criticality in one-dimensional models. In this work we focus on the transition between Z3 ferromagnet and Valence Bond Solid (VBS) in a 1d chain with a Z3xZ3 global symmetry. We use a model with alternating projective representations on the sites of the two sublattices. This allows the model to connect to an exactly solvable point which has VBS character as SU(3)-invariant singlets. We find a direct transition from this phase to a ferromagnetically ordered phase breaking Z3 symmetry. Numerical evidence suggests a second-order or extremely weak first-order transition. We characterize the apparent criticality using entanglement scaling and the critical scaling of lattice operators.

4:18PM D50.00010: Physical properties of the van der Waals material Fe$_5$GeTe$_2$  ANDREW MAY (Presenter), Oak Ridge National Lab, DMITRY OVCHINNIKOV, University of Washington, QIANG ZHENG, RAPHAEL HERMANN, STUART CALDER, CRAIG A. BRIDGES, Oak Ridge National Lab, XIAODONG XU, University of Washington, MICHAEL MCGUIRE, Oak Ridge National Lab — van der Waals bonded materials that possess magnetic order at high temperatures are of great interest for integrating magnetic effects into engineered heterostructures. Of the cleavable materials studied so far, Fe$_{5-x}$GeTe$_2$ possesses the highest reported Curie temperature $T_C$ in the bulk and maintains a high $T_C$ in exfoliated flakes. This presentation will discuss the physical properties of Fe$_{5-x}$GeTe$_2$ single crystals, with an emphasis on the metastable nature of the compound and how magnetism on one Fe sublattice dominates the transport properties. The ability to tune the magnetism through cobalt doping will also be briefly discussed.

*This research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division
**4:30PM D50.00011: The effect of Ge substitution on optical properties of FeGa$_3$ single crystals**

AASHISH POUDEL (Presenter), IHOR SYDORYK, Ramapo College of NJ, Mahwah NJ, 07430, RODICA M MARTIN, Montclair State University, Montclair NJ, 07043, USA, CEDOMIR PETROVIC, REN WEIJUN, Brookhaven National Laboratory, NY 11973, USA, CATALIN MARTIN, Ramapo College of NJ, Mahwah NJ, 07430 — Studied initially for its large thermopower effect, the intermetallic semiconductor FeGa$_3$ has recently been shown to provide a suitable platform for studying electron correlations, such as metal-insulator transition, non Fermi liquid behavior and ferromagnetism. In particular, with Ge-doping at Ga site the ground state is tuned from a Kondo insulator to a paramagnetic and further to a ferromagnetic metal. Here we present optical reflectance measurements on single crystals of FeGa$_{3-x}$Ge$_x$, for different values of x. The temperature was varied between 300 K and 5 K, and the frequency ranged from 80 cm$^{-1}$ to 50 000 cm$^{-1}$. From Kramers-Kronig transformation we obtained various optical functions and discuss here the effect of Ge substitution on optical conductivity across all three proposed ground states.

*C. Martin aknowledges NSF support through MRI Grant 1625882.
Work at Brookhaven National Laboratory was supported by the U.S. DOE-BES, Division of Materials Science and Engineering, under contract No. DESC00112704.

**4:42PM D50.00012: Intrinsically weak magnetic anisotropy of cerium in potential hard-magnetic intermetallics**

ANNA GALLER (Presenter), SILKE BIERMANN, LEONID POUROVSKII, Centre de Physique Théorique, Ecole Polytechnique, France — We study the magnetic properties of the "1-12" family of prospective hard-magnetic Ce-Fe intermetallics using an *ab initio* dynamical mean-field theory approach to treat the complex many-electron physics of the Ce 4f$^1$ shell. By considering the hypothetical binary compound CeFe$_{12}$, as well as the realistic compositions CeFe$_{11}$Ti and CeFe$_{11}$TiN, we show that the localization of the Ce 4f electron is strongly sensitive to alloying and interstitials. The onset of heavy-fermion behavior accompanied by a significant reduction of the Ce-4f moment—and concomitantly its contribution to the magnetic anisotropy—is found to occur in CeFe$_{12}$ for a wide temperature range up to about 400K. This 4f delocalization is moderately reduced by Ti substitution on the Fe site and, unexpectedly, markedly increased by nitrogen interstitials. However, even for localized Ce-4f electrons their contribution to the magnetic anisotropy is rapidly suppressed with increasing temperature.

*Agence Nationale de la Recherche (ANR), France
European Research Council
Austrian Science Fund (FWF), Austria
Thickness-dependent magnetic order in CrI$_3$ single crystals

YU LIU (Presenter), LIJUN WU, XIAO TONG, JUN LI, JING TAO, YIMEI ZHU, CEDOMIR PETROVIC

Brookhaven National Laboratory — Two-dimensional (2D) materials with intrinsic ferromagnetism provide unique opportunity to engineer new functionalities in nano-spintronics. One such material is CrI$_3$, showing long-range magnetic order in monolayer with the Curie temperature ($T_C$) of 45 K. Here we study detailed evolution of magnetic transition and magnetic critical properties in response to systematic reduction in crystal thickness down to 50 nm. Bulk $T_C$ of 61 K is gradually suppressed to 57 K, however, the satellite transition at $T^* = 45$ K is observed layer-independent at fixed magnetic field of 1 kOe. The reduction of thickness facilitates a field-driven metamagnetic transition around 20 kOe with out-of-plane field, in contrast to the continuous changes with in-plane field. The critical analysis around $T_C$ elucidates a three-dimensional (3D) long-range magnetic coupling in bulk CrI$_3$, then mean-field type interactions in microscale-thick flake, and evolves into 2D Ising-like ferromagnetism in monolayer.

*Work at Brookhaven National Laboratory was supported by US DOE, Office of Science, Office of Basic Energy Sciences under contract DE-SC0012704.

Magnetic-Competition-Induced Colossal Magnetoresistance in n-Type HgCr$_2$Se$_4$ under High Pressure

JIANPING SUN (Presenter), YUANYUAN JIAO, Institute of Physics, Chinese Academy of Sciences, SACHITH DISSANAYAKE, MASAAKI MATSUDA, Oak Ridge National Laboratory, YOSHIYA UWATOKO, Institute for Solid State Physics, University of Tokyo, YOU GUO SHI, YONGQING LI, ZHONG FANG, JINGUANG CHENG, Institute of Physics, Chinese Academy of Sciences — HgCr$_2$Se$_4$ is a well-known ferromagnetic (FM) semiconductor with $T_C = 106 \sim 120$ K$^1$ and it has received renewed interest recently. Here, we performed the first comprehensive high-pressure study on n-type HgCr$_2$Se$_4$ single crystals and surprisingly found that the FM metallic ground state is destabilized and gradually replaced by an antiferromagnetic (AF) insulating ground state under high pressure. Our combined magnetic susceptibility and neutron measurements under high pressure indicated that the AF order is most likely a spiral-type. On the other hand, the application of external magnetic fields can restore the FM metallic state again at high pressures, resulting in a colossal magnetoresistance as high as $\sim 3 \times 10^{11}$ % under 5 T and 2 K at 4 GPa. Our results demonstrate that HgCr$_2$Se$_4$ situates at a critical point where the competition between FM and AF exchange interactions can be easily tuned by pressure and magnetic field. Thus, our work provides a means for realizing novel state where the extremely large magnetoresistance can be obtained via switching between two distinct electronic ground states in a single-valent system$^2$.


*National Key R&D Program of China
Electronic band structures of FeGe driven by thermal-fluctuation

YANG XU (Presenter), ZIZHAO GONG, RUI SUN, LI NA, XINGQUN ZHANG, WEI HE, ZHAOHUA CHENG, State Key Lab. of Magnetism, Institute of Physics, Chinese Academy of Sciences — Fluctuation-induced first-order transitions have been discussed in superconductors, liquid crystals, and magnetic materials. Recently, chiral magnet, such as FeGe, were found thermal-fluctuation first-order transition above $T_C$, which forms fluctuation disordered state (FD) of magnetic structure. Here, we unveil the Fermi surface symmetry and the evolution of electronic structures across the transition temperature of helimagnetic-paramagnetic phase at $T_C$~274K by means of angle-resolved photoemission spectroscopy (ARPES) on high-quality FeGe(111) films epitaxially grown on Si(111) substrate. The evolution of electronic structures with temperature suggest that FeGe is a Stoner itinerant magnetism. In contrast to ordinary ferromagnetism, a small kink in the integral energy distribution curve (IEDC) at binding energy of 0.5eV in the regime of 274K≤$T_C$≤276K can be identified. This temperature range is the same with the range of FD measured by AC magnetic susceptibility. Therefore, the small kinks on IEDCs imply the contribution of Dzyaloshinskii-Moriya interaction (DMI) on electronic band structure. Our finding paves the path for the theory of the relationship between freedom of spin and electron in itinerant DM helimagnet.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D51 DCMP DMP: Graphene: Electronic Structure and Interactions II; moire and topology

Correlated Insulators in Twisted Double Bilayer Graphene

GREGORY WILLIAM BURG (Presenter), JIHANG ZHU, The University of Texas at Austin, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ALLAN MACDONALD, EMANUEL TUTUC, The University of Texas at Austin — We present a combined experimental and theoretical study of twisted double bilayer graphene with twist angles near 1°. Consistent with moiré band structure calculations, we observe insulators at integer moiré band fillings one and three. Within windows of finite transverse electric fields, the first moiré conduction band is separated from neighboring bands, and we observe correlated insulators at 1/4, 1/2, and 3/4 band filling. The insulators at 1/4 and 3/4 filling emerge in a parallel magnetic field, whereas the resistance at half band filling is weakly dependent on parallel magnetic field. These findings suggest that correlated insulators are favored when a moiré flat band is spectrally isolated, with spin polarization at 1/4 and 3/4 band fillings, and valley polarization at 1/2 band filling.

*This work was supported by the National Science Foundation grant EECS-1610008, Army Research Office under Award W911NF-17-1-0312, and the Welch Foundation. Work was partly done at the Texas Nanofabrication Facility supported by NSF grant NNCI-1542159. K. W. and T. T. acknowledge support from the Elemental Strategy Initiative conducted by the MEXT, Japan and JSPS KAKENHI Grant Numbers JP15K21722.
Correlated states in twisted trilayer graphene

SHAOWEN CHEN, Columbia Univ, VALERIE HSIEH, University of California, Berkeley, MATTHEW A YANKOWITZ, Columbia Univ, KENJI WATANABE, TAKASHI TANIGUCHI (Presenter), National Institute for Materials Science, CORY DEAN, Columbia Univ — Twisted bilayer graphene near the “magic angle” of 1.1 degrees can host low energy flat bands. Here we show tunable band hybridization and correlated states in twisted trilayer graphene, realized by placing monolayer graphene on top of a bernal bilayer graphene. Twisted monolayer-bilayer (tML-BL) devices were fabricated in a dual gate geometry allowing independent tunability of the carrier density and perpendicular displacement field D. For twist angle between 1.4 and 2 degrees the low energy band structure mostly preserves the monolayer and bilayer subbands, with an energy offset tunable with displacement field. At D = 0 the charge neutrality point is semi-metallic with compensated electrons and holes. Mapping the Landau levels as a function of density, D and magnetic field reveals transition between subbands, with a gapped monolayer subband. For twist angle ~ 1.2 degrees, we observed evidence of a flat band and emergent correlated insulating states, which are asymmetrically tunable with displacement field due to the lack of mirror symmetry.

Coexistence of ultraheavy and ultrarelativistic Dirac quasiparticles in sandwiched trilayer graphene.*

CHENYUAN LI (Presenter), STEPHEN CARR, ZIYAN ZHU, EFTHIMIOS KAXIRAS, SUBIR SACHDEV, ALEX KRUCHKOV, Harvard University — Electrons in quantum materials exhibiting coexistence of flat bands piercing dispersive bands can give rise to strongly correlated phenomena, and are associated with unconventional superconductivity. It is known that in twisted trilayer graphene steep Dirac cones can coexist with band flattening, but the phenomenon is not stable under layer misalignments. Here we show that such a twisted sandwiched graphene (TSWG) - a three-layer van der Waals heterostructure with a twisted middle layer - can have very stable flat bands coexisting with Dirac cones near the Fermi energy when twisted to 1.5 degrees. These flat bands require a specific high-symmetry stacking order, and our atomistic calculations predict that TSWG always relaxes to it. Additionally, with external fields, we can control the relative energy offset between the Dirac cone vertex and the flat bands. Our work establishes TSWG as a new platform for research into strongly interacting phases, and topological transport beyond Dirac and Weyl semimetals.

*This work was supported by SNSF Grant No. P2ELP2_175278, NSF Grants No. DMR-1664842 and No. DMR-1231319, and ARO MURI Award W911NF-14-0247. Computations were run on the Odyssey cluster supported by the FAS Division of Science, Research Computing Group at Harvard University.
3:06PM D51.00004: Periodically strained graphene lattice: flat bands*  SLAVISA MILOVANOVIC (Presenter), MISA ANDELKOVIC, LUCIAN COVACI, FRANCOIS M PEETERS, Univ of Antwerp — The conditions for the appearance of flat bands in periodically buckled graphene systems is determined. We use a tight-binding model to calculate the band structure of periodically strained graphene lattice. Three different strain configurations are considered: 1) triangular pseudo-magnetic field (PMF) mode - which is the first two-dimensional buckling mode where flat bands have been observed, 2) hexagonal buckling mode - as a common out-of-plane buckling mode in case of stacking different hexagonal lattices, and 3) herringbone buckling mode - as the lowest energy configuration in the case of large biaxial strains. We examine the band flattening versus the period of the buckling and the strength of the deformation and give predictions for the necessary conditions to access the regime of correlated phases. Our simulations show that the triangular PMF configuration is the most favourable for the appearance of flat bands due to the PMF-induced electron confinement. Similarly as in the case of energy levels of graphene quantum dots in the magnetic field, we find that flat bands show the same dispersion versus the strength of the deformation with energy separation that is inversely proportional to the buckling period.

*This work was supported by the Flemish Science Foundation.

3:18PM D51.00005: Experimental Discovery of High Dimensional Band Topology in Twisted Bilayer Graphene*  CHAO MA (Presenter), Yale University, QIYUE WANG, The University of Texas at Dallas, SCOTT MILLS, Stony Brook University, XIAOLONG CHEN, BINGCHEN DENG, SHAOFAN YUAN, CHENG LI, Yale University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, DU XU, Stony Brook University, FAN ZHANG, The University of Texas at Dallas, FENGNIAN XIA, Yale University — Recently twisted bilayer graphene (t-BLG) emerges as a strongly correlated physical platform near a magic twist angle, hosting the Mott-like insulating phases and unconventional superconducting behavior. Besides, band topology may be another critical element in strongly correlated twistronics. In this work, we performed a systematic nonlocal transport study and revealed the nontrivial high dimensional band topology in t-BLG. Pronounced nonlocal responses are observed both in the electron and hole superlattice gaps of t-BLG, which are robust to the interlayer electric field, twist angle, and edge termination. We elucidate that two high dimensional $Z_2$ invariants characterize the topology of the moiré bands. Our findings provide a new perspective for understanding the emerging strongly correlated phenomena in twisted van der Waals heterostructures.

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Office of Naval Research.
Army Research Office under Grant Number W911NF-18-1-0416.
Natural Science Foundation under Grant Number DMR-1921581 through the DMREF program. Elemental Strategy Initiative conducted by the MEXT, Japan and the CREST (JPMJCR15F3), JST.
3:30PM D51.00006: Flat bands and gaps in twisted double bilayer graphene  RODRIGO CAPAZ (Presenter), FRANCISCO CULCHAC, Federal University of Rio de Janeiro, LEONOR CHICO, Instituto de Ciencia de Materiales de Madrid, ERIC SUAREZ MORELL, Universidad Tecnica Federico Santa Maria — We present electronic structure calculations of twisted double bilayer graphene (TDBG): A tetralayer graphene structure composed of two AB-stacked graphene bilayers with a relative rotation angle between them. Using first-principles calculations, we find that TDBG is semiconducting with a band gap that depends on the twist angle, that can be tuned by an external electric field. The gap is consistent with TDBG symmetry and its magnitude is related to surface effects, driving electron transfer from outer to inner layers. The surface effect competes with an energy upshift of localized states at inner layers, giving rise to the peculiar angle dependence of the band gap, which reduces at low angles. For these low twist angles, the TDBG develops flat bands, in which electrons in the inner layers are localized at the AA regions, as in twisted bilayer graphene.

3:42PM D51.00007: Electric field tunable correlated insulating states and spin-polarized phase transitions in twisted bilayer-bilayer graphene  ORIOL RUBIES-BIGORDA (Presenter), YUAN CAO, DANIEL RODAN-LEGRAIN, JEONG MIN PARK, Massachusetts Institute of Technology MIT, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science (Japan), PABLO JARILLO-HERRERO, Massachusetts Institute of Technology MIT — Understanding how strongly correlated materials behave has been a challenge for the last decades. The recent discovery of superconductivity and correlated insulators in magic angle twisted bilayer graphene (MAGTB) has paved the way to realizing strongly correlated phases of matter using twisted van der Waals heterostructures. We report here on a new correlated platform, twisted bilayer-bilayer graphene (TBBG), which consists of two sheets of Bernal stacked bilayer graphene rotated by a small angle. This system exhibits tunable correlated insulating states at different commensurate fillings. In particular, these insulating states can be switched on and off if an electric displacement field is applied across the sample. The magnetic field response of the correlated insulators in TBBG points towards evidence of spin-polarized ground states. Besides, TBBG shows multiple flat bands near charge neutrality for small twist angles. This results into different correlated states that can be tuned by electric field and are located at half-filling of each flat band. This work contributes to the study of twist-angle and electric-field dependent correlated phases of matter.
3:54PM D51.00008: Lifshitz transitions in magic-angle twisted bilayer graphene*
ZHENGUAN ZHANG (Presenter), SHUANG WU, EVA ANDREI, Rutgers University, New Brunswick — In magic-angle twisted bilayer graphene, the flat band fosters the emergence of rich physics associated with strong correlations. Here we report on magneto-transport measurements of a twisted bilayer graphene device(1.17°±0.02°). From Hall measurements, we extract the Hall number $n_H$, which provides information about the Fermi surface topology as a function of doping within the flat band. At low filling, $|n/n_0| < 2$, we find $n_H = n$ as expected for a system with closed Fermi pockets. Here $n_0$ is the carrier density corresponding to one electron per moire cell. Upon approaching fillings of 2 carriers per moire cell, $n_H$ follows the logarithmic dependence predicted for a Lifshitz transition at a van-Hove singularity. Interestingly on the high doping side of the transition the linear dependence is restored but with an offset, indicating that the Fermi surface shrinks by 2 carriers per moire cell and a correlation gap opens. Moreover, a singular dependence around $±3n_0$ is observed suggesting a Lifshitz transition but without a gap. As the field is increased above 4T a gap opens at $n/n_0 = 3$ signaled by the appearance of a Landau fan and quantized $R_{xy}$ plateaus. At the same time $n_H$ suggests yet another change in the Fermi surface topology.

*Work supported by DOE-FG02-99ER45742, NSF DMR 1708158

4:06PM D51.00009: Chern insulators at odd fillings in magic-angle twisted bilayer
graphene* SHUANG WU (Presenter), ZHENYUAN ZHANG, EVA ANDREI, Rutgers University, New Brunswick — The interplay of magnetic field and the moire superlattice in magic-angle twisted bilayer graphene provides a rich playground for correlated electron physics. We report on magneto-transport measurements of a twisted bilayer graphene device(1.17°±0.02°). At high out-of-plane magnetic fields, we observe Landau fans at integer fillings with well quantized Hall plateaus: $\sigma_{xy}=ve^2/h$, corresponding to integer Chern numbers, $v\in \mathbb{Z}$. These are formally equivalent to the Chern bands of the Hofstadter butterfly formed by the single-particle spectrum of an electron in a periodic potential at high magnetic fields. At fillings of $n/n_0=-1$, we find $v=3$, while at $n/n_0=3, v=1$. Here, $n$ is the total carrier density. $n_0$ is the carrier density corresponding to one electron per moire cell. For these fillings, we find that the field dependence of the Hall number $n_H(B)$ extracted from the Hall resistivity, is non-monotonic indicating the opening of a gap at high fields($B>4T$). This finding is confirmed by measuring the field dependence of the thermal activation gaps for both in plane and out of plane magnetic fields. The linear field dependence of the gaps being consistent with Zeeman splitting, suggests the emergence of a spin-aligned ferromagnetic phase.

*Work supported by DOE-FG02-99ER45742, NSF DMR 1708158
4:18PM D51.00010: Nematicity in twisted bilayer graphene: impact of the moiré superlattice* RAFAEL FERNANDES (Presenter), University of Minnesota, J.W.F. VENDERBOS, Drexel University — Recent experiments have reported evidence that the threefold rotational symmetry of magic-angle twisted bilayer graphene is broken in several regions of the phase diagram, both in the normal state and in the superconducting state. Here, we theoretically investigate the coupling between electronic nematic and moiré superlattice degrees of freedom. Because the nematic transition is described in terms of a three-state Potts order parameter, we show that a true phase transition can still take place even in the presence of externally applied uniaxial strain. Moreover, the nature of the Potts-nematic transition is fundamentally altered by fluctuating strain modes associated with the domain walls separating AB/BA stacking regions of the triangular moiré superlattice. In particular, these fluctuations mediate an effective nemato-orbital coupling that not only renders the nematic transition mean-field and first-order, but also ties the orientation of the nematic director to certain soft directions in momentum space. Finally, we contrast our results to the more familiar case of Ising-nematic order in a tetragonal rigid lattice.

*RMF acknowledges support from the U. S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0020045

4:30PM D51.00011: Z2 topology and edge states of twisted bilayer graphene* CHAO MA, Department of Electrical Engineering, Yale University, QIYUE WANG (Presenter), Department of Physics, University of Texas at Dallas, SCOTT MILLS, Department of Physics, Stony Brook University, XIAOLONG CHEN, BINGCHEN DENG, SHAOFAN YUAN, CHENG LI, Department of Electrical Engineering, Yale University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, DU XU, Department of Physics, Stony Brook University, FAN ZHANG, Department of Physics, University of Texas at Dallas, FENGNIAN XIA, Department of Electrical Engineering, Yale University — Recently twisted bilayer graphene (tBLG) emerges as a new platform of strongly correlated electrons near a magic twist angle, which hosts many exciting phenomena such as the Mott-like insulating phase, unconventional superconducting behavior, and emergent Chern ferromagnetism. Besides the apparent significance of band flatness, band topology may be another critical element responsible for the strongly correlated phenomena (like in the fractional quantum Hall effect) yet receives much less attention. We demonstrate that, while an unusual symmetry of tBLG trivializes the Berry curvature, two Z2 invariants characterize the topology of the moiré Dirac bands. We further show that subtle gapless edge states can survive in the electron and hole superlattice gaps of tBLG and mediate universal nonlocal transport that are robust to the interlayer electric field, twist angle, and edge termination.

*This theoretical work at UTD is supported by Army Research Office under Grant No. W911NF-18-1-0416 and Natural Science Foundation under Grant No. DMR-1921581 through the DMREF program.
**4:42PM D51.00012: Topological Floquet engineering of twisted bilayer graphene**

MICHAEL SENTEF (Presenter), GABRIEL E. TOPP, GREGOR JOTZU, JAMES W MCIVER, LEDE XIAN, ANGEL RUBIO, Max Planck Inst Structure & Dynamics of Matter — We investigate the topological properties of Floquet-engineered twisted bilayer graphene above the magic angle driven by circularly polarized laser pulses. Employing a full Moiré-unit-cell tight-binding Hamiltonian based on first-principles electronic structure, we show that the band topology in the bilayer, at twisting angles above 1.05 degrees, essentially corresponds to the one of single-layer graphene. However, the ability to open topologically trivial gaps in this system by a bias voltage between the layers enables the full topological phase diagram to be explored, which is not possible in single-layer graphene. Circularly polarized light induces a transition to a topologically nontrivial Floquet band structure with the Berry curvature analogous to a Chern insulator. Importantly, the twisting allows for tuning electronic energy scales, which implies that the electronic bandwidth can be tailored to match realistic driving frequencies in the ultraviolet or midinfrared photon-energy regimes.

*DFG Emmy Noether program (No. SE 2558/2-1).
European Research Council (No. ERC-2015-AdG694097).
The Flatiron Institute is a division of the Simons Foundation.

**4:54PM D51.00013: Topological charge pumping by sliding moiré pattern**

MANATO FUJIMOTO (Presenter), Osaka Univ, HENRI KOSCHKE, Physics, Cologne Univ, MIKITO KOSHINO, Osaka Univ — We theoretically study the adiabatic topological charge pumping driven by interlayer sliding in the moiré superlattices. We show that, when we slide a single layer of the twisted bilayer system relatively to the other, a moiré pattern flow and a quantized transport of electrons occurs.[1] When the Fermi energy is in a spectral gap, the number of pumped charges in the interlayer sliding process is quantized to a sliding Chern number, which is related to the interlayer sliding degree of freedom and obeys a Diophantine equation analogous to the quantum Hall effect [2]. We apply the argument to the twisted bilayer graphene, and find that energy gaps above and below the nearly-flat bands has non-zero sliding Chern numbers. When the Fermi energy is in either of those gaps, the slide-driven topological pumping occurs perpendicularly to the sliding direction.


*The authors are supported by JSPS KAKENHI Grant Number JP17K05496.
Artificial gauge field in Moiré superlattices

CE SHANG, ADEL ABBOUT, XIAONING ZANG, UDO SCHWINGENSCHLOEGL, AURELIEN MANCHON (Presenter), King Abdullah Univ of Sci & Tech (KAUST) — Moiré superlattices, originating from rotational alignment or/and lattice constants mismatch between the individual layers, open up new strategies for engineering electronic properties [1]. Gauge fields unveil one of the most ubiquitous concepts which describes many branches of physics, ranging from the standard model to the general theory of relativity. In recent years, artificial gauge field for engineered systems extend their proven quantum simulation abilities further, e.g., to quantum Hall physics or topological insulators [2,3]. Here, we propose a method to create a tunable, artificial gauge potential in a periodically modulated Moiré superlattice. By imprinting Peierls phase on the hopping parameters between neighboring lattice sites, we present the realization of a Haldane-like model and investigate the characterization of its topological band structure. As an application, we also provide a methodology to directly measure topological order in such system from a dynamical quench process.


Multiple topological phases in graphene via magnetoelectric proximity effect

HIROYUKI TAKENAKA (Presenter), SHANE SANDHOEFNER, ALEXEY KOVALEV, EVGENY Y TSYMBAL, University of Nebraska - Lincoln — Topological antiferromagnetic (AFM) spintronics have been drawn special attention for the next generation of non-volatile, ultra-fast, and low-power memory and storage devices. The key to realize the spintronic applications is to manipulate the topological electronic states via switching the AFM order parameter. Here we propose a new approach to control the topological electronic states of a two-dimensional material by the proximity of a magnetoelectric antiferromagnet. Using density functional theory and tight-binding Hamiltonian approaches, we investigate an interface between graphene and AFM magnetoelectric Cr$_2$O$_3$ (0001). Due to the proximity effect, the interface electronic structure exhibits non-trivial band gap openings in the graphene Dirac bands asymmetric between the $K$ and $K'$ valleys. This gives rise to an unconventional quantum anomalous Hall effect (QAHE) and, in addition, the spin-polarized valley Hall effect (VHE). The quantum anomalous Hall effect (QAHE), the valley-polarized QAHE and the quantum valley Hall effect emerge in graphene across a 180 magnetic domain wall in chromia. We theoretically demonstrate that these topological properties are controlled by voltage through magnetoelectric switching of the AFM insulator with no need for spin-orbit torques.
2:30PM D52.00001: Eu intercalation in Highly Ordered Pyrolytic Graphite (HOPG)*  
CHRIS MASI (Presenter), AARON WANG, Univ of Wyoming, NATHAN GUISINGER, Argonne National Laboratory, TE-YU CHIEN, Univ of Wyoming — Recently, two-dimensional (2D) van der Waals (vdW) magnetic materials have been of significant interest. Beside the intrinsic magnetism in the 2D materials, synthesized 2D magnetic materials may provide a wider range of opportunities. To achieve this, we successfully prepared Europium (Eu) intercalated highly ordered pyrolytic graphite (HOPG) through thermal evaporation. The intercalation is evidenced by the atomic resolution scanning tunneling microscopy (STM) measurements. Observations of a shift in dI/dV spectra near the Eu intercalation site indicate the electron doping effect. Next step is to test the transport properties and seek for the magnetoresistance signal.

*US National Science Foundation, Division of Materials Research(DMR) (Grant no. DMR-1710512)

2:42PM D52.00002: First-principles study of electronic structures of two-dimensional Y₂C electride surfaces*  
GUNN KIM (Presenter), JUNSU LEE, GWAN WOO KIM, JINWOONG CHAE, Department of Physics and Astronomy, Sejong Univ — Electrides are attractive ionic compounds in which electrons confined to the narrow interior space in the material act as anions because of their exotic physical and chemical properties such as low work function and efficient electron transfer. In particular, in the case of two-dimensional electride, electrons gather at the interstitial space. In this talk, we report the electronic structure of a two-dimensional Y₂C surface using the first-principles study. We calculate the work function of Y₂C multilayers and analyze how the electronic structure of the material changes when the external electric field is applied. Finally, we discuss what happens to the electronic structure of the Y₂C surface if a Y (or C) atom is missing.

*This work was supported by the General Research Program through the National Research Foundation of Korea (NRF) ) funded by the Korea Government (Grant No. NRF-2019R1F1A1058177).
2:54PM D52.00003: The Moiré Superstructure of Graphene Intercalated with a Co Layer*
CLAUDIA CARDOSO (Presenter), DANIELE VARSANO, ANDREA FERRETTI, S3 Center, Istituto Nanoscienze, CNR, Consiglio Nazionale delle Ricerche — The moiré superstructure of graphene grown on metals can drive the assembly of molecular architectures, such as metal-phthalocyanine molecules, allowing for the production of artificial molecular configurations. A detailed analysis of the Gr/Co interaction upon intercalation (including the resulting moiré pattern) is performed here by density functional theory, providing an accurate description of the template as a function of the corrugation parameters. We pay special attention to the comparison with experimental photoemission data (X-ray Photoemission Spectroscopy, XPS). We then report on empty electron states in cobalt-intercalated graphene, studied by X-ray adsorption spectroscopy and angle-resolved inverse photoemission spectroscopy. The experimental data are compared with theoretical calculations to unveil the dispersion of empty states and the hybridization of graphene π bands at the Gr/Co/Ir(111) interface.

*This work was financially supported by the European Union H2020-EINFRA-2015-1 program (Grant No. 676598 and 824143, project MaX -- MAterials at the eXascale). Computational resources were provided by the ISCRA program (IsB19 ,PHINEGAN) on the Marconi machine at CINECA.

3:06PM D52.00004: A non-invasive SOI gating method for probing 2D transport on pristine chemically-terminated Si surfaces*
LUKE ROBERTSON (Presenter), BRUCE E KANE, University of Maryland, College Park — Silicon has a variety of surface terminations available to it in which surface states are passivated and where 2D electron inversion layers are possible through electrostatic gating. In the Kane lab, Si(111) surfaces are terminated with hydrogen using a simple wet-chemical treatment of high-purity, deoxygenated, aqueous NH₄F. Extremely high mobilities, in excess of 300,000 cm²/Vs [1], have been demonstrated in our previous generation devices, and further refinement of these techniques to preserve the pristine nature of these passivated Si surfaces is expected to yield even higher mobilities. To this end, we have developed a new technique to probe these pristine H-Si surfaces using a non-invasive SOI flip-chip gating assembly in which all critical device fabrication is performed on the SOI end. Additionally, our novel device architecture is fully process-compatible with existing UHV halogen-termination (Cl, Br, I) techniques providing a viable solution for 2D transport studies on these surfaces. Architecture details and 77K characterization of 4-terminal devices with newly-incorporated Au depletion gates will be discussed, as well as ongoing low temperature (4K and below) challenges.


*Laboratory for Physical Sciences
3:18PM D52.00005: Electronic Density of States of CrBr$_3$ studied by Scanning Tunneling Microscopy and Spectroscopy (STM/S)*

DINESH BARAL (Presenter), ZHUANGEN FU, ANDREI S. ZADOROZHNYI, RABINDRA DULAL, AARON WANG, NARENDRA SHRESTHA, JINKE TANG, YURI DAHNOVSKY, JIFA TIAN, TEYU CHIEN, Department of Physics and Astronomy, Univ of Wyoming — CrBr$_3$ is a van der Waals material exhibiting magnetism at the 2D limit. Despite the great attention on magnetic properties, the electronic properties of CrBr$_3$ are relatively unexplored. Here, the study of thin flakes of CrBr$_3$ exfoliated on Highly Ordered Pyrolytic Graphite (HOPG) surface was performed using STM/S. The atomic resolution topography, multi-peak $dI/dV$ measurements on the bulk CrBr$_3$ as well as at the monolayer limit will be presented and discussed. Topography agrees with the crystal structures while the multi-peak $dI/dV$ spectra agree extremely well with reported optical measurements. However, the observed energy gap extracted from the $dI/dV$ measurements is determined to be $\sim0.57$ eV, much smaller than the previously believed $\sim1.7$ eV observed by absorption spectrum. DFT calculated DOS failed to reproduce two peaks near the Fermi energy. Further studies are needed to explain the discrepancy. The mono- and bi-layer flakes depict degradation at the edges due to air exposure during sample transfer. These observations provide important information towards the fundamental understanding of CrBr$_3$.

*Academic Affairs Energy GA Fellowship, University of Wyoming.
U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering (DE-SC0020074)

3:30PM D52.00006: Two-dimensional conductive surface oxide on CrN(001) and Cr$_{1-x}$Al$_x$N(001) films

MARY E MCGAHAY (Presenter), DANIEL GALL, Rensselaer Polytechnic Institute — CrN is a Mott-Hubbard insulator but forms a conductive surface oxide with a sheet conductance $G_s = 5.9 \times 10^{-5}$ [Ω/sq]$^{-1}$ when exposed to oxygen. This is demonstrated by in situ transport measurements on epitaxial CrN(001) layers during a continuously increasing pressure $dp/dt = 0.05$ Pa/s of a 90% Ar - 10% O$_2$ mixture, suggesting the formation of a thin n-type doped layer through substitutional replacement of N surface atoms with O. Low-temperature transport measurements indicate incomplete carrier delocalization in the 2D conductive oxide. Alloying with AlN to form cubic Cr$_{1-x}$Al$_x$N(001) films results in similar conductive surface oxides for $x < 0.62$, an increase in the room temperature resistivity from $\rho = 0.070$ to 26 Ω-cm for $x = 0-0.46$, and an increase in the optical band gap from 0.8 to 4.0 eV for $x = 0-0.85$. Direct oxygen incorporation during reactive deposition in a Ar-N$_2$-O$_2$ mixture yields epitaxial CrN$_{1-x}$O$_x$(001) films with a sheet resistance that decreases by over two orders-of-magnitude from $4.4 \times 10^3$ to 7.5 Ω/sq with an increasing O$_2$ partial pressure $P_{O_2} = 0-0.060$ mTorr, and an insulator-to-metal transition at $P_{O_2} = 0.015$ mTorr. The overall results show that oxygen can be used to control transport in CrN, with potential applications in 2D electronics and thermoelectrics.
3:42PM D52.00007: Topological charge pumping in twisted bilayer graphene* YINHAN ZHANG (Presenter), YANG GAO, DI XIAO, Carnegie Mellon Univ —
We show that a sliding motion between the two layers of a \moire superlattice induces an electric current and realizes a two-dimensional version of the topological Thouless pump when the Fermi energy lies in one of the minigaps. Interestingly, a chiral charge pump, namely, a transverse current induced by the sliding motion, is possible in twisted homobilayers. This result is confirmed by a concrete calculation of the adiabatic current in twisted bilayer graphene. Our work reveals an interesting link between mechanical motion and electricity unique to \moire superlattices, and may find applications in nanogenerators and nanomotors.

*Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division, Pro-QM EFRC (DE-SC0019443).
Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division (DE-SC0012509).
Simons Foundation Fellowship in Theoretical Physics

3:54PM D52.00008: Edge states and no wetting layer in ultrathin Bi(110) films grown on graphene/6H-SiC(0001)* YANFENG LYU (Presenter), SAMIRA DANESHMANDI, SHUYUAN HUYAN, PAUL C. W. CHU, Texas Center for Superconductivity, University of Houston — Ultrathin Bi(110) films have attracted significant attraction recently as a potential candidate for two-dimensional topological insulators. Grown on different substrates, ultrathin Bi(110) films exhibit totally different topological properties. Clarifying charge doping from substrates and wetting layer existing or not will profoundly deepen our understanding of possible topological properties in ultrathin Bi(110) films, which are still under fierce debate. In this talk, we unambiguously demonstrate no wetting layer existing in epitaxial ultrathin Bi(110) films grown on graphene/6H-SiC(0001) using low-temperature scanning tunneling microscopy/spectroscopy (STM/S). Obvious moiré pattern and (6 × 6) reconstruction originating from SiC(001) are clearly observed on the three-monolayer Bi(110) islands, confirming sharp and clean interface between graphene and Bi(110). Gapless edge states are also detected on island edges and domain boundaries, showing a signature of topological nontrivial electronic states in ultrathin Bi(110) films.

*The work performed at Houston is supported by USAFOSR Grant FA9550-15-1-0236, TLL Temple Foundation, JJ&R Moores Endowment, and State of Texas through TCSUH.
4:06PM D52.00009: Superconductivity in monolayer graphene driven by Ca and K doping*

YUKIHIRO ENDO (Presenter), JEHONG JUNG, Department of Physics, Univ of Tokyo, TAKUSHI IIMORI, Institute for Solid State Physics (ISSP), The University of Tokyo, RYOTA AKIYAMA, Department of Physics, Univ of Tokyo, FUMIO KOMORI, Institute for Solid State Physics (ISSP), The University of Tokyo, SHUJI HASEGAWA, Department of Physics, Univ of Tokyo — Superconductivity (SC) induced in graphene has been attracting much attention recently [1, 2]. An example is Ca-intercalated bilayer graphene on SiC [1]. Our structural analysis has unveiled that Ca is intercalated in graphene-buffer interlayer [3], not in graphene-graphene interlayer as analogy of graphite intercalation. Because the position of Ca atoms is on the buffer layer, it can be expected to intercalate Ca atoms into monolayer graphene on SiC. In this study, we have fabricated three samples: Ca-intercalated monolayer graphene grown on SiC(0001), and K or Ca+K adsorbed one on it to change the carrier concentration. Transport measurements have been performed in situ in ultrahigh vacuum. The result shows SC transition at ($T_c =$) 5.5 K, 3.2 K and 1.6 K, respectively. This is the first report of SC in monolayer graphene which has Dirac electrons. The relation between the $T_c$ and the carrier density is different from that of the conventional SC. In the presentation, we will show the details of the experiments and discuss the mechanism of SC. This work was supported by JSPS KAKENHI Grant Number 18K18732, 18K19014, and JSPS fellows.


4:18PM D52.00010: Growth of Silicene on Iodine/Silver (111) studied by low temperature scanning tunneling microscopy

MICHAEL DREYER (Presenter), Physics, University of Maryland, College Park, JENNIFER DEMELL, ROBERT E BUTERA, Laboratory for Physical Sciences — Silicene is the 2D form of silicon. It grows readily on silver (111) as single layers or even bi-layers showing several surface reconstructions in scanning tunneling microscopy images. In an attempt to produce more insulated silicene sheets we grew ~ 0.5 ML of silicon on an almost fully iodine terminated Ag(111) single crystal. For the most part silicene seems to be forming underneath the iodine layer and appears as iodine terminated silicene. In several areas clean silicene sheets were observed. Topographic and spectroscopic data will be discussed.
**4:30PM D52.00011: Emerging electronic states in van der Waals hetero-bilayers** Xianghua Kong (Presenter), Hong Guo, McGill Univ — Bilayer heterostructures have received tremendous attentions in recent years. It is usually believed that electronic structures of stacked van der Waals (vdW) bilayers are simply superposition of their monolayer electronic structures. Here, we show that significant interlayer electronic hybridization occurs even for the most weak-interlayer coupled MoS$_2$/WSe$_2$ bilayer among MoS$_2$/WSe$_2$, MoSe$_2$/PtSe$_2$ and PtS$_2$/PtSe$_2$ bilayers. Several interface states originating from the interlayer S-Se or Se-Se hybridization are explicitly identified by our density functional theory calculations of up to 4000 atoms and confirmed by electrostatic force microscopy (EFM) imaging. In addition, our results also explained the found emerging states within the bandgap of the MoS$_2$/WSe$_2$ bilayer.

*This work is financially supported by the Natural Science and Engineering Research Council (NSERC) of Canada. We thank Compute Canada and the High Performance Computing Center of McGill University for substantial computational support which made this work possible.

**4:42PM D52.00012: Selective adsorption of Dy on intercalated epitaxial graphene** Cai-Zhuang Wang (Presenter), Minsung Kim, Myron Hupalo, Ames Laboratory, Michael C. Tringides, Department of Physics and Astronomy, Iowa State University, Pat A Thiel, Department of Chemistry and Department of Materials Science and Engineering, Iowa State University, Kai-Ming Ho, Department of Physics and Astronomy, Iowa State University — Manipulation of metal deposition and growth morphology on graphene is essential for promising applications of graphene, e.g., magnetic nanoislands for computer memory and stable nanoparticles for catalytic activity. In this study, we present an effective method to control the adsorption and nucleation property of metal ions on graphene via metal intercalation. We experimentally demonstrate that Dy adatoms show highly selective adsorption behavior on Dy-intercalated epitaxial graphene on SiC(0001) by scanning tunnelling microscopy. This adsorption selectivity is theoretically explained by comparing adsorption energies on graphene regions with different intercalation configurations using first-principles methods based on density functional theory. Our results show that the metal intercalation can be an effective way for the functional manipulation of graphene and enlarge the scope of graphene application.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering. The research was performed at Ames laboratory which is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358.
4:54PM D52.00013: Theory of Epitaxial Growth of Borophene on Layered Electride: Thermodynamic Stability and Kinetic Pathway*  XIAOJUAN NI (Presenter), HUAQING HUANG, KYUNG-HWAN JIN, University of Utah, ZHENGFEI WANG, University of Science and Technology of China, FENG LIU, University of Utah — Based on first-principles calculations, we propose that the layered electride can serve as an effective substrate, in place of metal substrate, to grow borophene. We first confirm the thermodynamic stability of B@Sr\(_{2}\)N heterostructures by energetics analysis. Then, kinetically, we identify the atomistic pathways for a preferred 2D growth mode with a mixed triangle-hexagon configuration over 3D growth on the surface of Sr\(_{2}\)N, indicating the feasibility of epitaxial growth of borophene on layered electrides. As a weak metal, the significantly reduced density of states from the electride at the Fermi level helps to retain the most intrinsic electronic and transport properties of borophene, a significant advantage over metal substrate. We envision that layered electrides provide an attractive family of substrates for epitaxial growth of a range of 2D materials that can otherwise only be grown on undesirable metal substrates.

*This work is supported by U.S. Department of Energy-Basic Energy Sciences (Grant No. DE-FG02-04ER46148).

D52.00014: Electronic structures of air-exposed few-layer black phosphorus by optical spectroscopy*  FANJIE WANG (Presenter), GUOWEI ZHANG, SHENYANG HUANG, CHAOYU SONG, CHONG WANG, QIAOXIA XING, YUCHEN LEI, HUGEN YAN, Fudan Univ — The electronic structure of few-layer black phosphorus(BP) sensitively depends on the sample thickness, strain and doping. Here, we show that it's also vulnerable to air-exposure. The oxidation of BP caused by air-exposure gives several optical signatures, including the broadening of resonance peaks and increased Stokes shift between infrared absorption and photoluminescence peaks. More importantly, air exposure causes blue shifts of all resonance peaks in infrared absorption and photoluminescence spectra, with more prominent effects for thinner samples and higher order subband transitions. Our study may provides a convenient and exotic way for band-structure engineering of few-layer black phosphorus through controllable air-exposure or defect creation.

*grants: 11874009, 11734007, 2016YFA0203900 and 2017YFA0303504, XDB30000000, 11804398, 11704075

Monday, March 2, 2020 2:30 PM - 5:18 PM

Session D53 DMP: Novel Phases and Phase Transitions in 2D Materials

Mile High Ballroom 1F - Liuyan Zhao, Univ of Michigan - Ann Arbor - Tag(s): Focus
2:30PM D53.00001: Imaging spinons in a 2D gapless quantum spin liquid [Invited] MICHAEL F CROMMIE (Presenter), University of California, Berkeley — Two-dimensional triangular-lattice antiferromagnets are predicted under some conditions to exhibit a quantum spin liquid ground state whose low-energy behavior is described by a spinon Fermi surface. This “ghost” Fermi surface (in an otherwise insulating material) is a key concept for understanding spin liquids and their relationship to other quantum phases. Directly imaging the spinon Fermi surface, however, is difficult due to the fractional and chargeless nature of spinons. I will discuss how we have used scanning tunneling microscopy (STM) to image density fluctuations arising from a spin liquid Fermi surface in single-layer 1T-TaSe2, a two-dimensional Mott insulator. Quantum spin liquid behavior was observed in isolated single layers of 1T-TaSe2 through long-wavelength modulations of the local density of states at Hubbard band energies. These modulations reflect a spinon Fermi surface instability in single-layer 1T-TaSe2 and allow direct experimental measurement of the spinon Fermi wavevector, in good agreement with theoretical predictions for a 2D quantum spin liquid. Our results establish single-layer 1T-TaSe2 as an ideal platform for studying novel two-dimensional quantum spin liquid phenomena.

3:06PM D53.00002: Intrinsic magnetic topological insulators: MnBi$_2$Te$_4$ and beyond [Invited] YONG XU (Presenter), Department of Physics, Tsinghua University — Intrinsic magnetic topological insulators are novel states of quantum matter possessing both inherent magnetic order and topological electronic states, which offer a fertile playground to explore emergent quantum physics. The antiferromagnetic topological insulator MnBi$_2$Te$_4$ [1-4] is a rapidly rising star in the research field. The material is theoretically predicted to host rich topological quantum states (e.g., topological axion states, magnetic Weyl semimetal, and quantum anomalous Hall (QAH) effect). In addition to theoretical proposals, I will also introduce recent experimental findings, including the discoveries of antiferromagnetic topological insulator states [1,4], QAH effect [5], robust axion insulator and Chern insulator phases [6], high-Chern-number and high-temperature QAH effect [7], helical Chern insulator phase [8], etc. An outlook for future work will be given. Importantly, the working temperature of MnBi$_2$Te$_4$ is limited by its rather weak ferromagnetic exchange, making superior material candidates desirable. In this perspective, I will briefly report an unexpected theoretical finding of room-temperature ferromagnetism and large-gap QAH insulators in lithium-decorated iron-based superconductor materials LiFeX (X=S, Se, Te) [9], which is awaiting for experimental proof.

Reference:
3:42PM D53.00003: Optically probing tunable topology in group V monolayers

GAOFENG XU (Presenter), TONG ZHOU, State Univ of NY - Buffalo, BENEDIKT SCHARF, University of Wurzburg, IGOR ZUTIC, State Univ of NY - Buffalo — Experiments on Bi monolayers on a SiC substrate reveal an interplay between a huge topologically nontrivial gap ~0.8 eV and strong spin-orbit coupling (SOC), leading to striking transport properties such as a robust quantum spin Hall effect (QSHE) [1]. With a suitable choice of substrates it is also possible to remove valley degeneracy and realize multiple Hall effects in a single materials system [2]. In contrast to transport properties, much less is known about how an optical response could yield topological signatures in these group V monolayers. By combining first-principles calculations for different substrates and a careful inclusion of strong SOC in effective models as well as the Coulomb interaction in these monolayers, we show that the changes in optical response reveal topological properties inherent to these systems. We explain how these findings offer new opportunities for proximitized materials [3].


*U.S. DOE, Office of Science BES, under Award No. DE-SC0004890

3:54PM D53.00004: Topological aspects of the band structure of monolayer \beta-Sb in flat and buckled form: Nodal line to unpinned Dirac cones.

SANTOSH KUMAR RADHA (Presenter), WALTER R.L LAMBRECHT, Case Western Reserve University — Monolayer antimonene in the beta structure has a buckled honeycomb structure with a semiconducting band structure. DFT calculations show that a flat honeycomb structure is a metastable state which has been stabilized epitaxially on Ag. In the flat form of Sb, the Fermi level occurs near linear dispersion band crossings, formed by the intersection of two warped Dirac cones, one derived from p_z orbitals and the other from p_x, p_y orbitals. This conical intersection corresponds to a nodal line with a Lissajous pattern in k-space leading to an interesting Fermi surface with electron and hole pockets in different in-plane directions, in other words an in-plane angle dependent carrier polarity (goniopolarity). Tight-binding as well as DFT calculations show that the nodal line breaks up into six individual symmetry protected Dirac points in the slightly buckled form. These Dirac cones are unpinned and can be moved with increasing buckling until Dirac points of opposite winding number annihilate beyond a critical buckling angle. Band structure calculations in the quasiparticle self-consistent GW approximation including spin-orbit coupling show that a gap opens at the various Dirac crossings but lead to an indirect zero gap situation.
4:06PM D53.00005: *Ab initio* study of pressure-driven phase transition in FePS$_3$ and FePSe$_3$*

YEXIN FENG (Presenter), YUESHAO ZHENG, Hunan University — In spite of recent findings about the pressure-driven insulator-to-metal phase transition, and emerging superconductivity of FePS$_3$ and FePSe$_3$, the knowledge about the atomic structures of them is still vague. Here, we investigate the pressure-driven structural phase transitions of FePS$_3$ and FePSe$_3$ from 0 to 35 GPa by using *ab initio* calculations. We find that FePS$_3$ B-I structure transforms to FePS$_3$ B-II phase at about 5 GPa. Then above 17 GPa, FePS$_3$ B-III phase becomes energetically favored. For FePSe$_3$, with increasing pressure, FePSe$_3$ transforms to B-II phase at around 6 GPa and further to B-III phase at about 15 GPa. Our calculation results are consistent with experimentally observed high-pressure induced cell volume collapse, spin-crossovers and insulator-metal transition in FePS$_3$ and FePSe$_3$, which shed new light on understanding the high-pressure physics and phase transitions of FePS$_3$ and FePSe$_3$.

*This study is supported by the National Basic Research Programs of China with grant No. 2016YFA0300901 and the National Science Foundation of China with grant Nos. 11974105, 11604092, 11774429. The computational resources were provided by the supercomputer TianHe in Changsha, China. We also thank Chaoyu He (Xiangtan University) for very useful discussions.

4:18PM D53.00006: Van-der-Waals layered ferroelectric CuInP$_2$S$_6$ I: a quadruple-well potential*

LEI TAO (Presenter), Chinese Academy of Sciences, JOHN A BREHM, Vanderbilt University, SABINE M. NEUMAYER, Oak Ridge National Laboratory, ANDREW O’HARA, Vanderbilt University, MARIUS CHYASNAVICHUS, Oak Ridge National Laboratory, MICHAEL SUSNER, Air Force Research Laboratory, MICHAEL MCGUIRE, SERGEI V. KALININ, STEPHEN JESSE, PANCHARAPAKESAN GANESH, Oak Ridge National Laboratory, SOKRATES T PANTELIDES, Vanderbilt University, PETRO MAKSYMOVYCH, NINA BALKE, Oak Ridge National Laboratory — CuInP$_2$S$_6$ (CIPS) is a van der Waals solid that is ferrielectric below room temperature and has polarization in the stacking direction. Using density-functional-theory calculations, we discovered that, instead of the usual double-well potential, CIPS features a unique quadruple-well potential, with two low-polarization and two high-polarization states, with the latter corresponding to large Cu displacements to the layer surfaces, where they bond to the adjacent layers.[1] The quadruple well is tunable by strain, which can eliminate one or the other of the polar states. Quantum molecular dynamics shed light on the nature of polarization switching in the CIPS environment. The predicted features have been verified by experiments utilizing scanning probe microscopy (next abstract, Maksymovych et al.). The new results and the propensity of CIPS for ionic substitution opens new opportunities to control and generate ferroelectric properties in layered materials.


*Work at CNMS, ORNL supported by DOE BES MSE. At Vanderbilt MSE Div. DE-FG02-09ER46554; LT partially funded by IoP, CAS, Beijing.
4:30PM D53.00007: Van-der-Waals layered ferroelectric CuInP$_2$S$_6$ II: negative
electrostriction and pressure-induced switching*  

JOHN A BREHM, Vanderbilt University,
SABINE M. NEUMAYER, Oak Ridge National Lab, LEI TAO, ANDREW O'HARA, Vanderbilt University,
MARIUS CHYASNAVICHUS, MICHAEL SUSNER, MICHAEL MCGUIRE, SERGEI V. KALININ, STEPHEN JESSE, PANCHAPAKESAN GANESH, Oak Ridge National Lab, SOKRATES T PANTELIDES, Vanderbilt University, PETRO MAKSYMOWYCH (Presenter), NINA BALKE, Oak Ridge National Lab — Layered ferroelectric CuInP$_2$S$_6$ (CIPS) is highly unusual in light of its negative longitudinal piezoelectric coefficient the recently predicted quadruple-well potential (previous abstract, Brehm et al.). Here we show an even larger spectrum of peculiar behaviors, obtained via systematic analysis of nanoscale electromechanical properties with scanning probe microscopy [1]: giant negative electrostriction, coexistence of high and low polarization phases with four distinct polarization orientations, and intrinsic pressure-induced polarization switching. These properties derive from the quadruple potential well for polar displacements, verifying its existence. The combination of unique properties enable deeper insight from microscopic measurements, such as imaging of inhomogeneous strain distribution. More broadly, the peculiarities of CIPS are in large part engendered by its van der Waals structure, thus opening new prospects at the intersection of ferroelectric and 2D materials. [1] J. A. Brehm et al. “Tunable quadruple-well ferroelectric van-der-Waals crystals” Nature Mater., in press.

*Funding: Work at CNMS, ORNL supported by DOE BES MSE. At Vanderbilt MSE Div. DE-FG02-09ER46554; LT partially funded by IoP, CAS, Beijing.
4:42PM D53.00008: Reversible electrical control of stacking order phase transition in few-layer graphene*  
HONGYUAN LI (Presenter), IQBAL UTAMA, SHENG WANG, WENYU ZHAO, SIHAN ZHAO, Department of Physics, University of California, Berkeley, XIAO XIAO, YUE JIANG, Department of Physics, The Chinese University of Hong Kong, LILI JIANG, Department of Physics, University of California, Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, ALEXANDER WEBER-BARGIONI, Lawrence Berkeley National Laboratory, ALEX ZETTL, FENG WANG, Department of Physics, University of California, Berkeley — The layer stacking order has profound effects on physical properties of two-dimensional (2D) van der Waals heterostructures. For example, graphene multilayers can have distinct electronic band structures and behaviors depending on their stacking orders. Fascinating physical phenomena -- such as correlated insulators, superconductors, and ferromagnetism -- can also emerge with a periodic variation of the layer stacking order, known as the moiré superlattice in van der Waals materials. In this work, we demonstrate that a reversible phase transition between different layer stacking orders can be induced globally in few-layer graphene by electrostatic gating. We directly image the gate-induced stacking orders phase transition with infrared near-field optical microscopy. We reveal that both the carrier doping and the vertical electrical field can drive the stacking order phase transition, but with different mechanisms, through a systematic study of dual-gated few-layer graphene. Our findings provide a reversible and non-invasive method to globally control the stacking orders of few-layer graphene, and they have important implications for the understanding of gate-dependent quantum phenomena in graphene moiré superlattices.

*DE-AC02-05-CH11231 (JPMJCR15F3), JST.

4:54PM D53.00009: Electronic Properties and Polarization Profiles of Janus Transition Metal Dichalcogenides*  
KAICHEN XIE (Presenter), TING CAO, University of Washington — In this talk, we will present our recent studies on the structural and electronic properties of Janus transition metal dichalcogenides by density functional theory calculations. For the structural properties, we identify a novel reaction path in the materials conversion from transition metal dichalcogenides monolayers to its Janus form. For the electronic properties, we calculate the electronic band structures and polarization profile of the Janus monolayer, and discuss how these electronic properties can be modified through interlayer interactions. We further connect our theoretical works to experimental measurements.

*This research was partially supported by NSF through the University of Washington Materials Research Science and Engineering Center DMR-1719797. T.C. acknowledges support from the Micron Foundation. Computational resources were provided by Hyak at UW, and the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation under Grant No. ACI-1053575.
**5:06PM D53.00010: Crystallography and Properties of Atomic Chirality in Two-dimensional Helical Crystal Tellurium**

CHANG NIU (Presenter), GANG QIU, Electrical and Computer Engineering, Purdue University, YIXIU WANG, Industrial Engineering, Purdue University, JINGKAI QIN, Electrical and Computer Engineering, Purdue University, JIE JIAN, HAIYAN WANG, Material Engineering, Purdue University, WENZHUO WU, Industrial Engineering, Purdue University, PEIDE (PETER) YE, Electrical and Computer Engineering, Purdue University — Chirality is a fundamental property of nature which is extensively studied in various of fields such as chemistry, material science and biology. In condensed matter physics, chiral crystals bring exotic optical, electrical and magneto properties due to the lack of mirror and inversion symmetry. Tellurium (Te) as one of the chiral materials is formed by van der Waals interaction between each one-dimensional helical chiral atom chains which determine the chirality of the whole crystal, and Te with opposite chiralities are described by different space groups: P3\(_1\)21 (right-handed) and P3\(_2\)21 (left-handed). Here we report that two dimensional tellurium twin flakes were identified with opposite chirality by electron crystallographic techniques (high-resolution transmission electron microscope image along different primary axes) and sulfuric acid etching method. These Te twin flakes offers an ideal platform to study the chirality-dependent material properties which can potentially be distinguished in electronic structure and transport properties. Our results pave a way for the research in fundamental properties of chiral materials in two-dimensional limit.

*The synthesis of 2D Te materials is supported by the National Science Foundation under Grant CMMI-1762698.

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**Monday, March 2, 2020 2:30 PM - 5:30 PM**

**Session D54 DCMP: Construction and detection of topological orders**

Mile High Ballroom 2A

**2:30PM D54.00001: A defect TQFT approach to fractons**

DAVID AASEN (Presenter), Microsoft Quantum, Microsoft Station Q, University of California, Santa Barbara, DANIEL BULMASH, University of Maryland, College Park, ABHINAV PREM, Princeton University, KEVIN SLAGLE, Physics, Caltech, DOMINIC WILLIAMSON, Physics, Stanford — We explore fracton phases from the perspective of topological quantum field theories. We argue that type I and type II gapped fracton models can be realized by a network of defects embedded into various 3+1D topological quantum field theories. The idea is that subdimensional excitations characteristic of fracton phases can appear due to mobility restrictions imposed by the defect network. We explicitly construct many well known examples of fracton phases and a few new models using the defect construction. As a byproduct the defect construction provides a generalized membrane-net condensate picture of fracton phases.

*This work was supported by a postdoctoral fellowship from the Gordon and Betty Moore Foundation, under the EPIQS initiative, Grant GBMF4304.
THOMAS SCHUSTER (Presenter), University of California, Berkeley, NATHANAN TANTIVASADAKARN, ASHVIN VISHWANATH, Harvard University, NORMAN YAO, University of California, Berkeley — Fractons are three-dimensional phases distinguished by the restricted mobility of their quasiparticles, and share many similarities to topological order in two dimensions. In this talk, we demonstrate that boundaries of well-known fracton models feature anomalous constraints arising from the emergent conservation laws that govern the bulk fracton order, in a manner similar to 2D topological orders such as the toric code. These constraints restrict the allowed boundary operators to those that commute with certain subsystem symmetry operations, determined both by the bulk fracton order and the direction of boundary termination. The constraints are anomalous in the sense that they cannot arise in any 2D local theory; we demonstrate this from a microscopic perspective, showing that the boundary operators' anticommutation relations are inconsistent with the constraints in any such theory. This gives rise to a rich phase diagram for the boundary theory, in correspondence with that of local 2D subsystem-symmetric systems.

ANDREY GROMOV (Presenter), Physics, Brown University — I will describe an effective field theory approach to the fracton order. In particular I will show how to construct a U(1) version of the Haah code from the principles of symmetry and gauge invariance.

HAN YAN (Presenter), Okinawa Inst of Sci & Tech — In this talk we reason that there is a universal picture for several different holographic toy model constructions, and a gravity-like bulk field theory that gives rise it. First, we observe that the perfect tensor-networks and hyperbolic fracton models are both equivalent to the even distribution of bit-threads on geodesics in the AdS space. Such picture is also a natural "leading-order" approximation to the holographic entanglement properties. Then, we argue that the rank-2 U(1) theory with linearized diffeomorphism as its gauge symmetry, also known as a case of Lifshitz gravity, is the bulk field theory behind such picture. The Gauss' laws and spatial curvature require the electric field lines along the geodesics to be the fundamental dynamical variables, which lead to geodesic string condensation. These results provide an intuitive way to understand the entanglement structure of gravity in AdS/CFT.

*HY is supported by the Theory of Quantum Matter Unit at Okinawa Institute of Science and Technology, and the Japan Society for the Promotion of Science (JSPS) Research Fellowships for Young Scientists.
Localized representation and surface signature of Hopf insulators.
ALEKSANDRA NELSON (Presenter), Physik-Institut, University of Zurich, ARIS ALEXANDRADINATA, Department of Physics, University of Illinois at Urbana-Champaign, ALEXEY SOLUYANOV, Physik-Institut, University of Zurich — The Hopf insulator is a 3D topological insulator that can't be described in terms of a 10-fold classification. It also differs from fragile topological insulators. The main requirement for its existence is a two-rank Hamiltonian. In case when Hopf Hamiltonian has a trivial first Chern class, it obeys Z classification.

In our work, we address two questions. Firstly, we study the possibility for the Hopf insulator to possess localized Wannier representation and the existence of its topological obstructions. We propose that Wannier functions are exponentially localized and preserve the symmetries of the system. What obstructs the equivalence of the Hopf insulator to the atomic limit is the finiteness of the Wannier function width.

The second part of our work is related to the surface signature of the Hopf insulator. We claim that the surface states can be gapped out by surface potential without violating the symmetry or closing the bulk gap. However, surface states have a nontrivial first Chern number that equals to the bulk Hopf invariant. This bulk-edge correspondence can be explained by a new type of bulk-to-boundary Berry curvature flow originating from gauge-invariant magnetoelectric polarizability.

Lattice models that realize $\mathbb{Z}_n$-1-symmetry protected topological states for even $n^*$
LOKMAN TSUI (Presenter), XIAO-GANG WEN, Massachusetts Institute of Technology MIT — We study the lattice model of $\mathbb{Z}_n$-1-symmetry protected topological states (1-SPT) in 3+1D for even $n$. We write down an exactly soluble lattice model and study its boundary transformation. On the boundary, we show the existence of anyons with non-trivial self-statistics. For the $n=2$ case, where the bulk classification is given by an integer $m \mod 4$, we show that the boundary can be gapped with double semion topological order for $m=1$ and toric code for $m=2$. The bulk ground state wavefunction amplitude is given in terms of the linking numbers of loops in the dual lattice. Our construction can be generalized to arbitrary 1-SPT protected by finite unitary symmetry.

*LT is supported by the Croucher Fellowship for Postdoctoral Research. XGW is partially supported by NSF Grant No. DMS-1664412.
3:42PM D54.00007: Strong 3D planar subsystem symmetry-protected topological phases and their dual fracton orders*  TRITHEP DEVAKUL (Presenter), Princeton University, WILBUR SHIRLEY, Department of Physics, California Institute of Technology, JUVEN C WANG, Center of Mathematical Sciences and Applications, Harvard University — We classify subsystem symmetry-protected topological (SSPT) phases in 3+1D protected by planar subsystem symmetries: short-range entangled phases which are dual to long-range entangled abelian fracton topological orders via a generalized `gauging' duality. We distinguish between weak SSPTs, which can be constructed by stacking 2+1D SPTs, and strong SSPTs, which cannot. We identify signatures of strong phases, and show by explicit construction that such phases exist. A classification of strong phases is presented for an arbitrary finite abelian group. Finally, we show that fracton orders realizable via p-string condensation are dual to weak SSPTs, while those dual to strong SSPTs do not admit such a realization.

*This work is supported by the Charlotte Elizabeth Procter Fellowship at Princeton University. W.S. is supported by the National Science Foundation under award number DMR-1654340 and the Institute for Quantum Information and Matter at Caltech. J.W. was supported by NSF Grant PHY-1606531, Institute for Advanced Study, NSF Grant DMS-1607871 `\Analysis, Geometry and Mathematical Physics", and the Center for Mathematical Sciences and Applications at Harvard University.

3:54PM D54.00008: Coupled wire constructions of 3D topological phases*  JOSEPH SULLIVAN (Presenter), Yale University — We present a general coupled wire construction in 3D in an effort to study novel topological phases of matter. Starting by stacking 1D quantum wires of free Dirac fermions into a rectangular array, interactions are added by introducing back scattering terms. The gapping terms are chosen to act on each plaquet of the array. By construction they mutually commute and hence completely gap out the bulk. The resulting theory is very rich, exhibiting many of the hallmarks of topological phases. We compute the ground state degeneracy on the 3 torus and study particular realizations which support fracton-like excitations.

*This work is supported by the NSF under award number DMR-1846109 and the Alfred P. Sloan research fellowship.
4:06PM D54.00009: Modeling Electron Fractionalization with Unconventional Fock Spaces

EMILIO COBANERA (Presenter), Department of Mathematics and Physics, SUNY Polytechnic Institute — It is shown that certain fractionally-charged quasiparticles can be modeled on D-dimensional lattices in terms of unconventional yet simple Fock algebras of creation and annihilation operators. These unconventional Fock algebras are derived from the usual fermionic algebra by taking roots (the square root, cubic root, etc) of the usual fermionic creation and annihilation operators. If the fermions carry non-Abelian charges like spin, then this approach fractionalizes the Abelian charges only. In particular, the mth-root of a spinful fermion is an operator that carries charge e/m and spin 1/2. While the exclusion statics is fixed by the root operation, there are several possible choices of quantum exchange statistics for fermion-root quasiparticles. These choices are tied to the dimensionality D = ... 1, 2, 3, of the lattice and the exchange statistics between fermions and fractionalized fermions. As an application of potential mesoscopic interest, I investigate numerically the hybridization of Majorana and parafermion zero-energy edge modes caused by fractionalizing but charge-conserving tunneling.


4:18PM D54.00010: Fractionalization and Anomalies in Symmetry-Enriched U(1) Gauge Theories

LIUJUN ZOU (Presenter), Perimeter Institute, SHANG-QIANG NING, University of Hong Kong, MENG CHENG, Yale University — We classify symmetry fractionalization and anomalies in a 3+1d U(1) gauge theory enriched by a global symmetry group G. We find that, in general, a symmetry-enrichment pattern is specified by 4 pieces of data: \( \rho \), a map from \( G \) to the duality symmetry group of this U(1) gauge theory, \( \nu \in H^2(\rho[G, U_T(1)]) \), \( p \in H^1(G, Z_T) \), and a torsor \( n \) over \( H^3(\rho[G, Z]) \). However, certain choices of \((\rho, \nu, p, n)\) are not physically realizable, i.e., they are anomalous. There are two levels of anomalies. The first level of anomalies, deconfinement anomalies, obstruct fractional excitations being deconfined. States with these anomalies can be realized on the boundary of a 4+1d long-range entangled state. In the absence a deconfinement anomaly, there can still be the more familiar ’t Hooft anomaly, which forbids certain types of symmetry fractionalization patterns to be implemented in an on-site manner. States with these anomalies can live on the boundary of a 4+1d short-range entangled state. We apply our results to some interesting physical examples.

* S.Q.N. is supported by NSFC (Grant Nos.11574392, 11574172), the Ministry of Science and Technology of China (Grant No. 2016YFA0300504). L.Z. is supported by NSF grant DMR-1608505. M.C. is supported by Alfred P. Sloan Research Fellowship and NSF CAREER (DMR-1846109).
4:30PM D54.00011: Coupled Wire Model of $\mathbb{Z}_2 \times \mathbb{Z}_2$ Orbifold Quantum Hall States*  POK MAN TAM (Presenter), Physics and Astronomy, University of Pennsylvania, YICHERN HU, Physics, University of Oxford, CHARLES L KANE, Physics and Astronomy, University of Pennsylvania — We construct a coupled wire model for a sequence of non-Abelian quantum Hall states occurring at filling factors $\nu = 2/(2M+q)$ with integers $M$ and even(odd) integers $q$ for fermionic(bosonic) states. They are termed $\mathbb{Z}_2 \times \mathbb{Z}_2$ orbifold states, which have a topological order with a neutral sector described by the $c=1$ orbifold conformal field theory (CFT) at radius $R^2 = p/2$ with even integers $p$. When $p=2$, the state can be viewed as two decoupled layers of Moore-Read (MR) state, whose neutral sector is described by the Ising $\times$ Ising CFT and contains a $\mathbb{Z}_2 \times \mathbb{Z}_2$ fusion subalgebra. We demonstrate that orbifold states with $p > 2$, also containing a $\mathbb{Z}_2 \times \mathbb{Z}_2$ fusion algebra, can be obtained by coupling an array of MR $\times$ MR wires together through local interactions. The corresponding charge spectrum of quasiparticles is also examined. The orbifold states constructed here are complementary to the $\mathbb{Z}_4$ orbifold states, whose neutral edge theory is described by orbifold CFT with odd integer $p$ and contains a $\mathbb{Z}_4$ fusion algebra.

*This work is in part supported by the Croucher Scholarship for Doctoral Study from the Croucher Foundation (PMT), grant EP/S020527/1 from EPSRC (YH) and a Simons Investigator grant from the Simons Foundation (CLK).

4:42PM D54.00012: Properties of the Dice-Lattice and its Ribbons  RAHUL SONI (Presenter), NITIN KAUSHAL, ELBIO DAGOTTO, SATOSHI OKAMOTO, University of Tennessee, Knoxville — Previous theoretical studies established the existence of nearly flat bands with non-zero Chern numbers in the dice lattice using non-interacting electrons in the presence of spin-orbit coupling and magnetic field [1]. To pave the way towards the introduction of Hubbard correlation effects via numerical methods here we explore if the main properties of the dice lattice survive in ribbons where one direction is made much shorter than the other [2]. Surprisingly, we find a rich eigenvalue spectrum that continues to display flat bands even for the smallest ribbon such as the $N \times 2$. Real-space charge currents moving along the edges clearly develop. We observed the presence of non-zero Hall-conductance ($\sigma_{xy}^H$) and associated Quantum Anomalous Hall effect for all the ribbons investigated [3]. Time allowing, preliminary results for the effects of interaction ($U$) at half-filling on these ribbons will also be discussed using DMRG. In particular, for the $N \times 2$ system when no magnetic field is present the ground state is ferri-magnetic increasing $U$. The evolution of the edge currents with increasing $U$ will be presented.

Anyonic partial transpose

HASSAN SHAPOURIAN (Presenter), Harvard University, ROGER MONG, University of Pittsburgh, SHINSEI RYU, University of Chicago — A basic diagnostic of entanglement in mixed quantum states is known as the positive partial transpose and the corresponding entanglement measure is called the logarithmic negativity. Despite the great success of logarithmic negativity in characterizing bosonic many-body systems, generalizing the partial transpose to fermionic systems remained a technical challenge until recently when a new definition that accounts for the Fermi statistics has been put forward. In this talk, I will present our attempts to generalize partial transpose to anyons with fractional statistics. It turns out that there is a connection between the partial transpose and braiding statistics. As an application, I will show how the braiding matrix can be used to reproduce many-body topological invariants of 1D time-reversal symmetric topological superconductors.

Detecting Topological Order at Finite Temperature Using Entanglement Negativity*

TSUNG-CHENG LU (Presenter), University of California, San Diego, TIMOTHY HSIEH, Perimeter Institute for Theoretical Physics, TARUN GROVER, University of California, San Diego — We propose a scheme to diagnose finite temperature topological order using the long-range component of entanglement negativity, dubbed topological entanglement negativity. As a demonstration, we study the toric code model in d spatial dimension for d=2,3,4, and find that a topological ordered state at finite temperature has non-zero topological entanglement negativity, whose value is equal to topological entanglement entropy at zero temperature. To calculate entanglement negativity, we develop a general tool for any commuting projector Hamiltonians to derive the spectrum of a thermal state under partial transpose, allowing us to map the calculation of negativity to a classical statistical mechanics problem. Relatedly, using the idea of minimally entangled typical thermal states, we derive necessary conditions for the existence of finite temperature topological order in any CSS code Hamiltonians.

*This project is supported by an Alfred P. Sloan Research Fellowship.

Aharonov-Bohm Effect without Using Vector Potential

XIANG LI (Presenter), Shanghai Jiao Tong University, HANS HANSSON, Stockholm University, WEI KU, Tsung-Dao Lee Institute — Aharonov-Bohm effect is a pure quantum effect that describes a phase shift of a quantum particle due to magnetic flux present in space inaccessible to the particle. Such a non-local effect appears to be impossible classically given the locality of coupling between a particle and magnetic field. Typically, this effect is accounted for via the use of a gauge-dependent vector potential, which extends to the entire space beyond the region with finite magnetic field and thus recovers the locality of the theory. This leads to a perspective of electromagnetic potential being more “fundamental” than the electromagnetic field in quantum mechanics, despite the gauge dependent nature of the vector potential. Here, we demonstrate that this effect can be completely accounted for by consideration of the gauge invariant magnetic field only, if the entire system is included in the analysis. This gauge invariant picture provides an alternative intuitive physical understanding that explicitly encapsulates the non-locality of quantum mechanics in the presence of magnetic field.
2:30PM D55.00001: Strain induced semimetal-insulator transition in monolayer 1T'-WTe₂
ZHAO CHENXIAO (Presenter), JINFENG JIA, Shanghai Jiao Tong Univ, JUNWEI LIU, department of physics, ust.hk — Monolayer 1T'-WTe₂ has exhibited clear quantized transportation originated from the quantum spin Hall phase, while the channel length with quantized conductance is restricted around 100 nm due to its semimetallic nature. To overcome this problem, it is crucial to find a way to engineer the electronic structure. Through a combined in-situ scanning tunneling microscopy/spectroscopy (STM/STS) and Density functional theory (DFT) study, we demonstrate that strain can effectively manipulate the band structure of monolayer 1T'-WTe₂ to realize a phase transition from a semimetal to an insulator upon application of a compressive strain along a axis or a tensile strain along b axis. Moreover, the topological edge states are found to be very robust against strains. Besides, we find that the out-of-plane distortions can also significantly change the band structure. Our results reveal the clear strain dependence of electronic properties and phases of monolayer 1T'-WTe₂, which provides an effective approach to realize the long-coherent quantized conductance for the further transport experiments verification.

2:42PM D55.00002: Finite-temperature spectroscopy in dirty helical Luttinger liquids*
TZU-CHI HSIEH (Presenter), Department of Physics, University of Colorado, Boulder, YANG-ZHI CHOU, Department of Physics, University of Maryland, College Park, LEO RADZIHOVSKY, Department of Physics, University of Colorado, Boulder — I will discuss a theory of finite-temperature momentum-resolved tunneling spectroscopy (MRTS) for disordered two-dimensional INTERACTING topological-insulator edges. The MRTS setup measures the spectral properties and THUS provides a complementary way (distinct from transport) to characterize helical Luttinger liquid edges of topological insulators. The (exact within bosonization) finite-temperature spectral function and the tunneling current of MRTS are derived in the presence of disorder and interaction. The theory provides a detailed analytical characterization of MRTS between helical edges, that should be of interest for corresponding experimental studies.

*Supported by the Simons Investigator Award through the James Simons Foundation (to LR)
2:54PM D55.00003: Atomically resolved study of the effect of back-gating on the band structure in monolayer WTe$_2$* YULIA MAXIMENKO (Presenter), YUEQING CHANG, LUCAS WAGNER, VIDYA MADHAVAN, University of Illinois at Urbana-Champaign — Two-dimensional topological materials have generated a lot of excitement as systems potentially exhibiting quantum spin Hall (QSH) effect, ballistic 1D transport, and helical edge modes. Monolayer 1T’-WTe$_2$ has been demonstrated to be both a QSH insulator and a superconductor upon doping using electronic transport and photoemission spectroscopy on single crystal flakes and epitaxial films. Atomically-resolved scanning tunneling microscopy (STM) also demonstrated clear edge states on WTe$_2$ monolayer islands. Here, we report the first STM study of monolayer 1T’-WTe$_2$ with in-situ tuning of carrier concentration using back-gating. We demonstrate band structure changes in response to doping and back-gating and use first principle calculations to explain the observed effects.

*The STM studies were supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award #DE-SC0014335, and in part by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4860.

3:06PM D55.00004: Resolving the topological classification of bismuth with topological defects ABHAY NAYAK (Presenter), JONATHAN REINER, RAQUEL QUEIROZ, HUIXIA FU, Weizmann Institute of Science, CHANDRA SHEKHY, Max Planck Institute for Chemical Physics of Solids, BINGHAI YAN, Weizmann Institute of Science, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, NURIT AVRAHAM, HAIM BEIDENKOPF, Weizmann Institute of Science — Bulk boundary correspondence has been the cornerstone in the study of topological quantum materials. It has enabled the exploration of electronic bulk properties through the investigation of topological boundary modes. However, the growing diversity and profusion of topological classes has lead to ambiguity between classes sharing similar boundary phenomenology. This is the current status of bismuth, for which recent studies have suggested nontrivial classifications like strong or higher-order TI, both of which hosts 1D helical modes on their boundaries. Here, we use a novel approach to resolve the topological classification of bismuth by spectroscopically mapping the response of a topological lattice defect like screw dislocation using a scanning tunneling microscope. We find a 1D edge mode, bound to the step edges of bismuth, extending to the core of the screw dislocation without gapping out. This signifies that the edge mode binds to the topological defect, characteristic of a material with nonzero weak indices. This work paves the way for the identification of novel electronic topological phases through the study of boundary modes associated with topological defects.
Domain walls as possible realization of edge state coupling in a quantum spin Hall insulator  RAUL STÜHLER, ANDRÉ KOWALEWSKI, FELIX REIS, JOHANNES WEIS, JOERG SCHAEFER, Universität Würzburg, Germany, GANG LI, ShanghaiTech University, China, WERNER R HANKE, DIMITRI JUNGBLUT, BENEDIKT SCHARF, FERNANDO DOMINGUEZ TIJERO, EWELINA M HANKIEWICZ, RALPH CLAESSEN (Presenter), Universität Würzburg, Germany — The recently discovered monolayer system bismuthene/SiC(0001) is a promising candidate for the realization of a room temperature quantum spin Hall (QSH) effect. Previous experiments have established a large fundamental band gap (0.8 eV) and the existence of one-dimensional metallic edge states [1]. As expected for a QSH insulator, the electronic edge channels do not show any signs of backscattering from kinky edge sections that would manifest in interference phenomena. Notwithstanding, topological protection against defect scattering may become lifted when two helical edge channels are brought into direct proximity, resulting in quantum interference. By scanning tunneling microscopy we study phase-slip domain boundaries (DB) that form as result of bismuthene being a rt3 x rt3 R30° reconstruction on SiC(0001) as substrate. Kinks and disorder limit the longitudinal extent of these quasi one-dimensional topographic defects. By spectroscopic means we scrutinize quasi-particle interference along the DB that points towards a linear electronic dispersion strongly reminiscent of a Fabry-Pérot resonator. We discuss our findings as possible quantum interference between coupled helical edge states that are formed in the vicinity of a DB.


Drumhead surface state in ZrSiTe probed by scanning tunneling microscopy  BRANDON A STUART, SEOKHWAN CHOI (Presenter), JISUN KIM, Stewart Blusson Quantum Matter Institute, University of British Columbia, RAQUEL QUEIROZ, Department of Condensed Matter Physics, Weizmann Institute of Science, LUKAS MUECHLER, Center for Computational Quantum Physics, The Flatiron Institute, LESLIE Schoop, Department of Chemistry, Princeton University, DOUGLAS ANDREW BONN, SARAH A BURKE, Stewart Blusson Quantum Matter Institute, University of British Columbia — The family of materials ZrSiX (X = S, Se, Te) are topological nodal-line semimetals characterized by linear band crossings in 1-dimensional lines or loops in momentum space, rather than discrete points as in Dirac or Weyl semimetals. ZrSiTe has a non-symmorphic crystal symmetry, protecting nodal lines at high symmetry lines in the Brillouin zone (BZ). ZrSiTe is host to four nodal lines, two of which form loops in the BZ, one encircling gamma and the other encircling Z, and the other two forming lines that extend through the BZ. It was theoretically predicted that in the surface projection of ZrSiTe, the area between the nodal loops would contain a drumhead state, an exotic, topologically protected 2-dimensional surface state that links the nodal loops together [1]. Surface states have long been probed by scanning tunneling microscopy (STM) using quasiparticle interference (QPI) measurements, and have also been able to provide additional information on the topological nature of these states. Here, we show the first observed signature of electronic scattering within the drumhead state using low-temperature STM and QPI measurements.

3:42PM D55.00007: Symmetry dictated grain boundary state in a two-dimensional topological insulator MoTe$_2$  HYO WON KIM (Presenter), Samsung Adv Inst of Tech, SEOUNG-HUN KANG, HYUN-JUNG KIM, KISUNG CHAE, Korea Institute for Advanced Study, SUYEON CHO, Ewha Womans University, WONHEE KO, Oak Ridge National Laboratory, SANGJUN JEON, Chung-ang University, SUNG WNG KIM, Sungkyunkwan University, YOUNG-KYUN KWON, Kyung Hee University, YOUNG-WOO SON, Korea Institute for Advanced Study — Structural imperfections such as grain boundaries (GBs) and dislocations are ubiquitous in solids and have been of central importance in understanding the nature of polycrystals. In addition to their classical roles, the advent of topological insulators (TIs) offers a chance to realize distinct topological states bound to them. Although dislocations inside three-dimensional TIs are one of the prime candidates to look for, their direct detection and characterization is challenging. Instead, in two-dimensional (2D) TIs, their creations and measurements are easier and, moreover, topological states at the GBs or dislocations are intimately related to their lattice symmetry. However, such roles of crystalline symmetries of GBs in 2D TIs have not been definitively measured yet. Here, we present the first direct evidence of a symmetry-enforced Dirac type metallic state along a GB in 1T'-MoTe$_2$, a prototypical 2D TI. Using scanning tunneling microscopy, we show a metallic state along a grain boundary with non-symmorphic lattice symmetry and its absence along another boundary with symmorphic symmetry. Our large-scale atomistic simulations demonstrate hourglass like nodal-line semimetallic in-gap states for the former, whereas the gap opens for the latter, explaining our observation well.

3:54PM D55.00008: Scanning Tunneling Microscopy Imaging of Electronic Waves on the Surface of Molecular Beam Epitaxy Grown Ag$_2$Se*  SAMIRA DANESHMANDI (Presenter), YANFENG LYU, HANMING YUAN, CHING (PAUL) W CHU, Univ of Houston — Recently, silver chalcogenide systems are being studied as possible candidates for topological insulators (TIs). While experimental works have been reported only on the electronic transport of anisotropic Dirac fermions in silver chalcogenides, no local scanning tunneling microscopy (STM) studies have been done on these materials. Here, we report the synthesis of epitaxial Ag$_2$Se nanostructures using molecular beam epitaxy (MBE) method. Based on atomic-resolved STM images, a new monoclinic structure is proposed for the MBE grown Ag$_2$Se, which was not seen in this system before. The electronic structures of the Ag$_2$Se have been investigated by means of scanning tunneling spectroscopy (STS). To test the unique feature of topological surface states (TSSs), we conducted a low-temperature STM/S study on the surface states of Ag$_2$Se films. On the selenium (Se)-terminated surfaces, evidence for TSSs are observed in the quasi-particle interference patterns. The existence of standing waves strongly supports the surface nature of topological states. Our results may help resolve the current controversy on the topological nature of Ag$_2$Se.

*The work performed at Houston is supported by USAFOSR Grant FA9550-15-1-0236, TLL Temple Foundation, JJ&R Moores Endowment, and State of Texas through TCSUH.
JIANFENG GE (Presenter), Leiden University, KAIYUAN GU, Peking University, ADITYA MAHADEVAN, Harvard University, HAIMEI ZHANG, Wellesley College, JIAOXUAN GUO, HAO TANG, Peking University, JENNIFER E. HOFFMAN, Harvard University — Topological surface states are unconventional two-dimensional electronic states that are protected from backscattering and overcome surface barriers. Previous experiments have shown that topological surface states have an enhanced transmission and a reduced reflection at the common bilayer step edges on the (111) surface of topological semimetal antimony (Sb), indicating the presence of backscattering against bilayer step edges. We use scanning tunneling microscopy and spectroscopy to investigate Sb(111) surface, which exhibits novel monolayer step edges. We demonstrate that topological surface states transmit through these monolayer step edges perfectly without backscattering. Furthermore, we discover localized states on these edges resembling the helical edge states originating from higher-order topology.

*Experiments were supported by National Science Foundation DMR-1410480.

CHI MING YIM (Presenter), DIBYASHREE CHAKRABORTI, LUKE RHODES, Univ of St Andrews, SEUNGHYUN KHIM, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, PETER WAHL, Univ of St Andrews — Rashba spin-splitting enables manipulation of spins with electric fields, opening avenues to transformative device concepts. In most materials where Rashba-spin splitting has been observed, the underlying electronic structure is uncorrelated and therefore well described by electronic structure calculations. This is not the case for correlated systems, in which electronic repulsion is needed to be accounted for. Here, we report a scanning tunnelling microscopy, quasiparticle interference (QPI) study of the two-dimensional electron gas (2DEG) at the surface of PdCoO$_2$, a correlated oxide system reported to exhibit giant Rashba-like spin-splitting [1] Our QPI data reveal a complex quasiparticle scattering pattern which, in particular, consists of a rounded-hexagon shaped, hole-like scattering band that disperses with averaged effective masses of $\sim -13.0$ m$_e$ and $\sim -11.1$ m$_e$ along the G-K and G-M directions, respectively. Through comparison with tight-binding calculations, we also show that the scattering is well described once the spin-selection rules are accounted for. Observation of quantized states in a 5-nm wide terrace region confined by a set of parallel step-edges is also discussed.
**4:30PM D55.00011: Observation of backscattering induced by magnetism in the topological hinge state of bismuth**

BERTHOLD JAECK (Presenter), YONGLONG XIE, ANDREI BERNEVIG, ALI YAZDANI, Princeton University — We have investigated the effects of time-reversal symmetry breaking on the topological hinge state of bismuth. Using spectroscopic imaging and spin-polarized measurements with an STM, we have compared quasiparticle interference (QPI) occurring in the hinge state of a pristine bismuth bilayer with that occurring in the hinge state of a bilayer, which is terminated by ferromagnetic iron clusters. Our experiments on the decorated bilayer edge reveal an additional QPI branch that can be associated with spin-flip scattering across the Brioullin zone center between time-reversal band partners. The observed QPI characteristics exactly match with theoretical expectations for a topological edge state having one Kramer's pair of bands and, thus provide spectroscopic evidence for back scattering in the topological edge states of bismuth.

*This work is supported by the ONR, the Moore foundation, NSF-DMR, NSF-MRSEC & the Humboldt foundation.

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**Monday, March 2, 2020 2:30 PM - 5:30 PM**

**Session D56 DCMP: Strontium and Calcium Ruthenates** Mile High Ballroom 2C -

Sung-Kwan Mo, Lawrence Berkeley National Laboratory

**2:30PM D56.00001: Van Hove singularity and stress-induced Fermi surface tuning in Sr$_2$RuO$_4$**

AARON CHRONISTER (Presenter), ANDREJ PUSTOGOW, University of California, Los Angeles, YONGKANG LUO, Huazhong University of Science and Technology, YUE-SHUN SU, University of California, Los Angeles, ANDREW MACKENZIE, CLIFFORD W HICKS, Max Planck Institute for Chemical Physics of Solids, ERIC BAUER, Los Alamos National Laboratory, NAOKI KIKUGAWA, National Institute for Material Science, Tsukuba Japan, STUART BROWN, University of California, Los Angeles — Application of in-plane uniaxial stress to the quasi-2D correlated material Sr$_2$RuO$_4$ results in pronounced changes to the physical properties; most familiar is a factor 2.5 increase in superconducting transition temperature. The normal state of Sr$_2$RuO$_4$ is also impacted. Specifically, the crossover temperature to standard Fermi Liquid properties can be tuned from T=30 K to almost 0 K with -0.44% strain. These anomalous properties are associated with the proximity of the Fermi energy ($E_F$) to a sharp singularity in the density of states, which can be tuned to $E_F$ and thus varies strongly on the scale of the Zeeman interaction and thermal energies. Reported here are $^{17}$O NMR hyperfine shifts over a wide range of stress, field, and temperature. Simple modeling of the results indicates that the difference between $E_F$ and the energy of the van Hove singularity plays a dominant role in the normal state properties for temperatures of order 300 K and below.

*Support from the National Science Foundation (DMR-1709304) and by the Laboratory Directed Research and Development (LDRD) programme of Los Alamos National Laboratory (20170204ER) is acknowledged.
2:42PM D56.00002: Density wave at the reconstructed surface of Sr$_2$RuO$_4$ and implications for quantum criticality  CAROLINA DE ALMEIDA MARQUES (Presenter), LUKE RHODES, Univ of St Andrews, VERONICA GRANATA, ROSALBA FITTIPALDI, ANTONIO VECCHIONE, CNR-SPIN, ANDREAS ROST, PETER WAHL, Univ of St Andrews — Many of the exciting properties of strongly correlated electron materials, including high-temperature superconductivity, are intricately linked to proximity to a quantum phase transition, a transition through which a material can be tuned as a function of an external control parameter other than temperature. Here, we propose that the reconstructed surface layer of Sr$_2$RuO$_4$ constitutes an ideal material to study the physics of quantum criticality. Using ultra-low temperature scanning tunneling microscopy, we observe the signature of a density wave in topographic images of the reconstructed surface of Sr$_2$RuO$_4$ which is linked with a sharp peak in the tunneling spectra, a few mV below the Fermi energy. We identify this peak as being the surface van Hove singularity (vHs) by comparing differential conductance ($dI/dV$) maps with a tight-binding model. Magnetic field splits the vHs peak, pushing one branch towards the Fermi energy. At 0T, the $dI/dV$ maps reveal a density wave with the periodicity of the reconstructed surface unit cell at the vHs peak energy. The energy at which this density wave occurs follows the field-split vHs. We discuss possible origins of this density wave as well as possible consequences for quantum criticality.

2:54PM D56.00003: QSGW+DMFT+BSE description of superconductivity in Sr$_2$RuO$_4$*  SWAGATA ACHARYA (Presenter), DIMITAR PASHOV, MARK SCHILFGAARDE, Physics, Kings College London — The nature of pairing in Sr$_2$RuO$_4$ continues to be widely debated, in particular, the possibility of a triplet origin of Cooper pairs. Its complexity, with multiple low-energy scales involving subtle interplay among spin, charge and orbital degrees of freedom, calls for advanced theoretical approaches which treat on equal footing all electronic effects. We present a novel approach, a detailed \emph{ab initio} theory, coupling quasiparticle self-consistent GW approximation with dynamical mean field theory (DMFT). We report that the superconducting instability has multiple triplet and singlet components. In the unstrained case the triplet eigenvalues are larger than the singlets. Under uniaxial strain, the triplet eigenvalues drop rapidly and the singlet components increase. This is concomitant with our observation of spin and charge fluctuations shifting closer to wave-vectors favoring singlet pairing in the Brillouin zone. We identify a complex mechanism where charge fluctuations and spin fluctuations co-operate in the even-parity channel under strain leading to increment in $T_c$, thus proposing a novel mechanism for pushing the frontier of $T_c$ in unconventional "triplet" superconductors.

*This work was supported by the Simons Many-Electron Collaboration.
Non-monotonic temperature dependence of the Hall coefficient in Hund's metals

MANUEL ZINGL (Presenter), Flatiron Institute, Center for Computational Quantum Physics, JERNEJ MRAVLJE, Department of Theoretical Physics, Institute Jozef Stefan, MARKUS AICHHORN, Institute of Theoretical and Computational Physics, Graz University of Technology, OLIVIER PARCOLLET, ANTOINE GEORGES, Flatiron Institute, Center for Computational Quantum Physics — A non-monotonic temperature dependence of the Hall coefficient has been reported for several strongly correlated materials, e.g. Sr$_2$RuO$_4$, Sr$_3$Ru$_2$O$_7$, LiFeAs and FeSe [1]. One common signature of these Hund’s metals is a strong orbital selectivity of electronic correlations. On the example of Sr$_2$RuO$_4$, where the Hall coefficient exhibits two sign reversals, we show that the behavior of the Hall coefficient is directly linked to the temperature dependence of the ratio of inelastic scattering rates between the different correlated orbitals [2]. In our picture the sign reversals reflect two important crossovers in the physics of this material: (I) from a high-T incoherent to a coherent regime at low-T associated with a remarkably large ratio of scattering rates, and (II) from inelastic to impurity-dominated scattering. This qualitative picture is supported by quantitative calculations using Boltzmann transport theory in combination with dynamical mean-field theory, taking into account the effect of spin–orbit coupling.


Fluctuation stabilised spin-density-wave order and the phase diagram of Sr$_3$Ru$_2$O$_7$

STEPHEN HAYDEN (Presenter), RICHARD WAITE, CHRIS LESTER, University of Bristol, UK, ROBIN PERRY, University College London, UK, SILVIA RAMOS, University of Kent, UK, DMITRY KHALYAVIN, FABIO ORLANDI, PASCAL MANUEL, ISIS, Rutherford Appleton Laboratory, UK — Sr$_2$Ru$_3$O$_7$ is a unique metal in which a magnetic field of about 8 Tesla can induce spin density wave (SDW) order [1]. There are two SDW ordered phases (A and B) with different incommensurate wavevectors. Here we use magnetic neutron diffraction to characterise the magnetic order as a function of magnetic field strength and direction. The order is observed for all field directions investigated. Our results suggest that the SDW is closely linked to Fermi surface nesting and is probably stabilised by magnetic fluctuations. Thus the SDW order explains many (magnetic, transport and thermal) anomalies in this material.

3:30PM D56.00006: Interplay between Spatially Modulated Nematic and Spin-Density Wave Order in Sr$_3$Ru$_2$O$_7$  JONATHAN CLEPKENS (Presenter), HAE-YOUNG KEE, Univ of Toronto — The anisotropic resistivity observed in Sr$_3$Ru$_2$O$_7$ [1] has led to a variety of theoretical studies proposing microscopic routes to a nematic phase in the material. However, the discovery of spin-density wave (SDW) order in the same region of phase space [2] has cast some doubt on this picture, even though there are open issues that cannot be understood within the SDW scenario. Here we study the interplay between spatially modulated nematic and SDW order from a microscopic viewpoint. Mean-field results illustrating the formation of the finite momentum nematic and SDW order will be presented. Implications towards the importance of bilayer coupling, spin-orbit coupling and the presence of a van-Hove singularity in Sr$_3$Ru$_2$O$_7$ will also be discussed.


3:42PM D56.00007: Metal-Insulator and Magnetic Phase Diagram of Ca$_2$RuO$_4$ from Auxiliary Field Quantum Monte Carlo and Dynamical Mean Field Theory*  HAO SHI (Presenter), Simons Foundation, HONGXIA HAO, Department of Chemistry, Brown University, ANTOINE GEORGES, ANDREW MILLIS, Simons Foundation, BRENTDA M RUBENSTEIN, Department of Chemistry, Brown University, QIANG HAN, Department of Physics, Columbia University — Layered perovskite ruthenium oxides exhibit a striking series of metal-insulator and magnetic-nonmagnetic phase transitions easily tuned by temperature, pressure, epitaxy, and nonlinear drive. In this work, we combine results from two complementary states of the art many-body methods, Auxiliary Field Quantum Monte Carlo and Dynamical Mean Field Theory, to determine the low-temperature phase diagram of Ca$_2$RuO$_4$. Both methods predict a low-temperature pressure-driven metal-insulator transition coincident with a structural transition and accompanied by a ferromagnetic-antiferromagnetic transition. The properties of the ferromagnetic state are dominated by the ruthenium xy orbital while properties of the antiferromagnetic state are dominated by the xz and yz orbitals. Differences of detail in the predictions of the two methods are analyzed. The work is theoretically important as an application of the auxiliary field quantum Monte Carlo method to an orbitally degenerate system with both Mott and Hund's physics and provides an important comparison of the dynamical mean-field and auxiliary field quantum Monte Carlo methods.

*Support by NSF, DOE, and the Alfred P. Sloan Foundation. The Flatiron Institute is a division of the Simons Foundation
3:54PM D56.00008: Spin-orbit interpretation of the Higgs mode in Ca$_2$RuO$_4$*  PAUL SARTE
(Presenter), California NanoSystems Institute/Materials, University of California, Santa Barbara, CHRIS STOCK, Univ of Edinburgh, BRENDEX ORTIZ, STEPHEN WILSON, California NanoSystems Institute/Materials, University of California, Santa Barbara — The role played by spin-orbit coupling in the determination of a system’s magnetism has recently been the subject of intense study, with particular interest being placed on magnets based on Ru$^{4+}$ and Ir$^{4+}$, revealing a wealth of novel emergent phenomena. Stemming from the complex interplay of comparable values for $J$ and $\lambda$, the parameterization for such phenomena has proven challenging. One particular example corresponds to the modeling of the low energy magnetic fluctuations, where conventional approaches often require complicated phenomenological Hamiltonians. Using the 4$d$ layered antiferromagnet Ca$_2$RuO$_4$ as a case study, we demonstrate that a mean-field multilevel spin-orbit exciton model employing a minimalist Hamiltonian captures the main features of the low energy magnetic excitation spectrum. Corresponding to a tetragonally-distorted $A$-centered antiferromagnetic unit cell, the model accounts for the softening and longitudinal polarization of the Higgs mode. The success of such a minimalist Hamiltonian in capturing such a rich spectrum for a 4$d$ magnet, suggests that the spin-orbit exciton model may be a suitable alternative to traditional approaches.

*We acknowledge financial support from the Elings Fellowship (CNSI), EPSRC, ERC, and the Carnegie Trust.

4:06PM D56.00009: Strain-mediated Mott transition in Ca$_2$RuO$_4$ induced by a dc current
ALFRED ZONG (Presenter), ANSHUL KOGAR, Massachusetts Institute of Technology MIT, HENGDI ZHAO, University of Colorado, Boulder, QIAN LI, Argonne National Laboratory, YIFAN SU, Massachusetts Institute of Technology MIT, SAMUEL D MARKS, Argonne National Laboratory and University of Wisconsin-Madison, GANG CAO, University of Colorado, Boulder, HAIDAN WEN, Argonne National Laboratory, NUH GEDIK, Massachusetts Institute of Technology MIT — In a Mott insulator, the delicate balance among several competing energy scales gives rise to a plethora of ground states, which may be tuned into one another by pressure, electric field, photoexcitation among other perturbations. Owing to many degrees of freedom present in the system, understanding Mott transitions remains difficult. Recently, Ca$_2$RuO$_4$ has emerged as a new platform for studying the insulator-to-metal Mott transition. A dramatic change in its structural and optical properties across the phase boundary allows a multimodal approach to investigate the transition in space and time. Here, we report *in situ* transport, optical, and X-ray microscopy measurements on current-induced Mott transition in Ca$_2$RuO$_4$. We find that lattice strain plays a central role in this spatially-inhomogeneous transition, whose temporal evolution is characterized by local fluctuations in temperature. The present work clarifies important aspects of the current-induced Mott transition and provides insights into future applications that harness such electromagnetic control.
4:18PM D56.00010: Tailoring the ferromagnetic easy axis of Ca$_2$RuO$_4$ via epitaxial strain

LUDI MIAO (Presenter), HARI NAIR, NATHANIEL SCHREIBER, JACOB RUF, MATTHEW FU, YONGHUN LEE, CELESTA CHANG, JACOB RUFF, DAVID MULLER, DARRELL SCHLOM, KYLE M SHEN, Cornell University — Magnetism in strongly correlated ruthenates has been a central topic in condensed matter physics, where the spin degree of freedom is has a strong interplay with lattice, charge and orbital degrees of freedom. For instance, the Mott insulator Ca$_2$RuO$_4$ (CRO) can be turned into a ferromagnetic metal under epitaxial strain or hydrostatic pressure. Here, we have grown coherently strained CRO thin films on various substrates including SrLaAlO$_4$ and YAlO$_3$ via molecular beam epitaxy and investigated the strain effect on their magnetic properties. We have used angle-resolved magnetoresistance measurements to characterize the ferromagnetic easy axes of these films, and found that they are also drastically different from CRO bulk, and show how the magnetic easy axes can be tuned as a function of epitaxial strain. Our results manifest the complex interplay between the spin, lattice and orbital degree of freedom in CRO, as well as demonstrate a practical approach to tailor the magnetic properties in strongly correlated oxide materials via epitaxial strain, in general.

4:30PM D56.00011: Imaging the current-driven metal–insulator transition in Ca$_2$RuO$_4^*$

GIORDANO MATTONI (Presenter), SHINGO YONEZAWA, Physics, Kyoto University, FUMIHIKO NAKAMURA, Education and Creation Engineering, Kurume Institute of Technology, YOSHITERU MAENO, Physics, Kyoto University — The flow of electric current is a powerful tool to alter the ground state of strongly correlated ruthenates, where novel material properties emerge in non-equilibrium steady states [1,2,3]. Despite the efforts to investigate these phenomena, the microscopic mechanism and the physical quantities responsible for the current-induced phase changes have not been clarified yet.

Here, I will present our recent results based on thermal imaging of single-crystal Ca$_2$RuO$_4$ while triggering its metal–insulator transition with the flow of direct current. By measuring the infrared thermal emission of the material and exploiting the different emissivity of the metallic and insulating state, we observe the formation of phase-separated regions which can be controlled and stabilised by current. We determine the correlation between current density and the metal–insulator transition, discussing the interplay between electronic effects and localised Joule heating. Our technique provides a fundamental step towards understanding the mechanism regulating current-induced phenomena in quantum materials.


*Dutch Research Council (NWO) through a Rubicon grant number 019.183EN.031
**4:42PM D56.00012: Pump-probe Nano-spectroscopy of Mott Insulating Ca$_2$RuO$_4$**
ROCCO VITALONE (Presenter), AARON STERNBACH, BEN FOUTTY, ALEXANDER MCLEOD, Physics, Columbia University, CHANCHAL SOW, Physics, Kyoto University, FUMIHIKO NAKAMURA, Department of Education and Creation Engineering, Kurume Institute of Technology, YOSHITERU MAENO, Physics, Kyoto University, ABHAY PASUPATHY, DMITRI BASOV, Physics, Columbia University — Ca$_2$RuO$_4$ is a Mott Insulator that exhibits a temperature-induced insulator to metal transition occurring slightly above room temperature. Further, Ca$_2$RuO$_4$ exhibits a current-driven IMT at room temperature and current-induced diamagnetism below 50K. These discoveries, particularly the latter, imply that the application of current can expose a previously hidden state in Ca$_2$RuO$_4$. Motivated by the current induced transition, we conducted nanoscale pump-probe measurements to explore the phase diagram further. In our experiments, we study both the static and photo-induced response with nano-FTIR measurements to interrogate the dynamics of the spectral response throughout the mid-IR. The static spectra reveal a large phonon resonance of the in-plane stretching mode of the Ru-O bonds in the insulating state, while the metallic state demonstrates a flat, Drude like response. The photo-induced spectra reveal an initial suppression of the phonon mode and a noticeable increase in the Drude response at later times. We interpret the response as an initial injection of charge carriers that screen the phonon mode while their thermalization at later times leads to the Drude-like response.

*NDSEG Fellowship*

**4:54PM D56.00013: Magnetic phase tuning in Ca$_2$Ru$_{1-x}$Fe$_x$O$_4$: A structural perspective**
SONGXUE CHI (Presenter), FENG YE, Neutron Scattering Division, Oak Ridge National Laboratory, GANG CAO, Physics, University of Colorado Boulder, HUIBO CAO, JAIME FERNANDEZ-BACA, Neutron Scattering Division, Oak Ridge National Laboratory — The crystalline and magnetic structures of Ca$_2$Ru$_{1-x}$Fe$_x$O$_4$ (x=0.02, 0.05, 0.08 and 0.12) have been studied using neutron scattering and X-ray diffraction. The Fe-doping reduces the Ru-O bond length in both apical and planar directions. The smaller Ru(Fe)O$_6$ octahedra leads to its reduced distortion. The Pbca space group is maintained and so is the apical flattening. Warming has similar effect as Fe-doping in releasing the distorted octahedra except an abrupt change of flattening across the Neel temperature in x=0.08. Two types of antiferromagnetic orders, A- and B-centered phases with the same in-plane spin arrangement but different stack sequences, have been found. The Fe induced structure with relaxed octahedra seems to prefer the B-phase to the A-centered one, which is systematically overwhelmed and replaced as the Fe-doping increases. The nature of the magnetic phase competition and its connection to its host structure is discussed.
5:06PM D56.00014: Emergence of Competing Stripe Phase near the Mott Transition in Ti-doped Bilayer Calcium Ruthenates*  ASHISH GANGSHETTIWAR (Presenter), University of Texas at Austin, YANGLIN ZHU, Physics, Penn State University, JIN PENG, Tulane University, YU WANG, Physics, Penn State University, ZHANZHI JIANG, University of Texas at Austin, ZHIQIANG MAO, Physics, Penn State University, KEJI LAI, University of Texas at Austin — The physics of nanoscale phase separation is at the heart of strongly correlated materials, where multiple degrees of freedom such as charge, spin, lattice, and orbital are simultaneously active. Using microwave impedance microscopy, we spatially resolved the coexisting phases on a Ca₃(Ru₀.₉Ti₀.₁)₂O₇ bulk crystal during the metal-insulator transition. Different from a typical first-order phase transition where coexistence of the two terminal phases takes place, a new stripe phase oriented along the in-plane crystalline axes emerges inside both the G-type antiferromagnetic insulating state and paramagnetic metallic state. The effect of this electronic state can be observed in macroscopic measurements, allowing us to construct a phase diagram that takes into account the energetically competing phases. Our work provides a model approach to correlate macroscopic properties and mesoscopic phase separation in complex oxides.

*U.S (DOE), award no. DE-SC0019025 and NSF (2DCC-MIP) award no. DMR-1539916

5:18PM D56.00015: Nano-resolved insulator-metal domain textures in a polar bilayer ruthenate  ALEXANDER MCLEOD (Presenter), RAN JING, JEDRZEJ WIETESKA, Physics, Columbia University, LEIXIN MIAO, Materials Science and Engineering, Penn State University, BEN FOUTTY, Physics, Columbia University, RUI ZU, Materials Science and Engineering, Penn State University, GIULIANO CHIRIACO, QIANG HAN, Physics, Columbia University, DANilo PUGGIONI, JAMES RONDINELLI, Materials Science and Engineering, Northwestern University, ANDREw MILLIS, Physics, Columbia University, VENKATRAMAN GOPALAN, Materials Science and Engineering, Penn State University, ZHIQIANG MAO, Physics, Penn State University, NASIM ALEM, Materials Science and Engineering, Penn State University, ABHAY PASUPATHY, DIMITRI BASOV, Physics, Columbia University — The 4d transition metal oxides of the Caₙ₊₁RuₙO₃ₙ₊₁ perovskite family have recently garnered interest for their correlated electron physics and strong sensitivity to external stimuli like strain, temperature, and even electric current. The bilayer ruthenate Ca₃Ru₂O₇ exhibits a structural distortion producing a polar metal and, under Ti substitution for Ru, a correlated antiferromagnetic insulator. Through low-temperature nano-infrared imaging, we reveal a spontaneous striped texture of coexisting insulating and metallic domains in single crystals across their insulator-metal phase transition at T=70-100K. Under in situ uniaxial strain, we image anisotropic nucleation and growth of these domains, rationalized through on-demand control of a spontaneous Jahn-Teller distortion. Through high resolution transmission electron microscopy, we also reveal the detailed interplay between this textured phase coexistence and the displacive orientations, volumetric structures, and domain boundaries among polar twin domains in these crystals. These novel imaging methods afford new insights into strain- and structure-mediated manipulation of the insulator-metal transition in 4d metal oxides and the ubiquity of phase coexistence even in pristine single crystals.

Monday, March 2, 2020 2:30 PM - 5:30 PM
2:30PM D57.00001: Ultra-high sensitive gas sensor based on graphene/carbon nanotube barristor  
YOUNGGYU YOU (Presenter), DO-HYUN PARK, JUN-HO LEE, INCHUL CHOI, KonKuk Univ, SUNG-IL JO, GOO-HWAN JEONG, Kangwon Univ, ELEANOR CAMPBELL, University of Edinburgh, HYUN-JONG CHUNG, JHANG SUNG HO, KonKuk Univ — We have investigated switching characteristics in graphene/semiconducting single-walled carbon nanotube (SWCNT) junction device, so-called graphene/SWCNT barristor. We modulated the Schottky barrier between the graphene and the carbon nanotube by using top and bottom gate electrodes, and achieved on-off ratio of $10^8$ and the subthreshold swing of 74 mV/dec with high current density. In addition, we demonstrated the potential of our device as a NO$_2$/NH$_3$ gas sensor. Graphene/SWCNT barristor showed the $10^7$ % of sensitivity for the 100 ppm NO$_2$ gas, and $10^5$ % of sensitivity for the 100 ppm NH$_3$ gas. Also, our device is sensitive enough to detect NO$_2$ gas down to 25 ppb concentration with 400 % sensitivity.

2:42PM D57.00002: Circular nanoelectromechanical resonators based on hexagonal boron nitride graphene heterostructures  
ROHIT KUMAR (Presenter), DERIC W SESSION, HARRISON PAAS, RYUICHI TSUCHIKAWA, VIKRAM V DESHPANDE, University of Utah — 2D materials like graphene and h-BN, to name a few, when layered on top of each other offer a new class of metamaterials. Especially, the twisting degree of freedom between two layers has opened the window for new phenomenon not explored before. The mechanical properties of these heterostructures in the form of nanoelectromechanical systems (NEMS) have not been studied extensively. Their exceptional attributes like ultra-low mass, robustness and high tunability make 2D materials suitable for NEMS which holds promise for various technological applications viz. ultrafast sensors, actuators etc. We report fabrication and characterization of hexagonal-boron nitride (h-BN) graphene heterostructure based circular nanoelectromechanical resonators on sapphire substrates. The device is measured at cryogenic temperatures and exhibits multiple mode frequencies which are highly tunable with gate voltage. A continuum mechanics model is employed to analyze the transmission ($S_{21}$) data of fundamental mode. Parameters like built-in tension obtained from the fit are used to identify the indices (m, n) of higher mechanical modes observed for the device. NEMS could offer a way to study the electronic phenomena such as superconductivity in twisted bilayer graphene heterostructures.
2:54PM D57.00003: Advances in MEMS based Strain Engineering of 2D Materials*  MOUNIKA VUTUKURU (Presenter), ZHUOFA CHEN, ANNA K SWAN, Boston Univ — Strain on 2D materials is an exciting avenue to explore material properties as well as induce novel phenomena, such as strain-dependent electron-hole plasma (EHP) formation in MoS2, or pseudo-magnetic field generation in graphene. In this work, we successfully incorporate MoS2 and graphene with microelectromechanical systems (MEMS) to controllably introduce strain, while simultaneously observing 2-terminal transport and electro-optical changes. We fabricate suspended 2D material integrated MEMS devices using a novel polymer transfer microstructure without damaging the MEMS or the 2D film. By electrically powering our devices, suspended 2D materials undergo controllable, reversible uniaxial strain which we characterize by optical spectroscopy. Equipped with two-terminal contacts, we explore the conductance of suspended 2D materials while simultaneously straining the material in air, with the goal of achieving different strain gradients for accessing novel physics.

*This work is supported by NSF DMR grant 141108.

3:06PM D57.00004: Probing layered magnets with graphene van der Waals heterostructures  JESSE BALGLE (Presenter), Physics, Washington University in St. Louis, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, ERIK HENRIKSEN, Physics, Washington University in St. Louis — Layered magnets are promising platforms for science and applications including novel quantum magnetic phases, nanoscale magnetic memory, and spintronics devices. However common bulk probes such as neutron and x-ray scattering or thermal probes are difficult or impossible to use to characterize these materials in the few-layer limit. We seek to develop new approaches for probing devices incorporating single-/few-layer magnets. Electronic transport in graphene can be influenced by both nearby and nonlocal scatterers. We have found that the resistance of graphene exhibits a nonmonotonic change with temperature when placed in contact with a material undergoing a magnetic phase transition. This is reminiscent of “critical resistivity” measurements in (anti-)ferromagnetic metals dating back over 50 years, which show that transport can be sensitive to spin-scattering. Motivated by these findings, we explore transport in graphene separated from layered magnets by thin hexagonal boron nitride (hBN). We find unusual nonmonotonic changes in graphene resistance persist even when the graphene is only in contact with hBN, suggesting that nearby magnetic materials impact transport. We show results for devices incorporating magnetic metals (Gd, Dy) as well as layered magnets α-RuCl3 and FePS3.
3:18PM D57.00005: NEGF simulations of metal contacts for graphene nanoribbon based device  
HANCHENG QIN (Presenter), WENCHANG LU, JERRY BERNHOLC, North Carolina State University — For nanoscale electronic devices, the precise atomic structure of the metal contact plays a significant role on the performance of the device. We use an accurate, DFT-based non-equilibrium Green's function method with variationally-optimized localized orbitals to study contacts between different metals and graphene and/or graphene nanoribbons (GNRs). For on-top metal contacts not chemically bound to graphene, we have found that Ti contacts have lower resistance than other metals, such as Au, Ca, Ir, Pt, and Sr. We will discuss channel length effects on the off-state current and the required minimum channel and metal-graphene contact lengths for applications. Other contact structures (side contacts with chemical bonds) will also be discussed.

3:30PM D57.00006: An ultra-high vacuum system for fabricating 2D material devices  
SHUAIFEI GUO (Presenter), Fudan University, SATORU MASUBUCHI, University of Tokyo, NAI ZHOU WANG, University of Science and Technology of China, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, XIANHUI CHEN, University of Science and Technology of China, TOMOKI MACHIDA, University of Tokyo, YUANBO ZHANG, Fudan University — Atomically thin two-dimensional (2D) materials exhibit a rich set of electronic properties that may impact future electronic and optoelectronic applications. Many 2D materials, however, are prone to degradation in the presence of trace amount of oxygen or water vapor. The study of the intrinsic properties of these 2D materials requires protection from degradation agents during sample fabrication process. To this end, we design and build an ultra-high vacuum (UHV) system, in which the entire sample fabrication is performed under a base pressure lower than $5 \times 10^{-10}$ mbar. We demonstrate the functionality of this UHV fabrication system by fabricating black phosphorus heterostructures completed with electrical contacts and gate electrode for transport measurements.

3:42PM D57.00007: Integration of 2D materials for Device applications [Invited]  
LAIN-JONG LI (Presenter), TSMC — Selected by Focus Topic Organizer (Deji Akinwande)
Towards the ideal diode: Half-metal spin-gapless semiconductor junctions based on 2D materials*  

ERSOY SASIOGLU (Presenter), THORSTEN AULL, Institute of Physics, Martin Luther University Halle-Wittenberg, STEFAN BLUEGEL, Peter Grünberg Institut, Forschungszentrum Jülich, INGRID MERTIG, Institute of Physics, Martin Luther University Halle-Wittenberg — Conventional semiconductor diodes have a junction barrier that electrons have to overcome and thus they have a threshold voltage \( V_T \), which must be supplied to the diode to turn it on. Using the half-metallic magnets (HMMs) and spin-gapless semiconductors (SGSs) we propose a new diode concept, which does not have a junction barrier and whose operation principle relies on unique spin-dependent transport properties of the HMM and SGS materials. We show that HMM and SGS materials form an Ohmic contact under any finite forward bias, while for the reverse bias current is blocked. Thus, the HMM-SGS junctions act as a diode with zero threshold voltage \( V_T \), linear current-voltage (I-V) characteristics as well as very high on/off ratio. We employ the nonequilibrium Greens function method combined with density functional theory to demonstrate the linear I-V characteristics of the proposed diode based on 2D spin-gapless semiconducting VS\(_2\) and half metallic Fe/MoS\(_2\) planar heterojunctions. Moreover, a reconfigurable magnetic tunnel diode [1] is also realized by vertically stacking the VS\(_2\) and Fe/MoS\(_2\) monolayers. [1] E. Sasioglu, S. Blügel, and I. Mertig, ACS Appl. Electron. Mater. 1, 1552–1559 (2019).

*Funding by the European Union (EFRE) is greatly acknowledged.

Improved broadband on-chip time domain terahertz spectrometer for van der Waals heterostructures  

ALEX POTTS (Presenter), JOSHUA O ISLAND, ERIC SPANTON, University of California, Santa Barbara, PETER KISSIN, Physics, University of California, San Diego, ANTHONY P MCFADDEN, LIAM COHEN, CHRIS J PALMSTROM, University of California, Santa Barbara, RICHARD AVERITT, Physics, University of California, San Diego, ANDREA YOUNG, University of California, Santa Barbara — Time domain THz spectroscopy is a powerful technique for studying low-energy excitations in quantum materials, but is typically restricted to samples physically larger than the electromagnetic diffraction limit (~0.3 mm). We present an on-chip THz time domain spectrometer based on transmission line-coupled photoconductive switches fabricated by aligned transfer of epitaxially grown ErAs superlattices. We benchmark our bandwidth and dynamic range, which shows significant improvement over radiation damaged silicon-based devices on silicon substrates, and anticipate the technique’s use in studying dynamics and non-equilibrium phases in exfoliable van der Waals materials and heterostructures.
Two-dimensional (2D) materials and heterostructures have emerged as promising candidates for post-Moore electronics due to their unique electronic properties and atomically thin geometry. I will start with our studies on 2D semiconductors with low lattice symmetry and type-II Weyl semimetals. In atomically thin Rhenium disulfide (ReS$_2$), we observed interesting low-symmetry-induced anisotropic transport and mechanical properties, and studied their electronic and optoelectronic applications.[1] In type-II Weyl semimetal Tungsten ditelluride (WTe$_2$), we observed planar-orientation-dependent negative longitudinal magnetoresistance (MR) which reveals important transport signatures of chiral anomaly and type-II Weyl fermions.[2] In the second part of my talk, I will show that 2D heterostructures could play important roles in future advanced memory, computing and optoelectronic applications. One example is robust memristors with good thermal stability based on a 2D heterostructure composed of graphene/MoS$_{2-x}$O$_x$/graphene, which show promising memory and neuromorphic applications. [3] Our latest results on the observation of ballistic avalanche phenomena in a thin 2D heterostructure made of black phosphorus and Indium Selenide (InSe), as well as their high-performance electronic and optoelectronic applications will also be presented.[4]


Graphene is a 2-dimensional plane of carbon and a zero-band gap material whose conduction and valence band meet at dirac point. This electronic band structure makes it possible that the graphene's fermi energy level is modulated with accumulated charges by ~0.5 eV [1]. In this study, the unique property of graphene, large modulation of fermi energy level, was used to realize a vertical transistor which is based on graphene/hexagonal boron nitride (hBN) heterostructure. This device controlled tunneling barrier height between graphene and hBN by modulating the graphene's fermi energy level, and $I_{on}/I_{off}$ up to $10^6$ was achieved at 300 K. We also confirmed that there was little change in performance of device at 300 K and 15 K.

Density Functional Theory (DFT) and Time-Dependent (TD) DFT allow us in principle to express observables as functionals of the density. Relatively efficient approximations exist for the ground state total energy, but major difficulties remain, for example to describe strongly correlated systems, or situations where long range correlation is important. For other observables, even less is known about how to build good density functionals.

One way of designing approximations is to use results of model systems. In this talk we will show how model results can be used in an in principle exact way, called “Connector Theory”, in order to describe observables and systems of interest. Within this approach, a quantity of interest is calculated for a model system as function of a parameter once and forever, and the results are stored. Under certain conditions, the result for an appropriate choice of parameter can then be used to replace a value of interest in a given real system. This choice of parameter is called “connector”.

We will discuss the principles and general properties of such an approach. Of course, in practice, the connector has to be approximated. We will show that formulating the problem in this way is a convenient starting point for approximations, and a strategy to build systematic approximations will be presented.

We will then focus more specifically on the use of the connector approach to design density functionals, both for DFT and TDDFT. Particular emphasis will be put on effects of non-locality in space and time, which are important to capture, e.g., image potentials or multiple excitations, respectively. Some discussion and results can be found in [1,2].

Nonadiabatic electron dynamics in time-dependent density-functional theory at the cost of adiabatic local density approximation.*

DMITRY GULEVICH (Presenter), YAROSLAV V. ZHUMAGULOV, ITMO University, ALEXEI V. VAGOV, ITMO University; University of Bayreuth, ILYA V. TOKATLY, University of the Basque Country, VASILI PEREBEINOS, University at Buffalo

— We propose a computationally efficient approach to nonadiabatic electron dynamics in time-dependent density functional theory (TDDFT) based on a representation of the frequency-dependent exchange correlation kernel as a response of a set of damped oscillators. The requirements to computational resources needed to implement our approach do not differ from those of the standard real-time TDDFT in the adiabatic local density approximation (ALDA). Our result offers an exciting opportunity to take into account temporal nonlocality and memory effects in calculations with TDDFT in quantum chemistry and solid state physics for unprecedentedly low costs. We present few simple approximations to nonadiabatic exchange-correlation kernels and their application to study nonadiabatic dynamics of electron liquid in semiconductor quantum wells and atoms.

References:

*The work is supported by the Russian Science Foundation under the grant 18-12-00429.

Imitating beyond-DFT calculations via external on-site potentials

NITIN KUMAR (Presenter), Colorado School of Mines, STEPHAN LANY, National Renewable Energy Laboratory

— Density functional theory (DFT) based methods are the basis for the high-throughput calculations of structural and electronic properties currently used in most Materials-by-Design approaches for materials discovery. To improve the accuracy of such predictive theory, it is now necessary to bridge the gap between efficient, but approximate, DFT calculations, and accurate, but computationally expensive, “beyond-DFT” approaches, such as GW electronic structure and random phase approximation (RPA) total energy calculations. In this direction, we aim to reproduce the beyond-DFT level by using angular-momentum and energy-dependent external on-site potentials. The problem of fitting the potential parameters is equivalent to solving a multi-objective optimization problem. Using VO2 as a model system, we develop a workflow for potential fitting via machine learning, so to explore the extensive multi-dimensional search space for the highly non-linear objective function.
3:30PM D58.00004: First Principles Derivation of the Effect of Geometric Noise on Distributions of Electronic Properties using the Effective Stochastic Kohn-Sham Potential Method  JEREMY SCHER (Presenter), ARINDAM CHAKRABORTY, Syracuse University — Obtaining ensemble averages by sampling many conformations is vital for an accurate description of temperature-dependent properties of chemical systems. However, constructing distributions of $10^5 - 10^6$ samples is computationally challenging due to the high computational cost of performing calculations. In this work, we present a new approach called the effective stochastic Kohn-Sham potential (ESKS) method to address this challenge. Using the classical nuclear-nuclear repulsion energy as a metric, we derive statistical relationships between the distribution of nuclear-nuclear repulsion energies and the distributions of ground state quantum mechanical properties for a general chemical system. The results from this analysis show that the geometric noise experienced by molecules due to solvent interaction and thermal motion can be effectively captured by an effective stochastic operator. This allows for introducing a stochastic variable in the Kohn-Sham potential. Comparison of the analytical results with numerical DFT calculations on small molecules, semiconductor clusters, and large organic molecules will be presented. Both analytical and numerical results demonstrate the advantage of using an effective stochastic operator for performing large scale sampling of conformations.

3:42PM D58.00005: Towards Spectroscopic Accuracy for In-Silico Materials Design*  ADA SEDOVA (Presenter), Oak Ridge National Lab, ANUP PANDEY, Los Alamos National Lab, ANIBAL J. RAMIREZ-CUESTA, Oak Ridge National Lab — We present a new approach for enabling highly accurate prediction of non-equilibrium behavior of large supramolecular organic systems for in-silico design of novel functional materials. Using datasets of INS measurements of organic molecular crystals from the high-throughput, high resolution neutron vibrational spectrometer at SNS (VISION), we obtain essential information for achieving spectroscopic accuracy in density functional theoretical descriptions of the forces acting on large organic supramolecular assemblies with strong non-covalent bonds, using high performance computing and massively parallel DFT calculations. The work will pave the way for an ability to design and test new materials using high-confidence in-silico methods.

*This work was supported by the U.S. Department of Energy (DOE), Office of Science and used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725. ORNL is managed by UT-Battelle, LLC for the U.S. DOE under contract DE-AC05-00OR22725.
3:54PM D58.00006: Understanding the interplay between hole localization and reactivity in photoionized water clusters using real-time Time-Dependent Density Functional Theory*
VIDUSHI SHARMA (Presenter), MARIVI FERNANDEZ SERRA, Department of Physics and Astronomy, and Institute for Advanced Computational Science, Stony Brook University — Photocatalytic water-splitting on semiconductor surfaces is of topical interest for renewable energy applications, and yet, the molecular intermediates and their mutual interactions underlying photocatalysis remain poorly understood. In this work, we examine the scope of rt-TDDFT-based methods for analyzing ultrafast processes in photoexcited systems. We study the response of a prototypical molecular system consisting of chains of H-bonded (H_2O)_n molecules (n=2-5) under photoionization. The time evolution of the photogenerated hole is captured by rt-TDDFT Ehrenfest dynamics. We use a generalized gradient approximation (GGA-PBE) for nonadiabatic electron-ion dynamics, justified by comparing dynamic hole densities computed at PBE with those at higher PBE0 level of the theory. We also compare results from rt-TDDFT dynamics with those from adiabatic Born-Oppenheimer molecular dynamics at the GGA level, elucidating the importance of incorporating explicit nonadiabatic effects in excited-state phenomena. The H-bond cooperativity effects in (H_2O)_n^+ chains are identified, emphasizing their role in facilitating hole localization. Finally, we also uncover new connections between the test system and the H-bond network formed at water-semiconductor interfaces.

*DOE grant DE-FG02-09ER16052

4:06PM D58.00007: Approaches for Non-Adiabatic Functional Approximations in TDDFT*
LIONEL LACOMBE, NEEPA MAITRA (Presenter), Rutgers University, Newark — Several examples of electron dynamics in the non-perturbative regime highlight the need to go beyond the adiabatic approximation to achieve even a qualitatively reasonable description. This includes charge-transfer dynamics out of the ground-state, resonantly-driven dynamics, and cases of pump-probe spectroscopy. We discuss different approaches to develop functionals that build in memory into new non-adiabatic exchange-correlation functionals. In one, we develop density-matrix coupled exchange-correlation approximations, starting from an exact expression for the time-dependent exchange-correlation functional. In another, a time-dependent extension of the adiabatic connection formula is developed to take advantage of coupling-constant integration.

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Department of Energy Office of Basic Energy Sciences DE-SC-0020044
Plasmon dispersion and the role of the exact constraints on exchange-correlation kernels within time-dependent density functional theory

ADRIENN RUZSINSZKY (Presenter), BIMAL NEUPANE, SHIQI RUAN, SANTOSH ADHIKARI, SANTOSH NEUPANE, NIRAJ K. NEPAL, Physics, Temple University — Small-wavevector excitations in Coulomb-interacting systems can be decomposed into the high-energy collective longitudinal plasmon and the low-energy single-electron excitations. The random phase approximation (RPA) is exact in the high-density limit but can capture the plasmonic dispersion reasonably even for densities with $r_s > 1$. The work by Tatarczyk et al. [1] found that the impact of the exchange-correlation kernels is significant and modifies the plasmon dispersion curve. There is however a large difference in the construction and performance of the kernels investigated earlier. Our current work for the jellium model introduces recent model exchange-only and exchange-correlation kernels and discusses the relevance of some exact constraints [2,3] in the construction of the kernel. This work could give a further hint toward a better plasmon dispersion in realistic metals where anomalous behavior was observed with RPA.


*Work is supported by National Science Foundation under Grant No. DMR–1553022.

Nonlocal energy optimized (NEO) kernel for the formation energies of alloys and surface energies of metals

BIMAL NEUPANE (Presenter), NIRAJ NEPAL, SANTOSH ADHIKARI, ADRIENN RUZSINSZKY, Temple Univ — Semi-local Density Functional Theory (DFT) includes the self-interaction error and misses the long-range van der Waals interaction. One possible remedy of these failures is the direct Random Phase Approximations (RPA). RPA stands on the highest rung of Jacob’s ladder of density functional approximations and includes the occupied and unoccupied Kohn Sham orbitals. However, the direct RPA is limited by neglecting the short ranged-correlation captured by an exchange-correlation kernel. Kernels based on the uniform electron gas model have shown some improvement over RPA and are computationally as affordable as RPA itself within PAW/pseudopotential codes. In this work, we are using the nonlocal energy-optimized (NEO) exchange-only kernel [1,2] to assess the formation energies of some intermetallic alloys and surface energies of some metals. These physical examples were chosen because they require a very delicate interplay of the short and long-range correlation in the kernel-corrected RPA and therefore a sophisticated way to construct the model kernel.


*National Science Foundation under Grant No. DMR–1553022.
The ground-state equilibrium properties of copper-gold alloys have been explored with the state-of-the-art random phase approximation (RPA) [1]. The PBE, PBE revised for solids, and revised Tao-Perdew-Staroverov-Scuseria functionals by Perdew et al. predict too-low formation energies, while the SCAN slightly overestimates it. The inclusion of thermal correction or the long-range dispersion provides a negligible contribution to the formation energies estimated with semilocal density functional theory. The spin-orbit coupling improves the formation energies of PBE only by 7-8 meV, while it intensifies the overestimation of SCAN. We found that the nonlocality present in RPA is able to describe the transition between two delocalized electron densities (bulk elemental constituents to crystallized alloys), as required to provide accurate formation energies without any further corrections.


* N.K.N. and A.R. acknowledge support by the National Science Foundation under Grant No. DMR-1553022. J.E.B. was supported by the A.R. Smith Department of Chemistry and Fermentation Sciences.
4:54PM D58.00011: Non-Adiabatic Quantum Molecular Dynamics Investigation of Hot Carrier Dynamics in Dielectric Polymers under High Electric Fields.* THOMAS LINKER (Presenter), SUBODH TIWARI, Collaboratory for Advanced Computing and Simulations, University of Southern California, HIROYUKI KUMAZOE, SHOGO FUKUSHIMA, Department of Physics, Kumamoto University, RAJIV KALIA, AIICHIRO NAKANO, Collaboratory for Advanced Computing and Simulations, University of Southern California, RAMAMURTHY RAMPRASAD, School of Materials Science and Engineering, Georgia Institute of Technology, FUYUKI SHIMOJO, Department of Physics, Kumamoto University, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, University of Southern California — Non-Adiabatic Quantum Molecular Dynamics (NAQMD) is a powerful tool typically used to model excited state electron-phonon dynamics under optical excitation. In this work we have ported NAQMD to study excited hot charge carriers involved in dielectric breakdown of organic polymers under high electric fields. Organic polymers offer many advantages over inorganic dielectrics, but they are severely limited by breakdown under the application of high electric fields. There also remains no mechanistic method for quantitative prediction of the breakdown field in polymers, unlike inorganic materials. Here we performed a systematic study of different electric fields on hot carrier dynamics and resulting chemical damage in a slab of archetypal polymer, polyethylene. We found a critical transition occurring near the experimentally reported intrinsic breakdown field marked by strong localization of electronic states at the slab surface and emergence of hot carrier C-H vibrational resonance. Such a localization transition may provide a critically-missing prediction method for computationally screening dielectric polymers with high breakdown fields.

*This work was supported by the Office of Naval Research through a Multi-University Research Initiative (MURI) grant (N00014-17-1-2656).
Electron-nuclear coupling in non-equilibrium dynamics plays a fundamental role in condensed matter physics, defining behavior from phase transitions to chemical reactions. Recently the dynamics of these processes have been able to be experimentally resolved in the time-domain, requiring a theoretical framework beyond the Born-Oppenheimer approximation to describe [1]. While approaches such as the multi-configuration time-dependent Hartree method have been successful at describing excited state dynamics of relatively small systems, the cost to precompute potential energy surfaces and non-adiabatic couplings becomes a significant bottleneck for larger systems. In this talk we develop a trajectory based variational ansatz which treats the electronic system at the level of time-dependent density functional theory, while simultaneously incorporating a nonadiabatic quantum mechanical description of the nuclei. This method is compared to multi-trajectory Ehrenfest dynamics in the resolution of nuclear effects within the optical spectrum of small molecules.


*We acknowledge funding from the ERC through the QSpec-NewMat Project
Localized and collective magnetic excitations in the magnetic topological insulator Sn$_{1-x}$Mn$_x$Te*  

ROBERT MCQUEENEY (Presenter), Iowa State University, DAVID VAKNIN, SANTANU PAKHIRA, Ames Laboratory, DANIEL M. PAJEROWSKI, Oak Ridge National Laboratory, DAVID C JOHNSTON, Iowa State University, DEBORAH SCHLAGEL, Ames Laboratory — The nature of the magnetism dilute magnetic topological insulators (MTIs), controlled by atomic disorder and/or clustering and the competition between short- and long-range magnetic interactions, is not well understood. MTIs that develop ferromagnetic (FM) long-range order can host dissipationless electronic transport via the quantum anomalous Hall effect. We studied the magnetic excitations in a prototypical MTI, Sn$_{0.95}$Mn$_{0.05}$Te, using inelastic neutron scattering. Neutron diffraction and magnetization data indicate that our Sn$_{0.95}$Mn$_{0.05}$Te sample has no FM long-range order. However, we observe slow, collective FM fluctuations (<70 μeV), indicating proximity to FM order. We also find a series of sharp peaks originating from excitations of antiferromagnetically coupled Mn-Mn dimers with J$_{AF}$ = 230 μeV. These dimers sit at next-nearest neighbor positions on the FCC sublattice, suggesting that Mn substitution is not completely random. The simultaneous presence of collective and localized components indicate that some Mn ions contribute to FM order and some form strongly-bound dimer singlets.

*This work was supported by the U. S. DOE, BES, DMSE, under Contract DE-AC02-07CH11358. This research used resources at SNS, a U. S. DOE User Facility operated by ORNL.

Topological insulator interfaced with ferromagnetic insulators: Bi$_2$Te$_3$ thin films on magnetite and iron garnets  

CHI-NAN WU (Presenter), VANDA M PEREIRA, SIMONE G ALTENDORF, SHENG-CHIEH LIAO, CHENG-EN LIU, ALEXANDER KOMAREK, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, MENGXIN GUO, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, HONG-JI LIN, CHIEN-TE CHEN, National Synchrotron Radiation Research Center, Hsinchu, Taiwan, MINGHWEI HONG, Department of Physics, National Taiwan University, Taipei, Taiwan, JUEINAI KWO, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, LIU TJENG, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — We have grown Bi$_2$Te$_3$ thin films on Y$_3$Fe$_5$O$_{12}$(111), Tm$_3$Fe$_5$O$_{12}$(111), Fe$_3$O$_4$(111), and Fe$_3$O$_4$(100) by molecular beam epitaxy with minimal chemical reaction at the interface. Electrical transport measurements were performed to study the magnetism induced by the proximity effect in the topological insulator in conjunction to the ferromagnetic insulators. We observed the anomalous Hall effect on these heterostructures. Magnetoresistance measurements at low temperature reveal a suppression of the weak antilocalization, indicating a possible topological surface state gap opening induced by the magnetic proximity effect. However, we did not observe any obvious x-ray magnetic circular dichroism (XMCD) on the Te M$_{45}$ edges. The results suggest that the ferromagnetism induced by the magnetic proximity effect via Van der Waals bonding in Bi$_2$Te$_3$ by is too weak to be detected by XMCD, but still can be observed by electrical transport measurements. This is consistent with published density-functional theory results on topological insulator/magnetic insulator heterostructure showing that only a small band gap of 9 meV is induced by the magnetic proximity effect.
Tailoring Hybrid Anomalous Hall Response in Engineered Magnetic Topological Insulator Heterostructures

PENG CHEN, YONG ZHANG, School of Information Science and Technology, ShanghaiTech University, QI YAO, School of Physical Science and Technology, ShanghaiTech University, THORSTEN HESJEDAL, Department of Physics, University of Oxford, SHILEI ZHANG, School of Physical Science and Technology, ShanghaiTech University, XUFENG KOU (Presenter), School of Information Science and Technology, ShanghaiTech University — Magnetic topological insulators (MTIs) have greatly broadened the research scope of topological quantum materials. Introducing MTIs into the field of spintronics defines a new trend of magnetic-based logic and memory applications. Engineering the anomalous Hall effect (AHE) in emerging MTIs has great potentials for quantum information processing and spintronics applications.

In this talk, we will present the MBE growth and exotic transport properties of Bi2Te3/MnTe heterostructures. RHEED, XRR and TEM have revealed the high quality and atomically flat interface of the film. Through transport measurements, we observed pronounced AHE signals from both layers combined together. The evolution of the resulting hybrid AHE intensity with the top Bi2Te3 layer thickness manifests the presence of an intrinsic ferromagnetic phase induced by the topological surface states at the heterolayer-interface. Surprisingly, we find the polarity of AHE can be switched by adjusting the Fermi level position of the Bi2Te3 layer via effective Sb-doping. Such flexibility in controlling the AHE strength, which depend on the specific band structure (i.e., Berry curvature), in our MTI heterostructures therefore opens up a multitude of opportunities to explore MTI-based spintronics devices.

Molecular Beam Epitaxy Growth and Magnetization Characterization of Fe-doped Bi2Se3

ZHENG REN (Presenter), HE ZHAO, HONG LI, BRYAN RACHMILOWITZ, ILIJA ZELJKOVIC, Boston College — Bi2Se3 is a prototypical 3D topological insulator (TI), which hosts gapless surface states protected by time-reversal-symmetry (TRS). When TRS is broken by doping with magnetic elements, this system can realize exotic electronic states, such as the quantum anomalous hall states (QAHS) (Rui Yu et al., Science 329 , 61 (2010)). We grow Fe-doped Bi2Se3 thin films on SrTiO3(001) substrates by molecular beam epitaxy (MBE), and characterize them using a combination of low-temperature scanning tunneling microscopy/spectroscopy (STM/S) and magnetization measurements. We find a large difference between the Fe concentration in the topmost layer determined from STM topographs and that inferred from magnetization measurements. Moreover we find an intriguing magnetic anisotropy of the thin films, different from that observed in their bulk counterparts. Our findings provide a fresh insight into the idea of doping Fe into Bi2Se3 as a route towards achieving QAHS.

*We gratefully acknowledge the funding from the Army Research Office, grant W911NF-17-1-0399.
Optically manipulating ferromagnetism in Cr-doped topological insulators (TIs)*

ADRIAN LLANOS (Presenter), Department of Applied Physics, Caltech, CHIEN-CHANG CHEN, MARCUS L TEAGUE, Department of Physics, Caltech, XIAOYU CHE, PENG ZHANG, LEI PAN, KANG L. WANG, Department of Electrical Engineering, University of California Los Angeles, NAICHANG YEH, Department of Physics, Caltech — Optically manipulating ferromagnetic materials has been shown to be a promising route to opto-spintronic applications. Using a combination of optically-enabled transport measurements and scanning tunneling spectroscopic (STS) measurements in the presence of circularly polarized (CP) light, we found an enhancement of magnetization in 10% Cr-doped (Bi\textsubscript{x}Sb\textsubscript{1-x})\textsubscript{2}Te\textsubscript{3} bilayer heterostructures which consisted of a pure layer (Bi\textsubscript{x}Sb\textsubscript{1-x})\textsubscript{2}Te\textsubscript{3} on top of a 10% Cr-doped (Bi\textsubscript{x}Sb\textsubscript{1-x})\textsubscript{2}Te\textsubscript{3} layer. Measurements of the anomalous Hall resistance revealed an increase in $R_{xy}$ and a decrease in longitudinal resistance $R_{xx}$ in the bilayer magnetic TI system under CP light (wavelengths $\lambda = 1600 \sim 1700$ nm). In contrast, both $R_{xx}$ and $R_{xy}$ were suppressed under CP light for uniformly Cr-doped (Bi\textsubscript{x}Sb\textsubscript{1-x})\textsubscript{2}Te\textsubscript{3}. To understand the microscopic origin of these results, we performed spatially resolved STS studies on the surface state of magnetic TIs as a function of temperature and magnetic field. We further conducted optically-assisted STS studies to spatially map out the CP light-induced spectral changes to the surface state. The physical implications from correlating the spatially resolved STS under CP light with findings from macroscopic $R_{xx}$ and $R_{xy}$ will be discussed.

*This work is jointly supported by ARO and NSF.
Magneto-transport properties of bulk-insulating topological insulators (Bi,Sb)$_2$Te$_3$ on thulium iron garnets

CHUN-CHIA CHEN (Presenter), SHANG RONG YANG, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, YU-TING FANCHIANG, Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei 10617, Taiwan, WEI-JHIH ZOU, MENGXIN GUO, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, CHAO-KAI CHENG, Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei 10617, Taiwan, SHENG-WEN HUANG, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, KENG-YUNG LIN, Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei 10617, Taiwan, KO-HSUAN CHEN, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, MINGHWEI HONG, Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei 10617, Taiwan, JUEINAI KWO, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan — Breaking time-reversal symmetry in topological insulators (TIs) via magnetic proximity effect attracted intense studies. The spin dynamics of magnetic insulators (MIs) interfacing with TIs has been investigated by ferromagnetic resonance,

High-temperature ferromagnetic topological crystalline insulating state induced by proximity effect in a EuS/SnTe heterostructure

RYOTA AKIYAMA (Presenter), KAZUKI WATANABE, Univ of Tokyo, YUTA TOMOHIRO, TAKERU SHIMANO, Institute of Material Sciences, Univ of Tsukuba, RYO ISHIKAWA, Ulvac, KAZUHIRO AKUTSU, KAZUKI IIDA, Comprehensive Research Organization for Science and Society, SHINJI KURODA, Institute of Material Sciences, Univ of Tsukuba, SHUJI HASEGAWA, Univ of Tokyo — Ferromagnetic topological insulators attract much attention because they enable us to realize the quantum anomalous Hall effect (QAHE), possibly useful for low-energy-consumption devices by using the chiral edge state. However, the temperature for QAHE is still low mostly due to degradation of crystallinity by doping magnetic atoms. To prevent it, using ferromagnetic proximity effect is one of the solutions [1,2]. We made and measured a EuS/SnTe heterostructure. As a result, intriguingly, the perpendicular magnetization (PM) reaches minimum at ~100 K and then increases with increasing temperature and keeps up to room temperature. A similar behavior was reported in EuS/Bi$_2$Se$_3$[1], and the explanation is that after disappearance of bulk magnetization in EuS ($T_C$=17 K), the direction of the interface magnetization becomes perpendicular from oblique with increasing temperature. On the other hand, when we use a trivial insulator PbTe: EuS/PbTe, the PM monotonically decreases with increasing temperature. This suggests that the anomalous interface ferromagnetism is induced by the non-trivial nature in SnTe. [1] F. Katmis et al., nature 533, 513 (2016). [2] R. Akiyama et al., arXiv 1910.10540 (2019).

*This work was partially supported by KAKENHI (18K18732, 18H01857 and 16H02108).
Ultrafast momentum-resolved study of electron-phonon coupling in an antiferromagnetic topological insulator

HARICHARAN PADMANABHAN (Presenter), VLADIMIR A STOICA, HUAIYU WANG, Pennsylvania State University, NATHAN KOOCHER, MINGQIANG GU, Northwestern University, XIAOZHE SHEN, MING-FU LIN, SLAC National Accelerator Laboratory, SENG HUAT LEE, ZHIQIANG MAO, Pennsylvania State University, AARON LINDENBERG, XIJIE WANG, SLAC National Accelerator Laboratory, JAMES RONDINELLI, Northwestern University, VENKATRAMAN GOPALAN, Pennsylvania State University — Elementary electronic and lattice excitations and their mutual interactions form the foundation of our understanding of condensed matter systems. In the context of topological insulators, the electron-phonon coupling determines in addition, the robustness of dissipationless surface states at finite temperatures. In this work, we consider the first discovered intrinsic antiferromagnetic topological insulator, MnBi$_2$Te$_4$, a system that is predicted to exhibit the quantum anomalous Hall effect [1]. We study the momentum-resolved electron-phonon coupling in this material at its inherent femtosecond timescale using ultrafast electron diffraction and coherent phonon optical spectroscopy. We find that electrons are strongly coupled to in-plane zone-boundary Eg optical phonons, resulting in a highly nonequilibrium phonon population for several hundreds of femtoseconds after excitation. The nonequilibrium phonon system subsequently relaxes by phonon-phonon coupling to zone-center transverse acoustic phonons. We simulate how the strongly coupled Eg phonons modulate the exchange interaction and magnetism using DFT calculations.


DOE grant 432 43 68KK

Pressurizing an antiferromagnetic topological insulator candidate

PRISCILA ROSA (Presenter), SEAN THOMAS, ERIC BAUER, JOE D THOMPSON, FILIP RONNING, Los Alamos National Laboratory — Intrinsic magnetic topological insulators hold the potential of hosting quantum anomalous Hall states, chiral Majorana fermions, and topological magnetoelectric effects. We have identified Zintl antiferromagnet Eu$_5$In$_2$Sb$_6$ as a candidate material which displays remarkable insulating behavior. Our previous results showed the presence of colossal magnetoresistance in this system, which is consistent with the presence of magnetic polarons. Here we investigate the effects of applied hydrostatic and uniaxial pressure on Eu$_5$In$_2$Sb$_6$ single crystals in an effort to drive the system through a topological phase transition. Our results show an exceptionally large decrease in resistivity under applied hydrostatic pressure as well as uniaxial pressure along the c axis.

*Work at Los Alamos was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering.
4:18PM D59.00010: Spin-to-charge conversion on the edge of quantum spin Hall insulator
YASUFUMI ARAKI (Presenter), Japan Atomic Energy Agency, TAKAHIRO MISAWA, The University of Tokyo, KENTARO NOMURA, Tohoku University — We present our theoretical work on dynamical spin-to-charge conversion at the edge of a quantum spin Hall insulator (QSHI), namely a two-dimensional topological insulator with helical edge states. Interconversion between spin- and charge-related quantities has been a key idea in making use of magnetic materials, especially in the context of spintronics. QSHI is a typical system showing a universal charge-to-spin conversion behavior, namely the quantum spin Hall effect, whereas the spin-to-charge conversion therein is still not clearly understood.

We here investigate the many-body dynamics of the electrons under the magnetization dynamics at the QSHI-ferromagnet(FM) junction. We analytically treat the electron dynamics in terms of the Floquet-Keldysh formalism, and compare the spin injection rate from the FM into the QSHI and the charge current induced along the edge. Whereas the edge current seen in the previous works is reproduced, we find that it is not proportional to the spin injection rate, especially when the exchange interaction at the junction is strong enough. This relation implies that the spin-to-charge conversion in this system cannot be considered as the inverse spin Hall effect, while it can be rather seen as the inverse Edelstein effect.

4:30PM D59.00011: Exchange interactions between topological and meta-magnetic insulators
YING WANG (Presenter), Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA, purdue university, VALERIA LAUTER, Thin Films and Nanostructures, Oak Ridge National Laboratory, JACEK K. FURDYNA, XINYU LIU, Department of Physics, Notre Dame University, LEONID ROKHINSON, Physics department and Birck Nanotechnology Center, Purdue university — The hallmark of 3D topological insulators(TIs) are topological surface states(TSS) protected by the time-reversal symmetry. One of the important goals is the ability to manipulate surface electron states and to lift the topological protection of TSS for the emergence of novel physical phenomena. Gapping of TSS has been demonstrated in TIs with bulk doping using the magnetic impurities and via exchange coupling to insulating magnetic or antiferromagnetic materials. Here we report an experimental study of exchange coupling in EuSe/Bi$_2$Se$_3$ and EuSe/Bi$_2$Se$_3$/EuSe heterostructures grown by MBE. Bi$_2$Se$_3$ is a typical TI and EuSe is a meta-magnetic insulator with a rich phase diagram of paramagnetic, antiferromagnetic, ferrimagnetic and ferromagnetic phases at low temperatures. Polarized neutron scattering experiments indicate enhanced exchange interaction between EuSe and Bi$_2$Se$_3$ and we observe finite in-plane magnetization at the interface even above the Néel temperature ($T_N$~5K) of EuSe. In transport measurement, we observe modulation of longitudinal and Hall resistance as a function of the magnetic field, which may be explained by the formation and re-arrangement of magnetic domains at the interface.

*Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy
We investigate the topological magneto-electric effect (TME) in Bi$_2$Se$_3$ topological insulator (TI) thin films, with a perpendicular exchange field applied to the top and bottom surfaces in the anti-parallel configuration. Here the system is in the axion insulator phase, which allows a direct probe of the quantized topological $\theta$-term of the axion electrodynamics. The $\theta$-term is a TI bulk property which gives the coefficient of proportionality between an applied electric field and the induced magnetization. We first consider an infinite slab and extract $\theta$ in a tight-binding framework, under the condition of weak electric field. In the second part of the work, we consider systems which are finite in one or more dimensions. By analyzing the dependence of $\theta$ on the system size and the strengths and profiles of the exchange fields on the two surfaces, we determine when the TME is expected to be quantized. Furthermore, we investigate possible deviations from exact quantization in the regime where the exchange field on one of two surfaces is progressively enhanced beyond a critical value. Our study sheds light on the fundamental issue of whether TME in a TI is completely determined by the bulk properties or it can be affected by how time-reversal symmetry is broken at the surfaces.

**4:54PM D59.00013: Electrically Tunable Anomalous Hall Effect in Topological Crystalline Insulator Films**

PENG DENG (Presenter), PENG ZHANG, XIAOYU CHE, KANG-LUNG WANG, Electrical and Computer Engineering, University of California, Los Angeles — Introducing ferromagnetism into topological crystalline insulator SnTe could lead to the high-Chern-number quantum anomalous Hall effect. Here we report the observation of magnetic proximity effect in heterostructures formed by the SnTe (111) and 2 quintuple layers thick Cr-doped (BiSb)$_2$Te$_3$ (CBST). Owing to the charge transfer between CBST and SnTe, the Fermi level of the latter can be tuned by adjusting the Bi/Sb ratio in the former. An anomalous Hall resistance as large as 0.08 $h/e^2$ is revealed. The transferred charges modify the electric field perpendicular to the film and change the critical thickness of topological phase transition in SnTe. Such property makes SnTe useful in realizing the topological transistor.
Large-Gap Quantum Anomalous Hall effect in a Magnetically doped Type-I Topological Heterostructure

ANH PHAM (Presenter), PANCHAPAKESAN GANESH, Oak Ridge National Lab — Current method of doping a topological insulator (TI) with magnetic element has only yielded low temperature quantum anomalous hall effect due to the small exchange energy of dopants and uncontrollable shifts in the Fermi-level due to band-bending effects [1]. To overcome the band-bending effect, Fermi-level can be pinned by creating a Type-I type TI/insulator band offset, while the magnetic exchange energy can be increased by searching over different potential magnetic dopants that remain neutral. Given the recent successes of growing high-quality TI-films on Cr$_2$O$_3$ heterostructure [2], we study different magnetically doped TI/Cr$_2$O$_3$ heterostructures using a combination of density functional theory and k.p modelling. We find Sb$_2$Te$_3$ to form a type-I interface with Cr$_2$O$_3$I, thereby making the heterostructure insulating, meanwhile maximizing the Zeeman energy due to the segeration of the dopants at the interface, suggesting possible room-temperature QAHE. We also compare our interfacial magnetism model with available experiments.


This research were financially supported by the Oak Ridge National Laboratory’s Laboratory Directed Research and Development project (Project ID: 8988).

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D60 DMP: Topological Materials: Topological Superconductors and Majorana States

WEI LI (Presenter), Tsinghua University — A possible topological superconductor 2M-WS$_2$ has been discovered and its superconducting transition temperature is ~ 8.8 K. By using low-temperature scanning tunneling microscopy, we have made direct observation of a clean Majorana zero mode in this transition metal dichalcogenide. The observed Majorana zero mode well separates in energy from the Caroli-de Gennes-Matricon bound states inside the vortex-core, therefore providing a good platform for the future quantum computing.

3:06PM D60.00002: Applications of a Novel Quantum Interband Index in Condensed Matter: Topological Insulators, Optical Selection Rules, and Beyond*  THARINDU WARNAKULASOORIYA FERNANDO (Presenter), TING CAO, Physics, University of Washington, CONGJUN WU, Physics, University of California, San Diego — The physical significance of a novel gauge-invariant interband index $T$ proposed in [1] is not immediately clear in condensed matter systems. In this talk, we present numerical calculations of the index $T$ in various systems. Calculations of $T$ in loops around valleys of the Haldane model for the anomalous quantum Hall effect give distinct integer numbers with behavior partly reminiscent of different types of Chern numbers (such as spin or valley). For loops containing more/less than 1 Dirac point, our calculations reveal perplexing results including a link to the sign of local Berry curvature. We further connect this index to recently discovered optical selection rules [2-4] and demonstrate other physical effects related to $T$.


*This work is supported by the Provost Fellowship from the Department of Physics at the University of Washington.

3:18PM D60.00003: Bulk superconductivity in FeTe$_{1-x}$Sex via physicochemical pumping of excess iron  LIANYANG DONG (Presenter), University of California, Santa Barbara, HE ZHAO, ILIJA ZELJKOVIC, Boston college, STEPHEN WILSON, JOHN W HARTER, University of California, Santa Barbara — The iron-based superconductor FeTe$_{1-x}$Sex has attracted considerable attention as a candidate topological superconductor owing to a unique combination of topological surface states and bulk high-temperature superconductivity. The superconducting properties of as-grown single crystals, however, are highly variable and synthesis dependent due to excess interstitial iron impurities incorporated during growth. Here we report a novel physicochemical process for pumping this interstitial iron out of the FeTe$_{1-x}$Sex matrix and achieving bulk superconductivity. Our method should have significant value for the synthesis of high-quality single crystals of FeTe$_{1-x}$Sex with large superconducting volume fractions.
3:30PM D60.00004: Molecular Beam Epitaxy Growth of Superconducting Sn\(_{1-x}\)In\(_x\)Te (0 ≤ x ≤ 0.67) Thin Films  MAKOTO MASUKO (Presenter), Department of Applied Physics, Univ of Tokyo, RYUTARO YOSHIMI, Center for Emergent Matter Science, RIKEN, ATSUSHI TSUKAZAKI, Institute for Materials Research, Tohoku University, MINORU KAWAMURA, KEI TAKAHASHI, Center for Emergent Matter Science, RIKEN, MASASHI KAWASAKI, Department of Applied Physics, Univ of Tokyo, YOSHINORI TOKURA, Center for Emergent Matter Science, RIKEN — Topological superconductivity has attracted increasing interest for not only its novel properties but also the possible application to quantum computing. One way to realize topological superconductivity is to induce superconducting gap in the surface states of topological insulators (TIs) by the proximity effect. To maximize the superconducting proximity effect, all-telluride based heterostructures consisting of TI (Bi,Sb)\(_2\)Te\(_3\) and Te-based superconductor (SC) may be a promising candidate. As the first step toward TI/SC heterostructures, epitaxial growth of Te-based SC is required.

In this work, we report the thin film growth of rock-salt type SC Sn\(_{1-x}\)In\(_x\)Te (SIT) by means of molecular beam epitaxy. By finely tuning the amount of Te supply especially in the high-doping region, we have achieved In-doping up to x = 0.66, which exceeds bulk solubility limit under ambient pressure x ~ 0.5. In the transport measurements, we have observed superconductivity in SIT thin films, and \(T_c\) shows dome-shaped dependence on x with the highest \(T_c\) = 4.25 K at x = 0.55. Our result may lead to the TI/SC heterostructures and interfacial topological superconductivity.

3:42PM D60.00005: Proximity-induced superconductivity in SnTe thin films*  BRYAN RACHMILOWITZ (Presenter), HE ZHAO, HONG LI, ALEXANDER LAFLEUR, Boston College, JOHN SCHNEELOCH, RUIDAN ZHONG, GENDA GU, Brookhaven National Lab, ILIJA ZELJKOVIC, Boston College — Superconducting topological crystalline insulators (TCIs) are theorized to host new types of topologically protected surface states distinct from those at the surface of superconducting Z\(_2\) topological insulators (TIs). While superconducting proximity effect has been widely used to induce superconductivity in Z\(_2\) TIs, the efforts to induce superconductivity in TCIs have been hindered by growth difficulties. Here we report the synthesis of heterostructures of a prototypical TCI SnTe(111) and high temperature superconductor Fe(Te,Se) using molecular beam epitaxy. Utilizing low-temperature scanning tunneling microscopy and spectroscopy as function of temperature and magnetic field, we show strong evidence of induced superconductivity at the surface of SnTe. Our work provides a new platform for studying emergent phenomena in superconducting TCIs.

*We gratefully acknowledge the support from the Army Research Office Grant No. W911NF-17-1-0399 and the NSF Grant No. 1654041
3:54PM D60.00006: Fractional disclination charge in two-dimensional \(C_n\)-symmetric topological crystalline insulators* TIANHE LI (Presenter), PENGHAO ZHU, University of Illinois at Urbana-Champaign, WLADIMIR A BENALCAZAR, Department of Physics, Pennsylvania State University, TAYLOR L HUGHES, University of Illinois at Urbana-Champaign — Robust fractional charge localized at disclination defects has been recently found as a topological response in \(C_6\) symmetric 2D topological crystalline insulators (TCIs). We thoroughly investigate the fractional charge on disclinations in \(C_n\) symmetric TCIs, with or without time-reversal symmetry, and including spinless and spin-1/2 cases. We find the disclination charge is fractionalized in units of \(e/n\) for \(C_n\) symmetric TCIs; and for spin-1/2 TCIs, with additional time-reversal symmetry, the disclination charge is fractionalized in units of \(2e/n\). Utilizing band representation theory, we construct topological indices of the fractional disclination charge for all 2D TCIs that admit a (generalized) Wannier representation. Moreover, we use an algebraic technique to generalize the indices for TCIs with non-zero Chern numbers, where a (generalized) Wannier representation is not applicable. Our results provide a quantitative and intuitive understanding of fractional charge at defects for 2D \(C_n\)-symmetric TCIs.

*This work is supported by NSF grants EFMA-1627184 (EFRI), DMR-1351895, the MRSEC program under NSF Award Number DMR-1720633 (SuperSEED) (TL, PZ, TLH), and Eberly Postdoctoral Fellowship at Penn State (WAB).

4:06PM D60.00007: Tuning the Edge States of Topological Crystalline Insulator Bismuthene via Substrate Effects* CHUTIAN WANG, YUEFENG YIN, Materials Science and Engineering, Monash University, MICHAEL FUHRER, Physics and Astronomy, Monash University, NIKHIL MEDHEKAR (Presenter), Materials Science and Engineering, Monash University — One of the key challenges in design of devices bases on topological materials is to conveniently turn the surface and edge states on and off. Two-dimensional (2D) topological crystalline insulators (TCI) are ideal materials for achieving this switch, as their edge states can be turned on/off by applying a symmetry-breaking field. However, it remains unresolved how 2D TCI phases can be integrated in experimental devices due to the difficulty in synthesis and the complex interactions between TCI and underlying substrates. In this theoretical study based on first principles calculations and Wannier tight-binding models, we show that the edge states of TCI bismuthene can be stabilized on some substrates (e.g. h-BN and SiC) when the stacking pattern does not break mirror symmetry. We can achieve fine tuning of the edge states of bismuthene by applying strain or an external electric field. This research provides guidelines for selection of appropriate substrates for the experimental realization of topological edge states and the methodology to tune the edge states in 2D TCIs.

*This work is supported by ARC Centre of Excellence in Future Low-Energy Electronics Technologies (CE170100039).
4:18PM D60.00008: Searching for ideal topological crystalline insulators and topological superconductors in Pb-Sn-In-Te system  GENDA GU (Presenter), RUIDAN ZHONG, YANGMU LI, QIANG LI, TONICA VALLA, JOHN TRANQUADA, Brookhaven National Laboratory — The discovery of 3D topological insulator materials and topological superconductor open up a new research field in the condensed matter physics. In order to search for the topological superconductor, we have grown a large number of the single crystals of Pb-system (Pb-Sn-In-Te) topological crystalline insulator and their topological superconductor. We have measured the physical properties on these single crystals by various techniques. We have studied the effect of crystal growth condition, impurity and composition on the bulk electrical conductivity of these single crystals. We try to find out which composition and crystal growth condition is the best for the ideal topological insulator, topological crystalline insulator and topological superconductor. We have got the bulk topological superconductor with $T_c=5K$.

4:30PM D60.00009: Superconducting proximity effect in InAsSb surface quantum wells with in-situ Al contacts*  WILLIAM SCHIELA (Presenter), WILLIAM MAYER, JOSEPH YUAN, MEHDI HATEFIPOUR, Department of Physics, New York University, WENDY L SARNEY, STEFAN P SVENSSON, ASHER LEFF, US Army CombatCapabilities Command, Army Research Laboratory, TIAGO DE CAMPOS, Department of Physics, University at Buffalo, KAUSHINI S WICKRAMASINGHE, MATTHIEU DARTIALH, Department of Physics, New York University, IGOR ZUTIC, Department of Physics, New York University, WENDY L SARNEY, STEFAN P SVENSSON, ASHER LEFF, US Army CombatCapabilities Command, Army Research Laboratory, TIAGO DE CAMPOS, Department of Physics, University at Buffalo, KAUSHINI S WICKRAMASINGHE, MATTHIEU DARTIALH, Department of Physics, New York University, IGOR ZUTIC, Department of Physics, New York University — We demonstrate a robust superconducting proximity effect in InAs$_{0.5}$Sb$_{0.5}$ quantum wells grown with epitaxial Al contacts, which has important implications for mesoscopic and topological superconductivity. Unlike more commonly studied InAs and InSb semiconductors, bulk InAs$_{0.5}$Sb$_{0.5}$ supports stronger spin-orbit coupling and a larger g-factor. Through structural and transport characterization we observe high-quality interfaces and strong spin-orbit coupling. We fabricate Josephson junctions based on InAs$_{0.5}$Sb$_{0.5}$ quantum wells and observe a strong proximity effect. These junctions exhibit products of normal resistance and critical current, $I_cR_N = 270\mu V$, and excess current, $I_{ex}R_N = 200\mu V$, at contact separations of 500nm. Both of these quantities demonstrate a robust and long-range proximity effect with highly-transparent contacts.

*This work was partially supported by NSF DMR 1836687, the US Army research office, US ONR N000141712793, NSF ECCS-1810266, the University at Buffalo Center for Computational Research, and the ARO/LPS Quantum Computing Graduate Research Fellowship (QuaCGR BAA W911NF-17-S-0002).
4:42PM D60.00010: Topological Properties of Superconducting PdTe  RAMAKANTA CHAPAI (Presenter), Louisiana State University, Baton Rouge, PERAM SREENIVASA REDDY, National Cheng Kung University, Taiwan, LINGYI XING, Louisiana State University, Baton Rouge, DAVID E GRAF, National High Magnetic Field Laboratory, Tallahassee, FL, AMAR B. KARKI, WEIWEI XIE, JOHN DITUSA, Louisiana State University, Baton Rouge, TAY-RONG CHANG, National Cheng Kung University, Taiwan, RONGYING JIN, Louisiana State University, Baton Rouge — PdTe is a superconductor with $T_c \sim 4.5$ K. We have investigated its normal-state electronic properties via both first principles calculations and magnetic torque measurements by applying magnetic field up to 35 Tesla. Detailed analysis of the de-Haas van Alphen (dHvA) oscillations allows us to identify four frequencies: $F_\alpha = 64$ T, $F_\beta = 658$ T, $F_\gamma = 1155$ T, and $F_\eta = 1867$ T. Using the Lifshitz-Kosevich equation to fit the experimental data, the effective masses are obtained with $m^*_\alpha = 0.305m_0$, $m^*_\beta = 0.288m_0$, $m^*_\gamma = 0.415m_0$, and $m^*_\eta = 0.451m_0$ ($m_0$ is the free electron mass). By constructing the Landau fan diagram for each band, we extract the Berry phase, which is non-trivial for the $\alpha$ and $\gamma$ bands. These experimental findings are consistent with the calculated results. This suggests that PdTe is a topological superconductor.

4:54PM D60.00011: Tuning topological hinge states of Bi by edge adsorption: first-principles study*  IVAN NAUMOV (Presenter), PRATIBHA DEV, Howard University — Recent studies have shown that bismuth is a crystalline topological insulator and, additionally, hosts two different second-order band topologies that are protected by twofold and the threefold rotational symmetries [1,2]. These second-order topologies manifest themselves in one-dimensional hinge states in samples whose shape preserve the corresponding rotational symmetry [1,2]. Using first-principles calculations we show that the hinge states can be significantly tuned by H and N adsorption. We discuss the changes in their dispersion curves, real-space charge distributions and spin texture. Our findings may have practical applications in future electronic devices.


*This research was supported by W. M. Keck Foundation.
5:06PM D60.00012: The edge theories of 2D fermionic symmetry protected topological phases

SHANGQIANG NING (Presenter), CHENJIE WANG, Department of Physics, The University of Hong Kong, QING-RUI WANG, ZHENGCHENG GU, Department of Physics, The Chinese University of Hong Kong — Abelian Chern-Simons theory, labeled by the so-called $K$ matrices, have been quite successful in characterizing and classifying Abelian fractional quantum hall effect (FQHE) as well as symmetry protected topological (SPT) phases, especially for bosonic SPT phases. However, there are still some puzzles in dealing with fermionic SPT phases. In this paper, we utilize the Abelian Chern-Simons theory to study the fermionic SPT phases protected by Abelian total symmetry $G_f$ that is a central extension of bosonic symmetry $G_b$ by fermion parity symmetry $Z^f_2$. In particular, we study the edge theories with the proper anomalous symmetry action on the edge fields for various examples. Moreover, we also discuss the construction of edge theories with central charge $n - 1$ for Type-III bosonic SPT phases protected by $(Z_n)^3$ symmetry.

*This work is supported by the Research Grant Council of Hong Kong (ECS 21301018), Direct Grant No. 4053346 from The Chinese University of Hong Kong and funding from Hong Kong's Research Grants Council (GRF No.14306918, ANR/RGC Joint Research Scheme No. A-CUHK402/18), the Ministry of Science and Technology of China (Grant 322 No. 2016YFA0300504), the NSF of China (Grant 323 No. 11574392 and No. 11974421).

5:18PM D60.00013: Selective Control of Surface Spin Current in Topological Pyrite OsX$_2$ (X= Se, Te) Crystals

YUEFENG YIN (Presenter), Materials Science and Engineering, Monash University, MICHAEL FUHRER, Physics and Astronomy, Monash University, NIKHIL MEDHEKAR, Materials Science and Engineering, Monash University — The development of next-generation spin-based nanoelectronic devices requires effective control and detection of spin polarization. Recently topological materials have shown promising potential in this field due to their unique spin textures. Here we report the discovery of highly anisotropic surface spin textures in the (001) surfaces of topological pyrite OsX$_2$ (X = Se, Te) crystals using first principles calculations and Wannier tight-binding models. The surface spin textures of topologically nontrivial OsX$_2$ features a transition from in-plane to out-of-plane spin polarization in the momentum space and are protected by local crystalline symmetries. The energy screening of bulk bands leads to selective filtering of the magnitude and orientations of the surface spin polarization. These results provide new physical insights for manipulating spin degree of freedom in spin logic devices and could inspire new strategies of search nonmagnetic materials hosting exotic spin properties.

*This work is supported by ARC Centre of Excellence in Future Low-Energy Electronics Technologies (CE170100039).
2:30PM D61.00001: Effect of pressure on the competing phases in FeSe and BaFe$_2$As$_2$:

Insights from specific heat measurements and beyond* [Invited] ELENA GATI (Presenter), LI XIANG, SERGEY L. BUD'KO, PAUL C CANFIELD, Iowa State University, Ames Laboratory —

Understanding the phase interplay in iron-based superconductors is considered to be crucial for unravelling the mechanism behind their superconductivity. In this talk, we focus on new insights into the phase interplay under pressure of two members, FeSe and BaFe$_2$As$_2$, from specific heat under pressures [1] up to ~ 2.5 GPa.

For FeSe [2], we show that superconductivity is bulk and competes with magnetism, whenever present. In addition, we conclude that, whenever magnetism is present, magnetic and superconducting fluctuations exist across wide ranges of pressure above their respective, bulk transition temperatures.

For Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ [3], we argue that the behavior of the nematic transition under pressure is intimately linked to changes of the Fermi surface topology. We complement these data by presenting the first study of elastoresistance under pressure [4] on BaFe$_2$As$_2$, which might allow to study the interplay of nematicity and superconductivity under pressure.


*The present work was done in collaboration with Anna Böhmer (KIT).

*This work was carried out at Iowa State University and supported by Ames Laboratory, US DOE, under Contract No. DE-AC02-07CH11358, by the Gordon and Betty Moore Foundation’s EPiQS Initiative and the W. M. Keck Foundation.
3:06PM D61.00002: Electronic phase diagram of FeSe$_{1-x}$Te$_x$ under high pressure  
KIYOTAKA MUKASA (Presenter), KOHEI MATSUURA, YUICHI SUGIMURA, MUKU OTANI, MINGWEI QIU, MIKIHIKO SAITO, YUTA MIZUKAMI, KENICHIRO HASHIMOTO, Department of Advanced Materials Science, University of Tokyo, JUN GOUCHI, YOSHIYA UWATOKO, Institute for Solid State Physics, University of Tokyo, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, University of Tokyo — FeSe has the simplest crystal structure among the iron-based superconductors and is known to have a nonmagnetic nematic order. When selenium is substituted by the isovalent element, sulfur, the nematic phase is suppressed and a nematic quantum critical point without magnetism appears. On the other hand, under pressure, a dome-shaped magnetic phase is induced and the superconducting transition temperature rises from 9 K to 37 K. In this study, we focus on FeSe$_{1-x}$Te$_x$ in which selenium is substituted by tellurium. In order to clarify the relationship between the nematic phase and the superconducting phase, we have synthesized bulk single crystals of FeSe$_{1-x}$Te$_x$ (0 < x < 0.22) by using the chemical vapor transport method. The temperature dependence of the electrical resistivity was measured on the FeSe$_{1-x}$Te$_x$ crystals under pressure up to 8 GPa using a constant loading cubic anvil high-pressure apparatus. As a result, we have established the three-dimensional electronic phase diagram; temperature against pressure and Te-substitution. The obtained phase diagram indicates that the tellurium substitution shifts the pressure-induced magnetic phase to a lower pressure side, which is in contrast to the sulfur substitution case.

3:18PM D61.00003: Multiple Magnetic Phases Hiding in Plain (and Out-of-Plane) Sight in Coexistence with Superconductivity in LaFeAs$_{1-x}$P$_x$O 1111 System*  
RYAN STADEL (Presenter), Northern Illinois Univ, DMITRY KHALYAVIN, PASCAL MANUEL, ISIS, Rutherford Appleton Laboratory, RAFAEL FERNANDES, MORTEN HOLM CHRISTENSEN, University of Minnesota, KEITH TADDEI, HFIR, Oak Ridge National Laboratory, CLARINA RELOJ DELA CRUZ, ASHFIA HUQ, SNS, Oak Ridge National Laboratory, SAUL LAPI DUS, APS, Argonne National Laboratory, DANIEL PHELAN, DUCK YOUNG CHUNG, MATTHEW KROGSTAD, RAYMOND OSBORN, STEPHAN ROSENKRANZ, Material Science, Argonne National Laboratory, OMAR CHMAISSEM, Northern Illinois Univ — Following the discovery of the microscopic co-existence of antiferromagnetic spin density waves and superconductivity in Ba$_{1-x}$K$_x$Fe$_2$As$_2$ and the low temperature structural re-entrance to the magnetic C$_4$ tetragonal phase in Ba$_{1-x}$Na$_x$Fe$_2$As$_2$, an effort was made to seek similar phases in the related LaFeAs$_{1-x}$P$_x$O 1111 system. Previous work had reported two superconducting domes as well as two distinct magnetic regions. While the low doping magnetic phase had been well characterized by neutron diffraction, the higher doped magnetic region had been deduced from short range $^{31}$P-NMR measurements. We present a detailed phase diagram with nuclear and magnetic structural characterization based on a combination of x-ray and neutron diffraction, as well as magnetic temperature dependence thoroughly mapped by muon spin resonance. This work demonstrates three distinct magnetic phases evolving from in-plane orthorhombic to in-plane tetragonal to out-of-plane tetragonal permeating the entire phase diagram from the parent LaFeAsO to superconducting LaFeAs$_{0.2}$P$_{0.8}$O.

*Work at the Materials Science Division at Argonne National Laboratory was supported by the US Department of Energy, Office of Science, Materials Sciences and Engineering Division.
3:30PM D61.00004: Wang-Landau simulations of the coupled magnetic and nematic transitions in disordered iron-based superconductors*  ANZUMAAN CHAKRABORTY (Presenter), Department of Physics, Missouri University of Science and Technology, WILLIAM J MEESE, RAFAEL FERNANDES, School of Physics and Astronomy, University of Minnesota, THOMAS VOJTA, Department of Physics, Missouri University of Science and Technology — In many iron-based superconductors, nematicity and magnetism are found to be closely related and occurring at comparable temperatures. While many works have discussed the character of these coupled transitions in clean systems, the impact of disorder, like random strain, has not been elucidated. Here we perform Monte Carlo simulations of an appealing model that captures these two transitions, namely, the 2D anisotropic Ising-O(3) model. For sufficiently large anisotropy in the exchange coupling, there is a direct first-order transition from the paramagnetic tetragonal phase to the low-temperature phase that displays both spin and nematic (Ising) orders. This transition splits into two separate transitions as the anisotropy decreases, giving rise to a nematic intermediate phase. We study both clean and disordered systems and compare conventional algorithms, such as Metropolis and Wolff, to an implementation using the Wang-Landau algorithm. The latter avoids the supercritical slowing down associated with the first-order transitions, providing an efficient way to probe the complicated free energy landscapes near the multi-critical point. Phase diagrams are obtained and compared to experimental results.

*Work supported by the NSF under Grant numbers DMR-1506152 and DMR-1828489.

3:42PM D61.00005: Coexistence of long-range magnetic ordering and superconductivity in FeSe/EuTiO$_3$ heterostructure  CHONG LIU (Presenter), HYUNGKI SHIN, RYAN ROEMER, KE ZOU, Stewart Blusson Quantum Matter Institute, University of British Columbia — Spin degree of freedom has played a key role in unconventional superconductivities. FeSe monolayer superconductors, with the highest transition temperature in Fe-based superconductors, remain not magnetically ordered, while spin density waves and nematicity have been observed in bulk FeSe. We grow heterostructures of FeSe on (001) antiferromagnetic EuTiO$_3$ (ETO) using molecular beam epitaxy. Transport measurements showed clear anomalous Hall effect in both ETO and FeSe/ETO samples. Simultaneously, superconducting transition was also observed in FeSe films on ETO. Our work provides a new platform for the interplay of spins and superconductivity, which may promote integration of superconductors in new spintronics.
Quasi-elastic scattering from short-range magnetic order in FeTe$_{1-x}$Se$_x$ compounds

GUANGYONG XU (Presenter), ZHIJUN XU, National Institute of Standards and Technology, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory, ROBERT J BIRGENEAU, University of California, Berkeley — We report neutron scattering measurements on single crystals of FeTe$_{1-x}$Se$_x$. Superconductivity (SC) and antiferromagnetic (AFM) order in these compounds can be tuned together by varying Se compositions and/or excess Fe. We show that in systems where long-range magnetic order develops, superconductivity is completely suppressed. The long-range magnetic order is static with long life-time. On the other hand, when the magnetic order is short-range and the system exhibits behaviors of a mixed phase or phase separation between AFM and SC, the energy profile of the magnetic order appears to be quasi-elastic with energy widths around 0.2 meV. We discuss the evolution of the quasi-elastic magnetic scattering with temperature and doping, and their implications on the understanding of the spin-glass/SC mixed phase in FeTe$_{1-x}$Se$_x$ systems.

*The work at Brookhaven National Laboratory and Lawrence Berkeley National Laboratory was supported by the Office of Basic Energy Sciences (BES), Division of Materials Science and Engineering, U.S. Department of Energy (DOE), under Contracts No. DE-SC0012704 and No. DEAC02-05CH1123, respectively.
Elastoresistance of CaK(Fe,Ni)$_4$As$_4$*  ANNA BOEHMER (Presenter), Karlsruhe Institute of Technology; Ames Laboratory, WILLIAM MEIER, MINGYU XU, GIL DRACHUCK, Ames Laboratory, Iowa State University, PAUL WIECKI, Karlsruhe Institute of Technology, SERGEY L. BUD'KO, Ames Laboratory, Iowa State University, CHRISTOPH MEINGAST, Karlsruhe Institute of Technology, FEI CHEN, MORTEN HOLM CHRISTENSEN, RAFAEL FERNANDES, University of Minnesota, PAUL C CANFIELD, Ames Laboratory, Iowa State University — Elastoresistance describes the resistance change induced by an elastic deformation. In the well-known compound BaFe$_2$As$_2$ with clear nematicity, a diverging elastoresistance has been taken as a measure of the nematic susceptibility [1]. In contrast to BaFe$_2$As$_2$, the related CaK(Fe,Ni)$_4$As$_4$ orders antiferromagnetically as a so-called spin-vortex crystal (SVC) [2], which does not entail any nematicity. Here, we have determined the elastoresistance of CaK(Fe$_{1-x}$Ni$_x$)$_4$As$_4$ ($x=0-0.05$), spanning the phase diagram from a superconducting sample with $T_c=35$ K and no magnetic order, to a sample with magnetic order at a high $T_N=51$ K having $T_c=10$ K. The nematic susceptibility for SVC order is analyzed theoretically via a Ginzburg-Landau expansion and compared with the elastoresistance data. Implications on the place of CaK(Fe,Ni)$_4$As$_4$ in the wider material class and the factors contributing to elastoresistance are discussed.


*Work at Ames Laboratory was supported by the U.S. DOE, BES, DMSE. Ames Laboratory is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358. WRM was supported by the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant GBMF4411.
**4:18PM D61.00008: Prediction of Antiferromagnetism in Chromium Analog (BaCr$_2$P$_2$) of Iron Pnictide Confirmed by Synthesis**  
RADI JISHI, JOSE RODRIGUEZ (Presenter), Physics and Astronomy, California State University Los Angeles, TIMOTHY HAUGAN, MICHAEL SUSNER, Aerospace Systems Directorate, Air Force Research Laboratory — We have performed density-functional theory (DFT) calculations for BaCr$_2$P$_2$. It is a chromium analog to the parent compound BaFe$_2$As$_2$ for a series of iron-pnictide superconductors. By combining evolutionary methods with DFT, we predict that BaCr$_2$P$_2$ has the same crystal structure as its iron-pnictide analog[1]. DFT also predicts Neel antiferromagnetic order over the chromium sites. A simple hopping model over a square lattice of chromium atoms that includes only the principal 3d$_{xz}$ and 3d$_{yz}$ orbitals suggests that such checkerboard antiferromagnetic order is due to residual nesting of the Fermi surfaces that is obscured by a Lifshitz transition[1]. The DFT prediction has been confirmed experimentally after the synthesis of polycrystalline samples of BaCr$_2$P$_2$. X-ray diffraction recovers the predicted crystal structure to high accuracy, while magnetic susceptibility and specific-heat measurements are consistent with an antiferromagnetically ordered state at temperatures below $T_N \sim 60$ K [1].


*This work was supported in part by the Air Force Office of Scientific Research and by the National Science Foundation.

**4:30PM D61.00009: Novel Fe-based superconductor LaFe$_2$As$_2$ in comparison with traditional pnictides**  
IGOR MAZIN (Presenter), Naval Research Laboratory (currently at George Mason University), HARALD JESCHKE, MAKOTO SHIMIZU, NAYUTA TAKEMORI, University of Okayama — The recently discovered Fe-based superconductor (FeBS) LaFe$_2$As$_2$ seems to break away from an established pattern that doping FeBS beyond 0.2 e/Fe destroys superconductivity. LaFe$_2$As$_2$ has an apparent doping of 0.5 e, yet superconducts at 12.1 K. Its Fermi surface bears no visual resemblance with the canonical FeBS Fermiology. It also exhibits two phases, none magnetic and only one superconducting. We show that the difference between them has nonetheless magnetic origin, the one featuring disordered moments, and the other locally nonmagnetic. We find that La there assumes an unusual valence of +2.6 to +2.7, so that the effective doping is reduced to 0.30-0.35 e. A closer look reveals the same key elements: hole Fermi surfaces near the $\Gamma$-Z and electron ones near the X-P lines, with the corresponding peak in susceptibility, and a strong tendency to stripe magnetism. The physics of LaFe$_2$As$_2$ is thus more similar to the FeBS paradigm than hitherto appreciated.
4:42PM D61.00010: Biaxial Strain Tuning of Strong Electronic Correlations in CsFe$_2$As$_2$  PAUL WIECKI (Presenter), AMIR-ABBAS HAGHIGHIRAD, THOMAS WOLF, ANNA BOEHMER, Karlsruhe Institute of Technology — CsFe$_2$As$_2$ is an iron-based superconductor with $T_c \approx 2.3$ K and a large Sommerfeld coefficient of 180 mJ / mol K, indicating strong electronic correlations at low temperature [1]. In addition, CsFe$_2$As$_2$ shows a coherence-incoherence crossover, reminiscent of heavy fermion systems [2,3]. In this contribution, using transport and x-ray diffraction measurements, we demonstrate that in-plane biaxial tension strain, applied by gluing the sample to a rigid substrate with a large mismatch in thermal expansivity, can modify the low-temperature electronic correlations as well as the coherence-incoherence crossover temperature in this material.


4:54PM D61.00011: Emergent electronic properties of FeTe by strain tuning  SOUMENDRA PANJA (Presenter), CRAIG V TOPPING, CHI MING YIM, CHRISTOPHER TRAINER, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, United Kingdom, SUPA, School of Physics and Astronomy, DORINA CROITORI, VLADIMI TSURKAN, ALOIS LOIDL, Center for Electronic Correlations and Magnetism, Experimental Physics V, University of Augsburg, D-86159 Augsburg, Germany, PETER WAHL, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, United Kingdom, SUPA, School of Physics and Astronomy, ANDREAS ROST, School of physics and astronomy, SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, United Kingdom; Max Planck Institute — FeTe is an ‘11’ non-superconducting parent compound with properties significantly different from those of other iron-based high-temperature superconductors. Most discernible is the double stripe antiferromagnetic order with the $(\pi,0)$ propagation vector contrary to the more typical $(\pi, \pi)$ order. That these properties can be significantly tuned by tensile strain has for example been shown by thin film experiments in which superconductivity was stabilised at 13K. In our research programme we explore the magnetic and superconducting phase diagram under uniaxial strain along [110]. We complement direct imaging of magnetic order by spectroscopic imaging STM with low-temperature magnetoresistivity measurements in force cell. We discuss the possibility of stabilising $(\pi, \pi)$ order both on the surface and in bulk under experimentally accessible strains and the potential to stabilise superconductivity in Fe$_{1+x}$Te via this route.
Unconventional charge density wave order in the pnictide superconductors $\text{Ba(Ni}_{1-x}\text{Co}_x\text{)}_2\text{As}_2$ and $\text{Ba}_{1-x}\text{Sr}_x\text{Ni}_2\text{As}_2$*  

SANGJUN LEE (Presenter), XIAOLAN SUN, XUEFEI GUO, University of Illinois at Urbana-Champaign, JOHN COLLINI, CHRIS ECKBERG, JOHNPIERRE PAGLIONE, University of Maryland, College Park, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — $\text{BaNi}_2\text{As}_2$ is a structural homologue of the pnictide high temperature superconductor parent compound, $\text{BaFe}_2\text{As}_2$, in which the Fe atoms are replaced by Ni. Superconductivity is highly suppressed in this system, reaching a maximum $T_c = 2.3$ K upon Co doping, compared to 24 K in its iron-based cousin, and the origin of this $T_c$ suppression is not known. Using x-ray scattering, we present the discovery of CDW order in $\text{BaNi}_2\text{As}_2$ and its evolution upon Co and Sr doping. The chemical doping suppresses the CDW, paralleling the behavior of antiferromagnetism in iron-based superconductors. Our study demonstrates that pnictide superconductors can exhibit CDW order which may be closely related to the $T_c$ suppression in this system. We also present the response of CDW in $\text{Ba}_{1-x}\text{Sr}_x\text{Ni}_2\text{As}_2$ under external strain and discuss how it relates to the strong nematic susceptibility recently discovered in these compounds via elastoresistivity measurements.

*X-ray work was supported by DOE grant DE-FG02-06ER46285 and crystal growth was supported by AFOSR grant FA9550-14-1-0332. P. A. and J. P. acknowledge Gordon and Betty Moore Foundation EPIQS grants GBMF4542 and GBMF4419, respectively.
Emergence of Fulde-Ferrell-Larkin-Ovchinnikov phase in FeSe in the BCS-BEC crossover*

SHIGERU KASAHARA (Presenter), YUKI SATO, Kyoto Univ, SALVATORE LICCIARDELLO, MATIJA ĆULO, High Field Magnet Laboratory (HFML-EMFL) and Institute for Molecules and Materials, Radboud University, STEVAN ARSENJEVIC, Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, THOM OTTENBROS, High Field Magnet Laboratory (HFML-EMFL) and Institute for Molecules and Materials, Radboud University, TAKAHITO TOMINAGA, Kyoto Univ, JAKOB BÖKER, ILYA EREMIN, Ruhr-Universität Bochum, JOACHIM WOSNITZA, Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, TAKASADA SHIBAUCHI, Univ. of Tokyo, NIGEL HUSSEY, High Field Magnet Laboratory (HFML-EMFL) and Institute for Molecules and Materials, Radboud University, YUJI MATSUDA, Kyoto Univ — The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase, predicted more than a half-century ago, is a highly exotic state of fermionic condensate, in which oscillations of the order parameter emerge in real space. Yet, quest of the FFLO phase has been a challenge for a broad range of scientists, including solid-state, ultracold atomic and high-energy physics. Here, via thermal transport measurements in intense magnetic fields up to 33 T, we present compelling evidence for a distinct high-field superconducting phase in an iron-chalcogenide superconductor FeSe for the field $H \parallel ab$-plane. A discontinuous downward jump in the quasiparticle thermal transport indicates the presence of a first-order transition line within the superconducting phase. We attribute the high-field phase to the FFLO phase, where planar nodes are formed. We discuss the importance of the extremely small Fermi energies, strong spin-orbit coupling and multiband nature for the FFLO phase in FeSe.

*This work is supported by Grants-in-Aid for Scientific Research (KAKENHI) (Nos. 15H03688, 15KK0160, 18H01177, 18H05227, 19H00649) and on Innovative Areas "Topological Material Science" (No. 15H05852) "Quantum Liquid Crystals" (No. 19H05824) from JSPS. This work is also supported by HFML-RU and HLD-HZDR, members of the EMFL.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D62 DMP: Nanostructures and Metamaterials III Mile High Ballroom 4C - Antoinette Taylor, Los Alamos Natl Lab - Tag(s): Focus
2:30PM D62.00001: Topological structures of and for light* [Invited] KOBUS KUIPERS (Presenter), Quantum Nanoscience, Kavli Institute of Nanoscience Delft — Topology is an invaluable tool to elucidate the properties of physical systems. Typically, it refers to instances where an entity has so-called topological protection, which means that the entity cannot disappear if small changes are made to the system. In this lecture I will address two illustrations of topological protection in light fields.

The first relates to optical singularities, which can have a topological charge. I will experimentally show that the charge of both phase- and polarization singularities plays a role in how they are distributed in space and also in the way they are created and annihilated. The second relates to the behavior of light in photonic nanostructures of which the properties have a non-trivial topology. We experimentally investigated the propagation of edge states between topologically non-trivial photonic crystals. I will show how the propagation direction is related to the far-field optical spin of the modes. Time allowing I will address the heterogeneity of the spatial distribution of the near-field optical spin of the mode, which is of importance to quantum optical application of these states.

* I would like to acknowledge funding from the European Research Council (ERC Advanced Grant No. 340438-CONSTANS).

3:06PM D62.00002: Topological phases of electromagnetic waves in superlattices of negative- and positive- epsilon materials AKIHIRO OKAMOTO (Presenter), Department of Physics, Tokyo Institute of Technology, YOSUKE NAKATA, Graduate School of Engineering Science, Osaka University, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology — Recently, a new topological invariant is proposed to classify electromagnetic waves in an isotropic medium with positive or negative permittivity and permeability, and various interface modes such as surface plasmons are interpreted as topological boundary modes [1]. We expect similar topological phases of electromagnetic waves even for metamaterials.

To this end, we consider the electromagnetic waves in a 1D multilayer consisting positive- and negative- epsilon layers, studied in [2]. Depending on the ratio of layer thicknesses and the values of the dielectric constants of the constituent layers, the spectra changes, and the dispersion opens a gap at the origin depending on the spatial average of the dielectric constant. We associate this with a change in the topological number proposed in [1]. In addition, we find that interface states appear at an interface between different topological phases as expected.

3:18PM D62.00003: Diverged photonic spin hall effect in Weyl Photonic metamaterial
WENHUI A. WANG (Presenter), Singapore University of Technology and Design, WENLONG GAO, University of Birmingham, SHENGYUAN YANG, Singapore University of Technology and Design, SHUANG ZHANG, University of Birmingham — Weyl semimetal is gaining increasing attention due to the unprecedented physical observables including the chiral magnetoresistance effect in condensed physics matter. In optics however, observables besides the detection of Weyl node and the Fermi arcs are still in lack. In this work, we discover that when circularly polarized beams are reflected by a Weyl medium, a handedness dependent spin hall effect can be realized due to the topological properties of the scattering matrix arises from the Weyl node. The scattering properties of the Weyl node could dramatically influence the trajectory of the light in real space resulting in a handedness dependent Imbert-Fedorov shift. More importantly, the shift is shown to be diverging in approximate to the Weyl node. Our discovery creates a whole new and readily available platform realizing diverged spin hall effect of optical Weyl medium.

3:30PM D62.00004: Optically tunable topological photonic structures [Invited] NATALIA LITCHINITSER (Presenter), MIKHAIL SHALAEV, WIKTOR WALASIK, Duke University, HOUCHEN LI, Nankai University, JIANNAN GAO, Duke University — Photonic topological insulators offer the possibility to eliminate backscattering losses and improve the efficiency of optical communication systems. We combine the properties of a planar silicon photonic crystal and the concept of topological protection to demonstrate dynamically controlled transmission in a topological photonic crystal that exhibits the valley Hall effect.

4:06PM D62.00005: Non-Hermitian landau damping and bulk Fermi arc in superlattice-gate-tuned graphene plasmons MINWOO JUNG (Presenter), Department of Physics, Cornell University, HANAN HERZIG SHEINFUX, ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, FENGYU LIU, Department of Electrical and Computer Engineering, University of Maryland, FRANK KOPPENS, ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, GENNADY SHVETS, School of Applied and Engineering Physics, Cornell University — Landau damping, in which a plasmon emits an electron-hole pair, has been considered as a hindering factor for low-loss nanophotonic applications of graphene surface plasmon-polaritons (GSP), and is usually avoided by Pauli-blocking at high doping. In contrast to this simple view against landau damping, here we unravel its ironic utility and show how significantly this loss mechanism can extend the existing framework of graphene nanophotonics. Given a properly designed spatial pattern, landau damping becomes a key element for exotic non-Hermitian band structure engineering of GSPs, without damaging their quality factor severely. We propose that periodic damping textures can be assigned by field-effect gating through a combination of two electrodes; a metagate, thin and periodically punctured, provides a superlattice photonic crystal structure to GSPs, and a backgate, placed far below the metagate, controls local carrier densities on graphene selectively on the regions above holes in the metagate. This setting allows us to use the backgate voltage as a switch for the bulk Fermi arc, a topological signature of an exceptional point pair in the band structure. Our work thus opens up a new regime of graphene plasmonics involving open systems and non-Hermitian topological physics.
4:18PM D62.00006: SAW interdigitated transducers as topological mechanical metamaterial

SEAN MCHUGH (Presenter), Resonant Inc. — A lattice model is developed to describe the mechanical displacement of and current through each electrode of a surface acoustic wave (SAW) interdigitated transducer (IDT). Each electrode of an IDT is treated as a mass connected mechanically to its neighbors with a spring and electrically with a capacitor. Simulations for the electrical admittance of a typical SAW IDT are performed and compared with the results of an accurate FEM simulation. The utility of this lattice model is demonstrated by simulating the admittance of an IDT structure known as a hiccup resonator, which has a mode in the center of the band gap. It is shown here that this mode is a topologically protected edge state described by the 1D Su-Schrieffer-Heeger (SSH) model. Hiccup resonators have been used in commercial products for decades, and as such it may considered the first mass-produced topological mechanical metamaterial.

4:30PM D62.00007: A polarization-actuated plasmonic circulator

TZU-YU CHEN, CHENBIN HUANG (Presenter), Natl Tsing Hua Univ — We show both by simulation and experiment, a plasmonic structure functions as a nanoscopic optical circulator when the input laser beam is properly polarized. Moreover, depending on the helicity of the spin angular momentum carried by the light, the circulation direction of surface plasmons could be correspondingly controlled.

*Ministry of Science and Technology in Taiwan (MOST) 106-2112-M-007-004-MY3.

4:42PM D62.00008: Integration of single layer MoSe2 with photonic rings for electrically switchable routing of light

ROBERT SHREINER (Presenter), KAI HAO, AMY BUTCHER, ALEXANDER A HIGH, University of Chicago — Semiconducting transition metal dichalcogenide monolayers exhibit pronounced optical signatures in the visible and near-infrared regimes due to strong excitonic resonances, which can be modulated significantly through electrostatic doping. When interfaced with such tunable dielectric environments, nanophotonic devices inherit gate-dependent functionalities. Here, we demonstrate an electro-optical switch composed of a titanium dioxide ring resonator fabricated on monolayer molybdenum diselenide. Gate-varying measurements reveal electrically tunable cavity transmission, suggesting future application in on-chip photonic circuitry.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1746045.
Diffraction of elastic waves is considered for a system consisting of two parallel arrays of thin (subwavelength) cylinders that are arranged periodically. The embedding media supports waves with all polarizations, one longitudinal and two transverse, having different dispersion relations. An interaction with defects mixes the in-plane longitudinal and transverse modes. It is shown that the system supports bound states in the continuum (BSC) that have no specific polarization, that is, there are standing waves localized in the scattering structure whose wave numbers lies in the first open diffraction channels for both longitudinal and transverse modes. BSCs are shown to exists only for specific distances between the arrays and for specific values of the wave vector component along the array. An analytic solution is obtained for BSCs containing coupled elastic waves with different dispersion relations. For distances between the parallel arrays much larger than the wavelength, the existence of BSCs is explained by a destructive interference similar to the interference in a Fabri-Perot interferometer.

*University of Florida College of Art and Sciences
Sergei Shabanov

5:06PM D62.00010: Strong nonreciprocal transmission self-induced by nonlinear PT-symmetric metamaterials  CHRISTOS ARGYROPOULOS (Presenter), BOYUAN JIN, University of Nebraska - Lincoln — Self-induced nonreciprocity based on optical nonlinear effects is a more appealing technique compared to other ways to achieve nonreciprocal response due to the absence of any kind of bias based on magnets, currents, or time modulation. We demonstrate strong self-induced nonreciprocal transmission by using a new compact nonlinear parity-time (PT) symmetric system based on epsilon-near-zero (ENZ) metamaterials photonically doped with gain and loss defects [B. Jin and C. Argyropoulos, “Nonreciprocal Transmission in Nonlinear PT-Symmetric Metamaterials Using Epsilon-near-Zero Media Doped with Defects,” Adv. Opt. Mat., p. 1901083 (2019)]. The strong self-induced nonreciprocal transmission arises from the extreme asymmetric field distribution achieved upon excitation from opposite incident directions combined with the boosted nonlinear effects at the nanoscale. The transmittance from one direction is kept exactly unity while the transmittance from the other direction is decreased to very low values, achieving very high optical isolation. The presented work can have a plethora of applications, such as nonreciprocal ultrathin coatings for the protection of sources or other sensitive equipment from external pulsed signals, circulators, and isolators without the use of bulk magnets.
5:18PM D62.00011: High-efficient harmonic generation via Plasmonic Tamm states
YINXIAO XIANG (Presenter), West Virginia Univ, CHENGLIN DU, Physics department, Nankai University, FAN SHI, YI LIANG, West Virginia Univ, WEI CAI, Physics department, Nankai University, CHENG CEN, West Virginia Univ — Plasmonic Tamm states in nanoscaled plasmonic waveguides can increase the electric and magnetic field intensity separately by three orders of magnitude via the spatial confinement and phase-matching. Theoretical or numerical models about plasmonic Tamm states have been proposed in metal-insulator-metal plasmonic waveguides and graphene plasmonic crystals. In this work, we experimentally realized plasmonic Tamm states by combining a nanoantenna with a plasmonic Tamm structure. The field enhancement was characterized by our home-made multi-photon microscope, in which highly efficient second and third harmonic generations were both observed. Our work demonstrates a promising potential for electromagnetic nanofocusing and nanosensing.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D63 DMP: Theory and Computation of Hybrid Perovskites Mile
High Ballroom 4D - Aron Walsh, National Renewable Energy Laboratory - Tag(s): Focus

2:30PM D63.00001: A Theoretical Study of Structure Property Relations in Photovoltaic Perovskites*
JORDAN COWELL (Presenter), NICHOLAS C. BRISTOWE, Materials for Energy and Electronics, University of Kent — Perovskite materials are a great example of systems with a multitude of structure-property relationships. For example, metal insulator transitions in the nickelates and manganites can be linked to breathing and Jahn-Teller distortions which allow for charge and orbital ordering, respectively. This study examines the relationship between atomic structure and electrical band-gaps in the promising photovolatics material A2Au2X6 (A = Cs, Rb, K, X = I, Cl), through first principles calculations based on DFT. We find that there is a complex competition between various structural degrees of freedom in the material, which can be manipulated through chemistry and pressure, and that each of the structural modes can strongly tune the band gap. For example, in the Rb2Au2I6 double perovskite, we predict that, contrary to expectation, hydrostatic pressure produces a polar phase. We argue that this is due to a) the cooperative coupling of the Jahn-Teller and tilt modes which are both reduced with pressure, and b) the competitive coupling of tilting and polar modes. We finally discuss the effect of each of these modes and chemical changes on the band gap, and how the polar mode could be helpful to separate photo-excited carriers via the photoferroic effect.

*University of Kent
**2:42PM D63.00002: Improved Accuracy Tight Binding Model for Finite Temperature Electronic Structure Dynamics in Methyl Ammonium Lead Iodide (MAPbI3)**  
DAVID ABRAMOVITCH (Presenter), Department of Physics, University of California, Berkeley, LIANG TAN, Molecular Foundry, Lawrence Berkeley National Lab — Halide perovskites are promising photovoltaic and optoelectronic materials. However, computing electronic properties and dynamics at finite temperature is challenging due to nonlinear lattice dynamics and prohibitive computational costs for ab initio methods. Tight binding models decrease computational costs, but current models lack the ability to accurately model instantaneous atom displacement and reduced symmetry at finite temperature. We present a parameterized tight binding model for MAPbI3 capable of predicting instantaneous electronic structures for large systems based on atomic positions extracted from classical molecular dynamics. Our tight binding Hamiltonian predicts instantaneous atomic orbital onsite energies and hopping parameters accurate to 0.1 to 0.01 eV compared to DFT across the orthorhombic, tetragonal, and cubic phases, including effects of temperature, reduced symmetry, and spin orbit coupling. This model allows for efficient calculation of instantaneous and dynamical electronic structure at the length and time scales required to address coupled electronic and ionic dynamics, as required for predicting temperature dependence of carrier mass, band structure, free carrier scattering, and polaron transport and recombination.

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**2:54PM D63.00003: Materials Property Database for Hybrid Organic-Inorganic Perovskites and Application to Stability and Electronic Structure of (PEA)\(_2\)PbI\(_4\)\(^*\)**  
XIXI QIN (Presenter), XIAOCHEN DU, SVENJA JANKE, RAUL LAASNER, TIANYANG LI, MANOJ KUMAR JANA, Duke University, CONNOR CLAYTON, Carnegie Mellon University, CHI LIU, Duke University, SAMPREETI BHATTACHARYYA, University of North Carolina at Chapel Hill, JULIANA MENDES, North Carolina State University, JUN HU, University of North Carolina at Chapel Hill, DOVLETGELDI SEYITLIYEV, North Carolina State University, RUYI SONG, Duke University, MATTI ROPO, University of Turku, FRANKY SO, KENAN GUNDOGDU, North Carolina State University, WEI YOU, YOSUKE KANAI, University of North Carolina at Chapel Hill, DAVID B. MITZI, VOLKER BLUM, Duke University — Hybrid organic-inorganic perovskites (HOIPs) are attracting significant attention as new semiconductor materials, due to their inherent tunability by varying both the organic and the inorganic components. However, keeping track of the dramatically increasing volume of materials data related to HOIPs is challenging. We here present an open database, "HybriD\(^3\)" (Design, discovery and dissemination (D\(^3\)) of data related to hybrid materials, https://materials.hybrid3.duke.edu), aiming to collect, curate, and make available materials data related to HOIPs. The database is open to the community and designed to accept community input for a broad set of data, i.e., experimental and computational, related to in principle any materials property. We demonstrate the use of the database for the widely investigated material phenethylamine lead iodide, (PEA)\(_2\)PbI\(_4\), for which several crystal structure refinements have been reported in past work. Using density functional theory including van der Waals effects, we identify the lowest-energy structure among them and provide the electronic band structure at a high level of theory (hybrid density functional theory including spin-orbit coupling).

\(^*\)NSF DMR-1729297, 1728921, 1729383, CHOOSE EFRC (DOE-BES), DFG 393196393.
3:06PM D63.00004: First-principles Study of Water Insertion Process on MAPbI$_3$ Surface

MD. ABDULLAH ASAD (Presenter), Okayama Univ, MASAKI HADA, Tsukuba Research Center for Interdisciplinary Materials Science, University of Tsukuba, KYOSUKE SATO, YOICHI HASEGAWA, RYOTA NAGAOKA, RYUJI MISHIMA, TAKEHI NISHIKAWA, YOSHIFUMI YAMASHITA, YASUHIKO HAYASHI, KENJI TSURUTA, Okayama Univ — We computationally investigate an insertion process of water into the methylammonium lead halide perovskite (MAPbI$_3$), which has been attracting considerable interest during recent years due to its high performance in solar-cell application [1]. The rapid decomposition of MAPbI$_3$ reaction with water has been recognized to be a major obstacle to outdoor applications [2]. To overcome this drawback process, it is important to identify the initial stage of water insertion into the MAPbI$_3$. The first-principles calculation based on the density-functional theory is performed to investigate the water insertion process on outer surface layer of MAPbI$_3$ slab model. Using the Nudged Elastic Band method, we find that the initial insertion process follows the three steps; approaching, re-orienting and finally sinking into the perovskite layer. This process requires approximately 0.60 eV to overcome an energy barrier, which agrees with an in situ X-ray diffraction (XRD) measurement of the reaction threshold of water molecules with the MAPbI$_3$ crystal at room temperature [3].

References:

3:18PM D63.00005: Theory of Layer Edge States in 2D Halide-Perovskites

JISOOK HONG (Presenter), DAVID PRENDERGAST, LIANG TAN, Lawrence Berkeley National Laboratory — Halide perovskites are one of the most promising candidate materials for photovoltaic and optoelectronic applications. Compared to the 3D organic-inorganic hybrid perovskites, the 2D layered perovskites exhibit greater tunability of band gaps and exciton binding energies, while solving the well-known stability issue of hybrid perovskites at the same time. Recent experimental observations suggest that extrinsic localized edge states are present in 2D layered perovskites. [1-3] The edge state facilitates extremely efficient electron-hole dissociation and long carrier lifetimes as much as those of 3D perovskites. However, the phenomenon has not been thoroughly investigated in a first-principles theoretical framework. In this talk, we will discuss electronic structures and the origin of the edge states studied using first-principles calculations. Understanding the mechanism for edge state formation and their role in carrier separation will pave the way for controlling the edge states in future applications such as efficient photovoltaic devices and high-performance photodetectors.

Halide perovskites (HaPs) exhibit intriguing optoelectronic properties that cannot yet be fully explained on a microscopic level. Understanding the characteristics of HaPs is possible with well-established conventional theoretical calculations, such as density functional theory (DFT), but their applicability to large-scale simulations is often limited by their computational costs. Here, building on previous work [1] we put forward a tight binding (TB) approach as a computationally efficient tool to model large-scale system sizes and calculate optoelectronic properties of HaPs. Parametrizing the TB model with DFT calculations and unifying it with force-field molecular dynamics, we compute dynamic band gap distributions for several HaPs as well as their dependence on temperature. This helps resolving confluences of small Urbach energies and large amounts of nuclear disorder in HaPs around room temperature.

References
**3:54PM D63.00008: Structural and transport studies from air-stable hybrid perovskite thin films**

RANDY BURNS (Presenter), Department of Physics and Astronomy, University of Missouri - Columbia, SIPHELO NGQOLODA, CHRISTOPHER ARENDSE, THEOPHILLUS MULLER, Department of Physics, University of Western Cape, SORB YESUDHAS, DEEPAK K SINGH, SUCHISMITA GUHA, Department of Physics and Astronomy, University of Missouri - Columbia — Traditionally, MAPbX$_3$ (X = Br, I, or Cl) hybrid organic-inorganic perovskite films have been deposited with spin coating techniques which cause degradation under ambient atmospheric conditions. We demonstrate the feasibility of stable MAPbI$_3$ thin films grown by a facile two-step low-pressure vapor deposition process in a single reactor. Absorption measurements confirm excellent stability after three weeks. In confluence with the absorption data, synchrotron x-ray diffraction experiments reveal good structural stability on the timescale of several months. Temperature dependent transport measurements show sharp inflection points of the resistance curve at distinct temperatures. One inflection point occurs precisely at the expected tetragonal to orthorhombic transition, however, another inflection deviates significantly from the expected tetragonal to cubic transition. Consequently, we conducted temperature dependent laboratory-based x-ray diffraction measurements that also suggest a transition below the commonly reported tetragonal/cubic transition temperature. Concerning device application, the MAPbI$_3$ films were incorporated into solar cells that maintained the majority of their efficiency and energy yield on the timescale of weeks.

*Supported by NSF under Grant No. ECCS-1807263

**4:06PM D63.00009: Frenkel-Holstein Hamiltonian Applied to Quaterthiophene-based 2D Hybrid Organic-Inorganic Perovskites**

SVENJA JANKE (Presenter), Mechanical Engineering and Material Sciences, Duke University, MOHAMMAD B. QARAI, Chemistry, Temple University, VOLKER BLUM, Mechanical Engineering and Material Sciences; Chemistry, Duke University, FRANK SPANO, Chemistry, Temple University — In two-dimensional hybrid organic-inorganic perovskites (HOIPs), both the organic and inorganic components can contribute to the electronic properties at the electronic frontier levels and hence open up a wide area for design of new materials with high tunability. For development of new devices like solar cells or light emitting diodes, the understanding of electronic excitations and their photophysical signatures plays a fundamental role. Here, we show by the example of quaterthiophene-based lead-halide HOIPs that the organic contribution to 2D HOIP absorption spectra can be theoretically appreciated employing a Frenkel-Holstein Hamiltonian that treats electronic coupling and electron-phonon coupling on equal footing. We relate changes in the spectra to structural changes in the organic layer that in turn are caused by variation of the halide anion. Specifically, we find that the strength of the excitonic coupling on the organic component decreases when the halide anion is varied from Cl to Br to I. Our research opens up a potential pathway for predicting optoeletronic properties of newly designed 2D HOIPs.

*Supported by the German Science Foundation (DFG), grant number 393196393 and NSF DMR-1729297.
Layered (so-called two-dimensional, 2D) hybrid organic-inorganic perovskites (HOIPs) can be created by combining a wide range of possible inorganic components with an even broader range of organic molecules, offering considerable flexibility to fine-tune their synthesizability and properties. This talk focuses on computational predictions of the electronic (carrier, i.e., electron- and hole-like) energy levels of new 2D HOIP materials. Such predictions pose a considerable challenge due to high required levels of theory and large unit cells (hundreds of atoms) associated with typical 2D HOIPs. We here use high-precision, all-electron hybrid density functional theory including spin-orbit coupling, showing that this combination provides descriptions of the quantum-well like energy level alignment in lead halide based oligothiophene perovskites in excellent agreement with experiments. We then employ the same approach to predictively address the electronic properties of a broad range of further 2D HOIPs, including lead-free (Ag-Bi) based ones. As a final point, we show that the details of the atomic structure used to predict electronic properties matter significantly, even in a qualitative sense, by determining energy level alignments and, therefore, which component (organic or inorganic) forms the band edges. A complete structural understanding of a given target 2D HOIP is thus essential for faithfully predicting the properties that can be leveraged within this promising new semiconductor materials space.

This work is enabled by the very large community of developers and users of the FHI-aims code as well as by close collaborations with leading experimental colleagues, particularly the group of David B. Mitzi (Duke University).

*NSF DMREF program, grant number DMR-1729297; Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE), an Energy Frontier Research Center funded by the U. S. Department of Energy, Office of Science, Basic Energy Sciences (BES).
4:54PM D63.00011: Compounds with high macroscopically-averaged symmetries and low local symmetries: The consequence of lone-pair nematicity on electronic properties*

XINGANG ZHAO (Presenter), ZHI WANG, ALEX ZUNGER, University of Colorado, Boulder — The knowledge of the appropriate unit cell for a compound is crucial for many physical studies e.g. band structure theory. Traditionally, one prefers to use the smallest cell consistent with the global symmetry, e.g. monomorphous cells containing a single structural motif. It is well known that at high temperatures local displacements have the well-known thermal origin due to dynamically thermal fluctuation. But besides thermal effects, some compounds have non-thermal intrinsic local displacements already at low temperatures (LT) due to the preference of chemical bonding for stabilizing certain low-symmetry structural motifs requiring for their representation larger than minimal unit cells. By calculating in DFT the relaxed total energies of numerous cubic phases of ABX₃ compounds (X=oxygen or halogen) we identify special cases where the energy per formula unit decreases due to atomic displacements as the cubic cell size increases. Examples include cubic CsMX₃ (M=Sn, Pb; X=Br, I), and PbMO₃ (M=Ti, Zr, Hf) etc. These intrinsic, LT polymorphous networks are interesting because their properties (band gaps, etc.,) can be very different than those gleaned from their macroscopic averaged counterparts represented as a minimal unit cell.

*Supported by NSF-DMREF.

5:06PM D63.00012: Ligand Design Rules for Improving 2-D Organic-Inorganic Hybrid Halide Perovskite Moisture Stability

STEPHEN SHIRING (Presenter), BRETT SAVOIE, Purdue Univ — Organic-inorganic hybrid halide perovskites are promising semiconductor materials due to their long carrier lifetimes, diffusion lengths, and tunable band gap. Two-dimensional (2-D) Ruddlesden-Popper halide perovskites are particularly interesting from an optoelectronics device standpoint due to broad range of organic ligands that can be incorporated into the perovskite lattice and ease of fabrication. However, a major challenge for perovskite optoelectronics is their sensitivity to moisture, leading to chemical instability and device reliability issues. Here, we show that judicious choice in selection of the surface cation for a 2-D perovskite prevents water from penetrating into and dissolving the inorganic layer. We use molecular dynamics simulations to elucidate general design rules for designing water-proofing surface cations, showing that the length/size of the surface ligand alone is not sufficient to suppress water penetration. Our results provide insight into the stability-enhancing mechanism and provide a path for designing perovskites with improved properties.
Interfacial Electromechanics Predict Phase Behavior of 2D Hybrid Halide Perovskites

CHRIS PRICE (Presenter), University of Pennsylvania, JEAN-CHRISTOPHE BLANCON, ADITYA MOHITE, Chemical and Biomolecular Engineering, Rice University, VIVEK SHENOY, University of Pennsylvania — Quasi-two dimensional mixed-cation hybrid halide perovskites (q-2DPK) have improved structural stability and device lifetime over their 3D perovskite counterparts. The addition of a large organic A’ cation to the bulk AMX$_3$ structure gives the q-2DPK chemical formula A’$_2$A$_{N-1}$M$_N$X$_{3N+1}$ and introduces new synthetic degrees of freedom through the composition index N. Ordered lamellar structures form via coordinated M-X bond breaking and peculiar critical phase behavior emerges as a function of N. We propose a thermodynamic model parametrized by first-principles calculations to generate a phase diagram for the q-2DPK. We find that the difficulty in synthesizing phase-pure samples in the high-N composition range arises from the energetic competition between electrostatic interactions of opposing interfacial dipole layers and mechanical relaxation of interfacial stress. Our model shows quantitative agreement with experimental observations and explains the non-monotonic evolution of the lattice parameters with composition index N. This model is generalizable to the entire family of q-2DPK and can guide the design of optoelectronic and photovoltaic materials with enhanced environmental stability and reduced excitonic degradations to carrier transport.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D64 DMP: Emerging Phenomena & Defects in Transition Metal Oxides and 2D Materials

Mile High Ballroom 4E - Alexandru Bogdan Georgescu, Simons Foundation -
Tag(s): Focus
Effect of local correlation and nonlocal exchange*  HRISHIT BANERJEE (Presenter), Insitut für Theoretische Physik–Computational Physics, Graz Univ of Technology, OLEG JANSON, Institute for Theoretical Solid State Physics, IFW Dresden, KARSTEN HELD, Institut für Festkörperphysik, TU Wien, TANUSRI SAHA-DASGUPTA, Condensed Matter Physics and Materials Sciences, S. N. Bose National Centre for Basic Sciences, MARKUS AICHHORN, Insitut für Theoretische Physik–Computational Physics, Graz Univ of Technology — Motivated by the puzzling report of a ferromagnetic insulating state in LaMnO$_3$/SrTiO$_3$ heterostructures, we calculate the electronic and magnetic state of LaMnO$_3$, strained to a SrTiO$_3$ square substrate. We use 3 different computational approaches: (a) density functional theory (DFT) with Hubbard U(DFT+U), (b) DFT + dynamical mean-field theory (DMFT), and (c) DFT + Hartree Fock (HF) as a hybrid functional. While the first two approaches include local correlations and exchange at Mn sites, treated in a static and dynamic manner, respectively, the last one takes into account the effect of nonlocal exchange at all sites. We find in all three approaches that the compressive strain induced by the square substrate of SrTiO$_3$ turns LaMnO$_3$ to a ferromagnet with suppressed Jahn-Teller distortion, in agreement with experiment. The hybrid calculations result in a ferromagnetic insulating solution, as observed in experiment. This insulating behavior is found to originate from an electronic charge disproportionation. Our conclusions remain valid when we investigate LaMnO$_3$/SrTiO$_3$ within the experimental setup of a superlattice geometry using hybrid functionals. DMFT calculations show the presence of a paramagnetic insulating state.


* DST, India, FWF, Austria

Ultimate strength measurements on freestanding SrTiO$_3$ thin films
VARUN HARBOLA (Presenter), Physics, Stanford University, SAMUEL CROSSLEY, PRASTUTI SINGH, RUIJUAN XU, HAROLD HWANG, Applied Physics, Stanford University — The last two decades have seen enormous growth in the field of nanoengineering and nanomechanics using thin sheets owing to the variety of 2D materials available to us (2D Mater. 5, 032005 (2018)). With new advances in thin film growth techniques(Nat. Mater. 15, 1255–1260 (2016)), a new class of functional oxide thin films which are freestanding can be produced and readily incorporated in such nanomechanical implementations. However functional oxides are rigid and brittle in bulk, so it becomes imperative to verify the feasibility of nanomechanical deformations by investigating the breaking strength of these thin films. Here we report measurements of the ultimate strength of SrTiO$_3$ thin films using an atomic force microscope (AFM) by impinging upon a freestanding drumhead with an AFM tip. We demonstrate that in the sub-20 nm thickness regime of these thin films, SrTiO$_3$ can withstand an elastic extension of ~ 6% which is more than an order of magnitude higher than that for bulk. Furthermore, we also show that the fracture point of these films with respect to applied force is robust thus demonstrating their potential for use in nanomechanical platforms and devices.
Local modification of superconductivity in few unit cell thick high-\(T_C\) \(\text{Bi}_{2}\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}\) superconductor

SANAT GHOSH (Presenter), Tata Institute of Fundamental Research (TIFR), JAYKUMAR VAIDYA, University of Virginia, SAWANI DATTA, RAM PRAKASH PANDEYA, DIGAMBAR A. JANGADE, KALOBARAN MAITI, A. THAMIZHAVEL, MANDAR M DESHMUKH, Tata Institute of Fundamental Research (TIFR) — High temperature superconductors are interesting systems to study from the point of views of basic understanding about the origin and the nature of their superconducting properties as well as their numerous applications. Here we report transport studies on one of the high \(T_C\) cuprate superconductors namely \(\text{Bi}_{2}\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}\), an easily exfoliable Van der Waals material having superconducting transition temperature of 85K. In thin layers of this material, we have found that one can tune its superconducting property locally. This can have many potential device applications like patterning 2D superconductors for making high temperature Josephson Junctions and superconducting quantum interference devices.

*We acknowledge funding from Department of Atomic Energy and Department of Science and Technology of India.

Proving High Temperature Superconductivity in Monolayer \(\text{Bi}_{2}\text{Sr}_{2-x}\text{La}_x\text{Cu}_6\text{O}_{6+\delta}\)

HENGSHENG LUO (Presenter), LIGUO MA, YIJUN YU, PENG CAI, Fudan Univ, DONGJOON SONG, National Institute of Advanced Industrial Science and Technology, RUIDAN ZHONG, Brookhaven National Lab, JIAN SHEN, Fudan Univ, GENDA GU, Brookhaven National Lab, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, XIANHUI CHEN, physics department, University of Science and Technology of China, YUANBO ZHANG, Fudan Univ — Dimensionality plays a fundamental role in cuprate high-temperature superconductivity; all high-temperature cuprate superconductors adopt a layered crystal structure, and much of high-temperature superconductivity theory is based on purely two-dimensional (2D) models. A monolayer Bi2201 contains only a single layer of CuO\(_2\) plane, and therefore represents a cuprate superconductor in the ultimate 2D limit. Here, we exfoliate La doped Bi2201 (Bi\(_{2}\)Sr\(_{2-x}\)La\(_x\)CuO\(_6+\delta\)) single crystals down to monolayer (i.e. half unit cell) for transport measurements. We are able to tune the doping level of Bi2201 by annealing the sample in vacuum or ozone, and study the strongly correlated electronic states in Bi2201 over the entire phase diagram in a single sample. In addition, we probe the electronic structure of monolayer Bi2201 at atomic scale using scanning tunnelling microscopy and spectroscopy.
3:18PM D64.00005: Single-domain to Multi-domain Transition Due to Phase Separation in (La$_{1-y}$Pr$_y$)$_{1-x}$Ca$_x$MnO$_3$ Thin Films*  ASHKAN PAYKAR (Presenter), A. BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — The perovskite manganite (La$_{1-y}$Pr$_y$)$_{1-x}$Ca$_x$MnO$_3$ exhibits complex electronic and magnetic behaviors caused by a phase competition between its ferromagnetic metallic (FMM) and charged order insulating (COI) phases. While La$_{0.67}$Ca$_{0.33}$MnO$_3$ ($x=0.33, y=0$) undergoes a transition from a paramagnetic insulator to a pure FMM below 250 K, (La$_{0.4}$Pr$_{0.6}$)$_{0.67}$Ca$_{0.33}$MnO$_3$ ($x=0.33, y=0.6$) shows electronic phase-separation between FMM and COI phases at temperatures approximately below 120 K. Thin films of (La$_{1-y}$Pr$_y$)$_{1-x}$Ca$_x$MnO$_3$ ($x=0.33, y=0, 0.5, 0.6$) were grown on (110) NdGaO$_3$ (NGO) using pulsed laser deposition. Among these thin films, (La$_{0.4}$Pr$_{0.6}$)$_{0.67}$Ca$_{0.33}$MnO$_3$ also shows a single-domain to multi-domain transition in the FMM regions as they percolate at low temperatures. This domain transition is partially due to the in-plane uniaxial magnetic anisotropy caused by the anisotropic substrate strain exerted by (110) NGO. To check if phase separation also plays a role in the domain transition, we measured the temperature dependence of the coercive field ($H_c$) for $y=0$ and $y=0.5$ thin films. These films show a monotonic increase in $H_c$ with lowering temperature showing that phase separation and a percolation of the FMM regions is required for the domain transition.

*NSF DMR-1410237

3:30PM D64.00006: Effects of epitaxial strain and oxygen underdoping on order parameter competition in manganite/cuprate thin-film heterostructures*  CHAO C ZHANG, HAO ZHANG (Presenter), Department of Physics, University of Toronto, ANH NGUYEN, THOMAS GREDIG, Department of Physics and Astronomy, California State University Long Beach, MIN GU KANG, RICCARDO COMIN, Department of Physics, Massachusetts Institute of Technology, JOHN Y.T. WEI, Department of Physics, University of Toronto — To distinguish the role of magnetism from other factors that affect superconductivity in c-axis La$_{2/3}$Ca$_{1/3}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-\delta}$ (LCMO/YBCO) heterostructures, we grow and characterize various perovskite/YBCO/perovskite trilayers, using ferromagnetic LCMO, paramagnetic LaNiO$_3$ (LNO), and orthorhombic PrBa$_2$Cu$_3$O$_{7-\delta}$ (PBCO) as the sandwiching layers. LCMO and LNO trilayers show similarly large superconducting $T_c$ reductions with decreasing YBCO layer thickness, whereas this $T_c$ reduction is not seen in the PBCO trilayers. Our results indicate that epitaxial strain has a stronger effect on the $T_c$ of LCMO/YBCO heterostructures than any long-range magnetic proximity effect present. Using this system, we also study how the $T_c$ reduction varies with oxygen underdoping by deoxygenating the cuprate layer. [1] We discuss our results in the wider context of multiple competing orders, in particular the recent observation by resonant x-ray scattering of robust charge-density-wave order in LCMO/YBCO multilayers. [2]


*Work supported by NSERC, CFI-OIT and the Canadian Institute for Advanced Research
Creating Emergent Phases in Transition Metal Oxides

MILAN RADOVIC (Presenter), Photon Science Division, Paul Scherrer Institut — Transition Metal Oxides (TMOs) exhibit unique and multifunctional physical phenomena directly related to the spin and orbital degrees of freedom of metal d-states and their interplay with the lattice. Importantly, the isostructure of TMOs permits realization of hetero-structures generating at their surfaces and interfaces new physical matters that radically differ from those of the constituent bulk materials. Through two examples, novel and fascinating properties emerged in TMO based hetero-structures and routes to control them will be presented:

1. Altering orbital ordering and band filling of the 2DEG at titanates surfaces. Employing Angle-Resolved Photoemission Spectroscopy (ARPES) we found ways to manipulate the 2DEG and, consequently, to tune electronic properties of titanates surfaces (SrTiO3, TiO2-anatase and CaTiO3).

2. Tuning electronic phases in ultra-thin NdNiO3 (NNO) films via the strain and the proximity to a magnetic layer. Our study reveals that substrate-induced strain tunes the crystal field splitting, consequently changing the Fermi surface, nesting conditions and spin-fluctuation strength. All of them thereby effect and control the Metal Insulator Transition (MIT). In addition, we found that the ferromagnetic metallic (FM-M) state can be induced while MIT is quenched in ultra-thin NNO via the proximity to the magnetically ordered manganite buffer layer.

Overall our studies establish different approaches to manipulate the properties of the two-dimensional electron gas and electronic phases in NNO signifying perspectives of TMO for novel applications.
Electrically Controlled Intrinsic Tunneling in Dynamically Phase Separated Manganites* AMBIKA SHAKYA (Presenter), A. BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — (La$_{1-y}$Pr$_y$)$_{1-x}$Ca$_x$MnO$_3$ (LPCMO) thin films grown on (110) NdGaO$_3$ (NGO) substrates show clear evidence of micrometer scale electronic phase separation. A static phase separated state is observed at low temperatures while at high temperatures (approximately above 50 K) a dynamic (fluid) phase separated state (DPS) is formed. It has been shown that in the DPS state, the ferromagnetic metallic (FMM) regions can be reorganized using a non-uniform external electric field. We used microstructured gold contact patterns on LPCMO thin films to apply a non-uniform electric field and simultaneously measure the resistance vs. temperature ($R$-$T$) behavior. The $R$-$T$ graph shows a temperature independent resistance plateau at low temperatures (from about 20 K - 50 K). This behavior is a signature of tunneling. We further confirmed this tunneling behavior using current vs. voltage ($I$-$V$) measurements at low temperatures. Warming the sample up to a temperature of dynamic phase separation leads to redistribution of the FMM regions due to the non-uniform electric field between the gold electrodes. This redistribution changes the $I$-$V$ characteristics from tunneling to ohmic behavior. Hence, the properties of these magnetic devices can be modified using non-uniform external electric field.

*NSF DMR - 1410237

Electronic and magnetic properties in three-component manganite films – the role of ordered interfaces and ionic size effects* CAITLIN KENGLE (Presenter), MAITRI WARUSAWITHANA, DAKOTA BROWN, JAMES PAYNE, THOMAS PEKAREK, University of North Florida — The mixed-valent manganite, La$_{1-x}$Sr$_x$MnO$_3$, with $x=1/3$ has been widely studied for its colossal magneto-resistive properties arising from the double exchange interaction. This material can be grown in thin-film form as a random alloy or an ordered superlattice. Here we grow films replacing 50% of the La with Y to make La$_{1/3}$Y$_{1/3}$Sr$_{1/3}$MnO$_3$ as both random alloys where La, Sr, and Y randomly occupy the A-site and ordered superlattices where the supercells comprise of single unit cells of LaMnO$_3$, YMnO$_3$, and SrMnO$_3$ stacked in sequence. While electronically La and Y are very similar, as both tend to be in a 3+ oxidation state in the crystal, we find contrastingly different electronic transport. The Y-substituted films exhibit a suppression of the metal-to-insulator transition compared to that of La$_{1/3}$Sr$_{2/3}$MnO$_3$. While the suppression is observed in both the ordered superlattice and the random alloy, we find it notably more amplified in the random alloy sample. We will discuss how ionic size effects and ordered interfaces affect the electronic and magnetic properties of these samples.

*This work was supported by NSF Grant No. DMR-16-26332. Select films were grown at Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM).
4:42PM D64.00010: Superconductivity in a Metal/Quantum Dimer Heterostructure*  ELI GERBER (Presenter), JIAN-HUANG SHE, Cornell University, CHOONG HYUN KIM, Seoul National University, CRAIG J FENNIE, MICHAEL J LAWLER, EUN-AH KIM, Cornell University — Recently we proposed a new approach to engineering exotic superconductors based on a metal/quantum spin ice heterostructure. However, pyrochlore materials are difficult to grow and current models of their spin fluctuation spectra remain incomplete. In contrast, weakly-interacting spin dimer compounds such as Ba3Mn2O8 are experimentally tractable and their spin correlations can be calculated explicitly. In this work we focus on a new example of such a setup, the spin dimer compound Ba3Mn2O8 in heterostructure with electron-doped Ba3Sb2O8, and predict interfacial p+ip pairing at a few Kelvin. We also provide criteria for materializing the heterostructure using ab initio calculations. Hence we present a concrete proposal based on a controlled calculation predicting p+ip superconductivity in a metal/quantum dimer heterostructure.

*The authors acknowledge support through the NSF MRSEC program (DMR-1719875) and the Materials Innovation Platform grant DMR-1539918.

4:54PM D64.00011: Investigation of the Defect-Tolerance of Chalcogenide Perovskites*  JIANG LUO (Presenter), ZHAOHAN I ZHANG, Washington University in St. Louis, BOYANG ZHAO, HUANDONG CHEN, JAYAKANTH RAVICHANDRAN, University of Southern California, ROHAN MISHRA, Washington University in St. Louis — Chalcogenide perovskites, such as BaZrS3, have been proposed as defect-tolerant materials — that can maintain their electronic properties even in the presence of defects. When combined with their novel electronic structure, they have been proposed as promising materials for application in solar cells and optoelectronic devices; however, a systematic investigation of the defect tolerance of such perovskites is missing. We have used BaZrS3 as a prototype chalcogenide perovskite and investigated its defect tolerance to intrinsic point defects using a combination of density-functional-theory calculations, spectroscopic and transport measurements. Based on the calculations, we find that most defects lead to shallow levels. However, we find that the sulfur vacancies have low formation energy. They lead to a deep transition level that is spatially localized to act as a non-radiative recombination center. Results of transport measurements with specimens annealed with S-rich and S-deficient conditions will be presented. Our work demonstrates that critical control over the chalcogen stoichiometry is necessary to improve the performance of these chalcogen perovskites.

*This work was supported by NSF DMR-1806147.
**5:06PM D64.00012: Variation of defect states with the number of layers in 2D materials**

DAN WANG (Presenter), RAVISHANKAR SUNDARARAMAN, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute — The high sensitivity of two-dimensional (2D) materials to surroundings makes layer number an important consideration in designing devices for opto-electronic and quantum applications. However, the theoretical prediction on the variation process of defect level with increasing layer number is challenging due to the high computational cost. Here, we used a recently developed continuum model[1] to explore the layer-dependent effects. The scheme removes the defect-free layers from the density-functional-theory (DFT) calculations and captures their effects on the defect by replacing the electrostatic effect of the defect-free layers with a continuum dielectric function. Application of this method to defects in multilayer hBN (from monolayer to five-layer and bulk) reveals that defect levels become shallower with increasing layer number due to the increased dielectric screening, and the reduction process of ionization energy is highly dependent on the level of theory (DFT or many-body perturbation theory) as a result of the presence of self-interaction error and the absence of non-local screening effect in DFT.


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**5:18PM D64.00013: Tunable High-Temperature Superconductivity in Monolayer Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$**  
YIJUN YU (Presenter), LIGUO MA, PENG CAI, Fudan University, RUIDAN ZHONG, Brookhaven National Laboratory, CUN YE, JIAN SHEN, Fudan University, GENDA GU, Brookhaven National Laboratory, XIANHUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Fudan University — Atomically-thin layered van der Waals crystals represent ideal material systems in the ultimate two-dimensional (2D) limit. Among all layered materials, high-temperature superconductors stand out for their fundamental importance in material research and potential impact on future technology. Here, we developed a fabrication process that enabled us to produce intrinsic monolayer crystals of high-temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi-2212; here monolayer refers to a half unit cell) and probe their transport properties. The lack of dimensionality effect on superconducting transition temperature $T_c$ defies expectations from Mermin-Wagner theorem; it also sharply contrasts with much reduced $T_c$ in conventional superconductors in 2D limit. Being atomically thin, monolayer Bi-2212 offers unprecedented tunability over its doping and disorder level across the superconductor-insulator transition (SIT). Finite size scaling analysis at SIT provides a unified picture for disparate observations in cuprate systems. Our results establish monolayer Bi-2212 as an ideal platform for studying high-temperature superconductivity and other strongly correlated phenomena in 2D.
Defect spin qubits in silicon carbide (SiC) combine near-telecom operation and long coherence with a host crystal amenable to wafer scale semiconductor device engineering[1]. In particular, the neutral divacancy ($VV^0$) in SiC has a spin-photon interface ideal for long distance quantum communications and repeater schemes[2]. Here, we isolate for the first time single $VV^0$ defects in functioning, doped semiconductor p-i-n diodes and use the device to control the charge states of these defects[3]. This integration of the single spin into the semiconductor junction not only allows for a drastic reduction in spectral diffusion of the emitter, but also a careful study of the defect's charge state under illumination. We focus on these photodynamics and demonstrate deterministic and optimized charge control of the defect, allowing for charge state stabilization and electrical gating of single photon emission. We discuss the outlook for electrical control, manipulation and readout of both the spin and charge degrees of freedom in these quantum emitters.

References:

*Supported by AFOSR, DARPA, NSF, ONR, VR, KAW
3:06PM D65.00002: Jahn-Teller Effects in Group IV Quantum Defects in Diamond*

CHRISTOPHER CICCARINO (Presenter), School of Engineering and Applied Sciences, Harvard University, JOHANNES FLICK, Center for Computational Quantum Physics, Simons Foundation, MATTHEW TRUSHEIM, PRINEHA NARANG, School of Engineering and Applied Sciences, Harvard University — Defects in diamond are leading solid-state candidates for a range of quantum technologies. Recent research has focused on identifying new color centers with properties that reach beyond the limitations of the well-known nitrogen-vacancy (NV\textsuperscript{−}) center. Group IV-vacancy centers have been a primary focus due to their symmetry-protected optical transitions and long-lived spin degree of freedom. A detailed understanding of the electronic structure of these emitters is paramount to their use in spin-photon systems. Here we detail the ground- and excited-state properties of the negative and neutral group IV color centers using first-principles methods. In particular, we outline the dynamic and product Jahn-Teller (pJT) effects expected in these defect systems, including their potential impact on zero phonon line energetics and spin-orbit coupling. We capture the interplay of spin-orbit and electron-phonon coupling in order to accurately describe the pJT-affected excited state manifold. These results provide a more accurate benchmark for comparison with experiment, especially for the group IV neutral centers, where many open questions remain.

*We acknowledge funding from the Army Research Office MURI (Ab-initio Solid-State Quantum Materials) Grant Number W911NF-18-1-0431.

3:18PM D65.00003: Group III Defects in Diamond for Quantum Information Applications

ISAAC HARRIS (Presenter), Massachusetts Institute of Technology, CHRISTOPHER CICCARINO, MATTHEW TRUSHEIM, Harvard University, JOHANNES FLICK, Flatiron Institute, DIRK R. ENGLUND, Massachusetts Institute of Technology, PRINEHA NARANG, Harvard University — Point defects in wide bandgap semiconductors have emerged as leading spin-photon interfaces for applications in quantum information science. In particular, several types of color centers in diamond have been characterised as promising candidates for spin-photon interfaces. However, no color center has yet demonstrated the required spin initialisation, spin coherence and optical stability required for easy integration into quantum devices. Here, we discuss theoretical and experimental results for a new class of color centers, the group III vacancy complexes in diamond, and in particular the negatively-charged gallium vacancy center. These group III color centers are predicted to be stable in an inversion-symmetric configuration, which makes their optical transition resilient to charge noise, and therefore well-suited to integration in nanostructures. Furthermore, they are thermodynamically stable in a spin-1 charge state, which gives them desirable level structures and spin coherence properties for quantum information applications. Based on these results, we comment on the suitability of these new color centers as spin-photon interfaces.
First-principles characterization of nitrogen-related spin-defects in 4H- and 6H-SiC

YIZHI ZHU (Presenter), GIULIA GALLI, University of Chicago — Optically active spin defects in wide-gap semiconductors are promising platforms for solid-state quantum technologies. For example, in the last few years several defect qubits with long coherence times have been realized in SiC, an attractive material due to its ease of growth and microfabrication, compared to diamond. Recent studies [1-3] have explored the possibility of realizing a nitrogen vacancy (NV) in SiC, in analogy with diamond. We used first-principles calculations based on density functional theory to identify fingerprints of nitrogen related spin-defects in SiC. We computed several properties of point-defects containing nitrogen impurities, including zero-fielding splitting, hyperfine tensors, and zero-phonon lines. In order to analyze the robustness of our results, we conducted sensitivity analysis to establish the effect of pseudopotentials, density functionals and optimized atomistic structures on the computed electronic and spectroscopic properties of the defects.


Vanadium spin qubits as telecom quantum emitters in silicon carbide

GARY WOLFOWICZ (Presenter), Center for Molecular Engineering, Materials Science Division, Argonne National Laboratory, CHRISTOPHER ANDERSON, BERK DILER, Pritzker School of Molecular Engineering, University of Chicago, OLEG G. POLUEKTOV, Chemical Sciences and Engineering Division, Argonne National Laboratory, JOSEPH P HEREMANS, Center for Molecular Engineering, Materials Science Division, Argonne National Laboratory, DAVID AWSCHALOM, Pritzker School of Molecular Engineering, University of Chicago — Solid state quantum emitters with addressable spin registers are promising platforms for quantum communication, yet few emit in the telecom band necessary for low-loss fiber networks. Here we create and isolate single vanadium dopants in silicon carbide (SiC) with emission in the O-band (~1300 nm) and with brightness allowing cavity-free detection, in a wafer scale CMOS-compatible material [1]. We demonstrate that their emission is stable and narrow near surfaces, enabling integration with nanoscale devices.

We characterize the complex $d^1$ orbital physics in vanadium ensembles in all five sites available in 4H- and 6H-SiC. The optical transitions are observed to be sensitive to mass shifts from the distribution of nearest neighbor silicon and carbon isotopes, enabling optically resolved nuclear spin registers. Optically detected magnetic resonance of ground and excited states’ spin transitions reveal diverse hyperfine interactions with the vanadium nuclear spin and offer clock transitions for use as quantum memories. Finally, we demonstrate coherent quantum control of the spin state at 3.3 K. These results provide a path for solid-state telecom emitters for quantum applications.


*This work is supported by AFOSR, DOE, DARPA and ONR.
Finite-size and Surface effects: Deep Defects in Nanostructured SiC

TAMANNA JOSHI (Presenter), PRATIBHA DEV, Howard University — Spin-active deep defects in wide-bandgap semiconductors like silicon carbide (SiC) are being studied for application in quantum technologies, such as quantum computing, and nanoscale field sensing. Often these applications involve nanostructuring of the host semiconductor. In a nanostructure, the electronical and optical properties are expected to be affected by surface and quantum confinement effects. In our work, we investigate these finite size effects by studying the properties of silicon vacancies with different charge states in 2H-SiC (wurtzite) nanowires. Defect properties like formation energy, spin, and spin polarization energies are shown to be site-dependent in the nanostructured host. Our results indicate that a surface acts as a sink for the defects, and the migration of defects towards the surface may lead to the loss of the signal from a defect placed in a nanostructured host.

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Formation and migration of vacancies in SiC

ELIZABETH LEE (Presenter), JUAN DE PABLO, GIULIA GALLI, Pritzker School of Molecular Engineering, University of Chicago — Divacancy spin defects in silicon carbide (SiC) are promising platforms for quantum information science applications. However, the formation mechanism and migration properties of point defects in SiC are poorly understood and hence difficult to control. Using advanced simulation techniques, we gain insight into the creation, interaction and migration of vacancies in SiC, aimed at deriving rules for the design of robust defects in scalable quantum materials. In particular, we used a combination of enhanced sampling methods (https://github.com/MICCoM/SSAGES-public) coupled with classical Molecular Dynamics, and Density Functional Theory to investigate the defect electronic properties. We compare our results with thermal annealing and photoluminescence experiments [1], and we discuss possible processing conditions for the formation of divacancy defects with favorable spin states.


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Coherent control and high-fidelity readout of chromium ions in commercial silicon carbide

BERK DILER (Presenter), Pritzker School of Molecular Engineering, University of Chicago, SAMUEL J WHITELEY, CHRISTOPHER ANDERSON, Department of Physics, University of Chicago, GARY WOLFOWICZ, Center for Molecular Engineering and Materials Science Division, Argonne National Laboratory, MARIE WESSON, Department of Physics, University of Chicago, EDWARD S BIELEJEC, Sandia National Laboratories, JOSEPH P HEREMANS, Center for Molecular Engineering and Materials Science Division, Argonne National Laboratory, DAVID AWSCHALOM, Pritzker School of Molecular Engineering, University of Chicago — Transition metal ions provide a rich set of optically active defect spins in wide bandgap semiconductors. Their extrinsic nature promises easy device integration through nano implantation. Specifically, chromium in the 4+ charge state (Cr^{4+}) in silicon carbide (SiC) produces an S = 1 ground state and an S = 0 excited state with a strain insensitive near-telecom Λ-like optical-spin interface. In previous demonstrations the ground state spin control was limited by material quality. In this work [1], we study the formation Cr^{4+} in a commercial SiC substrate through implantation and annealing, enabling optical and coherent spin characterization. We measure an ensemble optical hole linewidth of 31 MHz, an order of magnitude narrower compared to as-grown samples. Through a detailed investigation of the Cr^{4+} governing transition dynamics, we optimize for high readout fidelities (79%). We report $T_1$ times greater than 1 s at T = 15 K with a $T_2^* = 317$ ns and a $T_2 = 81$ μs limited by the ensemble density. These results demonstrate Cr^{4+} in SiC to be an optically active spin-qubit for integration within hybrid quantum devices.


*DOE
4:30PM D65.00009: Decoherence of diamond NV ensembles with varying nitrogen spin concentration: a cluster expansion study  HUIJIN PARK (Presenter), Ajou Univ, JUNGHYUN LEE, SANG-YUN LEE, KIST Center for Quantum Information, HOSUNG SEO, Ajou Univ — Nitrogen-vacancy (NV) centers in diamond have been developed into essential hardware units to develop a wide range of solid-state quantum technologies. For such applications, the long coherence time of NV centers is crucial. Numerous previous studies identified that the NV's decoherence is often governed by the magnetic noise produced by the $^{13}$C nuclear spin bath and the nitrogen (P1) electron spin bath in a diamond. While the $^{13}$C-induced decoherence has been well understood, understanding of the P1-driven decoherence is still incomplete. In this study, we aim at the systematic theoretical investigation on the P1-driven decoherence of NV ensembles with varying P1 concentrations from 1ppm to 100ppm. We employ a cluster correlation expansion method. We discuss our results in comparison with recently published experimental data [1,2] and previous theoretical results [3,4]. Our results provide not only a microscopic understanding of the NV decoherence but also useful information to optimize the NV's performance in various quantum applications such as NV-based magnetometry and NV-based quantum registers.


4:42PM D65.00010: Dynamics of Silicon-Vacancy Color Center in Nanodiamonds  CHUNJING JIA (Presenter), YAN-KAI TZENG, YU LIN, THOMAS DEVEREAUX, STEVEN CHU, Stanford University — Diamond-based color centers have emerged for a variety of applications in quantum communication, quantum photonics, and biological sciences, etc. Optical color center of SiV formed by one silicon atom sited in the middle of two vacancies shows great promise as a single-photon source. Unlike the NV center, which can be improved sufficiently for quantum applications by high-temperature annealing to mobilize only vacancies, SiV center may become unstable in diamond lattice under annealing. Upon annealing to temperatures up to 800 ºC, both SiVs and vacancies would become mobile to the surface of diamond. It is unclear during the annealing process whether SiV or vacancy impurity migration dominates and the relative time-scale of the two processes. In this talk, we are going to present our studies to unravel this problem. An AOM-modulated laser heating and annealing in a diamond anvil cell has been used. The fluorescent intensities of SiV center before and after the annealing were measured using fluorescent spectroscopy. ab initio DFT calculations were used to quantify the dynamics of two impurities. Both experimental and theoretical results suggest that SiV centers can be stabilized associated with the crystalline quality during the production of artificial SiV photonic centers.
4:54PM D65.00011: Study of the Structure-property Relationship in Diamond (100), (110) and (111) Surfaces  HECTOR GOMEZ (Presenter), MICHAEL GROVES, Chemistry, California State University, Fullerton, MAHESH R NEUPANE, SEDD, US Army Rsch Lab - Adelphi — Understanding the electronic and physical properties of reconstructed diamond (100), (110), and (111) is important for meeting the increasing demand for high-powered control electronics in harsh environments. By determining the electronic and structural properties of reconstructed diamond (100), (110), and (111) surfaces, the effect reconstruction has on its electronic properties versus an ideal surface is revealed. Using GPAW, a density-functional theory (DFT) and the AutoNEB package, a stepwise surface reconstruction for diamond (111) and (100) was modeled. Diamond (100) reconstruction demonstrated an exothermic reaction with no observable intermediates or transition states. Following reconstruction in the (100) phase, -0.254 eV/atom energetic variance was observed from the bulk-like surface. In the (111) phase, a never before predicted intermediate state, with per atom energy difference of -0.011 eV from the bulk-like 2X1 surface, was observed between the bulk-like and Pandey-chain surfaces. Observed stable Pandey-chain reconstructed state resulted in an energy difference of -0.109 eV/atom from its bulk-like counterpart. Lastly, the favorability of the reconstruction suggests that 2x1 diamond (100) and (111) will follow this configuration instead of the bulk-like surface.

5:06PM D65.00012: The Spin-Flip Bethe-Salpeter Equation approach, and applications to molecular magnets and defects in solids for quantum information*  BRADFORD BARKER (Presenter), DAVID STRUBBE, University of California, Merced — Molecular magnets containing transition metals (e.g. Cr, Mn, Fe) are promising candidates for qubits due to their unpaired spins. Description of their ground- and excited-state energies is quite challenging for electronic structure methods, as these systems are poorly described by single-reference electronic-structure methods. The “spin flip” approach allows such methods to describe open-shell states as an excitation -- up or down in energy -- from a related single-reference high-spin state. Spin-flip time-dependent density-functional theory (TDDFT) has shown moderate successes in describing their energies, as well as their Heisenberg exchange coupling constants. The GW/Bethe-Salpeter equations have a similar form to TDDFT, but provide an ab initio kernel that overcomes many problems of standard TDDFT approximations. We have implemented spin-flip Bethe-Salpeter, allowing more accurate calculations on molecules, and enabling spin-flip for extended systems such as defects in solids for quantum information. We consider transition-metal dimers Mn_2 and Cr_2, and other molecular magnets, as well as the well-known diamond NV^ center.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, CTC and CPIMS Programs, under Award DE-SC0019053.
5:18PM D65.00013: NV-color centers in nanodiamond as a photon emitter embedded in whispering-gallery-mode optical resonator*  SUNGWAN CHO (Presenter), ETRI, MUHAMMED KAAN YILDIZ, IN HWAN DO, DONG-IN JUNG, Department of Physics, KAIST, JUNG HYUN SHIM, KI SEOK HONG, HEE JIN LIM, JAE HOON LEE, HYUN GYU HONG, Korea Research Institute of Standards and Science, JUNG BAE YOON, DONG HUN LEE, Department of Physics, Korea University, HANSUEK LEE, Department of Physics, KAIST — Development of reliable and stable photon source is crucial for applications in quantum technology, as well as fundamental experiment and metrology. NV(Nitrogen-vacancy) color center in diamond, are among the promising candidate for photon source. Although coupling of color centers with an high-Q optical cavity has high potential, fabricating optical cavities embedding defect centers have been challenging tasks with recent initial demonstrations. Here, we present a novel approach to fabricate high-Q optical Whispering-Gallery-Mode resonator comprising NV-color center. Starting from disk resonator coated with nanodiamond particles, we also fabricate microtoroid optical resonator. Fabricated microtoroid resonator with NV-center shows Q-factor above $10^7$ at telecom wavelength. A scanning photoluminescence spectrum also confirms stable photoemission inside the microtoroid resonators. With further development of this hybrid UHQ resonator, we expect the realization of robust platform for cavity QED and quantum metrology

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Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D66 DCMP: Unconventional States and Excitations in the Fractional Quantum Hall Effect  Four Seasons 1 - Steven Kivelson, Stanford Univ - Tag(s): Invited
Precursors to Exciton Condensation in Quantum Hall Bilayers* [Invited]

JAMES EISENSTEIN (Presenter), physics, Caltech, LOREN PFEIFFER, KENNETH WEST, electrical engineering, Princeton — Bilayer two-dimensional electron systems at high magnetic field exhibit an interlayer coherent excitonic phase when the layer separation is sufficiently small, the temperature sufficiently low, and the total electron density in the bilayer equals the degeneracy of a single Landau level. This phase is well known to display exotic transport phenomena, notably Josephson-like interlayer tunneling and essentially dissipationless transport of excitons across the bulk of the 2D system. While first detected twenty years ago in GaAs-based double quantum wells, this and related interlayer correlated phases have recently been observed in graphene-based multilayer systems.

In spite of this long history, the nature of the quantum phase transition between the incoherent phase at large layer separation and the coherent excitonic phase at small separations remains poorly understood. In this talk I will report on recent experiments which shed new light on the transition. In particular, I will discuss tunneling spectroscopy measurements which reveal evidence for interlayer electron-hole correlations at layer separations near, but above, the transition to the exciton condensate at total Landau level filling $\nu_T = 1$. These correlations are manifested by a nonlinear suppression of the Coulomb pseudogap which inhibits low energy interlayer tunneling in weakly coupled bilayers. The pseudogap suppression is strongest at $\nu_T = 1$ and grows rapidly as the critical layer separation for exciton condensation is approached from above. These and other observations suggest that exciton-hole condensation fluctuations exist in the incoherent phase well above the critical layer separation, in a manner reminiscent of Cooper pair fluctuations above the superconducting critical temperature.

*This work was supported by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center, the Gordon and Betty Moore Foundation through Grants GBMF1250 and GBMF4420, and the NSF via MRSEC Grant No. 1420541.
3:06PM D66.00002: Parton theory of the fractional quantum Hall effect: New developments* [Invited] JAINENDRA JAIN (Presenter), Pennsylvania State University — In the parton construction [1], one divides each electron into fictitious particles called partons, places each species of partons into an IQH state, and then fuses the partons back into physical electrons. This produces candidate FQHE states that are products of IQH states. Some of the states so produced are predicted to have non-Abelian excitations [2]. I will review recent work on the applicability of such wave functions to physically observed states at ν=5/2 [3], ν=2+6/13 [4], and ν=1/4 in wide quantum wells [5]. Theory suggests that a non-Abelian "221" state may appear at ν=1/2 in bilayer and trilayer graphene [6]. I will also discuss exact Hamiltonians for a subclass of such states [6,7].


*The work was supported by the U. S. Department of Energy, Oce of Basic Energy Sciences, under Grant no. DE-SC0005042.

3:42PM D66.00003: Duality in Quantum Hall Compressible States* [Invited] EDUARDO FRADKIN (Presenter), University of Illinois at Urbana-Champaign — It has long been known (at least since 1997) empirically that quantum Hall plateau transitions enjoy an apparent self-duality symmetry. The meaning of this statement is that the current-voltage (I-V) curves are non-linear and are symmetric around their linear behavior at the quantum phase transition. This behavior was first observed in dirtier samples and is now known to occur in the compressible states at filling fractions 1/2 and 1/4. This empirical result was interpreted by Shimshoni, Sondhi and Shahar (PRB 55, 13730 (1997)) as a manifestation of a particle-vortex duality. Yet, the origin of this symmetry has been mysterious and has remained unexplained until quite recently. In a very recent paper (Hart Goldman and Eduardo Fradkin, PRB 98, 165137 (2018)) Goldman and myself used the recently developed dualities of Dirac fermions (D. T. Son Phys. Rev X. 5, 031027 (2015); N. Seiberg, T. Senthil, C. Wang and E. Witten, Ann. Phys. 374, 3095 (2016)) to show that the mirror symmetry of the Jain sequences converging on 1/2n compressible states explain the observed self-duality as a property of the compressible states. Hart Goldman was the lead author of this work.

4:18PM D66.00004: New unconventional plasmons in the N=1 Landau level* [Invited]  LINGJIE DU (Presenter), School of Physics, Nanjing University — In the partially filled second Landau level (SLL) emergent exotic quantum fluids overlap and interplay with fractional quantum Hall (FQH) liquids. Collective modes of the exotic quantum fluids uncover underlying physical mechanisms responsible for emerging new ground states [1-3]. Resonant inelastic light scattering (RILS) spectra access unprecedented collective modes in the FQH regime of the SLL: intra-Landau-level plasmons[3]. The plasmons herald rotational-symmetry-breaking (nematic) phases in the SLL and reveal the nature of long-range translational invariance in these phases. The intricate dependence of plasmon features on filling factor provides new insights on complex interplay between topological quantum Hall order and nematic electronic liquid crystal phases. A marked intensity minimum in the plasmon spectrum at Landau level filling factor v = 5/2 strongly suggests that the paired state, which may support non-Abelian excitations, overwhelms competing phases, revealing the robustness of the 5/2 superfluid state for small tilt angles. In contrast, a sharp and intense plasmon peak in the state at v=7/3 reveals that the macroscopic coherence of the FQH liquid coexists with nematic order, supporting the proposed model of a FQH nematic at 7/3. Other interpretations of the new collective mode, such as chiral graviton [4], will be discussed.


*Research supported by the National Science Foundation through grant NSF-DMR-1306976
Composite Fermions near Half-filled Landau Levels: Precise Experimental Tests of Luttinger Theorem, Particle-Hole Symmetry, and Fermi Sea Anisotropy

MANSOUR SHAYEGAN (Presenter), Princeton University — Composite fermions (CFs), exotic particles formed by pairing an even number of flux quanta to each electron, provide a fascinating description of phenomena exhibited by interacting two-dimensional electrons at high perpendicular magnetic fields and low temperatures. At and near Landau level half-fillings, CFs occupy a Fermi sea. In this talk, I will present our experimental results aimed at probing this Fermi sea directly and quantitatively. The probe consists of geometric resonance measurements, manifesting minima in the magneto-resistance when the CFs’ cyclotron orbit diameter becomes commensurate with the period of a periodic potential imposed in the plane. The data provide evidence that particle-hole symmetry and the Luttinger theorem are obeyed to very high precision for CFs, quasi-particles which themselves are a product of interaction. There are, however, quantitative differences from the predictions of the existing (Dirac and Halperin-Lee-Read) theories. We also report measurements of CF Fermi sea shape, tuned by the application of uniaxial strain. The strain-induced results reveal that the Fermi sea anisotropy for CFs ($\alpha_{CF}$) is less than the anisotropy of their low-field hole (fermion) counterparts ($\alpha_F$), and closely follows the relation $\alpha_{CF} = \alpha_F^{1/2}$.


Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D67 DCMP: Nematicity in Topological and Superconducting Materials Four Seasons 2-3 - Qimiao Si, Rice Univ - Tag(s): Invited
2:30PM D67.00001: Interacting multi-channel topological boundary modes in a quantum Hall valley system*  [Invited] MALLIKA RANDERIA (Presenter), Massachusetts Institute of Technology MIT — Two-dimensional quantum Hall systems offer a versatile platform to explore the interplay between topology and symmetry breaking facilitated by Coulomb interactions. Spontaneous valley ordering of bismuth surface states in a large magnetic field gives rise to the emergence of a nematic phase. We can directly visualize the rotational symmetry breaking of this nematic phase using a scanning tunneling microscope (STM) [1]. We further use an STM to image the formation of topological boundary modes in between nematic quantum Hall domains. By changing the valley flavor and number of modes at the domain wall, we realize strikingly different regimes where these boundary modes are either metallic or insulating. This behavior is a consequence of Coulomb interactions constrained by the valley flavor, making these channels a new class of interacting symmetry-protected Luttinger liquids [2,3].


*We acknowledge funding from the Gordon and Betty Moore Foundation, DOE and NSF.

3:06PM D67.00002: Odd-parity multipolar orders in the spin–orbit-coupled metal Cd$_2$Re$_2$O$_7$*  
[Invited] SATOSHI TAJIMA, DAIGOROU HIRAI, MASASHI TOKUNAGA, MASASHI TAKIGAWA, Univ of Tokyo, TATSUO C. KOBAYASHI, Okamaya University, TAKUMI HASEGAWA, Hiroshima University, ZENJI HIROI (Presenter), Univ of Tokyo — The pyrochlore oxide Cd$_2$Re$_2$O$_7$ is the only superconductor ($T_c = 1.0$ K) in the family of α-pyrochlore oxides [1]. Moreover, it exhibits two characteristic structural transitions losing the inversion symmetry below 200 K. Recently, it has attracted increasing attention as a candidate spin–orbit-coupled metal (SOCM), in which specific Fermi liquid instability can lead to odd-parity multipolar orders with spontaneous inversion-symmetry breaking [2] and parity-mixing superconductivity [3, 4]. More recent theoretical classifications based on the crystal symmetry reveal that the two parity-breaking phases are described by unconventional odd-parity multipoles, that are the electric toroidal quadrupoles (ETQs) with different components, $x^2−y^2$ and $3z^2−r^2$ [5]. These ETQs are unique as they are cluster multipoles defined on the tetrahedral unit of the pyrochlore lattice, distinguished from conventional atomic multipoles realized in f-electron systems [6]. Here we report our recent experimental progress and review the present understanding of the SOCM Cd$_2$Re$_2$O$_7$.


*This work was partly supported by KAKENHI Grant Number 18H01169 given by Japan Society for the Promotion of Science (JSPS).
3:42PM D67.00003: Nematic Superconductivity [Invited] VLADYSLAV KOZII (Presenter), Physics, University of California, Berkeley, LIANG FU, Physics, Massachusetts Institute of Technology, JORN VENDERBOS, Physics, University of Pennsylvania, HIROKI ISOBE, Physics, Massachusetts Institute of Technology — Nematic superconductivity refers to the spontaneous breaking of rotational symmetry of a system in superconducting state. Nematic superconductivity in topological insulator Bi2Se3 doped with Cu, Nb, or Sr atoms was observed in numerous experiments, including Knight shift, upper critical field, specific heat, magnetic torque, and STM measurements. Remarkably, such a nematic state appears to be a clear signature of topological superconductivity. In this talk, I will discuss the theoretically predicted properties of these compounds and their relation to the existing experiments. Furthermore, the recent measurements of the upper critical field in twisted bilayer graphene revealed strong two-fold anisotropy of the superconducting state, indicating nematic superconductivity. Motivated by these experiments, I will also briefly describe some theoretical proposals aiming to explain such an exotic state.

4:18PM D67.00004: Nematicity in normal and superconducting states of twisted bilayer graphene [Invited] PABLO JARILLO-HERRERO (Presenter), Massachusetts Institute of Technology MIT — In this talk I will review our recent experiments on magic-angle twisted bilayer graphene which show normal state and superconducting state anisotropies in the resistivity and critical magnetic field, respectively. These represent evidence for nematicity in this novel correlated system.

4:54PM D67.00005: Spin-polarized correlated insulator and superconductor in twisted double bilayer graphene.* [Invited] XIAOMENG LIU (Presenter), ZEYU HAO, ESLAM KHALAF, JONG YEON LEE, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, ASHVIN VISHWANATH, PHILIP KIM, Harvard University — In flat electronic bands, the effect of interaction is elevated, which may lead to the emergence of correlated electronic states. Recently, the discoveries of correlated insulator and interaction-driven superconductivity in the magic-angle twisted bilayer graphene (MATBG) sparked the search of flat band materials enabled by moire superlattices. In this talk, I will present our experimental study of moire flat band in twisted double bilayer graphene (TDBG). In TDBG, the flatness of the band is tunable by perpendicular electric fields, adding another experimental knob and eliminating the requirement of a precise twist angle. Correlated insulators and superconductivity are discovered in TDBG with a much larger energy scale than in MATBG. Intriguingly, these emergent phases are found to be spin-polarized by in-plane magnetic field dependence. Since ferromagnetism and superconductivity typically compete with each other, the finding of spin-polarization in a superconductor carries an implication of exotic paring mechanism and pairing symmetry.

*The major experimental work is supported by Department of Energy.

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D68 DPOLY: Highly Loaded and Morphologically Enhanced Polymer Nanocomposites Four Seasons 4 - Zahra Fakhraai, University of Pennsylvania - Tag(s): Invited
Conventional methods of nanocomposite fabrication involve mixing and dispersing nanoparticles into a polymer matrix, making it challenging to produce composites with extremely high volume fractions (> 50 vol%) of nanoparticles. Recently our group has shown that such nanocomposites in the forms of films and membranes can be produced by capillary rise infiltration (CaRI) by thermally annealing a bilayer of polymer and nanoparticle. CaRI induces imbibition of polymer into the interstices of the nanoparticle packing via capillarity. This method has been further extended to induce polymer infiltration into nanoparticle packings through solvent annealing and leaching from a elastomer network. While these methods provide powerful ways to produce highly loaded nanocomposites, they also provide a rich platform to study the behavior of polymers under extreme nanoconfinement. The chain dimension of the polymer, which depends on its molecular weight, can be comparable to or greater than the average pore size of the nanoparticle packing. In this talk, I will share our current understanding of the transport phenomena of polymers under such nanoconfinement using a combination of experimental and computational approaches. I will show that the dynamics of CaRI depends strongly on the confinement ratio as well as the molecular weight of the polymer. In particular, the effective viscosity of the polymer can decrease or increase depending on the extent of confinement and the molecular weight of the polymer. We also show that the structure and properties of the resulting nanocomposites also depend strongly on the processing parameters and the molecular weight of the polymer.
Biomimetic nanocomposites exemplified by nanostructured nacre-like assemblies, provide a generalized approach to engineer materials. Continuing this research, we learn that the unique mechanics of tooth enamel can be replicated combining out-of-plane nanoscale columns with molecular precision of layer-by-layer (LBL) assembly. These composites reveal remarkably high vibrational damping thought to be impossible for stiff materials.

The novel type of biomimetic nanocomposites are those based on aramid nanofibers (ANFs). They spontaneously assemble into three-dimensional percolating networks reminiscent of cartilage. The nanoscale structure of ANF composites reveal nanoscale porosity that can be controlled by nanofiber branching. The latest results from multiple groups demonstrate that ANF composites resolve some of the essential property bottlenecks for ion-selective membranes, dendrite-resistant electrolytes, and structural batteries.

One of the emerging fields for biomimetic nanocomposites are optical devices. The high strain and strong polarization rotation make possible metaoptical devices with kirigami composites with wide-angle diffraction gratings for LIDARs and highly efficient quarter wave plates for THz scanners. Chiroplasmonic composites with mirror-asymmetrical 3D shapes of gold nanoparticles represent the first dynamically reconfigurable metaoptical composites for visible, near-IR and THz ranges of electromagnetic spectrum.

*DoD Vannevar Bush Fellowship
National Science Foundation
Air Force Office of Scientific Research
3:42PM D68.00003: Polymer Processing at Liquid Crystal-Air Interfaces* [Invited]  
XIAOSHUANG WEI, LAURA BRADLEY (Presenter), Univ of Mass - Amherst — Fluid interfaces are unique environments for materials processing because, as inherently open systems, they promote dynamic transport from adjoining phases and offer anisotropic structures that give rise to strong directional interactions during assembly. Liquid crystal interfaces add further prospects for producing materials with directional ordering or anisotropic morphology. For example, colloids assembled at liquid crystal-air and liquid crystal-water interfaces can form chains or hexagonal lattices. In this talk, we demonstrate liquid crystal-mediated synthesis and assembly of polymer colloids at liquid crystal-air interfaces. The polymer colloids are produced by polymerization of acrylic monomers in non-reactive liquid crystal mesogens. We examine mechanisms governing the simultaneous polymer growth and assembly as a function of reaction time, initial monomer concentration, and liquid crystal director orientation. Results outline design rules to control the nucleation and growth of morphologically enhanced polymer composites.

*This work is supported by an NSF CAREER Award (#1845631).

4:18PM D68.00004: Driving and manipulating polymer degradation in nanocomposites via photothermal heating of the particle* [Invited]  
LAURA CLARKE (Presenter), Physics, North Carolina State University, HONGLU HUANG, Wilson College of Textiles, North Carolina State University, GABRIEL FIRESTONE, DANIELA FONTECHA, Physics, North Carolina State University, RUSSELL GORGA, Wilson College of Textiles, North Carolina State University, JASON R BOCHINSKI, Physics, North Carolina State University — We are interested in thermally-driving chemical reactions in small volumes within a solid material, where diffusion of reactants and products are limited. Such experiments are achieved by photothermally heating metal nanoparticles incorporated within a polymer, which creates significant heat generation at the particle and an inhomogeneous steady state temperature distribution across the solid. Specifically, polymer far from any particle is cool while in contrast, local regions surrounding a particle experience temperatures up to few 100s deg. C. Utilizing polymer degradation as a test reaction creates a detectable product as a permanent record of the temperature profile and, if localized, forms defects which dramatically alter mechanical properties. In general, manipulating the connection between the fraction of chemical degradation and mechanical strength as an object deteriorates is important for plastic waste management where microfragmentation may either be harmful or beneficial depending on the remediation strategy. Polyethylcyanoacrylate (PECA) degrades by depolymerizing and in confinement the monomer will repolymerize to form oligomers. Photothermal heating of PECA exhibits heterogeneous degradation, including defect formation and synthesis of a carbonaceous by-product localized around each particle. Polyethylene (PE) degrades via thermo-oxidative processes that rely on the presence of oxygen and pre-existing defects in addition to heat; consequently, photothermal heating of PE demonstrates homogeneous degradation due to the distributed nature of the reaction pathway.

*National Science Foundation CMMI-1462966
There is an increasing need for the development of multifunctional lightweight materials that are strong, tough, and reconfigurable. Natural systems have evolved efficient strategies, exemplified in the biological tissues of numerous animal and plant species, to synthesize and construct composites from a limited selection of available starting materials that often exhibit exceptional mechanical properties that are similar, and frequently superior to, mechanical properties exhibited by many engineering materials. These biological systems have accomplished this feat by establishing controlled synthesis and hierarchical assembly of nano- to micro-scaled building blocks that are integrated into macroscale structures. However, Nature goes one step further, often producing materials with that display multi-functionality in order to provide organisms with a unique ecological advantage to ensure survival.

In this work, we investigate a variety of organisms that have taken advantage of hundreds of millions of years of evolutionary changes to derive structures, which are not only strong and tough, but also demonstrate the ability to articulate as well as display multifunctional features including damage sensing and self-cooling. We discuss the mechanical properties and functionality stemming from these hierarchical features as well as how they are formed. From the investigation of synthesis-structure-property relationships in these unique organisms, we are now developing and fabricating cost-effective and environmentally friendly multifunctional engineering composites.

*AFOSR-FA9550-15-1-0009

Monday, March 2, 2020 2:30 PM - 5:30 PM

Session D70 DPOLY DSOFT GSNP DBIO: Rheology and Dynamics of Polymer Liquids and Glasses 208 - Thomas O'Connor, Sandia National Laboratories - Tag(s): Focus
2:30PM D70.00001: Molecular Simulations of Poly[n]catenane Dynamics and Rheology*
PHILLIP RAUSCHER (Presenter), University of Chicago, KENNETH SCHWEIZER, University of Illinois, STUART J ROWAN, JUAN DE PABLO, University of Chicago — With the recent synthesis of poly[n]catenanes – polymers composed of interlocking ring molecules – the possibility of incorporating catenated moieties into functional materials continues to grow. However, catenated polymers have been only sparsely studied, as previous investigations have primarily focused on statistical, topological, or structural features, rather than the dynamics. To characterize these new systems, we conducted molecular dynamics simulations of model poly[n]catenanes in the melt. We observe unusual monomer diffusion and present a Rouse-like model that can qualitatively explain the results. We show that this model fails to account for topological interactions and that various measures of friction in the system are not self-consistent. We examine the stress relaxation and find that the viscosity exhibits a surprising non-monotonic dependence on ring size. We briefly outline how these results may be applied to material design and synthesis.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. 1746045. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

2:42PM D70.00002: Graft Polymers and Entanglements: From Linear Chains to Filaments*
ANDREY DOBRYNIN (Presenter), HEYI LIANG, Univ of Akron, GARY GREST, Sandia National Laboratories — Dynamics of melts and solutions of high molecular weight polymers is controlled by topological constraints (entanglements) imposing sliding chain motion along an effective confining tube. For linear chains, the tube size is determined by a universal packing number Pe, the number of polymer strands within a confining tube required for chains to entangle. Using coarse-grained molecular dynamics simulations, it is shown that in melts of graft polymers, the packing number is not universal and depends on the molecular architecture. The packing number of graft polymers is a nonmonotonic function of the degree of overlap between side chains belonging to the same molecule. Below side chain overlap, it decreases with increasing grafting density, then begins to increase as side chains start to interpenetrate, finally, in the limit of densely grafted side chains it approaches Pe for linear chains. This dependence reflects a crossover from chain-like entanglements in systems with loosely grafted side chains to entanglements between flexible filaments. This is in agreement with the experimental data for dependence of plateau modulus on the molecular architecture of graft poly(n-butyl acrylates) and poly(norbornene)-graft-poly(lactide) melts.

*NSF DMR-1535412
2:54PM D70.00003: Effect of Head-to-Head Association/Dissociation on Relaxation of Entangled Chains  
HIROSHI WATANABE (Presenter), YUMI MATSUMIYA, Kyoto Univ, YOUNGDON KWON, Sungkyunkwan Univ — For entangled high-cis polyisoprene (PI-COOH) undergoing monofunctional, head-to-head association/dissociation through hydrogen bonding of COOH groups attached at the chain head, viscoelastic and dielectric relaxation behavior was examined in bulk state. The relaxation was found to deviate significantly from that of a simple mixture (blend) of non-associative unimer PI and dimer (PI)₂ having the same composition as the associative PI-COOH (determined from FTIR spectroscopy for the COOH group). This deviation is attributed to an association/dissociation-induced motional coupling between the PI-COOH unimer and its dimer. Analysis based on the reptation eigenfunction expansion lends support to this conclusion.

3:06PM D70.00004: Unified analytic expressions for the entanglement length, tube diameter, and plateau modulus in polymer melts*  
ROBERT HOY (Presenter), Univ of South Florida, MARTIN KRÖGER, ETH Zurich — By postulating that the contributions to the dimensionless plateau modulus from flexible-, semiflexible-, and stiff-chain entanglement mechanisms combine additively (in parallel), and testing this postulate with molecular dynamics simulations and topological analyses of Kremer-Grest bead-spring polymer melts, we obtain analytic expressions that quantitatively predict the plateau modulus $G$, the entanglement length $N_e$, and the tube diameter $a$ in melts that span three orders of magnitude in $l_K/p$, where $l_K$ and $p$ are respectively the Kuhn and packing lengths. Our expressions resolve conflicts between previous scaling predictions for the loosely entangled [Lin-Noolandi: $Gl_K^3/k_BT \sim (l_K/p)^3$] and tightly-entangled [Morse: $Gl_K^3/k_BT \sim (l_K/p)^{7/5}$] regimes.

*Support from NSF Award No. DMR-1555242 is gratefully acknowledged.

3:18PM D70.00005: The Source of Strain Hardening in Glassy Polymers Investigated by Molecular Dynamics and Brownian Dynamics Simulations*  
RONALD LARSON (Presenter), Chemical Engineering, University of Michigan, ROBERT HOY, Physcs, University of South Florida, SOROUSH MOGHADAM, WEIZHONG ZOU, Chemical Engineering, University of Michigan — Using both fine-grained Molecular Dynamics (MD) simulations and coarse-grained simulations we show how strain hardening in polymeric glasses under uniaxial extension arises from highly stretched strands that form as the polymer chains deform subaffinely on increasing length scales as strain increases. We find that although the HBD model ignores entanglements, it accurately predicts how the MD chain configurations evolve during deformation. Both models shows similar strain hardening modulus $G_R$ that is much larger than the melt plateau modulus $G_N$ because chain segments become highly stretched at modest Hencky strain (<1 ). Both models also capture the increase in strain hardening with increasing chain length that saturates in the long chain limit. We improve upon HBD’s ability to accurately capture stress-strain curves at small strains through yielding and strain softening by extending the theory to multiple segmental relaxation modes, whose strain-dependent relaxation times are obtained from small-molecule probe relaxation experiments by Ediger and coworkers [Bending, B. & Ediger, M. D. J. Polym. Sci. B 2016, 54, 1957-1967].

*We acknowledge funding by the National Science Foundation DMR-1707640
3:30PM D70.00006: Predicting time-temperature-superposition breakdown near the glass transition with the Heterogeneous Rouse Model*  DAVID SIMMONS (Presenter), Chemical and Biomedical Engineering, University of South Florida — Since pioneering work by Plazek in the 1960’s, it has been known that time-temperature superposition breaks down in many polymers upon approach to the glass transition. Because TTS is fundamentally rooted in the Rouse model prediction of a shared temperature dependence for chain and segmental relaxation modes, this breakdown implies a significant gap in our understanding of polymer dynamics at low temperature. Here, we report on predictions of TTS breakdown by the Heterogeneous Rouse Model, which generalizes the Rouse model to incorporate dynamic heterogeneity – the emergence of a distribution of segmental relaxation times at low temperature. Predictions are in good agreement with simulations and with available experimentally observed relaxation spectra in the TTS-breakdown regime, suggesting that this theory provides a promising model for dynamics in the TTS breakdown regime.

*This material is based in part on work supported by the National Science Foundation NSF Career Award grant number DMR1554920.

3:42PM D70.00007: Relationship Between Large Amplitude Oscillatory Strain (LAOS) Experiments and Commercial Pressure Sensitive Adhesives Applications Testing  ALAN NAKATANI (Presenter), SIPEI ZHANG, Core R&D Analytical Science, The Dow Chemical Company, SEHBAN OZAIR, ASGHAR PEERA, DOW Adhesives, Collegeville, PA 19446, The Dow Chemical Company, OWEN YOUNG, Core R&D Analytical Science, The Dow Chemical Company, KYLIE MANNING, CACHAE PEARSON, HIMAL RAY, DOW Adhesives, Collegeville, PA 19446, The Dow Chemical Company — Historically, analytical test methods on pressure sensitive adhesives (PSA’s) have shown poor correlation to applications test results. Since applications tests such as peel and shear involve large deformations of the adhesive, large amplitude oscillatory strain (LAOS) experiments may correlate more strongly to the applications test results than typical linear viscoelastic measurements. Here we report the applications and characterization results on nine different commercial PSA films. The primary applications test results are 90° stainless steel peel and stainless steel shear. Based on these results, the adhesives were classified as “tape”, “label”, or “removable”, with three samples in each category. The adhesives were characterized analytically by large amplitude oscillatory strain (LAOS) tests. The various LAOS parameters appear correlated to the applications peel and shear results indicating LAOS may provide a better indication of applications performance in a more efficient way than existing applications test protocols.
3:54PM D70.00008: Polymer rheology predictions from first-principles using the slip-link model*  DIEGO BECERRA, ANDRES CORDOBA, Chemical Engineering, Universidad de Concepcion, MARIA KATZAROVA, Chemical Engineering, University of Delaware, MARAT ANDREEV, Chemical Engineering, MIT, DAVID CHRISTOPHER VENERUS, Chemical Engineering, New Jersey Institute of Technology, JAY SCHIEBER (Presenter), Physics, Applied Math, Chemical Engineering, Illinois Institute of Technology — The discrete slip-link theory a hierarchy of strongly connected models that have great success predicting the linear and nonlinear rheology of high-molecular weight polymers. Three of the four parameters of the most detailed model can be extracted from primitive path analysis, which give quantitative experimental agreement for all examined chemistries (PS, PI, PBd and PE). Here we show that the remaining friction parameter can also be extracted from atomistic simulations. In particular, an available quantum chemistry-based force field for polyethylene oxide (PEO) was used to perform molecular dynamics simulations of a 12kDa melt. Once the four parameters are determined for any chemistry, all parameters for all members of the slip-link hierarchy are determined. Then, using a coarser member of the hierarchy the dynamic modulus and nonlinear rheology of a 256kDa PEO melt was predicted. The predictions are compared to experimental measurements performed at the same temperature. Unfortunately, the extracted friction differs by a factor of two from experiment, which presumably arises from insufficient accuracy in the force field. Nonetheless, the work demonstrates that theory predictions without adjustable parameters should be possible.

*Funded by FONDECYT grant 11170056 and NLHPC, ECM-02

4:06PM D70.00009: A priori Determination of the Extensional Viscosity of Polydisperse Linear Polymer Melts*  JOHN DORGAN, JOHN SZFRANSKI (Presenter), Michigan State Univ — Compared to coarse grained MD, the COMOFLO algorithm is 100,000 times faster. The steady-state extensional viscosity function is calculated in a parameter free completely a priori manner as previously done for shear (Parameter Free Prediction of Rheological Properties of Homopolymer Melts by Dynamic Monte Carlo Simulation, Dorgan et.al., Macromolecules, (2012) DOI: 10.1021/ma301307d). The algorithm captures molecular details of extensional flow in three dimensions for entangled polymer melts of arbitrary molecular weight distribution across multiple flow regimes from the correct low deformation limit, through the strain-hardening regime, to the high deformation rate strain softening region. Comprehensive a priori shear rheology of polydisperse systems was established earlier (Finding the Missing Physics: Mapping Polydispersity into Lattice-Based Simulations. Rorrer & Dorgan, Macromolecules, 2014, DOI: 10.1021/ma5001207 ). The ability to predict steady shear and elongational rheology for linear polymer melts of arbitrary molecular weight distribution can be considered a solved problem.

*Funding was provided by the Fluid Dynamics Program of the NSF under grant CBET-1067707 and by the David and Denise Lamp Endowment gift to the Michigan State University Foundation.
4:18PM D70.00010: Thinning and break up of freestanding polymer solutions* [Invited]  JAN VERMANT (Presenter), EMMANOUIL CHATZIGIANNAKIS, Materials, ETH Zürich — The stability and break-up of thin liquid polymer films is a fascinating subject and reflects a complex interplay between intermolecular forces, hydrodynamic and viscoleastic phenomena, osmotic pressure and the effects of confinement. We have studied the thinning dynamics of concentrated polymer-solutions liquid films experimentally using a modified thin film balance technique. The variation of the capillary pressure that is driving the thinning of the film allows us to control the ratio of the the competing timescales of drainage and rupture. It is shown that rupture occurs through the random evolution of thickness fluctuations, whereas the drainage dynamics are described well by continuum approaches, even down to length scales on the order of the radius of gyration of the films. Using time dependent positive, negative and oscillatory pressure jumps across the interface, a wide range of dynamical phenomena can be evidenced. The implications of these results on macroscopic stability of multiphase systems and modelling events such as coalescence will be discussed.

*We acknowledge funding of Shell, The Netherlands.

4:54PM D70.00011: Uniaxial Extensional Rheology of Associating Polymers: from Processing to Performance  ZACHARY HINTON (Presenter), NICOLAS ALVAREZ, Department of Chemical and Biological Engineering, Drexel University — Polymers which include associating groups show increased performance characteristics over the base backbone polymer. The tunable properties of associating polymers are desirable for a wide range of applications, including as self-healing materials. However, there is typically a loss of processability for strongly associating polymers. In this work, we use filament stretching uniaxial extension to probe the processing window of strongly associating polymers. We show that, processing is limited by melt fracture in a wide range of Weissenberg numbers. The presence of entanglements increases the level of processability both in terms of the maximum Hencky strain before failure and the minimum achievable strain at low temperatures. Furthermore, the mechanical performance of associating polymers is confirmed to depend strongly on the associating group strength. Both the processability and performance of associating polymers can be captured by a spectrum of relaxation timescales related to the polymer backbone and various states of the associating groups. By reducing the critical behaviors of associating polymers to key timescales, clear design and processing parameters can be addressed in terms of fundamental physics.
5:06PM D70.00012: Liquid to soft solid transition in block polymers via low strength magnetic fields*  KARTHIKA SURESH (Presenter), MICHELLE A CALABRESE, Chemical Engineering and Materials Science Department, University of Minnesota — Achieving magnetic field-induced orientation in block polymers (BCPs) has typically relied on large field strengths (B≥5 T), the addition of liquid-crystalline (LC) or rod-like blocks, substantial chain anisotropy, or combinations therein. BCP ordering upon application of low-strength fields (≤0.5 T) has only been reported in systems of over 60% wt LC mesogen by mass. Here, we identify substantial field-induced rheological and structural changes in several coil-coil BCP variants using magneto-rheology and small-angle neutron scattering (SANS). Linear viscoelastic temperature ramps combined with B≥0.1 T magnetic field show a liquid to gel transition where the increase by three-to-six orders of magnitude beyond a critical time (t_c). Here, t_c is a function of field strength, polymer concentration and molecular weight, temperature, and ionic strength. The resultant gel state is stable for several hours after field removal, where the structural relaxation time scales with the maximum achieved modulus. SANS detects distinct gelation mechanisms based on BCP variant. In addition to structure enhancement, this approach has the potential to discover new structures not accessible through traditional self-assembly routes with minimal input from external fields.

*Seed grant, UMN MRSEC

5:18PM D70.00013: Multiscale simulation of a well-entangled polymer melt flow in between two coaxial cylinders under non-isothermal condition*  YUJI HAMADA, TAKESHI SATO, TAKASHI TANIGUCHI (Presenter), Chemical Engineering, Kyoto University — We have successfully extended a multiscale simulation method to non-isothermal well-entangled polymer melt flows in between two coaxial cylinders. At the microscopic level, a dual slip-link model is employed as a model for well-entangled polymers. We found that the extended multiscale simulation method is quite effective to reveal the relation between non-isothermal polymeric flows and microscopic states of polymer chains expressed by primitive paths and slip-links. It is also found that the temperature-dependent reptation-time-based Weissenberg number is a suitable measure to understand how extent polymer chains are deformed in a range of the shear rate used in this study.

*We acknowledge support by the Japan Society for the Promotion of Science (JSPS) KAKENHI Grant No.19H01862 and by the Ogasawara Foundation.

Monday, March 2, 2020 5:45 PM - 6:45 PM

Session E01 APS: APS Prizes and Awards Ceremonial Session Hyatt Centennial

5:45PM E01.00001: APS Prizes and Awards Ceremonial Session —

Monday, March 2, 2020 5:45 PM - 7:00 PM
Session E19 APS: Connecting with Success: Networking Workshop for Physicists 207 - Tag(s): Careers, Undergrad Friendly

5:45PM E19.00001: Connecting with Success: Networking Workshop for Physicists — Out of 100 physics bachelors, fewer than 4 will actually go on to hold permanent academic physics jobs - the rest will work in private sector or national lab environments. Building a network that spans employment sectors is essential to finding a job. In this interactive workshop, students will learn about building and using their professional network to discover career opportunities. Students will have plenty of time to ask questions, and will even get the chance to practice networking skills during the workshop. Refreshments will be served.

Monday, March 2, 2020 5:45 PM - 6:45 PM

Session E34 DPOLY: Open Discussion on Polymer Science and Polymer Scientists in the Age of Global Plastics Pollution 506 - Andrew Lovinger, National Science Foundation

5:45PM E34.00001: Open Discussion on Polymer Science and Polymer Scientists in the Age of Global Plastics Pollution —

Monday, March 2, 2020 6:45 PM - 8:15 PM

Session E71 APS: Graduate School Fair 2020 I Exhibit Hall C/D - Tag(s): Careers, Education, Undergrad Friendly

6:45PM E71.00001: Graduate School Fair 2020 — Graduate schools are invited to distribute literature and meet with students about their graduate programs. Each participating school will receive a small table with signage in the undergraduate student lounge. Both powered and unpowered options are available.

Monday, March 2, 2020 6:45 PM - 8:15 PM

Session E72 APS: APS Welcome Reception (6:45pm - 8:15pm) Exhibit Hall C/D - Tag(s): Undergrad Friendly

6:45PM E72.00001: APS Welcome Reception (6:45pm - 8:15pm) —

Monday, March 2, 2020 8:00 PM - 9:00 PM

Session E36 DCOMP: DCOMP Business Meeting (8:00pm-9:00pm) 601
Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F01 DAMOP DQI: Hybrid/Macroscopic Quantum Systems, Optomechanics, and Interfacing AMO with Solid State/Nano Systems I

103 - Anja Metelmann, Princeton University - Tag(s): Focus

8:00AM F01.00001: Sensing and transduction with high-Q micromechanical membranes
[Invited] CINDY REGAL (Presenter), University of Colorado, Boulder —
I will present experiments probing micromechanical motion at quantum limits using SiN membranes. In particular I will discuss work in which we use ultra-high-Q patterned membranes in force sensing and in quantum transduction between microwave and optical signals.

8:36AM F01.00002: Improved optical cavity in microwave-mechanical-optical transducer*
MAXWELL URMEY (Presenter), BENJAMIN M BRUBAKER, SARANG MITTAL, PETER S BURNS, JONATHAN KINDEM, KONRAD LEHNERT, CINDY REGAL, JILA — Linking quantum computational nodes to form a long-distance network in an architecture based on superconducting qubits faces an inherent challenge: the low excitation energy of microwave photons precludes quantum signal propagation at room temperature. A quantum coherent transducer between microwave and optical frequencies would overcome this difficulty. By coupling both a superconducting LC resonator and an optical Fabry-Perot cavity to the same MHz-frequency mode of a SiN membrane micromechanical oscillator, we realize a converter with 47% efficiency \[1\]. The process adds 38 photons of noise which prevent its quantum operation, with a significant contribution associated with the optical pump mediating the optomechanical interaction. By redesigning the optical cavity, we have reduced misalignment-induced optical loss and enabled greater optomechanical coupling, allowing reduced pump powers.


*AFOSR MURI
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AFOSR PECASE
8:48AM F01.00003: Toward on-chip microwave to optical transduction using erbium doped crystals

JAKE ROCHMAN (Presenter), TIAN XIE, JOHN G BARTHOLOMEW, IOANA CRAICIU, JONATHAN KINDEM, KEITH SCHWAB, ANDREI FARAON, Caltech — Future quantum networks based on superconducting circuits that operate at microwave frequencies will strongly benefit from optical interconnects between the distant nodes. One promising platform to achieve bidirectional conversion between microwave and optical photons are ensembles of rare-earth ions (REIs) strongly coupled simultaneously to an optical and a microwave resonator. The strong interactions between the REIs and photons are critical to minimize the optical power required to mediate the conversion process and for potential operation at temperatures below 100 mK. Here, we present our progress towards a REI-based transducer using superconducting microwave resonators and amorphous silicon photonic crystal resonators patterned on the surface of an erbium-doped yttrium orthovanadate crystal. Both resonators are designed to maintain high quality factors while preserving the mode overlap between the optical and microwave fields required for high conversion efficiency. We present initial results characterizing the device performance at cryogenic temperatures.

*Jake Rochman acknowledges support from NSERC. The authors acknowledge support from the ONR Young Investigator Award and ARO/LPS CQTS.

9:00AM F01.00004: Constructing Perfect Quantum Transducers Using Multi-Mode Imperfect Transducers

MENGZHEN ZHANG (Presenter), SHOUMIK CHOWDHURY, Yale University, LIANG JIANG, University of Chicago — Quantum transducers can transfer quantum information between different bosonic physical platforms, which are crucial for hybrid quantum devices and quantum networks. In practice, however, transduction devices are not perfect, as there are systematic deviations and coupling to other bosonic modes. Recently, Lau and Clerk showed that combining finite single-mode squeezing and imperfect transduction operations we can implement desired perfect quantum transduction, but only restricted to two-mode. In this work, we generalize the previous results and show how to transform generic multi-mode imperfect transducers into perfect transducers requiring only finite-squeezing resources, based on a general protocol of decoupling irrelevant bosonic modes from the original system.
9:12AM F01.00005: A compact trampoline-in-the-middle system for acoustic frequency quantum optomechanics
CHRISTIAN PLUCHAR (Presenter), AMAN AGRAWAL, EDWARD SCHENK, DALZIEL WILSON, College of Optical Sciences, University of Arizona — Strained nanomechanical resonators can have extremely low mechanical loss at acoustic frequencies, spurring recent proposals for ultra-sensitive force detection and quantum experiments at room temperature. We present a quasi-monolithic membrane-in-the-middle system that incorporates a 10 ng Si$_3$N$_4$ trampoline resonator with a fundamental frequency of 40 kHz into a 100 um Fabry-Perot cavity with a finesse of 30,000. Prior to cavity assembly, we record a mechanical loss rate of 0.8 mHz (a quality factor of 50 million) for the fundamental trampoline mode, corresponding to a force sensitivity of 30 aN/√Hz and a zero-point displacement spectral density of 0.3 pm/√Hz. Mounting results in significant added loss; however, the large optomechanical cooperativity still reveals itself as Brownian motion exceeding the cavity linewidth by an order of magnitude. We present a technique to “load” the resonator into the cavity by radiation pressure feedback cooling. Eliminating mounting loss would result in a vacuum cooperativity of $10^4$, accessing a regime currently targeted with levitated nanoparticles.

9:24AM F01.00006: Reducing added-noise in a micro-mechanically mediated electro-optic converter
SARANG MITTAL (Presenter), BENJAMIN M BRUBAKER, MAXWELL URMEY, PETER S BURNS, JONATHAN KINDEM, CINDY REGAL, KONRAD LEHNERT, JILA — Bidirectional transduction of microwave and optical fields would be a useful resource in the toolbox of quantum technology. We have demonstrated a mechanically mediated electro-optic converter by coupling a micromechanical oscillator to a microwave circuit and an optical cavity simultaneously. Operating this device at T < 100 mK, we recorded a conversion efficiency of 47% and added noise of 38 photons [1]. While we have realized high efficiency, the added noise is still an order of magnitude too large. Here, we present our efforts to lower the added noise by designing phononic shielding of the mechanics and replacing our superconducting metal with NbTiN.


*AFOSR MURI
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AFOSR PECASE
9:36AM F01.00007: Towards quantum optomechanics using bulk acoustic wave resonators
HUGO DOELEMAN (Presenter), SILVAN VOLLENWEIDER, UWE VON LÜPKE, YIWEN CHU, ETH Zurich — Superconducting circuits are one of the most sophisticated architectures for quantum information processing to date. MW-to-optical conversion in the quantum regime could enhance their scalability and range of applications, since optical photons can be used as noise-free carriers of quantum information that connect circuits in different refrigerators. This requires conversion that is coherent, efficient, and with minimal added noise, which has not been demonstrated yet.

We present our advances in developing a cryogenic cavity optomechanical device based on a bulk-acoustic-wave (BAW) mechanical resonator, which can act as an essential part of a MW-to-optical transducer. Strong coupling to BAWs has been demonstrated both for microwave photons [1] and for optical photons [2]. Building on these works, we are developing an optomechanical system that is also compatible with coupling to superconducting circuits. We report on first experiments of BAW resonators cooled to millikelvin temperatures and coupled to optical cavity modes. As a first proof-of-principle, we discuss prospects for storage and retrieval of low-photon-number coherent optical states in the mechanical resonator.


9:48AM F01.00008: Towards entanglement and interconversion of single mm-wave and optical photons in a hybrid cavity-QED system with Rydberg atoms
AZIZA SULEYMANZADE (Presenter), MARK J STONE, LAVANYA TANEJA, ALEXANDER ANFEROV, JASMINE KALIA, DAVID I SCHUSTER, JONATHAN SIMON, University of Chicago — I will present our most recent progress towards entangling and interconverting single millimeter wave (mm-wave) and optical photons using Rydberg atoms as a transducer. Hybrid systems, which cross-couple optical and microwave regimes, can harness the unique strengths of optical systems for communication and microwave systems for quantum information processing, yielding a more powerful toolset for quantum information technology. The mm-wave band additionally offers access to single photon resolution at 1K, due to low thermal photon occupation at high frequencies. I will present our recent realization of a hybrid cavity with crossed mm-wave and optical modes, enabling smooth integration of cold atoms, laser beams and Rydberg excitations. The high-Q mm-wave cavity has a $Q_{tot} = 3 \times 10^7$ at 98GHz and mode volume of $V = 0.1 \lambda^3$, which allows strong coupling with cooperativity of $h=22000$ between single mm-wave photon and a single Rydberg atom on the 36S $\rightarrow$ 35P transition. I will report our first observations of intra-cavity vacuum Rabi Splitting, Rydberg Electromagnetically Induced Transparency (EIT) and outline our path towards creating strong interactions between single mm-wave and optical photons.
Large electromechanical coupling in inductively coupled electromechanics

PHILIP SCHMIDT, MOHAMMAD AMAWI, STEFAN WEICHSELBAUMER, DANIEL SCHWIENBACHER, STEFAN POGORZALEK, ACHIM MARX, RUDOLF O GROSS, HANS HUEBL (Presenter), Walther Meissner Inst — Light-matter interaction in optomechanical systems is the foundation for ultra-sensitive detection schemes measuring displacements, accelerations, and forces. In addition, this interaction enables the generation of mechanical quantum states and entangled states of photons and phonons. Electromechanical systems implement the field of optomechanics using microwave circuits. Most implementations realize the coupling using a mechanically compliant capacitance, demonstrating a maximum interaction rate of 280 Hz [1]. However, it was realized early on that inductive coupling schemes promise much higher interaction strengths even with the potential to reach the strong vacuum coupling regime. Here, we demonstrate electromechanical coupling based on a partly suspended SQUID combined with a coplanar microwave resonator exceeding a coupling rate of 1 kHz. This coupling enables force sensitivities on a sub-attonewton level using a single-photon ultra-low power readout. We discuss the performance of the concept including the tunability of this coupling with magnetic field.


This project is funded from the European Union’s Horizon 2020 programm (No 736943) and by the German Research Foundation (EXC-2111 – 390814868).

Laser cooling to the zero-point energy of a nanomechanical oscillator

LIU QIU (Presenter), ITAY SHOMRONI, Ecole Polytechnique Federale de Lausanne, PAUL SEIDLER, IBM Research -- Zurich, TOBIAS J. KIPPENBERG, Ecole Polytechnique Federale de Lausanne — Silicon optomechanical crystals enable coupling of photons at telecommunication wavelengths to GHz mechanical modes, giving rise to optomechanical dynamics that can extend well into the resolved-sideband regime. Despite these promising characteristics, high-fidelity ground state preparation has to date only been achieved using passive cooling in a dilution refrigerator. Moreover, heating due to optical absorption has limited measurement protocols to short, low-energy optical pulses. Here, we demonstrate continuous-wave laser sideband cooling of a silicon optomechanical crystal to the zero-point energy, reaching a mean thermal occupancy of $0.09^{+0.02}_{-0.01}$ quanta, or 92\% ground state occupation, self-calibrated via motional sideband asymmetry. Our results overcome previous limitations due to optical absorption heating and highlight optomechanical crystals for quantum-enhanced continuous displacement measurements, low-added-noise quantum transducers, and integration with superconducting qubit technology.

This work is supported by the Swiss National Science Foundation under grant No.~163387 and grant No.~51NF40-160591 (NCCR-QSIT), and the European Union's Horizon 2020 research and innovation programme under grant No.~732894 (FET Proactive HOT).
The possibility to operate mechanical systems close to the quantum regime has become central in both fundamental and applied science. A key parameter here is how strongly photons will impact the mechanics. The microwave regime offers the opportunity to achieve large couplings towards a regime where the coupling rate becomes the dominant time scale. In our ongoing experimental efforts to reach this single-photon strong coupling regime, we developed an approach based on a mechanical oscillator inductively coupled to a superconducting circuit. We place a NdFeB micromagnet on the tip of an AFM cantilever and align it on top of the SQUID of a tunable 3D microstrip resonator. When flux sensitive, the motion of the cantilever will result in a change in resonance frequency of the microstrip resonator, similar to typical cavity optomechanical setups. Varying the external flux allows us to tune the coupling strength from virtually zero to higher values, reaching single photon strong cooperativity, allowing for cooling with a single photon. Improving our current design, we hope to reach single photon strong coupling, allowing the quantum control of massive mechanical resonators.

*Funded by European Union’s Horizon 2020 – FET (No. 736943) and Austrian Science Fund FWF – DK-ALM (W1259-N27).
8:00AM F02.00001: Vortices in Rotating Bose-Einstein Condensate Shells  KARMELA PADAVIC (Presenter), University of Illinois at Urbana-Champaign, KUEI SUN, The University of Texas at Dallas - Richardson, COURTNEY LANNERT, Smith College, University of Massachusetts - Amherst, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign — We present a study of superfluid vortices in rotating shell-shaped Bose-Einstein condensates (BECs). Hollow spherical BECs are of interest in connection to ongoing experimental efforts on the International Space Station and they naturally occur in optical lattice systems of ultracold bosons and interiors of neutron stars. Fundamentally, they have interesting geometry (non-zero curvature) and topology (hollow center). When BECs are rotated, discrete vortices are generated in pairs, as a consequence of the quantum coherence and the closed shape of the system. Using a mean-field approach, numerical solutions of the Gross-Pitaevskii equation and insights from classical fluid dynamics, we find that hollow condensates have a lower energy barrier to emergence of vortices than fully filled BECs. Further, we show that the rotation frequency at which nucleation of vortex lines is energetically favorable increases with BEC shell thickness. At this frequency the first vortex line is generated as straight and extends along the rotation axis. We consider the possibility of bent vortex lines (off-axis vortex pairs of opposite circulations in the two-dimensional shell limit) and determine that they are unstable except at fast rotation.

8:12AM F02.00002: Dynamics of Quantum Gas in Non-Abelian Gauge Field  MEHEDI HASAN (Presenter), CHETAN MADASU, CHANG CHI KWONG, Nanyang Tech Univ, FRÉDÉRIC CHEVY, Laboratoire Kastler Brossel, Ecole Normale Supérieure, DAVID WILKOWSKI, Nanyang Tech Univ — We experimentally realize SU(2)-symmetric artificial gauge field with the tripod laser scheme. First, the non-Abelian nature of the artificial gauge field is revealed by performing loop operations, at different orders, in the parameter space [1]. It was found that the dynamics of internal states leads to a new thermometric scheme that exploits the interferometric-displacement of atoms [1]. Afterwards, the coupling dynamics of internal(i.e., spin)- and external(i.e., momentum)-degrees of freedoms, in a two-dimensional non-Abelian gauge field, is shown to exhibit an asymmetric expansion of the atomic cloud [2]. This spin-orbit-coupled gas breaks the Galilean invariance and modifies the usual reflection-laws, owing to its inherent peculiar dispersion relation. The density distribution of external dynamics markedly carries the signature of the non-Abelian nature of the underlying gauge field.

8:24AM F02.00003: Quantum simulation of Dynamical gauge field for ultra-cold atoms in a cavity*  SANKALPA GHOSH (Presenter), POORNIMA SHAKYA, Indian Inst of Tech-New Delhi — Quantum simulation of synthetic gauge field in ultra-cold atoms provides opportunity to realize the analogues of Landau levels of electrons and Quantum Hall Physics, Hofstadter-Harper Hamiltonian, and topological phases in a much more controlled environment. Where the initial studies were mostly on synthetic gauge fields that do not have dynamics of their own, a number of current studies aimed to create dynamical gauge field for neutral ultra-cold atoms to extend the scope of such analogue quantum simulations for condensed matter and high-energy physics related phenomena. 

In this work, we propose that ultra cold atoms in high finesse ring cavity of suitable geometry to create a non-uniform dynamical gauge field for neutral ultracold atom. The resulting energy spectrum is similar to the energy dispersion for an electron in a similar magnetic modulation that can effectively create one dimensional flow of such ultra-cold atoms. Starting with single atoms dynamics in such synthetically created dynamical non-uniform gauge field we extend this idea to the ultra-cold atomic Bose-Einstein condensates and study the corresponding dynamics.

*UGC Fellowship (PS) and S.G. and BRNS (DAE, Govt. of India) Grant no. 21/07/2015-BRNS/35041(SG) for DAE SRC Outstanding Investigator Award)

8:36AM F02.00004: Superfluidity and Bogoliubov excitations of a striped spin-orbit coupled BEC induced by a weak optical lattice*  GUANQIANG LI (Presenter), XIWANG LUO, JUNPENG HOU, CHUANWEI ZHANG, University of Texas at Dallas — We investigate the ground-state superfluidity and Bogoliubov excitations of a striped spin-orbit coupled Bose-Einstein condensate (BEC) with the momentum-space hopping induced by a weak optical lattice. The ground-state phase diagram and corresponding superfluid fraction are calculated for different system parameters. The Bogoliubov spectrum is studied and an exotic avoided band crossing between roton and Goldstone modes is revealed, which is very different from traditional spin-orbit coupled Bose-Einstein condensate with double-gapless Goldstone modes. We study the quantum depletion, which can be used to characterize the phase transitions.

*NSF,ARO,AFOSR
8:48AM F02.00005: Optical Vortex Braiding in Composite Bessels* ANDREW VOITIV
(Presenter), JASMINE ANDERSEN, MARK SIEMENS, Univ of Denver, MARK T. LUSK, Department of Physics, Colorado School of Mines — We theoretically propose and experimentally demonstrate the braiding of optical vortices in a laser beam with more than 2π rotation by superposing Bessel modes with a plane wave. Laser beams containing a single, centered vortex with integer-valued orbital angular momentum (OAM) have been extensively studied and engineered, but beams with two or more optical vortices have received less attention. Optical vortex braiding refers to the periodic rotation of two or more vortices around the central axis of propagation in a laser beam. Braiding is a topological feature in knot theory, but no physically-realizable scheme for optical vortex braiding beyond a ¼ - rotation has been identified, much less experimentally demonstrated. In this work, we present a theoretical proposition for braiding optical vortices in Bessel beams, along with analytical expressions for the braiding trajectories and braiding period. We accompany this work with the experimental realization of vortex braiding in physical laser beams, using Bessel-Gaussian beams. We show two vortices braiding completely three times, the most observed to our knowledge.

*W. M. Keck Foundation
National Science Foundation

9:00AM F02.00006: Spin Angular Momentum in Acoustic Field Theory LUCAS BURNS
(Presenter), Schmid College of Science and Technology, Chapman University, KONSTANTIN Y BLIOKH, Theoretical Quantum Physics Laboratory, RIKEN Cluster for Pioneering Research, JUSTIN DRESSEL, Institute for Quantum Studies, Chapman University — We construct a Lagrangian representation of acoustic field theory that accounts for the local radiation forces and torques experienced by subwavelength probe particles, analogous to those experienced by Rayleigh particles in optical fields. The traditional acoustic Lagrangian representation with a scalar potential is unable to reproduce these measured effects. By introducing a displacement vector potential, analogous to the electromagnetic vector potential, we derive the appropriate local momentum and spin densities directly as conserved Noether currents. The results agree with those proposed in recent analyses of intrinsic acoustic spin and are consistent with recent experiments.
Bose-Einstein condensation in effective Harper-Hofstadter bands: simulations of synthetic magnetic fields by optical lattice shaking

HAN FU (Presenter), FNU SETIAWAN, LOGAN W CLARK, University of Chicago, ANDREAS GLATZ, Argonne National Lab, KATHRYN LEVIN, University of Chicago — The cold atom field has been focused on generating topological and other exotic phases of quantum matter by, for example, creating strong synthetic magnetic fields. In the present work we use time-dependent Gross-Pitaevskii simulations to investigate the feasibility of these schemes. There are several key questions we numerically address: 1. Can one implement shaking so that a BEC will emerge, consistent with the effective energy minima of Bloch-Floquet bandstructure? 2. How realistic is it to experimentally enter the Harper-Hofstadter regime which involves extreme parameter values (such as for hopping and shaking frequency)? 3. An important attribute of applying these Bloch-Floquet recipes to cold atoms is that there are easily tunable many-body interactions present, which are necessary for equilibration. One can then be concerned that they undermine the single-particle Floquet bandstructure. In this talk we address these issues, and in the process provide advice for experimentalists in implementing these shaking recipes for arriving at a Hofstader BEC. Additionally, in our simulations we investigate what underlies “heating” and how it is affected by the strength of the interactions g.

Inhomogeneous mean-field approach for collective modes at the superfluid-Mott glass transition*

MARTIN PUSCHMANN (Presenter), Missouri Univ of Sci & Tech, JOSE A HOYOS, Universidade de São Paulo, THOMAS VOJTA, Missouri Univ of Sci & Tech — We employ an inhomogeneous mean-field approach plus Gaussian fluctuations to investigate disordered Bose-Hubbard models with particle-hole symmetry in two and three dimensions. Within this framework, the collective excitations, i.e., Goldstone mode and the Higgs (amplitude) mode, are described by two effective, decoupled, disordered single-particle Hamiltonians whose properties are determined by the underlying mean-field solution. Based on multifractal analysis, we investigate the localization properties of each mode separately as a function of energy and the distance from the superfluid-Mott glass transition. Furthermore, we calculate susceptibility functions and compare the results with Monte Carlo simulations and experiments.

*This work was supported by the NSF under Grant Nos. DMR-1506152, DMR-1828489, PHY-1125915 and PHY-1607611 as well as by the São Paulo Research Foundation (FAPESP) under Grant No. 2017/08631-0.
9:36AM F02.00009: Realizing $Z_2$ phases and Majorana Spectroscopy in extended Bose-Hubbard systems  SMITHA VISHVESHWARA (Presenter), University of Illinois at Urbana-Champaign, DAVID MINOT WELD, University of California, Santa Barbara — The connection between transverse XY spin chains and the fermionic Kitaev chain with nearest-neighbor hopping and pairing has been well known for decades, and has lately drawn attention for its rich phase diagram and relevance to realizations of Majorana fermions. Here, we study the novel system comprised of a Bose-Hubbard chain connected to a reservoir that can generate analogous pairing terms for bosons. We describe a cold-atom realization of such a system in a biased zig-zag optical lattice. We show that in certain limits, the Bosonic Kitaev chain maps on to the XY spin chain, resulting in an unusual $Z_2$ phase that has number fluctuation but no off-diagonal long range order associated with boson condensation. Noteworthy features include the possibility of a strongly correlated many-body qubit ground state and the potential for cold-atom measurements of the Kitaev chain energy spectrum, including zero-energy Majorana bound states.

9:48AM F02.00010: Dark states of multilevel fermionic atoms in doubly-filled optical lattices  ASIER PINEIRO ORIOLI (Presenter), ANA MARIA REY, JILA, NIST, University of Colorado — We propose to use fermionic atoms with degenerate ground and excited internal levels ($F_g \rightarrow F_e$), loaded into the motional ground state of an optical lattice with two atoms per lattice site, to realize dark states with no radiative decay. The physical mechanism behind the dark states is an interplay of Pauli blocking and multilevel dipolar interactions. The dark states are independent of lattice geometry, can support an extensive number of excitations and can be coherently prepared using a Raman scheme taking advantage of the quantum Zeno effect. These attributes make them appealing for atomic clocks, quantum memories, and quantum information on decoherence free subspaces.

10:00AM F02.00011: Numerical study of antiferromagnetic nearest-neighbor spin correlations of an SU(6) Fermi gas in an optical lattice*  EDUARDO IBARRA GARCIA PADILLA (Presenter), KADEN HAZZARD, Rice University, RICHARD THEODORE SCALETTAR, UC Davis, HAO-TIAN WEI, Fudan University, SHINTARO TAIE, NAOKI NISHIZAWA, YOSUKE TAKASU, YOSHIHITO KUNO, YOSHIRO TAKAHASHI, Kyoto University — Experimental progress with ultracold alkaline-earth-like atoms allows quantum simulation of novel phenomena and phases of matter. Many interesting SU($N$) phases are characterized by their magnetic correlations. Recently, the experiment at Kyoto has detected nearest-neighbor antiferromagnetic (AFM) spin-correlations in an SU(6)$^{173}$Yb Fermi gas loaded in 1D, 2D and 3D optical lattices. Such systems are effectively described by the SU($N$) Fermi Hubbard Model. We have developed and applied the Exact Diagonalization and Determinant Quantum Monte Carlo methods to solve such model in all of the relevant geometries. With these tools we calculate the density, double occupancy, entropy and magnetic correlations in a trapped gas under the local density approximation. We compare the calculated and measured nearest-neighbor AFM correlations, and we find they agree quantitatively. In 2D and 3D the experiments reach lower temperatures than is possible to accurately compute with theory, but in 1D, the temperature estimated from theory comparison is $k_B T/t = 0.08(2)$, being the lowest temperature ever reported for a Fermi gas in an optical lattice.

*RTS was supported by the Department of Energy, grant DE-SC0014671.
10:12AM F02.00012: Dynamics of an almost lattice gauge theory realized by an ultracold atom system  
DANIEL GONZALEZ CUADRA (Presenter), VALENTIN KASPER, ALEXANDRE DAUPHIN, ICFO, PHILIPP HAUKE, University of Trento, FRED JENDRZEJSKI, University of Heidelberg, MACiej LEWENSTEIN, ICFO — Recently carried out experiments with ultracold atoms have realized the first building blocks to simulate lattice gauge theories quantum. Despite the great progress, the influence of experimental imperfections on the phase structure or the non-equilibrium dynamics is unclear. In this thesis we study the effect of terms violating the local gauge invariance as they occur in a typical experimental setup. In particular, we focus on ultracold atom setups which exploit angular momentum conservation in order to realize local gauge invariance. We also study the influence of dissipation in these systems and compare the dynamics of a theory with exact and almost lattice gauge theory. Especially we determine the time scales and observables when the difference between the two theories becomes significant.

10:24AM F02.00013: $Z_2$ Lattice Gauge System and Dynamical Localization  
ZHIYUAN YAO (Presenter), CHANG LIU, PENGFEI ZHANG, HUI ZHAI, Tsinghua University — Gauge theory has been playing a fundamental role in our understanding of the deepest mysteries of physics. And recent advances in cold atom physics have also made the study of dynamical gauge systems a new frontier. Using Floquet approach, we propose to realize a one-dimensional $Z_2$ lattice gauge model, featuring extensive local constants of motions, using two specifies of Rb atoms. The resulting Floquet Hamiltonian turns out to be quite simple. Within a given symmetry sector of good quantum numbers, the system can be viewed as a 1D transverse quantum Ising model with a binary random longitudinal field. Therefore, the dynamics of the system is essentially controlled by disordered Hamiltonians, implying that the system can feature many body localization (MBL) as a result of dynamical localization. Numerical studies of energy level statistics and quench dynamics clearly demonstrate the existence of MBL phase in this system.

F02.00014: Unusual superfluid behavior of population imbalanced atomic Fermi gases in a two-dimensional optical lattice*  
LIN SUN (Presenter), Zhejiang university, QIJIN CHEN, University of Science and Technology of China — We study the superfluid behavior of population imbalanced ultracold atomic Fermi gases with a short range attractive interaction in a two-dimensional optical lattice (2DOL), using a pairing fluctuation theory, within the context of BCS-BEC crossover. We find that population imbalance now has highly unusual effects on the behavior of pairing and superfluidity, caused by the continuum-lattice mixing in 2DOL. We find that, in the presence of a finite population imbalance (p>0), the pair density at $T_c$ unexpectedly approaches zero towards to deep BEC regime and thus the transition $T_c$ is dramatically enhanced in the BEC regime and becomes proportional to the interaction strength $U$ in the BEC limit. This should be contrasted to the balanced case, for which $T_c$ decreases as $1/U$. And the system is an intermediate-temperature polarized superfluid state at unitarity and in the BCS regime. We perform stability analysis, and present complete phase diagrams along with the behavior of superfluid density. We show that a stable polarized superfluid emerges at relatively high temperature.

*Supported by NSF of China (Grant No. 11774309)

Tuesday, March 3, 2020 8:00 AM - 10:24 AM
Knowledge of the equation of state and chemical kinetics of materials under reactive conditions is needed for a wide number of research areas, including studies of planetary interiors, astrobiology, and high-pressure detonations of energetic materials. In this regard, we have developed a family of atomistic simulation models which yield similar accuracy to higher order quantum approaches (Kohn-Sham DFT) while yielding orders of magnitude increase in computational efficiency. This talk will focus on three different types of models in development in our research group: (1) semi-empirical quantum simulation approaches, (2) reactive force fields for molecular dynamics simulations, and (3) spin lattice models for solid phase reactivity. These efforts will be discussed in the context of corrosion on actinide and other metal surfaces, shock compression of organics and energetic materials, and prebiotic synthesis in impacting astrophysical ices. Our methods provide a straightforward way to conduct computationally efficient and highly accurate simulations over a broad range of conditions, where physical and chemical properties can be difficult to interrogate directly and there is historically a significant reliance on theoretical approaches for interpretation and validation of experimental results. Prepared by LLNL under Contract DE-AC52-07NA27344

Reactive molecular dynamics (MD) simulations can describe the complex physical and chemical processes in high energy density materials and ultimately contribute to a predictive understanding of their shock initiation under dynamical loading. However, computational intensity limits MD to the nanoscale, making it difficult to simulate hot spot formation and eventual shock to detonation transition. Thus, we developed a multiscale model that uses MD simulations to inform a continuum model capable of reaching the microstructural scales. We use dimensionality reduction via unsupervised learning to establish a two-step reduced-order chemistry model for the decomposition of RDX. From both homogeneous isothermal and adiabatic simulations, we extract chemical kinetics and heat of reaction parameters. The continuum model, capable of capturing chemistry, thermal transport and mechanics, is verified using homogeneous cook-off simulations and the multiscale approach validated from hot spot calculations. We find good agreement between the predicted critical temperatures from explicit MD simulations and the continuum model for nanoscale hot spots. Finally, we predict critical hot spot temperature as a function of size and quantify the effect of uncertainties for various materials’ parameters.
8:48AM F03.00003: Ultrafast Detonation of Hydrazoic Acid: Insights from Many-body Molecular Dynamics Force Fields*  HUY PHAM (Presenter), NIR GOLDMAN, LAURENCE FRIED, Lawrence Livermore Natl Lab — In this work, we present the development and application of the Chebyshev Interaction Model for Efficient Simulations (ChIMES) to the study of hydrazoic acid (HN₃) under detonation. Computational study of HN₃ is challenging due to its ultrafast detonation, i.e. the chemical decomposition to stable products is complete in less than 10 ps, and the system evolves through multiple thermodynamics (ambient and extreme conditions) and electronic (metal and insulator) states. We show that ChIMES, a generalized many-body reactive force field machine-learned to density functional theory (DFT) molecular dynamics trajectories, is able to retain the accuracy of DFT simulation in describing structural properties and chemistry for a wide range of thermodynamics states while increasing orders of magnitude in computational efficiency. Shock compression simulations show that the developed ChIMES model can capture the ultrafast chemical reactions of HN₃.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

9:00AM F03.00004: Reaction rates in shocked nitromethane from density functional tight binding simulations*  ROMAIN PERRIOT (Presenter), MARC CAWKWELL, ENRIQUE MARTINEZ SAEZ, EDWARD KOBER, SHAWN DAVID MCGRANE, Los Alamos National Laboratory — The chemistry of energetic materials (EM) is characterized by rapid exothermic reactions that lead to dramatic increase of the pressure and temperature on the pico- to nanosecond timescales. Under these conditions, experiments have struggled to provide detailed insights into early and intermediate processes, and simulations have thus become a valuable tool to help interpret experiments and parameterize mesoscale models. We have performed molecular dynamics (MD) cook-off simulations of nitromethane under pressure with DFTB, a parameterized form of DFT that allows to simulate systems with hundreds of atoms, over hundreds of picoseconds, with explicit treatment of the electronic interactions and an accuracy close to that of DFT. We find drastically different times-to-explosion, even for the same initial T/P conditions, due to multiple complex and competitive chemical pathways. However, a simple effective reaction rate can be extracted, as long as multiple simulations are performed at each T/P to account for the stochastic component of detonation chemistry in EM. We built a two-step model for NM detonation that can be compared to experimental results and used in higher scale models.

*LANL LDRD
9:12AM F03.00005: UQ-Driven Reactive Burn and EOS Parameterization, along with Particle Force Model Assessment for the Simulation of an Explosive Multiphase Experiment
JOSHUA GARNO (Presenter), SANGJUNE BAE, FREDERICK OUELLET, THOMAS L JACKSON, NAM-HO KIM, RAPHAEL HAFTKA, S BALACHANDAR, University of Florida — Recent results indicate that the Maxey-Riley-Gatignol (MRG) model is able to predict the force on a particle due to a passing air-shock and compressed flow. This work aims to assess the model’s predictive capability in the high-energy, post-detonation flow regime. Due to the tight coupling between the gas flow and particle motion, the evaluation of the particle force model necessitates high accuracy in the prediction of the gas flow. Therefore, modeling the detonation and rapid expansion of post-detonation product gases requires accurate models of reactive burn and the equation of state (EOS) for products of detonation. Using flow information extracted from experimental high-speed photographs as validation data, we make use of UQ methodologies to optimize the explosive-specific model parameters of the JWL EOS. With quantitative flow agreement between experiments and our finite-volume point-particle simulations, the MRG force model governing the motion of the particles is examined. Experimental X-ray data provides the trajectories of a few Tungsten particles for comparison with simulation results.

9:24AM F03.00006: Probing Intermediate Formation of Thin Film Explosives Through Ultrafast Broadband Infrared Spectroscopy
MICHAEL POWELL (Presenter), Purdue University/LANL, PAMELA BOWLAN, Los Alamos National Laboratory, STEVEN F. SON, Purdue University, CYNTHIA BOLME, KATHRYN E BROWN, DAVID STEVEN MOORE, MARC CAWKWELL, Los Alamos National Laboratory, ALEJANDRO H STRACHAN, Purdue University, SHAWN DAVID MCGRANE, Los Alamos National Laboratory — A first step to predicting explosive performance and safety is to understand the chemical pathways taken when high explosive materials are shocked. Unfortunately, there is insufficient data at relevant time and length scales to directly compare experiments to molecular level models. The intention of this work is to link experimental results to molecular dynamics models using ultrafast broadband mid-infrared and visible absorption spectroscopy to probe the chemical changes energetic materials undergo when shocked. PETN, a common HE, was shocked to the reactive regime and showed increased absorption near the anti-symmetric NO$_2$ stretch but not the symmetric NO$_2$ stretch. This change was attributed to absorbance from intermediate formation. These results were compared to molecular dynamics and accelerated chemistry models to interpret the shock chemistry. Comparing to gas phase calculations of the infrared absorption intensities, the intermediate was most likely HONO indicating H-ion and NO$_2$ elimination play an important role in early shock chemistry for PETN.
9:36AM F03.00007: Amorphous Explosives*  RAJEN PATEL (Presenter), VICTOR STEPANOV, Explosives Research Branch, US Army, CCDC-AC — Glassy amorphous organic energetics is a new field offering several novel areas for study. While practical application might be limited due to low density and propensity to crystallization of amorphous energetics, the scientific opportunities are fertile. For example, they allow an in depth view of crystallization in real time, even of novel systems such as cocryystals, and the in situ characterization of pores, cracks and other gross defects as they form. Amorphous energetic formulations with relatively low excipient (i.e. polymer used to inhibit crystallization) loadings offer a novel method of examining materials at extreme conditions. They can compared to their crystalline counterparts, and this could shed light on the processes of crystallization, shock induced phase transformations, and mechanically induced chemical reactions. While practical application will be limited for amorphous materials due to their low density, the scientific possibilities are quite exciting.

*This work is funded by a combination of OSD/US Army funds.

9:48AM F03.00008: Mechanical Stimulation of Gasless Reaction in Inorganic Systems: Overview*  ALEXANDER MUKASYAN (Presenter), University of Notre Dame — The phenomenon of a reaction, occurring in inorganic high energy density systems after it is stimulated by a shock wave, has been under investigation for a long time. The first experimental studies on the topic of chemical transformations in the inorganic substance under shock compression dated back to the late 1950s and a lot of work has been accomplished since. In this overview, we primarily consider reactive heterogeneous media that involves a powder mixture of the inorganic solid precursors, which, after mechanical stimulation, resulted in the synthesis of a new material. It is no doubt that such reactions can be initiated by sufficient mechanical impulse, but can they occur in the time scale of the high-pressure shock state? What mechanisms may be responsible for such rapid solid-state transformations? These and related questions are discussed based on the recent experimental findings.

*This work was supported by the Department of Energy, National Nuclear Security Administration, under the award number DE-NA0002377 as part of the Predictive Science Academic Alliance Program II.
10:00AM F03.00009: Dance of HMX molecule in conformational space by quasi-static heating: a combined Raman spectroscopy and theoretical study*  
YANGYANG ZENG  
(Presenter), National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China Academy of Engineering Physics, CHAN GAO, Department of Physics, University of Science and Technology of China, GUOYANG YU, National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China Academy of Engineering Physics, RUCHENG DAI, ZHONGPING WANG, The Centre for Physical Experiments, University of Science and Technology of China, ZENGMING ZHANG, Key Laboratory of Strongly-Coupled Quantum Matter Physics, Chinese Academy of Sciences, School of Physical Sciences, University of Science and Technology of China, XIANXU ZHENG, YANQIANG YANG, National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China Academy of Engineering Physics — The complexity of HMX polymorphs arises from conformers and molecular packing. In this study, HMX single crystal is heated at rates of 0.1 or 0.2 K/min during phase transitions. The sample is equilibrated at least 15 minutes at every step of increasing temperature to achieve the quasi-static condition. Raman spectroscopy is performed to monitor transitions between conformers by fitting position and full width at half maximum of the observed spectra. Conformers, transition states and IRC are verified at the level of DLPNO-CCSD(T)/cc-pVQZ//M062X-D3(0)/def2-TZVP for single HMX molecule. We attribute the response of spectra to ring puckering and nitro vibrations during phase transitions by analyzing Raman spectra and decomposition and identification of vibrational modes. Our results provide evidence of B-α and subsequent α-δ phase transition, which agree with recent thermodynamic model that α-HMX must be thermodynamically stable in phase diagram.

*This work was financially supported by the Science Challenge Project (Grant TZ2016001)

10:12AM F03.00010: DETONATION PROPERTIES OF PRESSED AND LIQUID HYDRAZINE NITRATE*  
ALEXANDER UTKIN (Presenter), VALENTINA MOCHALOVA, Institute of Problems of Chemical Physics RAS — In this work, the structure of the steady-state detonation waves, the critical diameter, detonation parameters and the dependence of detonation velocity on the charge diameter for pressed hydrazine nitrate (HN) and the HN/water solution were investigated by a VISAR laser interferometer. For pressed HN, it was found that the critical diameter drops with the initial density decrease. For pressed HN, the change of the detonation velocity with variation of the initial density is not monotonic, but has a characteristic s-shape. For the water solution of HN, the detonation velocity decreases linearly with increasing concentration of water. The limits of detonation propagation were found for HN/water solution. It doesn’t detonate at a water concentration exceeding 33 wt % at room temperature. Experiments on the determination of Hugoniot and initiation of detonation under shock wave action for pressed HN were carried out with samples of maximum density (1.68 g/cc). The results of the conducted experiments show the low shock wave sensitivity, which is much lower than that of TNT. A noticeable reaction rate behind the front of the initiating shock wave in charges of maximum density is observed only at a pressure above 20 GPa.

*This work was supported by the program of Presidium of RAS No 56.

Tuesday, March 3, 2020 8:00 AM - 10:48 AM
8:00AM F04.00001: Investigating graphene oxide-aqueous interfaces* [Invited] REVATI KUMAR (Presenter), ROLF DAVID, VISAL K. SUBASINGHEGE DON, Chemistry, Louisiana State University — Graphene oxides (GO) are nanosheets of graphene with oxygen bearing defects. The GO sheet is highly heterogeneous with the sp$^3$ carbons, connected to oxygen bearing functional groups, interspersed between the usual sp$^2$ carbons of graphene resulting in competition between aromatic regions and highly hydrophilic domains (from the oxygen containing functional groups, typically -OH and epoxy groups) at the GO-aqueous interface. GO materials are increasingly gaining traction for ion and molecule separations. The interfacial region between the GO material and aqueous solutions plays a key role in these applications. Our efforts are focused on gaining molecular level insight into the interfacial ordering using molecular simulations. Classical and Born-Oppenheimer molecular dynamics were performed to study the interfacial water structure, including hydrogen bonding environments, using different order parameters. The simulations were used to gain insight into the results from recent vibrational sum frequency generation experiments. The reactivity of the graphene oxide-neat water interface as well as in the presence of an acidic excess proton were also investigated. The results of this study will be presented and discussed.

*This work was funded by the National Science Foundation, Award #1845795

8:36AM F04.00002: Viscoelasticity and dynamics of nanoconfined water by atomic force microscopy* PETER HOFFMANN (Presenter), EDWARD KRAMKOWSKI, Wayne State Univ, SHAH H KHAN, Physics, University of Peshawar — Our group has conducted extensive measurements of the viscoelastic properties of nanoconfined water in hydrophilic environments using a specialized high-resolution dynamic atomic force microscopy technique. Here we will present an overview of our findings, including the observation of dynamic solidification, the effect of ions on ordering and dynamics, and the recent observation of the compression rate dependence of the effective viscosity.

*We acknowledge generous funding from NSF DMR-0804283 and Wayne State University.
8:48AM F04.00003: Hydrogen bonding structure of confined water templated by a metal-organic framework with open metal sites*  KELLY HUNTER (Presenter), University of California, San Diego, ADAM J. RIETH, MIRCEA DINCA, Massachusetts Institute of Technology, FRANCESCO PAESANI, University of California, San Diego — While the properties of bulk water are difficult to understand, water in confinement is even more poorly understood. Metal-organic frameworks (MOFs) are unique a class of materials that display high adsorption properties. Recently, the MOF Co$_2$Cl$_2$BTDD has been shown to adsorb water at low relative humidity, attracting interest for applications in harvesting water from air. Here, we investigate structural and dynamical properties of water adsorbed in Co$_2$Cl$_2$BTDD as a function of relative humidity using many-body molecular dynamics simulations with the MB-pol model. Comparisons of the experimental and theoretical infrared spectra allow us to elucidate the mechanism of pore filling, with water initially binding to the open metal sites and forming one-dimensional chains along the interior of the framework. These chains nucleate pore filling, establishing a three-dimensional hydrogen-bond network. As the pore fills, the spectroscopic features and orientational dynamics indicate a gradual transition from “ice-like” to “liquid-like” properties modulated by the heterogeneous confinement, with individual water molecules exhibiting distinct behavior depending on their specific location inside the pores. Nat. Commun. 2019, 10, 1-7.

*Department of Energy grant no. DE-SC0019333

9:00AM F04.00004: Vibrational dynamics and quantum tunneling of water molecules in bassanite*  ALEXANDER KOLESNIKOV (Presenter), LAWRENCE {LARRY} M. ANOVITZ, STEPHAN IRLE, Oak Ridge National Lab — Using inelastic neutron scattering (INS) we studied dynamics of bassanite (CaSO$_4$*0.5H$_2$O), a structure of which has channels formed by CaO$_8$ and CaO$_9$ polyhedra with water molecules residing in the channels and occupying two different positions. The INS spectra showed that at low temperature ($T=5$ K) intramolecular O-H stretching modes of water are at high energy, around 445 meV (compared to 410 meV in ice-Ih), and the intermolecular librational band is at low energies, 35-90 meV (65-125 meV in ice-Ih), indicating weak hydrogen bonds acting on water molecules. At lower energies we observed a peak at about 1 meV, which shows the behaviour of tunneling mode: its intensity decreases with temperature increase and shows nonmagnetic momentum transfer dependence. In the talk we will discuss the observed INS results and attempt to explain the tunneling of water molecule, which was not observed before in other INS experiments involved confined water molecules in the presence of hydrogen bonds.

*This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.
Carbon nanopores underpin a large array of materials systems and technological applications, including supercapacitors and water desalination. In these devices, understanding of the ion solvation and dynamics is essential for predicting and optimizing the performance; however, many mechanistic details remain enigmatic. Here, we employ first-principles simulations to unravel key features of the solvation structure of several common ions confined within graphene slit pores and carbon nanotubes (CNTs). We find that polarizable ions exhibit a stronger adsorption at the interfaces and these effects are found to be significantly enhanced under confinement. In addition, we find that confinement significantly influences ion selectivity and transport, i.e., ions with a small radius are found to yield a notably larger energy barrier to reach the pore entrance. Our study points to the complex interplay between confinement and specific ion effects, which has broad implications in optimizing nanopores for ion selectivity and energy storage.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344. Financial support is from CENT, an EFRC funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019112.
9:24AM F04.00006: One atom thick angstrom-scale capillaries: Water flow* [Invited] RADHA BOYA (Presenter), Univ of Manchester — It has been an ultimate but seemingly distant goal of nanofluidics to controllably fabricate capillaries with dimensions approaching the size of small ions and water molecules. But surface roughness makes it challenging to produce capillaries with precisely controlled dimensions. We have developed a method for fabrication of narrow and smooth angstrom (Å) scale capillaries through van der Waals assembly of 2D-materials, with atomically flat sheets at the top and bottom separated by spacers made of 2D-crystals with a precisely controlled number of layers. These capillaries can be envisaged as if individual atomic planes are removed from a bulk layered crystal leaving behind flat voids of a chosen height. Water transport through the channels, ranging in height from one to several dozen atomic planes, is characterized by unexpectedly fast flow (up to 1 metre per second) that we attribute to high capillary pressures of about 1000 bar and large slip lengths [1]. For channels that accommodate only a few layers of water, the flow exhibits a marked enhancement that we associate with an increased structural order. In this talk, I will also discuss about how ions reconfigure their hydration shell, becoming essentially “squashed” while flowing through these capillaries[2]. Water and ionic flows are coupled in such confinement, and the transport, driven by pressure and applied electric field, reveals a transistor-like electrohydrodynamic effect [3]. I will conclude the talk by showing our recent results where only one layer of water is confined in these channels, essentially leading to two-dimensional water [4]. Our results lay the basis for exploration of such Å-size channels in nanofluidics, molecular separation and other nanotechnologies.


*EPSRC UK, Royal Society Fellowship, ERC

10:00AM F04.00007: Nano-confined water and ions in cement pores ABHAY GOYAL (Presenter), Georgetown University, IVAN PALAIA, University Paris-Sud, KATERINA IOANNIDOU, University of Montpellier, EMMANUEL TRIZAC, University Paris-Sud, ROLAND JM PELLENQ, Massachussets Institute of Technology, EMANUELA DEL GADO, Georgetown University — We use numerical simulations to study the behavior of water confined by planar surfaces in the presence of divalent ions. The dynamics and mobility of the water are found to be strongly dependent on confinement. At large surface separations, most of the water behaves like in bulk conditions, but in high confinement the dynamics slow down and become coupled to the ions. This in turn increases the ion ordering and thus the overall attraction between two charged surfaces when the confinement is high. From these observations, we develop an analytical prediction of the attractive strength based on the formation of correlated ion-water structures. These results reveal a new mechanism for strong electrostatic cohesion of charged particles due to the restructuring of confined water. This effect is very relevant for the case of cement, where it explains the incredible strength of the material and could be the basis for intelligent design of cements.
**Microscopic study of proton kinetic energy anomaly for confined water**

MOHAMMAD MOID (Presenter), Indian Institute of Science - Dept of Physics, YACOV FINKESTEIN, Nuclear Research Center-Negev, Beer-Sheva, RAYMOND MOREH, Department of Physics, Ben-Gurion University of the Negev, Beer-Sheva, PRABAL K MAITI, Indian Institute of Science - Dept of Physics — Several anomalies, related to structural and dynamical transition, have been reported for water at different thermodynamic conditions and environments. Of particular interest, the reported anomalies of the proton mean kinetic energy, $K_{e}(H)$, in nanoconfined water, as measured by deep inelastic neutron scattering (DINS), are a longstanding problem related to proton dynamics in hydrogen-bonded systems. We used classical MD method to deduce $K_{e}(H)$ by calculating the proton vibrational density of states, $H$-VDOS, for the case of water inside single wall carbon nanotubes (SWCNT) of varying diameters. The mean vibrational density of states (VDOS) of protons in water nanoconfined inside single wall carbon nanotubes (SWCNTs) is calculated as a function of temperature and SWCNT diameter, $D_{CNT}$. The calculated VDOS are utilized for deducing the mean kinetic energy of the water protons, $K_{e}(H)$, by treating each phonon state as a quantum harmonic oscillator. The calculation depicts a strong confinement effect as reflected in the drop of the value of $K_{e}(H)$ at 5K for $D_{CNT} < \sim 12\text{Å}$, while absent for larger diameters. The results also reveal a very significant blue and red shifts of the stretching and bending modes respectively compared to those in bulk ice, in agreement with experiment.

*CSIR,IISc

**Water dynamics in Evaporating Nanodroplets**

LUIS RUIZ PESTANA (Presenter), Civil, Architectural, and Environmental Engineering, University of Miami, TERESA HEAD-GORDON, Chemistry, University of California, Berkeley — The evaporation of droplets on heated substrates has been intensively studied in the last several decades. As such, well validated continuum theories have been developed that describe the modes of evaporation, evaporating profiles, and also predict the internal convective flows compatible with the evaporating modes. The evaporation of small nanoscale droplets plays a key role in a myriad of scientific and technological applications from atmospheric chemistry to the cooling of nanoelectronics to catalysis, where evaporating nanodroplets produced by electro spray ionization are increasingly being used to accelerate chemical reactions. At the nanoscale, however, where large surface to volume ratios govern the behavior, and fluctuations play a major role, it remains unclear whether the continuum theories can be applied to predict the the response. Here, we put that to the test and use classical molecular dynamics simulations of water nanodroplets of two different sizes both suspended under isothermal evaporation conditions and on heated substrates with different levels of hydrophobicity. We focus on mapping the convective flows that develop within water nanodroplets and the resulting evaporating profiles, with the aim of assessing the predictive power of the continuum theories.
A molecular view of glycerol-water hydrogen bonding patterns

CAMERON MACKIE, University of California, Berkeley, BO XU, OLEG KOSTKO, Lawrence Berkeley National Laboratory, NIKHIL CHARI, EMILY ZHANG, MARTIN P HEAD-GORDON, University of California, Berkeley, MUSAHID AHMED (Presenter), Lawrence Berkeley National Laboratory — Photoionization dynamics of micro-hydrated molecules in the gas phase when combined with theory can reveal information on the solution phase. Synchrotron based molecular beam mass spectrometry of water-glycerol clusters in the gas phase and terahertz time domain spectroscopy in solution coupled to calculations reveal the nature of hydrogen bonding in glycerol water solutions and provides a general picture of the interaction of polyols with water. A novel hydrogen bonding pattern is theoretically observed at specific glycerol to water concentrations. A significant shortening (and strengthening) of hydrogen bond lengths (~1.6 Å) are observed between H$_2$O molecules where one of the H$_2$O molecules is held in a “tweezed” fashion by the two hydroxyl groups of glycerol. This hydrogen bond shortening is also observed to reach beyond the first hydration shell. Experimental results show a clear preference for certain clusters to retain two water molecules due to the enhanced hydrogen bonding strengths. This shortening of hydrogen bonds is also proposed to explain the experimentally observed decrease of excess molar volumes with concentrations for various polyols.

*DOE-BES-GPCP- DE-AC02-05CH1123

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F05 DCP DCMP DPOLY: The Chemical Physics of Molecular Polaritons III. Vibrational Strong Coupling 111 - Wei Xiong, University of California, San Diego - Tag(s): Focus
8:00AM F05.00001: Dynamics of Vibration-Cavity Polaritons* [Invited] JEFFREY OWRUTSKY (Presenter), ANDREA GRAFTON, ADAM DUNKELBERGER, BLAKE SIMPKINS, United States Naval Research Laboratory — Coupling vibrational modes to optical cavities results in vibration-cavity polaritons which can modify vibrational coherence and energy dynamics. Ultrafast infrared spectroscopy has been used to investigate vibration-cavity polaritons. We recently reported time resolved IR pump-probe studies on strongly-coupled vibration-cavity polaritons for tungsten hexacarbonyl (W(CO)$_6$) in hexane in a Fabry-Pérot cavity [1]. The results demonstrated that while much of the response is due to so-called reservoir or uncoupled excited state absorption as well as polariton contraction, a component of the observed signals is due to polariton state evolution. We observe saturable absorption as nearly complete polariton contraction not only in pump probe measurements but also in single pulse studies.[2] 2DIR spectroscopy was used to provide evidence of hybrid light-matter polariton evolution and clear indications of direct excitation of dark states.[3] We have further expanded the investigation of vibrational dynamics for strongly coupled vibration-cavity polaritons to W(CO)$_6$ in other solvents and to nitroprusside (Fe(CN)$_5$NO$_2$) in methanol. We explore salient features of the transient response, especially at short delay times, which show aspects of the response that are due to polaritons and are distinguished from uncoupled higher order excitations.


*This work was supported by the ONR through the NRL. ABG acknowledges a fellowship administered by the NAS.

8:36AM F05.00002: Kinetic effects of vibrational polaritons in electron transfer.* JORGE CAMPOS GONZALEZ ANGULO (Presenter), RAPHAEL RIBEIRO, JOEL YUEN-ZHOU, University of California, San Diego — Chemical kinetics has been modified for thermally activated reactions with molecules under vibrational strong light-matter coupling (VSC). These experiments are counterintuitive since VSC can only be achieved when a collectivity of vibrational modes ($N \approx 10^{10}$) simultaneously couples to a single confined electromagnetic mode, and, as a result, the normal modes consist of two polaritonic modes and $N - 1$ dark modes that behave as uncoupled vibrations. In this work, we show how VSC can induce catalysis in electron transfer, as described by the Marcus-Levich-Jortner formalism, by providing low activation energy channels that dominate the kinetics even when they are largely outnumbered by channels with unmodified activation energy.

*UC-MEXUS-CONACYT graduate scholarship ref. 235273/472318
AFOSR award FA9550-18-1-0289
8:48AM F05.00003: Molecular dipole moment drives the dynamics of vibrational polaritons in the strong and ultrastrong coupling regimes  JOHAN TRIANA GALVIS (Presenter), FEDERICO J. HERNÁNDEZ, FELIPE HERRERA, Univ de Santiago de Chile — Molecular polaritonics is a growing research topic both theoretically and experimentally. However, the underlying microscopic mechanisms for the modification of chemical reactions observed in experiments has yet to be fully understood. To improve our theoretical understanding, models such as the Holstein-Tavis-Cummings or the multi-level quantum Rabi model have been proposed to describe light-matter interaction between quantized fields and molecular transitions. In the strong coupling regime, effects induced by the light-matter coupling may have implications in the modification of chemical reactions, which demands an analysis beyond the RWA. We study the dynamics of anharmonic vibrational polaritons for polar (e.g. R-CO) and non-polar (e.g. CO$_2$) molecules at equilibrium. We show that the electric dipole function strongly determines the dynamics of vibrational polaritons, and we describe such dependence in detail. Our results hint to a possible mechanism for cavity catalysis of chemical reactions under vibrational strong coupling and the spectroscopy of vibrational polaritons in liquid phase. In addition, our analysis could serve as a benchmark for future developments in the study of polariton chemistry in high-dimensional nuclear configuration spaces and multi-mode cavities.

9:00AM F05.00004: Strong Coupling of Terahertz Fields to Collective Intermolecular Vibrations*  RAN DAMARI, OMRI WEINBERG, DANIEL KROTKOV, NATALIA DEMINA, KATHERINE AKULOV, ADINA GOLOMBEK, SHARLY FLEISCHER, TAL SCHWARTZ (Presenter), Physical Chemistry, Tel Aviv University — Several years ago, strong coupling of intra-molecular vibrations to mid-infrared resonators was introduced as a new paradigm in the field of polariton chemistry [1]. Such vibrational strong coupling allows the manipulation of molecular processes occurring at the electronic ground-state, by targeting a specific bond within the molecules [2]. Here, we demonstrate for the first time strong coupling of collective vibrations in organic molecule crystallites, occurring at THz frequencies. In our experiments, we performed THz time-domain spectroscopy on a metallic cavity filled with α-lactose crystallites, which exhibit a sharp absorption peak at 0.53 THz. We observed a Rabi-splitting of ~70 GHz, and directly probe the Rabi-oscillations in the coupled system. Our results take strong coupling and polariton chemistry into a new class of material, including polymers, proteins and other organic materials, in which collective, spatially extended degrees of freedom participate in the dynamics.


*This research was supported by Wolfson Family Charitable Trust, Israel Science Foundation and the Ministry of Science and Technology, Israel.
9:12AM F05.00005: Polariton-mediated vibrational ladder climbing  RAPHAEL RIBEIRO
(Presenter), JOEL YUEN-ZHOU, University of California, San Diego — Vibrational ladder climbing (VLC) happens when a dipole-active molecular vibration is promoted to a highly excited-state by undergoing multiphoton absorption. Applications of this phenomenon include chemical reaction control via optical generation of non-equilibrium molecular excited-state populations with an increased probability of undergoing bond-breaking events. In this work, we present a theoretical treatment of VLC under strong infrared coupling, where the collective vibrational polarization efficiently exchanges energy reversibly with the electromagnetic field of an optical microcavity and hybrid light-matter excitations (polaritons) emerge. We focus on the basic principles of polariton-mediated VLC, including how its efficiency can be modulated by a proper choice of mesoscopic material, and conclude by discussing potential applications to reaction dynamics control, and spectroscopy of highly-excited states.

9:24AM F05.00006: Exploring Vibrational Polariton Dynamics with Ultrafast Two-Dimensional Infrared Spectroscopy* [Invited]  RONG DUAN, VIVIAN CRUM, KEVIN KUBARYCH
(Presenter), Univ of Michigan - Ann Arbor — Vibrational strong coupling (VSC) offers a new approach to manipulate reaction thermodynamics, vibrational energy flow, and intermolecular interactions. The complex energy relaxation, transfer, and dephasing processes in vibrational polaritons are ideally suited for study by ultrafast infrared spectroscopy, particularly two-dimensional infrared (2D-IR), which has become a major tool to unravel vibrational dynamics in general. This talk will introduce and review the key principles and molecular observables central to 2D-IR, while demonstrating its application to a vibrational polariton system. For our first implementations of VSC we have chosen a tripodal transition metal carbonyl complex, methyl cycopentadienyl manganese tricarbonyl (MeCMT), which has two strong CO stretching bands near 2000 cm$^{-1}$ separated by roughly 80 cm$^{-1}$. Using a cavity with a free spectral range that closely matches this energy splitting, we establish strong coupling between the molecule and two adjacent cavity modes. The 2D-IR spectra show significant coupling between the two branches of polaritons, as well as extensive coherences and signatures for coherence transfer.

*This work was supported by the National Science Foundation (CHE-1836529)
**10:00AM F05.00007: Controling quantum pathways in the vibrational polaritons system**

ZIMO YANG (Presenter), WEI XIONG, BO XIONG, University of California, San Diego — Molecular vibrational polaritons are hybrid quasi-particles between molecular vibrations and photons, through strong coherent light-matter coupling. It has attracted many attentions, because of its potential to alter photonic properties and also change the course of chemical reactions. Molecular vibrational polaritons have been studied by 2D infrared (2D IR) spectroscopy, which has advanced our understanding of the roles of dark states, hot excited state energy relaxation, and manipulation of nonlinear interactions in cavities. However, the coherent nature of polaritons imposes many quantum pathways contributing to the 2D IR signal, which complicates its interpretation and precision manipulation of quantum states. Using mid-IR pulse shaper, we report a way to selectively excite quantum pathways, to directly measure polariton nonlinear responses involving either coherence or population states. Because vibrational polariton forms a two-level system, it can serve a toy model to study the importance of coherence in energy transportation in energy materials. Thus, this work lays the foundation to prepare arbitrary quantum states in polaritons, for further exploration of the phenomena of nonlinear photonics, chemistry and quantum phenomena.

*This work is supported by NSF DMR-1848215*

**10:12AM F05.00008: Remote of chemistry in optical cavities**

MATTHEW DU (Presenter), RAPHAEL RIBEIRO, JOEL YUEN-ZHOU, University of California, San Diego — Quantum states in different molecules can be hybridized by strong light-matter interaction. This phenomenon has been previously harnessed to realize long-range energy transfer between organic chromophores separated by optical length scales. Here, we propose a remote control of chemistry whereby photoexcitation of molecules in one optical microcavity influences the photochemical reactivity of molecules in another microcavity. For the infrared-induced \textit{cis}-to-\textit{trans} conformational isomerization of nitrous acid (HONO), we show that the proposed strategy leads to enhancement of the reaction efficiency by an order of magnitude.
10:24AM F05.00009: Cavity-Modified Chemical Reaction Kinetics and Electrochemical Modulation of Coupling Strength  BLAKE SIMPKINS (Presenter), United States Naval Research Laboratory, WONMI AHN, Excet, ADAM DUNKELBERGER, ANDREA GRAFTON, United States Naval Research Laboratory, JEREMY PIETRON, Lawrence Livermore National Laboratory, KENAN FEARS, JEFFREY OWRUTSKY, United States Naval Research Laboratory — Quantum emitters strongly coupled to optical cavities exchange energy inextricably, creating new hybrid polaritons. Recently, this half-light half-matter quasi-state has been demonstrated with molecular vibrations coherently coupled to optical modes. In this talk, we discuss (1) cavity-modified chemical reactivity and (2) modulation of the strong coupling phenomenon via electrochemical reaction. Specifically, we monitor transmission of a Fabry-Pérot microcavity filled with reactive species. Both reactants and products have strong molecular vibrations that couple to the optical cavity modes. We compare reaction rates in and out of the cavity to expose the influence of vibrational strong coupling on reaction kinetics. Secondly, we evaluate electrochemical switching of cavity coupling magnitude in both the visible and infrared regimes. Our results demonstrate full modulation of the Rabi splitting, a diffusion-limited redox process, and imaging of molecular adsorption/desorption processes on the metal surface. These results have important implications for chemical synthesis and catalysis.

10:36AM F05.00010: Ultrastrong coupling in hexagonal Boron Nitride microcavities*  UNAI MUNIAIN (Presenter), DIPC, MARIA BARRA-BURILLO, nanoGUNE, RUBEN ESTEBAN, DIPC and Ikerbasque, SARA CATALANO, MARTA AUTORE, nanoGUNE, LUIS HUESO, RAINER HILLENBRAND, nanoGUNE and Ikerbasque, JAVIER AIZPURUA, Centro de Física de Materiales-MPC (CSIC-UPV/EHU) — When the interaction between light and matter is very efficient, it is possible to attain the regime of ultrastrong coupling (USC), where a variety of quantum effects of considerable interest can be revealed [1]. In this contribution, we study an infrared Fabry-Perót microcavity formed by metallic mirrors, filled with hexagonal Boron Nitride (hBN) acting as a phononic material [2]. The optical response obtained within a transfer-matrix approximation can be interpreted with the use of a semi-classical model of coupled harmonic oscillators. As a consequence of the large Reststrahlen band of hBN, the Rabi splitting obtained is of the order of the frequencies of the bare cavity and the phonons. The system is thus in the USC regime. We also show that the calculations are in excellent agreement with experimental measurements, which suggests the interest of this configuration as a practical setup to explore USC.


*GV project PI2017-30
Resonant Rayleigh Scattering from Collective Molecular Excitations

MUKUNDAKUMAR BALASUBRAHMANIYAM (Presenter), ADINA GOLOMBEK, MARIA KAEEK, KEREN HADAR, TAL SCHWARTZ, Physical Chemistry Department, Tel Aviv University — Resonant Rayleigh scattering (RRS) is the pronounced elastic scattering of photons present at the vicinity of the natural resonances of sub-wavelength physical objects such as molecules, which otherwise scatter negligibly. Here, we study RRS from molecular ensembles strongly coupled to an optical microcavity. Under these conditions, the coherent interaction between the molecules and the cavity mode produces collective molecular states known as cavity polaritons and which can drastically modify the properties of these molecules. Our spectroscopic measurements reveal that strong RRS occurs at the polaritonic energies, reaching ~25% efficiency. Interestingly, this resonant scattering corresponds to the collective scattering of each photon from a macroscopically-large ensemble of molecules, rather than the scattering by individual ones, as in the usual case. We show that the scattering from the polaritonic states exhibit non-trivial behaviors, specifically a linear dependence of the scattering strength on their photonic component. We believe that these observations, together with further investigation, may lead to a deeper understanding of these delocalized, collective molecular excitations, their non-equilibrium transport and the role of disorder in their dynamics.

Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F06 GMED FIAP DAMOP DSOFT: Optics in Soft Matter and Medicine 113 - Joshua Dijksman, Wageningen University - Tag(s): Focus, Undergrad Friendly

Novel biomedical applications of lasers: dermatology, gynecology, and stomatology [Invited] MATJAZ LUKAC (Presenter), Complex Matter, Institute Jozef Stefan, MATIJA MILANIC, Faculty of Mathematics and Physics, University of Ljubljana, MATIJA JEZERSEK, Faculty of Mechanics, University of Ljubljana — Water is an important constituent of all soft and hard human tissues. For this reason, the Er:YAG laser is of a particular interest for tissue ablation since its wavelength coincides with the major absorption peak of the water molecule. By controlling the temporal structure of Er:YAG pulses it is possible to control the laser-tissue interaction from “cold” to coagulative ablation, thus optimizing the laser either for skin resurfacing or for precise and painless cutting of teeth. The high absorption of the Er:YAG in irrigation fluids has been utilized also for photo-acoustically induced cleaning and disinfection of dental root canals. On the other hand, the wavelength of the Nd:YAG laser lies in the skin’s optical window and is thus suitable for transcutaneous delivery of laser energy deep into the adipose tissue. This characteristic has been explored for a novel “fat reduction” procedure offering a less invasive alternative to surgical liposuction. Recently, it was discovered that the extremely short absorption depth of the Er:YAG laser in soft tissues can be utilized also to create extremely short and intense heat shock pulses within the superficial tissue layer without causing irreversible thermal damage or ablation of the tissue. The discovery has led to the development of novel minimally invasive methods in various medical areas, including for treating vaginal atrophy, urinary incontinence or snoring, thus in many cases replacing much more aggressive and risky standard surgical procedures.
8:36AM F06.00002: Understanding coronary plaque biomechanical properties with intravascular imaging* [Invited] BRET BOUMA (Presenter), Massachusetts Institute of Technology
MIT — The biomechanical properties of coronary artery atherosclerosis are vital in understanding acute myocardial infarction and the factors that contribute to plaque instability. Intravascular cross-sectional imaging, with a resolution approaching that of histopathology and with high speed to avoid motion artifacts that arise from the dynamic cardiac cycle, can provide a basis for mechanical modeling and analysis to identify the primary compositional and structural factors in lesion vulnerability. We have recently developed a novel approach for real-time modeling that can be used during procedures in the cardiac catheterization laboratory.

*This research was funded by the National Institutes of Health, Grants P41EB-015903 and R01HL-119065.

9:12AM F06.00003: Optical properties of silicone rubber tissue phantoms for biomedical optics applications* MATIJA MILANIC (Presenter), Univ of Ljubljana, JURE NOVAK, Dia-vit, PETER NAGLIČ, YEVHEN ZELINSKYI, LUKA ROGELJ, Univ of Ljubljana, BORUT KUMPERŠČAK, Dia-vit, JOST STERGAR, MIRAN BÜRMMEN, Univ of Ljubljana — In medical physics, tissue phantoms play important role in characterization, validation, calibration and optimization of medical devices. A useful phantom must be well characterized, namely its physical properties must be accurately measured using standard techniques.

A set of silicon rubber tissue phantoms was prepared for applications in biomedical optics. A black pigment served as an absorber and hollow silica micro-spheres as scatterers. Nine samples with different absorber and scatterer concentrations were prepared. Refractive indices of the samples were measured in the 430 – 660 nm spectral range and did not vary significantly (<0.02 %). Optical properties (absorption and scattering coefficients, and similarity parameter γ) were estimated using spatially resolved reflectance spectroscopy in the subdiffusive regime (400 - 1000 nm). The determined optical properties covered the range characteristic for biological tissues.

Silicon rubber tissue phantoms feature many advantageous properties in comparison to other common phantoms in biomedical optics (e.g., intralipid, agar). They are stable, solid, reproducible, and their optical properties can be adjusted according to the application demands. Therefore, they are promising tools for biomedical optics.

*ARRS: P1-0389, J2-8171.
9:24AM F06.00004: Laser induced jets in needle free drug delivery*  
FNU PANKAJ (Presenter), JEREMY O MARSTON, Texas Tech Univ — Various actuation mechanisms have been used in the past for needle-free injection systems, predominantly springs and compressed gas. However, recent innovation has seen use of pulsed and continuous wave lasers for precise injection of ultra-low doses. Here, we have investigated the feasibility of laser-induced micro-jets as a needle-free injection technique. Effect of various parameters such as capillary diameter, laser pulse energy and distance of the laser focal point on jet dynamics were studied in the past, however, we also varied the fluid viscosity and orifice stand-off relative to the target. To quantify the penetration dynamics and dispersion of the liquid delivered, both gelatin gel (in-vitro) and porcine tissue (ex-vivo) were used as skin models. Lastly, we also discuss the possibility of using a spark-cavitation system to generate high-speed micro-jets instead of pulsed lasers.

*NSF-CBET, Inovio Pharmaceuticals

9:36AM F06.00005: Fourier Transform Laser Speckle Imaging for art conservation  
JESSE BUIJS (Presenter), JASPER VAN DER GUCHT, JORIS SPRAKEL, Wageningen University — Laser speckle imaging is a powerful imaging technique that visualizes microscopic motion within turbid materials. At current two methods are widely used to analyze speckle data: one is fast but qualitative, the other quantitative but computationally expensive. We have developed a new processing algorithm based on the fast Fourier transform, which converts raw speckle patterns into maps of microscopic motion and is both fast and quantitative, providing a dynamic spectrum of the material over a frequency range spanning several decades. In this article we show how to apply this algorithm and how to measure a diffusion coefficient with it. We harness the potential of this new approach by constructing a portable laser speckle imaging setup that performs quantitative data processing in real-time on a tablet. We will show one of many possible applications of this method in the form of monitoring the cleanig process of artistic oil paintings.

9:48AM F06.00006: Doppler Functional Imaging of Cancer Drug Sensitivity in Living Tumor Biopsies  
ZHE LI (Presenter), Department of Physics and Astronomy, Purdue University, SHADIA I. JALAL, Department of Medicine, IU School of Medicine, JOHN TUREK, Department of Basic Medical Sciences, Purdue University, DAVID D NOLTE, Department of Physics and Astronomy, Purdue University — Biodynamic imaging is a deep-tissue digital holography imaging technique that captures the response of living tissue to applied therapeutics. Biodynamic metrics can predict patient clinical response with high accuracy. However, evaluating drug responses on a sample basis has high variance because of the underlying sample heterogeneity related to tissue features. We introduce a technique called tissue dynamics spectroscopic imaging (TDSI) to reveal drug response variations within small cubic millimeter biopsy samples. By performing tissue dynamics spectroscopy on a voxel basis and extracting biodynamic biomarkers, functional images are obtained of the heterogeneous spatial response of tumor tissue to anticancer drugs. Spatial maps of biodynamic biomarkers are created using a bivariate colormap to represent the spatial distribution of pairs of signed biomarkers. Time-lapse response maps provide further details into drug mechanisms.
**10:00AM F06.00007: Probing the interior dynamics of shear thickening colloidal suspensions using confocal line scans**  
JOIA MILLER (Presenter), DANIEL BLAIR, JEFFREY S URBACH, Georgetown University — Under high stresses, shear thickening suspensions transition from low viscosity to high viscosity or shear jammed states. While both the bulk rheology and the microscopic driving forces of such transitions are well-studied, the bridge between the microscopic and macroscopic scales is incomplete. Measurements at the boundaries indicate that dynamic high stress regions propagate through shear thickening suspensions of colloidal spheres, but the means of propagation within the suspension interior was inaccessible due to imaging limitations. Here we use line scans on a confocal microscope to visualize particle flows in a sheared suspension, increasing our temporal resolution by two orders of magnitude. These line scans reveal that high stress regions are correlated with significant changes in particle speed, density, and order that extend many particle diameters deep into the suspension.

*NSF Award DMR-1809890

**10:12AM F06.00008: Nanoscale Optical Imaging of Soft Matter Under Flow**  
ANISHA SHAKYA (Presenter), SEONG JUN PARK, JOHN KING, Center for Soft and Living Matter, Institute for Basic Science — Far-field fluorescence microscopy provides an enticing platform for spatially resolving equilibrium and nonequilibrium dynamics of soft matter systems, ranging from thin films to polymer solutions. However, several long-standing challenges, including limited spatial resolution and poor image contrast in densely labeled systems, have limited its application to such systems. Here, we develop a novel adaptation of super-resolution microscopy based on stimulated emission depletion (STED) coupled with fluorescence anisotropy detection to image concentration profiles of high molecular weight polyelectrolytes in semi-dilute solutions. We use this technique to study depletion layer formation and dynamics under Poiseuille flow, which remains an outstanding problem in fluid mechanics. While the inherently short length scales associated with depletion layer dynamics have traditionally prohibited direct imaging, STED-anisotropy imaging provides sufficient spatial resolution and contrast to measure small changes in polymer concentration over 10s of nanometers.

*Korean Institute for Basic Science, Project Code IBS-R020-D1.*
10:24AM F06.00009: Analyzing the Flow Drying Colloidal Suspensions Using Optical Coherence Tomography  LANFANG LI (Presenter), Physics Department and Emulsion Polymers Institute, Lehigh Univ, YONGYANG HUANG, Electrical&Computer Engineering, Lehigh Univ, ZHIYU JIANG, Physics, Lehigh Univ, CHAO ZHOU, Biomedical Engineering, Washington University in Saint Louis, HDANIEL OU-YANG, Physics Department and Emulsion Polymers Institute, Lehigh Univ — In this work, we present the visualization and analysis of flow in drying colloidal suspensions composed of colloidal polymer particles in water. The flow induced particle transport and deposition can influence the final structure of the polymer film deposited. Employing time-lapse, high-speed imaging, Optical Coherence Tomography was used to monitor the dynamic process of drying colloidal droplets. With the aid of high refractive index tracer particles, fluid flows were captured. The speckle contrast analysis differentiates the dynamics of particles, showing the packing process and particle transporting to the edge of droplet. In low particle concentration suspension, this resembles the coffee ring phenomenon. In high concentrations of particles, a situation in practical coatings or ink-jet applications, the viscosity plays an important role in the material flow and deposition, resulting in different flow pattern and final dry film structures, such as cracks, shear bands, and skin formation.

10:36AM F06.00010: Hyperspectral imaging as a technique to evaluate peritonitis in mouse models*  JOST STERGAR (Presenter), ROK DOLENEC, Univ of Ljubljana, KATJA LAKOTA, NEZA BREZOVEC, UMC Ljubljana, MARTINA PERSE, NIKA KOJC, Univ of Ljubljana, MATIJA TOMSIC, UMC Ljubljana, MATIJA MILANIC, Univ of Ljubljana — Hyperspectral imaging (HSI) is an optical technique that combines imaging and spectroscopy. Images can be processed spectroscopically, extracting information about tissue biochemistry and morphology that can be of importance to physicians. Peritonitis is an inflammation of the peritoneal cavity that can result in death. In animal model studies of the disease, golden standard is histology, while biomolecular techniques can also be used. These techniques only provide either good spatial resolution or area coverage. A technique with large area coverage and resolution is thus desired.

We present a classification method for determination of the state of peritonitis using HSI. The technique provides both good spatial resolution and coverage of the whole organ. Spectra are acquired in reflection geometry and processed using a custom model of light transport in thin samples. Tissue parameters including oxygenation and scattering properties are extracted from the images and used to assess disease state. Per subject scores are used to successfully separate control from model groups. HSI obtained scores are also compared with existing techniques (histology, PCR and Western blot) showing good concordance, meaning that HSI can be a useful tool for disease evaluation.

*ARRS P1-0389 and J2-8171

Tuesday, March 3, 2020 8:00 AM - 11:00 AM
**8:00AM F07.00001: Variational Quantum Fidelity Estimation**

MARCO CEREZO DE LA ROCA (Presenter), Los Alamos National Laboratory, ALEXANDER POREMBA, Computing and Mathematical Sciences, California Institute of Technology, LUKASZ CINCIO, PATRICK COLES, Los Alamos National Laboratory — We present an efficient, near-term algorithm for estimating the well-known fidelity, which quantifies the closeness of quantum states. Our algorithm is an important tool for verifying and characterizing states on a quantum computer. This work is timely given the industrial rise of quantum computing. Prior to our work, there was no efficient algorithm to estimate the fidelity that could be refined to arbitrary tightness. We solve this outstanding problem by introducing novel bounds on the fidelity that can be estimated with hybrid quantum-classical computation. We show that our approach can detect quantum phase transitions and cannot be classical simulated efficiently.

*This work was supported by the Center for Nonlinear Studies at Los Alamos National Laboratory (LANL) and by the LDRD program at LANL.

**8:12AM F07.00002: Variational Quantum Algorithm for Markovian Open Quantum Systems**

NOBUYUKI YOSHIOKA, University of Tokyo, YUYA O. NAKAGAWA (Presenter), QunaSys Inc., KOSUKE MITARAI, KEISUKE FUJII, Osaka University — We propose a quantum-classical hybrid variational algorithm to simulate the non-equilibrium stationary states of Markovian open quantum systems, named the dissipative-system Variational Quantum Eigensolver (dVQE) [1]. In order to employ the variational optimization technique for a unitary quantum circuit, we first map a density matrix into a wavefunction with the doubled number of qubits, and then design the unitary quantum circuit so that the physical requirements for a mixed state are fulfilled. This allows us to define a cost function that consists of the time evolution generator of the Markovian quantum master equation. After the optimization, physical observables are evaluated by a quantum circuit with the original number of qubits. Our dVQE scheme is demonstrated by both numerical simulation on a classical computer and actual quantum simulation that makes use of the device provided in Rigetti Quantum Cloud Service.


**KAKENHI Grant Numbers JP17J00743 (N. Y.), JP19J10978 (K. M.), and JP16H02211 (K. F.). K. F. is supported by JST PRESTO JPMJPR1668, JST ERATO JPMJER1601, and JST CREST JPMJCR1673, MEXT Q-LEAP JPMXS01180673. Y. O. N. is supported by MEXT Q-LEAP JPMXS0118068682.**
**8:24AM F07.00003: Variational Generation of Thermofield Double States and Critical Ground States with a Quantum Computer**

ANNE MATSUURA (Presenter), SONIKA JOHRI, Intel Corp - Santa Clara, DAIWEI ZHU, NORBERT M LINKE, KEVIN LANDSMAN, NHUNG NGUYEN, CINTHIA ALDERETE, University of Maryland, TIMOTHY HSIEH, Perimeter Institute, CHRISTOPHER ROY MONROE, University of Maryland — Finite-temperature phases of many-body quantum systems are fundamental to phenomena ranging from condensed-matter physics to cosmology, yet they are generally difficult to simulate. Using an ion trap quantum computer and protocols motivated by the Quantum Approximate Optimization Algorithm (QAOA), we generate nontrivial thermal quantum states of the transverse-field Ising model (TFIM) by preparing thermofield double states at a variety of temperatures. We also prepare the critical state of the TFIM at zero temperature using quantum-classical hybrid optimization. The entanglement structure of thermofield double and critical states plays a key role in the study of black holes, and our work simulates such nontrivial structures on a quantum computer. Moreover, we find that the variational quantum circuits exhibit noise thresholds above which the lowest depth QAOA circuits provide the best results.

*ARO through the IARPA LogiQ program, AFOSR MURIs on Quantum Measurement/Verification and Quantum Interactive Protocols, ARO MURI on Modular Quantum Circuits, DoE BES QIS Program, DOE HEP QuantISED Program, DoE ASCR Quantum Testbed program, NSF Physics Frontier Center at JQI, Industry Canada, the Province of Ontario through the Ministry of Research and Innovation, Intel Corporation.*

**8:36AM F07.00004: Exactly-solvable models as benchmarks for VQE**

KEN ROBBINS (Presenter), PETER LOVE, Tufts Univ — Perhaps the most promising application of Noisy Intermediate Scale Quantum (NISQ) computers is the Variational Quantum Eigensolver (VQE). Due to their namesake noise, NISQ computers performing VQE will need benchmarks to interpret their results. Exactly solvable models such as the Lipkin-Meshkov-Glick (LMG) model, a simple nuclear model of N fermions, can provide such benchmarks. We give circuits that produce low-N LMG eigenstates on a quantum computer with gate and qubit costs suited to the NISQ era. Further, we discuss how we might generalize the circuits for simulations of a higher number of particles.

*This project is supported in part by the Department of Energy under grant number DE-SC0019665.*
Variational Quantum Linear Solver: A Hybrid Algorithm for Linear Systems  
CARLOS BRAVO-PRIETO (Presenter), Barcelona Supercomputing Center, RYAN M LAROSE, Michigan State University, MARCO CEREZO, YIGIT SUBASI, LUKASZ CINCIO, PATRICK COLES, Los Alamos National Laboratory — Solving linear systems of equations is central to many engineering and scientific fields. Several quantum algorithms have been proposed for linear systems, where the goal is to prepare $|x\rangle$ such that $A|x\rangle \propto |b\rangle$. While these algorithms are promising, the time horizon for their implementation is long due to the required quantum circuit depth. In this work, we propose a variational hybrid quantum-classical algorithm for solving linear systems, with the aim of reducing the circuit depth and doing much of the computation classically. We propose a cost function based on the overlap between $|b\rangle$ and $A|x\rangle$, and we derive an operational meaning for this cost in terms of the solution precision. We also introduce a quantum circuit to estimate this cost, while showing that this cost cannot be efficiently estimated classically. Using Rigetti’s quantum computer, we successfully implement our algorithm up to a problem size of $32 \times 32$. Furthermore, we numerically find that the complexity of our algorithm scales efficiently in both $1/\kappa$ and $\kappa$, with $\kappa$ the condition number of $A$. Our algorithm provides a heuristic for quantum linear systems that could make this application more near term.

Variational Preparation of Quantum Hall States on a Lattice*  
ERIC JONES (Presenter), ELIOT KAPIT, Colorado Sch of Mines — Simulation of many-body quantum systems is one of the most promising applications of near-term quantum computers. The fractional quantum Hall states display fascinating many-body physics such as topological order and strong correlations and so are interesting candidates for quantum simulation experiments. We classically diagonalize for the low-energy spectrum of the Kapit-Mueller Hamiltonian for hardcore bosons on a lattice. The Laughlin state is an exact ground state of this long-range Hamiltonian for appropriate magnetic flux densities. In addition, we study the low-lying spectrum of a shorter-range proxy Hamiltonian and tune its hopping and interaction parameters in order to optimize the associated topological degeneracy and many-body gap. We then demonstrate a scheme for variational preparation of the Laughlin state on the lattice through a Trotterization of adiabatic state preparation with defect-pinned particles as the reference state. Such calculations suggest a way forward in the simulation of fractional quantum Hall states on quantum hardware.

*The authors would like to acknowledge funding from NSF grant PHY-1653820, Google Inc., and the National Renewable Energy Laboratory.
9:12AM F07.00007: Variational quantum simulation of the Fermi-Hubbard model*
ALEXANDRE CHOQUETTE (Presenter), AGUSTIN DI PAOLO, Universite de Sherbrooke, PANAGIOTIS BARKOUTSOS, IBM Research Zürich, DAVID SENECHAL, Universite de Sherbrooke, IVANO TAVERNELLI, IBM Research Zürich, ALEXANDRE BLAIS, Universite de Sherbrooke — Noisy intermediate-scale quantum devices have the potential to be useful for quantum simulation of materials. A prominent approach for near-term quantum simulation is based on variational quantum algorithms (VQAs). In this talk, we propose a VQA to prepare the groundstate of the Fermi-Hubbard model. In particular, we investigate various state-preparation circuits and benchmark their performance in presence of realistic noise. We find that Hamiltonian-inspired variational forms perform better than a hardware-efficient approach. This work constitutes a first step towards the simulation of strongly correlated fermionic systems.

*This work was undertaken thanks in part to funding from NSERC, FRQNT and the Canada First Research Excellence Fund.

9:24AM F07.00008: A Non-Orthogonal Variational Quantum Eigensolver*
WILLIAM HUGGINS (Presenter), Chemistry, University of California, Berkeley, JOONHO LEE, Chemistry, Columbia University, UNPIL BAEK, Physics, University of California, Berkeley, BRYAN O’GORMAN, Electrical Engineering and Computer Sciences, University of California, Berkeley, BIRGITTA K WHALEY, Chemistry, University of California, Berkeley — We present an extension to the variational quantum eigensolver that approximates the ground state of a system by solving a generalized eigenvalue problem in a subspace spanned by a collection of parametrized quantum states. This allows for systematic improvement of a logical wavefunction ansatz without significant increase in circuit complexity. To minimize the circuit complexity, we propose a strategy for efficiently measuring the Hamiltonian and overlap matrix elements between states parametrized by circuits that commute with the total particle number operator. We propose a classical Monte Carlo scheme to estimate the uncertainty in the ground state energy caused by a finite number of measurements of matrix elements and to adaptively schedule the required measurements. We apply these ideas to two strongly correlated systems, a square configuration of H$_4$ and the π-system of Hexatriene (C$_6$H$_8$).

*This work was supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Quantum Algorithm Teams Program, and a Quantum Algorithms Focused Award from Google LLC B.O. was supported by a NASA Space Technology Research Fellowship.
Variational quantum-classical algorithms (VQCAs) optimize the parameters of a quantum neural network, $V$, to minimize a cost function, $C$. Many researchers believe that VQCAs will enable the first practical applications of noisy quantum computers. However, VQCAs are heuristic methods with unproven scaling. Here, we rigorously prove two results related to the trainability of VQCAs. Our first result states that choosing $C$ to be a global function of $V$ leads to an exponentially vanishing gradient (i.e., a barren plateau) even when $V$ is shallow. This implies that many VQCAs proposed in the literature must revise their proposed cost functions. Our second results states that, under the same conditions, choosing $C$ to be a local function of $V$ leads to a non-vanishing gradient, i.e., with the gradient vanishing no worse than polynomially. This suggests that VQCAs have the potential to be trainable, if one chooses an appropriate cost function. We support these analytical results with numerics for large problem sizes.

We acknowledge funding from the Los Alamos National Laboratory (LANL) Laboratory Directed Research and Development (LDRD) program, and from the LANL Center for Nonlinear Studies (CNLS).

Scaling up variational quantum eigensolver (VQE) algorithms to practical applications utilizing quantum advantage with noisy intermediate-scale quantum (NISQ) devices is challenging. The expansive cost-function evaluation and demanding optimization quickly exhaust the precious quantum resource available on NISQ devices. In this work, we discuss the appropriate VQE strategy suitable for multi-site interacting boson systems, for example, the Holstein model and the Rabi lattice model. We investigate the cost-function setup and the optimization tactics to utilize the limited quantum resource efficiently. Our strategy illustrates that the scalable VQE algorithms of interacting bosons have a promising future.

This work has been authored by Fermi Research Alliance, LLC under Contract No. DE-AC02-07CH11359 with the U.S. Department of Energy, Office of Science, Office of High Energy Physics.
10:00AM F07.00011: Efficient Variational Generation of Thermofield Double States on a Superconducting Quantum Processor: Theory (Part 1)  SHAVIDRRA PREMARATNE (Presenter), SONIKA JOHRI, XING CHRIE ZOU, Intel Labs, Intel Corporation, RAMIRO SAGASTIZBAL, MICHEL ADRIAAN ROL, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, BEREND KLAVER, MIGUEL MOREIRA, CARMINA ALMUDEVER, QuTech, Delft University of Technology, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, ANNE MATSUURA, Intel Labs, Intel Corporation — Thermofield double (TFD) states are entangled pure states between two systems which yield a thermal state when one of the systems is traced out [1]. TFD state generation on larger qubit systems is relevant for studying the finite-temperature phase diagram of condensed matter systems. We implement a quantum-classical hybrid variational optimization algorithm to efficiently generate TFD states of the tranverse-field Ising chain. Unlike Variational Quantum Eigensolvers with a cost function that is known a priori, the success of our optimization hinges on choosing the best cost function which can generate the desired TFD state. Here, we discuss the benefits and drawbacks of various cost functions that can be used for the optimization, and show how our constructed cost function yields excellent agreement across the full temperature range.


10:12AM F07.00012: Efficient Variational Generation of Thermofield Double States on a Superconducting Quantum Processor: Experiment (Part 2)  RAMIRO SAGASTIZBAL (Presenter), MICHEL ADRIAAN ROL, BEREND KLAVER, MIGUEL MOREIRA, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, SHAVIDRRA PREMARATNE, SONIKA JOHRI, XING CHRIE ZOU, Intel Labs, Intel Corporation, CARMINA ALMUDEVER, QuTech, Delft University of Technology, ANNE MATSUURA, Intel Labs, Intel Corporation, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Recent progress on Near Intermediate Small Quantum devices has allowed the field of quantum simulation to experimentally investigate many interesting systems such as spin lattices, Fermi-Hubbard models and electronic orbitals of molecules. Most of this work focuses on preparing low-energy eigenstates of a known target Hamiltonian. Here, we experimentally investigate finite-temperature effects on a transverse-field Ising chain using four qubits of a seven-transmon quantum processor. Specifically, we variationally approximate thermofield double (TFD) states through minimization of the constructed cost function described in Part 1. We extract various correlation functions over a range of simulated temperatures, showing good agreement to those of an exact TFD.

*This research is funded by an ERC Synergy Grant, Intel Corporation, and IARPA (U.S. Army Research Office grant W911NF-16-1-0071).
Efficient Symmetry-Preserving State Preparation Circuits for the Variational Quantum Eigensolver Algorithm

LINGHUA ZHU (Presenter), BRYAN T. GARD, GEORGE S. BARRON, Department of Physics, Virginia Tech, NICHOLAS J. MAYHALL, Department of Chemistry, Virginia Tech, SOPHIA E. ECONOMOU, EDWIN BARNES, Department of Physics, Virginia Tech

The variational quantum eigensolver (VQE) is one of the most promising approaches for performing chemistry simulations using noisy intermediate-scale quantum (NISQ) processors. The efficiency of this algorithm depends crucially on the ability to prepare multi-qubit trial states on the quantum processor that either include, or at least closely approximate, the actual energy eigenstates of the problem being simulated while avoiding states that have little overlap with them. Symmetries play a central role in determining the best trial states. Here, we present efficient state preparation circuits that respect particle number, total spin, spin projection, and time-reversal symmetries. These circuits contain the minimal number of variational parameters needed to fully span the appropriate symmetry subspace dictated by the chemistry problem while avoiding all irrelevant sectors of Hilbert space. We show how to construct these circuits for arbitrary numbers of orbitals, electrons, and spin quantum numbers, and we provide explicit decompositions and gate counts in terms of standard gate sets in each case.

Noncontextuality as classicality in variational quantum eigensolvers

WILLIAM KIRBY (Presenter), PETER LOVE, Tufts University

In this talk we show how to use contextuality, an indicator of non-classicality in quantum systems, to evaluate the variational quantum eigensolver (VQE), a promising tool for near-term quantum simulation. We present an efficiently computable test to determine whether or not the Hamiltonian in a VQE procedure is contextual. We then show that we may construct a simple, global unitary mapping that diagonalizes a noncontextual Hamiltonian. The diagonal Hamiltonian resulting from this mapping is efficiently classically calculable, which proves that the noncontextual Hamiltonian problem is NP-complete. We also give a quasi-quantized model for variational quantum eigensolvers whose Hamiltonians are noncontextual. This provides a second sense in which noncontextual Hamiltonians are essentially classical. These results support the notion of noncontextuality as classicality in quantum systems.

WMK acknowledges support from the National Science Foundation, grant numbers DGE-1842474 and PHY-1818914. PJL acknowledges support from the National Science Foundation, grant numbers PHY-1720395 and PHY-1818914, and from Google Inc.
Variational hybrid quantum-classical algorithms (VHQCAs) seem likely to be the first useful algorithms in the era of near-term quantum computing. There is however a justified concern that the number of measurements needed for these algorithms to converge might become prohibitive when scaling up to non-trivial problem sizes. We address this issue by adapting results from classical optimization to the problem of shot-frugal optimization of VHQCAs. Specifically, we present new techniques and compare them with standard methods to demonstrate the potential for improvement both with noiseless and noisy quantum devices.

*This work was supported by the U.S. Department of Energy (DOE) through a quantum computing program sponsored by the Los Alamos National Laboratory (LANL) Information Science & Technology Institute, the LDRD program at LANL, and the LANL ASC Beyond Moore's Law project. This work was also supported by the U.S. DOE, Office of Science, Office of Advanced Scientific Computing Research, under the Quantum Computing Application Teams program.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F08 DQI: Control and Modelling of Open Quantum Systems 104 - Sophia Economou

Experimental simulation of a two-level open system based on Trotter decomposition

Quantum simulation is one of the promising applications on a fully controlled quantum system. Such tasks can be solved with either high dimensional ancillary systems or deep feedback control network. We demonstrate a hardware-efficient repetitive Trotter scheme of open system simulation, which allows efficient simulation of arbitrary noisy environments for a two-level system. The scheme only requires an ancillary superconducting qubit, and real-time feedback control is not necessary. We verify that our implementation can be further strengthened in two ways: higher-order Trotter operation sequencing and error mitigation, which are straight forward with the controllability of our system. Our results show the feasibility to perform quantum simulation tasks on small systems and with restricted experimental resources.
**8:12AM F08.00002: Arbitrary quantum channel simulations of a superconducting qudit system**
WEIZHOU CAI (Presenter), JIA XIU HAN, LING HU, YU WEI MA, YUAN XU, XIANGHAO MU, YIPU SONG, Center for Quantum Information, Institute for Interdisciplinary Information Sciences, Tsinghua University, CHANG-LING ZOU, Key Laboratory of Quantum Information, CAS, University of Science and Technology of China, LUYAN SUN, Center for Quantum Information, Institute for Interdisciplinary Information Sciences, Tsinghua University — Unitary operations of closed quantum systems have been well studied. However, practical quantum systems are open and their evolution is described by quantum channels. So exploring arbitrary quantum channel simulation with minimum resources is of great importance for both fundamental understandings of open systems and mitigating of quantum noise. In this talk, we will introduce our recent experimental efforts on arbitrary quantum channel simulations of a high dimensional photonic qudit (cavity), with the assistance of a transmon qubit. First, continuous evolutions of an open quantum system are simulated by digitally and repetitively implementing Lindblad operators. Two interesting channels, odd parity stabilization channel and two-photon dissipation channel, have been demonstrated with this method. Then, the quantum channel that directly maps the input to output is simulated based on adaptive control. By using this method, preparation of arbitrarily mixed states and state tomography by symmetric informationally complete positive operator-valued measures are demonstrated.

**8:24AM F08.00003: Adiabaticity in non-Hermitian dynamics of a superconducting qubit**
WEIJIAN CHEN (Presenter), MARYAM ABBASI, Physics, Washington University, St. Louis, MAHDI NAGHILOO, Electrical engineering and computer science, Massachusetts Institute of Technology MIT, YOGESH JOGLEKAR, Physics, Indiana University - Purdue University Indianapolis, KATER MURCH, Physics, Washington University, St. Louis — In general, a quantum system subject to slow parameter variation will closely follow its instantaneous eigenstates. This well-known adiabatic theorem, however, has been shown to break down in recent studies of open systems with gain or loss. Such systems are effectively described by non-Hermitian Hamiltonians and thus possess complex eigenvalues and nonorthogonal eigenstates. In this talk, I will present our study of adiabaticity in non-Hermitian dynamics of a single dissipative superconducting qubit, where we tune the frequency and amplitude of microwave drives to vary the system Hamiltonian. The resulting dynamics is determined by the nonadiabatic coupling between eigenstates as well as their complex-eigenvalue-induced growth or decay. Our understanding of adiabaticity in the presence of complex eigenvalues will be important in harnessing non-Hermiticities for quantum sensing and control.

*This work was supported by NSF Grant PHY-1607156 and PHY-1752844 (CAREER), and NSF Grant DMR-1054020 (CAREER). W. Chen acknowledges the support from Center for Quantum Sensors at Washington University.*
8:36AM F08.00004: Encircling exceptional points of a single dissipative qubit*  MARYAM ABBASI (Presenter), WEIJIAN CHEN, physics, Washington University, St. Louis, MAHDI NAGHILOO, Electrical engineering and computer science, Massachusetts Institute of Technology MIT, SCOTT HERSHBERGER, physics, Washington University, St. Louis, YOGESH JOGLEKAR, physics, Indiana University - Purdue University Indianapolis, KATER MURCH, physics, Washington University, St. Louis — We study the behavior of a single dissipative qubit which is described by a non-Hermitian Hamiltonian. This system exhibits a degeneracy known as an exceptional point (EP) where both eigenvalues and eigenstates coalesce. According to the adiabatic theorem, slow variation of the system parameters in a closed loop transports the system back to its initial state. Surprisingly, in a loop encircling an EP the eigenstates of the system will switch. Moreover, this behavior is chiral due to its dependence on the encircling direction and the initial state. We experimentally explore these phenomena by varying the drive parameters in a superconducting transmon circuit, creating closed loops in parameter space with one or two EPs. Our study shows how non-Hermiticities enable novel methods of quantum control.

*This work was supported by NSF PHY-1607156, NSF PHY-1752844 (CAREER)), and NSF grant DMR-1054020 (CAREER).

8:48AM F08.00005: Dissipative processs to generate entangled state in solid state system  WANG XIN (Presenter), Tsinghua University — When the target system interacts with the environment with some dissipative process, this process may be engineered to generate and protect the quantum state. Dissipation can be used to engineer some strongly correlated state, and also help one to understand the dynamics of the system and reservoir. Former work has been completed to design the dissipation in many experimental system, for example, ion trap, superconductor and atomic ensembles system. We demonstrate firstly that by utilizing a designed dissipative protocol one can generate a maximum entangled state in Nitrogen-vacancy solid spin system. Meanwhile, the fidelity of target state will stay steady and not change with the generation sequence number increasing.

9:00AM F08.00006: Shortcuts to adiabaticity in open systems: thermalization of an open quantum oscillator  AURELIA CHENU (Presenter), LEONCE DUPAYS, Donostia International Physics Center (DIPC), INIGO LOUIS EGUSQUIZA, Physics, Universidad del Pais Vasco (UPV), ADOLFO DEL CAMPO, Donostia International Physics Center (DIPC) — The dynamical control of quantum systems is a necessity to advance quantum sciences and technology. Techniques known as shortcuts to adiabaticity (STA) provide an alternative to adiabatic driving, and have proven useful in a wide diversity of applications. However, they are currently restricted to the control of closed systems. We introduce STA in open quantum systems, and develop a technique to control the thermalization of a driven open quantum oscillator. We provide the time modulation of the trap frequency and dephasing strength that allow for the preparation of an arbitrary thermal state in a finite time. Thereby, the super-adiabatic control of Gaussian states in non-unitary processes is demonstrated. Experimental implementation in the laboratory relies on stochastic parametric driving, which is readily accessible in a variety of platforms. The possibility to control cooling and heating of thermal states finds applications in finite-time thermodynamics.
9:12AM F08.00007: Modeling non-Markovian dynamics with augmented CPTP maps* KEVIN YOUNG (Presenter), ROBIN BLUME-KOHOUT, Sandia National Laboratories, STEPHEN D BARTLETT, University of Sydney — Markovian quantum processes on qubits can be perfectly described with completely-positive, trace-preserving (CPTP) maps. However, real physical systems are replete with non-Markovian effects. Trapped ions experience heating, microwave sources display power instabilities, and resonators take time to relax. Fluctuating magnetic fields display large spatial correlations, qubits experience leakage, and quantum gates that occur early in a circuit can impact the performance of those occurring later. CPTP maps on qubits capture none of these memory effects. In this talk, we propose a family of augmented CPTP maps that enable simple models of a wide variety of non-Markovian dynamics. We provide a number of numerical examples demonstrating that that these maps are easy to construct and interpret. Furthermore, we show that we can estimate the parameters of these maps from experimental data.

*This work funded in part by Sandia National Laboratories' Laboratory Directed Research and Development program.

9:24AM F08.00008: Learning the dynamics of open quantum systems from local measurements EYAL BAIREY (Presenter), Technion - Israel Institute of Technology, CHU GUO, Quantum Intelligence Lab (QI-Lab), Supremacy Future Technologies (SFT), DARIO POLETTI, Science and Mathematics Cluster and EPD Pillar, Singapore University of Technology and Design, NETANEL LINDNER, ITAI ARAD, Technion - Israel Institute of Technology — The increasing complexity of engineered quantum systems and devices raises the need for efficient methods to verify that these systems are indeed performing the desired quantum dynamics. Due to the inevitable coupling to external environments, these methods should obtain not only the unitary part of the dynamics, but also the dissipation and decoherence affecting the system's dynamics. Here, we propose a method for reconstructing the Lindbladian governing the Markovian dynamics of open many-body quantum systems, using data obtained from local measurements on their steady states. We show that the number of measurements and computational resources required by the method are polynomial in the system size. For systems with finite-range interactions, the method recovers the Lindbladian acting on each finite spatial domain using only observables within that domain. We numerically study the accuracy of the reconstruction as a function of the number of measurements, type of open-system dynamics and system size. Interestingly, we show that couplings to external environments can in fact facilitate the reconstruction of Hamiltonians composed of commuting terms.
9:36AM F08.00009: Noise Memory Kernel Reconstruction via the Post-Markovian Master Equation*  
HAIMENG ZHANG (Presenter), DANIEL A LIDAR, Univ of Southern California — Understanding and combating decoherence is one of the central topics in realizing quantum computation. Correlated, non-Markovian noise presents a particularly relevant challenge in superconducting qubit systems. This talk will present results on the construction of a bath memory kernel function from the experimentally measured state dynamics of a superconducting qubit. This phenomenological memory kernel arises in the post-Markovian master equation (PMME) [A. Shabani and D. A. Lidar, PRA 71, 020101 (2005)]. The memory kernel as constructed is of practical interest for quantum computation tasks as it provides insight into the noise origin and the characteristic timescales associated with bath memory effect. It also illuminates how the non-Markovian property of the noise can potentially be utilized to extend coherence timescales relative to the Markovian limit.

*The research is based upon work supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.

9:48AM F08.00010: Scalable Bayesian learning of local Hamiltonians and Lindbladian*  
TIMOTHY EVANS (Presenter), ROBIN HARPER, STEVEN FLAMMIA, Univ of Sydney — As the size of quantum devices continues to grow, the development of scalable methods to characterise and diagnose noisy devices is becoming an increasingly important problem. Recent results demonstrate how a local Hamiltonians and Lindbladians can be reconstructed from a single, arbitrary steady state with a number of measurements that scales efficiently in the size of the system. These methods, however, can only characterise the system up to scalar factor and lack sufficient robustness to noise, both of which are imperative to be of practical use. In this talk I will present a Bayesian method that addresses both of these issues by making use of any, or all, of the following: experimental control of Hamiltonian couplings, the preparation of multiple states and the availability of any prior information we may already have for the Hamiltonian couplings. Moreover we provide an adaptive measurement protocol that can be performed online, updating estimates and their corresponding uncertainties as experimental data becomes available.

*This work was supported by the Australian Research Council via EQuS project number CE170100009 and by the US Army Research Office grant numbers W911NF-14-1-0098 and W911NF-14-1-0103.
10:00AM F08.00011: Parametric Quantum Noise Spectroscopy Using SchWARMA
KEVIN SCHULTZ (Presenter), GREGORY QUIROZ, DAVID CLADER, Johns Hopkins University Applied Physics Lab — Markovian noise is a fundamental assumption in many characterization and analysis protocols for quantum circuits. However, this assumption is generally not valid in reality, which has led to considerable efforts to characterize and alleviate temporally correlated errors. Here, we adapt techniques from classical time series analysis to model, simulate, and estimate non-Markovian noise. We call this family of techniques Schrodinger Wave ARMA (SchWARMA), and show that it is not only a flexible method for representing noise spectra, but that it is a powerful statistical model that can be used for estimating noise and predicting the effects of non-Markovian noise on quantum circuits.

*Army Research Office, DOE Office of Science

10:12AM F08.00012: Experimental Realization of Noise Injection using SchWARMA
ANDREW MURPHY (Presenter), KEVIN SCHULTZ, JACOB EPSTEIN, KYLE P MCELROY, GREGORY QUIROZ, BRIAN S TIEN-STREET, JOAN AUDREY HOFFMANN, DAVID CLADER, TIMOTHY SWEENEY, Johns Hopkins University Applied Physics Laboratory — We develop a noise-injection scheme applied to an experimental qubit system in order to validate protocols that characterize and mitigate noise. We use a technique known as Schrodinger Wave Autoregressive Moving Average (SchWARMA) to mimic phase noise on a qubit. This is realized by imparting SchWARMA generated errors on the phase of the RF drive that is used to generate control pulses. The accumulation of phase errors mimics dephasing a qubit might experience relative to a perfect drive. We use quantum noise spectroscopy techniques to perform spectral estimation of the noise power spectrum and evaluate the efficacy of the noise injection approach. Our results show SchWARMA is a powerful tool for mimicking correlated phase noise processes in a superconducting qubit system. The power of SchWARMA can be shown to go beyond our initial experiments, extending to multi-axis noise models and arbitrary qubit systems.

*Funded by Laboratory for Physical Sciences and IARPA

10:24AM F08.00013: Continuous feedback of a controllable nonlinear cavity with Deep Reinforcement Learning
RICCARDO POROTTI (Presenter), MICHAEL ZWERGER, FLORIAN MARQUARDT, Max Planck Institute for the Science of Light — Many tasks in quantum information processing require numerical methods to identify the best control sequence to achieve a specific goal. Deep Reinforcement Learning (DRL) has been applied with great success to many other fields, thanks to its ability to identify the best strategy in problems involving a competition between short and long-term rewards.
We focus on one of the simplest quantum systems highly relevant for quantum information processing, namely a controllable nonlinear cavity. We show how DRL can find the correct feedback control to stabilize a desired state (e.g. a particular Fock state), subject to dissipation and weak measurements.
The few existing DRL applications in physics rely mostly on discrete action spaces, but we show how continuous control sequences can be easily plugged in in such framework, which is the most natural way to handle feedback control sequences in physics. Finally, we exploit Long short-term memory (LSTM) networks to account for non-Markovianity in the master equation.
10:36AM F08.00014: Quantum Machine Learning using a Dissipative Quantum Reservoir*  
JOHN MILLER (Presenter), MARTHA VILLAGRAN, Univ of Houston — Recurrent neural networks (RNNs) are often slow learners, requiring extensive training of their hidden layers. In reservoir computing, the RNN's hidden layers are replaced by a reservoir, which can be a complex circuit (e.g., echo state network, or ESN) or physical system. The reservoir transforms recent temporal data into output patterns that can be read by a trainable single layer of neurons. The quantum reservoir, with just a few qubits and including dissipation, has recently been shown outperform a much larger classical ESN. Here we discuss the charge density wave (CDW) - a correlated electron-phonon system - as a candidate quantum reservoir. Some CDW materials (e.g., NbSe3) show learning, such as a pulse-duration memory effect, where 1-3 training pulses are needed experimentally vs. 100's to 1000's in classical simulations. This occurs in a highly dissipative environment with many normal electrons. Related materials (e.g., NbS3) have optimum CDW transport properties at room temperature, suggesting the possibility of certain types of quantum machine learning at high temperatures.

*This work was supported by the State of Texas through the Texas Center for Superconductivity and the University of Houston Health Research Institute.

10:48AM F08.00015: Decoherence Properties of Qubits and Oscillators Coupled to Minimal Environments*  
KEVIN RANDLES (Presenter), Weber State University, DAVID DIAZ, Stony Brook University, JEAN-FRANCOIS VAN HUELE, TY BEUS, MANUEL BERRONDO, Brigham Young Univ - Provo — Decoherence refers to the loss of quantum coherence through contact with the environment. We are interested in characterizing this decoherence in models of simple quantum systems interacting with a minimal environment, following the work of Vidiella-Baranco [Physica A 402, 209 (2014) & Physica 459,78 (2016)]. We work out the full exact dynamics or approximations to the exact dynamics for coupled systems of qubits, oscillators, and mixed systems of qubits with oscillators. We then trace over the environment degrees of freedom and extract the decoherence of the reduced system as characterized by its linear entropy and visualize the results with Bloch spheres and Husimi functions. We relate decoherence rates to coupling strength. We also observe similarities and differences between solutions for couplings corresponding to the rotating and counter-rotating wave approximations. We notice in particular the disappearance of periodicity above a critical coupling strength in the counter rotating coupling in the oscillator case.

*Supported by NSF award #1757998

Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F09 DQI: General Quantum Algorithms 106 - Peter Love, Tufts Univ
8:00AM F09.00001: Novel Trotter formulas for digital quantum simulation*  
YI-XIANG LIU  
(Presenter), Massachusetts Institute of Technology MIT, JORDAN H HINES, University of California, Berkeley, ZHI LI, University of Pittsburgh, ASHOK AJOY, University of California, Berkeley, PAOLA CAPPELLARO, Massachusetts Institute of Technology MIT — Quantum simulation promises to address many challenges in fields ranging from quantum chemistry to material science and high-energy physics, and could be implemented in noisy intermediate scale quantum devices. A challenge in building good digital quantum simulators is the fidelity of the engineered dynamics given a finite set of elementary operations. The goal of this work is to find a proper ordering of elementary operations so that they approximate as well as possible the desired evolution. However, when the quantum system is large, even calculating one elementary operation is computationally expensive. In this talk, I will introduce a geometric framework for optimizing the order of operations without considering the details of the operations themselves, thus achieving computational efficiency. Based on the geometric framework, I will present two alternative orderings. One has optimal fidelity at a short time scale, and the other one is robust at a long time scale. Thanks to the improved fidelity at different time scales, the two different orderings can form the basis for experimental-constrained digital quantum simulation.

*This work was supported in part by DARPA DRINQS, NSF grant EECS1702716, and PHY1734011.

8:12AM F09.00002: Quantum Simulation of Quantum Field Theory with Qubit Models*  
ALEX BUSER (Presenter), Caltech, TANMOY BHATTACHARYA, Los Alamos National Laboratory, SHAILESH CHANDRASEKHARAN, HERSHEYDEEP SINGH, Duke University, RAJAN GUPTA, Los Alamos National Laboratory — Quantum computers are expected to outperform classical methods in the simulation of strongly-coupled quantum field theories, as they permit the calculation of dynamic quantities in real-time and avoid the notorious sign-problem. We consider a class of qubit models which can be simulated efficiently on a fault-tolerant quantum computer, and present evidence that these models possess a rich phase diagram. One of the quantum critical points in the phase diagram may help define the traditional asymptotically free O(3) non-linear sigma model. We discuss implementation of these qubit models on both NISQ and fault-tolerant quantum computers, and provide numerical results on adiabatic ground state preparation for the O(3) sigma model. This work serves as a stepping stone towards simulating non-Abelian Kogut-Susskind type gauge theories with quantum devices.

* - Department of Energy (DOE) Office of Science - High Energy Physics Contract #89233218CNA000001  
- Los Alamos National Laboratory Quantum Computing Summer School Fellowship
8:24AM F09.00003: Quantum Simulation of Nonlinear Classical Dynamics*  ILON JOSEPH
(Presenter), ALESSANDRO ROBERTO CASTELLI, JONATHAN L. DUBOIS, VASILY GEYKO, FRANK R
GRAZIANI, STEPHEN BERNARD LIBBY, JEFFREY PARKER, YANIV J. ROSEN, YUAN SHI, Lawrence
Livermore Natl Lab — Nonlinear classical dynamics can be simulated by a quantum computer with
enough resources to approach the semiclassical limit. There is an exact embedding of a classical
system of $N$ ordinary differential equations (ODEs) within an enlarged quantum mechanical
system with $2N$ degrees of freedom. Any set of ODEs can be derived from a classical Hamiltonian
that is a sum over a set of $N$ constraints, thereby yielding $2N$ equations of motion. Quantizing the
constrained system leads to a Schrodinger equation that is equal to the classical Liouville
equation which ensures conservation of phase space density for the original set of ODEs.
Heisenberg’s uncertainty principle is satisfied by each variable and its canonically conjugate
momentum, the Lagrange multiplier, on the extended phase space. Hence, there is no
uncertainty in a simultaneous measurement of any of the variables of the original ODE. An
appropriate choice of Planck’s constant can be used to reduce the uncertainty in the degrees of
freedom of interest to a width on the order of the level spacing. Thus, excellent fidelity to the
classical system can be achieved.

*This work was performed by LLNL under US DOE contract DE-AC52-07NA27344, DOE-FES

8:36AM F09.00004: Predicting Features of Quantum Systems from Very Few Measurements
HSIN-YUAN HUANG (Presenter), RICHARD KUENG, JOHN PRESKILL, Caltech —
Predicting features of complex, large-scale quantum systems is essential to the characterization
and engineering of quantum architectures. We present an efficient approach for constructing an
approximate classical description, called the classical shadow, of a quantum system from very
few quantum measurements that can later be used to predict a large collection of features. This
approach is guaranteed to accurately predict $M$ observables with bounded Hilbert-Schmidt norm
from only order of $\log(M)$ measurements. This is completely independent of the system size and
saturates fundamental lower bounds from information theory. A distinct realization of the
concept can also be used to predict $M$ few-body observables using classical descriptions
constructed from single-qubit measurements on $\log(M)$ copies of the system. These protocols
have applications in variational quantum algorithms, estimating quantum fidelity, or inferring
entanglement properties of the quantum system. We support our theoretical findings with
numerical experiments over a wide range of problem sizes (2 to 162 qubits). These highlight
advantages compared to existing machine learning approaches.
8:48AM F09.00005: Characterizing quantum phase transitions by the entanglement of high symmetric points: A quantum computational investigation*  XIAO XIAO (Presenter), ALEXANDER F KEMPER, North Carolina State University — Quantum phase transitions play fundamental roles in our understanding of various properties of quantum materials. Therefore, how to characterize quantum phase transitions efficiently is pursued, especially for topological quantum phase transitions, which have no well-defined order parameters. Here we demonstrate that the entanglement of a small subset of a product state can be used as an indicator for quantum phase transitions. Moreover, this strategy can be easily applied with the near-term quantum computers, in which the number of qubits is highly limited. As examples, we demonstrate with IBM quantum computers for the transverse Ising and Kitaev spin model that the entanglement of product states formed by the states at the high-symmetric points of the Brillouin zone, which are subsets of the real ground state, can be used to determine different ground state phases.

*The Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Grant No. de-sc0019469

9:00AM F09.00006: CnNOT gates for implementing random quantum walks*  SELIM SOUFARGI, IYED BEN SLIMEN, SysCom Lab, National Engineering School of Tunis, ENIT, University of EL Manar, 1002 Le Belvédère, Tunis, Tunisia, AMOR GUEDDANA (Presenter), Green & Smart Communication Systems Lab, Gres’Com, Engineering School of Communication of Tunis, Sup’Com, University of Carthage, Ghazela Technopark, 2083, Ariana, Tunisia, VASUDEVAN LAKSHMINARAYANAN, University of Waterloo — Quantum walks have been investigated for traversing graphs with certain oracles. This is important for building quantum routers on future quantum computers. Building quantum walk circuits benefit from the exponential increase in speed when compared to classical random walks. Here we investigated CnNOT based implementation of quantum walks along different length cycles and 2-D hypercycle. We decomposed the circuits into a set of series and parallel combinations of elementary CNOT and single qubit gates and simulated them theoretically taking into consideration the deterministic functioning of the gates. In addition, we ran a Python code simulating the same circuits on an IBM-Q supercomputer implemented with superconducting qubits. Based on the outputs, we highlight the physical constraints behind the real backend results and give numerical approximations for the errors for higher qubit number systems.

*Vasudevan Lakshminarayanan was supported by a DISCOVERY grant from NSERC, Canada
9:12AM F09.00007: Isolated Vertices in Continuous-Time Quantum Walks on Dynamic Graphs* THOMAS WONG (Presenter), Creighton University — It was recently shown that continuous-time quantum walks on dynamic graphs, i.e., sequences of static graphs whose edges change at specific times, can implement a universal set of quantum gates. This result treated all isolated vertices as having self-loops, so they all evolved by a phase under the quantum walk. In this paper, we permit isolated vertices to be loopless or looped, and loopless isolated vertices do not evolve at all under the quantum walk. Using this distinction, we construct simpler dynamic graphs that implement the Pauli gates and a set of universal quantum gates consisting of the Hadamard, $T$, and CNOT gates, and these gates are easily extended to multi-qubit systems. For example, the $T$ gate is simplified from a sequence of six graphs to a single graph, and the number of vertices is reduced by a factor of four. We also construct a generalized phase gate, of which $Z$, $S$, and $T$ are specific instances. Finally, we validate our implementations by numerically simulating a quantum circuit consisting of layers of one- and two-qubit gates, similar to those in recent quantum supremacy experiments, using a quantum walk.

*This work was supported by startup funds from Creighton University.

9:24AM F09.00008: Enhancing Quantum Linear System Algorithm by Richardson Extrapolation ALMUDENA CARRERA VAZQUEZ (Presenter), IBM Research - Zurich, ALBERT FRISCH, DOMINIK STEENKEN, HARRY BAROWSKI, IBM Systems - Germany, RALF HIPTMAIR, ETH Zurich, STEFAN WOERNER, IBM Research - Zurich — We present a complete implementation of the HHL algorithm to solve tridiagonal Toeplitz systems of linear equations of size $N$ with $O(\log(N)\log^3(1/\varepsilon) + \log(\kappa)\lambda_{\text{min}}/\varepsilon)$ gates, where $\varepsilon$ is the accuracy, $\kappa$ the condition number and $\lambda_{\text{min}}$ the smallest eigenvalue, an exponential improvement in the size of the system over classical methods. In particular, we present efficient oracles for preparing a quantum state where amplitudes are specified by a given function, Hamiltonian simulation and solution observables, and we show that the Euclidean norm of the solution can be obtained deterministically.

The main result is the use of Richardson extrapolation for general product formulae Hamiltonian simulation, resulting in an implementation of the quantum phase estimation part at $\text{polylog}(1/\varepsilon)$ complexity instead of $\text{poly}(1/\varepsilon)$.

For each result we provide detailed mathematical analysis that do not restrict to tridiagonal matrices, and analyze whether it is possible to obtain a quantum advantage taking into account different classes of right hand sides and quantum algorithms.

All the procedures presented are implemented with Qiskit and tested on a quantum simulator. We demonstrate our algorithm for a small illustrative problem and two different observables on real hardware of the IBM Quantum Computing Center.
9:36AM F09.00009: Universality and conformal invariance in hybrid quantum circuits

YAODONG LI (Presenter), University of California, Santa Barbara, XIAO CHEN, Kavli Institute for Theoretical Physics, ANDREAS W LUDWIG, MATTHEW P A FISHER, University of California, Santa Barbara — We establish the emergence of conformal field theories (CFT) in (1+1)-dimensional hybrid quantum circuits right at the measurement-driven entanglement transition, by revealing the remarkable space-time conformal covariance of entanglement entropies and mutual information, computed numerically for various subregions at all time steps within Clifford circuits of up to \( L = 512 \) qubits and \( T = 1024 \) time steps. Though the evolution takes place in real-time, the time dimension of the circuit becomes “imaginary” or “space-like” – to be consistent with conformal invariance – as a result of measurements that break unitarity. Throughout the paper we investigate Clifford circuits with several different boundary conditions by injecting physical qubits at the spatial and/or temporal boundaries, all giving consistent characterizations of the “Clifford CFT”. We emphasize universal results that are consequences solely of the conformal invariance and do not depend crucially on the precise nature of the CFT. Among these are the infinite “entangling speed” as a manifestation of “many-body entanglement swapping”, and the critical decaying behavior of the thermal entropy of a mixed state at the recently discovered “purification transition”.

*Heising-Simons Foundation
IQIM
Gordon&Betty Moore Foundation
NSF

9:48AM F09.00010: Time Complexity Reduction for Gate-Model Quantum Computers

LASZLO GYONGYOSI (Presenter), Univ of Southampton, SANDOR IMRE, Budapest University of Technology and Economics — A method is defined for the time complexity reduction of near-term gate-model quantum computers. The proposed solution evaluates the reduced time complexity equivalent of a reference quantum circuit and recovers the reference output quantum system of the reference quantum circuit via quantum operations on the output of the reduced time complexity quantum circuit. We prove the complexity of the proposed quantum algorithm and the achievable reduction in time complexity. We define the auxiliary cost of the proposed quantum algorithm and show that it is significantly lower than the gainable reduction in time complexity. The algorithm provides a tractable solution to reduce both time complexity and the economic cost of implementing the physical-layer quantum computer by reducing quantum hardware elements. The results are useful for experimental gate-model quantum computations and the near-term quantum devices of the quantum Internet.

*The research has been supported by the National Research, Development and Innovation Fund (TUDFO/51757/2019-ITM), by the National Research Development and Innovation Office of Hungary (2017-1.2.1-NKP-2017-00001), by the Hungarian Scientific Research Fund - OTKA K-112125 and in part by the BME Artificial Intelligence FIKP grant of EMMI (BME FIKP-MI/SC).
10:00AM F09.00011: Green's functions of molecules using a quantum computer  
TAICHI KOSUGI (Presenter), YUICHIRO MATSUSHITA, Tokyo Institute of Technology — Given the recent rapid development of techniques for quantum computation of electronic structures[1], we propose an algorithm for the construction of one-particle Green's function (GF) of an interacting electronic system via statistical sampling on a quantum computer for quantum chemistry.[2] By avoiding the difficulty coming from the non-unitarity of creation and annihilation operators for the electronic spin orbitals, we provide quantum circuits equipped with at most two ancillary qubits for obtaining all the components of GF. We perform simulations of such construction of GFs for LiH and H2O molecules based on the unitary coupled-cluster (UCC) method and compare the quasiparticle and satellite spectra exact within UCC and those from full configuration interaction calculation.


10:12AM F09.00012: Quantum Phase Estimation with Time-Frequency Qudits in a Single Photon*  
ZIXUAN HU, HSUAN-HAO LU, MOHAMMED S ALSHAYKH, ALEXANDRIA J. MOORE, YUCHEN WANG (Presenter), POOLAD IMANY, ANDREW M WEINER, SABRE K AIS, Purdue Univ — In this work, we report an experimental realization of a qudit-based PEA on a photonic platform, utilizing the high dimensionality in time and frequency degrees of freedom (DoFs) in a single photon. The controlled-unitary gates can be realized in a deterministic fashion, as the control and target registers are now represented by two DoFs in a single photon. We also proposed a systematic scheme to decompose an arbitrary unitary matrix into smaller d-level unitary matrices. Representing and connecting these d-level unitary matrices with photonic qudit gates is our plan for future research.

*This work was supported in part by the National Science Foundation under award number 1839191-ECCS.

10:24AM F09.00013: Implementing single-qubit POVMs on a circuit-based quantum computer  
YORDAN YORDANOV (Presenter), Univ of Cambridge — We present a deterministic protocol to implement general single-qubit POVMs on near-term circuit-based quantum computers. The protocol has a modular structure, such that an n-element POVM is implemented as a sequence of (n-1) circuit modules. Each module performs a 2-element POVM. Two variations of the protocol are suggested, one optimal in terms of number of ancilla qubits, the other optimal in terms of number of qubit gate operations and quantum circuit depth. We use the protocol to implement 2- and 3-element POVMs on two publicly available quantum computing devices. The results we obtain are positive, and suggest that implementing non-trivial POVMs could be within the reach of current noisy intermediate scale quantum computing devices.
OLEG OLENSKI (Presenter), Department of Applied Physics and Astronomy, University of Sharjah — One-parameter functionals of the Renyi $R_{\rho,\gamma}(\alpha)$ and Tsallis $T_{\rho,\gamma}(\alpha)$ types are calculated in the position (subscript $\rho$) and momentum (subscript $\gamma$) spaces for the 2D nanoring placed into the combination of the uniform magnetic field $B$ and the AB flux $\Phi_{AB}$. Ring potential is modelled by the superposition of the quadratic and inverse quadratic dependencies on the radius $r$.

Position (momentum) Renyi entropy depends on $B$ as a negative (positive) logarithm of $\omega_{\text{eff}} = (\omega_0^2 + \omega_c^2/4)^{1/2}$, where $\omega_0$ determines the quadratic steepness of the confining potential and $\omega_c$ is a cyclotron frequency. This makes the sum $R_{\rho nm}(\alpha)+R_{\gamma nm}(\alpha/(2\alpha-1))$ a field-independent quantity that increases with the principal $n$ and azimuthal $m$ quantum numbers and satisfies corresponding uncertainty relation. In the limit $\alpha\to1$ both entropies in either space tend to their Shannon counterparts along, however, different paths. Analytic expression for the lower boundary of the semi-infinite range of the dimensionless coefficient $\alpha$ where the momentum entropies exist reveals that it depends on the ring geometry, $\Phi_{AB}$ and $m$. There is the only orbital for which both uncertainty relations turn into the identity at $\alpha=1/2$ and which is not necessarily the lowest-energy level. At any coefficient $\alpha$, the $R_{\rho}\cdot\Phi_{AB}$ curve mimics the energy variation with $\Phi_{AB}$.

Tuesday, March 3, 2020 8:00 AM - 10:12 AM

Session F10 GIMS: Advances in Scanned Probe Microscopy 3: Scanning Probes Spectroscopic Techniques 108 - Stephen Jesse, University of Tennessee - Tag(s): Focus
Direct and converse flexoelectricity: the effect of strain and electric field gradients on nanoscale electromechanical responses

NEUS DOMINGO (Presenter), Institut Català de Nanociència i Nanotecnologia (ICN2), AMIR ABDOLLAHI, Universitat Politècnica de Catalunya (UPC), KUMARA CORDERO EDUARDS, DQMP, Université de Geneve, JORDI SORT, Universitat Autònoma de Barcelona (UAB), IRENE ARIAS, Universitat Politècnica de Catalunya (UPC), GUSTAU CATALAN, Institut Català de Nanociència i Nanotecnologia (ICN2) — Surface electromechanics at the nanoscale are typically studied by Piezoresponse Force Microscopy (PFM), based on the inverse piezoelectric effect. As a first approach, generally only homogeneous responses are taken into account, but it has been realized that the effect of gradients in electro-mechanical phenomena at the nanoscale can become dominating: the generation of electrical signals after the application of mechanical strain gradients with an AFM tip has been proved, and it has been shown that it is possible to write ferroelectric domains [1] or to move oxygen vacancies and charges.

In this talk, I will review how gradient-based electro-mechanical effects couples and affects the quantification of PFM measurements. I will start by showing the asymmetry in mechanical properties induced by the coupling of flexoelectricity to ferroelectricity leading to ferroelectrics as smart mechanical materials [2], and opening new opportunities to mechanically read ferroelectric polarization states in both, thin films and single crystals, on the base of Contact Resonance Frequency AFM mode. Then, I will show how converse flexoelectric effect [3] due to the presence of strong local electric field gradients at the tip end can induce a mechanical strain of the sample in dielectric centrosymmetric materials with magnitudes comparable to piezoelectric $d_{33}$ coefficient.

References:

*Financial support from MINECO Grant MAT2016-77100-C2-1-P and FIS2015-73932-JIN and support of Generalitat de Catalunya (Grant No. 2017-SGR-579). ICN2 acknowledges support from the Severo Ochoa Program (MINECO, Grant SEV-2017-0706)
New modalities for cryogenic nano-imaging and spectroscopy

Sven A. Doenges (Presenter), Kyung-Duck Park, Tao Jiang, Fabian Menges, Markus B. Raschke, Department of Physics, Department of Chemistry, and JILA, University of Colorado, Boulder — Scanning nano-optical imaging and spectroscopy have emerged as powerful tools in investigating and understanding heterogeneities and underlying physics in a wide range of organic, layered van der Waals, and correlated electron materials. However, the extension to variable and low temperatures has remained a major experimental challenge, yet highly desirable with many fundamental properties and phase transitions only emerging far below room temperature. Here, we present the development of cryogen-free variable temperature infrared nano-imaging and spectroscopy, as well as variable temperature tip-enhanced photoluminescence and nano-Raman spectroscopy in different instruments based on closed cycle cryocoolers with an exchange gas cooled low vibration interface. At the example of surface plasmon polariton nano-imaging in graphene, we establish infrared scattering scanning near-field optical microscopy (s-SNOM) at temperatures as low as 15 K with spatial resolution of 10 nm. Further, we demonstrate tip-enhanced photo-luminescence (TEPL) and tip-enhanced Raman spectroscopy (TERS) of different excitonic systems based on 2D transition metal dichalcogenide (TMD) heterostructures.

Bulk ferromagnetic tips for spin-polarized scanning tunneling microscopy

Masahiro Haze (Presenter), Hung-Hsiang Yang, Kanta Asakawa, Ryosuke Yamamoto, Nobuyuki Watanabe, Yasuo Yoshida, Yukio Hasegawa, Univ of Tokyo-Kashiwanoha — To develop nano-controlled magnetic materials for condensed matter physics and device applications, it has been required to investigate magnetic structures in atomic scales. While spin-polarized scanning tunneling microscopy (SP-STM) is one of the powerful tools, the usage is still hampered because of the issue on its probe. Tips coated with magnetic thin films are often used, but fabricating stable and reliable ones is not easy unless well equipped. Among the bulk magnetic probes, which can be prepared rather easily, chemically etched antiferromagnetic Cr tips are most commonly used. However, antiferromagnetic probes have disadvantages that the magnetization direction cannot be controlled and defined. On the other hand, bulk ferromagnetic probes are good choices if target materials are robust against stray fields such as antiferromagnetic materials.

In this study, we demonstrate that chemically etched bulk ferromagnetic Ni and Fe tips are ones of the best choices for reliable SP-STM probes using an antiferromagnetic spin-spiral sample; Mn double layers formed on W(110). We also demonstrated that their magnetization direction can be easily controlled by external magnetic fields. This work provides new options for the magnetic probes, opening up versatility of SP-STM.
9:00AM F10.00004: Fourier transform infrared scanning tunneling microscopy: Measuring vibrational modes at the nanoscale  KRISTOPHER BARR (Presenter), NAIHAO CHIANG, ANDREW IRA GUTTENTAG, PAUL S WEISS, University of California, Los Angeles — Scanning probe microscopy has enabled unprecedented surface imaging capability down to atomic resolution. Recent advances in photon technologies has led to successful integration of optical spectroscopy with various scanning probe microscopy. In this work, we use the scanning tunneling microscope tip as a nano antenna and a multiplexed signal from a bench-top Fourier-transform interferometer to discover vibrational modes at the nanoscale. By back illuminating our gold on sapphire samples, we are able to excite molecular self-assembled monolayers into vibrationally excited states evanescently, thus creating a perturbation in the conductance of the STM junction. We use cyanide on gold as a proof-of-concept system because of its distinct vibrational spectra, its stability under ambient conditions, and our control of the molecules interactions. In previous work, we have demonstrated direct control of the gold cyanide molecular packing structures – cubic or hexagonal close packed – and can contribute a vibrational mode from Raman and infrared spectroscopy to each phase. This custom-built instrument performs operates at ambient temperature and pressure, enabling us to image chemical structure with single-molecule resolution on a variety of systems.

9:12AM F10.00005: Role of steps on Pb atomic-layer superconductivity  YUDAI SATO (Presenter), FUMIKAZU OGURO, KANTA ASAKAWA, Institute for Solid State Physics, The University of Tokyo, TAKASHI UCHIHASHI, International Center for Materials Nanoarchitectonics, National Institute for Material Science, YUKIO HASEGAWA, Institute for Solid State Physics, The University of Tokyo — Atomic-layer superconductors [1] exhibit various unique characteristics. One of the features is the enhancement of the in-plane critical magnetic field. The presence of steps, which work as a Josephson barrier [2], is inevitable. It is thus expected that the weakened coupling between terraces confines cooper pairs within the terraces and modifies superconductivity depending on the terrace width. Pb monolayers on a Si(111) substrate is known to form various superconducting phases. Using scanning tunneling microscopy (STM), we found a√3×√43 superconductivity phase still remains on narrow terraces (< 150 nm) even under out-of-plane magnetic fields above its critical magnetic field (190 mT). In addition, on a striped incommensurate (SIC) phase formed on a 1.1 degrees tilted vicinal Si(111) substrate, where 15 nm-narrow terraces covers the whole surface, we observed suppression of the superconductivity breaking against out-of-plane magnetic field. Our results open up the possibility of creating superconducting materials whose the critical magnetic fields of all directions are enhanced in a macroscopic level.

References:
9:24AM F10.00006: GHz-THz near-field imaging of extreme subwavelength metal structures

XINZHONG CHEN (Presenter), State Univ of NY - Stony Brook, XIAO LIU, University of Shanghai for Science and Technology, XIANGDONG GUO, National Center for Nanoscience and Technology, SHUCHEN, CIC nanoGUNE, HAI HU, National Center for Nanoscience and Technology, ELIZAVETA NIKULINA, CIC nanoGUNE, ZIHENG YAO, State Univ of NY - Stony Brook, HANS BECHTEL, MICHAEL MARTIN, Lawrence Berkeley National Laboratory, G CARR, Brookhaven National Laboratory, QING DAI, National Center for Nanoscience and Technology, SONGLIN ZHUANG, University of Shanghai for Science and Technology, QING HU, Massachusetts Institute of Technology, YIMING ZHU, University of Shanghai for Science and Technology, RAINER HILLENBRAND, CIC nanoGUNE, MENGKUN LIU, State Univ of NY - Stony Brook, GUANJUN YOU, University of Shanghai for Science and Technology — Modern scattering-type scanning near-field optical microscopy (s-SNOM) has become an indispensable tool in material research. In this talk we present a home-built GHz-THz s-SNOM using Schottky diodes as both light source and detector, achieving unprecedented spatial resolution at long wavelength (~2 mm). We systematically investigated a series of extreme subwavelength metallic nanostructures at the micrometer scale. The near-field material contrast is found to be greatly impacted by the lateral size and connectivity of the nanostructures, which is drastically different from the cases at shorter wavelengths (e.g. IR s-SNOM). The observed phenomena can be explained by a quasi-static analysis and full-wave electromagnetic simulations. Our results reveal that s-SNOM with long wavelength excitation is an ideal candidate for investigating the electrostatic behavior of metallic devices.

9:36AM F10.00007: Ultrafast infrared nano-spectroscopic imaging of heterogeneous photoinduced dynamical processes

JUN NISHIDA (Presenter), SAMUEL C. JOHNSON, SVEN A. DOENGES, Department of Physics, Department of Chemistry and JILA, University of Colorado, Boulder, AMANI H ALFAIFI, National Renewable Energy Laboratory, SEAN SHAHEEN, Renewable and Sustainable Energy Institute, University of Colorado, Boulder, MARKUS B. RASCHKE, Department of Physics, Department of Chemistry and JILA, University of Colorado, Boulder — Low-energy responses and interactions at mid-infrared frequencies often play central roles in photoinduced dynamical phenomena, ranging from phase transitions in quantum materials to polaron formations in photovoltaic materials. However, the spatial heterogeneities and temporal evolution associated with such low-energy processes in the photoinduced transient state has remained elusive. Here, we develop and apply ultrafast infrared scattering scanning near-field optical microscopy (IR s-SNOM) to characterize photoinduced dynamics with far-from-equilibrium excitation and ultrahigh spatio-temporal-spectral resolution. For unambiguous determination of nano-scale phase and spectral responses, we develop optical pump - infrared probe nano-imaging with heterodyne detection. We demonstrate the performance of ultrafast IR s-SNOM to probe transient quantum states of the photoinduced heterogeneous metallic phase in vanadium oxide microrods, as well as spatially varying polaron-molecule coupling in lead halide perovskite films. The approach of ultrafast heterodyne IR s-SNOM with strong pump excitation is generally applicable to a wide range of strong transient field phenomena, providing for fundamental insight into heterogeneous electronic, structural, and dynamical properties of materials.
9:48AM F10.00008: Calibrating atomic force microscope detectors on soft surfaces  DANIEL FORCHHEIMER (Presenter), KTH Royal Inst of Tech, DANIEL PLATZ, MST, TU Wien, RICCARDO BORGANI, DAVID HAVILAND, KTH Royal Inst of Tech — Quantitative force microscopy requires independant means of calibrating both cantilever stiffness and detector responsivity (i.e. the factor mapping cantilever deflection in nanometers to photo-detector signal in Volts). The conventional methods slowly approach the surface while observing either static bending or change in oscillation amplitude. Detector responsivity is then obtained under the assumption that the surface does not deform during the region of approach used for calibration. This assumption may be satisfied for large force and stiff sample, both of which risk damaging the tip. Here we present a new method for detector calibration based on Intermodulation AFM where the tip-surface force versus cantilever deflection is continuously monitored during the slow approach. This method allows us to calibrate the detector without the previously mentioned assumptions. We can therefore calibrate on any surface, hard or soft, or directly on the sample with the same magnitude of force used for quantitative imaging. We present the theory of this method and its experimental implementation on a variety of different surfaces.

10:00AM F10.00009: The influence of time and temperature on viscoelastic properties of nanoscale domains within polymer composites  BEDE PITTENGER (Presenter), SERGEY OSECHINSKIY, JOHN THORNTON, SOPHIE LOIRE, THOMAS MUELLER, AFM Unit, Bruker Nano Surfaces — The behavior of polymer composites is controlled by the properties of the components as well as the microstructure of the material. Because confinement effects and interphase formation can alter properties of the microphases, only measurements performed directly on the composite can provide the needed local property distribution. Mechanical properties of polymers are generally time dependent, so a full understanding requires measurements over a range of frequencies and temperatures. Ideally, one would like to observe the mechanical behavior of these microscopic domains while they pass through their glass transitions to appreciate the influence of size effects and confinement on time dependent mechanical properties.

Recently, Atomic Force Microscopy based nano-Dynamic Mechanical Analysis (AFM-nDMA) was introduced. Like bulk DMA, this mode provides spectra of storage and loss modulus across frequency and temperature, allowing construction of master curves through Time Temperature Superposition (TTS). In addition, it allows high resolution measurements localized to the microscopic structures within heterogeneous samples. This presentation will examine the capabilities of this new mode with examples in a wide range of polymers and composites.
F10.00010: Cryogenic Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) has become an important branch of modern optical techniques in the past decade, which allows nanoscale imaging over a broad spectral range. This informative technique is feasible to study the electrodynamics of correlated quantum materials with a spatial resolution down to 10 nm. As a powerful scanning probe microscopy, although the importance of cryo-SNOM has been universally recognized, the realization remains to be a challenging task. Based on the experience of cryo-AFM, we built a set of s-SNOM operating with variable sample temperature down to 10 K. The scanning probe is located in ultra high vacuum chamber with He-bath cryostat maintaining low temperature and combined with a molecule beam epitaxy (MBE) system. The nine home-made positioners of the scanning system function well at low temperature. The system is equipped with CO\(_2\) laser which can provide long-time stable light source. Our cryo-SNOM has been tested at liquid nitrogen temperature, which shows good performance and is promising to work well below 10K.

Tuesday, March 3, 2020 8:00 AM - 10:36 AM

Session F11 APS/SPS: Undergraduate Research VI

8:00AM F11.00001: Measuring the Glass Transition in Dense 2D Colloidal Fluids* WILLIAM MOORE (Presenter), ORRIN SHINDELL, Trinity University — We use Total Internal Reflection Fluorescence Microscopy (TIRF) to analyze dense colloidal fluids fully restricted to two dimensions near their glass transition. Our experiments use 40-100 nm diameter phospholipid vesicles (nanospheres) produced in the lab and commercially manufactured 500 nm and 1000 nm diameter fluorescent polystyrene spheres (microspheres). The microspheres are individually resolvable under TIRF, which allows us to measure their instantaneous positions in both a fluid and a glass state. For both the nanospheres and the microspheres, the position of the colloidal particles is tracked as a function of time, which allows us to measure the viscosity of the colloidal fluid at a range of particle densities. We are thus able to obtain both structural and dynamical information about two-dimensional dense fluids near their glass transition.

*Murchison Fellowship and Mach Fellowship from Trinity University
8:12AM F11.00002: Minimum flow rate in electro-coflow* BENJAMIN OVERLIE (Presenter), JOSEFA GUERRERO MILLAN, Augusta University — Controlled generation of micron and sub-micron sized drops continues to be of strong interest for the scientific community due to the variety of applications in many different fields. Emulsion drops can be generated by flowing two immiscible liquids inside a glass-based microfluidic device. Their minimum size will be of the order of the tip size. To create smaller drops, an external electric field can be used, similarly to what it is done in the classical electrospray. In electrospray, a liquid is issued into air from an electrified needle. When the flow rate of the liquid is controlled, there is a minimum flow rate below which a cone-jet cannot be formed regardless of the applied voltage. This minimum flow rate gives you the minimum drop size that can be generated, usually one or two orders of magnitude smaller than the tip size. We explore this lower limit in electro-coflow using pressure control instead, and we have found a different result than in electrospray, with a more complex behavior. The use of pressure control and the presence of an outer moving fluid, enrich the dynamics in the minimum flow rate limit.

*Acknowledgment is made to the donors of the American Chemical Society Petroleum Research Fund for support (or partial support) of this research (60302-UR9).

8:24AM F11.00003: Energy spectra for turbulent Rayleigh-Bénard convection MICHAEL KWAN (Presenter), JANET D SCHEEL, Occidental Coll — We investigated the scaling behaviors for numerically simulated, turbulent Rayleigh-Bénard convection by determining the kinetic and thermal energy spectra. The systems have aspect ratio 1, Prandtl numbers 0.7, 0.021 and 0.005, and various Rayleigh numbers ranging from $10^5$ to $10^{10}$. Whereas in previous studies the frequency spectra from a time series were considered, we calculated the energy spectra from spatial fields. In particular, we performed Fourier analysis on two-dimensional cross sections of the temperature and velocity fields. We also computed the velocity and temperature structure functions on the same cross sections to verify our findings. Lastly, we tested whether Kolmogorov's 1941 (K41) scaling law or the Bolgiano-Obukhov (BO) scaling law applied to both the kinetic and thermal energy spectra for the various systems.

8:36AM F11.00004: The Effect of Short Range Attractions on Sequence Defined Polyelectrolyte Coacervation NATALIA MARKIEWICZ (Presenter), TYLER LYTLE, CHARLES SING, University of Illinois at Urbana-Champaign — Complex coacervation is the liquid-liquid phase separation of polyelectrolytes in aqueous salt solution into a polymer-dense phase, the coacervate, and a polymer-dilute phase, the supernatant. Previous work using Monte Carlo simulations demonstrated that changing the sequence of charged and neutral monomers on polyelectrolytes while keeping the charge fraction constant alters the extent of phase separation. However, previous data does not account for the hydrophobicity of different neutral monomers. To understand the coacervation of polymers with various chemical structures, van der Waals interactions at various strengths are included in Monte Carlo simulations to show hydrophobic effects in the system. Comparisons are made to existing Monte Carlo simulations and experimental data. Understanding these patterning effects will enhance the knowledge of biomacromolecule phase separation, as well as expand the understanding of sequence-dependent polymer physics.
8:48AM F11.00005: Measurement of Low Temperature Strain in 3D Printed Materials
JOESEPH MOORE (Presenter), MICHAEL RAY, California State University, Sacramento — The versatility and ease of use of 3D printing provides access for custom built parts to be quickly manufactured for experimental applications. However, not much is currently known about the behavior of these materials at low temperatures. In this project we measured the thermal properties of a 3D printed material in a cryogenic environment in order to determine its suitability for use in low temperature applications. Specifically, we used a strain gauge to measure the thermal contraction of Polylactic Acid, which is a common material used in 3D printing. We will present our results and discuss the implications for its use in low temperature experiments.

*This work is supported by the National Science Foundation under grant DMR-1807476

9:00AM F11.00006: Measurement of the Low Temperature Porosity of 3D Printed Materials
KEVIN COAN (Presenter), MICHAEL RAY, California State University, Sacramento — Over the past decade, 3D printing has become popular due to its ease of manufacturing and low cost. This work will explore the possibility of using 3D printers to design custom components for use in low temperature experiments. Specifically, we designed an experiment to test the low temperature porosity of Polylactic Acid, a common 3D printed material. We will present the methods used in this experiment, the results obtained, and then discuss its implications for low temperature use.

*This work is supported by the National Science Foundation under grant DMR-1807476

JOHN REVELLE (Presenter), ANKIT KUMAR, ALEXANDER F KEMPER, Department of Physics, North Carolina State University — Time-resolved optical conductivity is an oft-used tool to interrogate quantum materials driven out of equilibrium. Theoretically calculating this observable is a complex topic with several approaches discussed in the literature. Using a non-equilibrium Keldysh formalism and a functional derivative approach to the conductivity, we present a comparison of two particular approaches to the calculation of the optical conductivity, and their distinguishing features, as applied to a pumped superconductor. The two methods are distinguished by the relative motion of the probe and gate times; either the probe or gate time is kept fixed while the other is swept. We find that both the methods result in same qualitative features of the time-resolved conductivity after pump is over. However, calculating the conductivity by keeping the gate fixed removes artifacts inherent to the other method. We provide software that, based on data for the first method, is able to construct the second approach.

*This material is based upon work supported by the National Science Foundation under Grant DMR-1752713.
9:24AM F11.00008: Superconductor-based light detection*  KYRIL KAVETSKY (Presenter),
Department of Physics & Astronomy, Rowan University, HARISH KRISHNAMOORTHY, CESARE SOCI,
Division of Physics and Applied Physics, Nanyang Technological University, MICHAEL LIM, Department of
Physics & Astronomy, Rowan University — The ability to detect a single photon could have powerful
applications in high-precision object location and quantum information encryption. A
superconducting nanowire single-photon detector (SNSPD) is a promising solution that is smaller
than the period at the end of this sentence. While they are commercially available now, there is
still some room for improvement of efficiency, particularly when a wider operational bandwidth
is required, which could be achieved by improving the light absorption. This research presents
finite-element-method-based simulations to enhance the absorption in superconducting thin
films by utilizing plasmonic nanostructures with broadband absorption response.

*The authors acknowledge support from NSF-IRES 1559410.

9:36AM F11.00009: Phenomenological description of excitonic complexes in tip-enhanced
photoluminescence of 2D materials  ZACHARY WITHERS (Presenter), DMITRI VORONINE,
Department of Physics, University of South Florida — Two dimensional materials exhibit different
electronic and optical properties than the corresponding bulk materials. Transition metal
dichalcogenides (TMDs) are semiconducting 2D crystals that exhibit unusually strong
photoluminescence (PL) signals due to the stability of excitons at room temperature. However,
many factors can effect the measured intensity of PL signals including charge doping or the
presence of a plasmonic AFM tip. Here we present a set of phenomenological rate equations in
order to model the intensity of PL in tip-enhanced experiments involving tip-sample distance
dependent measurements and near field imaging. Furthering the understanding of exciton
dynamics around heterojunctions of TMDs may lead to the engineering of new optoelectronic
devices such as optical transistors, novel optomechanics, and controllable signaling on the
nanoscale.
Double Resonant Local Fields Appreciably Enhance Third Harmonic Generation in Core-shell Nano-cavity  

WENBO ZANG, ZHUO CHEN, ZHONGWEI WANG  
(Presenter), Physics Department, Nanjing University — We simulate the intensity of third harmonic generation (THG) in a metallic core-shell nanostructure in double resonant conditions, where the corresponding wavelength of two cavity modes are tuned in to couple with the wavelength of the pump light and the THG signal simultaneously by adjusting the refractive index of the dielectric. It turns out that the double resonant condition is crucial to our discovery.

Numerical simulations show that if the fundamental wavelength of the pump light is adjusted to 1390nm, which is the corresponding eigen wavelength of TM$\text{2}_{1}$ mode, and the frequency of a higher-order cavity mode, say, TE$\text{3}_{2}$ mode was also adjusted to the frequency of THG, the THG signal was more intensified than the single resonant condition on which only TM$\text{2}_{1}$ mode was tuned in to the fundamental frequency. What's more, when the two cavity modes involved, e.g., TM$\text{2}_{1}$ and TM$\text{2}_{3}$ mode, have the same multipolar moment (as indicated by the first number), the final THG efficiency will be enhanced up to 3 magnitudes, much more than the enhancement in situations where two cavity modes have different multipolar moment, for instance, TM$\text{2}_{1}$ and TM$\text{1}_{3}$ mode. It can be believed that this phenomenon is important and will open new opportunities in nonlinear optics.

Developing and controlling single-photon emitters by tip-enhanced photoluminescence nanospectroscopy and nano-localized force control  

JUN YAN  
(Presenter), CHUANLIN LI, MOLLY A. MAY, TAO JJANG, MARKUS B. RASCHKE, Department of Physics, Department of Chemistry, and JILA, University of Colorado - Boulder — Strain-induced single-photon emitters in two-dimensional (2D) materials associated with deterministically located quantum wells could pave the way for quantum state transfer in solid state qubits. However, far-field optical techniques can neither spatially resolve these highly localized emitters nor allow for deterministic control of the light-matter interaction. Here, we develop plasmonic tip-induced, nano-localized force control to generate, tune, and control nano-localized quantum states in monolayer WSe$_2$ by tuning the strain gradients and the plastic deformation depth with sub-nanometer precision. We investigate exciton funnelling behavior and strain-induced bandgap modification from spectral peak shift and intensity of the indented nanostructures, which could possibly help to reveal the deterministic formation of single-photon quantum emitter. In addition, we provide a perspective on this tip-based nanocavity approach, which has been used to probe in photoluminescence bright and dark exciton emissions, localized states, and interlayer excitons in 2D heterostructures.
10:12AM F11.00012: *Velocity, Release and Attack Angle and Distance of an Ultimate Frisbee Disc* ANDREW POLCARI (Presenter), Ithaca Coll — This study is exploring how an ultimate frisbee disc rotates and acts while in flight using high-speed video. The relationship between angular speed and flight stability and optimal release angle and flight distance will be explored. The methods used will all be physical methods as opposed to a re-creation of a computer program. By attaching a disc to a motor and spin it at varying speeds, we will be able to determine the optimal angular velocity and relate those measurements to flight stability. To measure the distance, this project will use a high-speed camera to measure the angle of release and then correlate those data to the distance travelled by that specific throw. The results explore pitch, roll, and velocity. This project will show that physics can be related to any topic and discipline. It relates a sport, hobby and past time all together and shows how physics affects the classic piece of plastic we toss between us.

*Ithaca College Physics and Astronomy Department*

10:24AM F11.00013: Study on the Apparent Weight of Hourglass Caused by Sand Flow CHUNZHEN LI (Presenter), Nankai University — Due to the acceleration of the sand centroid, the hourglass's apparent weight will change slightly with time in the process of sand flow, which is the sum of the effects of each part of the sand in the hourglass. By establishing an hourglass model, in this paper we can get the relationship between the centroid position vector of each part of the sand and the time, and then get the time-dependent acceleration of the overall centroid of the sand. According to the shape of the hourglass itself and the parameters of each part, the process of sand flow can be divided into five stages. Then the mismatch between theoretical and experimental values is analyzed, and the imperfect elastic collision between sand and the bottom of the hourglass is used to explain and further revise the previous theory.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F12 APS/SPS: Undergraduate Research VII 112 - Matthew Wright, Adelphi University - Tag(s): Undergrad Friendly
8:00AM F12.00001: netQuil: A quantum playground for distributed quantum computing simulations*  MATTHEW RADZIHOVSKY (Presenter), ZACHARY ESPINOSA, Stanford Univ — NetQuil is an open-source Python framework for quantum networking simulations built on the quantum computing framework pyQuil, by Rigetti Computing. NetQuil is built for testing ideas in quantum network topology and distributed quantum protocol. This platform allows users to create multi-agent networks, connect parties through classical and quantum channels, and introduce realistic noise and device models. NetQuil also makes running multiple trials for non-deterministic experiments, reviewing traffic in real-time, and synchronizing agents based on local and master clocks simple and easy. We provide an overview of the state of distributed quantum protocol, as well as a basic introduction to netQuil's framework. We present several demonstrations of canonical quantum information protocol built using netQuil's distributed quantum gates and pyQuil. We hope netQuil allows users to explore the quantum playground and the possibilities of distributed quantum computing.

*We wish to thank Yewon Gim, the entire team at AT&T Foundry for providing support and helpful feedback throughout development.

8:12AM F12.00002: Hardware and Software for Qubit Control*  GREGORY PENN (Presenter), Department of Physics, Temple University, ALESSANDRO LANDRA, Centre for Quantum Technologies, National University of Singapore, RAINER DUMKE, Division of Physics and Applied Physics, Nanyang Technological University, MICHAEL LIM, Department of Physics & Astronomy, Rowan University — Quantum computers have the potential to exponentially increase the speed of certain algorithms. Such a quantum information processor is currently under construction at the Centre for Quantum Technology, Singapore. It is based on Josephson-junction qubits, the basic unit of quantum information. A crucial part of this system is the control of the individual qubits and their interaction. We describe the experimental setup for qubit spectroscopy to measure the excitation energy of each qubit. Modular hardware was realized to initialize and read out qubit states using a phase measurement technique.

*The authors acknowledge support from NSF-IRES 1559410.
8:24AM F12.00003: Nonlinear Optical Properties of Janus 2D Materials: A First Principles Study*  ALEX STRASSER (Presenter), HUA WANG, XIAOFENG QIAN, Texas A&M Univ — Two-dimensional (2D) transition metal dichalcogenides (TMDCs) have provided a unique materials platform with a variety of interesting optoelectronic properties and great potential for device applications. Janus 2D TMDCs is a new class of 2D materials with lower symmetry. Here we present our first-principles study of nonlinear optical properties in Janus 2D TMDCs. Electronic structures such as linear and nonlinear optical properties were calculated using first-principles density functional theory and analyzed in combination with group theory. The microscopic origin of these nonlinear optical properties of Janus TMDs is elaborated by k-point resolved absorption, shift current, and shift vector. We found that the absence of horizontal mirror plane enables the out-of-plane second harmonic generation (SHG) and other nonlinear optical phenomena, such as shift photocurrent and circular photocurrent. Janus 2D materials, therefore, offer a unique platform for exploring nonlinear optical phenomena and designing configurable layered nonlinear optical materials.

*This work was supported by the National Science Foundation (NSF) under award no. DMR-1753054. First-principles calculations were conducted with advanced computing resources provided by Texas A&M High Performance Research Computing.

8:36AM F12.00004: Reflectance of Graphene Coated Metals: Copper & Nickel*  MATTHEW CRITCHLEY (Presenter), DANIEL FINKENSTADT, STEVEN MONTGOMERY, RAJRATAN BASU, US Naval Academy — Accelerator technology often requires the presence of a photocathode electron source. Unfortunately, these materials are often very volatile. In order to improve the lifetime of materials without compromising their quantum efficiency, we look at the optical effects of monolayer graphene coatings on known substances. This project looks at the optical effects a monolayer coating of graphene has on copper and nickel surfaces. We analyze the optical effects via theory by developing an effective dielectric medium model, computation by using Density Functional Theory, and experiment with graphene coated copper samples. In addition, we plan to conduct specular reflection for graphene off nickel. These methods allow us to compare the reflectivity and dielectric constant between pure and graphene coated metals over the visible light spectrum.

*Office of Midshipman Research U.S. Naval Academy
Bowman Scholars Program U.S. Naval Academy
8:48AM F12.00005: Modeling the Progression of Women in STEM Fields  JESSICA JENSEN (Presenter), Engineering, Roger Williams University, DARRELL VALENTI, Mathematics, Roger Williams University, JULIETTE M CAFFREY, Engineering, Roger Williams University, JENNIFER PEARCE, Physics, Roger Williams University — Creating a mathematical model to predict participation in STEM fields would allow social scientists to quantitatively examine their theories, as well as provide a multitude of simulated populations to explore. Furthermore, these models can be used to predict the result of interactions between populations. One model that simulates the progression of women through male-dominated academic fields explores the idea of homophily between women as the driving force for their advancement. We propose an alternate model that simulates the progression of women in these male-dominated fields as a predator-prey type system. We believe that such a model more effectively describes the population dynamics.

9:00AM F12.00006: Deep Learning for Engineering Problems  ANANYANANDA DASARI (Presenter), Mechanical Engineering, INDIAN INST. OF TECH MADRAS, DEEPAK SOMASUNDARAM, Mechanical Engineering, College of Engineering, Guindy, VISHAL V.R. NANDIGANA, Mechanical Engineering, INDIAN INST. OF TECH MADRAS — In this paper, we propose a data driven deep learning model to solve transport phenomenon without incorporating physics based PDEs. Here, a deep Recurrent Neural Network (RNN) with Long Short Term Memory (LSTM) is used to solve a general 2D heat conduction phenomenon. The problem is solved for square and circular geometries. The model is trained on 1670 cases for square domain and 3000 cases for circular domain. The cases include both Dirichlet boundary conditions and Neumann boundary conditions. The model was then tested on 610 cases for square geometry and 1000 cases for circular geometry. Our proposed RNN-LSTM model shows a 3-order speed up in computational time compared to conventional finite difference method. Moreover, the predicted solution shows 99.9% accuracy. Also, our proposed model can easily be generalized and extended for other transport phenomenon problems, both linear and nonlinear. We test this by considering a simple nonlinear advection-conduction phenomenon. We believe the RNN-LSTM deep learning method has the ability to predict transport phenomenon in applications like aerospace, automobile, semiconductor and thermal management domains like electronic cooling applications, without incorporating physics based PDEs.

9:12AM F12.00007: The phenomenon of nonlinear coupling in an asymmetric pendulum  QIUHAN JIA (Presenter), YAO LUO, Nanjing Univ — We investigate the nonlinear effect of a pendulum with the upper end fixed to an elastic rod which is only allowed to vibrate horizontally. The pendulum will start rotating while oscillating without initial angular momentum. We explain it as amplitude and phase modulation due to nonlinear coupling between the two dimensions. We build the theoretical model and obtain the pendulum's equations of motion. The pendulum's motion patterns are solved numerically and analytically using the method of multiple scales. In the analytical solution, the conversion period not only depends on the dynamical parameters, but also on the pendulum's initial releasing positions, which is a typical nonlinear behavior. The analytical approximate solutions are consistent with numerical solutions with good accuracy.
9:24AM F12.00008: Individual and Collective Transient Behavior near Daido's Aging Transition  AUSTIN HOWARD (Presenter), DAVID MERTENS, Physics, Eckerd College — We report on individual and collective behavior of an ensemble of electronic oscillators near the Daido aging transition. Work by Diado and others indicate that the collective response in an aging transition of identical oscillators should possess dynamics that are nearly identical to that of the individuals. Theoretical calculations for our oscillators predict a Hopf transition, which we have confirmed with measurements of individual transient behavior. However, it was previously reported that the collective behavior of these oscillators near the aging transition exhibited an intriguing discontinuity, seemingly contradicting the above conjecture. It turns out that this seeming contradiction arose from a high sensitivity to the system bifurcation value. We will explore the boundaries of Daido's hypothesis and examine how variation in non-bifurcation parameters across the population lead to collective behavior that differs from that of an individual oscillator.

9:36AM F12.00009: A Theoretical Study of Chaos in Higher Dimensions*  JOSE PACHECO (Presenter), AJIT HIRA, DAVID NUNN, ARRICK GONZALES, RAMKRISHNA KHALSA, RUBEN RIVERA, Northern New Mexico College — We use the computational tools available to us to explore the possibility of creating chaos in four dimensions and in higher dimensions. Even basic physics leads to unexpected results, when we go beyond 3-dimensional space. In four dimensions, we can create Klein bottles, can tape the edges of two Möbius strips together, and can invent sailing knots of stunning complexities: all of the knots that work in 3 dimensions will fall apart in higher dimensions. Our calculations for gravitational force reveal that the force drops as $1/(R^D - 1)$, where $D$ is the dimension and $R$ is the distance between the interacting objects. We first review generalizations of the Li and Yorke definition of chaos to difference equations in $\mathbb{R}^n$, and the higher dimensional conditions leading to the existence of chaos. Then we consider many 3-D, 4-D, 5-D, and 6-D Generalized Henon Maps (GHMs). We look for fixed points that are locally stable. We find that for many values of the parameter $\alpha$, chaotic behavior exists in dimensions $D = 4, 5$ and 6. We also discuss the possibility of uncovering the existence of some of the higher dimensions, by delineating the 3-D projections of chaotic behavior from higher dimensions.

*New Mexico AMP program, funded by NSF, provided some financial support for this research.
9:48AM F12.00010: Fractional derivative of composite functions: exact results and physical applications*  GAVRIL SHCHEDRIN, NATHAN C SMITH, ANASTASIA GLADKINA, JOSHUA LEWIS (Presenter), JOEL BEEN, LINCOLN CARR, Physics, Colorado School of Mines — We examine the fractional derivative of composite functions and present a generalization of the product and chain rules for the Caputo fractional derivative. We derive the product rule with the expression of the Caputo fractional derivative as an infinite expansion of integer order derivatives and the chain rule as a generalization of di Bruno's formula. Unlike the Leibniz and di Bruno formulae that characterize an integer-order derivative of a product of functions and composite functions, respectively, and which result in a finite series of lower order derivatives, the fractional analogs of these formulae produce an infinite series of fractional derivatives of the constituent functions. These results are important for a comprehensive description of transport phenomena through multiscale physical systems and biological structures, e.g., porous materials, disordered media, and neuron clusters. We demonstrate the utility of these results by the evaluation of the Caputo fractional derivative of hyperbolic tangent and suggest that the application of the derived chain and product rules to elementary functions, whose Caputo fractional derivative is expressible as a generalized hypergeometric function, leads to an infinite series of generalized hypergeometric functions.

* Funded by NSF

10:00AM F12.00011: Why Polygons are Mostly Pointless  JOHN CHRISTENSEN (Presenter), JEREMY JORGENSEN, GUS HART, Brigham Young Univ - Provo — When performing materials calculations, one of the most computationally expensive calculations is performing an integral of the electronic band structure of a material. For reasons explained in the talk, integration techniques that rely on non-uniform sampling cannot utilize the full symmetry of the system. To ensure optimal symmetry reduction, calculations should be performed in the symmetrically irreducible Brillouin zone (IBZ). We present an algorithm for finding the IBZ for an arbitrary lattice.

10:12AM F12.00012: Transform as a vector? Tying functional parity with rotation angle of coordinate axes  SAYAK BHATTACHARJEE (Presenter), Department of Physics, Indian Institute of Technology Kanpur — A vector is defined as a quantity which remains unchanged under a rotation of coordinate axes. This definition is associated with the phrase 'transform as a vector'; however, students are frequently confused about the meaning of the phrase and seldom realize its significance. To remedy this, an exposition to this definition is pursued. As a central notion, quantities (triplets) of the form \( C = (\Phi(x), \Phi(y), \Phi(z)) \) (where \( x, y \) and \( z \) are coordinate points and \( \Phi \) is a real valued function) are investigated using the definition. This novel approach employs elementary mathematics to determine possible value(s) of rotation of axes angle \( \theta \) at which \( C \) may transform as a vector, even if it does not for all \( \theta \). A notable correspondence between the parity of function and rotation angle(s) is observed. The analysis, initially carried out in an orthogonal coordinate system, is subsequently generalized for skew coordinate systems. This work was accepted for publication in the European Journal of Physics in October 2019 [1].

Expansion of fractional derivatives in terms of an integer derivative series: physical and numerical applications*  
ANASTASIA GLADKINA, GAVRIL SHCHEDRIN, Colorado School of Mines, U. AL KHAWAJA, Physics, United Arab Emirates University, JOEL BEEN (Presenter), JOSHUA LEWIS, LINCOLN CARR, Colorado School of Mines — We use the displacement operator to derive an infinite series of integer derivatives for the Grünwald-Letnikov fractional derivative and demonstrate that the infinite series of integer order derivatives is the same for Grünwald-Letnikov, Riemann-Liouville, and Caputo fractional derivatives. With the first few terms of the infinite series, we find that for functions with a finite radius of convergence of their Taylor series, the corresponding integer derivative expansion has by an infinite radius of convergence. Specifically, we demonstrate a robust convergence of integer derivative expansion for the hyperbolic secant and tangent functions, characterized by a finite radius of convergence of the Taylor series R=pi/2. Moreover, for a plane wave with an infinite radius of convergence, we show the truncation error decreases as the number of terms in the expansion increases. We find that our numerical results closely approximates the exact solutions given by the Mittag-Leffler and Fox-Wright functions. Thus, we demonstrate that the truncated expansion is a powerful method for solving linear fractional differential equations.

*funded by NSF

Nonlinear tuning curves of a tuning fork  
LINTAO XIAO (Presenter), QIUHAN JIA, CHENYU BAO, Nanjing Univ — Cantilever beams of a tuning fork have both hardening and softening oscillation modes. Yet, teaching experiments concerning tuning forks usually only demonstrate their linear resonance. In this work, we introduce a simple experiment that can be used to measure the nonlinear tuning curve of a regular tuning fork. Using double-grating Doppler interferometry, our measurement accuracy reaches tens of micron. With this experimental setup, we observed typical nonlinear phenomena of the tuning fork such as the bent tuning curve and "jump phenomena". Our experiment is inexpensive and easy to operate, so it can readily be used as a lecture demonstration for undergraduate students.
10:48AM F12.00015: Anti-Cancer targeting and treatment using nanocarriers based drug delivery system  PRAGATI GUPTA (Presenter), Indian Inst of Technology Roorkee — Cancer is the second leading cause of death globally and recurring disease. Main problems associated with anti-cancer drugs is that it targets healthy cells along with cancer cells. Others include multidrug resistance, poor water solubility. Even small drug molecules get eliminated by the liver and kidneys. Cancer drugs need to have higher activity and selectivity and be non-toxic to healthy cells. Nanotechnology has the potential to revolutionize cancer diagnosis and therapy and they provide a great alternative for the classical drug delivery techniques. The reasons being improved drug tolerability, efficacy, decreased toxicities, enhanced solubility, stability and controlled release. Advances in protein engineering and material science have contributed to novel nanoscale targeting approaches that bring new hope to cancer patients. However, to date, there are only a few clinically approved nanocarriers that incorporate molecules to selectively bind and target cancer cells. This review examines some of the advanced formulations and discusses the challenges in translating basic research to the clinic and emphasizing the challenges in cancer treatment
References

Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F15 DFD DBIO: Swimming, Motility, & Locomotion 210/212 - Alison Patteson, Syracuse University

8:00AM F15.00001: Scattering of a fast-swimming bacterium off of a surface  ALEXANDER PETROFF (Presenter), SCHUYLER MCDONOUGH, BENJAMIN ROQUE, Clark University — The sediment bacterium Thiovulum majus is one of the fastest known bacteria. Each bacterium is spherical and covered in approximately 200 flagella, which propel cell at a speed of 600 micron/sec. When a cell collides with a surface, it often becomes hydrodynamically trapped. A bound cell exerts a force normal to the surface and rotates. These cells self-organize into active two-dimensional crystals of rotating cells. Here we present the first experimental observations of the scattering of a fast-swimming bacterium off of a flat surface. We show that the probability that a cell becomes bound decays exponentially with the angle at which the cell approaches the surface; cells colliding head on with the surface are most likely to become trapped. We examine the stability of bound cell and measure the timescale over which the cell orients normal to the surface. Finally we show that when a cell escapes, it leaves the surface at a fixed angle. These results give insight into the the ecology of fast-swimming sediment microbes as they navigate the water saturated pore spaces in which they live.
8:36AM F15.00002: Optically-Powered Microscopic Bubble Rockets*  SAMANTHA NORRIS (Presenter), MICHAEL REYNOLDS, ALEJANDRO CORTESE, PAUL L MCEUEN, Cornell University — Artificial microswimmers have attracted great interest recently, especially for applications in sensing and biology. In particular, micro-propulsion by producing bubbles using decomposition of a chemical fuel is an attractive method, but it requires a fuel source. In this talk, we demonstrate a new optically-powered approach to catalyst-free bubble self-propulsion that works in a broad range of fluids, including deionized water. These devices, approximately 100 microns in size, consist of encapsulated silicon photodiodes connected in series with two external electrodes. Under standard illumination conditions in a microscope, the photovoltaics drive water splitting at the electrodes and eject the resulting bubbles preferentially in one direction, propelling the device through fluid. These devices are fabricated and released in parallel using standard semiconductor technologies. We discuss the fabrication and characterization of these devices, demonstrate working bubble rockets, and discuss their efficiency and potential applications.

*This work is supported by the Air Force Office of Scientific Research (MURI: FA9550-16-1-0031), the National Science Foundation Graduate Research Fellowship Program (DGE-1650441), and the Cornell Center for Materials Research (DMR-1719875).

8:48AM F15.00003: Antagonism in multiple-cue chemotaxis in breast cancer cells*  SOUTICK SAHA (Presenter), Department of Physics and Astronomy, Purdue University, HYE-RAN MOON, BUMSOO HAN, School of Mechanical Engineering, Purdue University, ANDREW MUGLER, Department of Physics and Astronomy, Purdue University — Chemotaxis is defined as biased cell motion towards an external chemical gradient. It is a pivotal step in cancer metastasis where cancer cells move towards chemical cues and spread to different parts of the body. We used triple-negative breast cancer cells to study chemotaxis towards cues formed by multiple growth factors and found, surprisingly, that the bias in the movement was less pronounced when we combine two attractant gradients compared to when we have individual gradients. We study this antagonism using stochastic simulations and a simple analytic model.

*This work is supported by a Phase I Concept Award from the Purdue Center for Cancer Research.
9:00AM F15.00004: A universal mechanism for chiral swimming at low Reynolds number
DARIO CORTESE (Presenter), KIRSTY WAN, Living Systems Institute, University of Exeter — Eukaryotes evolved radically new ways to sense and respond to a constantly changing environment. Even single-celled microorganisms display near-deterministic navigation towards sensory cues. Helical alignment towards gradients is a ubiquitous mechanism by which ciliated and flagellated organisms achieve reorientation in three-dimensional space. This navigational strategy usually requires the presence of a specialised organelle which detects stimulus direction and an about-axis rotation of the organism. Here, we consider the biflagellate green alga *Chlamydomonas reinhardtii* which has an eyespot photosensor and rotates steadily at 2Hz in the absence of stimuli. We combine theory and experiment to reveal how *Chlamydomonas* actively modulates asymmetries in flagellar beating to produce axial rotation and steering. In previous models, helical swimming is usually assumed rather than derived. In contrast, in our model chiral axial rotation emerges naturally from the 3D flagellar dynamics. We perform high-speed imaging to measure key simulation parameters, which successfully reproduce the experimentally observed dynamics. Finally, we demonstrate how this coupling between signal detection and motor output constitutes a universal strategy for responding to an arbitrary, vectorial stimulus.

9:12AM F15.00005: Bacterial swarming: Motion under extreme forces?  IRAKLI GUDAVADZE (Presenter), JANELLE KORF, ERNST-LUDWIG FLORIN, University of Texas at Austin — Bacterial swarming is a rapid, collective movement of bacteria over a surface powered by rotating flagella [1]. Unlike swimming, swarming takes place in thin liquid films, constraining bacteria to two dimensions. So far, it always has been assumed that the film is thicker than the diameter of a bacterium, but its exact thickness has never been measured. Here we present a novel method for measuring film thickness with tens of nanometer precision. For *Bacillus subtilis* colonies grown on agar gels, we find film thicknesses as thin or even thinner than the diameter of a single bacterium. For thicknesses thinner than a single bacterium, surface tension forces are expected to be on the order of tens of nanonewtons. These forces are about 4 orders of magnitudes greater than forces bacteria experience during swimming [2]. It remains unclear how flagella driven motility can be achieved under such strong confinement.


9:24AM F15.00006: Analysis of run-reverse-reorient motility of Helicobacter pylori and its ΔChePep mutant

WENTIAN LIAO, Boston Univ, MAIRA A CONSTANTINO, National Institutes of Health, MANUEL RICARDO AMIEVA, Stanford University School of Medicine, RAMA BANSIL (Presenter), Boston Univ — The gastric disease causing bacteria, Helicobacter pylori utilize flagella driven motility and chemotaxis to detect external signals as they swim away from acid to cross the mucus layer and colonize the epithelial surface of the stomach. The lack of the chemotaxis regulator protein ChePep leads to increased reversal frequency (Howitt et al2). We analyze translational and cell body rotational motility data obtained by phase contrast microscopy to compare the speed and turn angle distribution of the wild type (WT) with the ΔChePep mutant and compare with run-reversal-reorient model and Resistive Force Theory calculations of torque. We observe higher reversal frequency of ΔChePep in agreement with previous observation, however the cell body rotational rate and torque are not influenced by the lack of protein ChePep. Interestingly, both WT and ΔChePep are most likely to maintain their initial run speed after a reorientation or a reversal event, although the distribution of the change in speed indicates that large speed changes by factor of two and beyond are possible.

*1Supported by NIH 1R01 GM131408-1: subaward from Univ. of Utah No. 10047369-S1 (R.B).

9:36AM F15.00007: Force and torque on a rotating helical flagellum near a boundary

BRUCE RODENBORN (Presenter), CESAR ROMERO, JIN LEE, Centre College, HOA NGUYEN, ORRIN SHINDELL, Trinity University — As a free swimming bacterium approaches a boundary, both the propulsive force and torque on its helical flagellum increase rapidly. Though a constrained helical swimmer pumps the fluid, a similar increase in force and torque occur near a boundary (Das et al. 2018). We use scaled macroscopic experiments to measure this functional dependence of the force and torque as a constrained rotating helical flagellum approaches a boundary. We keep the Reynolds number in the experiments much less than unity to model bacterial fluid dynamics. These Reynolds-number-scaled experiments are compared with numerical simulations that use the method of images for regularized Stokeslets (Ainley et al. 2008). The computations find a similar functional dependence of force and torque on boundary distance. We also compare the results to biological measurements that use total internal reflection fluorescence microscopy to simultaneously measure the distance to the boundary and the dynamics of the bacteria. We show that all of the data can be collapsed onto a single curve by non-dimensionalizing the force, torque and boundary distance appropriately.

*Centre College Faculty Development Committee
The Alcock Fund
9:48AM F15.00008: A minimal neural reaction-diffusion model which generates *C. elegans* undulation  HAROLD HASTINGS (Presenter), Physics, Bard College at Simon's Rock, JENNY MAGNES, Physics, Vassar College, KATHLEEN SUSMAN, Biology, Vassar College, CHERIS C CONGO, MIRANDA R HULSEY-VINCENT, Physics, Vassar College, ANSHUL SINGHVI, RIFAH TASNIM, NAOL NEGASSA, Physics, Bard College at Simon's Rock — The small (1 mm) nematode *Caenorhabditis elegans* has become widely used as a model organism; in particular the *C. elegans* connectome has been completely mapped and *C. elegans* locomotion has been widely studied (c.f. http://www.wormbook.org/). We describe a minimal reaction-diffusion model for the *C. elegans* central pattern generator (CPG) (c.f. Xu et al. 2018, Wen et al. 2012). We use simulation methods to show that a small network of FitzHugh (1961)-Nagumo (et al. 1962) neurons (one of the simplest neuronal models) can generate key features of *C. elegans* undulation (c.f. Magnes et al. 2017) and thus locomotion. Compare the neuromechanical model of Izquierdo and Beer (2015). We also investigate dynamics and stability of the model. References
Xu T et al. 2018. PNAS USA 115 E4493.

10:00AM F15.00009: Swimmers at low Reynolds number driven by Quincke rotation  ENDAO HAN (Presenter), LAILAI ZHU, JOSHUA SHAEVITZ, HOWARD A STONE, Princeton University — In biological systems, the rotation and oscillation of flagella and cilia play important roles in realizing certain functions, such as self-propulsion and fluid mixing. Most previous attempts to build artificial small swimmers use an oscillatory drive. Here we present an artificial swimmer at low Reynolds number driven by an elasto-electro-hydrodynamic instability [1] based on Quincke rotation: a sphere in oil rotates in the presence of a high DC electric field. In our experiments, by attaching thin elastic fibers to a solid plastic sphere, we created swimmers that exhibit diverse behaviors when varying different control parameters. We demonstrate that the flexibility of the fibers leads to multiple stable states, where the swimmer can have unidirectional rotation or oscillatory motion controlled by the applied field. Furthermore, we relate these modes of motion to the kinematic properties of the swimmer such as the rotational speed and the ability to generate locomotion.

10:12AM F15.00010: Aerotaxis in Sinorhizobium meliloti, a soil bacterium* JULIEN BOUVARD (Presenter), FREDERIC MOISY, HAROLD AURADOU, University of Paris Sud — The legume family needs the help of soil bacteria to fix the atmospheric nitrogen they need to grow. In order to do so, such bacteria, called rhizobia, are swimming towards the plants by following the chemical gradient created by their roots. One of the most common member of the rhizobia family, Sinorhizobium meliloti, is displaying this chemotactic behaviour as well as an aerotactic one. To study and compare this not yet referenced aerotaxis to the already found chemotaxis, we made a few experimental set-ups. The first one consists of a sealed chamber containing S. meliloti, in which we insert an air bubble. The second one is a capillary filled with bacteria, sealed at one end and closed with PDMS at the other. In these experiments, we notice the formation of a profile of motile bacteria peaked at the interface with the air bubble or the PDMS. We also uses microfluidic devices to control the oxygen gradient in which the bacteria are swimming. The characterization of the swimming behaviour in presence of oxygen will help us understand the motility of S. meliloti in situ, and thus could lead us to some culture optimizations.

*This work benefited from the funding Investissements d'Avenir of PALM LabEx (ANR-10-LABX-0039-PALM).

10:24AM F15.00011: Pairwise and Collective Interactions of a Model Swimmer at Intermediate Reynolds Numbers* THOMAS DOMBROWSKI (Presenter), Univ of NC - Chapel Hill, AMNEET PAL SINGH BHALLA, San Diego State University, BOYCE E. GRIFFITH, DAPHNE KLOTSA, Univ of NC - Chapel Hill — In between the two extremes of Stokes flow, home to microorganisms, and inviscid flow, home to human swimmers and large fish, resides the less studied intermediate Reynolds regime where millimeter to centimeter sized organisms thrive. Here, both viscosity and inertia play a role in an organism’s movement, and few models have been developed which relate movement to general underlying physical mechanisms. In this presentation, we investigate pairwise interactions between reciprocal, asymmetric dumb-bell swimmers at intermediate Reynolds numbers (Re). Even for a single swimmer we find interesting behavior: a transition in the swimming direction from a small-sphere-leading to a large-sphere-leading regime. Their pairwise interactions are just as surprising. We computationally vary a broad range of parameters and find a wealth of states: steady pairs that cooperatively swim differently from individual swimmers under identical conditions, bi-stable pairs, orbits, and diverging paths. Averaged flow fields are analyzed to further understand these configurations. We continue by studying the collective behavior of large numbers of swimmers (up to a hundred) in order to identify pairwise versus many-body emergent behaviors.

*This work is supported by NSF-CAREER DMR-1753148
10:36AM F15.00012: Hydrodynamics of biomimetic propulsion using externally and internally actuated fins*  ERSAN DEMIRER (Presenter), ALEXANDER ALEXEEV, Georgia Institute of Technology — We combine experiments and computer simulations to examine the hydrodynamics of two different actuation types that can be used to actuate an elastic plate to serve as a biomimetic propulsor in robotic fish. In the first case the elastic palate is actuated to perform sinusoidal plunging at the root, whereas in the second case the actuation is due to a distributed internal bending moment that represents piezoelectric actuation of smart materials such as macro fiber composites. The Morison equation is often used to characterize the forces acting on oscillating submerged bodies in terms of two parameters: the inertia and drag coefficients. We evaluate these parameters using our simulations and experiments. We find close agreement between the experiments and simulations for both actuation types. We find that the inertia coefficient depends strongly on the actuation type and the magnitude of the trailing edge displacement. We rationalize this dependency by analyzing the differences in the kinematics of the plates with different actuation types. Our results are useful for developing efficient propulsors for biomimetic underwater locomotion.

*The work is supported by NSF CBET 1705739

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F16 DQI: Superconducting Qubit Materials, Fabrication, and Coherence I

8:00AM F16.00001: T1 of transmons with electrodes that have different gaps.*  KUNGANG LI (Presenter), FREDERICK C WELLSTOOD, CHRISTOPHER J LOBB, SUDEEP DUTTA, RUI ZHANG, SHAHRIRI KESHVARI, DYLAN POPPERT, University of Maryland, College Park — Using double-angle evaporation we fabricated a transmon which had one electrode formed by deposition of nominally pure aluminum and the counter-electrode formed by deposition of oxygen-doped aluminum. On the same sapphire chip, during the same pump-down of the evaporator we deposited a second transmon with both electrodes made from nominally pure aluminum. The energy gaps of the electrodes depend on the film thickness and the grain size, which is affected by the oxygen doping. Measurements of the relaxation time $T_1$ of the first device at 10 mK revealed a typical lifetime of about 200 microseconds while the second device had a typical $T_1$ of about 90 microseconds. When $T_1$ was measured as a function of temperature up to 300 mK, the two devices showed significantly different onset temperatures for the appearance of thermal quasiparticles. We compared our $T_1$ vs T results to a model based on the behavior of nonequilibrium quasiparticles residing in the electrodes and extracted the energy gap and the density of the non-equilibrium quasiparticles.

* This work was supported by the Maryland Quantum Materials Center, the Joint Quantum Institute, and the Laboratory for Physical Sciences.
8:12AM F16.00002: Power and temperature dependence of High Q superconducting resonators
ASHISH ALEXANDER (Presenter), CHRISTOPHER WEDDLE, CHRISTOPHER RICHARDSON, Laboratory of Physical Sciences, University of Maryland, College Park — An integrated power and temperature dependent model of resonator quality factor predicts loss contributions from two-level systems and quasiparticles simultaneously. At millikelvin temperatures, in the presence of external power, the weak electron-phonon coupling between the phonons and quasiparticles may lead to quasiparticles thermalizing at a different temperature than phonons. Here we propose a two temperature power and temperature dependent model to evaluate resonator losses that considers quasiparticle and phonon temperatures to be different. Resonators fabricated from epitaxial molecular beam epitaxy grown aluminum and titanium nitride on float-zone refined silicon are evaluated to have quality factors above 1M. These results are analyzed with the proposed model and the contribution of various loss mechanisms will also be explored.

8:24AM F16.00003: Integration of InAs-Al Heterostructures into Microwave Circuit
JOSEPH YUAN (Presenter), MATTHIEU DARTIAILH, WILLIAM MAYER, NOAH GOSS, TRI D NGUYEN, KAUSHINI S WICKRAMASINGHE, KASRA SARDASHTI, JAVAD SHABANI, New York Univ NYU — Semiconductor-based Josephson junctions provide a platform to study the proximity effect and for the realization of topological superconductivity. Recently our group has demonstrated the possibility of having highly transparent contact between a superconductor and a semiconductor by combining high mobility Indium Arsenide (InAs) surface two dimensional electron gases (2DEGs) with epitaxially grown aluminum (Al) [1]. This allows for gate-tunable superconducting Josephson Junctions and consequently gate-tunable Transmons [2]. Here we present the integration of these InAs-Al heterostructures into microwave circuits such as Gatemon Qubits. The steps needed to fabricate on III-V material platform while mitigating microwave losses and microwave response will be discussed.


*We acknowledge support from the US Army Office of Research and the ARO/LPS QuaCGR fellowship.
**8:36AM F16.00004: Preprocessing Method for Microwave Resonator Fitting**  
KEEGAN MULLINS (Presenter), University of Colorado Boulder, COREY RAE MCRAE, DAVID PAPPAS, National Institute of Standards and Technology Boulder, JOSH Y MUTUS, Google Inc., HAOZHI WANG, National Institute of Standards and Technology Boulder, DAVID FORK, Google Inc. — We present a preprocessing method for S21 data from superconducting microwave resonators. In the field of quantum computing, it is becoming increasingly necessary to characterize loss in superconducting circuits to a higher degree of accuracy. The goal of the code implemented is to provide a rigorous standard for characterizing this loss. The method is implemented in python where the Diameter Correction Method, Inverse S21 method and Closest Pole and Zero method are all used in conjunction with the preprocessing. Accuracy of the preprocessing method is tested by comparing results from computer simulated resonator data from circuit elements to calculated values from the circuit elements of the simulated data. The preprocessing method entails a removal of the S21 data background by linear fit of the end points for both magnitude and phase, as well as the option to remove background from a user background file (a dataset of the same format without resonator behavior to establish a baseline). Testing the preprocessing method across varying parameters of circuit elements allows us to view correlation between preprocessing and error in determination of parameters.

*We acknowledge support from NIST Boulder, JILA labs CU Boulder and Google Quantum Computing.*

**8:48AM F16.00005: Materials Engineering in Superconducting Qubits**  
ALEXANDER PLACE (Presenter), BASIL M SMITHAM, LILA RODGERS, PRANAV MUNDADA, MATTIAS V FITZPATRICK, SARA SUSSMAN, ANJALI PREMKUMAR, JACOB BRYON, BERTHOLD JAECK, GUANGMING CHENG, HARSHVARDHAN BABLA, TRISHA MADHAVAN, AUSTIN FERRENTI, ANDRAS GYENIS, ROBERT J. CAVA, NAN YAO, NATHALIE DE LEON, ANDREW HOUCK, Princeton University — During the early days of superconducting qubits, increases in coherence times were frequently driven by improvements in materials and fabrication techniques. More recent advances have focused on manipulating capacitive, inductive, and Josephson energy scales, as well as engineering favorable qubit environments. In this talk we again focus on materials engineering of qubits. We explore how new materials and surface treatments can improve coherence times. Furthermore, we correlate the results of materials spectroscopy and time domain measurements to provide insight into relaxation mechanisms.

*Army Research Office Grant W911NF1910016, National Science Foundation MRSEC Grant DMR-1420541, National Defense Science and Engineering Graduate Fellowship*
9:00AM F16.00006: Observation of individual two-level defects at material surfaces using circuit QED  
TIMOTHY KOHLER (Presenter), CHIH-CHIAO HUNG, University of Maryland, College Park, KEVIN OSBORN, NEDA FOROUZANI, Laboratory of Physical Science —  
The coherence of superconducting qubits have grown exponentially over the last decade. However, the coplanar electrodes used to shunt the JJ capacitance contain ubiquitous two-level system (TLS) defects on its surfaces. These defects are a major source of loss and decoherence in general, and the characteristics of the surface TLS are largely unknown. In an aluminum thin film on sapphire substrate we observe individual surface TLS using a DC electric-field bias in an interdigitated shunting capacitor with a submicron linewidth and line spacing. We use an electrical bridge of capacitors to apply the dc bias to manipulate the TLS energies allowing us to observe a hyperbolic dependence as well as splittings with the resonator. This technique allows us to capture the TLS average dipole moment as well as coherence time.

9:12AM F16.00007: TBD [Invited]  
DANNA ROSENBERG (Presenter), Massachusetts Institute of Technology — tbd

9:48AM F16.00008: The dielectric dipper: a differential technique to measure dielectric loss tangents with high sensitivity*  
ALEXANDER P READ (Presenter), KAICHENG LI, BENJAMIN J. CHAPMAN, CHAN U LEI, VIJAY JAIN, Yale University, CHRISTOPHER AXLINEN, ETH Zurich, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Yale University — Dielectric loss is suspected to limit superconducting qubit lifetimes. This could be tested by a measurement capable of detecting bulk dielectric loss smaller than the bound inferred from recent experiments (i.e., loss tangent less than $10^{-7}$). We have devised a method for characterizing bulk dielectric loss with a sensitivity on the order of $10^{-8}$. The method is compatible with cryogenic temperatures and single-photon powers and does not require lithographic processes. This allows for rapid comparison of isolated substrates, processing techniques, and their statistical variations. Such comparisons will inform designs and practices to better minimize dielectric loss. We present experimental comparisons of common dielectric substrates measured using this method.

*This research is supported by US Army Research Office modular grant W911NF-18-1-0212.
10:00AM F16.00009: Transmon qubit in a magnetic field: Evolution of coherence and transition frequency

MARTIN WEIDES (Presenter), University of Glasgow, ANDRE SCHNEIDER, TIM WOLZ, MARCO PFIRRMANN, MARTIN SPIEKER, HANNES ROTZINGER, ALEXEY V. USTINOV, Karlsruhe Institute of Technology — We report on spectroscopic and time-domain measurements on a fixed-frequency concentric transmon qubit in an applied in-plane magnetic field to explore its limits of magnetic field compatibility. We demonstrate quantum coherence of the qubit up to field values of $B=40mT$, even without an optimized chip design or material combination of the qubit. The dephasing rate $\Gamma_\phi$ is shown to be unaffected by the magnetic field in a broad range of the qubit transition frequency. For the evolution of the qubit transition frequency, we find the unintended second junction created in the shadow angle evaporation process to be non-negligible and deduce an analytic formula for the field-dependent qubit energies. We discuss the relevant field-dependent loss channels, which cannot be distinguished by our measurements, inviting further theoretical and experimental investigation. Using well-known and well-studied standard components of the superconducting quantum architecture, we are able to reach a field regime relevant for quantum sensing and hybrid applications of magnetic spins and spin systems.

*European Research Council (No. 648011), Deutsche Forschungsgemeinschaft (WE4359/7-1, INST121384/138-1), Helmholtz Association, Carl-Zeiss-Foundation, Helmholtz International Research School for Teratonics.

10:12AM F16.00010: Design of The Merged Element Transmon Qubit

SUNGOH PARK (Presenter), University of Colorado Boulder, RUICHEN ZHAO, COREY RAE MCRAE, National Institute of Standard and Technology Boulder, JUNLING LONG, TONGYU ZHAO, University of Colorado Boulder, RUSSELL LAKE, Bluefors, MUSTAFA BAL, HAOZHI WANG, DAVID PAPPAS, National Institute of Standard and Technology Boulder — Transmon qubits are one of the most promising candidates for building a universal quantum processor. They consist of two discrete elements: a nanoscale Josephson junction (JJ) and a coplanar capacitor. In conventional transmon designs, the plates of the shunt capacitor have to be very large to achieve low participation ratio of the lossy interfaces. To circumvent this issue, we propose to engineer the device so that the electric field distribution is confined to junction dielectric by merging the capacitor and JJ into a single superconductor/dielectric/superconductor trilayer structure such that the frequency, anharmonicity, and $E_J/E_C$ parameters are in the transmon regime. We refer to this architecture a mergemon to distinguish it from conventional designs. We explore different low-loss dielectrics such that the trilayer itself would provide not only the nonlinear inductance but also most of the capacitance of the transmon qubit. By FEM based simulation, we design the mergemon qubit-readout resonator to be in the strong dispersive regime. We also verify that this design can be realized with standard optical lithography process. Finally, we also discuss possibility of leveraging the state-of-the-art molecular-beam epitaxy technology to enhance the coherence of the mergemon.
10:24AM F16.00011: Improving the performance of superconducting coplanar waveguide resonators using interface engineering*  ARCHAN BANERJEE (Presenter), Lawrence Berkeley National Laboratory, MOHAMMED ALGHADEER, AHEMD HAJIR, King Fahd University of Petroleum and Minerals, JOHN MARK KREIKEBAUM, University of California, Berkeley, FRANK OGLETREE, VIRGINIA ALTOE, Lawrence Berkeley National Laboratory, SALEEM RAO, King Fahd University of Petroleum and Minerals, IRFAN SIDDIQI, University of California, Berkeley — Superconducting resonators are a key component in quantum circuits. While extensive research has explored techniques to improve the quality factor of such devices, the precise structure of amorphous dielectric layers on surfaces and interfaces and their associated loss mechanism remains a topic of active discussion. In this study, we explore the characterization and the fabrication of niobium coplanar waveguide resonators with more than $10^6$ internal quality factor at single-photon-excitation power (measured at 100 mK) for a variety of different surface treatments. Following electrical measurements, resonator samples have been probed using a suite of structural characterization tools (XPS, TEM and AFM) in order to correlate the efficacy of surface treatment with resonator quality factor. We also compare our measurement results with numerical simulations.

*This work was funded by U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05-CH11231 within the QISLBNL program.

10:36AM F16.00012: Reliable Growth of TaN Superconducting Film with Atomic Layer Deposition for Quantum Circuit Applications*  WONHO SONG (Presenter), Ulsan Natl Inst of Sci & Tech, SUNGCHUL JUNG, SK Hynix, JUNHYUNG KIM, Ulsan Natl Inst of Sci & Tech, GAHYUN CHOI, JOONYOUNG LEE, YONUK CHONG, Korea Research Institute of Standards and Science, KIBOG PARK, Ulsan Natl Inst of Sci & Tech — Atomic layer deposition (ALD) is a well-known method to grow a thin film which can ensure the uniformity and conformality of the grown film. In this work, several different thicknesses of TaN thin films are grown on SiO$_2$/Si or Si substrates with plasma enhanced ALD process using the Tris(diethylamido)(tert-butylimido)tantalum(TBTDET) precursor reacted with H$_2$ gas. The grown TaN films show superconductivity reproducibly and their transition temperatures vary in the range of 3-5 K depending on the film thickness. The superconducting transition temperature and microwave transmission properties of TaN films will be analyzed in terms of their correlation with DC transport parameters including carrier type, carrier density, and carrier mobility obtained from Hall effect measurements.

*NRF-2019R1F1A1057767, NRF-2019M3E4A1080198
10:48AM F16.00013: Microwave Loss in High-Q Titanium Nitride Resonators  RUI ZHANG (Presenter), ASHISH ALEXANDER, University of Maryland, College Park, CHRISTOPHER RICHARDSON, Laboratory of Physical Sciences, FREDERICK C WELLSTOOD, University of Maryland, College Park, BENJAMIN PALMER, Laboratory of Physical Sciences — We have measured the loss in a superconducting thin film titanium nitride microwave resonator from 20 mK to 1 K and at different stored microwave powers. The titanium nitride film had a superconducting transition temperature of $T_c = 5.5$ K and was grown in an MBE by reactively reacting evaporated titanium in a nitrogen plasma. The measured internal loss of the resonator is found to decrease by approximately a factor of 10 from $Q^{-1} = 2.5 \times 10^{-6}$ at low applied microwave powers and low temperatures to $Q^{-1} = 2.5 \times 10^{-7}$ at large applied powers and a temperature of 600 mK. We compare the measured $Q$ data to a model based on loss from the interaction of the superconducting resonator with lossy two-level systems and separately to a model we have developed based on non-equilibrium quasiparticles accumulating in regions of the TiNx film with a lower superconducting gap ($D$). To distinguish between these competing models, we will also discuss results where we apply superconducting pair-breaking infrared light directly to the resonator device and measure the loss.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F17 DQI: Focus Semiconductor Spin Qubit Readout 203 - Jason Petta, Princeton University - Tag(s): Focus

8:00AM F17.00001: Readout of small-scale semiconductor spin-qubit arrays [Invited]  ANASUA CHATTERJEE (Presenter), Niels Bohr Institute, University of Copenhagen — The engineering of readout methods becomes crucial as single qubits are scaled up in linear and two-dimensional arrays to form NISQ processors. In particular, fast, high-fidelity and simultaneous measurements across these small arrays are essential. I will present our work on readout techniques and scaling efforts, in particular involving RF-reflectometry, in small two-dimensional arrays of quantum dots in GaAs and silicon. In these systems we utilize techniques such as crosstalk mitigation, multi-qubit DC and pulse calibration, sensor compensation, virtual gates, and adaptive searching in high-dimensional spaces. First, I will discuss simultaneous, single-shot, and interlaced measurements for singlet-triplet spin qubits, performed via four independent sensors spaced across a GaAs chip. I will also show single-shot reflectometry measurements via compact gate-based dispersive sensing, carried out in a two-dimensional CMOS silicon array. These methods, combined with pulsed-gate techniques, enable deterministic single-electron shuttling within the array, and may be beneficial for many other quantum-dot devices or spin- and charge-based hybrid systems.

*In collaboration with Fabio Ansaloni, Federico Fedele, Heorhii Bohuslavskyi, Saeed Fallahi, Geoffrey C. Gardner, Michael J. Manfra, Louis Hutin, Maud Vinet, Yann-Michel Niquet, Silvano De Franceschi, and Ferdinand Kuemmeth.
Cascade-Based Fast, High-Fidelity and Scalable Spin Readout

CORNELIS VAN DIEPEN (Presenter), TZU-KAN HSIAO, UDITENDU MUKHOPADHYAY, Delft University of Technology, CHRISTIAN REICHL, WERNER WEGSCHEIDER, ETH Zürich, LIEVEN M VANDERSYPEN, Delft University of Technology — Spin-qubits based on gate-defined semiconductor quantum dots are a promising platform for quantum computation and simulation. An important advantage of quantum dots is their small footprint. The dot pitch is about 100 nm, hence 100 million dots fit on 1 mm². A problem is that qubit readout with charge sensing based on capacitive coupling only enables to sense nearby quantum dots and placing charge sensors within the quantum dot array hosting the qubits is detrimental for connectivity. Here, we report on cascade-based fast, high-fidelity and scalable spin readout. The cascade consists of an initial charge transition, far away from the sensor, and subsequent charge transitions induced by Coulomb repulsion, with the final transition nearby the sensor. Combined with spin-to-charge conversion a cascade enables the readout of charge and spin occupation of quantum dots remote from the charge sensor. We demonstrate fast and high-fidelity spin readout by performing Pauli spin blockade with a cascade implemented in a quadruple dot with a sensing dot. The cascade-based readout is a promising alternative for readout of large quantum dot arrays compared to gate-dispersive readout or state transfer via either shuttling or logical operations.

*The work is supported by NWO, ERC and SNF.

Fast charge sensing in undoped silicon quantum dots with radio-frequency reflectometry

AKITO NOIRI (Presenter), KENTA TAKEDA, JUN YONEDA, TAKASHI NAKAJIMA, Center for Emergent Matter Science (CEMS), RIKEN, TETSUO KODERA, Department of Electrical and Electronic Engineering, Tokyo Institute of Technology, SEIGO TARUCHA, Center for Emergent Matter Science (CEMS), RIKEN — Fast and sensitive charge sensing is an essential ingredient in quantum dot (QD) based spin qubit experiments. A performance of the charge sensing can be drastically improved by embedding the sensor in a radio-frequency (rf) tank circuit [1]. While the technique is commonly used in depletion-mode devices, applying it to accumulation-mode devices is a challenge due to a large parasitic capacitance by accumulation gates [2]. In this presentation, we report how to reduce this capacitance and realize charge sensing by the rf reflectometry in undoped Si/SiGe QDs. To this end, we introduce a specially designed device geometry comprising a small accumulation gate area [3]. We observe that the reflected rf power changes more than 30 dB by modulating the sensor conductance, which allows sensitive charge sensing. We achieve single-shot singlet-triplet readout with a SNR of 6 in an integration time of 0.8 μs.

References:

*This work was partially supported by CREST, JST (JPMJCR15N2, JPMJCR1675), Q-LEAP project initiated by MEXT (JPMXS0118069228), JSPS KAKENHI Grants Nos. 26220710, 17K14078, 19K14640, 18H01819.
9:00AM F17.00004: Rapid high-fidelity spin state readout in Si/SiGe quantum dots via radio-frequency reflectometry*  
JJ NELSON (Presenter), ELLIOT CONNORS, JOHN NICHOL, University of Rochester — Radio-frequency (rf) reflectometry, while enabling rapid high-fidelity readout of GaAs spin qubits, is challenging to implement in accumulation-mode Si quantum dot devices. The difficulty arises when a large parasitic gate capacitance is distributed along a relatively large resistance two-dimensional electron gas (2DEG). Here we will present minor design changes that when implemented in a Si/SiGe quantum dot device enable charge readout fidelity above 99.9% in 300ns using rf reflectometry. The rf compatible Si design can perform single-shot readout of spin states via spin-selective tunneling in microsecond integration times. We will also show high fidelity singlet and triplet readout of a double quantum dot via Pauli spin blockade. With the use of a charge latching mechanism we achieve a maximum fidelity of 99.0%.

*Research was sponsored by the Army Re-search Office and was accomplished under Grant Num-bers W911NF-16-1-0260 and W911NF-19-1-0167.

9:12AM F17.00005: Repetitive Quantum Nondemolition Measurement of a Silicon Spin Qubit Using Different Decodings  
XIAO XUE (Presenter), Delft University of Technology, BENJAMIN D’ANJOU, McGill University and University of Konstanz, THOMAS F WATSON, Delft University of Technology, DAN R. WARD, DONALD E SAVAGE, MAX G LAGALLY, MARK G FRIESEN, SUSAN NAN COPPERSMITH, MARK ALAN ERIKSSON, University of Wisconsin-Madison, WILLIAM COISH, McGill University, LIEVEN M VANDERSYPEN, Delft University of Technology — Silicon spin qubits show great promise for fault-tolerant quantum computing. As an essential step towards practical quantum error correction, quantum nondemolition (QND) measurements are needed to efficiently detect the state of a logical qubit without totally losing track of its state. Here we implement QND measurements in a Si/SiGe two-qubit system [1], with one qubit as the logical qubit and the other as the ancilla. Making use of a two-qubit controlled-rotation gate, the state of the logical qubit is mapped onto the ancilla, followed by a destructive readout of the ancilla. In contrast, QND measurement does not destroy the logical qubit but keeps it at the same state after the collapse caused by the first measurement, which allows us to enhance the readout fidelity by multiple QND measurements. Moreover, we also make use of a new analysis method called soft decoding to extract additional information on the state of the logical qubit [2]. We compare the two methods and discuss the conditions for which soft decoding provides an advantage.

Single-shot single-electron spin readout with a single-lead quantum dot charge sensor

MARK R HOGG, ANDREY V TIMOFEEV, PRASANNA PAKKIAM, SAMUEL KEITH GORMAN, MATTHEW HOUSE (Presenter), MICHELLE Y SIMMONS, Univ of New South Wales — “Gate-based”, or dispersive, charge sensors for the readout of semiconductor spin qubits have been growing in popularity because these compact sensors integrate readout capability into electrical control structures. However, dispersive readout can only directly measure a spin state in a double quantum dot, either by Pauli blockade or with a large magnetic field gradient. Here we demonstrate a dispersively-probed single-lead quantum dot (SLQD) charge sensor which senses the charges on four quantum dots, each defined with P atoms in Si using scanning tunnelling microscope lithography. With this charge sensor we demonstrate single-shot, single-spin readout via energy-selective tunnelling. We achieve a voltage signal-to-noise ratio of 8 for charge detection with a measurement bandwidth of 15 kHz and demonstrate spin readout with high fidelities of up to 97.4% at 2.5 Tesla. The capacitive coupling between all four quantum dots and the charge sensor is strong enough that there is no loss of sensitivity for detecting the more distant quantum dots, up to about 100 nm away from the sensor. Good sensitivity, compact geometry, and long-range sensing makes the SLQD a promising choice of sensor for scaling up future atomic-precision single-spin qubit devices to larger numbers of qubits.

Theory of Pulsed Spectroscopy in Quantum Dots: Interdot Dynamics

ANDREW PAN (Presenter), HRL Laboratories, LLC — Understanding the energy structure and dynamics of excited states in quantum-dot qubits is critical for device design and operation. Incoherent methods for probing these quantities typically call for loading from neighboring baths or applying large external magnetic or RF fields. These methods may be problematic if they require operating conditions far from the intended qubit environment. We have developed a technique to characterize these quantities using typical tune-up conditions, relying on the incoherent dynamics of interdot charge transitions. In the first half of this two-part talk, we examine theoretically how tunneling, dephasing, and detuning-dependent relaxation affect the time-dependent populations near charge transition points and allow excited states to be resolved. We compare these expectations to experimental results in Si/SiGe quantum dots. Potential connections to the dynamics relevant for spin qubit readout are considered.

Pulsed Spectroscopy of Si/SiGe Quantum Dots: One- and Two-Electron Valley-Orbit Excited States

KATE RAACH (Presenter), HRL Laboratories, LLC — The one- and two-electron energy spectra of silicon quantum dots can be complicated due to the interplay of valley and orbital degrees of freedom, affecting all aspects of spin qubit operation. For instance, in exchange-only qubits, low-lying single electron excitations are relevant during coherent evolution, while the two-electron singlet-triplet splitting limits the initialization and readout fidelity. In the second half of this two-part talk, we present experimental data and analysis of this energy structure using pulsed techniques to simultaneously probe multiple valley and orbital states of double quantum dots. We discuss the variations in one- and two-electron structure across dots and as a function of bias and how they compare with theoretical expectations.
10:00AM F17.00009: Developing Monolithic Superconducting Resonators for Gate-Based Quantum Dot Readout  ZAC BARCIKOWSKI (Presenter), University of Maryland, College Park, MICHAEL DAVID STEWART, MUSTAFA BAL, National Institute of Standards and Technology, CHRISTOPHER RICHARDSON, Laboratory for Physical Sciences, DAVID PAPPAS, JOSHUA POMEROY, National Institute of Standards and Technology — Gate-based sensing using resonant circuitry has been identified as a promising path towards high fidelity, fast, and compact readout for semiconductor quantum computing architectures. By coupling a quantum dot (QD) system to an LC resonator, the state is inferred via the reflected phase response. The resistive loss in the discrete inductors and loss associated with wirebonds often limit measurement sensitivity. In contrast to oft used surface mount components, we have fabricated Nb superconducting resonators to reduce resistive loss and will explore additional high kinetic inductance materials. The resonators are intended for monolithic integration with QD gates to reduce resonator-gate loss. We present transmission and reflection data used to assess our ability to deterministically fabricate resonators with designed inductance and capacitance values. Efforts to optimize resonance quality factor and integrate resonators with QDs are discussed.

10:12AM F17.00010: Non-Markovian qubit spectroscopy in cavity QED  ZOÉ MCINTYRE (Presenter), WILLIAM COISH, McGill Univ — The strong-coupling regime of cavity quantum electrodynamics (QED) can be identified spectroscopically from a peak splitting (~qubit-cavity coupling) that is large compared to the qubit decoherence and cavity decay rates. This interpretation normally relies on a Markovian model of qubit dynamics together with input-output theory. A Markovian description may however break down for charge qubits (coupling to ~1/f noise) or spin qubits (coupling to a slow nuclear-spin bath). Motivated by very recent work showing strong coupling of spin/charge qubits coupled to superconducting microwave resonators, we use a generalized input-output theory to account for a generic non-Markovian environment. This allows us to calculate a spectroscopic lineshape that fully accounts for non-Markovian features and which may be relevant to recent experiments.
10:24AM F17.00011: Low-magnetic field single-spin qubit operation in isotopically enriched silicon* RUICHEN ZHAO (Presenter), TUOMO TANTTU, University of New South Wales, KUAN YEN TAN, Aalto University, BAS HENSEN, KOK WAI CHAN, JASON HWANG, ROSS LEON, CHIH-HWAN YANG, WILL GILBERT, FAY E. HUDSON, University of New South Wales, KOHEI M ITOH, Keio University, ANDREY KISELEV, THADDEUS D LADD, HRL Laboratories, ANDREA MORELLO, ARNE LAUCHT, ANDREW STEVEN DZURAK, University of New South Wales — Single-spin qubit readout traditionally relies on selective tunneling to a neighboring reservoir. It requires sophisticated microwave engineering to deliver high-frequency qubit drives to the quantum chip from room-temperature electronics, which will be a challenge for scaling of a silicon-based quantum processor. Here we present an alternative scheme where we use high-fidelity Pauli spin blockade readout to enable single-spin qubit operation in a magnetic field as low as 150mT. We discover the qubits decohere faster in low magnetic fields due to the background (800 ppm) $^{29}$Si nuclear spins in the isotopically enriched substrate. A simulation modeling the nuclear spin induced qubit frequency fluctuation produced results consistent with our experimental data. This work indicates that further isotopic enrichment may be needed to achieve the high fidelities required for a scalable quantum processor.

*This research is funded by the Australian Research Council (CE170100012), the US Army Research Office (W911NF-17-10198), and, in part, by Silicon Quantum Computing Proprietary Limited.

10:36AM F17.00012: Adiabatic conversion for qubit readout: Optimal pulse shapes and dephasing FELIX FEHSE (Presenter), Physics, McGill University, Montreal, Canada, MICHEL PIORO-LADRIERE, Physics, Université de Sherbrooke, Sherbrooke, Canada, WILLIAM COISH, Physics, McGill University, Montreal, Canada — Adiabatic conversion schemes are commonly used to measure quantum states. These schemes may include, e.g., spin-to-charge conversion for spins in quantum dots or parity-to-charge conversion for qubits based on Majorana zero modes. In all of these schemes, a common element is that dephasing is minimized at an "operating point" (e.g., for the 'spin' or 'parity' quantum number), but measurement-induced dephasing is maximized at the "measurement point". The balance between 'adiabaticity' and dephasing can be optimized to improve performance of these readout schemes. We give an explicit construction that allows for optimal state conversion in qubit readouts. Applying this scheme to the specific case of spin qubits in quantum dots, we show that a high-fidelity (better than 99.9%) single-shot all-electrical readout is possible.
Recent advances towards employing quantum dots (QD) as a platform for quantum computation and simulation have shown promising results [1]. However, as the control parameters space grows significantly with increasing number of QDs, working with large QD arrays is challenging. Thus, finding a scalable and non-heuristic control approach to tune the electronic configuration in QDs is necessary. Due to high-dimensional patterns defining dot states, machine learning (ML) algorithms present a natural solution.

In this project, we extend a recent proposal [3,4] of employing a ML-based auto-tuner to linear QD devices to the more general case of 2D arrays. We use a Thomas-Fermi solver to establish an ensemble of simulated measurements for 2x2 QD arrays. This data set allows us to train and evaluate an image-based classifier that maps the charge stability diagrams showing the electronic configuration of the QD device into classes defining the number of dots formed in the system. This work will set foundations for research on machine learning-based control of 2D QD devices.


Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F18 DSOFT: Non-Equilibrium Bioinspired Modes of Assembling Materials 205 - Cecilia Leal, University of Illinois at Urbana-Champaign - Tag(s): Invited
Bioinspired liquid crystal patterns to command living matter*
OLEG D LAVRENTOVICH (Presenter), Department of Physics, Chemical Physics Interdisciplinary Program, and Advanced Materials and Liquid Crystal Institute, Kent State University — Microscale biological systems such as swarms of swimming bacteria and cell tissues demonstrate fascinating out-of-equilibrium dynamics. This dynamics is difficult to control by factors other than transient gradients, such as gradients of nutrients; visual, acoustic and tactile communication channels that humans use to control large animals are not effective. To establish communication with microscale biological systems, we propose to use special class of nontoxic lyotropic chromonic liquid crystal with a long-range orientational order. The anisotropy axis of the liquid crystal can be designed as uniform or be pre-patterned into various structures. We describe how the patterned liquid crystals can be designed to command dynamics of two systems, (i) swimming bacteria; (ii) tissues formed by human dermal fibroblast cells. Topological defects in liquid crystals are demonstrated to impact the biological microstructures most strongly, causing spatial variation of bacterial concentration and cell phenotype. The control of active matter by patterned liquid crystals might result in new approaches to harness the energy of collective motion for micro-robotic, biomechanical, and sensing devices.

*The work is supported by DOE DE-SC0019105, NSF DMS-1729509, CMMI-1663394 grants.

Reaction-Diffusion Driven Pattern Formation in Soft Materials*
NANCY SOTTOS (Presenter), EVAN M LLOYD, LEON DEAN, JEFFREY MOORE, Beckman Institute, University of Illinois at Urbana-Champaign — Reaction-diffusion processes are versatile, yet underexplored methods for manufacturing that provide unique opportunities to control the spatial properties of materials, achieving order through broken symmetry. The mathematical formalism and derivation of equations coupling reaction and diffusion were presented in the seminal paper by Alan Turing [Phil. Trans. R. Soc. Lond. B 237, 37, 1952], which describes how random fluctuations can drive the emergence of pattern and structure from initial uniformity. Inspired by reaction-diffusion systems in nature, this talk will describe a new processing strategy predicated on the exploitation of an advancing polymerization front sustained through coupled reaction and thermal diffusion. The system uses the exothermic release of energy to provide a positive feedback to the reaction. In turn, this stimulates further exothermic energy release and a self-propagating reaction “front” that rapidly moves through the material – a process called frontal polymerization. We recently reported the frontal ring-opening metathesis polymerization (FROMP) of dicyclopentadiene (DCPD) that exhibits the high energy density, high reactivity, relatively long pot life, and low viscosity required for the synthesis of high-performance thermosetting polymers and composites [Robertson et al., Nature, 557 (2018)]. This talk will describe several novel methods to control thermal transport in this system, giving rise to symmetry breaking events that enable complex, emergent pattern formation and control over growth, topology, and shape.

*AFOSR Grant # FA9550-16-1-0017

Silvia Vignolini Invited Talk

Jay Groves Invited Talk
Programming dynamic pathways to colloidal self-assembly using DNA nanotechnology* [invited]  WILLIAM ROGERS (Presenter), ALEXANDER HENSLEY, Brandeis Univ — DNA is not just the stuff of our genetic code; it is also a means to build new materials. For instance, grafting DNA onto small particles can, in principle, 'program' the particles with information that tells them exactly how to put themselves together--they 'self-assemble.' Recent advances in our understanding of how this information is compiled into specific interparticle forces have enabled the assembly of crystalline phases. However, programmable assembly of other user-prescribed structures, such as aperiodic solids, liquids, or other mesophases remains elusive. Furthermore, the dynamic pathways by which DNA-based materials self-assemble are largely unknown. In this talk, I will present experiments showing that: (1) combining DNA-grafted particles with free DNA oligomers dispersed in solution can create suspensions with new types of assembly pathways; and (2) we can quantify the dynamic pathways to self-assembly, such as nucleation and growth, using a combination of microfluidics, video microscopy, and image analysis. Whenever possible, I will describe attempts to understand and model our observations using simple physical arguments. In the future, this work could prove especially useful in nanomaterials research, where a central goal is to manufacture functional materials by growing them directly from solution.

*We acknowledge funding from the National Science Foundation (NSF DMR-1710112) and the Brandeis MRSEC (NSF DMR-1420382)

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F19 GMAG: Correlated and Magnetic Topological Materials

8:00AM F19.00001: Three-dimensional correlated topological semimetals* [Invited]  JOHANNES GOOTH (Presenter), Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — The physics of topological materials is typically well described by the band theory of non-interacting fermions. In contrast, some of the most fascinating effects in condensed matter physics merely emerge from electron correlations. Here, we will present two recent examples of phases of matter, arising from the interplay of interaction and non-trivial topology: an axionic charge density wave and three-dimensional quantum Hall states. Our electrical transport measurements reveal a positive longitudinal magnetoconductance in the sliding mode of the quasi-one-dimensional CDW–Weyl semimetal (TaSe₄)₂I, a signature that is linked to the presence of an axionic phason. In addition, we report the observation of integer and fractional quantum Hall plateaus in the bulk semimetal HfTe₅.

*European Union’s Horizon 2020 research and innovation program under Grant Agreement ID 829044 “SCHINES”.
The advent of Topological Quantum Chemistry (TQC) and Magnetic Topological Quantum Chemistry (MTQC) provides a straightforward approach to look at the topological properties of a material through ab-initio calculations. Combined with the non-magnetic material database from the Inorganic Crystal Structure Database and the Bilbao Magnetic Material Database, this allows for a systematic search of topological materials. In this talk, we will present the two databases of topological materials that we now provide to the community. Overall more than 37000 non-magnetic and 470 magnetic unique materials are available with a full topological characterization.
Weyl semimetals are gapless topological materials, breaking either spatial inversion or time reversal symmetry, that host Weyl fermions in the bulk and topological Fermi arc states on their surface. The time reversal symmetry broken Weyl semimetals are particularly attractive since they enable to study the interplay between magnetism, electron correlations, and topology. While several inversion symmetry broken Weyl semimetals have been verified experimentally, showing unambiguous evidence for a time reversal symmetry breaking Weyl semimetal is quite challenging. We used scanning tunneling spectroscopy to study the ferromagnetic semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$ and verified spectroscopically its classification as a time-reversal symmetry-broken Weyl semimetal [1]. In my talk I will describe how we visualize the topological “Fermi arc” states using quasiparticle interference measurements and show that the measured band structure of $\text{Co}_3\text{Sn}_2\text{S}_2$ exhibits direct signature of time reversal symmetry breaking, induced by the magnetic order of the Co atoms. By investigating three distinct surface terminations of the sample we examined complementary aspects of the surface and bulk band structure. I will describe the various surface and bulk electronic properties we extracted from each of the terminations. In particular I will demonstrate that the three different terminations of $\text{Co}_3\text{Sn}_2\text{S}_2$ exhibit not only distinct Fermi-arc contours, but also distinct connectivity between the Weyl nodes. The observed Weyl node connectivity changes from intra Brillouin zone connectivity on the Sn termination to a cross Brillouin-zones on the Co termination. This has significant implication on the magneto-transport properties of the Weyl electrons. Finally, the S termination allowed us to extract the extent of the Weyl gap by following the surface state dispersion. This provides a clear demonstration of the surface bulk correspondence in Weyl semimetals.

Chiral and magnetic topological semimetals

(NIELS SCHRÖTER)
(Invited)

Paul Scherrer Institute — Chiral topological semimetals (which possess neither mirror nor inversion symmetries) are expected to host numerous novel phenomena, such as multifold fermions with large topological charge, long Fermi-arc surface states, unusual magnetotransport and lattice dynamics, and a quantized response to circularly polarized light. Until recently, all experimentally confirmed topological semimetals crystallized in space groups that contain mirror operations, which means that the aforementioned phenomena vanish [1].

Here, I will present evidence from angle-resolved photoelectron spectroscopy that a family of intermetallic catalysts, including PtAl and PdGa [1,2], are chiral topological semimetals. We directly visualize the exotic multifold fermions in these materials and show that they carry the largest possible Chern number that is available in any material. We also show experimentally that there is a direct relationship between the handedness of the crystal structure and the electronic chirality (i.e. the Chern number sign) of the multifold fermions. This finding demonstrates that structural chirality can be used as a tuning knob to control the direction of topological photocurrents, which is sensitive to the Chern number sign.

Furthermore, I present evidence for multifold fermions in structurally chiral magnetic materials and show that CoS$_2$ - a putative half-metal - is in fact not-half metallic, but may host topological surface states that could affect its performance as a spin-injector.


Chiral spin textures: anti-skyrmions, elliptical skyrmions and Néel skyrmions

(STUART PARKIN)
(Invited)

Max Planck Inst Microstructure — Magnetic non-collinear spin textures that are chiral are of great current interest. We discuss various spin textures that range from chiral domain walls in synthetic antiferromagnetic racetracks to anti-skyrmions and elliptical skyrmions in inverse tetragonal Heusler compounds to Néel skyrmions in a non-centro-symmetric hexagonal ternary compound. We compare the properties of these distinct spin textures to skyrmions and to magnetic bubbles. We show that the symmetry of the Dzyaloshinskii-Moriya exchange that stabilizes many of these spin textures strongly influences the properties of the spin textures including especially their size, which in some cases, strongly depends on the thickness of the lamella in which they are observed. Using a combination of Lorentz transmission electron microscopy and magnetic force microscopy we show that for anti-skyrmions, which we have observed in several inverse tetragonal Heusler compounds, the diameter of the anti-skyrmion can be varied by more than an order of magnitude from <100 nm to more than 1 micron. This tunability is related to the important role of magnetic dipole-dipole interactions.

*European Research Council (ERC) advanced grant # 670166 & Deutsche Forschungsgemeinschaft project # 403505322.
Information extraction, analysis and feedback for directing matter by design [Invited] BOBBY SUMPTER (Presenter), Oak Ridge National Laboratory — Recent technical advances in the area of nanoscale imaging, spectroscopy and scattering/diffraction have provided tremendous capabilities for investigating materials structural, dynamical and functional characteristics. At the same time, advances in computational algorithms, including deep learning approaches, and computer capacities that are orders of magnitude larger and faster, have enabled extreme-scale simulations and deep data analytics of materials properties and processes starting with nothing but the identity of the atomic species and the basic principles of quantum and statistical mechanics and thermodynamics. This powerful confluence of capabilities/advances and the information bound in large volumes of high-quality data, offers new opportunities for advancing materials and chemical sciences. In this talk I will discuss how we are probing in-situ, chemical reactions and materials transformations, including hierarchical assembly, as a modality for direct feedback to an experiment in order to precisely impart directed energy (electrons, ions, photons, thermal) that manipulates a material at the nanoscale. This approach is enabled via the dual capability of high-resolution imaging and focused energy in-situ, with data rates, quality and volumes that allow for a deep learning framework to efficiently identify structures and dynamics across broad length and time scales. We have found that the approach can provide efficient mapping of solid-state reactions and transformations and overall allows a major step toward directing matter by design.

This research was conducted at the Center for Nanophase Materials Sciences, which is a US Department of Energy Office of Science User Facility.
8:36 AM F20.00002: High throughput search for plasmonic semiconductors using DFT databases*  ETHAN SHAPERA (Presenter), Physics, University of Illinois at Urbana-Champaign, ANDRE SCHLEIFE, Materials Science and Engineering, University of Illinois at Urbana-Champaign — The field of plasmonics aims to manipulate light via choice of materials and nanoscale structuring. Finding materials which exhibit low-loss responses to applied optical fields while remaining feasible for widespread use is an outstanding challenge. Online databases have compiled structural and electronic data for of tens of thousands of materials, but lack the expensive optical response calculations needed for selection of plasmonic materials. Understanding the optical response of semiconductors within DFT is complicated due to the DFT bandgap error and the influence of carrier doping density. We describe, validate, and demonstrate an approach which rapidly screens existing online databases to identify high quality factor plasmonic semiconductors. Using DFT bandstructures, we tabulate material bandgaps, optical transition energies, and effective masses. From correlations between bandstructure features and quality factor computed for a restricted set of semiconductors we predict CaMg$_2$N$_2$, InGaO$_3$, and LiInO$_2$ as candidate high quality factor plasmonic semiconductors. Quality factors are verified with DFT to describe optical absorption and the Drude model for intraband transitions.

*Blue Waters Sustained-Petascale Computing Project (OCI-0725070, ACI-1238993), NSF DMR-1555153.

8:48 AM F20.00003: Combined High-Throughput and Machine Learning Approach for Prediction of Lattice Thermal Conductivity  RINKLE JUNEJA, GEORGE YUMNAM, SWANTI SATSANGI, ABHISHEK SINGH (Presenter), Indian Institute of Science — Search for materials via explicit evaluation of thermal conductivity ($\kappa_l$) either experimentally or computationally is very challenging. We carried out high-throughput screening on a dataset containing total of 2691 binary, ternary, and quaternary compounds. The $\kappa_l$ values of 120 dynamically stable and nonmetallic compounds are calculated. Among these, 11 ultrahigh and 15 ultralow $\kappa_l$ materials are identified. For the machine learning prediction models, the descriptor set is usually tuned via conventional algorithms such as least absolute selection and shrinkage operator (LASSO). However, we generated an extensive property map from high-throughput calculations to design a minimal set of descriptors directly related to the physics of $\kappa_l$. These simple descriptors are maximum phonon frequency, integrated Grüneisen parameter up to 3 THz, average atomic mass, and volume of the unit cell. Using these descriptors, a Gaussian process regression-based machine learning (ML) model is developed. The model predicts room temperature log-scaled $\kappa_l$ with a very small root mean square error. The superior performance of the ML model can ensure a reliable and accelerated search for a multitude of low and high $\kappa_l$ materials.

Reference: Chem. Mater. 31, 14, 5145-5151, 2019
9:00AM F20.00004: Machine Learning-Assisted Design and Discovery of Next Generation 2D Materials  VICTOR VENTURI (Presenter), HOLDEN LOW PARKS, ZEESHAN AHMAD, VENKAT VISWANATHAN, Carnegie Mellon Univ — Atomically thin two-dimensional materials have attracted interest in the fields of electrochemistry, catalysis, and photonics due to the ease with which their properties may be tuned. First-principles calculations have proven an essential tool in the quest for new 2D materials with tailored properties. However, an exhaustive exploration of the parameter space is infeasible even in the monolayer case. In this work, we use a novel machine learning technique – Crystal Graph Convolutional Neural Networks (CGCNN) [1] – to train accurate models that can predict monolayer 2D material properties more efficiently than density functional theory simulations. Previously, CGCNN architectures have been demonstrated to successfully predict properties of solid electrolytes [2]. Here, we leverage their power to find design principles for 2D materials in light-absorbing and water-splitting applications.


9:12AM F20.00005: Revealing the Spectrum of Unknown Layered Materials with Super-Human Predictive Abilities  GOWOON CHEON (Presenter), Applied Physics, Stanford University, EKIN DOGUS CUBUK, Google Brain, EVAN ANTONIUK, Chemistry, Stanford University, JOSHUA GOLDBERGER, Chemistry, The Ohio State University, EVAN J. REED, Materials Science and Engineering, Stanford University — We use semi-supervised learning to discover over 1000 new two-dimensional layered materials that have yet to be discovered or synthesized. We accomplish this by combining physics with machine learning on experimentally obtained data and verify a subset of candidates using density functional theory. Our model accelerates the discovery of layered materials by 13 times compared to random trial-and-error approaches. Even compared to expert scientists working in the field of two-dimensional materials, it is five times better than practitioners in the field at identifying layered materials and is comparable or better than professional solid-state chemists. We also find that our model is orders of magnitude faster than any human.

To achieve super-human performance, we employ semi-supervised learning techniques for the first time in materials discovery. Semi-supervised learning utilizes unlabeled data in addition to labeled data, which is powerful in cases where labels are expensive to obtain or are noisy. We find that semi-supervised learning provides benefits over supervised learning in identifying layered materials, and it may be applicable to a wide range of problems in materials science.
9:24AM F20.00006: Probing the microscopic origin of magnetism in two-dimensional materials using machine learning*  TREVOR DAVID RHONE (Presenter), Physics, Rensselaer Polytechnic Institute, EFTHIMIOS KAXIRAS, Physics, Harvard University — Magnetic ordering in two-dimensions is at the forefront of research since the discovery of magnetism in monolayer CrI$_3$ in 2017. We study two-dimensional (2D) materials with intrinsic magnetic order and explore the microscopic origins of magnetism in these novel materials. The Mermin-Wagner theorem asserts that magnetic ordering cannot occur in 2D without the presence of magnetocrystalline anisotropy (MCA), which arises due to spin-orbit coupling. 2D materials with magnetic order provide a platform with which to study magnetism in low dimensions – the positions of all the atoms are known in theoretical studies and some experimental studies. This contrasts studies of magnetism in thin films. We use data analytics to study the magnetic and thermodynamic properties of 2D materials. Crystal structures based on monolayer CrI$_3$, are studied using density functional theory (DFT) calculations and machine learning. Magnetic properties, such as MCA and the magnetic moment are determined. We show that machine learning, combined with DFT, provides a means to learn patterns in 2D magnetic materials data, thereby providing insights into the microscopic origins of magnetic ordering in 2D. This approach to materials research also facilitates the rapid discovery of 2D magnets.

*DOE DE-AC02-06CH11357

9:36AM F20.00007: Topological data analysis for magnetic domain structure characterization*  MASATO KOTSUGI (Presenter), Tokyo Univ of Science, Katsushika — Analysis of the magnetic domain structure is an important process in the development of advanced magnetic materials. A number of successful studies have been carried out by high-resolution magnetic imaging or LLG simulations. However, the treatment of the information of the whole image, especially the shape of the magnetic domain structure, has not been sufficiently discussed.

We here executed the topological data analysis (TDA) to extract the feature of the shape in a magnetic domain structure [1, 2]. Maze magnetic domain structure was analyzed by TDA to visualize the pinning site during the magnetization reversal process. We utilized persistent homology to extract the topological feature of the magnetic domain structure, and principal component analysis was used to construct the correlation between persistence diagram and a magnetic hysteresis loop. As a result, we could automatically visualize the pinning site as a topological defect in the original magnetic domain structure for the first time.


*A part of this research was supported by MI2I-NIMS, KAKENHI-MEXT, Hitachi Metals Materials Science Foundation.
9:48AM F20.00008: Extracting Interpretable Physical Parameters from Spatiotemporal Systems using Unsupervised Learning* PETER LU (Presenter), Department of Physics, Massachusetts Institute of Technology, SAMUEL KIM, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, MARIN SOLJACIC, Department of Physics, Massachusetts Institute of Technology — Real-world data from spatiotemporal systems is often difficult to analyze and interpret due to complex dynamics as well as uncontrolled experimental variables. We demonstrate an unsupervised machine learning technique for extracting interpretable physical parameters from noisy spatiotemporal data and for building a transferable predictive model of the system. This is accomplished without prior knowledge of the underlying dynamics or the governing partial differential equation (PDE). Numerical experiments using simulated data governed by PDEs show that our method accurately identifies and extracts relevant parameters that characterize independent variations in the system dynamics. Our method for discovering interpretable latent parameters in spatiotemporal systems will allow us to better understand real-world phenomena by analyzing datasets with varying dynamical behaviors that are difficult to disentangle.

*This work is supported in part by the U.S. Department of Defense through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program, the MIT-SenseTime Alliance on Artificial Intelligence, the Army Research Office under Cooperative Agreement Number W911NF-18-2-0048, and the Defense Advanced Research Projects Agency (DARPA) under Agreement No. HR00111890042.

10:00AM F20.00009: Prediction of Seismic Wave Arrivals Using a Convolutional Neural Network* JORGE GARCIA (Presenter), LAUREN WASZEK, Department of Physics, New Mexico State University — Seismology uses energy from earthquakes to image the deep interior of Earth. Large amounts of seismic data are required in order to obtain detailed observations of the its internal structure; typical datasets comprise over 100,000 seismic records. With the exception of some basic processing methods, compilation of the data is performed by hand using simple visualization software. The most significant and time-consuming task is the identification and picking of seismic phases. Previous attempts at automating this procedure involve algorithms that generally underperform compared to a human expert. However, even among human-compiled datasets, consistency of phase arrival across and within datasets is a problem. The variation in decisions results in disagreement between obtained images, and subsequent interpretation of Earth's structure and processes. We employ a Convolutional Neural Network (CNN) to predict the arrival time of the mantle shear-wave phases in a seismogram in an effort to accelerate and make consistent the task of data processing. We approach strategies to ensure correct prediction of arrival time and polarity of the seismic phase, as well as applying the model for identification of precursor signals of the same phase.

*Work supported by NSF Award 1853662.
10:12AM F20.00010: Using Reinforcement Learning to Optimize Crystal Structure Determination*  WILLIAM RATCLIFF (Presenter), National Institute of Standards and Technology, KATE MEUSE, Montgomery Blair High School, JESSICA OPSAHL-ONG, Mclean High School, JOSEPH RATH, Rowan University, PAUL KIENZLE, National Institute of Standards and Technology, TELON YAN, RYAN CHO, Montgomery Blair High School, ABIGAIL WILSON, Tufts University — The first step to understanding the microscopic origins of the properties of a material is to determine the crystal structure. This can be accomplished with neutron diffraction. However, there are a small number of neutron sources in the world and thus it is critical to perform measurements as optimally as possible. We use reinforcement learning to address this problem. We compare several approaches within this framework including epsilon-greedy, Q-learning, and actor-critic. We find that in toy models, it is possible to measure a significantly smaller fraction of measurements than would commonly be performed to determine structural properties with the same accuracy.

*Support for Abigail Wilson, Joseph Rath, Kate Meuse, Jessica Opsahl-Ong, Ryan Cho, and Telon Yan was provided by the Center for High Resolution Neutron Scattering, a partnership between the National Institute of Standards and Technology and the National Science Foundation under Agreement No. DMR-1508249.

10:24AM F20.00011: Active Learning for Quantum Experimental Controiling  YADONG WU (Presenter), HUI ZHAI, Tsinghua University — Experimental control problems are popular task for experimental physicists in quantum experiments. Generally human tune the experimental parameters step by step, hand by hand to fine the suitable experimental parameters to set up the experimental system. While this way of tuning parameters is not efficient and may miss the ‘global minimum’. Here we apply one semi-supervised machine learning method, active learning, to this parameters tuning task to find the suitable parameters automatically. We will show the advantage of this machine learning method by two simulated examples. First we set the Efimovian expansion as a benchmark. Putting the unitary fermi gases into a harmonic trap with time dependent trapping frequency $\omega(t)$, active learning told us the most efficient way to release the trap is $\omega(t) \propto 1/t$ which is assistant with the theory. Then we apply this active learning to evaporative cooling issue. Comparing to the simulated result, this active learning can give us a better cooling trajectory which can reach to a lower temperature during less time.
International Radiological Information Exchange (IRIX) Standards for Emergency Radiation Monitoring Data Reporting

SANJOY MUKHOPADHYAY (Presenter), International Atomic Energy Agency — The Incident and Emergency Centre (IEC) of the International Atomic Energy Agency (IAEA) has developed a web application, the International Radiation Monitoring Information System (IRMIS). IAEA Member States (MS) can share and visualize large quantities of radiation monitoring data (viz. gamma dose rate, isotope specific ground depositions and air concentrations) using IRMIS. The radiation monitoring data may be uploaded into IRMIS in the International Radiological Information Exchange (IRIX) format. IRIX is a technical standard developed by the IAEA, in cooperation with the MSs and the European Commission (EC). IRIX enables the development of interoperable systems and solutions for exchanging emergency information and data between organisations at both national and international level during a nuclear or radiological emergency. IRIX is an open format based on the Extensible Markup Language (XML), which makes it both machine and human readable. The system interface specification (or web-service specification) enables organizations to interconnect their emergency information systems to automate information exchange. The XML provides a software- and hardware-independent way of storing, transporting, and sharing data. The article will discuss applications of IRIX in IRMIS.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F21 GERA: Towards Realizing the Energy Future

Undergrad Friendly
Three terminal tandem (3TT) solar cells can overcome some of the limitations of two terminal (current matched) and four terminal (independently operated) solar cell designs. This design is a compelling platform for tandem cell integration because 3TTs based on Si bottom cells with interdigitated back contacts enable the same robust performance of four terminal tandems but do not require lateral current extraction between the cells, which can become challenging when scaling devices to large areas. However, the coupled nature of 3TT devices adds a degree of complexity to the devices themselves and the ways that their performance can be measured and reported. While many different configurations of 3TT devices have been proposed, there is no standard taxonomy to discuss the device structure or loading topology. I will discuss a proposed taxonomy for classifying 3TT devices and explaining how to rigorously measure their performance. I will show how TCAD models agree with simple physical models and experimental results to explain the trends in the behavior of 3T tandems.

*Funding for this work was provided by the Department of Energy Office Solar Energy Technologies Office under contract SETP DE-EE00034911.*
Tremendous progress has been made in wide-bandgap (WBG) power electronic devices. Most WBG devices today are based on silicon carbide (SiC) or gallium nitride (GaN). However, the most mature GaN-based power device, the high electron mobility transistor (HEMT), falls short of the full potential of GaN for several reasons: (1) internal stress due to the growth of thick buffer layers on non-native substrates; (2) the lateral architecture of the HEMT produces a non-ideal internal electric field distribution; and (3) avalanche ruggedness is lacking. GaN-based HEMTs are thus unacceptable for higher-voltage applications such as the electric grid and vehicle drivetrain electrification. In contrast to GaN HEMTs, vertical GaN power devices grown on native GaN substrates do not suffer from these shortcomings. However, materials challenges exist for vertical GaN, such as the quality of native substrates and the epitaxial growth of thick (tens of microns or more), low-doped (< 10^16 cm^-3 n-type) drift layers required for high breakdown voltage. Processing challenges also exist, such as the ability to selectively dope GaN and to activate buried p-layers. This talk will present progress in the design, fabrication, and evaluation of vertical GaN power devices. The fundamental material properties relevant for such devices will be discussed, including how they enable devices superior to those fabricated from other semiconductors. Challenges and progress associated with substrates and epitaxial growth will be covered, as will design trade-offs and processing challenges (including yield and reliability) for various types of diodes and transistors.

*This work was supported by the ARPA-E OPEN+ Kilovolt Devices Cohort managed by Dr. Isik Kizilyalli, and by the US Department of Energy Vehicle Technologies Office Electric Drivetrain Consortium. Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.*
9:12AM F21.00003: Advancements in soft magnetic materials for future energy needs*

[Invited]  TODD MONSON (Presenter), Sandia National Laboratories — Power electronics and motor drives are now transitioning to wide band gap semiconductors, operating at higher frequencies, and enabling faster rotational speeds in electrical machines. This is creating a need for improved soft magnetic materials that can sustain higher flux densities with lower losses. Many different materials and strategies are being pursued and it is almost certain that a mix of soft magnetic materials will be required to meet all current and emerging applications. I will provide a brief overview of the history of soft magnetic materials and discuss some of the most promising approaches to meet the needs of future power electronics and rotating machines.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

9:48AM F21.00004: Data-Driven Discovery of Materials for Photocatalytic Energy Conversion

[Invited]  ARUNIMA SINGH (Presenter), Department of Physics, Arizona State University — Photocatalytic fuel production, e.g. generation of hydrogen from water splitting or the conversion of the greenhouse gas carbon dioxide to chemical fuels, promises us alternative energy sources that are clean, environmentally friendly and renewable. Advancements have been made in improving the efficiencies and product selectiveness of currently known photocatalysts, but the attempts for finding new photocatalytic materials have been few and based largely on trial and error.

In this talk, I will show how we can design first-principles simulations based descriptors for synthesizability, corrosion resistance, visible-light absorption, and compatibility of the electronic structure for the catalytic reaction and use them for a rational photocatalytic materials screening. I will present two examples here, first where we have performed the largest CO$_2$ photocathode search to date, starting with 68,860 candidate materials and found that only 52 materials meet the stringent requirements for CO$_2$ reduction photocatalysts.\textsuperscript{1} The photocathode materials identified include 9 materials previously reported as CO$_2$ photocathodes, as well as the discovery of a set of 43 new candidate photocathodes. In the other example, I will show how we discovered five manganese-based ternary metal-oxides for oxygen evolution through a joint computational and experimental photocatalyst screening.\textsuperscript{2}

Solvent-in-salt (SIS) electrolytes differ substantially from the traditional electrolytes: in such systems amounts of the dissolved salt is equivalent or more by weight/volume of that of the solvent. As a result, SIS systems feature a number of unique properties and provide electrochemical performance advantages that could not be attained by usage of the traditional electrolytes. One of the notable examples of SIS electrolytes are highly concentrated “water-in-salt”, WIS, systems which were demonstrated to be highly attractive electrolytes for aqueous batteries since they can offer significantly extended stability window, improved coulombic efficiency and cycling stability.\textsuperscript{1,2,3,4} Yet, while it is clear that such an extreme increase in salt concentration would result in highly modified interactions of the ionic and molecular components of the electrolyte a detailed our understanding is still lacking.

Here we present on multi-technique study of the two distinct WIS systems based on i) lithium salts of organic imides and ii) potassium acetate. Using a combination of the X-Ray Absorption Spectroscopy, wide angle X-Ray scattering and molecular dynamics simulations we reveal effects of the solution concentration and introduction of the multivalent cations such as Zn\textsuperscript{2+} on the solvation structure of the ionic species, local order within electrolytes and nano-heterogeneity within the studied WIS systems.

References

*This work was fully supported by the Joint Center for Energy Storage Research (JCESR).
8:00AM F22.00001: The avian eggshell: evolution and engineering of a tough, lightweight biological material [Invited]  MARY CASWELL STODDARD (Presenter), Princeton University, ZHIFEI DENG, ZI'AN JIA, LING LI, Virginia Tech, JAMES WEAVER, Harvard University — The eggs laid by modern birds are the products of more than 150 million years of evolution, resulting in a sophisticated package designed to balance a range of competing demands. The egg must be tough enough to prevent external damage but weak enough to permit a chick to hatch. It must resist bacterial contamination but allow gas exchange between the chick and the outside environment. The egg satisfies these requirements, which is remarkable given that it forms in under 24 hours. From an evolutionary perspective, bird eggs are fascinating because they come in a great variety of shapes, sizes, colors, and structures despite the fact that they serve the same essential function: to nourish and protect a chick until it hatches. What selective pressures influence the diversity of egg phenotypes? From an engineering perspective, eggshell is impressive because it is a strong, lightweight material, yet we understand relatively little about eggshell biomechanical properties outside of those from domestic chickens. What is the relationship between the structure and function of eggshell? In addition, how do eggs form in the avian oviduct? Here, we explore these questions through the lenses of evolutionary biology, biophysics and mechanical engineering, which together provide an integrative picture of the form and function of avian eggs.

8:36AM F22.00002: Misorientation and enhanced hardness in tooth enamel* CAYLA STIFLER (Presenter), CHANG-YU SUN, University of Wisconsin - Madison, ELIA BENIASH, University of Pittsburg, PUPA GILBERT, University of Wisconsin - Madison — Teeth are subjected to extreme, repetitive forces on a daily basis. Human enamel exerts forces up to 770 Newtons, hundreds of times per day, and must remain functional for decades\(^1\). By comparison, great white shark enameloid exerts 7400 Newtons of force when biting, but they shed their teeth regularly\(^2\). The mechanical stress the teeth undergo suggests there are structural features in enamel that prevent catastrophic failure. We used PIC (polarization-dependent imaging contrast)\(^3,4\) mapping at the calcium L-edge\(^5\) to reveal the crystal orientations within rods in mammalian enamel and in bundles in fish enameloid. Analysis of PIC maps from the enamel(oid)\(^6\) of diverse animals indicates that c-axis orientations of adjacent crystals are slightly misoriented by small angles. The observed misorientation is positively correlated with the hardness and elastic modulus, suggesting that crystal misorientation is related to, and possibly causes, these enhanced properties.

1 S Varga 2010, 10.1093/ejo/cjq097
3 P Gilbert 2011, 10.1073/pnas.1107917108
4 C Killian 2011, 10.1002/adfm.201001546
5 C Stifler 2018, 10.1021/jacs.8b05547
6 M Marcus 2017, 10.1021/acsnano.7b05044

*U.S. DOE Office of Basic Energy Sciences, CSGB Division, Award DE-FG02-07ER15899
8:48AM F22.00003: Crystallographic Parameters Of Rod And Interrod Enamel Crystallites Differ Systematically*  
ROBERT FREE, KAREN DEROCHER, STUART STOCK, DERK JOESTER  
(Presenter), Northwestern University — Dental enamel has evolved to bear large masticatory forces, resist mechanical fatigue, and withstand wear over decades of use. Functional impairment or loss, as a consequence of developmental defects or tooth decay, has a dramatic impact on health and quality of life. Enamel formation and its degradation remain incompletely understood. This is in part due to its hierarchical architecture. Our objective was to test the hypothesis that crystallographic features of two microstructural features of enamel, rod and interrod enamel, differ as a consequence of their developmental origin. Towards this goal, we mapped crystallographic order/disorder by azimuthal autocorrelation of WAXS patterns recorded at 500 nm spot size and correlated this information with crystallite size, lattice parameters, and microstrain at each point. We find that there are systematic variations in these parameters for rod and interrod crystallite populations that suggest differences in composition and imply that there are distinct crystallization environments during amelogenesis.

*NIH-NIDCR R03 DE025303-01, R01 DE025702-01,

9:00AM F22.00004: Characterization of a Novel Antimicrobial Agent for Endodontic Applications*  
ARIS ZHU (Presenter), JEFFREY WOLBERG, FARZAD KOOSHA, Dentistry, Stony Brook University, KARENA ETWARU, MIRIAM RAFAILOVICH, Materials Science, Stony Brook University — Recurrent endodontic infections are primarily caused by persistent bacteria Enterococcus faecalis and are more challenging to treat, compared to primary infection of the root canal system. Current treatment, calcium hydroxide (CaOH), is used despite its inefficacy against E faecalis and other common endodontic pathogens, so we developed a more effective composite material named “CASA”. This study characterizes the antimicrobial properties, cytotoxicity, and differentiation potential of CASA for dental pulp stem cells (DPSCs). To determine antimicrobial properties, agar plates were inoculated with common endodontic pathogens. Then, CASA or CaOH was inserted into wells in the agar plate with a diameter of 6 mm. They were incubated for 24 hrs, and then zones of inhibition were measured. CASA produced larger zones of inhibition than CaOH for all species tested. Cytotoxicity studies indicated a high tolerance for DPSCs for CASA, with a measured IC50 of 1.0 mg/ml, a far higher dose than tissue would be exposed to during standard treatment. Addition of 0.25 mg/ml of CASA to DPSCs in osteogenic culture, in the absence of dexamethasone, was observed to hinder differentiation and preserve stemness of the culture.

*We acknowledge support from the Morin Foundation Trust
Evolutionary patterns in skeletal biomineralization* [Invited] SUSANNAH PORTER (Presenter), JOHN MOORE, LEIGH ANNE RIEDMAN, Earth Science, University of California at Santa Barbara — Mineralized skeletons evolved many times within eukaryotes, providing multiple independent data points for testing hypotheses about skeletal evolution. We have identified >80 acquisitions of mineralized skeletons in eukaryotes along with their time of first appearance and their mineralogy, and have found several interesting patterns. First, the distribution of skeletal mineralogies tends to be non-uniform: most animals and archaeplastidans, for example, chose carbonate, whereas most rhizarians and stramenopiles chose silica. Whether this reflects functional constraints, e.g. related to uni- vs. multicellularity, or phylogenetic constraints, e.g. related to homologous genes involved in nucleation/inhibition of these minerals, is unclear. Second, acquisitions of phosphatic skeletons are clustered in the Cambrian, perhaps due to high PO$_4^{3-}$ in the oceans at this time. Finally, more than 60% of animal acquisitions occurred in the early Cambrian, whereas those of other eukaryotes are distributed more uniformly in time, supporting the view that factors affecting only animals, e.g., the appearance of carnivores, rather than factors affecting all marine organisms, e.g., increased Ca$^{2+}$, drove widespread biomineralization in the early Cambrian.

*This research is supported by NSF EAR-1411594.

Biomineralization by particle attachment in early animals* PUPA GILBERT (Presenter), Physics, University of Wisconsin - Madison, SUSANNAH M PORTER, Geosciences, University of California - Santa Barbara, CHANG-YU SUN, Physics, University of Wisconsin - Madison, SHUHAI XIAO, Geosciences, VA Tech, BRANDT M GIBSON, Geosciences, Vanderbilt University, NOA SHENKAR, Life Sciences, Tel-Aviv University, ANDREW H KNOLL, Organismic and Evolutionary Biology, Harvard University — Crystallization by particle attachment (CPA$^1$ of amorphous calcium carbonate (ACC) was demonstrated in modern biominerals from diverse animals. Precisely the same precursors, hydrated and anhydrous ACC, have been observed spectromicroscopically in echinoderms$^{2-4}$, molluscs$^5$, cnidarians$^6$. This is surprising, as these three phyla have no common ancestor that formed biominerals, and have, therefore, evolved carbonate biomineralization independently ~100 million years after diverging from one another$^7$. Here we correlate the occurrence of CPA of ACC precursor particles with nanoparticulate fabric and then use the latter to investigate the antiquity of the former. SEM images of the oldest known animal biominerals show that these animals used attachment of ACC particles to form their biominerals. The convergent evolution of biomineral CPA may have been dictated by the same thermodynamics and kinetics as we observe today.

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2 Y Politi 2008 DOI: 10.1073/pnas.0806604105
3 YUT Gong 2012 DOI: 10.1073/pnas.1118085109
4 M Albéric 2019 DOI: 10.1016/j.yjsbx.2019.100004
5 RT DeVol 2015 DOI: 10.1021/jacs.5b07931
6 T Mass 2017 DOI: 10.1073/pnas.1707890114
7 PUPA Gilbert 2019 doi/10.1073/pnas.1902273116

*DOE grant DE-FG02-07ER15899, NSF grant DMR-1603192.
10:00AM F22.00007: Applications of molecular taphonomy to the invertebrate fossil record  
[Invited] CORINNE MYERS (Presenter), Earth and Planetary Sciences, University of New Mexico, KRISTIN BERGMANN, Earth, Atmospheric, and Planetary Sciences, MIT, PUPA GILBERT, Physics, University of Wisconsin-Madison — Recently several studies have demonstrated the utility of PhotoEmission Electron spectroMicroscopy (PEEM) to observe exceptional preservation of organic matrix components and shell microstructure in fossil mollusks. Comparisons to modern representatives suggests very strong similarity and potential links to paleoenvironmental conditions (e.g., temperature). Current work must focus on replicating these results across additional time periods and types of biomineralizing species. Future work on the utility of hyperspectral imaging, the geography of preservation, and complementary analyses (e.g., Raman spectroscopy), will provide additional clues into the molecular and structural preservation of biominerals, as well as their evolution through geologic time.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F23 DBIO GSNP: Physics of Microbiomes and Bacterial Communities 304 - Raghuveer Parthasarathy, Univ of Oregon

8:00AM F23.00001: A statistical-mechanics approach to microbiome data analysis* ROBERT MARSLAND (Presenter), PANKAJ MEHTA, Boston Univ — Next-generation sequencing, high-throughput metabolomics and other measurement technologies have opened vast new horizons for collecting data on the structure and function of microbial communities. But it remains unclear how to leverage this data for effective intervention in medical and agricultural applications. We do not know which quantities can be reliably predicted, which are hopelessly contingent, and what the predictors are for the former. In this talk, I will draw on conceptual tools from statistical physics, which were designed to answer precisely these sorts of questions. In particular, I will argue that the key features of community structure are encoded in a susceptibility matrix, which contain the response of species population sizes to small changes in growth rates. I will show how to estimate this matrix in different scenarios from existing data sets, and then explain how it can be used to cluster species into functionally redundant groups for enhanced predictability of community composition.

*This work was supported by NIH NIGMS grant 1R35GM119461, Simons Investigator in the Mathematical Modeling of Living Systems (MMLS) to PM.
8:12AM F23.00002: Quantifying multi-species bacterial interactions in larval zebrafish
DEEPIKA SUNDARRAMAN (Presenter), EDOUARD HAY, DYLAN MARTINS, DREW SHIELDS, NOAH PETTINARI, KAREN GUILLEMIN, RAGHUVEER PARTHASARATHY, Univ of Oregon — The microbial communities resident in animal intestines are composed of many species and play an important role in host development, health and disease. The complex nature of these diverse communities makes it challenging to determine the driving forces behind microbial composition. Further, it is unclear for many multi-species consortia whether species-level makeup can be predicted solely on pairwise inter-species interactions, or whether higher-order interactions are needed to explain the composition of these communities.
To address this, we consider commensal intestinal microbes in larval zebrafish, initially raised germ-free to allow introduction of controlled combinations of bacterial species. Using dissection and plating assays we demonstrate the construction of communities of 1 to 5 bacterial species and show that the outcomes from the 2-species competitions do not contain enough information to predict the abundances in more complex communities. Furthermore, we observe a dampening of strong negative interactions as the microbial composition of the gut becomes more diverse. Our data suggests higher order interactions are important in the zebrafish gut, possibly due to changes in spatial organization that ongoing live imaging experiments are illuminating.

8:24AM F23.00003: Species covariance in *C. elegans* microbiome demonstrates existence of bacteria-bacteria and host-bacteria interactions*  
K. MICHAEL MARTINI (Presenter), MEGAN TAYLOR, ILYA M NEMENMAN, NICOLE MARIE VEGA, Emory University — The structure and internal dynamics of complex microbial communities in the guts of organisms is poorly understood. Here we analyze a simplified community of bacteria in the gut of *Caenorhabditis elegans*, a roundworm. Initially germ-free adult *C. elegans* are introduced into an environment with equal concentrations of eight bacterial species from a native worm microbiome. After four days, we examine individual worm gut communities and calculate the covariance structure of the bacterial abundances. We find statistically significant off-diagonal covariances. We demonstrate that a simple model only considering migration, birth, death, and competition for space among the bacteria can capture the mean values of bacterial abundances and their variances. However, it is incapable of explaining the off-diagonal covariances. We also show that the positive off-diagonal covariances can be partially explained by variation of the birth rate and other bacterial parameters among the worm hosts. However, to explain the off-diagonal negative covariances observed in the experiment requires interactions between bacteria beyond competition for space. We thus show that the structure of the microbiome is affected by both bacteria-bacteria and bacteria-host interactions.

*NIH: R01EB022872. NSF: BCS-1822677*
Evidence for a multi-level trophic organization of the human gut microbiome  

TONG WANG (Presenter), University of Illinois at Urbana-Champaign, AKSHIT GOYAL, Physics of Living Systems, Massachusetts Institute of Technology, VERONIKA DUBINKINA, SERGEI MASLOV, University of Illinois at Urbana-Champaign — The human gut microbiome is a complex ecosystem, in which hundreds of microbial species and metabolites coexist, in part due to an extensive network of cross-feeding interactions. However, both the large-scale trophic organization of this ecosystem and its effects on the underlying metabolic flow, remain unexplored. Here, using a simplified model, we provide quantitative support for a multi-level trophic organization of the human gut microbiome, where microbes consume and secrete metabolites in multiple iterative steps. Using a manually-curated set of metabolic interactions between microbes, our model suggests about four trophic levels, each characterized by a high level-to-level metabolic transfer of byproducts. It also quantitatively predicts the typical metabolic environment of the gut (fecal metabolome) in approximate agreement with the real data. To understand the consequences of this trophic organization, we quantify the metabolic flow and biomass distribution and explore patterns of microbial and metabolic diversity at different levels. The hierarchical trophic organization suggested by our model can help mechanistically establish causal links between the abundances of microbes and metabolites in the human gut.

Regime shifts in a phage-bacterial ecosystem and strategies for its control*  

SERGEI MASLOV (Presenter), University of Illinois at Urbana-Champaign, KIM SNEPPEN, Niels Bohr Institute — We show [1] that phage-bacterial ecosystems can have several alternative species compositions separated by abrupt regime shifts. In one of these states the fast-growing bacteria competitively exclude the slow-growing species by depleting common nutrient. In the other state the slow-growing bacteria with a large burst size make so many phages that the other species cannot survive. This scenario can be realized e.g. if two bacterial strains are protected from the same phage by, respectively, abortive infection or CRISPR, and partial resistance defence mechanisms. Alternative stable states and regime shifts greatly complicate the task of manipulation of microbial communities. We propose and study a successful control strategy via short population pulses aimed at inducing the desired regime shifts. In particular, we predict that a fast-growing pathogen could be eliminated by a combination of its phage and a slower-growing susceptible host.


*This project funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme under grant agreement No 740704.
9:00AM F23.00006: Biophysical consequences of sublethal antibiotics on gut bacterial persistence and transmission*  BRANDON SCHLOMANN, TRAVIS J WILES, ELENA S WALL, KAREN GUILLEMIN, RAGHUVEER PARTHASARATHY (Presenter), Univ of Oregon — Antibiotics induce large changes in the composition of the gut microbiome even at sublethal concentrations, by mechanisms that have remained elusive. Using larval zebrafish, which allow controlled studies of microbial dynamics, we found that sublethal doses of the common antibiotic ciprofloxacin cause severe drops in bacterial abundance. Contrary to conventional expectations, disruption was more pronounced for slow-growing, aggregated bacteria than for fast-growing, motile species. Three-dimensional live imaging revealed that antibiotic treatment promoted physical aggregation of bacteria in both planktonic and cohesive species and increased susceptibility to intestinal expulsion. Intestinal mechanics therefore amplify antibiotics effects on resident bacteria. A biophysical model, reminiscent of models of polymer growth and gelation, describes microbial dynamics and makes testable predictions of aggregation properties. The antibiotic-induced expulsion of live bacteria from the host influences the transmission of microbes to new hosts, which we suggest may contribute to the spread of antibiotic resistance.

*We acknowledge support from the NIH (P50GM09891 and P01GM125576-01), NSF (1427957), and the Kavli Foundation.

9:12AM F23.00007: Delayed antibiotic exposure induces population collapse in enterococcal communities with drug-resistant subpopulations  KELSEY HALLINEN (Presenter), JASON KARSLAKE, KEVIN WOOD, Biophysics, University of Michigan — The molecular and genetic causes of bacterial antibiotic resistance are increasingly understood, while less is known how these molecular events influence population dynamics. In this work, we show the dynamics of E. faecalis communities exposed to antibiotics can be surprisingly rich, as increasing population size or delaying drug exposure can promote population collapse. We combine experiments in computer-controlled bioreactors with simple mathematical models to reveal density-dependent feedback loops, coupling growth and antibiotic efficacy of populations with drug-resistant (β-lactamase) subpopulations. With a wide range of behavior—population survival, collapse, or one of two qualitatively distinct bistable behaviors where either small or large populations survive—competing density-dependent effects arise: drug-sensitive cell growth increases while drug-resistant cell growth decreases drug efficacy. We experimentally show how populations receiving immediate drug influx may thrive, while identical populations exposed to delayed drug influx (and lower average drug concentrations) collapse. These results illustrate the spread of drug resistant determinants—even in single-species communities—may be governed by counterintuitive dynamics driven by population-level interactions.
9:24AM F23.00008: Predicting microbial community metabolic function from genomic structure* KARNA GOWDA (Presenter), DEREK J PING, LAURA B TROYER, Physics, University of Illinois at Urbana-Champaign, MADHAV MANI, Engineering Sciences and Applied Mathematics, Northwestern University, SEPPE KUEHN, Physics, University of Illinois at Urbana-Champaign — The genes and organisms present in microbial communities determine metabolic flows that drive global nutrient cycles. A primary objective of microbial ecology is therefore to predict the metabolic function of a community from its genomic structure. We approach this prediction problem using denitrification as a model metabolic process. Denitrification is mediated by bacterial consortia that convert nitrate to dinitrogen gas. Using metabolite measurements and sequencing of denitrifying bacteria isolated from local soils, we develop a statistical-empirical approach to predicting community function from genomic structure. We show that for each strain in monoculture, the dynamics of denitrification are parameterized by a consumer-resource model. With some well-defined exceptions, we then find that the metabolite dynamics of simple communities are predictable from monoculture dynamics. This means we need only predict single-strain metabolite flows from genomes to successfully predict community-level metabolism. We solve this by predicting consumer-resource parameters via regression onto the presence/absence of each strain's denitrification genes, thereby providing a complete map from community genomic structure to metabolic function.

*NSF PHY 0822613,1430124; JSMF 220020499; SF 597491

9:36AM F23.00009: Cross-feeding is not necessarily evolutionarily stable BO LIU (Presenter), Harvard University, ZHIYUAN LI, Peking University, NED WINGGREEN, Princeton University — Cross-feeding is widely observed in microbial communities. Intuitively, cross-feeding provides mutual benefits: one species exports metabolic waste which can be taken up and utilized by another species. However, it remains unclear whether mutually beneficial cross-feeding is evolutionarily stable in the face of mutations, invasion by other species, and the cost of transporting metabolites. To address this question, we constructed a minimum metabolic model of cross-feeding, with trade-offs in enzyme allocation and reversible energy-producing reactions. The population dynamics of this system in a chemostat reveal that cross-feeding is evolutionarily unstable. Instead, we find stable coexistence between a species that exports an intermediate and a species that consumes the same nutrient but processes the intermediate. We show why cross-feeding is unstable for this system, and generalize our results for the coexistence of different consumption strategies to multi-step reactions. Further, we identify a scaling relation for the population ratios of coexisting species at large nutrient supply. In summary, our model reveals that cross-feeding is not necessarily evolutionarily stable, and identifies a mechanism for coexistence based on species polluting their own metabolic environment.
Percolation transition of pusher-type microswimmers*  
FABIAN JAN SCHWARZENDAHL (Presenter), School of Natural Sciences, University of California, Merced, MARCO G. MAZZA, Interdisciplinary Centre for Mathematical Modelling, Loughborough University — In this talk I will present the presence of a continuum percolation transition in model suspensions of pusher-type microswimmers. The clusters dynamically aggregate and disaggregate resulting from a competition of attractive and repulsive hydrodynamic and steric interactions. As the microswimmers' filling fraction increases, the cluster size distribution approaches a scale-free form and there emerge large clusters spanning the entire system. We characterize this microswimmer percolation transition via the critical exponents, analytical arguments, and scaling relations known from percolation theory. This finding opens new vistas on microswimmers' congregative processes.

*We thank the Deutsche Forschungsgemeinschaft (SFB 937, project A20) and from the Max Planck Society.

Biphasic Chemotaxis of E. coli to the Microbiota Metabolite Indole*  
JINGYUN YANG, RAVI CHAWLA, KATHY RHEE, RACHIT GUPTA, MICHAEL MANSON, ARUL JAYARAMAN, PUSHKAR LELE (Presenter), Texas A&M Univ — Bacterial chemotaxis to microbiota metabolites in the GI tract is important in the development of microbial communities. A prominent metabolite is indole, which has received wide attention for its role in regulating a broad range of bacterial phenotypes including virulence. The basis of chemotaxis to indole however, remains poorly understood. With a combination of flagellar motor and FRET assays, we have discovered a time-dependent inversion from a chemorepellent to chemoattractant response to indole. Such an inversion caused a bipartite response – wild-type cells were attracted to regions of high indole concentration if they had previously adapted to indole but were otherwise repelled. Interestingly, the flagellar motor itself mediated a repellent response independent of the chemoreceptors. I will discuss analytical models to explain these and other physiological responses to indole. The spatial filtering of cells by indole is likely important in repelling invaders while recruiting beneficial resident bacteria to growing microbial communities within the GI tract.

*PPL acknowledges support from the National Institute of General Medical Sciences (R01-GM123085) and the DOD ACC-APG-RTP Division (W911NF1810353).
Dynamic motility selection drives population segregation in a bacterial swarm*  

YILIN WU (Presenter), WENLONG ZUO, Chinese Univ of Hong Kong — Ecological models usually take growth rate fitness as the essential driver of population dynamics. However, as a widespread natural phenomenon, population expansion in space (or range expansion) is often governed by both motility and growth. Microbial communities offer unique systems to study how individual’s motility contributes to space competition among heterogeneous microbial populations during range expansion. Here we show that motility heterogeneity can promote the spatial segregation of sub-populations in structured microbial communities via a dynamic motility selection mechanism. Our findings are relevant to microbial stress response and microbial ecology. The results may also provide new insight to range expansion in other biological systems, such as tumor invasion and collective stress tolerance of cancer cells in densely packed environments.

*This work was supported by the National Natural Science Foundation of China (NSFC 21473152; to Y.W.) and by the Research Grants Council of Hong Kong SAR (RGC Ref. No. GRF 14322316; to Y.W.) as well as CUHK Direct Research Grants.

Continuum modeling of bacterial biofilm development*  

CHENYI FEI (Presenter), RICARD ALERT, BOYANG QIN, ANDREW BRIDGES, BONNIE BASSLER, NED WINGREEN, Princeton University — Biofilms are surface-associated bacterial communities embedded in an extracellular matrix. *Vibrio cholerae*, a rod-shaped bacterium, forms biofilms starting from a single cell and growing into a three-dimensional structure. Recent advances in single-cell imaging reveal the kinematics of this developmental process with single-cell resolution. To understand the role of mechanics in shaping the biofilm, we develop a multiphase continuum model of biofilm development. We find that the kinetic friction between the growing biofilm and the surface leads to a universal “fountain-like” flow of material within the biofilm, in good agreement with experimental data. Using a phase-field approach, we study how cell-cell and cell-matrix mechanical interactions affect the internal organization of cells in the growing biofilm.

*This work was supported by NIH Grants R01 GM082938 and 1R21AI146223-01, and by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030).

E. coli Bacteria near "Black Hole"*  

TRUNG PHAN (Presenter), Princeton University, RYAN MORRIS, University of Edinburgh, MATTHEW BLACK, KE-CHIH LIN, Princeton University, JULIA BOS, Pasteur Institute, ROBERT AUSTIN, Princeton University — In microfluidic environment, we create hydrodynamic horizon from which no E. coli bacteria can escape ("black hole") to study the collective behaviors of those organisms under the influence of such background, probing for their strategy to avoid potentially harmful region where part of the population disappears.

*This work was supported by NSF PHY-1659940.
10:48AM F23.00015: Microbial communities governed by interplay of bacterial interaction and biofilm mechanics*  GABI STEINBACH (Presenter), MICHAEL NG SIULUNG, CRISTIAN CRISAN, BRIAN K. HAMMER, PETER YUNKER, Georgia Inst of Tech — Biofilms are highly structured, densely packed bacterial consortia. Their structures are often explained as the result of social interactions between bacteria, e.g. cooperation and competition. Others concentrate on the role of local mechanics in biofilm formation. These two lines of argumentation are typically treated separately. Here, we show that mechanics and social interactions can be strongly interrelated and their combination can crucially impact biofilm formation and dynamics. Using Vibrio cholerae strains that kill each other on contact, we examine how bacterial antagonism impacts biofilm mechanics, and vice versa. We find that this interplay leads to counterintuitive results. For example, killing produces dead cells, which can prevent subsequent killing, and, thus, stabilizes coexistence.

*Funded by the German National Academy of Sciences Leopoldina.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F24 GSNP DBIO: Noise-Driven Dynamics in Far-From-Equilibrium Systems I  401 - Stephen Teitsworth, Duke University - Tag(s): Focus

8:00AM F24.00001: Climate variability: a manifestation of fluctuations in a nonequilibrium steady state* [Invited]  JEFFREY B. WEISS (Presenter), University of Colorado, Boulder, BAYLOR FOX-KEMPER, Brown University, DIBYENDU MANDAL, University of California, Berkeley, ARIN D. NELSON, University of Michigan, Ann Arbor, ROYCE ZIA, Virginia Polytechnic Institute and State University — The climate system is forced by incoming solar radiation, is damped by outgoing long-wave radiation, and is, apart from time-dependent natural and anthropogenic forcing, approximately in a nonequilibrium steady state. The natural variability about the time-mean climate state takes the form of coherent, preferred, spatio-temporal patterns with names such as the El-Niño Southern Oscillation, the Madden-Julien Oscillation, the Atlantic Multidecadal Oscillation, and the Pacific Decadal Oscillation. These climate oscillations have large human impacts and their response to anthropogenic climate change is uncertain. Nonequilibrium steady states can be characterized by persistent currents in phase space and we interpret climate oscillations as the physical space manifestation of those phase space currents. We describe a new diagnostic for phase space currents, the phase space angular momentum, which describes the rotational flow of trajectories in phase space by analogy to the mass angular momentum of a fluid rotating in physical space. One advantage of the phase space angular momentum is that it can be readily calculated from an observed time series with no assumptions about an underlying model. We find that the phase space angular momenta in simple stochastic models of the El-Niño Southern Oscillation and the Madden-Julien Oscillation agree surprisingly well with that seen in observations of the climate system. We propose that the phase space angular momentum might be a useful general metric to describe fluctuations in nonequilibrium steady states.

*This work was supported in part by NSF INSPIRE Award #1245944 and NSF DMR #1507371.
8:36AM F24.00002: Critical Dynamics of Anisotropic Antiferromagnets in an External Field*
UWE CLAUS TAUBER (Presenter), RIYA NANDI, Department of Physics & Center for Soft Matter and Biological Physics, Virginia Tech — We numerically investigate the non-equilibrium critical dynamics in three-dimensional anisotropic antiferromagnets in the presence of an external magnetic field. The phase space of this system exhibits two critical lines which meet at a bicritical point. In this system, the non-conserved components of staggered magnetization order parameter couple dynamically to the conserved component of the magnetization density along the direction of the external field. By employing a hybrid computational algorithm that combines reversible spin precession with relaxational Monte Carlo updates, we study the aging scaling dynamics for the model C critical line, identifying the critical initial slip, decay and aging collapse exponents, thus also verifying the dynamic critical exponent. We also probe the dynamic exponent of the model F critical line by investigating the system-size dependence of the characteristic spin wave frequencies near criticality. Furthermore, we investigate the aging scaling behavior of the slow order parameter and conserved field near the bicritical point.

*Research was sponsored by the U.S. Army Research Office and was accomplished under Grant Number W911NF1710156.

8:48AM F24.00003: Current fluctuations in presence of time-periodic metabolic conditions*
DANILO FORASTIERE (Presenter), GIANMARIA FALASCO, MASSIMILIANO ESPOSITO, University of Luxembourg Limpertsberg — We address the current response to periodic driving of a crucial biochemical reaction network, namely, substrate inhibition. We focus on the conversion rate of substrate into product under time-varying metabolic conditions, modelled by a periodic modulation of the product concentration. Coarse-graining the original model to a minimal solvable one by means of a projection technique, we study the leading behavior of the time averaged current and its fluctuations using a large deviations approach. We show that there exist different regimes, depending on the kinetic rates, in which positive and negative amplitude resonant effects take place, and we provide interpretations for the role that these nonequilibrium effects can play in the metabolic network.

*This work was funded by the European Research Council project NanoThermo (ERC-2015-CoG Agreement No. 681456).
While the biochemistry of metabolism in many organisms is well studied, details of the metabolic dynamics are yet fully explored.

Unless the parameters of a vast number of enzyme-catalyzed reactions happened to fall into very special ranges, a kinetic model on a large metabolic network would fail to reach a steady state.

Acquiring adequate in vivo kinetic parameters experimentally has always been an obstacle.

Approach:
A stable metabolic network can be systematically established via a biologically/evolutionally motivated regulatory process.

May be understood via a landscape description of metabolism as a stochastic system, which draws enzymatic parameters towards stable phase spaces.

Allows explicit thermodynamics constraints on concentrations and optimal balance of efficiency vs viability (i.e. stability/fitness/robustness).

The strategy was applied successfully to the central metabolism of Methylobacterium extorquens AM1 and the secondary metabolism and metabolic switches in Streptomyces xiamenensis 318.

*The work was partially supported by the Natural Science Foundation of China No. 91329301 and No. 91529306 (PA), No. 81273404 and No. 81473105 (MJX).
9:12AM F24.00005: Temperature interfaces in the Katz-Lebowitz-Spohn driven lattice gas* 
RUSLAN MUKHAMADIAROV (Presenter), PRIYANKA ., UWE CLAUS TAUBER, Virginia Tech — We explore the intriguing spatial patterns that emerge in a two-temperature Katz-Lebowitz-Spohn (KLS) model in two dimensions, a driven lattice gas with attractive nearest-neighbor interactions and periodic boundary conditions. The domain is split into two regions with hopping rates governed by different temperatures $T > T_c$ and $T_c$, respectively, where $T_c$ indicates the critical temperature for phase ordering. When the temperature boundaries are oriented transverse to the drive, the hotter region experiences an unexpected phase separation caused by the lower sustained current in the cooler region. The resulting density profiles in both hot and cold subsystems are similar to the well-characterized coexistence and maximal-current phases in (T)ASEP models with open boundary conditions, yet display marked fluctuation corrections. In contrast, when the temperature boundaries are oriented along the drive, the KLS dynamics is crucially determined by the choice of hopping rates across the temperature interfaces. In particular, when the latter break particle-hole symmetry, we observe particle influx from the cooler into the hotter region.

*Research was sponsored by the Army Research Office and was accomplished under Grant Number W911NF-17-1-0156.

9:24AM F24.00006: Anomalous heating in a colloidal system: Observation of the inverse Mpemba effect* 
AVINASH KUMAR (Presenter), JOHN BECHHOEFER, Simon Fraser Univ — We present the first experimental observation of anomalous heating in colloidal systems, a phenomenon known as the inverse Mpemba effect. In particular, under certain conditions, we observe that an initially cold system heats up faster than an identical warm system when coupled to the same thermal bath. We study the effect in a system consisting of a Brownian particle in a tilted double-well potential set in an asymmetric domain. We also study the forward Mpemba effect, where an initially hot system cools faster than an identical warm system. We observe the forward effect for a wide range of temperatures and domain sizes (region in space explored by the particle). By controlling the relative sizes of the basins of attraction of the stable and metastable potential wells, we can provide a direct kinetic path between the hot initial state and the cold equilibrium. We then observe exponentially faster cooling. This is the first experimental evidence for the strong Mpemba effect.

*This research work has been supported by Discovery and RTI Grants from the National Sciences and Engineering Research Council of Canada (NSERC).
9:36AM F24.00007: Decomposition of anomalous diffusion in generalized Lévy walks into its constitutive effects*  VIDUSHI ADLAKHA (Presenter), Department of Physics and TcSUH, Univ of Houston, PHILIPP G. MEYER, EREZ AGHION, HOLGER KANTZ, Max Planck Institute for the Physics of Complex Systems, KEVIN E. BASSLER, Department of Physics and TcSUH, Univ of Houston — Anomalous diffusion is observed in a variety of physical and social systems, including blinking quantum dots, animal locomotion, intra-day trades in financial markets and cold atoms in dissipative optical lattices. Generalized Lévy walks can be used to model their dynamics. We show that the anomalous diffusive behavior found in these systems can be decomposed into three fundamental constitutive causes. These causes, or effects, are related to ways that the Central Limit Theorem fails. The increments generated through the stochastic process can have either long-time correlations, infinite variance, or be non-stationary. Each of these properties can cause anomalous diffusion and is characterized by what is known as the Joseph, Noah and Moses effects, respectively. In generalized Lévy walks, a complex combination of these effects leads to the observed sub- and super-diffusive behaviors. We analytically calculate the scaling exponents determining each of the three constitutive effects and confirm the results with numerical simulations. The results satisfy a fundamental scaling relation between the exponents.

*This work was supported by the NSF through grant DMR-1507371.

9:48AM F24.00008: A coupled two-species model for the pair contact process with diffusion*  SHENGFENG DENG (Presenter), UWE CLAUS TAUBER, Department of Physics, Virginia Tech — The contact process with diffusion (PCPD) defined by the pair reactions $2B \rightarrow 3B$, $2B \rightarrow 0$ and diffusive particle spreading exhibits an unusual active to absorbing phase transition whose universality class has long been disputed. Multiple studies indicated that further coarse-graining of the model may be needed for its effective long-time, large-scale description. We introduce a coarse-grained two-species representation for the PCPD in which single particles $B$ and particle pairs $A$ are coupled according to the processes $2B \rightarrow A$, $A \rightarrow A+B$, $A \rightarrow 0$, $A \rightarrow 2B$, with each type of particles diffusing independently. We employ Monte Carlo simulations in one, two, and three dimensions to demonstrate that this model consistently captures the pertinent features of the PCPD. In the inactive phase, $A$ particles die out rapidly, effectively leaving the $B$ species to undergo pure pair annihilation kinetics. At criticality, both $A$ and $B$ densities decay with similar exponents to those measured for the PCPD and display mean-field scaling above the critical dimension $d_c=2$. In one dimension, exponents for the $B$ species obtained from seed simulations also agree well with previously reported ranges.

*Research was sponsored by the Army Research Office under Grant No. W911NF-17-1-0156 and CSC fellowship (No. 201806770029).
10:00AM F24.00009: Anomalous Diffusion with an Absorbing Wall*  ALEX WARHOVER
(Presenter), THOMAS VOJTA, Missouri Univ of Sci & Tech — Fractional Brownian Motion and the Fractional Langevin Equation, random processes characterized by long-time power law correlations in the noise, are prototypical models for anomalous diffusion. We employ large scale Monte Carlo simulations to investigate these models in the presence of an absorbing wall. In the limit of vanishing correlations, our findings reproduce the well-known results for normal diffusion. In contrast, the interplay between the absorbing wall and the long-range power correlations leads to a singular probability density close to the wall. We compare our results to those of Fractional Brownian Motion [1] as well as the Fractional Langevin Equation [2] in the presence of a reflecting wall, and we discuss implications of our results.


*This work was supported in part by the NSF under Grant No. DMR-1506152 and DMR-1828489.

10:12AM F24.00010: Diffusion in dynamic crowded spaces  DAVID YLLANES (Presenter), HARRY BENDEKGEY, GREG HUBER, LE YAN, Chan Zuckerberg Biohub — Brownian motion in disordered media is now well understood in the case of immobile hard obstacles. In many practical applications, however, the space itself can be dynamic. An important example is transport inside the cell, a very crowded environment with obstacles of varying sizes and complicated shapes that are constantly being rearranged. This situation has received comparatively little attention. With the ever-increasing quality of microscopy techniques, allowing for the tracking of particles inside living cells, the need for a quantitative model is clear.

Here we propose an extension of commonly used "Swiss-cheese" models to include moving obstacles and study it with numerical simulations in one, two and three dimensions. The motion of our tracer particles is anomalous over many decades in time, before reaching a diffusive steady state with an effective diffusion constant that depends on the obstacle density and diffusivity. Moreover, we find that the scaling behaviour of the effective diffusivity, above and below a critical regime at the percolation point for void space, can be characterised by two critical exponents: the conductivity $\mu$, also found in models with frozen obstacles, and a new exponent $\psi$ that quantifies the effect of the obstacle diffusivity.
10:24AM F24.00011: Trajectories and transport characteristics of a Brownian particle in a 1D potential subject to bias.*  TREV JIRON (Presenter), JARROD SCHIFFBAUER, Physical and Environmental Sciences, Colorado Mesa University — We investigate one-dimensional driven, diffusive motion of a single Brownian particle moving through a periodic lattice potential and subject to a constant, uniform bias using a Langevin equation of motion. The model yields explicit trajectories with bias-dependent trapping, hopping, and linear response regimes at sufficiently low temperatures and the statistical behavior generated by an ensemble of trajectories are essentially those of an asymmetric simple exclusion process. Moreover, we find that, at low bias, the system exhibits a negative differential mobility, decreasing with applied bias, to a distinct local minimum in the hopping transport regime. In the context of the dynamical model, we argue the non-monotonic behavior of the transport coefficient can be explained by the role of friction as the particle passes through the minima in each well. Such a model may be employed to describe a wide variety of intriguing transport behaviors. As an example, we show that experimental data on the transition from static to kinetic friction through a plastic regime can be described by such a model.

*The authors acknowledge support from the Department of Physical and Environmental Sciences and Colorado Mesa University.

10:36AM F24.00012: Fluctuation theorem for geometric pumping processes*  HISAO HAYAKAWA (Presenter), Yukawa Institute for Theoretical Physics, Kyoto University — We derive an extended fluctuation theorem for an open quantum system coupled with two reservoirs under one-cycle modulation. We confirm that the geometric phase caused by the Berry-Sinitsyn-Nemenman curvature in the parameter space generates non-Gaussian fluctuations. This non-Gaussianity is enhanced for the instantaneous fluctuation relation when the bias between the two reservoirs disappears.

*This work is partially supported by a Grant-in-Aid of MEXT for Scientific Research (Grant No. 16H04025).
**Stochastic Line Integrals as Metrics of Irreversibility and Heat Transfer**

STEPHEN TEITSWORTH (Presenter), Physics, Duke University, JOHN NEU, Math, UC Berkeley —

Stochastic line integrals provide a powerful tool for quantitatively characterizing irreversibility and detailed balance violation in noise-driven dynamical systems. A particular realization of such integrals, the stochastic area, was recently introduced for linear systems and has been tested experimentally in coupled linear electrical circuits [1,2]. In this talk, we provide a framework for understanding general properties of stochastic line integrals and clarify their implementation for experiments and simulations as well as their utility as metrics for quantifying non-equilibrium behavior. Theoretical results are supported by numerical studies of an overdamped, two-dimensional mass-spring system driven out of equilibrium. In this case, the stochastic area can be concisely expressed in terms of a streamfunction the sign of which determines the orientation of probability current loops. Furthermore, the stream function allows one to analytically understand the dependence of stochastic area on key parameters such as the noise strength (equivalently temperature) for both nonlinear and linear springs.


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**Session F25 GSNP: Mechanical Metamaterials II**

**Tuesday, March 3, 2020 8:00 AM - 11:00 AM**

**8:00AM F25.00001: On the design of multi-stable metastructures with rotational degrees of freedom**

YONG ZHANG (Presenter), MARCEL TICHEM, FRED VAN KEULEN, Department of Precision and Microsystems Engineering, Delft Univ of Tech —

Buckling-induced multi-stable metastructures are rationally designed structures whose unit cells exhibit bi-stable or multi-stable configurations. Apart from achieving transitions between two stable states at the unit cell level, metastructures composed of bi-stable beams are also able to realize rotations due to the spatial arrangement of beams. In this work, the design space of the geometric parameters for metastructures exhibiting both rotational and translational motions is explored on the basis of both theoretical and experimental studies. First, numerical results demonstrate that beam thickness, height and length play key roles in determining the rotational snapping. To quantify the effects of these structural parameters, we analytically model the rotational snapping behavior of a representative element that consists of two beam units. Furthermore, we conduct a comprehensive parametric survey based on the proposed model. This study reveals that the rotational stability is highly dependent on the ratio between beam thickness and height. In order to allow for rotational stable states, this ratio should be constrained within a specific range. Finally, we validate these effects by measuring the mechanical response of 3D-printed specimens with different geometric parameters.
8:12AM F25.00002: Prediction of Elastic Wave Propagation Characteristics of Composites via Strong-Contrast Expansions*  JAEUK KIM (Presenter), SALVATORE TORQUATO, Princeton University — The preponderance of previous treatments to predict the effective elastic properties of composites assume the purely static limit. Here we derive exact expressions for effective elastodynamic properties of two-phase composites at intermediate wavelengths by extending the "strong-contrast" expansion approach previously applied to the static problem. The resulting series expansion explicitly incorporates complete microstructural information about the composite via \( n \)-point correlation functions and is endowed with excellent convergence properties, even for high contrast ratios of phase moduli. The fast convergence of this series enables us to extract an accurate approximation that depends on the microstructure via the two-point correlation function or its Fourier counterpart, which we call the "spectral density." Our formula thus extends previous "mean-field" treatments that typically do not account for nontrivial microstructural information and/or are limited to small phase contrasts. We apply our spectral-density formula to a variety of models of disordered composites and discuss how to engineer composites with prescribed attenuation properties for elastic waves.

*This work was supported by the Air Force Office of Scientific Research Program under award No. FA9550-18-1-0514.

8:24AM F25.00003: What is the bending rigidity of a book? Stacked plates as a dissipative structured beam  SAMUEL POINCLoux (Presenter), TIAN CHEN, FlexLab, Ecole Polytechnique Federale de Lausanne, BASILE AUDOLY, Laboratoire de mécanique des solides, CNRS, Institut Polytechnique de Paris, PEDRO REIS, FlexLab, Ecole Polytechnique Federale de Lausanne — Multi-layered structures have long been exploited in engineering to design stiff and lightweight structural elements. For example, sandwich-structured composites involve an interplay between the mechanical properties of the individual layers and the inter-layer interactions through the matrix. In the absence of a matrix, when the layers are free to slide with respect to one another, energy is dissipated by frictional interactions. Here, in the context of designing high-performing metamaterial dampers, we focus on providing a quantitative description of the mechanical response of stacks composed of a large number (\( n \sim 50 \)) of elastic plates interacting through friction. In essence, we ask: “What is the bending rigidity of a book?” The mechanical response of our stacks is assessed experimentally through precision nonlinear bending tests. Naturally, our findings deviate from the purely linear elastic case, exhibiting surprising stiffening effects and hysteretic behavior. Taking friction as a perturbation, we develop a predictive model involving the coupling between the geometric nonlinearities, elasticity and friction that is in excellent agreement with experiments.
8:36AM F25.00004: The effect of dualities on elastic moduli
MICHEL FRUCHART (Presenter), VINCENZO VITELLI, University of Chicago — Elasticity describes how a rigid object like a rubber duck goes back to its original form when slightly deformed. Microscopic symmetries impose strong constraints on the elasticity of a crystalline solid. For instance, the elasticity of a 2D crystal with triangular symmetry is isotropic, and hence has only two independent elastic moduli (instead of six without any symmetry). This is because the elastic tensor relating stress and deformation transforms as a tensor under spatial transformations. Hence, it is surprising to encounter a family of anisotropic microscopic crystals devoid of any symmetry that however exhibits isotropic elasticity. We will show that a duality lies at the root of this riddle.

In addition to usual spatial symmetries, non-spatial symmetries can occur microscopically, that are not captured in the tensorial character of the elastic tensor. Such additional symmetries can emerge in families of microscopic systems where a duality transformation relates pairs of different systems: in self-dual systems (mapped to themselves by the duality), the duality can become an new symmetry different from spatial operations. These relations can constrain the elastic tensor, reducing the number of independent moduli both in self-dual systems and away from the self-dual point.

8:48AM F25.00005: Emergent plasticity and hysteresis in disordered packings of filaments.*
NICHALAS WEINER (Presenter), HUNTER KING, University of Akron, YASHRAJ R BHOSALE, MATTIA GAZZOLA, University of Illinois at Urbana-Champaign — A bird's cup-nest can be viewed as a disordered packing of slender grains, defined by average quantities -- coordination number and packing fraction; and dependent on grain properties -- flexibility, friction, and aspect ratio. Experimental data from packings of varying aspect ratio grains, subject to cyclic, quasi-static, oedometric compression reveal two distinctly meta-mechanical responses: plasticity associated with rearrangement without damage; and hysteresis associated with static friction rather than viscoelasticity. These qualitative behaviors appear to be common across systems of round grains to extremely fine fibers. One-to-one numerical simulations allow us to relate otherwise inaccessible micromechanical quantities such as contact distributions to bulk behaviors, confirming underlying assumptions regarding their origin.

*NSF CMMI #1825924
9:00AM F25.00006: Viscoelasticity and plasticity in the formation of creases in thin sheets
BUWANETH DHARMADASA (Presenter), University of Colorado, Boulder, CHINTHAKA H.M.Y. MALLIKARACHCHI, University of Moratuwa, FRANCISCO LOPEZ JIMENEZ, University of Colorado, Boulder — Origami inspired folding, which enables the transformation of a flat sheet into different geometries, has recently become a topic of interest among the engineering community as it helps solving problems ranging from deployable structures for space engineering to micro scale grippers for bio-medical applications. However, the mechanics of a folded sheet are not only governed by the sheet properties and the folding pattern, but also by the properties of the creases. We study them by performing experiments exploring the influence of different control parameters, such as the applied force and the time the film was pressed. We rationalize the experimental results with numerical simulations: a 1D elastica beam model and a high-fidelity finite element analysis, both accounting for elasto-plastic behavior and non-linear geometry. By considering the curvature localization, we can define a crease length that depends on the properties of the film and the fold control parameters. We found that non-dimensionalized results provide a robust scaling that enables to extend the results to other geometries and material properties. We also explore the effect of viscoelasticity of the sheet material.

9:12AM F25.00007: Viscoelastic Metamaterials
DAVID DYKSTRA (Presenter), JORIS BUSINK, Institute of Physics, University of Amsterdam, ALEKSI BOSSART, School of Engineering, École polytechnique fédérale de Lausanne, JOP VAN DER LAAN, Institute of Physics, University of Amsterdam, BERNARD ENNIS, Materials Design Department, Tata Steel Europe R&D, CORENTIN COULAIS, Institute of Physics, University of Amsterdam — We show how viscoelasticity can be harnessed to increase functionality in mechanical metamaterials. First, we explore experimentally the mechanical snap-through response of metamaterials that are made of constituents that exhibit large viscoelastic relaxation effects, encountered in the majority of rubbers [1]. Second, we demonstrate that we can rationally design multimode mechanical metamaterials, featuring viscoelastic and elastic elements. By altering the loading rate, we can switch between the two modes of deformation. Our findings bring a novel understanding of metamaterials in the dynamical regime and opens up avenues for the rational design of multifunctional viscoelastic metamaterials.


9:24AM F25.00008: Memory of a mechanical metamaterial
HADRIEN BENSE (Presenter), MARTIN VAN HECKE, FOM Inst - Amsterdam — Many disordered systems – granular suspensions, spin-glasses, crumpled paper – present history dependent features. However, their complex geometry makes observing, understanding and controlling such memory effects challenging. We introduce a class of patterned thin sheets that, when forced, exhibit controlled crumpling via elastic snap-through instabilities. Individual snap-through events act as `hysterons' that can be observed directly, and that lead to complex yet fully observable deformation pathways. We explore a variety of memory effects in these system, and connect memory to pathways.
**9:36AM F25.00009: Amplitude-dependent input to reprogram static and dynamic properties of multistable structures**

HIROMI YASUDA (Presenter), LUCIA KORPAS, JORDAN R. RANEY, University of Pennsylvania — Phase transformations can be observed from the nanometer scale of crystalline order to macroscale mechanical structures. These transformations are often associated with dramatic reconfigurations and changes to properties. Here, we study a tunable mechanical structure composed of a 1D chain of rotating squares and embedded magnets, with each cell along the chain capable of being in any of three possible stable phases, defined by the angular orientation of the square. We demonstrate the ability to change the static and dynamic responses, particularly linear/nonlinear wave dynamics, by reversibly reconfiguring the structure via controlled use of transition waves. We numerically and experimentally demonstrate the propagation of transition waves in a 1D chain. We then analyze the dynamic properties of the chain, including the opening/closing of a frequency band gap, and the coupling behavior between rotational and translational motion as a function of the phase. We demonstrate that transition waves with opposite rotational directions can be generated, and that a collision between such waves results in the formation of a phase boundary.

*This work was supported by ARO grant number W911NF-17-1-0147, and by NSF MRSEC DMR-1720530.

**9:48AM F25.00010: Porous Inclined Auxetic Structural Material**

MATHEUS C FERNANDES (Presenter), John A. Paulson School of Engineering and Applied Sciences, Harvard University, SAURABH MHATRE, OLGA MESA, Graduate School of Design, Harvard University, KATIA BERTOLDI, John A. Paulson School of Engineering and Applied Sciences, Harvard University, MARTIN BECHTHOLD, Graduate School of Design, Harvard University — Porous structural materials with well-defined periodicity are ubiquitous not only in nature but also in synthetic structures and devices. These types of materials have been proven to offer various types of auxetic behavior, ranging from negative Poisson's ratio to high energy absorption and excellent acoustic damping. Yet, here we present a novel auxetic behavior harnessed by introducing angled cuts into a periodic porous material. Using this approach, we utilize out-of-plane behavior with the potential to control friction, light emission and reflection, as well as fluid flow properties. Using a combination of physical experiments and non-linear finite element analysis, we study the effects of geometry on creating and propagating this out-of-plane auxetic behavior.

*NSF-GRFP Fellowship Grant DGE-1144152 (for M. C. F.)
10:00AM F25.00011: Engineering auxetic geometry design for flexible and stretchable devices  YU-KI LEE (Presenter), Department of Materials Science and Engineering, Seoul National University, YOUNG-JOO LEE, Department of materials science and engineering, University of pennsylvania, YOUNG-CHANG JOO, IN-SUK CHOI, Department of Materials Science and Engineering, Seoul National University — In this talk, we present how the auxetic design can be used to flexible and stretchable electronic devices. An auxetic structure called 'fractal cut', which means that the basic rotating units can be subdivided into a self-similar hierarchy, enables us to develop extremely and omni-directionally deformable batteries. During stretching or crumpling, deformation occurs only at hinges between two adjacent units while the units did not undergo distortion. In addition, a re-entrant auxetic elastomer used for capacitive-type stretchable strain sensor can overcome the theoretical limit of the conventional capacitive-type strain sensor. We believe that our auxetic geometry design can provide a strategy to apply mechanical metamaterials for fabricating flexible and stretchable electronic devices.

10:12AM F25.00012: Auxetic foam revisited: understanding the origin of negative Poisson's ratio using micro-CT and pore structure analysis*  LAMEI DU, SIDA LUO, YE XU (Presenter), BeiHang University — Porous foam with negative Poisson's ratio, namely auxetic foam, is a typical mechanical metamaterial. One of the commonly used approach in producing auxetic foam is the thermomechanical compression of porous thermoplastic materials such as Polyurethane (PU) foams. While qualitatively it is well understood that the negative Poisson's ratio arises from the reentrant cell shape, quantitative relation between the auxetic behavior and pore structure is still lacking. Using micro-CT, we systematically quantify the pore structures of a series of auxetic PU foams prepared with various degrees of thermomechanical compression, and correlate with their mechanical behaviors measured from tensile tests. We find that the fraction of bucked ribs of the pore structure is related to the initial value of Poisson's ratio upon stretching while the extent of buckling is related to the maximum tensile strain for negative Poisson's ratio. Our findings can shed light in designing mechanical metamaterials with targeted auxetic behaviors.

*This work is supported by National Natural Science Foundation of China (Grant No. 11674019)
10:24AM F25.00013: Dynamics and Topology of Non-Hermitian Elastic Lattices with Non-Local Feedback Interactions* MATHEUS NORA ROSA (Presenter), Georgia Inst of Tech, MASSIMO RUZZENE, Department of Mechanical Engineering, University Of Colorado Boulder — We investigate a family of non-Hermitian 1D elastic lattices whereby feedback control is used to establish non-local, non-reciprocal strain based interactions. We demonstrate that wave propagation is largely non-reciprocal for all frequencies within the dispersion bands, manifesting as either gain or loss for opposite propagation directions. The non-reciprocal bands are tunable based on the non-local interactions, which can define multiple frequency bands with opposite non-reciprocal behavior. The large non-reciprocity also manifests in finite lattices whereby all the bulk eigenmodes are localized at a boundary, which is known as the non-Hermitian skin effect. In analogy to recent work in quantum lattices, we show that the winding numbers of the dispersion bands on the complex plane predict the localization edge of the skin modes of finite lattices, which can be interpreted as a bulk-bulk correspondence principle. Finally, we investigate wave propagation in 2D lattices where directional non-reciprocity is demonstrated, and show preliminary results that suggest a 2D manifestation of the non-Hermitian skin effect in the form of corner modes for finite lattices.

*The authors acknowledge funding from the National Science Foundation (NSF) through the EFRI 1741685 grant.

10:36AM F25.00014: Non-Commuting Mechanical Metamaterials AMITESH SINGH (Presenter), Leiden University, MATTHIEU LABOUSSE, ESPCI Paris, MARTIN VAN HECKE, Leiden University — Strategies for programmable metamaterial design need to be sensitive to the order of input signals. Here, we introduce a non-commuting mechanical metamaterial that consists of a quasi-1D chain of weakly symmetry-broken beams. We demonstrate, via simulations and experiments, that its response depends on the order of external actuation. Our work opens a new route to mechanical memory and reprogrammable metamaterials.

10:48AM F25.00015: Bounds on resonant bandgap limits in a branched 1D lattice modeled by Bloch’s theorem MARY BASTAWROUS (Presenter), MAHMOUD I. HUSSEIN, Ann and H.J. Smead Department of Aerospace Engineering Sciences, University of Colorado Boulder — Elastic metamaterials exhibit unique properties associated with local resonance band gaps. A 1D lattice unit cell comprising a monatomic chain connected to a branch is examined leading to mathematical relations relating the vibration behavior of the independent branch to the dispersion of the entire unit cell. This perspective is distinct from studying the resonances of the full system and relating them to the local-resonance band gaps. The closed-form relation, based on Bloch’s theorem, determines the dependence of the upper and lower band-gap limits on the resonances and antiresonances of the frequency response of the separate branch. This offers a formal approach for identifying bounds for the location of band-gap edges. Moreover, it demonstrates that local resonance band gaps form as a result of a balance between the inertia and restoring forces of the main chain and the branch effective restoring force. This framework is further employed to study a special case where the branch is constructed out of a finite number of repeating diatomic units where the periodic branch's Bragg band gaps are exploited. Conditions are derived for a global unit-cell dispersion exhibiting super-wide local resonance band gaps or pass bands, super narrow pass bands, and tailored fano-resonances.
8:00AM F26.00001: **Vimentin intermediate filament biomechanics in 3D cell motility** [invited]

ALISON PATTESON (Presenter), Physics, Syracuse University — The migration of cells through confining spaces in tissues is important for many biological processes and depends on the mechanical properties of a cytoskeleton made up of three different filaments: F-actin, microtubules, and intermediate filaments. The signaling pathways and cytoskeletal structures that control cell motility on 2D are often very different from those that control motility in 3D. Previous studies have shown that intermediate filaments can promote actin-driven protrusions at the cell edge, but have little effect on overall motility of cells on flat surfaces. They are however important for cells to maintain resistance to repeated compressive stresses that are expected to occur *in vivo*. Using mouse embryonic fibroblasts derived from wild-type and vimentin-null mice, we find that loss of vimentin increases motility in 3D micro-channels even though on flat surfaces it has the opposite effect. Atomic force microscopy and traction force microscopy experiments reveal that vimentin enhances perinuclear cell stiffness while maintaining the same level of acto-myosin contractility in cells. We propose a minimal model in which a perinuclear vimentin cage constricts along with the nucleus during motility through confining spaces, providing mechanical resistance against large strains that can damage the structural integrity of cells and their nuclei.

8:36AM F26.00002: **Confined cell migration - a dynamical systems perspective**

DAVID BRÜCKNER (Presenter), ALEXANDRA FINK, MATTHEW SCHMITT, NICOLAS ARLT, JOACHIM O RÄDLER, CHASE BROEDERSZ, Faculty of Physics and Center for NanoScience, Ludwig Maximilian University Munich — In many biological phenomena, cells migrate through confining environments. However, a quantitative conceptual framework for confined migration has remained elusive. To provide such a framework, we employ a data-driven approach to infer the dynamics of cell movement, morphology and interactions of cells confined in two-state micropatterns. In this confinement, cells stochastically migrate back and forth between two square adhesion sites connected by a thin bridge. By inferring a stochastic equation of motion directly from the experimentally determined short time-scale dynamics, we show that cells exhibit intricate non-linear deterministic dynamics that adapt to the geometry of confinement. This approach reveals that different cell lines exhibit distinct classes of dynamical systems, ranging from bistable to limit cycle behavior. To connect these findings to underlying migratory mechanisms, we track the evolution of cell shape and develop a framework for the dynamics of cell morphology in confinement. Our approach yields a conceptual framework for the motility and morphology of confined cells which can be generalized to more complex environments including multiple interacting confined cells.
Finite element simulation of a cell entering a pipette: Effects of large deformation and frictional contact

XIAOHAO SUN (Presenter), Mechanical Engineering, University of Colorado, Boulder, KE WANG, Institute of Electronics, Chinese Academy of Sciences, HENGAN WU, Modern Mechanics, University of Science and Technology of China, JIAN CHEN, Institute of Electronics, Chinese Academy of Sciences, RONG LONG, Mechanical Engineering, University of Colorado, Boulder — The process of single cells entering a confined channel under pressure is widely seen in cell mechanics experiments (e.g., micropipette aspiration) and biological process (e.g., tumor cell migration in capillaries). Finite element method that models the cell as a continuum solid has been extensively used to study this process. However, most previous modeling studies suffered from limitations including inaccurate pressure and frictional boundary conditions, therefore making it challenging to simulate the complete entry process involving large deformation of the cell. Here we present a simulation approach that can continuously update the boundary condition according to the contact status as the cell enters the channel, thus enabling more accurate description of the pressure and frictional conditions. Using a quasi-linear viscoelastic solid model for the cell, we show that the detailed pressure boundary condition and interface friction coefficients can significantly affect the cell entry process.

Modeling the effect of vimentin on confined cell motility.

SARTHAK GUPTA (Presenter), ALISON PATTESON, JENNIFER SCHWARZ, Physics, Syracuse University — As a cell moves in a strongly confined geometry, its cytoskeleton undergoes changes as does the peri-nuclear cage. How do these changes affect cell motility? The cytoskeleton is made up of three different semi-flexible polymers: actin, microtubules, and intermediate filaments, such as vimentin. Recent studies demonstrate that the loss of vimentin enhances cell motility through micro-channels and confining spaces, though it has the opposite effect in 2D. We are, therefore, modeling the effects of intermediate filaments on cell motility in confinement to understand these latest experiments. We have developed a biophysical model for a cell moving through various confined geometries based on Brownian dynamics. It includes an intracellular network along with a peri-nuclear cage, both of which involve vimentin. We explore a possible mechanism behind the enhanced motility of vimentin-null cells, irrespective of channel width, in comparison to wild-type. We also characterize the increased speed of vimentin-null cells with increasing confinement and the minimal effect on the speed of wild-type cells under the same conditions. We also investigate the effects of flexible confinement walls on cell motility to better mimic the physiological conditions.

NSF-DMR-1832002
9:12AM F26.00005: Regulation of nuclear architecture, mechanics, and nucleocytoplasmic shuttling of epigenetic factors by cell geometric constraints* [Invited] FARID ALISAFAEI, University of Pennsylvania, DOORGESH SHARMA JOKHUN, GV SHIVASHANKAR, National University of Singapore, VIVEK SHENOY (Presenter), University of Pennsylvania — Cells sense mechanical signals from their microenvironment and transduce them to the nucleus to regulate gene expression programs. To elucidate the physical mechanisms involved in this regulation, we developed an active 3D chemomechanical model to describe the three-way feedback between the adhesions, the cytoskeleton, and the nucleus. The model shows local tensile stresses generated at the interface of the cell and the extracellular matrix regulate the properties of the nucleus, including nuclear morphology, levels of lamin A,C, and histone deacetylation, as these tensile stresses 1) are transmitted to the nucleus through cytoskeletal physical links and 2) trigger an actomyosin-dependent shuttling of epigenetic factors. We then show how cell geometric constraints affect the local tensile stresses and subsequently the three-way feedback and induce cytoskeleton-mediated alterations in the properties of the nucleus such as nuclear lamina softening, chromatin stiffening, nuclear lamina invaginations, increase in nuclear height, and shrinkage of nuclear volume. We predict a phase diagram that describes how the disruption of cytoskeletal components impacts the feedback and subsequently induce contractility-dependent alterations in the properties of the nucleus. Our simulations show that these changes in contractility levels can be also used as predictors of nucleocytoplasmic shuttling of transcription factors and the level of chromatin condensation. The predictions are experimentally validated by studying the properties of nuclei of fibroblasts on micropatterned substrates with different shapes and areas.

*This work is supported by National Cancer Institute Awards U01CA202177 and U54CA193417 (to V.B.S.), National Institute of Biomedical Imaging and Bioengineering Award R01EB017753 (to V.B.S.), the NSF Center for Engineering Mechanobiology (CMMI-154857), and Ministry of Education (MOE)-Tier3 grant Singapore (to G.V.S.).

9:48AM F26.00006: Effective pressure in a dense cell monolayer and collective cell migration EVGENIY KHAIN (Presenter), Physics, Oakland University — A system of dividing and growing cells provides an intriguing example of active matter far from equilibrium. Living cells in a dense system are all in contact with each other. The common assumption is that such cells stop dividing due to a lack of space. Recent experimental observations have shown, however, that cells continue dividing for some time, even after a dense cell monolayer is formed. Effective pressure is introduced in order to model the experimentally observed phenomenon in which the average cell size dramatically decreases over time, and cell area distribution becomes narrower. For a non-uniform system, I will consider the cell shift due to the gradient of the effective pressure and examine its effect on the average cell area profiles. Then I will discuss collective cell migration where cells maintain contact with their neighbors. This migration can be described in terms of a novel front propagation phenomenon; the front speed and effective pressure profile are found both numerically and analytically.
10:00AM F26.00007: Effects of cell-cell adhesion on collective migration of multicellular clusters*  USHASI ROY (Presenter), ANDREW MUGLER, Physics and Astronomy, Purdue University — Collections of cells exhibit directional coherent migration during morphogenesis, cancer-metastasis, and wound healing. Often during migration, bigger clusters split, smaller sub-clusters collide and reassemble, and gaps continually emerge. This leads to the formation of protrusions by some inner cells which eventually act as “leaders”, along with the cells at the leading edge, pulling the cluster towards the favorable direction. Large populations like neural crest cells are known to exhibit such phenomena. We hypothesize that the cells may have an optimal adhesion among themselves, rather than very strong or weak, to favor the formation of gaps and achieve an effective faster migration. We test this hypothesis for one- and two-dimensional cell clusters that collectively track chemical gradients using a mechanism based on contact inhibition of locomotion. We develop both a minimal framework based on the lattice gas model of statistical physics, as well as a more realistic framework based on the cellular Potts model. Results from both frameworks support our hypothesis, suggesting that intermediate adhesion leads to optimal migration. We discuss the mechanisms behind this optimum and relate our results to specific cellular systems.

*This work is supported by the Simons Foundation

10:12AM F26.00008: Plasticity of cell migration resulting from mechanochemical coupling*  ELISABETH GHABACHE (Presenter), YUANSHENG CAO, WOUTER-JAN RAPPEL, University of California, San Diego — Eukaryotic cells can migrate using different modes, ranging from amoeboid-like, during which actin filled protrusions come and go, to keratocyte-like, characterized by a stable actin wave at the front of the cell and persistent motion. How cells can switch between these modes is not well understood but waves of signaling events that lead to actin waves propagation are thought to play an important role in these transitions. Our experiments, performed with Dictyostelium discoideum, show that systematically reducing the protrusion force of the actin network using a drug, latrunculin B, leads to different migration modes including amoeboid-like and keratocyte-like. We find that a sufficient decrease of the protrusion force can destabilize keratocyte-like cells, resulting in cells that employ amoeboid-like migration. We then present a simple two-component biochemical reaction-diffusion model based on relaxation oscillators and couple this to a model for the mechanics of cell deformations. Predictions of the model are in good agreement with the experiments. Our results indicate the importance of coupling signaling events to cell mechanics and morphology and may be applicable in a wide variety of cell motility systems.

*Work supported by the NSF (PHY-1707637) and HFSP (LT000371/2017C).
10:24AM F26.00009: Collective Cell Migration in Wound Healing  KELLY VAZQUEZ (Presenter), JACOB NOTBOHM, University of Wisconsin - Madison — Following a wound, epithelial cells migrate collectively to heal. During healing, “leader cells” begin to form at the free edge and migrate as finger-like, multi-cellular protrusions into the wound boundary. While the presence of leader cells is well documented, factors contributing to their formation is not well understood. Standard wound healing assays often culture cells against a physical barrier, and cells migrate to the free space once the barrier is removed. However, the role of time in culture against a barrier in leader cell formation has not been studied. To address this, a monolayer of Human Keratinocytes (HaCaTs) is seeded against PDMS barriers. The time in culture is varied to study its effect on cell force, motion, wound closure, distribution of actin, and the presence of leader cells following barrier removal by using traction force microscopy and fluorescent imaging. With increased time against a barrier, the number of leader cells increased, a multi-cellular actin cable was formed at the leading edge, and cell migration speeds decreased. The resulting data point to the importance of time in culture in altering cellular mechanics to affect wound healing and add new understanding of factors affecting formation of leader cells in collective cell migration.

10:36AM F26.00010: Traction dynamics in collective cell migration  AASHRITH SARASWATHIBHATLA (Presenter), University of Wisconsin - Madison — Recent theoretical models have emphasized cell motility force as a key driver of collective cell migration. In experiments, the equivalent to the motility force is traction applied by each cell to the substrate, which can be measured by traction force microscopy. Previous experiments have measured tractions in groups of cells but have not tracked tractions applied by individual cells. As a result, there is a lack of information on single-cell tractions over time, which makes it difficult to bridge the gap between single cell and collective cell dynamics. Here, we designed experiments to follow cells in a Lagrangian frame of reference, tracking each cell using fluorescent imaging of its nucleus. To investigate the evolution of traction of each cell over time, we built a Voronoi tessellation based on the centroids of cell nuclei and mapped tractions obtained from traction force microscopy onto each cell's Voronoi-based polygon. The resulting data can be used to compute different metrics of traction dynamics of each cell such as the persistence of both direction and magnitude of traction. This new approach helps to investigate theoretical predictions of cell motility force on collective cell migration, thus bridging the gap between single cell and collective cell dynamics.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F27 FIAP: Electronic Structure: Theory & Spectra  404 - Maicol Ochoa, National Institute of Standards and Technology
8:00AM F27.00001: Extracting Electron Densities in n-Type GaAs from Raman Spectra.
MAICOL OCHOA (Presenter), IREAP, University of Maryland College Park, JAMES E MASLAR, HERBERT S. BENNETT, National Institute of Standards and Technology — Raman measurements can be utilized as a non-destructive method for determining carrier density in compound semiconductors. Rigorous determination of carrier density involves comparing measured and simulated coupled phonon-plasmon Raman spectra. Theories of varying degrees of complexity have been employed for simulating spectra in which spectra are generated as a function of Fermi energy (or carrier density in the degenerate limit). In general, previously utilized spectral models are strictly valid only for a temperature near 0 K and either for the classical or degenerate doping limit. However, such models cannot necessarily capture all spectral information. To overcome this limitation, we have developed a model that is valid at any temperature, any doping level, and for arbitrary values of the ratio $Q^2/\alpha$ (where $Q$ is the magnitude of the normalized wavevector, and $\alpha$ is the normalized frequency used in the Raman measurements). We compare measured n-type GaAs spectra, obtained from epilayers with different carrier concentrations, with simulated spectra obtained with this new spectral model employing different descriptions of the band structure as a function of Fermi energy.

8:12AM F27.00002: Microscopic perspective on the magnetoelectric response of an insulator*
PERRY MAHON (Presenter), JOHN EDWARD SIPE, University of Toronto — We implement a microscopic theory of polarization and magnetization to calculate the magnetoelectric response of an insulator at zero temperature. To first order in the applied fields the free charge and current densities vanish, and as a consequence the response of the system is characterized by the first-order corrections to the microscopic polarization and magnetization fields arising from the applied electric and magnetic fields. Associated with the dipole moment of the microscopic polarization (magnetization) field is a macroscopic polarization (magnetization), for which we extract various response tensors. The magnetoelectric tensor is composed of two distinct parts: the Chern-Simons and cross-gap contributions. We compare our results for these with those of earlier work. We analyze the origin of both the Chern-Simons and cross-gap terms from the perspective of our microscopic theory, and find the former to arise from more “localized” contributions to the response, while the latter to arise from more “extended” contributions.

*We thank the Natural Sciences and Engineering Research Council of Canada (NSERC) for funding.
8:24AM F27.00003: Accurate, Ground State Electronic and Transport Properties of h- BN
YURIY MALOZOVSKY (Presenter), CHEIK BAMBA, ANTHONY STEWART, LASHOUNDA T FRANKLIN, DIOLA BAGAYOKO, Southern Univ & A&M Coll — We present an ab-initio, density functional theory (DFT) description of ground state electronic and related properties of hexagonal boron nitride (h-BN). We used a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO) formalism. We implemented the Bagayoko, Zhao, and Williams method, as enhanced by Ekuma and Franklin (BZW-EF). The method leads to the ground state of the material, in verifiable manner, without employing over-complete basis sets. Consequently, our results possess the full, physical content of DFT, as per the second DFT theorem [AIP Advances, 4, 127104 (2014)]. We report the ground state band structure, band gap, total and partial densities of states, and electron and holes effective masses. Our calculated, indirect band gap of 4.3 eV is in excellent agreement with the measured value. The valence band maximum is slightly to the left of the K point, while the conduction band minimum is at the M point. Our calculated total width of the valence, total and partial densities of states are in agreement with corresponding, experimental findings.

*This work was funded in part by the US Department of Energy – NNSA (Award No. DE-NA0003679), the NSF (Award No. HRD-1503226), LaSPACE, and LONI-SUBR.

8:36AM F27.00004: Electronic structure of p-type transparent conducting oxide CuAlO₂
MOHAMED SALAH (Presenter), ALS, Lawrence Berkeley National Laboratory, JOONSEOK YOON, Department of Physics, Yonsei University, XIAOSONG LIU, WANLI YANG, ALS, Lawrence Berkeley National Laboratory, BONGJIN SIMON MUN, Department of Physics and Photon Science, Gwangju Institute of Science and Technology, MOHAMED MAHMOUD EL-DESOKY, Physics Department, Suez University, ZAHID HUSSAIN, ALS, Lawrence Berkeley National Laboratory, HONGLYOUL JU, Department of Physics, Yonsei University, SUNG-KWAN MO, ALS, Lawrence Berkeley National Laboratory — Transparent Conducting Oxides (TCOs) are generally considered to be very distinctive material because of their combining of electrical conductivity with the visible light transmission in a single material. The delafossite oxide CuAlO₂ is a p-type TCO which can be used to fabricate transparent p-n junction from TCO materials. In this work, we combine angle-resolved photoemission spectroscopy (ARPES) and X-ray emission and absorption spectroscopies (XES & XAS), to visualize the low-energy electronic structure. Fermi surface topology, detailed band structure, the effective mass of valence electrons, and the band gap size of the single crystal CuAlO₂ were examined experimentally. The electronic structure obtained from ARPES measurements are compared with theoretical calculations. These results indicate that CuAlO₂ is a good p-type TCO that may serve as a platform for optoelectronic applications.
A higher-dimensional electronic superstructure in a misfit chalcogenide (PbSe)_{1.16}(TiSe_2)_2

YUHKO KOHSAKA (Presenter), RIKEN, TEPPEI UENO, Okayama University, TADASHI MACHIDA, TETSUO HANAGURI, RIKEN, JUN AKIMITSU, KAYA KOBAYASHI, Okayama University — Aperiodic crystals, despite lack of translational invariance, are characterized by the primitive vectors as periodic crystals. A characteristic of aperiodic ones is number of the primitive vectors, which is larger than the physical dimension. This represents higher-dimensional nature of aperiodic crystals, resulting in exotic phenomena in atomic quasicrystals, light, and ultracold atom. However, no higher-dimensional phenomena have been found in electronic matters, where inner degrees of freedom and strong correlation are involved to yield rich phenomena. Here we show a higher-dimensional electronic modulation in a misfit chalcogenide (PbSe)_{1.16}(TiSe_2)_2 with spectroscopic imaging scanning tunneling microscopy. We find that the local density-of-states exhibits an aperiodic superstructure while the periodic charge density wave of 1T-TiSe_2 is completely suppressed. Our finding demonstrates that the interplay between hexagonal and tetragonal sublattices provides the electronic matters with extra degrees of freedom from higher dimensions and higher-dimensional electronic properties can be explored in a wider range of materials including artificial heterostructures.

*This work was supported by JSPS KAKENHI Grant numbers 18K03540 and 15H05886.

Experimental Observation of Hidden Berry Curvature in Inversion-Symmetric Bulk 2H-WSe_2

SOOHYUN CHO (Presenter), Yonsei University, SEUNG RYONG PARK, Incheon National University — We investigate the hidden Berry curvature in bulk 2H-WSe_2 by utilizing the surface sensitivity of angle resolved photoemission (ARPES). The symmetry in the electronic structure of transition metal dichalcogenides is used to uniquely determine the local orbital angular momentum (OAM) contribution to the circular dichroism (CD) in ARPES. The extracted CD signals for the K and K' valleys are almost identical, but their signs, which should be determined by the valley index, are opposite. In addition, the sign is found to be the same for the two spin-split bands, indicating that it is independent of spin state. These observed CD behaviors are what are expected from Berry curvature of a monolayer of WSe_2. In order to see if CD-ARPES is indeed representative of hidden Berry curvature within a layer, we use tight binding analysis as well as density functional calculation to calculate the Berry curvature and local OAM of a monolayer WSe_2. We find that measured CD-ARPES is approximately proportional to the calculated Berry curvature as well as local OAM, further supporting our interpretation.
9:12AM F27.00007: Theoretical study on symmetries and properties of three-dimensional valleytronic systems  MANABU TAKEICHI (Presenter), SHUICHI MURAKAMI, Tokyo Inst of Tech - Tokyo — Materials with spin-split valleys showing direct bandgaps, such as transition metal dichalcogenides, have been attracting interest in the context of valleytronics. All such materials known so far are two-dimensional. In this talk, we show a list of space groups to realize three-dimensional materials with such a valley degree of freedom. For this purpose, we made some criteria for space groups allowing valleys with good properties for valleytronics, and we find that there are only a few space groups that satisfy all of these criteria. Moreover, we propose a model which possesses inequivalent six valleys, and reveal its properties in the context of valleytronics, such as spin-valley coupling, nonzero Berry curvature, and some ways of controlling these valleys.

9:24AM F27.00008: Atomic and Electronic Structure of the Edges of multilayer and Monolayer Tin disulfide (SnS$_2$)  TAO YAN (Presenter), Materials Science and Engineering, Worcester Polytechnic Institut — Because of its two-dimensional structure and semiconducting properties, tin disulfide (SnS$_2$) is of interest for applications in electrochemical catalysis and sensing, as an electron transport layer for photovoltaics, and as an active material in photodetectors and thin film transistors. While the atomic and electronic structure of the basal planes of bulk and monolayer SnS$_2$ are well known, the same is not known for the edges, which could have a major influence on the performance of SnS$_2$ in the aforementioned applications. This paper reports on density functional theory (DFT) simulations and experimental measurements of the atomic and electronic structure of the edges of multilayer and monolayer SnS$_2$ under different chemical conditions. We found that the band gap of the SnS$_2$ edges becomes smaller with increasing sulfur coverage, and thereby determined the influence of chemical synthesis conditions on the electronic structure of the edges. We also found that as-synthesized SnS$_2$ has unpaired electrons at the edges, which suggests a direction to solve the degradation issue of SnS$_2$ as a catalyst in aqueous electrolytes.
9:36AM F27.00009: Theoretical and experimental measurements for the \((\text{Eu}_{1-x} \text{Sc}_x)^2 \text{Zr}_2 \text{O}_7\)

**Zirconate pyrochlore**

MOURAD BOUJNAH (Presenter), Institute of Materials Research - UNAM —

The interest to study pyrochlores was the diver’s optical, electric and magnetic properties. Theoretical work was done by using density functional theory (DFT). We studied the electronic properties to see the effect of Scandium in \(\text{Eu}_2 \text{Zr}_2 \text{O}_7\) for several percentage of Sc doping in the Zirconate pyrochlore and we see that we shift from half metal with an important magnetic moment to predicting semiconductor with 2.8 eV as band gap. Moreover, we observed that these doping present a significant coefficient absorption and transmission in the visible range which are around \(10 \times 10^4 \text{ cm}^{-1}\) and 88 % respectively. To understand that we calculated the electrical properties. For the experimental results, when \(x = (0, 0.5 \text{ and } 1)\) we observed by thermal analysis an interesting behavior in air. Generally gone mass and exhibits exothermic and endothermic conduct. Each thermal change, it is analysed with X-ray powder diffraction also the reagents. We detected a substitutional solid solution with complex mechanism, in air and oxygen flux.

Summary, \(\text{ZrO}\) unit cell accept oxygen and exist cationic substitution in \(\text{Sc}\) and \(\text{Eu}\) ions.

*No specific funding for this work*

9:48AM F27.00010: ACCURATE, SELF – CONSISTENT DENSITY FUNCTIONAL THEORY

**DESCRIPTION OF ROCK-SALT MAGNESIUM SELENIDE (MgSe)**

BLAISE AYIRIZIA (Presenter), UTTAM BHANDARI, YURIY MALOZOVSKY, LASHOUNDA T FRANKLIN, DIOLA BAGAYOKO, Southern Univ & A&M Coll — We report comprehensive results from density functional theory (DFT) calculations of electronic, transport, and bulk properties of magnesium selenide (MgSe) in the rock-salt crystal structure. We used a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO) method. We performed a generalized minimization of the energy using successive, self-consistent calculations with augmented basis sets. We verifiably attain the ground state of the material. Therefore, our results possess the full physical content of DFT. With a room temperature lattice constant of 5.460Å, our calculated, indirect band gap is 2.49 eV. We present the ground state band structure and the total (DOS) and partial (pDOS) densities of states. Our results are practically in agreement with available, corresponding experimental data and with some previous, theoretical findings. We found a value of 63.1GPa for the bulk modulus, in excellent agreement with the experimentally determined 62.8 ±1.6 GPa.

*This work was funded in part by the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE- NA0003679), the National Science Foundation (NSF) (Award No. HRD-1503226), LaSPACE, and LONI-SUBR.*
10:00AM F27.00011: First principle investigation of electronic, transport, and bulk properties of zinc-blende magnesium sulfide (MgS)*

**UTTAM BHANDARI (Presenter), BLAISE AYIRIZIA, YURIY MALOZOVSKY, LASHOUNDA T FRANKLIN, DIOLA BAGAYOKO, Southern Univ & A&M Coll** — We have studied the electronic, structural, and transport properties of the zinc-blende magnesium sulfide (zb-MgS), using Density Functional Theory (DFT). We employed a Local Density Approximation (LDA) potential with a Linear Combination of Atomic Orbitals (LCAO) approach. Our computational method leads to the ground state of the materials without utilizing over-complete basis sets. The calculated direct band gap of zb-MgS is 4.43 eV, in excellent agreement with the experimental band gap of 4.45 ± 0.2 eV. We also report the total and partial densities of states, the electron effective masses, the equilibrium lattice constant, and the bulk modulus.

*Work funded in part by the US Department of Energy (DOE), National Nuclear Security Administration (NNSA) (Award No.DE-NA0003679), the National Science Foundation (NSF) (Award No, 1503226), LaSPACE, and LONI-SUBR.

10:12AM F27.00012: Towards a Th-229 Nuclear Clock: Measurements of the Bandgap of ThF$_4$ by Electron Spectroscopy Techniques

**ROBERTO CACIUFFO (Presenter), THOMAS GOUDER, RACHEL ELOIRDI, Joint Research Centre, European Commission, Karlsruhe (Germany), MIKHAIL OSIPENKO, Istituto Nazionale Fisica Nucleare, Genova, Italy, MAURO GIOVANNINI, Department of Chemistry, University of Genova, Italy, RICHARD L. MARTIN, Theoretical Division, Los Alamos National Laboratory, NM** — The existence of an excited nuclear state at about 8.3 eV in Th-229 has stimulated enormous interest, because it opens the possibility to develop solid-state optical nuclear clocks with unparalleled accuracy and stability. In such a device, Th-229 should be embedded in a crystalline matrix with a band gap larger than the isomer energy, in order to suppress decay by internal conversion. The crystal matrix should also be able to host Th-229 atoms in regular lattice positions, in order to minimize color center defects. Here, we present an experimental determination of the bandgap of ThF$_4$ performed by two different techniques. The first one is based on a combination of x-ray photoemission spectroscopy and bremsstrahlung isochromat spectroscopy. The second measurement exploited the position of the inelastic threshold in reflection electron energy loss spectroscopy. Both measurements gave compatible values of the bandgap, with the average $\Delta E = 10.2(2)$ eV [1]. This value is in excellent agreement with theoretical calculations. The measured bandgap is significantly larger than the $^{229}\text{m}^\text{Th}$ excitation energy making ThF$_4$ a possible candidate material for a solid-state nuclear clock based on the vacuum ultraviolet $\gamma$ decay.

10:24AM F27.00013: Analysis of pre-edge of oxygen K-edge X-ray absorption spectra of transition metal oxides*  RUIMIN QIAO, SUBHAYAN ROYCHOUDHURY (Presenter), DAVID PRENDERGAST, WANLI YANG, Lawrence Berkeley National Laboratory — The recently developed MBXAS[1] formalism is a powerful tool for inexpensive, accurate simulation of X-ray absorption spectroscopy (XAS). By approximating the final (initial) many-body state as a Slater determinant of all electronic orbitals obtained in presence (absence) of the core hole, one can accurately simulate the electronic relaxation resulting from core-excitation, while maintaining computational advantage by staying within a mean-field framework, such as density functional theory (DFT). In collaboration with experimentalists, we used MBXAS to simulate the oxygen-K edge XAS of 3-d transition metal oxides (TMO). The onset-energy of each spectrum is determined from total energy differences of ground and excited state DFT calculations. For a given transition-metal, the first O K-edge pre-peak energy decreases with increasing valence, indicating strong contribution of metal 3-d levels in the conduction band edge via hybridization. Unlike transition-metal L-edge spectra, which are dominated by local atomic ligand field effects, the O K-edge essentially maps the conduction bands. The oxygen-K edge offers us an opportunity to plot the first-peak positions of all TMOs with a common energy scale.

*Research supported by LDRD funding from Berkeley Lab.

10:36AM F27.00014: A detailed Raman study of the photochemical oxidation process of monolayer CVD grown graphene  MOHD MUSAIB HAIDARI (Presenter), JIN HONG KIM, JIN SIK CHOI, KonKuk Univ — Although graphene oxide (GO) has emerged as a promising material in the semiconductor industry, optimization of oxidation conditions to meet industrial needs had remained a challenge for researchers. We prepared a monolayer GO sheet by photochemical treatment of CVD graphene within 80 s using UV irradiation. TEM data confirms that there were no structural defects through the optimized oxidation condition with 20% oxygen content. Comparing to conventional GO flakes, this large area GO layer shows higher homogeneity in functional group distribution. Comparison of Amplitude and Area intensity ratios of Raman peaks and XPS data show a correlation between changes in D’ (~1620 cm−1), G (~1587 cm−1), and 2D (~2678 cm−1) peaks with C sp3 (C-O), epoxide (C-O-C), and C sp2 (C=C) bonding. Moreover, although patterned graphene and GO regions are imperceptible by optical illuminance, they are distinguishable by Raman D and/or G-peak mapping. According to AFM data, our GO samples show the average thickness of 0.79 nm in its optimized condition with an ultra-clean surface comparable to that of exfoliated graphene. This work reveals some details about the oxidation process of graphene and sets the ground for transparent flexible optical and electrical applications of functionalized graphene.
10:48AM F27.00015: Realization of BaZrS$_3$ chalcogenide perovskite thin films for optoelectronics

**XIUCHENG WEI** (Presenter), HAOLEI HUI, State University of New York at Buffalo, MENGJIAO HAN, Southern University of Science & Technology, Shenzhen, SAMANTHE PERERA, University of Science and Arts of Oklahoma, JUNHAO LIN, Southern University of Science & Technology, Shenzhen, YI-YANG SUN, Shanghai Institute of Ceramics, Chinese Academy of Sciences, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, HAO ZENG, State University of New York at Buffalo — BaZrS$_3$, a prototypical chalcogenide perovskite, has not yet been deeply explored despite being first synthesized in the mid-1950s. In recent years, several publications on powder samples reveal that BaZrS$_3$ has a direct band gap of 1.7 to 1.8 eV, a high stability against moisture and pressure, and a very strong interaction with light. However, many of the fundamental properties still remain unknown due to the lack of film samples. Here we report the fabrication of BaZrS$_3$ thin films, by sulfurization of corresponding BaZrO$_3$ films deposited by pulsed laser deposition. Transport measurements indicate the films are n-type semiconductors with carrier densities in the range of $10^{19}$ to $10^{20}$ cm$^{-3}$. The hall mobility ranges from 2.1 to 13.7 cm$^2$/Vs depending on the sulfurization temperature. UV-Vis result shows an absorption coefficient of $>10^5$ cm$^{-1}$ at a photon energy of $>1.97$eV and temperature dependent conductivity measurements reveal shallow donor level with an activation energy of several milli-electron volts. Our results assure that BaZrS$_3$ is a promising candidate material for optoelectronics.

*Work supported by NSF CBET-1510121, CBET-1510948 and MRI-1229208.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F28 FIAP FECS: Seeing Your Career In a New Light 405-407 - Benjamin Ueland, Ames Lab - Tag(s): Careers, Industry, Invited, Undergrad Friendly

8:00AM F28.00001: Life as a PhD/MBA in the Optics and Photonics Industry [Invited] YURI SIKORSKI (Presenter), Excelitas Technologies Corp. — TBD

8:36AM F28.00002: When your protagonist is a Hamiltonian: A career in physics writing and editing [Invited] JESSICA THOMAS (Presenter), American Physical Society — Physics (physics.aps.org) is the online magazine for the Physical Review journals. We write and edit articles about top papers from the journals; we also work on news features, Q&As, and a variety of stories related to physics research and its influences. This talk is aimed at anyone who wants to learn more about a career in science writing and editing. Using a few examples of recent Physics articles, I'll give you an inside look at what we do and where we get our ideas. I'll also explain how the members of our team broke into this line of work and the skills we seek when hiring.

9:12AM F28.00003: From the Study of Physics to Entrepreneurship [Invited] JERAMY HUGHES (Presenter), FieldLine Inc. — Sit back as I take you on a journey that starts with working in the labs of Nobel Laureates and continues with founding FieldLine, a company that is creating world changing medical technologies. There will be plenty of failure, restarts, and advice for success as you learn how you can make the most of your opportunities.
9:48AM F28.00004: Navigating a National Lab Career [Invited]  JOHN SARRAO (Presenter), Los Alamos Natl Lab — The Department of Energy’s seventeen National Laboratories provide a career path that’s in between academia and industry. And the National Labs are hiring, with a number of Labs having hiring needs that are greater than 1000 staff/year. Nevertheless, the National Labs are relatively unknown to many students (and faculty) in academia. In this presentation, an overview of the Department of Energy National Laboratories is provided as well as a description of possible trajectories that span from graduate student for the duration of one’s career (as in the case of the speaker) to a variety of short-term internships, post-doc appointments, and staff positions.

10:24AM F28.00005: Trailblazing an Industrial Physics Career: Three Case Studies on Getting Hired Outside Your Subfield [Invited]  MATTHEW THOMPSON (Presenter), BAE Systems — You have probably heard that physicists are very employable and most of us find positions in the private sector. That is great news but making the transition can seem daunting when you are wrapping up your academic research on a hyper-specific topic in a narrow specialty. In this talk, I will recount how I switched subfields three times since leaving graduate school along with the lessons I learned about succeeding in the job market along the way. Moving between areas as diverse as particle accelerator physics, magnetic confinement fusion, and aerospace has been a fascinating journey I look forward to sharing.

Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F29 DSOFT DBIO DFD GSNP: Active Matter in Complex Environments IV  501 - Tapomoy Bhattacharjee, Princeton University

8:00AM F29.00001: Nonequilibrium phases in mixtures of active and passive particles  JUNANG LI (Presenter), SHREYAS GOKHALE, Massachusetts Institute of Technology MIT, ALEXANDRE SOLON, Physics, Sorbonne Université, JEFFREY GORE, NIKTA FAKHRI, Massachusetts Institute of Technology MIT — Active systems composed of self-propelled particles are intrinsically out of equilibrium. Due to the breaking of detailed balance at the individual particle level, they exhibit complex dynamic phenomena not observed in their equilibrium counterparts. For instance, distinct nonequilibrium phases such as a demixed state and motility induced phase separated state (MIPS) can arise in a binary mixture of passive and active particles. Here, we map the computational phase diagram of a binary mixture of active and passive particles as a function of orientational interactions and Peclet number and observe new emergent behavior of dynamical clustering and a polar band of active particles. This computational study helps us to illuminate observations of experiments we developed consisting of passive colloid particles immersed in a bath of bacteria. By quantifying fluctuations and correlations between passive particles in both simulations and experiments, we quantify how far the system is from equilibrium.
8:12AM F29.00002: Tuning the self-organization of confined active particles by the steepness of the trap  SHUBHASHIS RANA (Presenter), Univ of Houston, MD. SAMSUZZAMAN, ARNAB SAHA, Physics, Savitribai Phule Pune University — We consider the collective dynamics of self-propelling particles in two dimensions. They can align themselves according to the direction of propulsion of their neighbours, together with small rotational fluctuations. They also interact with each other via soft, isotropic, repulsive potentials. The particles are confined in a circular trap. The steepness of the trap is tuneable. The average packing fraction of the particles is low. When the trap is steep, particles flock along its boundary. They form a polar cluster that spreads over the boundary. The cluster is not spatially ordered. We show that when the steepness is decreased beyond a threshold value, the cluster becomes round and compact and eventually spatial order (hexagonal) emerges in addition to the pre-established polar order. We investigate the kinetics of such ordering. We find that while rotating around the centre of the trap along its circular boundary, the cluster needs to roll around its centre of mass to be spatially ordered. We have studied the stability of the order when the trap is suddenly switched off. We find that for the particles with velocity alignment interaction, the decay of the spatial order is much slower than the particles without the alignment interaction.

8:24AM F29.00003: Active matters: broken symmetries and response  SARA DAL CENGIO (Presenter), DEMIAN LEVIS, Univ de Barcelona, IGNACIO PAGONABARRAGA, EPFL — We address the question of how interacting active systems in a non-equilibrium steady-state respond to an external perturbation. We establish an extended fluctuation-dissipation theorem for Active Brownian Particles (ABP) which highlights the role played by the local violation of detailed balance due to activity. By making use of a Markovian approximation we derive closed Green-Kubo expressions for the diffusivity and mobility of ABP and quantify the deviations from the Stokes-Einstein relation. We compute the linear response function to an external force using unperturbed simulations of ABP and compare the results with the analytical predictions of the transport coefficients. Our results show the importance of the interplay between activity and interactions in the departure from equilibrium linear response.

8:36AM F29.00004: Spontaneous symmetry breaking induced unidirectional rotation of a chain-grafted colloidal particle in the active bath*  WENDE TIAN (Presenter), Soochow Univ — Exploiting the energy of randomly moving active agents such as bacteria is a fascinating way to power a microdevice. Here we show, by simulations, that a chain-grafted disk-like colloidal particle can rotate unidirectionally and hence output work when immersed in a thin film of active particle suspension. The collective spontaneous symmetry breaking of chain configurations is the origin of the unidirectional rotation. Long persistence time, large propelling force and/or small rotating friction are keys to sustaining the collective broken symmetry and realizing the rotation. In the rotating state, we find very simple linear relations, e.g. between the mean angular speed and the propelling force. The time-evolving asymmetry of chain configurations reveals that there are two types of non-rotating state. The basic phenomena are also observed in the macroscopic granular experiments, implying the generic nature of these phenomena. Our findings provide new insights into the collective spontaneous symmetry breaking in active systems with flexible objects and also open the way to conceive new soft/deformable microdevices.

*This work is supported by the NSFC with NO. 21474074 and 21674078.
8:48AM F29.00005: Temperature dependence of microtubule-based active fluid  TEAGAN BATE (Presenter), EDWARD J JARVIS, MEGAN VARNEY, KUN-TA WU, Worcester Polytech Inst — Kinesin molecular motors step along microtubules in cells to transport cargos with a stepping speed that increases with temperature. This temperature-dependent speed was reported to follow the Arrhenius Law. Kinesin was also used to drive microtubule-based active fluid; however, whether the flow of the fluid follows the Arrhenius Law to accelerate with temperature remains unclear. Here, we systematically characterized the flow speed of kinesin-driven active fluid as a function of temperature, followed by fitting the data to the Arrhenius equation. We characterized the temperature dependence of the flow speed in three different motor systems: (1) processive motors, (2) non-processive motors, and (3) an even mixture of both, finding that these systems followed the Arrhenius Law and developed faster flows with increasing temperature. However, we found that the relation between the flow speed and temperature could be reversed by introducing a depleting agent that had a temperature-dependent micelle formation, causing the active fluid to flow more slowly when heated. Finally, we heated and cooled the fluid repeatedly to accelerate and decelerate the flow sequentially, demonstrating the ability to control the flow speed in real time.

9:00AM F29.00006: Elasticity mediated attraction between active polar particles*  RAHUL GUPTA (Presenter), TIFR Centre for Interdisciplinary Sciences, RAUSHAN KANT, HARSH SONI, AJAY SOOD, SRIRAM RAMASWAMY, Physical Sciences, Indian Institute of Science — We investigate in experiments and simulations the interaction between a pair of motile granular rods moving through a dense monolayer of beads. Vibration of the supporting surface provides the energy source for motility. Above a critical value of the bead area fraction we find that the rods reorient in such a way as to be drawn towards each other. We present a theory for this active attraction based on the forcing imposed by the motile rods on the crystalline medium of beads, and the action of the medium on the rod orientation. Our theoretically calculated the displacement field around a single rod compares favourably with measurements in simulations. We also discuss the segregation instability for the case of many rods.

*SR was supported by SERB (India) and the Tata Education and Development Trust
9:12AM F29.00007: Light-regulated swimming motility induces cell aggregation in confinement
ALEXANDROS FRAGKOPOULOS (Presenter), JÉRÉMY VACHIER, JOHANNES FREY, FLORA-MAUD LE MENN, MICHAEL WILCZEK, Department of Dynamics of Complex Fluids, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany, MARCO G. MAZZA, Department of Mathematical Sciences, Loughborough University, Leicestershire LE11 3TU, United Kingdom, OLIVER BAEUMCHEN, Department of Dynamics of Complex Fluids, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — A highly concentrated suspension of self-propelled particles can form large-scale concentration patterns, separating into regions of high and low particle concentrations. This phenomenon is induced by the activity of the particles and mediated by their mutual interactions. We observe that a suspension of freely swimming Chlamydomonas reinhardtii cells, a unicellular soil-dwelling microalgae and a model organism of puller-type microswimmers, forms such large-scale aggregations under confinement in specific light conditions. We find that the cell's motility changes under different light conditions. Through active Brownian particle simulations, we show that the change of the motility is sufficient to regulate cell aggregation. Finally, we show evidence that the extent of the photosynthetic activity controls the cell's motility, and consequently, the aggregation formation.

9:24AM F29.00008: Undulatory intruder dynamics in water-saturated granular beds*
ARSHAD KUDROLLI (Presenter), TRINH HUYNH, Clark University — We will report an investigation of active intruder dynamics through complex media with Lumbriculus variegatus moving through water saturated granular beds which are refractive index matched to enable observation of their motion inside the bed. These common marsh and pond dwelling worms display dual longitudinal peristaltic and transverse undulatory strokes. We will demonstrate that only the undulatory stroke plays a role in locomotion while swimming in water and in very shallow sediment layers which do not permit anchoring. The greater drag anisotropy of the rod like body in the sediments is shown to enable faster locomotion speeds compared to water because of drag-assisted propulsion. By constructing a magnetically driven soft filament robot, we will then describe the observed speeds as a function of undulatory strokes under prescribed conditions which include the undulation frequency and amplitude and the rheology of the medium.

*Supported by NSF Grant CBET-1805398.
9:36AM F29.00009: Pressure of bacterial suspensions on confining walls and freely moving chains

XIAOLEI MA (Presenter), SHUO GUO, Department of Chemical Engineering and Materials Science, University of Minnesota, XINLIANG XU, Complex Systems Division, Beijing Computational Science Research Center, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota — An active matter consists of a large number of self-propelling units capable of taking in, employing and dissipating energies. Different from equilibrium systems with detailed balance, active matter exhibits many unusual properties, highlighting the nonequilibrium nature of the system. In particular, mechanical pressure, a state variable in equilibrium systems, shows a nontrivial dependence on system boundary as well as specific measurement methods. Here, we experimentally study the mechanical pressure of bacterial suspensions by exploring the interactions between swimming Escherichia coli and confining walls of different shapes, as well as flexible chains of colloids linked by DNA in a quasi-two-dimensional space. We find that the pressure exerted by *E. coli* depends nonmonotonically on the apex angle of the V-shaped confining walls. We further characterize the interactions between *E. coli* and the freely-moving particle chains via imaging the fluctuation of the configuration of the particles and explore their dependence on the rigidity and the length of the chains. A hydrodynamic model is finally proposed to explain our results. Our study sheds light onto the mechanical properties of active matter and provides new understanding on the pressure exerted by swimming microorganisms.

9:48AM F29.00010: Active surfers on a vibrating bath: self-propulsion and interactions

ANAND OZA (Presenter), New Jersey Inst of Tech, IAN HO, School of Engineering, Brown University, GIUSEPPE PUCCI, Institut de Physique de Rennes, DANIEL M HARRIS, School of Engineering, Brown University — We present a combined experimental and theoretical investigation of a newly discovered active matter system consisting of objects floating on a vertically vibrating fluid bath. Recent experiments have demonstrated that such "surfers" oscillate vertically while self-propelling at constant horizontal velocity on the fluid interface. Multiple surfers may self-organize through the collective interfacial deformation in the form of propagating capillary waves. The experiments are complemented by a theoretical model for the surfer's positional and orientational dynamics. The model predictions exhibit good agreement with experimentally observed interaction modes between two surfers. Generally, this work shows that self-propelling objects coupled by interfacial flows constitute a tunable platform for expanding our understanding of active systems.
10:00AM F29.00011: Nutrient depletion thresholds in 3D printed cell assemblies  CAMERON MORLEY (Presenter), THOMAS ANGELINI, University of Florida — Energy consumption is an essential part of active matter; in biological systems energy consumption is often limited by the delivery of oxygen and glucose. Within tissues, these molecules are delivered to cells by a combination of flow through vasculature and intra-tissue diffusion. For dense tissues, the rates of oxygen and glucose diffusion compete with the rates at which they are metabolized, creating a threshold distance from a blood vessel, beyond which cells will become starved. It is almost universally accepted that in tissues of living organisms and in engineered tissues, all cells must be within 200 microns of vasculature because of this competition between diffusion and consumption. However, this rule cannot apply generally to all tissues because cellular metabolic rates are highly variable across cell types and cell densities. In this talk, we will describe experiments that test the 200 micron rule in which we 3D print controlled distributions of hepatocytes into 3D culture medium made from jammed granular microgels. By monitoring cell viability and the consumption of oxygen and glucose, we identify the diffusion-limited crossover to nutrient or oxygen deprived conditions. We vary the size of 3D printed structures and the cell density within them.

10:12AM F29.00012: Control of Active Nematics through Friction*  KRISTIAN THIJSSEN (Presenter), LUUK METSELAAR, University of Oxford, TYLER N SHENDRUK, Loughborough University, AMIN DOOSTMOHAMMADI, The Niels Bohr Institute, JULIA YEOMANS, University of Oxford — Using continuum simulations, we study the impact of anisotropic friction and of position-dependent friction on the emergent flows of active nematics. We show that, depending on whether the active particles align with or tumble in their collectively self-induced flows, anisotropic friction can result in markedly different patterns of motion. For a flow-aligning system with high anisotropic friction, the otherwise chaotic flows are streamlined into flow lanes, reproducing the experimental laning state, which has been obtained by interfacing microtubule-motor protein mixtures with smectic liquid crystals. However, this state is not possible in the flow-tumbling regime, emphasising the role of the flow-tumbling parameter in the dynamics of active nematics. Furthermore, we show that position-dependent friction in active nematic layers allows for the control of the active flows by creating effective hydrodynamic boundaries. Our work demonstrates novel methods to control active matter without the introduction of invasive solid bounding walls.

*This project has received funding from the European Union's Horizon 2020 research and innovation programme Marie Skłodowska-Curie Grant Agreement No. 722497
10:24AM F29.00013: Inertial effects on trapped active matter* MARIO SANDOVAL-ESPINOZA (Presenter), LORENZO GUTIERREZ, Department of Physics, Universidad Autonoma Metropolitana — So far, the effect of translational and rotational inertia in the field of active matter has been almost neglected. Here, we analytically find the effect of inertia on the mean-square displacement and mean-square speed of a system of inertial active Brownian particles subject to a weak and a strong harmonic trap. To validate our analytical results, Brownian dynamics simulations are also performed showing an excellent agreement between our theoretical predictions and the numerical results.

* M. S thanks Consejo Nacional de Ciencia y Tecnologia, CONACyT Grant: CB 2014/237848 for support.

10:36AM F29.00014: Wiggling arthropods induce flow in granular materials* MELIA KENDALL, SHIH-YUAN CHEN, KAREN DANIELS (Presenter), North Carolina State University — Just as heating a viscous fluid causes its viscosity to drop, we observe that the introduction of active particles into a passive granular material can increase its flowability. This effect can be observed, for instance, in the historical practice of aging Milbenkäse cheese in mixtures of flour and mites. In our experiments, we examine this effect by introducing flour beetle larvae (Tribolium confusum) into agricultural grains of various sizes. We measure the timescale for bulk flow via the relaxation of a sloping pile, and the timescale for particle-scale rearrangements via diffusing wave spectroscopy. We find that the macroscopic and microscopic timescales are approximately proportional; both timescales decrease as the fraction of larvae increases, but only for samples in which the grains are smaller than the larvae. For samples in which the larvae and grains are of similar size, these two timescales decouple.

*National Science Foundation

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F30 DSOFT DPOLY DBIO: Self-Limiting Assemblies II: Programmable Assemblies 502 - Efi Efrati, Weizmann Institute of Science - Tag(s): Focus
8:00AM F30.00001: Finite-Size Colloidal Constructs Designed through Self-Assembly of Defective Colloidal Molecules*  

NISHAN PARVEZ (Presenter), MEHDI ZANJANI, Miami University — Engineering various types of structures through self-assembly of colloidal particles is a powerful approach in material design and processing. While simple colloidal building blocks provide a number of well-known structures, more complex building blocks, such as colloidal molecules, are needed to create novel structures with desired functionalities and tunable properties.

In this study, we use computational techniques to identify, investigate, and exploit self-assembly paradigms that are made possible through the use of defective colloidal molecules. Specifically, we study how defective units, which are typically missing one or two particles compared to the regular units, can be taken advantage of to build finite-size constructs that would otherwise be inaccessible. We further demonstrate different types of finite-size, self-limiting, ‘supermolecules’ that can be assembled through engineered directional interactions between defective and regular colloidal molecules. We use Molecular Dynamics (MD) simulations to study the thermodynamics and kinetics of self-assembly, and investigate the phase behavior of the resulting colloidal constructs as a function of building block particle size ratio.

*We acknowledge support form the Ohio Supercomputer Center (Grant Number PMIU0139).

8:12AM F30.00002: Self-assembly of protein-made structures  

AGNESE CURATOLO (Presenter), CARL GOODRICH, OFER KIMCHI, MICHAEL PHILLIP BRENNER, Harvard University, YANG HSIA, ZIBO CHEN, SCOTT BOYKEN, DAVID BAKER, University of Washington — Living organisms create complex protein based materials with remarkable properties. Inspired by those, one could ask if it would be possible to design protein-based materials from scratch for specific human uses, with applications ranging from medicine to biomaterials.

To achieve this goal, we need to understand and re-design the rules used by nature to encode specificity in protein interactions. Sophisticated techniques for designing proteins de novo have been developed recently in David Baker's lab. These proteins interact via designed hydrogen-bonding networks and can be used as building blocks to fabricate functional materials. The drawback is the enormous space of interactions that can be designed.

In order to explore this space and identify the interactions leading to specific mechanical properties, we need to understand the link between the protein building blocks and the target structures to assemble. Here I will present different approaches that one can take to predict the yield of protein-made structures and address the difficulties of relating statistical mechanics models and real world experiments.
8:24AM F30.00003: Programmable self-assembly of DNA origami capsids based on the principles of virus structure.  
* [Invited] SETH FRADEN (Presenter), Brandeis Univ — We provide a general and modular solution for building synthetic icosahedral shells on the scale of 100 nm, motivated by the 1962 Caspar and Klug theory of virus structure. Strategies were explored for controlling the pathways, kinetics, and the yield by which subunits arrange themselves into icosahedral symmetry. The methods of DNA origami were employed to produce accurately-designed and rigid building blocks. We created multiple large virus-like capsids and validated the structures using cryo electron microscopy and studied the capsid assembly process experimentally and with a computational model to elucidate how the kinetics and yield of target structures depends on control parameters. Our capsid building blocks represent a near-ideal manifestation of patchy particles whose geometry and interactions can be designed with sub-nanometer and kBT precision, thus achieving a long sought after goal in soft matter physics.

*European Research Council Consolidator Grant (GA no. 724261), the Deutsche Forschungsgemeinschaft (Gottfried-Wilhelm-Leibniz Program), the SFB863 TPA9 (H.D.), the NSF Brandeis University MRSEC DMR-1420382 (S.F., M.F.H), NIHGMS R01GM108021 NSF XSEDE (MCB090163), and the Brandeis HPCC DMR-1420382 (M.F.H).

9:00AM F30.00004: Functionalized DNA origami shells for cargo encapsulation*  
S.ALI AGHVAMI (Presenter), Physics, Brandeis University, CHRIS SIGL, ELENA WILLNER, HENDRIK DIETZ, Physics, TUM, SETH FRADEN, Physics, Brandeis University — Inspired by the efficient design of virus particles, we develop self-assembling DNA origami icosahedral nanostructures for cargo encapsulation and delivery. Our design is based on the Casper and Klug (CK) geometric principles of virus structure. We demonstrate a robust method for self-assembly of virus like DNA origami capsids of various sizes by designing specific capsomers with programmable shape complementary lock and key interactions. The building blocks are designed and constructed according to the CK symmetry principles that dictate the minimal number of distinct bonds per capsid. These DNA nanostructures are highly modular, allowing us to successfully functionalize them for encapsulation of organic and non-organic cargo particles. We study self-assembly of capsid and encapsulation of different types of particles with TEM and electrophoretic mobility assays to elucidate different aspects of assembly pathways and encapsulation yield. These DNA origami structures are biocompatible and have highly controllable size and shape, making them candidates for biomaterial engineering purposes such as drug delivery and gene therapy.

*We acknowledge financial support from NSF MRSEC DMR-1420382.
9:12AM F30.00005: Structural and mechanical properties of nucleic acid nanotubes: A combined all-atom and coarse-grained molecular dynamics study*  
SUPRIYO NASKAR (Presenter), HIMANSHU JOSHI, MOUNIKA GOSIKA, Indian Institute of Science - Dept of Physics, BANANI CHAKRABORTY, Department of Chemical Engineering, Indian Institute of Science, NADRIAN C SEEMAN, Department of Chemistry, New York University, PRABAL K MAITI, Indian Institute of Science - Dept of Physics — In this work, we introduce a computational framework to model nucleic acid nanotubes and estimate their mechanical properties using various levels of theory. Using atomistic molecular dynamics (MD) simulations, we report the enhancement of the structural and mechanical stability of DNA nanotube (DNT) by changing the salt concentrations. The calculated persistence length ($L_p$) of the DNTs is ~1-2 μm which is an order of magnitude higher than that of a single dsDNA. DNTs have stretch modulus ($\gamma$) value in the range of ~6-8 nN. We find that, with the gradual increment of salt concentration, an increase in $L_p$ and $\gamma$ which reaffirms the structural and mechanical stability of the DNT at higher salt concentrations. We also model DNT using two widely used coarse-grain (CG) models – namely Martini and oxDNA. We compare and contrast the all-atom MD and experimental results with the results obtained using these CG models. We also propose a model of hexagonal nanotubes made of dsRNA connected by double crossover at different positions. The calculated $\gamma$ and $L_p$ of the in silico modeled RNTs are in the same range of values as in the case of DNTs. Using helicoidal parameters of individual base pairs, we explain the relative flexibility and rigidity of the RNTs having different sequences.

*CSIR IISc

9:24AM F30.00006: Self-assembly of DNA origami particles into self-limited surfaces*  
DAICHI HAYAKAWA (Presenter), Physics, Brandeis University, DOUGLAS HALL, Polymer Science and Engineering, University of Massachusetts Amherst, CHRIS SIGL, Physics, Technische Universität München, GREGORY GRASON, Polymer Science and Engineering, University of Massachusetts Amherst, WILLIAM ROGERS, Physics, Brandeis University — The combination of proteins’ unique folded shapes and specific interactions enable them to self-assemble into functional, nanostructured materials, such as viral capsids and microtubules. In this talk, I will present experimental results showing that we can mimic these features using DNA origami. We devise a scheme for designing synthetic building blocks with prescribed shapes and specific interactions. Our building blocks are DNA origami triangles, which bind via DNA base stacking interactions between shape-complementary edges. The dihedral angles between neighboring building blocks can be tuned independently by designing the building-block geometry. We illustrate our design approach by making triangular building blocks that assemble into self-limited structures, like a zigzag nanotube which is limited in size along one dimension. Molecular dynamics simulations, gel electrophoresis, and electron microscopy verify the three-dimensional structures of the individual building blocks as well as their assemblies. Going forward, our design method will enable us to create other building blocks that self-assemble into surfaces with user-prescribed curvatures.

*We acknowledge financial support from NSF MRSEC DMR-1420382.
9:36AM F30.00007: Frustration in the absence of Gaussian Curvature: what we learned from colloidal crystallization on a cylinder*  NABILA TANJEEM (Presenter), WILLIAM H WILKIN, CHRISTOPHER RYCRFT, VINOTHAN MANOHARAN, Harvard University — We demonstrate the effects of a closure constraint on a crystal in the absence of Gaussian curvature. Most studies on closure constraints have focused on crystals on the surface of a sphere, in which case both Gaussian curvature and topology affect the crystallization dynamics. To separate the effects of topology from Gaussian curvature, we study crystallization of colloidal spheres on the surface of a cylinder experimentally, because a cylinder has zero Gaussian curvature, but has a surface that loops back on itself. We find that chiral structures and line-slip defects emerge owing to the closure constraint. We also find that owing to anisotropic crystal growth on a thin and long cylinder, line-slip defects with smaller chiral angles become frustrated, incorporating kinks and fractional vacancies that do not relax in experimental timescale. We show a connection between crystal morphology and growth dynamics, which may elucidate the assembly mechanism of tubular crystalline materials, such as rod-like viruses, bacterial S-layers, and nanotubes.

*This work was supported by Harvard MRSEC (NSF DMR 1420570).

9:48AM F30.00008: Self-Assembly of Triply-Periodic Minimal Surfaces, An “Inverted” Caspar-Klug Approach*  CARLOS DUQUE (Presenter), DOUGLAS HALL, Univ of Mass - Amherst, BOTOND TYUKODI, MICHAEL HAGAN, Physics, Brandeis University, GREGORY GRASON, Univ of Mass - Amherst, CHRISTIAN SANTANGELO, Physics, Syracuse University — The seminal work of Caspar and Klug paved the way to deepen our understanding of the formation of viral shells. Since then, many efforts have been put into understanding the structural properties of a wide variety of viruses. Recently, with the development of DNA nanotechnology, it has been possible to program DNA nanoparticles to self-assemble into intricate shapes by carefully designing some elemental building blocks. In this work, we are interested in studying an “inverted” Caspar-Klug problem, focussed primarily on structures with negative Gaussian curvature. More specifically, we study a family of surfaces called triply periodic minimal surfaces (TPMS). During this talk I'll describe our efforts to discretize these surfaces using a Caspar-Klug approach. Furthermore, I’ll discuss how we can encode some simple rules on the programable matter in order to self-assemble into the desired structures. We perform Monte Carlo simulations to test the validity of the matching rules and finally touch upon the robustness of the assembled structures with the introduction of imperfections in the assembly process.

*NSF grant DMR-1507377
10:00 AM F30.00009: Colloidal crystallization on a cone* JESSICA SUN (Presenter), NABILA TANJEEM, VINOTHAN MANOHARAN, Harvard University — We study the self-assembly of colloidal spheres on the surface of a cone, which has zero Gaussian curvature but varying mean curvature. Therefore, we expect that a colloidal crystal growing on a cone must self-intersect at an angle and is limited to a finite size. In our experimental system, colloidal particles assemble by short-ranged depletion interactions onto a pulled microcapillary tube. For a cylindrical tube of constant mean curvature, defects form where the crystalline grain self-intersects. These defects, called line-slip defects, consist of particle pairs with five-fold coordination along the defect line. However, as we increase the cone angle of the tube, a gap opens up along the defect line. This gap, or fractional vacancy, has varying width along the length of the defect. We show that the varying width of the fractional vacancy corresponds with the cone angle. When we increase the cone angle to a critical value, the system reaches a jammed state.

*Supported by the National Science Foundation through the Harvard Materials Research Science and Engineering Center (DMR-1420570)

10:12 AM F30.00010: Programming extrinsic geometry to control membrane self-assembly* DOUGLAS HALL (Presenter), Univ of Mass - Amherst, MARK STEVENS, Sandia National Laboratories, GREGORY GRASON, Univ of Mass - Amherst — Advancements in nanotechnology have furthered the ability for tailoring shape of building blocks for self-assembly. A current challenge is to develop theories of self-limiting assembly of distinct superstructures, e.g. to create ribbons with robustly self-regulating and finite dimensions that are much larger than the building block dimensions. Previous work successfully describes helical nanoribbon assembly and how molecular shape is related to the programmed intrinsic geometry of the assembly (i.e. the preferred Gaussian curvature), resulting in self-limitation via frustration-induced stresses.

In this talk, we show how an additional molecular shape parameter separately controls the extrinsic geometry (i.e. the directionality of curvature axis relative to inter-block packing directions), modulates the intrinsic frustration energetics and influences the size scale over which frustration stress accumulate in the assembly. We derive a continuum elastic description of intrinsic- and extrinsic-programmed membranes, relate it to a coarse-grained model that realizes these shape parameters and verify the role of extrinsic geometry with simulations.

*We acknowledge NSF DMR-1608862, NSF MRSEC DMR-1420382 and the DOE CINT User facility.
10:24AM F30.00011: Dynamical and equilibrium calculations of self-limited assembly through geometric frustration*  BOTOND TYUKODI (Presenter), FARZANEH MOHAJERANI, Brandeis University, GREGORY GRASON, UMass Amherst, MICHAEL HAGAN, Brandeis University — The self-assembly of subunits into large structures with well-defined finite sizes is ubiquitous in biology. Understanding how to engineer self-assembling structures that exhibit such self-limiting assembly would have important applications in developing functional materials. Recent theoretical arguments have proposed a broad mechanism for self-limiting, geometrically frustrated assembly, in which the preferred local packing of subunits is frustrated by an incompatibility with the preferred global order of the assembly process.

In this talk, we use a recently developed dynamical MC algorithm and free energy calculations to study the assembly of subunits that undergo frustrated assembly. We consider triangular elastic subunits that assemble into a 2D sheet with local hexagonal packing, which is frustrated by the fact that the preferred inter-subunit binding angle favors a negative Gaussian curvature. This incompatibility induces a strain which grows with the size of the assemblage, in some cases leading to a finite size equilibrium assembly with open boundaries. We characterize the relationship between subunit geometry, material properties, the assembly size, and its robustness to parameter variations.

*Work supported by R01GM108021 from NIH and NSF MRSEC, DMR-1420382.

10:36AM F30.00012: Emergence of fiber in frustrated self assembly  HUGO LE ROY (Presenter), MARTIN Lenz, MERT TERZI, University of Paris Sud — Self-organization is an essential characteristic of life at all scales. Mistakes in self-organization at the protein level can lead to severe diseases such as Alzheimer’s, in which normally soluble proteins aggregate into fibril structures that interfere with the protein’s initial biological role. We try to understand the general mechanism behind these aggregation phenomena, which are exhibited by a wide variety of proteins. If surface tension energy would drive aggregation, it would do so at the cost of elastic energy due to protein deformation from there ill-fitting shape. Previous studies have found that fiber-like aggregates can have an energetic benefit over other shapes, representing a trade-off between surface tension and elastic energies. In this work, we use statistical physics tools to investigate the thermodynamic stability of such fibers in more realistic conditions.
10:48AM F30.00013: Role of Geometrical Frustration in Self-limiting Enantioselective Synthesis of Chiroptical Helices  PRASHANT KUMAR (Presenter), JIAO YAN, ALEXANDER F SIMON, DANIEL KATZ, Univ of Michigan - Ann Arbor, DOUGLAS HALL, GREGORY GRASON, University of Massachusetts Amherst, NICHOLAS KOTOV, Univ of Michigan - Ann Arbor — Tunable rotation of light polarization across a wide wavelength spectrum is a desired property for optoelectronic materials. Nanoscale helices and their segments (bow-ties) are expected to exhibit some of the strongest chiroptical activity among nanoscale structures with mirror asymmetry. Successful efforts for fabrication of helices with desired geometry (pitch, length, width, twist angle and thickness) have been focused on top-down approaches such as ion-beam lithography. However, lithographic methods are limited by the fabrication efficiency of the instrumentation involved, thereby hindering bulk production. Herein, we present a colloidal synthesis route for enantiopure bow-ties by guiding the electrostatic and coordination interactions between cadmium ions and chiral amino acid cysteine (Cys). Cd-Cys bow-ties are self-assembled from sheet-like monomeric units, with individually controllable length, width and pitch, leading to tunable chiroptical activity across 500 nm to 3 μm wavelength range. This self-limiting structure of bow-ties can be described within the theoretical framework of geometrical frustration and provide chemical design rules for controlling the interaction and bending energy of monomeric units.

Tuesday, March 3, 2020 8:00 AM - 10:24 AM

Session F31 DSOFT GSNP DPOLY: Wetting and Adhesion of Soft Materials: Dynamics and Instability II 503 - Etienne Barthel, ESPCI Paris

8:00AM F31.00001: Multiphase Flow Through Hairy Channels  CHRISTOPHER USHAY (Presenter), ETIENNE JAMON-PUILLET, PIERRE-THOMAS BRUN, Princeton University — Surfaces textured with long, flexible fibers are ubiquitous in nature and often serve vital functions in multiphase systems. Cilia in lung epithelia transport mucus along airways, while the fur of semiaquatic mammals entrains air for insulation while swimming. Inspired by their versatility, we fabricate “hairy” elastic surfaces by casting a curing elastomer in laser-cut acrylic molds. Specifically, we apply arrays of deformable posts in model systems for the displacement of immiscible phases in a Hele-Shaw cell patterned with elastic features, wherein the buckling of the obstacles modifies the local geometry and thus has a strong effect on drainage. By displacing the oil with water at \( \text{Ca} \ll 1 \), we study the geometry and contact line dynamics of the evolving interface and the impact of confinement on oil removal. Models for depth-averaged fluid flow and the deflection of elastic beams are adapted to our problem to describe the deformation of the host medium due to interfacial and viscous forces. We find the oil phase captured in bundles, in quantities that differ significantly from the undeformed reference case; this has implications towards both enhanced oil recovery and the development of liquid-infused surfaces, which possess properties such as omniphobicity and drag reduction.
8:12AM F31.00002: Rate control of blister inflations and the skin patterns*  TONG SHEN
(Presenter), EDUARD BENET CERDA, FRANCK J. VERNEREY, University of Colorado, Boulder — Surface blistering is commonly observed in various biological processes such as cell apoptosis and locomotion. Despite the variety between systems, blister formation and growth are characterized by the delamination of a thin viscoelastic membrane from its substrate, followed by its large deformation (>100 %) as it is inflated by the infiltration of interstitial fluid. The dynamic of this process is controlled by three rates: the inflation rate, the skin’s viscoelasticity and the delamination rate. Through a combination of experiment and theoretical modeling, we find that competition between these time scales may trigger two instabilities, namely the membrane’s thinning instability and the delamination instability. Utilizing the interplay between these two mechanisms, we are able to control the equilibrium shape of a blister by simply mediating its inflation rate. These findings are then used to understand the surface blisters observed on thermo-sensitive hydrogels as they quickly deswell during their volume phase transition. By understanding the mechanism that governs the interplay between blister inflation and solvent transport, one can explain a diversity of skin patterns observed on the gel surface for different temperature and the gel's crosslink density.

*NSF Award No. 1761918

8:24AM F31.00003: Rupture noise of a moving contact line*  CAISHAN YAN (Presenter),
Department of Physics, Hong Kong University of Science and Technology, DONGSHI GUAN, State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, CAS, China, PIK-YIN LAI, HSUAN-YI CHEN, Department of Physics, National Central University, Taiwan, PENERG TONG, Department of Physics, Hong Kong University of Science and Technology — Many disordered systems exhibit crackling noise when driven by an external force or filed, such as Barkhausen noise in magnetization of ferromagnetic materials, acoustic emission in plastic deformation and seismic activity in earthquakes. Here, we report the avalanche statistics of a moving contact line (CL) pulled by an AFM-based hanging glass fiber through a liquid-air interface. The measured capillary force acting on the circular CL between the liquid-air interface and fiber surface exhibits zig-zag fluctuations, resulting from stick-slip motion of the CL. In the stick state, the measured capillary force increases linearly with CL displacement. Once it reaches a critical value, the CL slips quickly in the form of avalanches, accompanied by a loss of capillary force $\delta f$. We found that the measured $\delta f$ follows a power-law distribution and the power-law exponent agrees with the predicted value by the ABBM model. The experimental results reveal novel features of the stick-slip dynamics and can help to understand other stick-slip phenomena.

*Work supported in part by the Research Grants Council of Hong Kong SAR.
8:36AM F31.00004: Soft Wetting and Phase Separation on Swollen Polymer Networks
ZHUOYUN CAI (Presenter), JONATHAN PHAM, Univ of Kentucky — When a water drop is deposited on a soft adhesive substrate, the surface tension of water drives deformation of the substrate to increase contact area; this is commonly known as soft wetting. In recent soft wetting theories, elastic forces and surface stress oppose substrate deformation. However, very soft, crosslinked materials often contain a liquid phase (i.e. solvent) and is can be considered a swollen network. For a covalently crosslinked network, solvent may separate from network near the contact line to minimize the elastic energy. Although phase separation near contact lines have been considered, the phase distribution at the contact zone is not well understood, and the condition required for phase separation is unclear. We implement confocal microscopy to visualize the crosslinked polymer and solvent phase separately during soft wetting. By controlling the degree of crosslinking and swelling ratio, we investigate both the solvent leeching and the deformation of the network. We find that phase separation does not clearly occur when the swelling ratio is small. We expect that examining the microscale contact zone will help in developing a theory for wetting of soft gels.

8:48AM F31.00005: Spreading dynamics of water onto soluble polymer coatings with hydrophobic insoluble patterns
SOLOMON S. MELIDES, CPE, U.Surrey, JONATHAN E. BROWN, Food Science and Nutrition, U.Surrey, JOSEPH L. KEDDIE, Physics, U.Surrey, MARCO RAMAIOLI (Presenter), UMR 782, Institut National Recherche Agronomique (INRA) — The wetting of many food powders is affected by hydrophobic ingredients present at the surface, such as fat. Instant beverages, soups and infant formulas are typical examples. The spreading of sessile droplets on homogeneous soluble polymer films is dominated by the hydration resulting from water evaporation and condensation ahead of the moving contact line\textsuperscript{1,2,3}, resulting in a strong dependence of the contact angle ($\theta$) on the contact line speed ($U$), film thickness and local water content. This study introduced surface heterogeneity by inkjet printing hydrophobic fat patterns at controlled area fractions 0-50% onto thin soluble polymer coatings of maltodextrin to assess the impact on the water spreading dynamics, at controlled ambient RH. Increasing the area coverage increased strongly $\theta$, for every $U$. A surface coverage of 26.3% was found to halve $U$ after 10 s of spreading. Fat patterns were shown to alter both the interface shape and the contact line length. A theory is proposed to describe the impact of these hydrophobic insoluble patterns on the water spreading dynamics.

REFERENCES:

*The authors thank EPSRC for partial funding.
9:00AM F31.00006: Tape Loop Adhesion  THERESA M ELDER, TIMOTHY J TWOHIG, ANDREW CROLL (Presenter), North Dakota State Univ — A common method of adhering two parallel surfaces to each other is to place a tape loop between them. Despite the tape loop’s prevalence there has, to our knowledge, been no full description of the mechanics of this system to date. We attack the problem experimentally using a reduced half-loop geometry, which is moved through a compression-retraction (sticking then peeling) cycle from which force-displacement curves are measured. We also imaged the shape of the loop during the experiment with photography and laser scanning confocal microscopy. By using both polydimethylsiloxane (PDMS) and polycarbonate (PC) as ‘tape’ materials, we explored the mechanics of both ‘tacky’ and dry adhesive systems. Notably, we find that the compression curve is completely insensitive to surface interactions. Adapting the ‘sticky-elastica’ model of Majidi and Vella, we show how the entire cycle can be described using only an elastic modulus and critical energy release rate as inputs. Remarkably, a complete model of the cycle allows us to create an incredibly simple measurement of adhesion, involving only a ruler.

9:12AM F31.00007: Elastocapillarity and Rolling Dynamics of Solid Nanoparticles*  YUAN TIAN (Presenter), HEYI LIANG, ANDREY DOBRYNIN, Polymer Science, The University of Akron — We use molecular dynamics simulations of rolling dynamics of solid nanoparticles with size $R_p$ in contact with soft elastic substrates to elucidate effect of capillary, elastic and friction forces on rolling motion. Our simulations have shown that a nanoparticle can be in stationary, steady rolling, and accelerating states depending on the nanoparticle-substrate work of adhesion, $W$, the magnitude of the net applied force, $F$, and the substrate shear modulus $G$. In the stationary state, the restoring torque produced in the contact area balances the torque due to the external force. The crossover rolling force $F_r$ is proportional to $WR_p$. In the steady rolling state, $F > F_r$, the nanoparticle maintains a constant rolling velocity which is a manifestation of the balance between the rolling friction force and the applied force. The observed scaling relationships between the applied force and nanoparticle velocity reflect a viscoelastic nature of the substrate deformation dynamics. A nanoparticle begins to accelerate when the energy supplied to the nanoparticle exceeds the energy dissipated in the contact area due to viscoelastic substrate deformation. Using these simulation results, we have constructed a diagram of states in terms of dimensionless parameters $F/WR_p$ and $W/GR_p$.

*NSF DMR-1624569
9:24AM F31.00008: Understanding Elastomeric Contact Interfaces in the Presence of Water*

NITYANSHU KUMAR (Presenter), SUKHMANJOT KAUR, SIDDHESH DALVI, ALI N DHINOJWALA, Univ of Akron — The traction of tires in the rain or sticking a bandage on wet skin involves understanding the role of interfacial water in adhesion and friction. In most cases, the contact interfaces are not completely dry or wet and instead show patchy contact. Even for smooth surfaces, the contact can be patchy due to difficulty in draining the water upon contact. In this work, we have studied the contact interface between hydrophobic PDMS and hydrophilic sapphire substrate in dry and wet conditions using infrared-visible sum-frequency generation (SFG) spectroscopy and macroscopic Johnson-Kendall-Roberts (JKR) adhesion measurements. SFG spectroscopy provides information on interfacial water and shows direct spectral peaks associated with the surface -OH groups in contact with either water or PDMS elastomers. This molecular information can be directly correlated with the macroscopic work of adhesion, adhesion hysteresis, and friction. We will discuss how the presence of interfacial water is affected by normal load and velocity.

*We acknowledge the financial support from the National Science Foundation (NSF) DMR-1610483.

9:36AM F31.00009: Universal Scaling Behavior of the Tackiness of Polymer Melts

YOU WANG, AIPING ZHOU, XIAORONG WANG (Presenter), School of Chemical Science and Engineering, Tongji University — This presentation describes the measurement of stickiness or tackiness, as measured by the peak force to pull off a cylindrical probe from neat polyisoprene melts, the latter of varying materials and surface roughness, over a range of separation speeds. The polymers were either linear or star-branched, with the molecular weights of the former ranging from 84 to 476 kg/mol and of the latter from 609 to 1130 kg/mol. Dynamic mechanic measurements of the polymers showed normal and classic behavior to this well-characterized system. We find that when the pulling speed ($V_s$) is greater than a critical speed ($V_c$), the maximum tack force ($F_{max}$) can be generally described by the following scaling relationships: $F_{max} \sim V_s^{1/3}$ and $F_{max} \sim t_{max}^{-1/2}$, where $t_{max}$ the time when the maximum force is reached in the force-time profile. Remarkably, this scaling behavior of the tackiness appears to be universal as it is independent of the adhered surface, the molecular weight distribution, and the linear or branched chain architecture of the polymer melt. We connect these relations to the physics whereby the tack is controlled by the crack propagation along the interface.
9:48AM F31.00010: Spreading dynamics of water droplets on hydrophilic surfaces*  MESFIN TSIGE (Presenter), SELEMON BEKELE, Univ of Akron — In the early stage of droplet spreading, the inertia of the drop resists the capillary driven motion, and for liquids with low viscosity the spreading radius has been observed to grow with time as \( r(t) \sim t^{1/2} \), independent of surface wettability. In the final stages, the effect of viscous forces acting in the neighbourhood of the three phase contact line become relevant and the competition between surface tension and viscous forces results in extremely slow spreading dynamics and follows what is called Tanner's law, \( r(t) \sim t^{1/10} \). In this work, we will present results on the spreading behaviour of water droplets of varying sizes on a completely wetting surface investigated using fully atomistic molecular dynamic simulations. The spreading observed is characterized by a monolayer of molecular dimensions that moves ahead of the main bulk part of the droplet. Interestingly, the bulk part initially spreads over the monolayer with increasing radius until a characteristic time \( t^* \); thereafter, the bulk radius shrinks maintaining a constant contact angle until it disappears altogether. We will show that a first principle model based on hydrodynamic theory describes the spreading data rather well in the regime where the low contact angle approximation holds.

*Was supported by NSF CHE-1665284.

10:00AM F31.00011: Multi-scale model of gas transport through soap-film membranes used for Artificial Photosynthesis* GABRIELE FALCIANI (Presenter), Politecnico di Torino, RICARDO FRANKLIN, ALI HASSANALI, International Centre for Theoretical Physics, ELIODORO CHIAVAZZO, Politecnico di Torino — This activity is part of the recently funded SoFiA project aiming at a new concept of soap-film photosynthetic membrane for carbon dioxide conversion into fuel [1]. Here, we specifically focus on gas transport through those membranes realized in the form of functionalized soap-films. Diffusion phenomena in the water core and surfactant monolayers are described by Fick's law [2, 3]. Molecular dynamics is used to compute the surfactant distribution and orientation in the membrane monolayers assuming hexaethylene glycol monododecyl ether (C12E6). The obtained atomistic details are then incorporated in a continuum model describing transport phenomena at a larger scale. Numerical predictions are validated against experimental data from literature and used to estimate the characteristic time for fuel-oxygen mixing when separated by photosynthetic soap film membranes.


*This project is funded by the European Union under the grant agreement #828838
The role of crystallization, dewetting, and contact angle in the formation of high aspect ratio crystals

MATHEW GISO (Presenter), Physics & Astronomy, Tufts University, HAODA ZHAO, PATRICK T SPICER, Chemical Engineering, University of New South Wales, TIM ATHERTON, Physics & Astronomy, Tufts University — High aspect ratio crystals have many applications including improved delivery of important ingredients in consumer products. We present a process to produce crystals with a controllable aspect ratio using just oil and water in an easily scalable process. When an oil in water emulsion crystallizes, generally crystallization occurs so quickly the droplets do not deform. By adding surfactants the remaining liquid fraction can be forced to eject the crystals as they grow resulting in an elongated crystal. The contact angle the oil droplet makes with the crystal does not remain constant during this process. The rate of dewetting can be tuned by varying the surfactant concentration. The rate of crystallization can be controlled by vary how quickly the system cools. We examine the crystallization and dewetting behaviors by using a non-equilibrium Monte Carlo model. We examine the behavior of the contact angle using a semi-analytical geometric model. Our results give insight into how the contact angle changes and the dependence of the final crystal morphology on the dewetting and crystallization rates.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1654283.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F32 DPOLY DSOFT DBIO: Responsive Polymers, Soft Materials, and Hybrids II

504 - Jinho Bae, University of California, San Diego - Tag(s): Focus

8:00AM F32.00001: BREAK
Detection of Polypeptide Conformational Transitions in Solution via Sound Velocity and Optical Rotation

*ALYSSA BLAKE (Presenter), GRAHAM PARKINSON, PAUL RUSSO, Georgia Inst of Tech — Of the many different core-shell particles being designed for drug delivery, protein sequestration, and other applications, polypeptide-coated silica is among the most promising. The combination of a configurable, chiral surface and a wide spectrum of surface moieties is difficult to match using conventional polymers. A model system for such polypeptide-silica composite particles (PCPs) has been constructed by covalent attachment of poly (ε-carbobenzyloxy-L-lysine) (PCBL) to silica microbeads. PCBL exhibits a reversible coil-helix transition when dissolved as a pure polymer in m-cresol, but the use of conventional optical methods (e.g., circular dichroism) to confirm such a transition for particles tethered to silica beads is confounded by solvent opacity and strong scattering. Sound velocity measurements provided comparable results to the conventional methods, such as optical rotation, but allows for optically active solvents and strongly scattering samples to be more easily measured. The combination of these two methods provides a new way to understand polypeptide transitions in complex environments and real-world formulations.

*National Science Foundation under Grant No 1505105 (DMR)

Giant hyaluronan polymer brushes display polyelectrolyte brush polymer physics behavior

*JESSICA FAUBEL (Presenter), School of Physics, Georgia Institute of Technology, RHIDDI P PATEL, School of Materials Science and Engineering, Georgia Institute of Technology, JENNIFER CURTIS, School of Physics, Georgia Institute of Technology, BLAIR K BRETTMANN, School of Materials Science and Engineering, Georgia Institute of Technology — We report on the polyelectrolyte brush behavior of extra-large hyaluronan polymer brushes (~15 microns) recently developed using an enzyme-mediated growth process. The giant height of the brushes enables direct characterization of 3D structure and time-dependent behavior. In this study, we explored the stimulus response of the brush to ionic strength and solvent changes. The brush displays classic osmotic brush and salted brush regime behaviors. In poor solvent (ethanol), the brush collapse by 96%. The collapse is rapid when changing from a good to a poor solvent, but re-expansion is extremely slow when changing back to a good solvent. The observed brush behavior is similar to that seen for smaller polyelectrolyte brushes, indicating that these ultra-thick brushes will serve well as model systems to study more complex phenomena, including dynamics, through confocal microscopy

*The authors gratefully acknowledge funding from NSF DMR #1709897.
9:00AM F32.00004: Detecting Bacteria with Plasmonic Microcapsules* REMI DREYFUS (Presenter), CNRS, CÉLINE BUREL, Solvay, CHRISTOPHER B MURRAY, UPENN, BERTRAND DONNIO, CNRS — Assembling nanoparticles into dispersible colloidal pH-sensitive sensors remains a challenge. Here, we show how to combine optically active plasmonic gold nanoparticles and pH-responsive thin shells into “plasmocapsules”. Upon pH change, plasmocapsules swell or shrink. Concomitantly, the distance between the gold nanoparticles embedded in the polymeric matrix varies, resulting in an unambiguous color change. Billions of micron-size sensors can thus be easily fabricated. They are non-intrusive, reusable, and sense local pH changes. Each plasmocapsule is an independent reversible microsensor over a large pH range. Finally, we demonstrate their potential use for the detection of bacterial growth, thus proving that plasmocapsules are a new class of sensing materials

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NSF MRSEC program under award No DMR-1720530
ANRT

9:12AM F32.00005: Enzyme-Responsive Materials for Regenerative Medicine [Invited] SARAH HEILSHORN (Presenter), Stanford Univ — In living materials, the tissue-level structure is constantly being remodeled through the molecular action of cell-secreted enzymes. Bioactive materials have been designed previously to respond to these enzymes through cleavage of individual molecular bonds. However, the resulting changes in the tissue-level material architecture has been underappreciated as a potential material design parameter that can impact cell function. Combining our experimental measurements of chemical reaction rates with a simple model of percolation network theory, we were able to accurately predict how tissue-level network structure evolves in an engineered biomaterial over time. We then demonstrated that encapsulated human endothelial cells respond to these tissue-level structural changes by forming vascular-like networks. In another example of molecular-level design enabling control of tissue-level structure and cell biology, we engineered a material for proliferating neural stem cells. Upon encapsulation, neural stem cells only maintained their stem-like behavior if they could sufficiently remodel the material through the action of a cell-produced enzyme. We further demonstrated that neural stem cell differentiation into more mature cell types is also dependent on tissue-level structure. Thus, this body of work has introduced material remodeling and tissue-level structural dynamics as key design criteria for the field of biomaterials.
Shape Control of Charge-patterned Nanocontainers

Nicholas Brunk (Presenter), Vikram Jadhao, Intelligent Systems Engineering, Indiana University — Stimuli-responsive control of the shape of nanoparticle (NP) containers enables their application as adaptive drug-delivery carriers. NP shape adaptation also provides dynamic building blocks in the design of reconfigurable, biomimetic materials. Molecular dynamics (MD) simulations are used to explore the role of surface charge patterning in controlling electrostatically-driven shape deformation of hollow, elastic NPs. Charge patterns investigated include those commonly synthesized in inverse patchy colloids: Janus particles with (N = 2) patches, striped charge patterns (N > 2), and polyhedral patterns. For Janus patterns, transitions to convex bowl, flattened hemisphere, and concave spinning-top-like conformations occur depending on the salt concentration screening the electrostatic drive to deform. As the number of stripes increases (N > 2), NPs with charged terminating ends adopt disc and rod conformations. However, (N > 2) striped particles with neutral terminating ends form concavities reminiscent of lock-and-key colloids. We also explore the shapes of polyhedrally-patterned nanocontainers and discuss the intersection between pattern-driven and buckling-driven shape control.

This work is supported by the National Science Foundation through Awards 1720625 and DMR-1753182.

A simple mechanical model for synthetic catch bonds

Kerim Dansuk (Presenter), Sinan Keten, Department of Mechanical Engineering, Northwestern University — Catch bonds are protein-ligand bonds which become more difficult to break as the applied force increases, a counterintuitive phenomenon that has not yet been reproduced in synthetic systems. Here, we have demonstrated that a simple mechanical design based on a tweezer-like mechanism can exhibit catch bond characteristics under thermal excitations. The tweezer has a force-sensitive switch which controls the transition of the system to a high-ligand-affinity state with additional ligand-tweezer interactions. Applying kinetic theory to a two-mass-two-spring idealized model of the tweezer, we show that by tuning the shape of the switch and the ligand-tweezer interaction energy landscapes, we can achieve greater lifetimes at larger force levels. We validate our theory with molecular dynamics simulations and produce a characteristic lifetime curve reminiscent of catch bonds. Our analysis reveals minimal design guidelines for reproducing the catch bond phenomenon in synthetic systems such as molecular switches/foldamers, DNA linkers, and nanoparticle networks.

Office of Naval Research Early Career Award, PECASE, grant # N00014-16-1-3175
10:12AM F32.00008: Towards Tumor pH Detection Using Plain Radiography: An Injectable pH-Responsive Polyacrylic Acid Based Hydrogel Biosensor*  
SACHINDRA KIRIDENA (Presenter), UTHPALA WIJAYARATNA, MD, ARIFUZZAMAN, JEFFREY N. ANKER, Department of Chemistry, Clemson University — A pH responsive polyacrylic acid hydrogel based injectable biosensor was developed to measure local tumor pH using plain radiography in order to study cancer pathophysiology, track tumor progression, and determine effectiveness of drugs in vivo. Although plain radiography is unable to detect local chemical concentrations directly, a chemically responsive hydrogel was synthesized to move a tantalum bead and thus report the local concentration. The hydrogel was synthesized by free radical co-polymerization of acrylic acid and n-octyl acrylate and a 13 mm disk of the gel with embedded radiopaque wire had a range of pH 4–8 with a precision of 0.065 pH units. A preliminary study was carried out to miniature this hydrogel sensor and fit it into an injectable porous metal sleeve, all fitting within a breast cancer biopsy marker needle. The 10 mm sensor showed repeatable response to pH cycling in the range of pH 4–8. We are optimizing the sensor for sensing in the pH 6.5 to 7.5 range most relevant to tumor acidosis in order to track tumor physiology and assess response to chemo/radiotherapy.

*NIH awarded grants R-01 (5R01AR070305) and SCBioCRAFT, COBRE (5P20GM10344407) and Wallace R. Roy Distinguished Professorship Funds

10:24AM F32.00009: Modulation of hydrogel biophysical properties using photoadaptable chemistry improves formation of intestinal organoids*  
MAX YAVITT (Presenter), TOBIN BROWN, ELLA HUSHKA, Department of Chemical and Biological Engineering, University of Colorado Boulder, PETER DEMPSEY, Department of Pediatrics, University of Colorado Anschutz Medical Campus, KRISTI ANSETH, Department of Chemical and Biological Engineering, University of Colorado Boulder — There is increasing interest to develop well-defined platforms for organoid growth and expansion. It is known that organoid formation from single intestinal stem cells (ISCs) in synthetic hydrogels is influenced by matrix stiffness and can be initiated by hydrogel degradation. Understanding these forces is key to improving efficiency of organoid growth. We use the adaptable allyl sulfide (AS) photochemistry to tune hydrogel biophysical properties through on demand network reorganization. We show that reorganization is dependent on the protonation state of a soluble, monofunctional thiol species. The rate of degradation can therefore be tailored by controlling the thiol pKa or the solution pH. This understanding then guides the selection of conditions that allow for more rapid degradation. Formed using a biorthogonal conjugation reaction, the AS hydrogels support organoid growth from ISCs, which show maintenance of stem cell markers. Intermittent light exposure will be applied in situ to tune the modulus of cell laden hydrogels and the resulting influence on growth, morphology, and presentation of mechanosensitive biochemical markers will be assessed. This understanding can be leveraged to optimize growth of colonies for development of intestinal organoids.

*NIH R01 DK120921
10:36AM F32.00010: Biosensor physics: DNA folding in a crowded environment* MARK TAYLOR (Presenter), Dept. of Physics, Hiram College, WOLFGANG PAUL, Institute for Physics, Martin-Luther-University — At the molecular level, biological systems operate in very crowded environments. It has long been recognized that crowding can affect the stability and phase transitions of the biopolymers comprising such systems. Similar issues arise in developing biotechnology applications based of dense arrays of surface-tethered polymers. In our recent work we directly measure the entropy reduction resulting from crowding/confinement using Wang-Landau computer simulation techniques [1]. Here we discuss the folding transition of a specific stem-loop forming, single-stranded DNA oligomer that has been studied extensively by the Plaxco group [2]. We develop a coarse-grained model for ssDNA (based on a flexible hard-sphere chain with square-well patch interactions that accounts for both H-bonding and base-pair stacking) and use it to examine the entropic effects associated with surface crowding. For the tethered ssDNA oligomer crowded by other tethered oligomers, we find, in agreement with experiment, that both stabilization and destabilization of the folded state are possible depending on the conformational state of the crowders. [1] Taylor, Macromolecules 50, 6967 (2017); J. Chem. Phys. 147, 166101 (2017); [2] Watkins et al, JACS 134, 2120 (2012); JACS 136, 8923 (2014).

*Funding: NSF DMR-1607143

10:48AM F32.00011: Effect of Nanoparticle Surface Functionality on Magnetic and Interfacial Properties of Iron Oxide–Poly(ethylene oxide) Nanocomposites* DONOVAN WEIBLEN (Presenter), Materials Science and Engineering, Rensselaer Polytechnic Institute, GRACE L GIONTA, Chemical and Biological Engineering, Rensselaer Polytechnic Institute, DENIZ RENDE, Center for Material, Devices, and Integrated Systems, Rensselaer Polytechnic Institute, PINAR AKCORA, Chemical Engineering and Materials Science, Stevens Institute of Technology, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Magnetically susceptible nanoparticles (NPs) have shown promise in diverse application areas such as shape memory polymers, membranes, and drug delivery. In the current work, the impact of surface coating of iron oxide (Fe₃O₄) NPs on interfacial heat transfer, bulk magnetization properties, and structure of poly(ethylene oxide), PEO, nanocomposites was explored. Bare, poly(ethylene glycol) (PEG), and amine coated 10–nm-diameter Fe₃O₄ NPs were dispersed at concentrations less than 1% by weight in PEO. When exposed to an alternating magnetic field (AMF), temperature increases for all PEO/Fe₃O₄ nanocomposites. Amine and PEG coated NPs showed an improved heat generation efficiency. Analysis of magnetization curves revealed an unusual result. Amine coated NPs had the strongest magnetization, however, bare NPs showed a stronger magnetization than the PEG coated NPs. Disagreement between magnetization and magnetic heating results implies that interfacial heat transfer is impacted by NP surface modification. Simulations and experiments were carried out to identify the interfacial structure. Specific attention was paid to how the interface changes with applied AMF and how it affects the mechanism of heat transfer.

*This material is based upon work supported by the NSF Grant 1825254.
In many polymers, the connection between morphology and performance is complex, and conventional materials structure measurements are not sufficient to provide a predictive structural model. Nanoscale variations in molecular orientation and composition, particularly in amorphous regions, are thought to be critical, but few techniques can probe them. I will describe our approach to polarized resonant soft X-ray scattering (P-RSoXS), which combines principles of soft X-ray spectroscopy, small-angle scattering, real-space imaging, and molecular simulation to produce a molecular scale structure measurement for soft materials and complex fluids. I will provide a complete description of our newly-constructed P-RSoXS measurement station at NIST beamlines of the National Synchrotron Light Source II. Results from model systems including commodity plastics, block copolymers, and semiconducting polymers will be discussed. An emphasis will be placed on connections between P-RSoXS and small angle neutron scattering (SANS), especially similarities in contrast variation approaches. I will conclude with our progress toward a forward-simulation framework that describes scattering length density at the nanoscale as a three-dimensional tensor. Results from this approach provide previously inaccessible orientation measurements of nanoscale amorphous regions in polymers.

X-ray scattering is a powerful tool to study the structure and dynamics of soft matter on length scales from nanometers to millimeters and time scales from picoseconds to seconds. In the presentation, I will give a brief overview of the scattering techniques and instruments available at the new, high-brightness, NSLS-II synchrotron to study soft and biomaterials and then present the detailed design, parameters and the status of the Soft Matter Interfaces (SMI) beamline. SMI beamline capabilities on the tender x-ray regime will be highlighted since it enables resonant x-ray scattering measurements at the K-edges of key elements to bring new perspectives to the soft matter community: such as the P, Cl for water membrane problematics; Sulfur edge for organo-electronic filed; as well as K, Ca and more edges. The second part of the presentation will focus on a broad overview of the first results obtained at the beamline on a wide range of material, from organo-photovoltaic polymer to liquid membranes. Finally, the development of new in-situ stages, such as heating, shearing opens a wide field of possibilities.

*The author aknowledge the U.S. Department of Energy (DOE) Office of Science User Facility operated by Brookhaven National Laboratory under Contract No. DESC0012704.
Molecular orientation in polyamide reverse osmosis membranes revealed by polarized resonant soft x-ray scattering

PETER BEAUCAGE (Presenter), National Institute of Standards and Technology — Despite their broad application for water desalination, little is known about the fundamental interplay of synthesis, structure, and water transport in polyamide thin film composite membranes. The active layers of these materials are produced by interfacial polymerization atop a porous support resulting in films of typical thickness 100 nm with > 50 nm RMS roughness, making characterization by conventional techniques extremely challenging. Using polarized resonant soft x-ray scattering, a uniquely sensitive probe of molecular orientation and structure, we observe a striking degree of polarization-induced anisotropy in both commercial and model polyamide films. This anisotropy is likely due to local molecular orientation of C=C and C=O π* electron systems. We compare orientation distributions and optical constants from P-RSoXS with those obtained by angle-dependent NEXAFS and demonstrate a new strategy for signal enhancement of interfacially oriented scattering. This previously-unreported molecular orientation may play a key role in connecting the processing and structure in polyamide thin film composite membranes to their water transport mechanisms, enabling enhanced performance in these important devices.

PAB thanks the NIST-NRC postdoctoral fellowship for support.

Label-free characterization of aqueous molecular micelle nanostructure and dynamics via in-situ RSoXS

TERRY MCAFEE (Presenter), BRIAN AKIRA COLLINS, Washington State Univ, ISVAR CORDOVA, CHENG WANG, Lawrence Berkeley National Laboratory, THOMAS FERRON, Washington State Univ, PHILLIP PICKETT, University of Southern Mississippi — Micelles are key to applications from drug delivery to commercial paints. Their nanostructure and dynamics are of critical importance to their macroscopic properties and functions, but are difficult to measure. Here we demonstrate a novel technique capable of such measurements based on Resonant Soft X-ray Scattering (RSoXS), which is uniquely capable of probing organic materials using their intrinsic chemical bonds rather than laborious and potentially disruptive labeling. Our customized nanofluidic cell enables RSoXS to be performed in liquid environments, allowing structure and dynamics to be measured in-situ for the intended application. We first apply the technique to a model system, Pluronic F127 micelles. Resonant energy contrast tuning allows the internal structure and composition to be measured quantitatively. We further investigate a novel amphiphilic statistical copolymer, “polysoap”, designed for oil spill remediation. Dynamic dual flow reveals an unexpected concentration dependence of the corona, which was not observed with traditional visible light scattering. We further show that despite aggregation, the unimeric core structure is retained, crucial for its application.

*NSF MRI grant 1626566

ISVAR CORDOVA (Presenter), MSD, Lawrence Berkeley National Lab, LUKE LONG, Physics, UC Berkeley, GUILLAUME FREYCHET, NSLS-II, Brookhaven National Lab, CHENG WANG, ALS, Lawrence Berkeley National Lab, PATRICK NAULLEAU, MSD, Lawrence Berkeley National Lab — With the adoption of extreme ultraviolet (EUV) lithography across the semiconductor industry, there comes a need to develop new resist materials that will become the mainstay enabling technology. This development places pressure on the metrology community to develop adequate non-destructive techniques capable of measuring the sub-10 nm patterns that such resists are meant to produce. Recent progress in grazing incidence and resonant x-ray scattering techniques have shown particular promise at being able to address part of these characterization challenges.¹,²

In this work, we show how resonant scattering contrast can harness spatially distributed chemical heterogeneities within exposed resist in order to probe their buried profile. Specifically, by focusing on a novel photoresists containing both organic and inorganic components, we demonstrate the insights into critical parameters gained by performing resonant scattering measurements at various energies and configurations.


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**10:00AM F33.00007: Revealing Strain-Induced Conjugated Polymer Behaviors with Soft X-Ray Scattering and Spectroscopy**

WENKAI ZHONG (Presenter), GREGORY SU, QIN HU, Lawrence Berkeley National Laboratory, FENG LIU, Shanghai Jiaotong University, WANLI YANG, THOMAS RUSSELL, CHENG WANG, Lawrence Berkeley National Laboratory — Conjugated polymers have generated great interest due to their potential in the fabrication of deformable logic circuits that can be integrated into portable/wearable electronics. Here, we developed a beamline setup that can be capable of probing the bulk- and surface-sensitive data of polymer thin films during tensile test using soft x-ray. The combination of experimental and simulated x-ray spectroscopies assists to uncover the fingerprint of molecular behaviors under strain-stress measurement. Furthermore, to establish the relationship of the molecular evolution and device performances, the charge transport properties of the static strained thin film are also evaluated. We expect this work can contribute to understand the molecular origins of mechanical behaviors associated with the resulting device performances.
10:12AM F33.00008: Polarized resonant soft X-ray scattering reveals local chain orientation in polymer-grafted nanoparticles  SUBHRANGSU MUKHERJEE (Presenter), National Institute of Standards and Technology, JASON STREIT, RICHARD ARTHUR VAIA, Air Force Research Laboratory, DEAN DELONGCHAMP, National Institute of Standards and Technology — Polymer-metal nanocomposites that are based on blends of metal NPs and matrix polymers face numerous design limitations and processing challenges. Polymer-grafted nanoparticles (PGNs) are of interest for applications ranging from structural to photonic and electrical. Many of the potential applications (coatings, adhesives, membrane separators, energy storage, etc.) necessitate co-optimization of functional performance with yield stress and toughness. An understanding of how the micro-architecture determines plasticity and failure modes in PGN assemblies is incomplete largely due to lack of tools to fully characterize the microstructure including local interfacial orientation. Here we show the measurement of local chain orientation in a PS-Au PGN system using polarized resonant soft X-ray scattering. The scattering anisotropy was observed at X-ray energies where the anisotropic contrast was affected by the Carbon K-edge 1s-π* resonance of the polystyrene phenyl group. Simple models of the particle geometry with forward simulation of the scattering pattern are consistent with phenyl ring orientation being ‘face on’ relative to the particle.

10:24AM F33.00009: Combining spectroscopy with DFT for optical models of polarized RSoXS to reveal molecular alignment in nanostructures*  VICTOR MURCIA (Presenter), BRIAN AKIRA COLLINS, Washington State Univ — Polarized Resonant Soft X-ray Scattering (pRSoXS) is uniquely sensitive to local molecular orientation regardless of crystallinity, making it a powerful tool in characterizing various types of nanostructures. Unfortunately, it is difficult to interpret the scattering patterns due to a lack of appropriate optical models. Building block models (BBM), used to measure global orientation in X-ray absorption spectroscopy (XAS) won't work for pRSoXS as it assesses differences in local ordering and means that XAS measurements alone will not provide enough information for an optical model. We have developed a model that combines angle-dependent XAS with density functional theory (DFT) to algorithmically create a biaxial optical tensor for molecules. We first show how the uniaxial approximation (UA) can be applied to the scattering anisotropy (SA) of Copper(II)Phthalocyanine (CuPc) films as measured by pRSoXS by expanding upon the BBM informed by DFT calculations. Then we show how the UA fails to describe the SA measured on poly-3-hexylthiophene (P3HT) films implying the need for a lower symmetry model. By combining DFT calculations with XAS, a model that enables extraction of additional details of local molecular orientation through pRSoXS can be developed.

*DOE Career Award DE-SC0017923
10:36AM F33.00010: Control of solvent aggregation to impact active layer morphology and enhance performance in non-fullerene organic solar cells  GUOYAN ZHANG (Presenter), SINTU RONGPipi, BROOKE KUEI, ENRIQUE D GOMEZ, Penn State — The use of solvent additives in the active layer casting solution has proved to be an effective strategy to enhance the performance of solar cells. Solvent additives often have high boiling points, can enhance or reduce solubility, and thereby promote polymer aggregation in solution prior to spin-coating. As a consequence, the use of solvent additives can facilitate the crystallization process. The resulting ordered structure can remarkably increase charge photogeneration, carrier lifetime, and carrier mobility.

Recently, we have found that volatile solvent additives can also improve the performance of organic solar cell fabricated with solution-processed non-fullerene acceptors, including Y6 to achieve device efficiencies in excess of 10%. We examined the effects of solvent quality on the structure in solution of both the donor and acceptor, and the resulting effects on film morphology and performance in solar cell devices. A combination of resonant soft X-ray scattering, grazing-incidence wide-angle X-ray scattering, energy-filtered TEM, and ultrafast spectroscopy reveal the complex interplay between solution structure and subsequent film structure through perturbations induced by solvent additives.

10:48AM F33.00011: Controlling Ionomer Phase Separation Through Side-Chain Engineering  GREGORY SU (Presenter), ISVAR CORDOVA, Lawrence Berkeley National Laboratory, WILLIAM WHITE, University of California, Irvine, MATTHEW LINDELL, MICHAEL YANDRASITS, 3M Corporation, LAWRENCE RENNA, University of California, Irvine, JUN FENG, Lawrence Berkeley National Laboratory, SHANE ARDO, University of California, Irvine, CHENG WANG, AHMET KUSOGLU, Lawrence Berkeley National Laboratory — Phase separation in perfluorinated ion-conducting polymer, or ionomer, membranes defines pathways for ion transport and controls overall conductivity. However, this phase-separated morphology is difficult to characterize and challenging to control based on molecular-level insights. Herein, we show two strategies to control phase-separation and domain spacing in perfluorinated ionomers, and resonant X-ray scattering is used to provide enhanced contrast and chemical sensitivity to decipher nanoscale morphology. Perfluoro ionene chain extended ionomers containing two or three ionic groups per side-chain exhibit tunable domain spacing based on side-chain length. Furthermore, the chain extended ionomers have greater long-range order and higher proton conductivity and water uptake compared to conventional perfluorinated sulfonic acid ionomers. Perfluorinated sulfonic acid ionomers with photoacid dyes covalently bound to side-chain ends, which are promising for light-driven ion conduction, reveal a phase-separation length scale that increases with increasing dye content. Overall, these studies provide insights into detailed connections between polymer chemistry and phase-separated morphology to inform molecular-level design of next-generation membranes.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F34 DPOLY DSOFT GSNP DFD: 3D Printing of Polymers and Soft Materials I 506 - Anthony Kotula, National Institute of Standards and Technology - Tag(s): Focus
8:36AM F34.00002: Re-Printable, Self-Healing Polymer Networks*  
SVETLANA SUKHISHVILI (Presenter), Department of Materials Science and Engineering, Texas A&M University, FRANK GARDEA, Army Research Laboratory South, U.S. Army Combat Capabilities Development Command, QING ZHOU, Department of Materials Science and Engineering, Texas A&M University — We report a versatile approach to designing 3D printable, re-processable dynamic covalent networks with controllable mechanical properties. The approach involves synthesis of epoxy-based oligomeric building blocks of controllable length which are then reversibly crosslinked using the Diels-Alder (DA) reaction. The networks demonstrate several features which are beneficial for additive manufacturing, such as reversible dissociation to liquids at temperatures above 110 °C and fast curing during fused deposition modeling. Moreover, DA reactivity of the precursor material improved interlayer adhesion during printing and enabled self-healing. Using this approach, a series of networks with glass transition temperatures controlled between -10 and 35 °C and the elastic moduli between 10 MPa and several GPa were demonstrated. Finally, the 3D printed networks exhibited shape-memory effects which are based on the stereochemical characteristics of DA adducts.

*We acknowledge the financial support from U.S. Army Research Laboratory and Oak Ridge Associated Universities, subaward W911NF-18-2-0232.

8:48AM F34.00003: Reactive Processing in Extrusion based Polymeric 3D Printing with Surface Segregating Additives*  
NEIKO LEVENHAGEN, MARK DADMUN (Presenter), University of Tennessee, Knoxville — Fabricating complex geometries with isotropic, robust mechanical properties by fused deposition modeling (FDM) remains a key target in expanding additive manufacturing towards the production of large scale commercially relevant structures. Due to the large size of polymer chains and the complex thermal environment experienced by the printed filament in FDM, entanglement of polymers between layers is incomplete, resulting in weak inter-layer interfaces and unsatisfactory Z-strength. Recently, our group has addressed these issues by developing novel polymer materials for FDM that revolve around the introduction of low molecular weight surface segregating additives (LMW-SuSAs) to the filament. We have recently expanded this concept to reactive additives, including methacrylate terminated linear and 3-arm PLA LMW-SuSAs. These reactive additives can now form inter-layer crosslinks by rational introduction of UV photo-initiators and fiber-optic based UV illumination. In situ reactive processing of the printed layers results in drastic increases in the transverse tensile stresses of the printed layers up to ~140% and ~200% for the linear and 3-arm LMW-SuSAs respectively to create essentially isotropic materials.

*Honeywell Corporation
9:00AM F34.00004: 3D Printing Polylactic Acid: modelling residual alignment, annealing and templated crystallinity*  CLAIRE MCILROY (Presenter), School of Mathematics & Physics, University of Lincoln, RICHARD S GRAHAM, School of Mathematical Sciences, University of Nottingham, DARIO CAVALLO, University of Genoa, JON SEPPALA, ANTHONY KOTULA, National Institute for Standards and Technology — Polylactic acid is a semi-crystalline polymer melt commonly used in extrusion-based 3D printing applications. This involves extruding molten polymer through a nozzle and depositing filaments layer-by-layer. Rapid cooling and solidification ensures the structural integrity of the printed part.

Since the crystallization kinetics are typically slow, there is insufficient time above the glass transition for crystallinity to develop. Thus, deposited filaments usually have an amorphous micro-structure upon solidification. Moreover, the deposition flow stretches and orients the polymer molecules, and residual alignment becomes trapped in the weld regions between deposited filaments at the glass transition. We propose that this micro-structure leads to reduced weld strength.

Post-processing thermal annealing may be employed to increase the crystal content and improve mechanical properties. However, we find that non-uniform properties are inevitable. Residual polymer stretch can "template" flow-induced nuclei into the weld regions. Upon annealing these nuclei grow into much smaller spherulites, whose size depend on both print speed and temperature.

*CM acknowledges funding from Royal Commission for the Exhibition of 1851 and Royal Society Exchange Scheme.
9:12AM F34.00005: Determination of polymer chain orientation in 3D printed filaments using Polarized Raman spectroscopy and Birefringence* NORA HASSAN (Presenter), JONATHAN SEPPALA, ANTHONY KOTULA, ANGELA HIGHT WALKER, KALMAN MIGLER, National Institute of Standards and Technology (NIST) — To study orientation and alignment of molecular chains in 3D printed polycarbonate filaments, we used a combination of polarized Raman spectroscopy and birefringence measurements. By changing the orientation of the sample with respect to polarization of incident radiation, we probe changes in the ratio between orientation-dependent vibration modes and orientation-independent modes. Raman measurements show that in 3D printed filaments, little to no orientation at the monomer level was detected, supporting molecular dynamics simulation results [1]. Birefringence measurements were compared to the intrinsic birefringence of 0.2, to estimate the degree of orientation. Measured values of birefringence suggest minimal orientation in agreement with the results of Raman measurements. 3D printed filaments were pulled at different draw ratios after annealing to estimate the limit of Raman measurements’ sensitivity to chain orientation in 3D printed fibers through comparison with birefringence measurements.

References
[1] Private communications with Marco Galvani and Mark Robbins

*This material is based upon work supported by the National Science Foundation under Grant No. 614374

9:24AM F34.00006: Mechanical Properties of an Additively Manufactured Cyanate Ester
MARISSA GIOVINO (Presenter), National Research Council, HILMAR KOERNER, JEFFERY BAUR, Air Force Research Lab - WPAFB — Additive manufacturing is a recent processing method that allows facile fabrication of complex geometries. Additive manufacturing of thermoset composites is commonly done using an extrusion based method termed direct ink writing. Most direct ink writing materials systems have been epoxy based. Epoxy has good mechanical properties but poor thermal stability. To improve the thermal stability a high temperature thermoset resin, bisphenol e cyanate ester, was selected for 3d printing. The cyanate ester was filled with fumed silica to enable direct ink writing. The high temperature thermoset is a brittle material. Inorganic nanoparticles were used to toughen the cyanate ester composite.
Effect of Chain Alignment and Entanglements on Thermal Welding in Fused Filament Fabrication

MARCO GALVANI (Presenter), MARK ROBBINS, Johns Hopkins University — 3D printed structures are often substantially weaker than those made with conventional techniques, but the reason has been unclear. Indeed alignment from flow during deposition was expected to reduce the number of entanglements and thus accelerate welding of filaments through interdiffusion. To address this puzzle we performed molecular dynamics simulations of welding between polymer melts with different degrees of initial alignment. Standard measures of the entanglement density, such as primitive path analysis, indicate significant entanglement loss with increasing alignment, but contrary to existing theories there is no change in the rate of interdiffusion or reorientation. The distance polymers have diffused and the number of entanglements formed across the interface are independent of initial alignment, and chain reorientation always occurs on the equilibrium disentanglement time. Despite this, mechanical tests show that parts welded from aligned states are weaker. We show that this is due to residual alignment in regions near the weld that yield before the weld. The maximum shear strength and fracture energy of systems containing a weld are the same as systems starting from uniform melts with the same alignment.

Supported by NSF through CMMI-1628974 and by CNPq-235249/2014-9.

3D Printing of Polymers and Soft Materials [Invited]

JON SEPPALA (Presenter), National Institute of Standards and Technology — Soft matter 3D printing (3DP) is a rich and diverse research area with new technologies, materials, and processes entering the literature at a rapid pace. Advancements in “traditional” soft 3DP and materials are giving way to hybrid or entirely new processes and materials designed for 3DP. These advancements have been supported by improvement of in-situ process characterization, a more complete understanding of critical material physics, and focused modeling efforts. Soft 3DP processes can now create function from structure and new materials allow the combination of 3DP and self-assembly, producing features at unprecedented length scales. Models, tuned with in-situ process measurements, predict voxel-by-voxel changes in material properties and combining modeling and multi-material printing has enabled advancements in soft robotics, stimuli-responsive materials, and 4D printing. Further, these advancements are pushing the field toward realizing one of the original promises, complete design freedom. This talk will cover “traditional” and emerging soft 3DP processes, material physics, measurement and modeling challenges, and opportunities.
10:24AM F34.00009: Using Eigenvector Centrality to Predict the Mechanical Properties of Structured Materials  CYNTHIA WELCH (Presenter), PAUL WELCH, BRIAN PATTERSON, MATTHEW HERMAN, LINDSEY KUETTNER, Los Alamos National Laboratory — We seek to link mesoscale organization to macroscopic mechanical response using a combination of 3D printing, mechanical testing, and theory. Our ultimate objectives are to provide a simple reduced-order model for predicting mechanical parameters for tailored structures and to better inform engineering models. Here, we report our efforts toward accomplishing these objectives by examining a set of lattice structures with controlled strut deletion. Octet lattice structures overlaying body-centered cubic unit cells were 3D-printed at two different length scales, using either the two-photon polymerization (2PP) method or the vat photopolymerization method with commercially available acrylate-based resins. A set of 10 lattice structures were printed in which struts were randomly removed to give a fraction of deleted struts up to 0.35, and each sample was compression-tested to obtain the Young's modulus. We applied graph theoretical tools typically used in complex network theory to analyze this set of samples. In particular, we propose that the bulk mechanical properties are dictated by a network free energy calculated from the principle eigenvector of the adjacency matrix encoding the mesoscopic structure.

10:36AM F34.00010: Mechanical Enhancement of Polydopamine Nano-Coatings via Thermal Annealing*  KATERINA G MALOLLARI, PEYMAN DELPARASTAN (Presenter), University of California, Berkeley, TANNER FINK, HELEN ZHA, Rensselaer Polytechnic Institute, PHILLIP B MESSERSMITH, University of California, Berkeley — Inspired by the adhesive proteins of mussels, polydopamine (pDA) has become one of the most widely employed methods for functionalizing material surfaces, powered in part by the versatility and simplicity of pDA film deposition. Despite the widespread adoption of pDA as a multifunctional coating for surface modification, it exhibits poor mechanical performance and it still remains a challenge to improve its mechanical properties without sacrificing functionality and versatility of pDA. Here, we demonstrate thermal annealing at a moderate temperature (130 °C) as a facile route to enhance mechanical robustness of pDA coatings. Chemical spectroscopy, x-ray scattering, molecular force spectroscopy and bulk mechanical analyses indicate that monomeric and oligomeric species undergo further polymerization during thermal annealing, leading to fundamental changes in molecular and bulk mechanical behavior of pDA. Considerable improvements in scratch resistance and elastic modulus were noted for the annealed pDA coating, indicating the enhanced ability of the annealed coating to resist mechanical deformations, possibly due to cross-linking and increased intermolecular and cohesive interactions in the pDA structure.

*This work was supported by NIH grant R37 DE014193.
10:48AM F34.00011: The Role of Ionization in Thermal Transport of Solid Polyelectrolytes
TENGFEI LUO (Presenter), XINGFEI WEI, Aerospace and Mechanical Engineering, University of Notre Dame — Amorphous polymers are known as thermal insulators, but increasing their thermal conductivity has not been guided by fully understood physics. In this work, we use molecular dynamics simulations to study the thermal transport mechanism of solid polyelectrolytes, poly(acrylic acid) (PAA) and its ionized forms. The thermal conductivity of PAA increases monotonically with the ionization strength. Although stronger ionization induces larger Coulombic interactions, the Coulombic interaction does not directly contribute to the thermal conductivity enhancement. Instead, it enhances thermal transport through the Lennard-Jones (LJ) interaction. The strong Coulombic force between the counterion and the ionized carboxylic group shifts the LJ force to the stronger LJ repulsive regime, which is mainly responsible for the improved thermal conductivity.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F35 DPOLY DSOFT: Biopolymer Structures and Assemblies 507 -
John Dorgan, Michigan State Univ - Tag(s): Focus

8:00AM F35.00001: BREAK —

8:36AM F35.00002: From Modeling Free Chains with the Rosenbluth Algorithm to Modeling Rigid, Compact, and Overlapped Chains with Our Developed Algorithm EBTISAM ALDAIS (Presenter), Biomedical Engineering, Imam Abdulrahman bin Faisal University, SCOTT RUSSELL CRITTENDEN, Physics & Astronomy Department, University of south Carolina — In 1955, Rosenbluth developed a chain-growth technique for Self-Avoiding Random Walk (SARW) with a set of weights that allows one to approximate all possible configurations of a real chain in a cubic or square lattice. We incorporate the Boltzmann factors for intermolecular bending energy into the monomer growth direction choice in the Rosenbluth algorithm to model chains of arbitrary nearest-neighbor rigidity. This allows for the consideration of compact, free, or extended chains. We validate against, and compare to, various other results, showing very good agreement with known results for short chains and demonstrate the ability to model chains up to 500 segments long, far beyond the length at which the normal Rosenbluth method becomes unstable for reasonable non-zero bending energies. Furthermore, we incorporate the Boltzmann factors for finite overlap energy to model chains that allow only two segments to overlap, Single-Overlapped Random Walk (SORW), into our algorithm. Again, we validate our results with a complete set of SORW for short chains. Our developed algorithms can be easily modified to model any configuration, stiff, free, compact, or overlapped, of polymer-like molecules in biological and non-biological systems.
8:48AM F35.00003: Simulations of Grafted Methylcellulose Chains in Solution*
VAIDYANATHAN SETHURAMAN (Presenter), KEVIN D DORFMAN, University of Minnesota — Recent experiments on methylcellulose chain grafted with polyethylene glycol in solution showed inhibition in methylcellulose fibril formation at high grafting density. We utilize coarse-grained molecular dynamics simulations to understand the influence of grafting on methylcellulose chains. The interaction between the grafts and the methylcellulose chains, as well as the grafting density, are systematically varied. Single chain simulations show that the precursor toroidal structure responsible for fibril formation is hampered by the graft, while Multi chain simulations show that the distance between the centers of masses of the chains increase beyond the minimum capture radius required for fibril formation at high grafting densities. We further demonstrate that conformational fluctuations are suppressed with increasing grafting density. Together, our results support the suppression in fibril formation in grafted methylcellulose systems.

*Materials Science Research and Engineering Center under Award No. DMR-1420013

9:00AM F35.00004: Random Copolymer Complexation with Proteins and Possible Applications*
JEREMY WANG (Presenter), BAOFU QIAO, TRUNG NGUYEN, JOHN TORKELSON, MONICA OLVERA DE LA CRUZ, Northwestern University — Random copolymers are polymers made of two or more monomer components, with their properties determined by the statistical distribution of the monomer sequence. Generally, these properties are understood to be averages of the different components, but recent work from the Olvera de la Cruz group has shown that the statistical distribution of random copolymers make them uniquely suited to form complexes with proteins, which have a heterogenous surface composed of hydrophilic, hydrophobic, and charged domains. This discovery allows us to develop novel and cost-effective techniques to enhance the properties of certain proteins, such as those with enzymatic functions, and increase their stability in demanding environments. The basic principles and potential applications of such techniques will be discussed.

*This work is funded by the Sherman Fairchild Foundation.
9:12AM F35.00005: Synthesis and Self-assembly of Saccharide-Polystyrene Hybrid Block Copolymers  MINJI SEO (Presenter), SHENG LI, KAIST — Oligosaccharide based block copolymers are a new class of hybrid polymers containing both natural and synthetic segments. Due to the large segregation strength between the hydrophilic saccharide block and the hydrophobic synthetic block, the resulting block copolymers are expected to microphase separate at small molecular weights, yielding ordered morphologies with sub-10nm feature sizes. In this contribution, a series of saccharide-containing diblocks and triblocks were prepared by combining maltotriose with polystyrene of different chain lengths. The polymer conjugates were synthesized via copper(I)-catalyzed 1,3-dipolar azide-alkyne cycloaddition of alkyne-functionalized maltotriose and azido-functionalized polystyrene. Additionally, bifunctional initiators were used to prepare triblocks of polystyrene center block and maltotriose end blocks. Despite the small size of maltotriose, the resulting block copolymers were found to microphase separate to form well-ordered microdomain structures. Their bulk morphologies as well as order-disorder transition behavior were examined to illustrate the complex phase behavior of these hybrid materials.

9:24AM F35.00006: Polyvinyl alcohol composite hydrogels containing mixtures of cellulose nanocrystals and chitin nanofibers*  CAMERON IRVIN, School of Materials Science and Engineering, Georgia Institute of Technology, CHINMAY SATAM, School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, PAUL RUSSO, School of Materials Science and Engineering, Georgia Institute of Technology, JAMES CARSON MEREDITH, School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, MEISHA SHOFNER (Presenter), School of Materials Science and Engineering, Georgia Institute of Technology — Among bio-based polymers, cellulose and chitin are abundant and available in a variety of forms, including nanofibers. Due to their anticipated mechanical properties and anisotropic structure, nanofibers of cellulose and chitin are desirable reinforcing fillers in polymers. These nanofibers are also dispersible in water, making them desirable as reinforcing fillers in polymer hydrogels as well. In this work, we have examined how cellulose nanocrystals (CNCs) and chitin nanofibers (ChNFs) may be used separately and as mixtures to affect the properties of poly(vinyl alcohol) (PVA) hydrogels. CNCs and ChNFs have negative and positive surface charges, respectively, providing opportunities for bonding between the nanofibers when used as mixtures and modifying the hydrogel properties further. The results of this work suggested that the types of networks formed were different with different filler types and these differences were observed through swelling behavior of the hydrogels and mechanical properties. Overall, these results demonstrate that nanoparticle mixtures may be used as effective reinforcements for polymer nanocomposites when compatible surface interactions are present between all the components.

*This work was funded by the Renewable Bioproducts Institute at Georgia Tech.
Hierarchically Organized Structure of Electrospun Nanofibers from Computationally Designed Peptide Bundlemers

KYUNGHEE KIM (Presenter), CHRISTOPHER J. KLOXIN, Univ of Delaware, JEFFERY G SAVEN, University of Pennsylvania, DARRIN JOHN POCHAN, Univ of Delaware — Fiber materials made from natural or synthetic polymers can be used as high performance materials exhibiting high stiffness, strength, and/or elongation, all while being light weight. The ability to create a desired internal nanostructure with controllable molecular interactions in the fibers is paramount to a construction of new materials with unique structural features and a remarkable combination of high stiffness, strength, and elongation. Herein, peptides are computationally designed to self-assemble into coiled coil bundles that serve as supramolecular monomers, or “bundlemers”, to create a hierarchical structure for high performance nanofibers. The bundlemers have chemical functionality for desired covalent interactions between bundles to facilitate hierarchical chain growth that displays rigid-rod character. The rigid rods are employed to fabricate uniform nanofibers via electrospinning. The rod chains are observed to be aligned along the fiber axis due to their molecular rigidity and the solution flow during electrospinning process, which impacts the eventual mechanical properties of the nanofibers. The mechanical properties of electrospun rod fibers are investigated as a function of rod length and intra- or inter-chain interactions in the rod chains.

DOE DE-SC0019355

Chitin Nanocrystals confined to polymer microgels.

SUJIN LEE (Presenter), ELSA REICHMANIS, JUNG O PARK, MOHAN SRINIVASARAO, Georgia Inst of Tech — Chitin is the second most abundant polysaccharide after cellulose, which can be extracted from exoskeletons of crustaceans and also from cell walls of fungi and insects. Similar to cellulose nanocrystals, chitin nanocrystals can be isolated through acid hydrolysis and form cholesteric phase. We investigate chitin nanocrystals confined to pnipam microgels using microfluidics device. The twisted structure of chitin nanocrystals are preserved within the polymer spheres, as characterized by optical microscopy. The droplet radius, R of the microgels can be adjusted by changing the volumetric flow rate of oil phase in a microfluidics device. Interestingly, the fabricated microgels shows bipolar structure with the shape of prolate spheroids. They exhibit swelling-deswelling behavior upon temperature change along the axis of helix.
10:00AM F35.00009: Enhanced mechanical properties of fatty acid-derived thermoplastic elastomers through incorporation of ionic interactions* MEGAN ROBERTSON (Presenter), WENYUE DING, JOSIAH HANSON, Univ of Houston — Vegetable oils and their fatty acids are attractive resources for polymers, due to their worldwide abundance, yet the presence of long alkyl chains greatly impacts the resulting polymer properties. The incorporation of ionic interactions in the unentangled poly(n-alkyl methacrylate) midblock of a fatty acid-based thermoplastic elastomeric triblock copolymer was explored as a method of improving its mechanical properties. Poly(methyl methacrylate-b-(lauryl methacrylate-co-tert-butyl methacrylate)-b-methyl methacrylate), which exhibits low tensile strength and elongation at break, was modified by hydrolysis to form poly(methyl methacrylate-b-(lauryl methacrylate-co-methacrylic acid)-b-methyl methacrylate). The methacrylic acid group in the midblock was further neutralized with sodium hydroxide to introduce ionic crosslinks into the system. Increased relaxation time was observed by increasing ion and acid contents. The triblock copolymer mechanical properties were improved significantly by the incorporation of ionic interactions. Enhancement of mechanical properties was correlated with the relaxation time of the midblock.

*National Science Foundation

10:12AM F35.00010: Characterizing Network Structure in Lignin-Based Hydrogel Composites for Aqueous Separations NICHOLAS GREGORICH (Presenter), JUNHUAN DING, MARK C. THIES, ERIC M DAVIS, Clemson University — Lignin-based hydrogels have garnered attention for use in a variety of aqueous separations as lignin is a sustainable, naturally abundant biopolymer with a high concentration of hydroxyl groups, which can be utilized as crosslinking sites during hydrogel fabrication. However, to date, widespread use of these materials is hindered by our limited understanding of how the addition of lignin alters the network structure of these composite hydrogels. Herein, lignin–poly(vinyl alcohol) (PVA) composites were synthesized using lignins of prescribed molecular weights (MWs) and low dispersity using two different crosslinking agents (CLA) – ammonium persulfate and glutaraldehyde. The permeability of various pollutants through the hydrated composites was measured via ultraviolet-visible spectroscopy, where penetrant permeability was found to depend on the MW of lignin and PVA, as well as the concentration of CLA utilized during membrane fabrication. In addition, poroelastic relaxation indentation was used to characterize both the mechanical and transport properties of the composites. Results from this work indicate that transport of pollutants through the composite hydrogels is governed by a combination of the network structure and strength of interaction between the pollutant and lignin.
MCKENZIE COUGHLIN (Presenter), JERRICK EDMUND, Chemical Engineering and Materials Science, University of Minnesota, S. PIRIL ERTEM, SVETLANA MOROZOVA, Chemistry, University of Minnesota, PETER SCHMIDT, Chemical Engineering and Materials Science, University of Minnesota, THERESA M REINEKE, Chemistry, University of Minnesota, FRANK S BATES, TIMOTHY LODGE, Chemical Engineering and Materials Science, University of Minnesota — Methylcellulose (MC) is a commercially relevant cellulose ether. As a water-soluble polymer, MC is used in a variety of applications from food to construction materials. Many applications exploit the thermoreversible gelation of MC at ca. 60 °C, which has been correlated with the formation of nanofibrils upon heating. Previously, we have shown that grafting poly(ethylene glycol) (PEG) chains onto MC modifies the fibril structure, including suppression of fibrils at high enough grafting densities. To expand our understanding of fibril formation, we have grafted poly(N-isopropylacrylamide) (PNIPAm) onto MC at various grafting densities. PNIPAm is water-soluble at room temperature, however, it displays a lower critical solution temperature at ca. 32 °C and phase separates upon heating. The chain conformation of PNIPAm-grafted MC was studied using dynamic and static light scattering as a function of temperature and grafting density. Cryogenic electron microscopy and small-angle X-ray scattering revealed changes in fibril structure and formation. Utilizing small-amplitude oscillatory shear, we characterized the change in modulus and gelation behavior. The effects of PNIPAm-grafting on MC gelation and fibril formation will be compared to the results obtained with PEG-grafted MC.

SUSAN KOZAWA (Presenter), ANNE WALKER, JONAH SCOTT-MCEAN, Case Western Reserve University, JEANETTE GARR, Youngstown State University, CHRIS FLASK, MICHAEL HORE, ALBERTO COSTA, GARY WNEK, Case Western Reserve University — Poly(acrylate) gels have been shown to exhibit electrical potentials in the range normally afforded by living cells. We have unexpectedly found that bathing poly(acrylate) gels in aqueous solutions of monovalent salts such as KH₂PO₄ in a narrow concentration range (ca. 8-16 mM) leads to a softening of gels without measurable volume changes. Moreover, electrical potentials of the gels in KH₂PO₄ solutions show an abrupt increase in gel potential concomitant with the mechanical softening transition. Magnetic resonance imaging experiments reveal an increase in water spin-spin relaxation time (T₂) at this range and small angle neutron scattering demonstrate a structural change at this transition, indicating increased water mobility due to a change in mesh size. This leads us to suggest additional considerations toward a more comprehensive theory of polyelectrolytes, namely ion site and affinity.

*This material is supported by the National Science Foundation under Grant No. NSF #1743475
10:48AM F35.00013: Strain-Field Analysis of Subsonic and Supersonic Cracks in Filled Elastomers  THANH-TAM MAI (Presenter), KENJI URAYAMA, Kyoto Institute of Technology — In the present study, the transition in the characteristics of local crack-tip strain-field from the subsonic ($V/C_s < 1$) to supersonic ($V/C_s > 1$) cracks in filled elastomers is investigated, where $V$ and $C_s$ are crack-growth velocity and shear wave speed, respectively. The crack propagation of the specimens stretched by pure shear deformation is observed by a digital high-speed camera. The crack-tip strain-field is evaluated by the two-dimensional digital image correlation technique (DIC) on the basis of the captured speckle images. The critical behavior of the vertical strain field ($e_{yy}$) near the crack-tip is characterized by the exponent $\alpha$ in the power law, $e_{yy} \sim (1/r)^\alpha$, known as a crack-tip singularity field. The exponent $\alpha$ in the subsonic crack is constant and larger than those of the linear elastic fracture mechanics (LEFM, $\alpha = 0.5$) as well as weakly nonlinear fracture mechanics (WNLM, $\alpha = 1$). In contrast, the exponent $\alpha$ in supersonic crack significantly increases with an increase in the crack growth rate.

**Tuesday, March 3, 2020 8:00 AM - 11:00 AM**

Session F36 DCOMP: Molecular Dynamics Ex Machina: Successes and Challenges 601/603 - Tag(s): Invited
Bayesian optimization is employed to build N-dimensional surrogate models for the energy or property landscapes and infer global minima. The models are iteratively refined by sequentially sampling DFT data points that are promising and/or have high information content. Representing heterogenous materials with compact chemical ‘building blocks’ allowed us to build in prior knowledge and reduce search dimensionality. The uncertainty-led exploration/exploitation sampling strategy delivers global minima with modest sampling, but also ensures visits to less favorable regions of phase space to gather information on rare events and energy barriers.

We applied this active learning scheme to study adsorption at the organic/inorganic interfaces: C\textsubscript{60} on TiO\textsubscript{2}(101) anatase and camphor on Cu(111). Global minima in 6 dimensions are identified with reasonable computational efficiency. BOSS produces chemically-intuitive adsorption energy landscapes that are parsed for local minima and the minimum energy paths between them, allowing us to extract complex barrier-related atomistic pathways. With a recent batch implementation for active learning, BOSS can make use of exascale computing resources to solve large-scale structural problems without sacrificing quantum-mechanical accuracy.


*This work is supported by the Academy of Finland through the AIPSE project number no. 316601 (AIMSS).
8:36AM F36.00002: Construction and simulation proofs of reliable high-dimensional neural network atomic potentials* [Invited] SATOSHI WATANABE (Presenter), KOJI SHIMIZU, The University of Tokyo, WENWEN LI, YASUNOBU ANDO, AIST, EMI MINAMITANI, Institute for Molecular Science, SEUNGWU HAN, Seoul National University — High-dimensional neural network atomic potentials (HDNNP) [1] has attracted attention because of their potential to achieve reliability and computational efficiency simultaneously. In this talk, we show our attempts to apply the HDNNP to several different topics, and discuss how to construct reliable HDNNP and verify the reliability through simulation proofs.
We show our results on Li ion diffusion in amorphous Li$_3$PO$_4$ [2] and thermal conductivities of wurtzite GaN and silicon crystals [3]. In both cases, we achieved good agreement with calculations within the density functional theory. Then we discuss the atomic energy mapping inferred by HDNNP [4]. We show that the energy mapping can be improved by choosing the training set carefully and monitoring the atomic energy during the training procedure. In addition, we will also touch on the HDNNP to examine the atomic structures of a complex four-element system, Au/Li$_3$PO$_4$ interfaces [5].


*The works were supported in part by MI$^2$I project of the Support Program for Starting Up Innovation Hub from JST, Japan, CREST-JST (JPMJCR1523), PRESTO-JST (JPMJPR1717), JSPS KAKENHI (17H05330), Japan, Technology Innovation Program (10052925) by Ministry of Trade, Industry & Energy, Korea and Creative Materials Discovery Program by the National Research Foundation of Korea (2017M3D1A1040689).

9:12AM F36.00003: Embedding physics in machine learning potentials [Invited] GÁBOR CSÁNYI, Department of Engineering, University of Cambridge, ALBERT BARTOK (Presenter), Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick — The last decade has seen an expansion in machine learning methods applied to atomistic modelling problems. Utilising the flexible functional form allowed by different flavours of machine learning approaches and thanks to the abundance of electronic structure data, it is now possible to fit highly predictive potential energy surfaces. However, transferability of these models is often limited, and predictive accuracy may only be expected in structural domains where the training data is concentrated. In the case of complex materials, where the accessible configurational space is significantly larger, data requirements could be prohibitive, and there is a need to place constrains on the interaction model. In this talk, I will discuss machine learning potentials in a Bayesian framework, and how physical knowledge and intuition can be embedded in the Bayesian prior of the model.
Automated training of machine learned potentials with Bayesian active learning

JONATHAN VANDERMAUSE (Presenter), YU XIE, LIXIN SUN, JIN SOO S LIM, STEVEN B TORRISI, SIMON BATZNER, Harvard University, ALEXIE KOLPAK, Massachusetts Institute of Technology, BORIS KOZINSKY, Harvard University — Machine learned interatomic potentials are often manually trained and restricted to single-component and nonreactive systems, severely limiting the practical application of these models. We present an adaptive Bayesian inference method for automating the training of multi-element interatomic potentials using structures drawn “on the fly” from molecular dynamics simulations. Within an online active learning algorithm, the internal uncertainty of a Gaussian process (GP) regression model is used to decide whether to accept the model prediction or to perform a first principles calculation to augment the training set of the model and reoptimize its hyperparameters. Model uncertainties are derived from the variance of the predictive posterior distribution of the GP, which is shown to correlate with true model error on independent test sets. The GP models are based on low-dimensional, explicitly multi-element two- and three-body kernels that can be mapped onto highly efficient cubic spline models suitable for large scale molecular dynamics simulations. Applications to a range of single- and multi-element systems will be discussed, including vacancy and adatom migration in Aluminum, fast-ion diffusion in AgI, and surface segregation in Pd/Ag alloys.

B.K. and J.V. acknowledge funding support from Bosch Research. A.M.K. and S.B. acknowledge funding from the MIT-Skoltech Center for Electrochemical Energy Storage. S.B.T. is supported by the Department of Energy Computational Science Graduate Fellowship under grant DEFG02-97ER25308.

Machine-learning interatomic potentials: a story about how a Big Data approach compensates for our incomplete understanding of interatomic interaction

ALEXANDER SHAPEEV (Presenter), Skolkovo Institute of Science and Technology — Machine learning, an approach to create models based on large amounts of data, is transforming many fields of research. This approach allows us to compensate for our incomplete understanding of a phenomenon by incorporating big data into a model. In my talk I will illustrate how this ideology works in the field of models of interatomic interaction.

Namely, in the first part of my presentation I will give a brief introduction to machine-learning potentials and present some of their success stories. The second part will be devoted to methodological foundations of machine-learning potentials and their successes. In particular, I will formulate the problem of construction of an interatomic potential as a model reduction problem with respect to a quantum-mechanical model (such as DFT). I will then discuss what modeling assumptions are made in classical potentials, identify which ones cause uncontrollable errors, and show how machine learning helps to lift some of those assumptions while still benefiting from physical knowledge. I will conclude by discussing the existing challenges related to those modeling assumptions that are difficult to lift or those cases in which common assumptions fail.

This work is supported by the Russian Science Foundation (Grant No. 18-13-00479).
Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F37 GSNP: Onsager/Apker/Oppenheim/Kadanoff Prize Session
605 - Tag(s): Invited, Undergrad Friendly

8:00AM F37.00001: The flocking theory: The early developments and a new perspective
[Invited] YUHAI TU (Presenter), IBM Tj Watson Research Center — In this talk, I will first describe some of the "accidental" events over 25 years ago that led to the early developments of the flocking theory. I will then discuss a possible new perspective on the flocking theory by looking at the non-equilibrium thermodynamics of collective motion in active matter.

8:36AM F37.00002: Title: Birth, Death, and Flight: the hydrodynamics of Malthusian flocks
[Invited] JOHN TONER (Presenter), Univ of Oregon — Abstract:

I'll present the hydrodynamic theory of ` `Malthusian Flocks": moving aggregates of self-propelled entities (e.g., organisms, cytoskeletal actin, microtubules in mitotic spindles) that reproduce and die. Long-ranged order (i.e., the existence of a non-zero average velocity \( \langle \vec{v}(\vec{r}, t) \rangle \neq \vec{0} \)) is possible in these systems, even in spatial dimension \( d = 2 \). Their spatiotemporal scaling structure can be determined exactly in \( d = 2 \); furthermore, they lack both the longitudinal sound waves and the giant number fluctuations found in immortal flocks. Number fluctuations are very \{it persistent\}, and propagate along the direction of flock motion, but at a different speed. I'll also present recent results for the three dimensional version of this problem, which required the first full blown dynamical renormalization treatment of a flocking system in its ordered phase.

9:12AM F37.00003: Dynamics of the Outer Solar System: from Neptune to Planet Nine
[Invited] TALI KHAIN (Presenter), Physics, University of Michigan, University of Chicago — The Kuiper belt, found beyond the orbit of Neptune, consists of a population of small, icy bodies that orbit the Sun. Due to perturbations from the giant planets (Jupiter, Saturn, Uranus, Neptune), the orbits of these objects slowly evolve with time. In this talk, we will analyze the orbital dynamics of the Kuiper belt objects (KBOs) both with numerical simulations and with a theoretical Hamiltonian approach. We will discuss the structure of the outer Solar System and focus on the most extreme sub-population of objects: the long-period high eccentricity class. The orbits of these extreme KBOs all appear to point in the same direction in physical space; this anomalous signal cannot be explained by the currently known eight-planet Solar System. In order to understand their origin and dynamics, we introduce the hypothesized Planet Nine to the distant Kuiper belt. We find that the presence of Planet Nine allows for two stable populations of objects - the aligned and anti-aligned KBOs - in agreement with observations. We will discuss the mechanisms that lead to this stability, and focus on a fascinating process called resonance hopping, in which a KBO rapidly transitions from one resonance to another with Planet Nine. By tying together studies of observed KBOs with more general analyses of the evolution of synthetic test particles, we elucidate the dynamics of the outer Solar System in and out of the Planet Nine context.
9:48AM F37.00004: Irwin Oppenheim Award talk: What is the simplest model of an amorphous solid? [Invited] ERIC DEGIULI (Presenter), Ryerson Univ — From glasses and emulsions to colloids and granular matter, amorphous solids show surprising universality in correlations, vibrational properties, and rheology. It has become increasingly clear that constraints of mechanical equilibrium control these universal features. Is there a simple model, analogous to the Debye model for crystals, able to explain this? I will review attempts to answer this question from jamming, large-dimension, and field-theoretic approaches, and argue that the latter is useful and parsimonious. Future challenges and gaps in understanding will be outlined.

10:24AM F37.00005: Something from (almost) nothing: complex lessons from simplicity* [Invited] NIGEL GOLDENFELD (Presenter), University of Illinois at Urbana-Champaign — I describe the use of minimal renormalization-group inspired/justified models in non-equilibrium statistical physics and biology. Using examples chosen from my own work in pattern formation, turbulence and biology, I point out that minimal models are able to make specific parameter-free predictions of appropriately-chosen experimental quantities, an outcome of universality in somewhat surprising settings. I argue that these considerations account for the unreasonable effectiveness of theoretical physics in describing seemingly complex phenomena.

*My work has been continuously funded by the National Science Foundation for 34 years, and by other agencies of the US government including NASA, the Department of Energy and the National Institutes of Health. I am grateful for their long-term support.

Tuesday, March 3, 2020 8:00 AM - 10:24 AM

Session F38 FHP DCOMP: Computation in the History of Physics 607 -

8:00AM F38.00001: Physics in the History of Computing: A Case Study from NSF [Invited] PETER FREEMAN (Presenter), Georgia institute of Technology — The histories of computation and of physics since the 1930s have had an essential co-dependency with each other. Without the most powerful computers and optical networks, many of the most important investigations in physics would be impossible. At the same time, the advancement of computer science and its applications that pervade modern life would also be impossible without the advancements in physics. A recent book, Peter A. Freeman, W. Richards Adrion, and William Aspray, Computing and the National Science Foundation, 1950-2016: Building a Foundation for Modern Computing (ACM Books, 2019, 407 pp.) yields some interesting examples of this co-dependency and areas for further historical research.
8:36AM F38.00002: On the status of Landauer's principle [Invited] KATHERINE ROBERTSON (Presenter), Univ of Birmingham — Maxwell's demon is a creature who cunningly violates the second law of thermodynamics. In what sense is such a demon possible? Whilst thermodynamics legislates against such a creature, the demon looks eminently possible according to the underlying classical or quantum dynamics: Poincare's recurrence theorem and Loschmidt's reversibility objection reveal that entropy can decrease in certain situations.

The orthodoxy is that Maxwell's demon is vanquished by Landauer's principle, according to which there is an entropy cost to reset the demon's memory - a vital step in the cyclic process that supposedly leads to a violation of the second law. But the status of Landauer's principle is controversial: some take it as obviously true, others (such as John Norton) have criticised the proofs of this principle.

In this talk, I clarify the status of Landauer's principle. First I discuss which assumptions are required to establish Landauer's principle, and argue that establishing to which theory (thermodynamics, statistical mechanics or quantum mechanics) these principles belong reveals the status of Landauer's principle. I then consider one of Norton's counterexamples to Landauer's principle, and discuss how it depends on certain views about the physical implementation of computation.

9:12AM F38.00003: Simulation Model Skill in Cosmology. [Invited] ERIC WINSBERG (Presenter), Univ of South Florida — What role can/could simulation play in supporting, puzzle-solving, modifying, disconfirming, or falsifying ΛCDM and its competitors? I review some of the problems cosmologists have solved or hope to solve using computer simulation, and examine some of problems and successes that have emerged. I draw some conclusions regarding the kind of simulation model skill we should expect to find in Cosmology.

9:48AM F38.00004: Cosmology in Silico [Invited] MARIE GUEGUEN (Presenter), University of Pittsburgh — Simulations play an ineliminable role in contemporary cosmology. Given the enormous range of processes involved—from stars forming to clusters of galaxies and cosmic filaments—and their non-linear nature, only numerical simulations can tell us what the standard cosmological model implies for structure formation. Simulations are thus indispensable to extract predictions from models, but also to supplement sparse or non-existing observations, and to help designing the observational surveys.

This ubiquity of simulations in cosmology raises an important concern. Indeed, a few astrophysicists have insisted that simulations suffer from numerical artefacts that none of the traditional methods to assess their reliability have successfully detected. These artefacts significantly impact our ability to track the logical consequences of the physical model implemented. As a result, when simulations fail to reproduce observations, there is no tool available to determine whether this discrepancy stems from numerical artefacts or constitutes a genuine failed prediction, and thus a motivation to revise our models. Yet, not only this concern has been neglected, but the race to an ever-increased resolution and more realistic simulations have made the problem even more complex. In this talk, I present a new method for evaluating the reliability of cosmological simulations, based on the reasoning of these astrophysicists who have contested traditional procedures for verifying simulations.
8:00AM F39.00001: **Nonlinear optics from first-principles real-time approaches** [Invited] MYRTA GRÜNING (Presenter), Atomistic Simulation Centre, Queen's University Belfast, CLAUDIO ATTACCALITE, Centre Interdisciplinaire de Nanoscience de Marseille, CNRS/Aix-Marseille Université — In the past decades, many-body approaches based on the GW approximation and the Bethe-Salpeter equation have become state-of-the-art for calculating optical absorption in solids and nanostructures. In this talk, I’ll first present a real-time approach derived from the non-equilibrium Green’s function, that allows extending the GW+BSE approach beyond the linear regime.[1,2] Using this approach, I’ll address the importance of many-body effects and in particular of excitonic effects for nonlinear optical properties.[3] For example, I’ll look at the case of single-layer monochalcogenide whose strong Second Harmonic Generation cannot be reproduced within the independent-particle approximation.[4] In the second part of the talk, I’ll then discuss the possibility of a real-time approach based on time-dependent density-functional theory, that can describe excitonic effects.[5]


8:36AM F39.00002: **Exciton bandstructure in carbon nanotubes from many-body perturbation theory** DANA NOVICHKOVA (Presenter), Materials and Interfaces, Weizmann Institute of Science, DIANA QIU, Mechanical Engineering and Materials Science, Yale University, SIVAN REFAELY-ABRAMSON, Materials and Interfaces, Weizmann Institute of Science — Understanding exciton decay processes and lifetimes in solid-state materials is of great interest, with emerging applications such as material characterization and energy conversion and storage. A predictive theoretical assessment of the involved underlying interaction mechanisms is, however, highly challenging. A computational scheme that supplies reliable excited-state properties in crystals is many-body perturbation theory within the GW approximation and the Bethe-Salpeter equation (BSE) approach (GW-BSE). This method allows a predictive evaluation of exciton wavefunctions and excitation energies, and recently also exciton bandstructures. In this study, we explore the excitonic bandstructure of a quasi 1D system – single wall carbon nanotubes (SWCNTs), a well-examined material due to its unique electronic properties and application in optoelectronic devices. We further explore the relation of the exciton dispersion to excitonic decay processes.

*This research is supported by the Israel Science Foundation.
Exciton and Spin Dynamics for Quantum Defects in Two-dimensional Materials from First-principles

YUAN PING (Presenter), University of California, Santa Cruz — Spin defects in 2D materials such as ultrathin hexagonal boron nitride (hBN) have been found to be promising single-photon emitters and potential candidates for qubits. However, first-principles prediction of accurate defect properties in 2D materials remains challenging, mainly because of the highly anisotropic dielectric screening in 2D materials and strong many body interactions. This work shows how we solve the numerical convergence issues for charged defect properties in 2D materials at both the DFT and many body perturbation theory (GW/Bethe-Salpeter equation), and how we tackle the complex many body interactions including electron-electron, electron-phonon and defect-excitons for the excited state dynamics of spin defects in 2D materials. We are also developing first-principles spin dynamics through Lindblad dynamics for open quantum systems. With our methods, we will design spin defects that have deep defect levels, weak electron-phonon coupling, high radiative recombination rates, and long spin relaxation and coherence time as future materials platforms for quantum information technologies.

This work was funded by NSF DMR-1760260.

Local Field Effect on Non-local Dielectric Screening of Two-Dimensional Interface Systems: A First-principles Study

CHUNHAO GUO (Presenter), JUNQING XU, University of California, Santa Cruz, USA, DARIO ROCCA, University of Lorraine, LPCT, UMR 7019, 54506 Vandœuvre-lès-Nancy, France, YUAN PING, University of California, Santa Cruz, USA — Two-dimensional (2D) materials have provided platforms for exotic physics and emerging applications by forming van-der Waals interfaces. Non-local dielectric screening by substrates play an important role in modifying the quasiparticle properties of these interface systems. While several studies have been performed for the substrate screening of 2D materials, the underlying approximations and the connection between different methods have not been investigated in detail. We derived the effective polarizability of the interfaces from each monolayer sub-system, and showed its equivalence to sum over irreducible polarizability at the Random Phase Approximation level. We used this method to calculate prototypical 2D interface systems (heterojunctions and bilayers) and compared with explicit calculations. We compared different existing methods and discussed the local field effect on quasiparticle energies and absorption spectra. Our study shows good consistency between single layer calculations with effective interface screening and explicit interface calculations, and provides careful evaluation of approximations involved in studying substrate screening and interface quasiparticle properties.

This work is supported by the National Science Foundation under grant number 1760260.
9:12AM F39.00005: Microscopic Theory of Plasmons in Substrate-supported Borophene* 
ANUBHAB HALDAR (Presenter), Boston Univ, CRISTIAN CORTES, PIERRE DARANCET, Center for Nanoscale Materials, Argonne National Laboratory, SAHAR SHARIFZADEH, Boston Univ — Two-dimensional boron, or borophene, is a metallic monolayer material which hosts low-loss, high-confinement, visible light plasmons, with possible applications in nanoplasmonic devices. In contrast with graphene, borophene cannot be exfoliated and has been synthesized on a variety of metallic substrates. In this talk, we present first-principles density functional theory calculations of the dielectric and plasmonic properties of borophene grown on Ag(111). We systematically investigate the linear response and the momentum-dependent polarizability of borophene as a function of its proximity to the metallic substrate. Our calculations indicate that the plasmons in borophene are damped by the substrate, which we explain via a simple electrodynamic model of coupled polarizabilities between the monolayer and substrate. Using this model, we predict the plasmonic properties of borophene on a variety of substrates that minimize plasmon damping.

* S.S. and A.H acknowledge funding from DOE BES Award #DE-SC0018080. This material is based upon work supported by LDRD funding from Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Use of the Center for Nanoscale Materials was supported by DOE under Contract No. DE-AC02-06CH11357.

ARIELLE COHEN (Presenter), KIRK LEWIS, TIANLUN HUANG, SAHAR SHARIFZADEH, Boston Univ — Germanium Selenide (GeSe) and other Group IV monochalcogenides are van der Waals-bonded layered materials with potential applications in sensing, solar energy and spintronics. Importantly, their band gaps can be tuned via strain, doping, and chemical modification. Due to the reduced dimensionality and reduced screening environment in the monolayer, these modifications have a significant impact on the optoelectronic properties. We apply density functional theory (DFT) and many-body perturbation theory to understand the electronic and optical properties of point vacancies in monolayer GeSe. We find that a Selenium vacancy in the -2 charge state induces mid-gap “trap states,” which strongly localize the electron and hole density. These trap states result in a sharp optical absorption peak below the predicted pristine optical gap and a localized exciton wavefunction around the defect. Overall, these results suggest that the vacancy is a strong perturbation to the system, demonstrating the importance of considering defects in the context of materials discovery and device design.

* The authors acknowledge funding support from the U.S. Department of Energy, Office of Science, Award #DE-SC0018080 and computational resources from DOE NERSC and NSF-XSEDE.
9:36AM F39.00007: Investigating the Role of Electron-Phonon Interactions and Reduced Dimensionality on Optical Excitations in Monolayer GeSe*  
TIANLUN HUANG (Presenter), KIRK LEWIS, ARIELLE COHEN, SAHAR SHARIFZADEH, Boston Univ — Two-dimensional (2D) van der Waals-bonded layered materials are promising as inexpensive, light-weight solar energy conversion materials. Better understanding the role of electron-phonon interactions in 2D will be necessary for understanding the optical properties of this class of materials. Here, we use first-principles theory to investigate the role of electron-phonon interactions on the optical absorption spectrum of monolayer germanium selenide GeSe, a direct gap 2D semiconductor with promising optoelectronic properties. We utilize density functional theory, density functional perturbation theory, and many-body perturbation theory to study both bulk and monolayer GeSe. We determine that the optical gap at room temperature is lower than that of the zero temperature for both systems. For the bulk, an indirect gap semiconductor, this reduction is mainly due to phonon-assisted transitions. For the monolayer, we attribute the reduced gap to the localization of the excited-state in the presence of phonons. The significant influence of electron-phonon interactions in the monolayer suggests that this phenomenon should be better understood for 2D material technology.

*We acknowledge funding from U.S. Department of Energy, Office of Science, Award #DE-SC0018080

9:48AM F39.00008: Dielectric embedding GW for weakly coupled molecule-substrate interfaces*  
ZHENFEI LIU (Presenter), Department of Chemistry, Wayne State University — Molecule-substrate interfaces are ubiquitous in many areas of nanoscale materials science. Accurate characterization of their electronic structure from first principles is key in understanding material properties. Although the first-principles GW approach is state-of-the-art and can yield accurate quasiparticle energy levels and interfacial level alignments that are in agreement with experiments, it is computationally challenging for large-scale interfaces. In this work, we develop a dielectric embedding approach based on GW, which significantly reduces the computational cost of direct GW for interfaces without sacrificing accuracy. We perform explicit GW calculations only in the simulation cell containing the molecular adsorbate, in which the dielectric effect of the substrate is effectively embedded. The embedding of the dielectric environment is made possible via a real-space truncation of the Kohn-Sham polarizability. Here, we focus on the interfacial level alignments, i.e., relative positions between molecular frontier orbital resonances and the Fermi level of the substrate, at weakly coupled molecule-substrate interfaces. We demonstrate our approach using a few interfaces of experimental interest.

*Computational resources are provided by NERSC and Argonne National Laboratory.
KEIAN NOORI (Presenter), FENGYUAN XUAN, SU YING QUEK, Natl Univ of Singapore — As the technological applications of 2D material-based electronics continue to rise, an understanding of the physical underpinnings of the energy barriers between metal-2D material contacts becomes critically important. Experimentally, these interfaces are often found to be controlled by Fermi-level pinning, which prevents the tuning of Schottky barrier heights by the modification of the contact metal work function. Theoretically, the high computational cost of these systems has largely restricted first principles studies to DFT-level calculations. The effects of dielectric screening, which are important even in atomically thin 2D materials$^1$, are therefore also ignored. Moreover, the small unit cells considered do not allow for the inclusion of defects, which can affect the energy-level alignment at the interface.

In this work we use the newly-developed XAF-GW approach$^2$ to study large supercells at the many-body GW level, thus including the full effects of dielectric screening. We examine the origin of the Schottky barrier heights of metal-2D material interfaces, including the effects of dielectric screening, structural reconstruction, and defects.

(1) Noori; Cheng; Xuan; Quek 2D Mater. 2019, 6 (3), 035036
(2) Xuan.; Chen.; Quek J. Chem. Theory Comput. 2019, 15 (6), 3824

NOCONA SANDERS (Presenter), EMMANOUIL KIOUPAKIS, University of Michigan — Given the successful synthesis of 2D GaN and investigations into the properties of freestanding 2D nitrides, heterostructures of these materials are now of particular interest. Extreme quantum confinement is a viable method to shift light emission to shorter wavelengths, but in 2D nitrides this is counteracted by the quantum-confined Stark shift due to the strong inherent polarization perpendicular to the 2D plane. We report the electronic and optical properties of 2D BN, GaN, AlN, and InN in various stacking orientations, such that the electric fields are either aligned or anti-parallel in two possible configurations. We employ density functional theory and quasiparticle corrections with the GW method, as well as the Bethe-Salpeter Equation, to derive accurate band structures, exciton binding energies, and luminescence energies. Through understanding how the stacking arrangement influences the underlying electronic and optical properties, critical insight will be gained in how to improve 2D III-nitride-based optoelectronics through accessing the additional degree of freedom provided by polarization.

*This work was supported by the NSF ECCS-CDS&E program (1607796). Computational resources were provided by the DOE NERSC facility under Contract No. DE-AC02-05CH11231.
10:24AM F39.00011: Optical trap for two-dimensional excitons* HIROKI KATOW (Presenter), AIST, RYOSUKE AKASHI, University of Tokyo, YOSHIYUKI MIYAMOTO, AIST, SHINJI TSUNEYUKI, University of Tokyo — For its potential optical controllability as quantum degrees of freedom, the exciton in two-dimensional system has attracted much attentions. In this presentation, we propose an optical trapping technique for the exciton. Exploiting the energy shift mechanism of excitonic system coupled to the electromagnetic field, spatial confinement potential can be implemented. The dimensionality and symmetry of the potential can be dynamically tunable. We performed an \textit{ab initio} calculation of the excitonic states in graphane, a two-dimensional wide gap semiconductor with $D_{3d}$ symmetry, based on GW+BSE method by using \textit{BerkeleyGW} package. The lowest excitonic state belongs to $E_u$ representation, followed by $E_g$ and $A_{2g}$ excitons of which energy levels are 500meV and 650meV apart from $E_u$ exciton, respectively. Two- and three-level systems can be implemented by coupling these levels with optical fields. We will report the possible depth and polarization dependency of the potential by applying nearly infrared laser light.

*This work is supported by a NEDO project “Development of advanced laser processing with intelligence based on high-brightness and high-efficiency laser technologies (TACMI project) and the use of the Supercomputer Center facilities, the ISSP the University of Tokyo.

10:36AM F39.00012: Accurate and approximative many-body methods for optical gap of semiconducting 2D materials* FRANTISEK KARLICKY (Presenter), Department of Physics, University of Ostrava — Many-body GW approximation and Bethe-Salpeter equation (BSE) are considered as state-of-the-art methods for reliable prediction of quasiparticle (QP) and optical gaps of bulk materials, respectively. On the other hand, GW and BSE methods are still computationally challenging and its usage for a larger supercell is almost unfeasible. We show which factors are important to obtain accurate QP and optical gaps by GW+BSE approach and we evaluate the magnitudes of such factors [1-3]. We also show that several computationally cheap approximations based on time-dependent DFT can be used as accurate alternative to GW+BSE approach and promising applications on selected vdW heterostructures are demonstrated [3-4].


*Czech Science Foundation (18-25128S), Institution Development Program of the University of Ostrava (IRP201826)
The Zeeman effect of excitons in two-dimensional transition metal dichalcogenides (TMDs) has attracted much recent attention. A g-factor can be associated with the valley splitting of the band structure in the presence of a weak out-of-plane magnetic field. Experimentalists have measured g-factors of -4 and -16 for excitons in monolayer and twisted bilayer TMDs. Theoretical interpretations of the g-factors have largely focused on monolayer TMDs, relying on a phenomenological model or a k.p model. The phenomenological model assumes that the g-factor is a sum of orbital, spin and valley terms, while the k.p model uses effective masses extracted from tight-binding calculations. Here, we start from the Luttinger-Kohn approximation to treat the magnetic field as a perturbation in a periodic system, and show that the g-factor cannot be written as a sum of only orbital, spin and valley terms. We compute the g-factors for TMD materials using density functional theory (DFT) and include self-energy corrections within many-body perturbation theory (MBPT). Using these results, we comment on the exciton g-factors measured in both monolayer and twisted bilayer TMDs, and show that the MBPT results agree better with experiment than DFT. The effects of spin-orbit coupling are also discussed.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F40 DCOMP DCMP DAMOP DMP: Building the bridge to exascale: applications and opportunities for materials, chemistry, and biology IV 705 - James Belak, Lawrence Livermore Natl Lab - Tag(s): Focus
8:00AM F40.00001: Towards Exascale Electronic Structure and Quantum Transport Calculations [Invited] JERRY BERNHOLC (Presenter), North Carolina State University — The development of robust, adaptive software and algorithms that can fully exploit exascale capabilities and future computing architectures is critical to designing advanced materials and devices with targeted properties. We have developed an open-source code that discretizes the DFT equations on real-space grids that are distributed over the nodes of a massively parallel system via domain decomposition. Multigrid techniques are used to dramatically accelerate convergence while only requiring nearest-neighbor communications. The real-space multigrid (RMG) code achieves full plane wave accuracy and scales from desktops and clusters to supercomputers consisting of ~200k cores and 20k GPUs, including the Cray XE-XK systems and the new IBM-NVIDIA pre-exascale Summit. Multilevel parallelization with MPI, threads and/or Cuda/HIP programming enables adaptation to future exascale supercomputers. RMG is distributed via www.rmgdft.org, with over 3,800 downloads do date. Advanced functionalities are provided through interfaces to other codes, including QMCPACK, BerkeleyGW, Phonopy, and ALAMODE. RMG is also being used for high throughput vibrational analysis of large systems at the Spallation Neutron Source. We will also describe the non-equilibrium Green's function module based on variationally-optimized localized orbitals, by which quantum transport properties can be studied for devices containing tens of thousands of atoms with full DFT accuracy. For a system with ten thousand atoms, our initial implementation scales linearly from 100 to 1000 nodes on Summit, already gaining ~4x speed-up from GPUs over CPU-only calculations. Several applications will be described as time permits, including a nanocircuit that could potentially enable electrical sequencing of DNA, and a novel experimentally realizable graphene-nanoribbon-based negative differential resistance device.


8:36AM F40.00002: Towards first-principles design of quantum devices JACEK JAKOWSKI (Presenter), Oak Ridge National Lab, JERRY BERNHOLC, North Carolina State University, MINA YOON, DAVID LINGERFELT, Oak Ridge National Lab, WENCHANG LU, EMIL BRIGGS, North Carolina State University — With the Moore's Law in high-performance computing approaching limits, future progress relies on harnessing quantum effects. Modeling quantum behavior at device scale requires an exascale computer and software that fully utilizes its extraordinary capabilities. Much of current research exploring future directions for nanoscale electronics is focused on two-dimensional materials. Evaluation of future nanodevices is very difficult and it it requires simulations involving thousands of atoms. Advanced quantum-mechanical simulations can be used to develop novel device concepts and identify the appropriate combinations of atomic constituents and nanoscale structures, thereby radically accelerating progress. We discuss the implementation of time-dependent electron dynamics in the real-space multigrid (RMG) density functional theory software package. The use of multiresolution grids permits real-space description of the electronic structure of systems comprised of hundreds-to-thousands of atoms, allowing atomistic description of systems approaching realistic device scales that can include arbitrary defects/impurities. Some results for quantum materials are presented that we believe could be the focus of future quantum computing and quantum information technologies.
GPU-Acceleration of the ELPA2 Distributed Eigensolver for Applications in Electronic Structure Theory*  
VICTOR YU (Presenter), Department of Mechanical Engineering and Materials Science, Duke University, JONATHAN MOUSSA, The Molecular Sciences Software Institute, VOLKER BLUM, Department of Mechanical Engineering and Materials Science, Duke University — The solution of eigenproblems is often a key computational bottleneck that limits the tractable system size of electronic structure theory. For large systems, these eigenproblems can easily exceed the capacity of a single computer, thus must be solved on distributed-memory parallel computers. The ELSI library facilitates large-scale electronic structure calculations by providing a unified interface to various fast and scalable eigensolvers and density matrix solvers, including the EigenExa, ELPA, libOMM, NTPoly, PEXSI, and SLEPc libraries. The ubiquitous adoption of hybrid CPU-GPU nodes in supercomputing opens up new opportunities to accelerate electronic structure calculations. We here present GPU-oriented optimizations of the ELPA two-stage tridiagonalization eigensolver (ELPA2). On top of its existing cuBLAS-based GPU offloading, we add a CUDA kernel to speed up the back-transformation of eigenvectors, which was known as the main bottleneck of the two-stage tridiagonalization algorithm. CPU, GPU, and MPI activities are overlapped wherever possible. Robust choices that maximize the GPU compute intensity are identified. We demonstrate the performance of this GPU-accelerated eigensolver by a set of benchmark calculations.

*This work is supported by NSF under grant number 1450280.

Driving exascale computational science with AiiDA  
SEBASTIAAN HUBER ( Presenter), GIOVANNI PIZZI, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne — The ever-growing availability of computational power and sustained development of advanced computational methods have contributed much to recent scientific progress. This progress presents new challenges regarding the sheer amount of calculations and data that has to be managed.

Next-generation exascale computing infrastructures will harden these challenges and we believe will require automated and scalable solutions.

Therefore, we have developed a comprehensive, robust, open source, high-throughput infrastructure AiiDA (http://aiida.net) dedicated to address the challenges in automated workflow management and data provenance storage.

We discuss how AiiDA's engine can now sustain throughputs of ~100’000 processes/hour, while automatically storing full data provenance.

The provenance is stored in relational database that makes the data queryable, traversable, and directly enables high-performance data analytics.

Any simulation software can be interfaced to AiiDA via its plugin system, and AiiDA's workflow language provides advanced automation and error handling features, as we demonstrate through one of our high-throughput projects.

We highlight how the resulting data can be disseminated by and to the wider community in a FAIR way on the Materials Cloud (http://materialscloud.org).
**9:12AM F40.00005: DMFTwDFT: A free-license DMFT package interfaced with various DFT implementations**

HYOWON PARK (Presenter), VIJAY SINGH, Univ of Illinois - Chicago, UTHPALA HERATH, West Virginia University, BENNY WAH, XINGYU LIAO, Univ of Illinois - Chicago, ALDO H ROMERO, West Virginia University — The electronic and structural characterization of strongly correlated materials (SCMs) is one of the most difficult problems in computational materials science. Dynamical Mean Field Theory (DMFT) has been successful in treating local many-body effects of correlated orbitals in SCMs, particularly when it is combined with density functional theory (DFT). In this talk, we present an open-source computational package (DMFTwDFT) combining DMFT with various DFT codes interfaced to a Wannier90 package for adopting maximally localized Wannier functions as local orbitals to describe a correlated subspace. We also provide the library mode for computing a DMFT density matrix such that our package can be efficiently linked to various DFT codes and achieves the charge-self-consistency within DFT+DMFT loops. We used our code for the study of well-known correlated materials, namely LaNiO3, SrVO3, and NiO to compute the density of states, the band structure, the total energy, the atomic force, and the Fermi surface within DFT+DMFT, and also compared our results to those obtained from other DFT+DMFT codes.

*This work is supported by the NSF SI2-SSE Grant 1740112.*

**9:24AM F40.00006: Scaling and Performance of Real-Space Electronic Structure Calculations on Exascale Architectures**

EMIL BRIGGS (Presenter), WENCHANG LU, JERRY BERNHOLC, North Carolina State University — Electronic structure calculations are hard to scale on massively parallel systems, and these challenges are compounded on CPU-GPU exascale architectures. Real-space formulations enable easy parallelization via domain decomposition, which has been implemented in our open-source real-space multigrid code (RMG). RMG has been designed to perform well on leading-edge supercomputers from inception. However, scaling to extreme sizes and to distributed multi-CPU-GPU architectures requires careful consideration of data distribution and flow, including inter-node transfers as well as between CPUs and GPUs located on the same node. The large mismatches between CPU and GPU clock speeds and FLOP rates provides additional constraints as well as optimization opportunities. We will discuss efficient and scalable implementation of distributed data flow and key electronic structure algorithms on exascale class machines in RMG, as well as methods for addressing MPI scalability constraints and data bottlenecks. RMG source code and build scripts for pre-exascale Summit, Cray XE-XK, clusters, Linux, Windows, and MacOS workstations are available at [www.rmgdft.org](http://www.rmgdft.org) together with help files and examples.
9:36AM F40.00007: From LSMS to MuST: Large scale first principles materials calculations at the exascale*  
MARKUS EISENBACH (Presenter), XIANGLIN LIU, Oak Ridge National Lab,  
KHORGOLKHUU ODBADRAKH, University of Tennessee, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University — We present recent advances in our Locally-selfconsistent Multiple Scattering (LSMS) code for scalable first principles density functional calculations of materials. A fundamental science drivers for large scale calculations is the need to understand materials beyond periodic crystalline lattices. Due to the large simulation cells of many thousands of atoms needed to describe complex electronic and magnetic ordering, defect states or disorder in alloys, the cubic scaling of traditional first principles methods has prevented direct first principles calculations. The real space formalism of LSMS enables calculations for $O(100,000)$ atom. In preparation for exascale systems, we are extending the use of accelerators to the calculation of forces and embedding methods for disordered systems. We will present results and performance measurements for defects in high entropy alloys and non-collinear magnetism in disordered systems. The computational capabilities will be available in our Multiple Scattering Theory suite (MuST) [https://github.com/mstsuite]

*Research supported in parts by the Office of Science of DOE and by the NSF Office of Advanced Cyberinfrastructure and the Directorate of Mathematical and Physical Sciences. It used resources of the Oak Ridge Leadership Computing Facility.

9:48AM F40.00008: Mixed precision sampling of quantum states of matter*  
THOMAS MAIER (Presenter), Oak Ridge National Laboratory, GIOVANNI BALDUZZI, URS R HAEHNER, ETH Zürich, YING WAI LI, Los Alamos National Laboratory, ARGHYA CHATTERJEE, ED D'AZEVEDO, Oak Ridge National Laboratory — Monte Carlo simulations are widely used throughout all areas of science. In materials science, they provide an important framework to unravel the mechanisms that give rise to complex behavior and different quantum states of matter. The DCA++ code is a high-performance research application that solves quantum many-body, materials problems with a cutting edge quantum Monte Carlo based dynamic cluster approximation (DCA). Here we discuss how mixed precision arithmetics finds a natural home in statistical sampling based Monte Carlo, and how it is being used in DCA++ to boost performance on ORNL’s Summit supercomputer.

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.
Towards finite-temperature tensor network simulations of the two-dimensional Hubbard model

ALEXANDER WIETEK (Presenter), MILES STOUDENMIRE, Center for Computational Quantum Physics, Flatiron Institute — The phase diagram of the two-dimensional Hubbard model at finite temperature poses one of the most interesting conundrums in contemporary condensed matter physics. Tensor network techniques, such as matrix-product based approaches as well as 2D tensor networks (PEPS), yield state-of-the-art unbiased simulations of the 2D Hubbard model at zero temperature and are capable of giving unbiased results at finite temperature as well. A promising approach for applying tensor networks to study finite-temperature quantum systems is the minimally entangled typical thermal state (METTS) algorithm, which is a Monte Carlo technique that samples from a family of entangled wavefunctions, and which offers favorable scaling and parallelism. We demonstrate how the METTS algorithm in combination with modern time-evolution algorithms for matrix-product states, like the time-dependent variational principle (TDVP) method, allows simulating the Hubbard model at finite temperature for cylinder geometries approaching the two-dimensional limit.

Comparison of systematically improvable DMC and AFQMC for condensed matter

ANOUAR BENALI (Presenter), Argonne Natl Lab, FIONN MALONE, MIGUEL A MORALES, Lawrence Livermore National Laboratory, LUKE SHULENBURGER, Sandia National Laboratories — Diffusion Monte Carlo (DMC) and Auxiliary Field Quantum Monte Carlo (AFQMC) can both have their approximations systematically improved by applying successively more accurate trial wavefunctions. In this work we assess the cost and feasibility of determining exact total energies for solid state Hamiltonians by studying primitive cells of four representative materials, Al, LiF, C and TiO2. Specifically, we utilize multideterminant trial wavefunctions generated via selective CI techniques with various sizes of single particle basis. Attention is paid to the rate at which the error decreases as the trial wavefunction includes more determinants and also to the cost as the basis increases in size. In this way, we are able to compare both DMC and AFQMC on equal terms at identical levels of approximation.

*Supported by US DOE BES, Mat. Sci. and Engn. Div., Comput. Mat. Sci. Prog. and Center for Predictive Simulation of Functional Materials. Calculations used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357 and the Livermore Computing Facilities. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525
Quantum Monte Carlo with orbital optimization applied on solids

YE LUO (Presenter), Argonne Natl Lab — The accuracy and efficiency of quantum Monte Carlo (QMC) methods can be improved directly by improving many body wavefunction. Full wavefunction optimization introduced a decade ago enabled solving scientific challenges beyond chemical accuracy. Recently algorithmic development pushed the computational efficiency of wavefunction derivatives and thus paved the way for simulation with large electron counts although demonstrations are mostly limited to molecular systems. When applying QMC in solids, using fixed orbitals calculated by density functional theory (DFT) together with variationally optimized Jastrow factors is still the common practice. Recent study on bandgaps shows qualitative improvement by simply adding limited multi determinant expansion. This hints the necessity of improving single particle orbitals restricted by DFT. Thus, we enable orbital optimization schemes like mixing occupied and unoccupied orbitals or directly optimizing orbital shapes and study their strength and weakness on solid state systems.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, as part of the Computational Materials Sciences Program and Center for Predictive Simulation of Functional Materials.

Auxiliary-Field Quantum Monte Carlo Applied to Correlated Materials

FIONN MALONE (Presenter), Lawrence Livermore Natl Lab, JOONHO LEE, Department of Chemistry, Columbia University, SHUAI ZHANG, Laboratory for Laser Energetics, University of Rochester, MIGUEL A MORALES, Lawrence Livermore Natl Lab — In this talk we investigate the application of auxiliary-field quantum Monte Carlo (AFQMC) to correlated materials. Focusing on elemental transition metals and their oxides we systematically investigate the effect of trial wavefunction and basis set quality on the energetics and static properties computed from AFQMC. We show how recent algorithmic developments allow us to reliably reach the thermodynamic limit and compare directly to experiment.

*The work of FDM, SZ and MAM was performed under the auspices of the U.S. Department of Energy (DOE) by LLNL under Contract No. DE-AC52-07NA27344. FDM, SZ and MAM acknowledge funding support from the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, as part of the Computational Materials Sciences Program and Center for Predictive Simulation of Functional Materials (CPSFM).
10:48AM F40.00013: Magnetic and charge orders in the ground state of the 2D repulsive Hubbard model

HAO XU (Presenter), William & Mary College, MINGPU QIN, School of Physics and Astronomy, Shanghai jiao tong University, HAO SHI, YUAN-YAO HE, SHIWEI ZHANG, Center for Computational Quantum Physics, Simons foundation — Using the auxiliary field quantum Monte-Carlo (AFQMC) method combined with a self-consistent constraint [1], we systematically study the ground state of the two-dimensional repulsive Hubbard model as a function of doping and interaction strengths. We focus on the spin and charge correlations, applying pinning fields to break translational symmetry and computing the spin and charge densities to probe the emergence of long-range order and collective modes. A phase diagram of spin-density and charge-density waves (including stripes) is obtained.


*The work is supported by Simons Foundation.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F41 GMAG DMP: Skyrmion Crystals 707 - Lingfei Wang, Seoul National University

8:00AM F41.00001: Skyrmion crystal from RKKY interaction mediated by 2DEG ZHENTAO WANG (Presenter), University of Tennessee, Knoxville, YING SU, SHIZENG LIN, Theoretical Division, T-4 and CNLS, Los Alamos National Laboratory, CRISTIAN BATISTA, University of Tennessee, Knoxville — Skyrmion crystals have been found in centro-symmetric itinerant magnets, where the long-range Ruderman-Kittel-Kasuya-Yoshida (RKKY) effective coupling is believed to be the dominant interaction between the local moments. In this work we show that the RKKY interaction mediated by a dilute ($k_F \ll 1$) 2D electron gas (2DEG) on a C$_6$ invariant lattice stabilizes a magnetic skyrmion crystal in the presence of magnetic field and easy-axis anisotropy. A remarkable aspect of this mechanism is that the ordering wave vectors of the resulting skyrmion crystal are dictated by the Fermi wave vector: $|Q_\nu| = 2k_F$ ($\nu = 1, 2, 3$). Consequently, the topological contribution to the Hall conductivity of the 2DEG becomes very large within the weak-coupling regime: the quantized value $e^2/h$ is reached when $J$ becomes comparable to the Fermi energy $E_F$. 
Magnetic hedgehog lattices in noncentrosymmetric metals* SHUN OKUMURA (Presenter), Department of Applied Physics, University of Tokyo, SATORU HAYAMI, Department of Physics, Hokkaido University, YASUYUKI KATO, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo — Recently, three-dimensional topological spin textures called the magnetic hedgehog lattices (HLs) were discovered in the B20-type compounds MnSi_{1-x}Ge_x [1]. The HLs have periodic arrays of magnetic monopoles and anti-monopoles, which induce interesting transport phenomena, such as the topological Hall effect and the topological thermoelectric transport. However, their stabilization mechanism has not been fully understood thus far. Here we investigate the ground state of an effective spin model with long-range interactions arising from the itinerant nature of electrons by variational calculations and simulated annealing. We find that the HLs are stabilized even at zero field by the synergetic effect of symmetric and antisymmetric interactions from the spin-charge and spin-orbit couplings, respectively. We also clarify the full phase diagram in the magnetic field, which includes multiple phase transitions with changes in the number of monopoles and anti-monopoles [2].


Ordering in magnetic skyrmion lattices* JAMES STIDHAM (Presenter), MICHEL PLEIMLING, Virginia Tech — Ordering in magnetic skyrmion lattices is an active area of research for skyrmion systems. In this talk, we present recent results obtained using Langevin molecular dynamic simulations, based on a previously derived particle model of skyrmions. Using a Voronoi cell algorithm, we examine the effect of the Magnus force present in skyrmion systems and how it affects ordering when noise is both present and absent in the system. We observe power-law behavior during late time ordering in these skyrmion systems. We also find power-law behavior when looking at the difference in time of consecutive events as the system orders.

*This research was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Grant No. DE-SC0002308.
Formation of square skyrmion lattice in a centrosymmetric magnet without geometrical frustration

Khanh Nguyen (Presenter), Taro Nakajima, Xiuwen Yu, Shang Gao, Max Hirschberger, Riken Center for Emergent Matter Science, Yuichi Yamasaki, Nims, Hajime Sagayama, Hiromi Nakao, KEK, Licong Peng, Kiyomi Nakajima, Riken Center for Emergent Matter Science, Kiyou Shibata, Rina Takagi, The University of Tokyo, Taka-Hisa Arima, Riken Center for Emergent Matter Science, Yoshinori Tokura, Shinichiro Seki, The University of Tokyo — Magnetic skyrmion, a topologically stable swirling spin texture, has attracted attention as a particle-like object potentially suitable for high-density information bit. The previous observation of skyrmions has mostly focused on noncentrosymmetric systems with Dzyaloshinskii-Moriya interaction, while the further search of novel mechanisms to realize smaller skyrmion is highly demanded. Here, we report the observation of square skyrmion lattice for a centrosymmetric non-frustrated tetragonal magnet GdRu$_2$Si$_2$ by performing resonant x-ray scattering and Lorentz TEM experiments. The possible origin of observed skyrmion formation has been discussed in terms of four-spin interaction mediated by itinerant electrons. The present results demonstrate that skyrmions can be stabilized even without geometrical frustration and inversion symmetry breaking, and suggest that rare-earth intermetallics with highly-symmetric crystal lattice may be ubiquitously platforms to explore nanometric skyrmions of exotic origins.

*This work was partly supported by Grants-In-Aid for Scientific Research Scientific Research (A) (Grant No. 18H03685) and Grant-in-Aid for Scientific Research on Innovative Area, "Nano Spin Conversion Science" (Grant No.17H05186) from JSPS, and PRESTO (Grant No. JPMJPR18L5) from JST.
**8:48AM F41.00005: Dramatic enhancement of the skyrmion phase-space of Cu$_2$OSeO$_3$ driven by high pressure**

LIANGZI DENG (Presenter), HUNG-CHENG WU, ALEXANDER LITVINCHUK, Texas Center for Superconductivity and Physics Department at the Univ of Houston, NOAH YUAN, Massachusetts Institute of Technology, JEY-JAU LEE, National Synchrotron Radiation Research Center, Taiwan, RABIN DAHAL, Texas Center for Superconductivity and Physics Department at the Univ of Houston, LIANG FU, Massachusetts Institute of Technology, HELMUTH BERGER, Institute of Physics of Complex Matter, Switzerland, HUNG-DUEN YANG, Department of Physics, National Sun Yat-sen University, Taiwan, ZHENG WU, MELISSA GOOCH, PAUL C. W. CHU, Texas Center for Superconductivity and Physics Department at the Univ of Houston — Generally, the skyrmion phase in a bulk helimagnet occurs only over a very restricted magnetic-field – temperature phase space and often at low temperatures. We have expanded and enhanced the skyrmion phase region from the small range of (55-58.5 K) to (5-300 K) in single crystal Cu$_2$OSeO$_3$ by pressures up to 42.1 GPa through a series of phase transitions from the cubic $P2_13$, through orthorhombic $P2_12_12_1$ and monoclinic $P2_1$, and finally to the triclinic $P1$ phase, using our newly developed ultrasensitive high pressure magnetization technique. The results are in agreement with our Ginzburg - Landau free energy analyses that pressure tends to stabilize the skyrmion states and at higher temperatures. These observations also show that the skyrmion state can be achieved at higher temperatures in various crystal symmetries, suggesting the insensitivity of skyrmions to the underlying crystal lattices and thus the possibility of finding more ubiquitous presence of skyrmions in helimagnets.

*The work performed at the Texas Center for Superconductivity at the University of Houston is supported by US Air Force Office of Scientific Research Grant FA9550-15-1-0236, the T. L. L. Temple Foundation, the John J. and Rebecca Moores Endowment, and the State of Texas through TcSUH.*
9:00AM F41.00006: Detection of magnetic skyrmion tubes in cubic B20 FeGe nanostructures

NITISH MATHUR (Presenter), MATTHEW JOHN STOLT, Department of Chemistry, 1101 University Avenue, Madison, WI-53706, University of Wisconsin Madison, FEHMI YASIN, RIKEN CEMS, Wako Japan - 3510198, PHILIPP RYBAKOV, Royal Institute of Technology (KTH), Stockholm, NIKOLAI S. KISELEV, Forschungszentrum Jülich, Germany, XIUZHEN YU, RIKEN CEMS, Wako Japan - 3510198, SONG JIN, Department of Chemistry, 1101 University Avenue, Madison, WI-53706, University of Wisconsin Madison —

In chiral helimagnets with the non-centrosymmetric cubic B20 crystal structure, such as FeGe, host magnetic Bloch-type skyrmions due to the Dzyaloshinskii-Moriya interaction (DMI). Although magnetic skyrmions are depicted as two-dimensional spin textures in bulk crystals, in reality, they possess a three-dimensional structure of skyrmions that looks like elongated tubes extending throughout the thickness of the sample. We have synthesized single-crystal FeGe nanowires (NWs) and Fe_{1-x}Co_xGe (x<0.1) nanoplates (NPLs) via chemical vapor deposition (CVD) to explore these magnetic skyrmion tubes (SkT) in geometrically confined nanostructures. Lorentz transmission electron microscopy imaging as well as magnetotransport measurements confirmed that skyrmions are stabilized in a wider magnetic field (B_{ext}) and temperature region in these nanostructures in comparison to the bulk materials. Furthermore, magnetoresistance measurements on FeGe nanostructures have shown some unusual features when B_{ext} is parallel to the current direction. In conjunction with magnetic contrast imaging techniques and micromagnetic simulations, we have further explored the spin modulation of SkT with the variation of in-plane applied magnetic field in FeGe nanostructures.
Spectroscopic-imaging STM measurement of magnetic skyrmions in a centrosymmetric crystal

YUUKI YASUI (Presenter), CHRISTOPHER BUTLER, KHANH NGUYEN, Center for Emergent Matter Science, RIKEN, TAKUYA NOMOTO, Department of Applied Physics, The University of Tokyo, SATORU HAYAMI, Department of Physics, Hokkaido University, TETSUO HANAGURI, Center for Emergent Matter Science, RIKEN, YUKITOSHI MOTOME, RYOTARO ARITA, Department of Applied Physics, The University of Tokyo, TAKA-HISA ARIMA, Department of Advanced Material Science, The University of Tokyo, YOSHINORI TOKURA, SHINICHIRO SEKI, Department of Applied Physics, The University of Tokyo — The magnetic skyrmion, vortex-like magnetic swirling structure, has attracted attention as a topological quasi-particle. The Dzyaloshinskii-Moriya interaction originating from broken inversion symmetry in the crystal structure is considered to be the key to stabilize the skyrmion. However, a mechanism to stabilize magnetic skyrmions even in centrosymmetric crystals has been proposed [1, 2]. For such centrosymmetric systems, experiments to show how the itinerant electrons interact with the magnetic structure are highly desired for further understanding.

We performed spectroscopic-imaging scanning tunneling microscopy (SI-STM) measurements for a centrosymmetric crystal GdRu$_2$Si$_2$, which is expected to host magnetic skyrmions. As a result, we found that the density of states near the Fermi energy (0.1 eV) varies in different magnetic phases including the skyrmion phase. Besides, we also observed periodic modulation in the electronic states with the same period as the magnetic skyrmion.

In the presentation, we will discuss a possible skyrmion formation mediated by itinerant electrons.


This work was supported by JST CREST Grant No. JPMJCR16F2

Helical and skyrmion phases in amorphous Fe-Ge thick films

XIAOQIAN CHEN (Presenter), ROBERT STREUBEL, Lawrence Berkeley National Laboratory, DINAH SIMONE BOUMA, University of California Berkeley, ROLAND KOCH, STEPHEN DOUGLAS KEVAN, Lawrence Berkeley National Laboratory, FRANCES HELLMAN, University of California Berkeley, PETER FISCHER, SUJOY ROY, Lawrence Berkeley National Laboratory — Magnetic skyrmions are topologically protected solitons with the potential to revolutionize future spintronics and computing due to its low energy cost of manipulation. Skyrmion phase, now found in various single crystals including ferrimagnet FeGe, has recently predicted to also manifest in vector spin frustrated amorphous films. We studied amorphous Fe-Ge films using coherent resonant soft x-ray scattering. We observed magnetic Bragg peaks associated with the helical and skyrmion periodicity and mapped out their field-temperature phase diagram. We also observed spontaneous dynamics for a large range of temperatures. We calculate the respective one-time correlation functions of this fluctuation, whose characteristic curvatures indicate the distinct dynamical behavior of the helical and skyrmion textures.

*This work was primarily funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05-CH11231 within the NEMM program (MSMAG).
Observation of Robust Néel Skyrmions in Metallic PtMnGa

SRIVASTAVA (Presenter), Nano-Systems from ions, spins and electrons, Max Planck Institute of Microstructure Physics, PARUL DEVI, Solid State Chemistry, Max Planck Institute for Chemical Physics of Solids, ANKIT SHARMA, TIANGPING MA, HAKAN DENIZ, HOLGER MEYERHEIM, Nano-Systems from ions, spins and electrons, Max Planck Institute of Microstructure Physics, CLAUDIA FELSER, Solid State Chemistry, Max Planck Institute for Chemical Physics of Solids, STUART PARKIN, Nano-Systems from ions, spins and electrons, Max Planck Institute of Microstructure Physics — Bloch[1] and anti-skyrmions[2] have attracted much attention since their first observation. Bulk Néel skyrmions have been observed in two compounds, GaV4S8[3] and VOSe2O5[4], but at low temperatures only. Here we report the first observation of bulk Néel skyrmions in a non-centrosymmetric metallic compound PtMnGa by means of Lorentz Transmission Electron Microscopy (LTEM)[5]. Skyrmions in PtMnGa are found to be stable over a wide temperature range up to its Curie temperature (~220K). By contrast with skyrmions observed to date, we find that the skyrmion size in PtMnGa is strongly influenced by the thickness of the lamella in which the skyrmions are observed. Their size increases by a factor of 7 when the thickness is increased from ~90 nm to ~4 µm. Moreover, skyrmions can be stabilized at zero field after suitable field cooling processes and are highly robust against large in-plane magnetic fields (~1 T). These properties make PtMnGa and related compounds an extremely exciting system for future spintronic applications.

5. Srivastava, A.K. et al., (under consideration)
New low temperature phases in chiral cubic magnets

CATHERINE PAPAS (Presenter), FENGJIAO QIAN, LARS J. BANNENBERG, ANKIT LABH, Applied Sciences, Delft University of Technology, HERIBERT WILHELM, Helmholtz Institute Ulm, ROBERT CUBITT, EDDY LELIÈVRE-BERNA, Institut Laue-Langevin, Grenoble, France, GREGORY CHABOUSSANT, Laboratoire Léon Brillouin, CEA-Saclay, Gif sur Yvette, France, LISA DEBEER-SCHMITT, Oak Ridge National Laboratory, Oak Ridge, USA, MARCUS P. SCHMIDT, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, MAXIM MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen, Netherlands, ANDREY LEONOV, Chiral Research Center, Hiroshima University, Japan — Chiral and skyrmion-hosting cubic magnets have so far been described in terms of a universal magnetic phase diagram composed of helical spiral, conical spiral, and skyrmion crystal phases. A remarkable deviation from this universal behavior occurs in Cu2OSeO3 revealed by neutron scattering and magnetization measurements. Below the upper critical field at which the conical spiral state disappears, the spiral wave vector rotates away from the magnetic field direction. We discuss the physical origin of this new state and suggest that it provides the inhomogeneous magnetic environment required to stabilise new low temperature skyrmionic phases. We discuss the different stabilization and nucleation mechanisms and the thermodynamic stability of these low temperature skyrmionics phases, as they have been investigated by neutron scattering.

*The work is financially supported by The Netherlands Organization for Scientific Research through project 721.012.102 (LARMOR), the Vrije FOM-programma ‘Skyrmionics’ (Netherlands) as well as the JSPS Core-to-Core Program, Advanced Research Networks (Japan) and JSPS Grant-in-Aid for Research Activity Start-up 17H06889 (Japan).
10:00AM F41.00011: Weak crystallization of fluctuating skyrmion textures in MnSi* JONAS KINDERVATER, IOANNIS STASINOPOULOS, ANDREAS BAUER, FRANZ XAVER HASLBECK (Presenter), FELIX RUCKER, ALFONSO CHACON, Physics Department, Technical University of Munich, Germany, SEBASTIAN MÜHLBAUER, CHRISTIAN FRANZ, Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Germany, MARKUS GARST, Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Germany, DIRK GRUNDLER, Institute of Materials and Laboratory of Nanoscale Magnetic Materials and Magnonics, École Polytechnique Fédérale de Lausanne, Switzerland, CHRISTIAN PFLEIDERER, Physics Department, Technical University of Munich, Germany — We report an experimental study of the emergence of non-trivial topological winding and long-range order across the paramagnetic to skyrmion lattice (SkL) transition in the transition metal helimagnet MnSi. Combining measurements of the susceptibility with small angle neutron scattering, neutron resonance spin echo spectroscopy and all-electrical microwave spectroscopy, we find evidence of skyrmion textures in the paramagnetic state exceeding $10^3 \text{Å}$ with lifetimes above several $10^{-9} \text{s}$. Our experimental findings establish that the paramagnetic to SkL transition in MnSi is well-described by the Landau soft-mode mechanism of weak crystallization, originally proposed in the context of the liquid to crystal transition. As a key aspect of this theoretical model, the modulation-vectors of periodic small amplitude components of the magnetization form triangles that add to zero. In excellent agreement with our experimental findings, these triangles of the modulation-vectors entail the presence of the non-trivial topological winding of skyrmions already in the paramagnetic state of MnSi when approaching the SkL transition. J. Kindervater et al., Phys. Rev. X (accepted for publication)

*We gratefully acknowledge financial support through DFG, ERC, BMBF, IAS, and TUM graduate school.
10:12AM F41.00012: Surface Effects in the Magnetic Textures of B20 MnGe Thin Films

JACOB REPICKY (Presenter), JOSEPH P CORBETT, TAO LIU, ADAM S AHMED, Ohio State Univ - Columbus, JONATHAN GUERRERO-SANCHEZ, Physics, Universidad Nacional Autónoma de México, ROLAND KAWAKAMI, JAY A GUPTA, Ohio State Univ - Columbus — Bulk MnGe hosts a three-dimensional skyrmion state with a period of only 3 nm. Using low-temperature (5K) spin-polarized scanning tunneling microscopy, we show that this magnetic texture is modified at the surface of MnGe thin films. We observe a stripe-like phase with a 6-8 nm period and a propagation vector that is not strongly pinned to any direction, but is influenced by step edges, surface termination, and atomic lattice strain. We also report the observation of target skyrmions with triangular shape that is set by the atomic lattice vectors, and a core size of 15 nm. We observe the target state is much more sensitive to magnetic fields than the stripe phase, and that pulses with the STM tip demonstrate the texture can be ‘switched’ between states with different topological charge. By analyzing the voltage and current applied during switching events we can determine their dependence on thermal energy of tunneling electrons, injection of spin-polarized current, or electric fields. Finally, we explore the magnetic texture in different film thicknesses and compare their larger scale film morphology to distinguish between thin film effects and true surface effects.

*Funding for this research was provided by the Defense Advanced Research Projects Agency Grant No. 18AP00008

10:24AM F41.00013: Equilibrium Skyrmions and Antiskyrmions in Strained Bulk Ferromagnets at Room Temperature

DANIIL KITCHAEV (Presenter), ANTON VAN DER VEN, University of California, Santa Barbara — Control over skyrmion formation and topology at room temperature is foundational to the realization of skyrmion-based spintronic devices. Strained bulk ferromagnets are a rich platform for achieving both goals as strain can precisely adjust the effective magnetic Hamiltonian and thereby control the stability of emergent phases. We use phenomenological and symmetry arguments to identify simple strain fields which may stabilize chiral skyrmions over wide temperature ranges for all crystallographic point groups. We then use first-principles calculations, cluster-expansions and Monte Carlo analysis to computationally demonstrate the strain-induced formation of equilibrium skyrmions and antiskyrmions at room temperature in a proof-of-concept material. Finally, we demonstrate how strain may be used to control the relative stability of skyrmions and antiskyrmions, or engineer a state where these topologies are degenerate.

*The research reported here is supported by the Materials Research Science and Engineering Center at UCSB (MRSEC NSF DMR 1720256) through IRG-1.
10:36AM F41.00014: Investigating skyrmions using muon-spin spectroscopy*  TOM LANCASTER (Presenter), Physics, Durham University, GEETHA BALAKRISHNAN, Physics, University of Warwick, STEPHEN BLUNDELL, Physics, University of Oxford, MATJAZ GOMILSEK, Jozef Stefan Institute, THOMAS HICKEN, BENJAMIN HUDDART, Physics, Durham University, ALES STEFANCIC, Paul Scherrer Institut, MURRAY N WILSON, Physics, Durham University — We present the results of muon-spin relaxation measurements on materials hosting a skyrmion lattice (SkL) phase. We argue that the muon is primarily sensitive to the dynamics of the SkL and we have used this property to probe the local magnetism of several distinct skyrmion systems. Here we discuss our recent results on the effect of disorder on the Néel-skyrmion system GaV$_4$S$_{(8-y)}$Se$_y$ [1], where we have used low-level substitution to assess the stability of the SkL. We also discuss Zn-substituted Cu$_2$OSeO$_3$, where we show that the splitting of the SkL phase that was previously reported is only observed in polycrystalline samples and reflects the occurrence of several coexisting phases with different Zn content, each distinguished by different magnetic behavior [2]. We support our results with density functional theory calculations of the muon stopping states, that allow us an additional insight into the local environment of the muon probe.


*This work is supported by EPSRC (UK) under grants EP/N024028/1 and EP/N032128/1.

10:48AM F41.00015: Imaging the internal spin structures of skyrmions by Lorentz scanning transmission electron microscopy*  ZHEN CHEN (Presenter), Cornell University, TENG XU, Department of Physics, Tsinghua University, GREGORY FUCHS, Cornell University, WANJUN JIANG, Department of Physics, Tsinghua University, DAVID MULLER, Cornell University — Magnetic skyrmions are noncollinear spin textures that have been detected and studied using many different techniques. However, a detailed characterization of the internal spin structures of skyrmions, especially for skyrmions with diameters smaller than 100 nm, is experimentally challenging. These experiments are extremely important for defining the chirality and spin topology. Recent experiments show that Lorentz scanning transmission electron microscopy with a high-dynamic-range pixel array detector - Lorentz 4D-STEM, allows direct imaging of magnetic structures at a spatial resolution down to a few nanometers. Here we first show that Lorentz 4D-STEM technique combining with ptychography can be used to detect the detailed spin structures inside skyrmions and spin singularities in skyrmion lattices. We subsequently demonstrate the direct determination of the chirality of Néel-type skyrmions from the magnetic induction field distribution in an inclined sample setup. Using both fast, wide-field Lorentz TEM and quantitative, high-resolution Lorentz STEM, we are able to perform real-space imaging of magnetic spin textures at length scales that span microns down to a few nanometers.

*Supported by DARPA TEE program (D18AC00009).

Tuesday, March 3, 2020 8:00 AM - 11:00 AM
8:00AM F42.00001: Distinct magneto-Raman signatures of spin-flip phase transitions in CrI$_3$

AMBER MCCREARY (Presenter), THUC MAI, National Institute of Standards and Technology, FRANZ UTERMOHLEN, Ohio State University, JEFFREY SIMPSON, Towson University, KEVIN GARRITY, National Institute of Standards and Technology, XIAOZHOU FENG, Penn State University, DMITRY SHCHERBAKOV, Ohio State University, YANGLIN ZHU, Penn State University, JINHU, University of Arkansas, DANIEL WEBER, Ohio State University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, JOSHUA GOLDBERGER, Ohio State University, ZHIQIANG MAO, Penn State University, CHUN NING LAU, YUANMING LU, NANDINI TRIVEDI, ROLANDO VALDES AGUILAR, Ohio State University, ANGELA HIGHT WALKER, National Institute of Standards and Technology — The discovery of 2-dimensional (2D) materials, such as CrI$_3$, that retain magnetic ordering at monolayer thickness has resulted in a surge of research in 2D magnetism from both pure and applied perspectives. Here, we report a magneto-Raman spectroscopy study on multilayered CrI$_3$, focusing on two new features in the spectra which appear at temperatures below the magnetic ordering temperature and were previously assigned to high frequency magnons. We observe a striking evolution of the Raman spectra with increasing magnetic field in which clear, sudden changes in intensities of the modes are attributed to the interlayer ordering changing from antiferromagnetic to ferromagnetic at a critical magnetic field. Our work highlights the sensitivity of the Raman modes to weak interlayer spin ordering in CrI$_3$. In addition, we theoretically examine potential origins for the new modes, which we deduce are unlikely single magnons.

8:12AM F42.00002: Probing Tunneling Magnetoresistances in Chromium Trihalide Junctions via First Principles Calculations*

JONATHAN HEATH (Presenter), MARCELO KURODA, Auburn University — The demonstration of magnetic tunnel junctions in heterostructures formed with two-dimensional materials has spawned research ventures regarding spin transport in these layered systems. Efforts that initiated with CrI$_3$ have now been expanded to other chromium trihalides such as CrBr$_3$ and CrCl$_3$. Owing to their nanometer thicknesses, the electronic and magnetic properties of chromium trihalide systems are affected by quantum confinement effects along with their environments. Here we characterize physical properties of multilayer chromium trihalide/graphene junctions using density functional theory (DFT) and Landauer's formalism for ballistic transport. We find that band alignments in few-layer chromium trihalide (CrX$_3$ with X = F, Cl, Br and I) slabs change based on the metamagnetic state of the junctions and differ from those of isolated layers. We also delve into metamagnetic dependent complex band structures as well as discuss changes in the band structures of chromium trihalide junctions beyond DFT. Our results suggest that tunneling magnetoresistance values as high as 4,000% can be attained in bilayer heterojunctions.

*We gratefully acknowledge the financial support from NSF DMR-1848344 grant.
8:24AM F42.00003: Optically probing low energy magnetic excitations in bilayer CrI$_3$
HONGCHAO XIE (Presenter), University of Michigan - Ann Arbor, ZHIPENG YE, Texas Tech University, SHANGJIE TIAN, HECHANG LEI, Renmin University of China, RUI HE, Texas Tech University, LIUYAN ZHAO, University of Michigan - Ann Arbor — Study of spin waves, collective magnetic excitations, in two-dimensional (2D) magnets emerges as one key yet new topic in the research of 2D magnetism. Among all the 2D magnets studied so far, bilayer CrI$_3$ stands out because of the realization of the layered antiferromagnetism, in which the spins order ferromagnetically within each layer and antiferromagnetically between the two layers. So far, the magnetic excitations in natural bilayer CrI$_3$ have been rarely studied, with the exception of inelastic magneto-tunneling spectroscopy results. A further question of how such magnetic excitations depends on the angular alignment between the two layers and the resulted long-range Moiré superlattice remains totally unexplored. Here, I will first present our ultra-low frequency Raman spectroscopy studies on the spin waves in natural bilayer CrI$_3$ and discuss its comparison to the inelastic magneto-tunneling spectroscopy. I will further show the magnetic field dependence of the spin waves in natural bilayer CrI$_3$. Furthermore, I will explore how these low energy spin waves depend on the twist angle between bilayer CrI$_3$.

8:36AM F42.00004: Current Control of Magnetism in Two-Dimensional Fe$_3$GeTe$_2$ [Invited]
ARNE BRATAAS (Presenter), Norwegian Univ Tech (NTNU) — The recent discovery of magnetism in two-dimensional van der Waals systems opens the door to discovering exciting physics. We investigate how a current can control the ferromagnetic properties of such materials. Using symmetry arguments, we identify a recently realized system in which the current-induced spin torque is particularly simple and powerful. In Fe$_3$GeTe$_2$, a single parameter determines the strength of the spin-orbit torque for a uniform magnetization. The spin-orbit torque acts as a contribution to the out-of-equilibrium free energy and introduces new in-plane magnetic anisotropies to the system. Therefore, we can tune the system from an easy-axis ferromagnet via an easy-plane ferromagnet to another easy-axis ferromagnet with increasing current density. This finding enables unprecedented control and provides the possibility to study the Berezinskii-Kosterlitz-Thouless phase transition in the 2D XY model and its associated critical exponents.

9:12AM F42.00005: Enhanced magnetoresistance in mixed van der Waals magnetic tunnel junctions
DAHLIA KLEIN (Presenter), DAVID MACNEILL, Massachusetts Institute of Technology MIT, MÄRTA TSCHUDIN, Universität Basel, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology MIT — Since the recent isolation of monolayer CrI$_3$, there has been a surge of interest in van der Waals heterostructures incorporating 2D magnets. Studies have demonstrated large tunneling magnetoresistances in van der Waals magnetic tunnel junctions fabricated from the insulating layered chromium trihalides (CrX$_3$) due to the spin filter effect. Here, we report electron tunneling in graphite/CrCl$_3$/CrBr$_3$/graphite van der Waals heterostructures to study the effect of the CrCl$_3$/CrBr$_3$ interface. We find that the magnetoresistance persists above the Néel temperature of the in-plane antiferromagnet CrCl$_3$ with enhanced values compared to magnetic tunnel junctions fabricated from CrCl$_3$ alone. We interpret these data as resulting from the out-of-plane ferromagnet CrBr$_3$ acting as a spin-polarizing layer.
The recent advent of atomically-thin ferromagnetic crystals has allowed experimental studies of two-dimensional (2D) magnetism that not only exhibits novel behavior due to the reduced dimensionality but also often serves as a starting point for understanding of the magnetic properties of bulk materials. However, the experimental techniques that were used to explore two-dimensional ferromagnetism could not probe the magnetic field directly. Here we show that ballistic Hall micromagnetometry provides a reliable and convenient way to measure magnetization of individual two-dimensional ferromagnets. Our devices are made by van der Waals assembly in such a way that the investigated ferromagnetic crystal is placed on top of a multiterminal Hall bar made from encapsulated graphene. We apply the micromagnetometry to study atomically-thin chromium tribromide (CrBr$_3$). The material remains ferromagnetic down to monolayer thickness and exhibits strong out-of-plane anisotropy. Magnetic response of CrBr$_3$ varies little with the number of layers and its temperature dependence cannot be described by the simple Ising model of two-dimensional ferromagnetism.

9:36AM F42.00007: The quantum non-Heisenberg nature of two-dimensional CrI$_3$ magnets

ELTON SANTOS (Presenter), DINA WAHAB, MATHIAS AUGUSTIN, Queens Univ Belfast, SAMUEL MAÑAS-VALERO, Instituto de Ciencia Molecular, Universidad de Valencia, WENJUN KUANG, Physics, University of Manchester, SARAH JENKINS, Physics, University of York, EUGENIO CORONADO, Instituto de Ciencia Molecular, Universidad de Valencia, IRINA GRIGORIEVA, IVAN JESUS VERA MARUN, Physics, University of Manchester, EFREN NAVARRO-MORATALLA, Instituto de Ciencia Molecular, Universidad de Valencia, RICHARD F. L. EVANS, Physics, University of York, KOSTYA S. NOVOSELOV, Physics, National University of Singapore — Higher-order exchange interactions and quantum effects are widely known to play an important role in describing the properties of nano magnets. Here we show that the magnetism of recently discovered 2D CrI$_3$ cannot be captured at the level of a simple Ising model as initially thought. Using a complementary suite of magneto-optical Kerr effect microscopy, magnetic force microscopy, correlated first-principles methods and Monte Carlo techniques including higher-order exchange interactions, we identify CrI$_3$ as a quantum non-Heisenberg material. We find that biquadratic exchange interactions are essential to quantitatively describe the magnetism of CrI$_3$ but requiring quantum scaling corrections to reproduce its thermal properties. The quantization of spin-wave excitations at the low temperature regime is reflected on the fluctuations of the magnetization which follow Bose-Einstein rather than the Boltzmann statistics. These fluctuations induce the formation of metastable magnetic domains stabilizing into a single macroscopic magnetization over large surface areas. Such domains have characteristics of N'eel and Bloch types with a narrow domain wall width (3-5 nm). Similar behavior is expected for the majority of 2D vdW magnets where higher-order exchange interactions are appreciable.

9:48AM F42.00008: Substrate-assisted asymmetric electronic gap in artificial magnetic honeycomb lattice*

JIASEN GUO (Presenter), YIYAO CHEN, GEORGE YUMNAM, QUINN CUNNINGHAM, DEEPAK K SINGH, Univ of Missouri - Columbia — An artificial magnetic honeycomb lattice was prepared via physical vapor deposition. Asymmetric electronic gaps with increasing breadth were observed in the differential conductivity when applying in-plane current at low temperatures ranging from 27K to 40 K. Electrical hysteresis behavior was also observed and became more profound with increasing temperature. It was seen that an in-plane magnetic field parallel or antiparallel to the applied current tends to narrow the aforementioned gaps and reduce the degree of asymmetry drastically. Resistance measurement with applied magnetic field up to 8.5 T shows a temperature-dependent transition from positive magnetoresistance to negative magnetoresistance, which we suspect, is subject to the effect of the substrate. The observed negative magnetoresistance can be explained as the giant magnetoresistance effect due to the ordering of magnetic moment on the artificial honeycomb lattice.

*The research at MU is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Grant No. DE-SC0014461.
10:00AM F42.00009: Magneto-Raman study of the Neel-type Antiferromagnet MnPSe$_3$*

THUC MAI (Presenter), National Institute of Standards and Technology, JOSHUA ARGO, Materials Science and Engineering, The Ohio State University, AMBER MCCREARY, National Institute of Standards and Technology, ROLANDO VALDES AGUILAR, Physics, The Ohio State University, VICKY DOAN-NGUYEN, Materials Science and Engineering, The Ohio State University, ANGELA HIGHT WALKER, National Institute of Standards and Technology — The discovery of 2D magnetism in van der Waals materials such as CrI$_3$ and Cr$_2$Ge$_2$Te$_6$ demonstrated that long range magnetic ordering can survive in the monolayer limit, given that the material has sufficiently large anisotropy. MnPSe$_3$ is a layered material with Neel-type antiferromagnetic spins lying parallel to the basal plane. We perform a systematic magneto-Raman study of MnPSe$_3$. Multiple excitation laser wavelengths were used. With resonant Raman condition, we study the temperature and magnetic field dependence of the Raman spectrum of single crystal MnPSe$_3$. A drastic shift in the phonon spectrum across T$_{\text{Neel}}$ is observed. We compare the spin-phonon coupling between bulk and thin samples.

*The work at the National Institute of Standards and Technology was supported by National Research Council Postdoctoral Research Associateship Program and NIST-STRS (Scientific and Technical Research Services) for funding. Work at OSU was supported by the Center for Emergent Materials, an NSF MRSEC under grant DMR-1420451. This was also supported in part by The Ohio State University Institute for Materials Research. X-ray diffraction was performed at the Center for Electron Microscopy and Analysis (CEMAS) at The Ohio State University.

10:12AM F42.00010: Magnetic structure determination of transition metal dichalcogenide Fe$_{1/3}$NbS$_2$*

SHAN WU (Presenter), University of California, Berkeley, ZHIJUN XU, (NCNR, National Institute of Standards and Technology), ERAN MANIV, ARANI ACHARYA, SPENCER DOYLE, CAOLAN JOHN, JAMES ANALYTIS, ROBERT J BIRGENEAU, University of California, Berkeley — In layered transition metal dichalcogenides (TMD) MA$_2$ (M = Ta, Nb, A = S, Se), the weak van der Waals bonding between adjacent layers allows easy intercalation of transition metal atoms. Intercalated magnetic ions, such as T = Fe, Co, Mn, Cr, occupy the vacant octahedral sites between the layers and form an ordered triangular superlattice. This introduces in the magnetic degree of freedom, giving rise to a class of layered magnetic materials with a rich array of magnetic phenomena. Recently, the current-induced switching and magnetic memory effects were reported in FexNbS$_2$ with x close to 1/3 that exhibits an antiferromagnetic transition at T$_N$ ~ 45 K. This provides a new avenue to realize the spintronic device. From neutron diffraction experiment, we determined a stripe-type order that develops into three magnetic domains, which is strongly coupled to three nematic domains. The magnetic order parameter can be explained with the development of canted moment, which is associated with competing exchange interactions in the frustrated lattice and the effect of Dzyaloshinskii-Moriya interaction because of the lack of the inversion symmetry.

*This work is funded by the U.S. DOE, Materials Sciences and Engineering Division under Contract No. DE-AC02-05-CH11231 within the QM Program (KC2202).
Magnetic interactions and excitations in magnetic 2D van der Waals materials* LIQIN KE (Presenter), Ames Laboratory — Magnetic 2D van der Waals (m2DvdW) materials add new functionality, leading to novel new magnetic 2D devices. Using linear-response ab initio methods, we investigate the magnetic interactions and spin excitations in various m2DvdW systems. Dynamical spin susceptibility is calculated using single-particle Hamiltonians constructed within density-functional theory (DFT) and the quasiparticle self-consistent GW (QSGW) methods. Results are compared with available Inelastic Neutron Scattering (INS) measurements. We found that the more elaborate description of electron interactions better describes the magnetic interactions within 2D van der Waals systems. For example, plain DFT overestimates the exchange couplings in CrI3, while the spin-wave spectrum calculated in QSGW is closer to experiments. The effects of Dzyaloshinskii-Moriya interaction on spin excitations are also discussed.

*This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, and Early Career Research Program. Ames Laboratory is operated for the U. S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358.

Is 2H-MoTe₂ an intrinsically magnetic semiconductor?* JONAS A. KRIEGER, ZURAB GUGUCHIA, TONI SHIROKA, THOMAS PROKSCHA, ANDREAS SUTER, VLADIMIR STROKOV, ZAHER SALMAN (Presenter), Paul Scherrer Institute — Layered transition metal dichalcogenides are currently intensively investigated due to their opto-electronic, superconducting and topological properties as well as their potential usage as mono-layer building blocks. However, despite their layered nature they often exhibit three dimensional (3D) properties in the bulk. A recently detected long-range magnetic order in semiconducting 2H-MoTe₂ was attributed to defects [1]. Here we present results of complementary spectroscopic techniques to elucidate the nature and origin of the reported magnetic order. We find that the magnetism is intrinsic with a layered-antiferromagnetic ground state. Our results also show that this magnetism remains unchanged near the surface, opening new possibilities for applications of 2H-MoTe₂ in interface engineering.


*Swiss National Science Foundation (SNF-Grant No. 200021_165910)
Patterning-induced ferromagnetism of Fe₃GeTe₂ van der Waals materials beyond room temperature

MENGMENG YANG (Presenter), QIAN LI, CHENG GONG, University of California, Berkeley, RAJESH V CHOPDEKAR, ALPHA T. N'DIAYE, JOHN TURNER, Lawrence Berkeley National Lab, GONG CHEN, University of California-Davis, ANDREAS SCHOLL, PADRAIC SHAFER, ELKE ARENHOLZ, ANDREAS SCHMID, Lawrence Berkeley National Lab, SHENG WANG, University of California, Berkeley, KAI LIU, University of California-Davis, NAN GAO, University of California, Berkeley, ALEMAYEHU S ADMASU, SANG-WOOK CHEONG, Rutgers University, New Brunswick, CHANYONG HWANG, Korea Research Institute of Standards and Science, JIA LI, Peking University, FENG WANG, XIANG ZHANG, ZI Q. QIU, University of California, Berkeley — Magnetic van der Waals (vdW) materials have emerged as promising candidates for spintronics applications especially after the recent discovery of intrinsic ferromagnetism in monolayer vdW materials. There has been a critical need for tunable ferromagnetic vdW materials beyond room temperature. Here we report a real space imaging study of itinerant ferromagnet Fe₃GeTe₂ and the enhancement of its Curie temperature well above ambient temperature. We find that the magnetic long-range order in Fe₃GeTe₂ is characterized by an unconventional out-of-plane stripe domain phase. In Fe₃GeTe₂ microstructures patterned by focused ion beam, the out-of-plane stripe domain phase undergoes a surprising transition at 230 K to an in-plane vortex phase that persists beyond room temperature. The discovery of tunable ferromagnetism in Fe₃GeTe₂ materials opens up vast opportunities for utilizing vdW magnets in room temperature spintronics devices.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F43 DCOMP DAMOP DCMP: Precision many-body physics III: Non-perturbative QFT 702 - James LeBlanc, Memo Univ of Newfoundland - Tag(s): Focus

Particle transmutations in flat-band lattices: bosons to fermions, fermions to composite fermions [Invited] SAURABH MAITI (Presenter), Concordia Univ, TIGRAN SEDRAKYAN, Physics, University of Massachusetts, Amherst — Understanding new quantum states and exotic quasiparticles can often be facilitated by approaching the problem in a different basis. One such example, amongst many, is viewing hard core bosons as fermions coupled to a special gauge-field (called the Chern-Simons gauge field). The non-Maxwellian nature of this gauge field introduces new challenges in treating such a problem. However, progress has been made by treating the problem via various mean-field schemes. In this talk, we will draw our attention to the consequences of one particular scheme that is designed to be applicable for various interesting 2D lattices. We will see how this scheme leads to a particular intra-unit cell flux distribution that provides a natural description of the system in the parameter space where a chiral spin-liquid is stabilized for bosons residing in either a Honeycomb lattice or a Kagome lattice. We will view these results in light of other numerical works in the literature. Interestingly, we will also see that when the same scheme is applied to fermions in a lattice, subject to an external magnetic field, we can make interesting predictions related to the composite fermion state: in particular the theory suggests that Graphene with next nearest neighbor hopping at the half-filling condition should be a doped Haldane-Chern insulator of composite fermions.
8:36AM F43.00002: Coherent states, Gram matrix, and Hofstadter butterfly with flat band
YOUJIANG XU (Presenter), HAN PU, Rice Univ — Through a concrete example, we illustrate that the correspondence between Gram matrices and Hamiltonians may open up grand opportunities to discover novel systems. We find that the Gram matrices of certain subsets of coherent states, whose associating eigenvalues form a lattice on the complex plane, can be interpreted as Hamiltonians which govern the dynamics of a particle hopping around the lattice under a gauge field. The completeness of the subsets of coherent states guarantees massive degeneracy of the ground states of the Hamiltonians, which is independent from the shape of the lattice, while different types of lattice result in different Hofstadter-butterfly-like patterns in the excitation spectrum. The models also feature ground state wave functions in universal form whose dynamics is special. Numerical evidence suggests that it is highly possible to study the models experimentally.

8:48AM F43.00003: Chern-Simons fermionization approach to the chiral spin liquid on a frustrated square lattice with moat band*
RUI WANG (Presenter), Nanjing Univ, Z. Y. XIE, Renmin Unvi, HAIYUAN ZOU, Shanghai Jiao Tong Univ, WEI SU, Nanjing Univ, TIGRAN SEDRAKYAN, Umass, Amherst, BAIGENG WANG, D. Y. XING, Nanjing Univ — We utilize the Chern-Simons (CS) fermionization to study quantum spin XY models on a square lattice in the regime where the lattice dispersion exhibits a moat-like structure. We analytically derive the low-energy effective field theory, and predict a possible non-uniform chiral spin-liquid (CSL) ground state. Using high-precision numerical calculations such as the tensor network renormalization group based on projected entangled paired state (PEPS), we obtain numerical evidences that further suggest the stabilization of the non-uniform CSL. Finally, we show that the CS fermionization approach is also able to describe the magnetically ordered phases, which are captured by a CS superconducting state with condensation of Cooper pairs of CS fermions. By comparing the Goldstone mode of the magnetically ordered phase and that of the CS superconductor, we found high-precision agreements that suggest the equivalence of the two states in terms of the low-energy excitations.

*This work was supported by the National Key R&D Program of China (Grant No. 2017YFA0303200), and by NSFC under Grants No. 11574217 and No. 60825402. H.Z. acknowledges support from Science and Technology Commission of Shanghai Municipality (Grants No. 16DZ2260200). T.A.S. acknowledges startup funds from UMass Amherst.
9:00AM F43.00004: Viscous Topological Electromagnetic Phases of Matter* ZUBIN JACOB (Presenter), Purdue Univ — We present the fundamental model of a topological electromagnetic phase of matter: viscous Maxwell-Chern-Simons theory. We solve both continuum and lattice regularized systems to demonstrate that this is the minimal (exactly solvable) gauge theory with a nontrivial photonic Chern number for electromagnetic waves coupled to matter $C \neq 0$. Physically, our predicted electromagnetic phases are connected to a dynamical photonic mass in the integer quantum Hall fluid. This arises from viscous (nonlocal) Hall conductivity and we identify the nonlocal Chern-Simons coupling with the Hall viscosity. The electromagnetic phase is topologically nontrivial $C \neq 0$ leading to unidirectional transverse electromagnetic edge waves when the Hall viscosity inhibits the total bulk Hall response. Our work bridges the gap between electromagnetic and condensed matter topological physics while also demonstrating the central role of spin-1 quantization in nontrivial photonic phases.

*DARPA Nascent Light-Matter Interactions Program

9:12AM F43.00005: Imaging impurities at quantum Hall edges in graphene: Dissipation rings induced by forward scattering GU ZHANG (Presenter), IGOR GORYNI, ALEXANDER MIRLIN, Karlsruhe Institute of Technology — Motivated by the recent experiment by Marguerite et al. on imaging in graphene samples, we investigate theoretically the dissipation induced by resonant impurities in the quantum Hall regime. Briefly, the impurity induced forward scattering of quantum Hall particles leads to an enhanced phonon emission, which reaches its maximum when the impurity state is fine tuned to its resonance by an applied tip voltage. Our analysis of the effect of a tip potential on the dissipation thus reveals peculiar thermal rings near the impurity, in consistency with experimental observations. This thermal ring behavior, while appearing similar as that in two dimensional materials, turns out to be physically novel and contains features that are unique in quantum Hall systems.

9:24AM F43.00006: Repulsive Casimir force in time-reversal symmetry broken media* ZHOU LI (Presenter), ZUBIN JACOB, Purdue Univ — In quantum field theory, a vacuum is not empty but full of fluctuating electromagnetic waves. If two dielectric mirrors (silicon plates) are placed facing each other in vacuum, it is well known that there exists an attractive Casimir force between them. When one of the silicon plates is replaced by a medium with time-reversal symmetry breaking (usually achieved by an external magnetic field), we show that the Casimir force can become repulsive. This opens the possibility of controlling the quantum vacuum with non-reciprocal media.

*DARPA NLM
9:36AM F43.00007: Supersymmetry approach to interacting disordered systems: the SYK model
TIGRAN SEDRAKYAN (Presenter), Univ of Mass - Amherst, KONSTANTIN EFETOV, Theoretical Physics, Ruhr-University, Bochum, Germany — In this talk, we propose a new, supersymmetric sigma-model representation for interacting disordered fermion systems. To derive it, we decouple the interaction Hamiltonian using the conventional Hubbard-Stratonovich approach. Then we notice that the Hubbard-Stratonovich field can, in some situations, be gauged out from the denominator. This enables one to supersymmetrize the interacting theory. The new formalism is tested by calculating the fermion Green's function in the SYK model at large times and is argued to be effective for other interacting models with the disorder.

9:48AM F43.00008: Spin and charge correlations across the metal-to-insulator crossover in the half-filled 2d Hubbard model*
AARAM J. KIM, FEDOR SIMKOVIC, EVGENY KOZIK (Presenter), King's College London — The 2d Hubbard model with nearest-neighbour hopping on the square lattice and an average of one electron per site is known to undergo an extended crossover from metallic to insulating behavior driven by proliferating antiferromagnetic correlations. We study signatures of this crossover in spin and charge correlation functions and present results obtained with controlled accuracy using diagrammatic Monte Carlo in the range of parameters amenable to experimental verification with ultracold atoms in optical lattices. The qualitative changes in charge and spin correlations associated with the crossover are observed at well-separated temperature scales, which encase the intermediary regime of non-Fermi-liquid character, where local magnetic moments are formed and non-local fluctuations in both channels are essential.

*EPSRC grant EP/P003052/1
Simons Foundation: Simons Collaboration on the Many-Electron Problem

10:00AM F43.00009: Equation of state and entropy of the doped 2d Hubbard Model*
CONNOR LENIHAN (Presenter), AARAM J. KIM, EVGENY KOZIK, FEDOR SIMKOVIC, Kings Coll — We study thermodynamic properties of the doped Hubbard model with nearest-neighbour hopping on the square lattice by Diagrammatic Monte Carlo and obtain results with controlled error bars in the thermodynamic limit. The behaviour of entropy reveals signatures of the insulating regime developing near half-filling at larger interactions: a maximum in the entropy as a function of density appears as the coupling strength is increased, along with an inflection point near half-filling evidencing a metal to insulator crossover. Cold atom simulations of the Hubbard model which prepare the sample adiabatically will find our data useful for thermometry.

*EPSRC grant EP/P003052/1,
Simons Foundation: Simons Collaboration on the Many-Electron Problem
10:12AM F43.00010: Pseudogap effects in the unitary Fermi gas and in strongly interacting 2D Fermi gases*  SCOTT JENSEN (Presenter), YORAM ALHASSID, Yale University, CHRISTOPHER GILBRETH, Central Washington University — Understanding of the unitary Fermi gas of infinite scattering length presents a major challenge owing to the presence of strong correlations. In particular, the existence and extent of a pseudogap regime, in which pairing correlations persist above the superfluid critical temperature, has been extensively debated in the literature. We address the pseudogap question using auxiliary-field quantum Monte Carlo methods on the lattice, optimized to enable large lattice calculations of thermodynamic observables. In particular, we calculate a model-independent energy-staggering pairing gap, which avoids an ill-posed numerical analytic continuation. We extrapolate to the continuum limit, thereby removing finite effective range effects. We use similar methods to study pseudogap effects in interacting 2D Fermi gases along the Bardeen-Cooper-Schrieffer (BCS) to Bose-Einstein condensation (BEC) crossover. Our results provide a benchmark for experiments and other strong coupling methods.

*This work was supported in part by the U.S. DOE grant Nos. DE-SC0019521, DE-FG02-91ER40608, and DE-FG02-00ER41132.

10:24AM F43.00011: Implicit renormalization approach to the problem of Cooper instability*  ANDREY CHUBUKOV, Physics, University of Minnesota, NIKOLAI PROKOF'EV (Presenter), BORIS SVISTUNOV, Univ of Mass - Amherst — In the vast majority of cases, superconducting transition takes place at exponentially low temperature $T_c$ out of the Fermi liquid regime. We discuss the problem of determining $T_c$ from known system properties at temperatures $T \gg T_c$, and stress that this cannot be done reliably by following the standard protocol of solving for the largest eigenvalue of the original gap-function equation. However, within the implicit renormalization approach, the gap-function equation can be used to formulate an alternative eigenvalue problem, solving which leads to an accurate prediction for both $T_c$ and the gap function immediately below $T_c$. With the diagrammatic Monte Carlo techniques, this eigenvalue problem can be solved without invoking the matrix inversion or even explicitly calculating the four-point vertex function. [Phys. Rev. B 100, 064513 (2019)]

*The work by AVC was supported by the Office of Basic Energy Sciences U. S. Department of Energy under award DE-SC0014402.
The work by NP and BS was supported by the Simons Collaboration on the Many Electron Problem, the National Science Foundation under grant DMR-1720465, and the MURI Program “Advanced quantum materials -- a new frontier for ultracold atoms” from AFOSR.
10:36AM F43.00012: Photoinduced superconducting-like properties: \( \eta \)-pairing and charge stiffness in optically driven Mott-Hubbard systems*  TATSUYA KANEKO (Presenter), Department of Physics, Columbia University, SEIJI YUNOKI, RIKEN, ANDREW MILLIS, Department of Physics, Columbia University, Center for Computational Quantum Physics, Flatiron Institute — We theoretically investigate the electron-electron (superconducting) pairing correlations and charge stiffness in the one-dimensional Hubbard model subjected to a pump electric field. By employing unbiased numerical methods, we show that irradiation of the Mott insulating state of the Hubbard model induces strong pair density-wave-like correlations. The pair density-wave correlations induced here are due to \( \eta \)-pairing states, which are preferentially generated by photoexcitation and possess staggered off-diagonal long-range correlations in the excited states of the Hubbard model. We show that the optically induced \( \eta \)-pairing states give rise to the nonzero charge stiffness, in contrast to the Mott insulating state, where the charge stiffness vanishes. We also discuss the system size dependence associated with the \( \eta \)-pairing state and show that the pairing correlations decay very slowly with system size.

*This work is supported by Grants-in-Aid for Scientific Research from JSPS (Projects No. JP18K13509 and No. JP18H01183) and the Basic Energy Sciences program of the US Department of Energy under grant DE-SC0018218. T.K. was supported by the JSPS Overseas Research Fellowship.

10:48AM F43.00013: Pairing tendencies in two-orbital Hubbard models with reduced sign problem  EDWIN HUANG (Presenter), University of Illinois at Urbana-Champaign, ABOLHASSAN VAEZI, Stanford University and Sharif University of Technology — How unconventional superconductivity arises from strong repulsive interactions is a central question in the study of high-temperature superconductivity. Here we study two-orbital Hubbard models with orbital-dependent interaction strength by large-scale Determinantal Quantum Monte Carlo (DQMC) simulations. When one orbital is strongly interacting and the other is weakly or non-interacting, the fermion sign problem is significantly reduced. Temperatures more than two orders of magnitude below the Fermi energy are accessible by DQMC. We present results for the superfluid stiffness and pairfield susceptibilities of such models and comment on their relevance to unconventional superconductors, including the recently discovered superconducting nickelates.

Tuesday, March 3, 2020 8:00 AM - 10:36 AM

Session F44 DCOMP: Van Der Waals Interactions in Molecules, Materials, and Complex Environments I  704 - Noa Marom, Carnegie Mellon Univ - Tag(s): Focus
8:00AM F44.00001: Quantum-mechanical van der Waals Interactions from Atoms to Asteroids [invited] ALEXANDRE TKATCHENKO (Presenter), University of Luxembourg — Noncovalent van der Waals (vdW) interactions arise from quantum-mechanical electronic and atomic fluctuations and they are ubiquitous in essentially all molecules and materials [RMP 88, 045003; Chem. Rev. 117, 4714; Science 351, 1171]. Intergrain vdW interactions have even been hypothesized to explain cohesion in kilometer-sized rubble pile asteroids in space [Nature 512, 174]. I will review the substantial progress in our understanding of everpresent quantum vdW forces at the atomic, nano, and mesoscopic scales achieved during the last two decades. Then I will turn to big gaps in our knowledge where intensive research is required, including (i) the unification of vdW methods with semilocal density functionals, (ii) the scaling of vdW forces with topology, dimensionality, size, and electronic properties of materials, (iii) the interplay between atomic vibrations and electronic fluctuations in the vdW forces, (iv) the delicate transition between vdW and Casimir physics in complex systems.

8:36AM F44.00002: Dispersion-corrected MP2 for improved descriptions of inter- and intramolecular interactions in organic molecular crystals* GREGORY BERAN (Presenter), University of California, Riverside — Reliably modeling polymorphic molecular crystals requires a careful balance between intra- and intermolecular interactions. Density-functional theory models have made tremendous progress in modeling such interactions, but a number of failures for conformational polymorphs and other systems can be found in the literature. A dispersion-corrected MP2 model, MP2D, will be presented which provides more accurate descriptions of non-covalent interactions in these challenging polymorphic crystals. The MP2D dispersion correction is expressed in terms of atom-centered dispersion coefficients which are computed via Grimme's D3 scheme. This approach has the benefits that the dispersion correction can be computed for any organic system with negligible computational cost, it can be applied to both intra- and intermolecular interactions, and analytical gradients can be implemented trivially. The performance of MP2D for both benchmark data sets and in challenging polymorphic molecular crystals will be presented.

*Funding for this research from the National Science Foundation (CHE-1665212) and XSEDE supercomputer time (TG-CHE110064) are gratefully acknowledged.
8:48AM F44.00003: Van der Waals Attraction and Pauli Repulsion: Learning New Tricks from an Old Dog
ORNELLA VACCARELLI (Presenter), DMITRY FEDOROV, ALEXANDRE TKATCHENKO, University of Luxembourg Limpertsberg — The structure and stability of molecular systems bonded by van der Waals (vdW) interactions are governed by the interplay between dispersion attraction and Pauli repulsion [Hermann et al., Chem. Rev. 117, 4714 (2017)]. Arising due to different physical origins, these forces do not seem to have a simple connection. Here, we present a coarse-grained approach for evaluating the exchange energy based on the multipole expansion of the Coulomb interaction. This allows us to reveal an unexpected compensation between attractive dispersion and repulsive exchange forces for closed-shell dimers at equilibrium distance, valid for each term of the multipole expansion. This effect explains the surprisingly simple relationship between the vdW radius and atomic polarizabilities discovered recently [Fedorov et al., PRL 121, 183401 (2018)]. The obtained recipe to build coarse-grained models for the exchange-repulsive forces in vdW-bonded systems could be used to develop next-generation quantum force fields. Therefore, our findings hint on a hidden symmetry between exchange and correlation interactions and suggest a surprising connection between electronic and geometric properties of atoms.

9:00AM F44.00004: Characterization of van der Waals Interactions with Energy Decomposition Analysis*
COLIN EGAN (Presenter), FRANCESCO PAESANI, CHINGLIN CHAN, JOSHUA FIGUEROA, Chemistry, UC San Diego — Van der Waals (vdW) interactions are ubiquitous in nature, and represent important contributions to the structure, stability, and function of many chemical systems. The absolutely localized molecular orbital energy decomposition analysis method (ALMO-EDA) allows for the characterization and quantification of intermolecular interactions such as London dispersion, the predominant attractive vdW component which is due to correlated fluctuations of the electron densities between molecules, and Pauli repulsion, the predominant repulsive vdW component which is a consequence of the antisymmetry of fermionic wave functions. Here we discuss our work studying vdW interactions calculated with ALMO-EDA in small and large molecular systems, and our findings regarding the role of nonlocal terms in approximate exchange-correlation density functionals in predicting vdW interaction energies, as well as many-body cooperativity in vdW interactions.


*This work was supported by NSF grant CHE-1453204.
9:12AM F44.00005: Introducing vdW-DF3 — an accurate van der Waals Density Functional*
DEBAJIT CHAKRABORTY (Presenter), Department of Physics, Wake Forest Univ, KRISTIAN BERLAND, Centre for Material Sciences and Nanotechnology, University of Oslo, TIMO THONHAUSER, Department of Physics, Wake Forest Univ — Recently, we identified the shape of the switching function in the original van der Waals density functional vdW-DF as the key to control the relative contributions of dispersion interactions at different separations (PRB 99, 195418, 2019). Building on this development, we introduce a reformulation that results in significantly higher accuracy for several different classes of systems, in particular for separations beyond the binding distance. This is achieved through tuning the switching function (and thus the non-local correlation) as well as the (semi)local exchange to a set of molecular dimers. Our new formulation provides better binding energies at the equilibrium distance and binding curves of molecular dimers, more accurate interlayer binding energies and lattice constants for layered systems, and improved binding energies for adsorption systems such as small-molecule-adsorption in MOFs and benzene on coinage metals.

*This work was funded by NSF grant No. DMR-1712425 and the Norwegian Research Council, project No. 250346.

9:24AM F44.00006: Experimental determination of van der Waals forces between two-dimensional materials in air and water [Invited]  
PAVLO GORDIICHUK (Presenter), Department of Chemical Engineering, Massachusetts Institute of Technology MIT — Two-dimensional (2D) materials have rather diverse properties and are therefore of high interest for applications in material science, physics, chemistry, and biology. Since many of these applications rely on interfacial stacking, a fundamental understanding of the interactions between 2D materials is of paramount importance. In this work, we describe a strategy which enables rapid and high-throughput determination of the forces between 2D materials (both in air and in liquids) using atomic force spectroscopy. While our experiments demonstrate strong adhesive forces between two graphene sheets with binding energies close to theoretical values, the scaling of the van der Waals (vdW) force with the separation distance differs quite substantially from theoretical predictions. In addition, our experiments in purified water demonstrate that the water confined between two hydrophobic surfaces leads to repulsive interactions, with increasing ionic strength reverting this behavior. These experiments challenge our current understanding of the vdW force and provide much needed experimental benchmarks for the further development of theoretical vdW methodologies.
**10:00AM F44.00007: Influence of Pore Size on the van der Waals Interaction in Two-Dimensional Molecules and Materials**

YAN YANG (Presenter), KA UN LAO, ROBERT DISTASIO, Cornell University — Despite the importance of porous two-dimensional (2D) molecules and materials in advanced technological applications, the question of how the void space in these systems affects the van der Waals (vdW) scaling landscape has been largely unanswered. In this work [1], we present a series of analytical and numerical models demonstrating that the mere presence of a pore leads to markedly different vdW scaling across non-asymptotic distances, with certain relative pore sizes yielding effective power laws ranging from simple monotonic decay to the formation of minima, extended plateaus, and even maxima. These models are in remarkable agreement with first-principles approaches for the 2D building blocks of covalent organic frameworks (COFs), and reveal that COF macrocycle dimers and periodic bilayers exhibit unique vdW scaling behavior that is quite distinct from their nonporous analogs. These findings extend across a range of distances relevant to the nanoscale, and represent an unexplored avenue towards governing the self-assembly of complex nanostructures from porous 2D molecules and materials.


*NSF MRSEC program (Grant No. DMR-1719875)*

**10:12AM F44.00008: Ultra Long-Range Interactions in the Delamination of Atomically-Thin Layers from Substrates**

PAUL HAUSEUX (Presenter), STÉPHANE BORDAS, ALEXANDRE TKATCHENKO, University of Luxembourg — Anomalous proximity effects have been experimentally observed in systems ranging from proteins, bacteria, and gecko feet suspended over semiconductor surfaces to interfaces between graphene and different substrate materials (Si, SiO2, Cu). In the latter case, long-range forces are evidenced by measurements of a non-vanishing stress that extends up to micrometer separations between graphene and the substrate. State-of-the-art models to describe adhesive properties are unable to explain these experimental observations, instead underestimating the measured distance range by 2-3 orders of magnitude. Here we develop an analytical and numerical variational approach that combines continuum mechanics and elasticity with quantum many-body treatment of van der Waals dispersion interactions between two extended objects. A full relaxation of the coupled adsorbate/substrate geometry as a function of separation leads us to conclude that wavelike atomic deformation is responsible for the observed ultra long-range stress in delamination of graphene from various substrates. Remarkably, the observed long-range proximity effect seems to be a general phenomenon for thin membranes and its correct theoretical description requires a direct coupling between quantum and continuum mechanics.
Recent atomic force microscopy experiments [ACS Nano 2014, 8, 12410–12417] conducted on graphene (G)-coated SiO$_2$ demonstrated that monolayer G can effectively screen dispersion van der Waals (vdW) interactions deriving from the underlying substrate. This G vdW opacity has far reaching implications, encompassing stabilization of multilayer heterostructures, micromechanical phenomena and heterogeneous catalysis. By quantum many-body analysis and ab-initio Density Functional Theory, here we provide theoretical rationalization of the observed G vdW screening on weakly interacting substrates: despite single atom thickness, the strong non-locality of G density response ensures large compensation between standard attractive vdW terms and many-body repulsive contributions, enabling effective vdW opacity over a broad range of distances. By virtue of combined theoretical/experimental validation, G hence emerges as a promising ultrathin shield for modulation and switching of vdW interactions and electrostatic fields at interfaces and complex nanoscale devices.

*We acknowledge financial support from Cassa di Risparmio di Padova e Rovigo (Cariparo) grant EngvdW. Computational resources were granted by CINECA

Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F45 DCOMP DCP: Modeling the electrochemical interface and aqueous solutions I 706 - Alexandre Rocha, Universidade Estadual Paulista - Tag(s): Focus
Addressing electrified water-metal interfaces with Non-Equilibrium Green's Functions* [Invited]  
PABLO ORDEJON (Presenter), Theory and Simulation, Catalan Institute of Nanoscience and Nanotechnology — The TranSIESTA method and code [1,2] were developed within the SIESTA project [3] to study problems involving steady-state non-equilibrium problems in nanoscale costrictions, where an external electric bias is applied between the two sides of the constriction, establishing a steady electric current. Non-equilibrium Green's Functions are used there to solve the problema, as they can deal with open, non periodic systems (leads plus nanoconstriction) driven out of equilibrium (external applied bias). This machinery can be also used to study electrified solid/liquid interfaces [4], where an external bias is applied to the solid electrode. Here, one is not concerned with the quantum electronic transport, but with the effect of the external bias on the properties and the chemical reactions induced at the metal/liquid interface. I will show examples of application of this idea, as a proof of concept for future realistic, atomistic first-principles simulations of electrochemical processes.

References:

*The author acknowledges collaborations with L. Medondjio, Z. Zanolli and M. Pruneda, members of the Theory and Simulation group at ICN2, and M.V. Fernández-Serra (Stony Brook) and Nick Papior (DTU). This work was supported by Spanish MICIU, AEI and EU FEDER (Grant No. PGC2018-096955-B-C4). ICN2 was supported by the Spanish MICIU and AEI Severo Ochoa Centers of Excellence Program (Grant No. SEV-2017-0706), and by Generalitat de Catalunya (CERCA Programme).
8:36AM F45.00002: First principles simulations of electrified silicon/water interfaces

ZIFAN YE (Presenter), BOZHI TIAN, GIULIA GALLI, University of Chicago — Si-based materials have been used in a myriad of devices, including light-activated systems such as cathodes in photoelectrochemical cells and p-i-n junctions in optoelectronic biomodulators. In both cases, Si surfaces are in contact with water, and the interface is under bias (e.g. under the effect of an electric field). Here we report a study of electrified Si/water interfaces aimed at understanding charge transfer mechanisms between the solid and the liquid, and their influence in determining the performance of optoelectronic devices. In particular, we carried out ab-initio molecular dynamics simulations of the hydrogenated Si(100)/water interface using the Qbox code (http://qboxcode.org), and we investigated the effect of an applied electric field on the band offsets at the interface. We compared our results with patch clamp measurements and we further investigated the modification of the structural properties of water at the interface, induced by an applied bias.

*This work was supported as part of the Advanced Materials for Energy-Water Systems (AMEWS) Center, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences.

8:48AM F45.00003: Ion Pairing in Liquid Water: An Ab Initio Study

ALEC WILLS (Presenter), MARIVI FERNANDEZ SERRA, Physics & Astronomy, Stony Brook University — Potentials of mean force are widely used to study solvation characteristics as a function of a particular reaction coordinate of interest. In particular, ion-pair association in water is of great importance to many scientific and industrial applications, but is not widely understood. Here we present a detailed study of NaCl solvation properties in the dilute limit. We examine in detail the sources of discrepancies between simulation results, with the objective to separate approximation and statistical errors from physical interpretations. It is found that the choice of water model and simulation time step has a notable effect on the solvation state stability. Moreover, solution density also has a large effect on energetically favorable configurations. We show how the underlying description of liquid water has important consequences on the inter-ionic potential of mean force, and how the solute ions affect the solution's equilibrium properties. Our results shed light into how ions in water affect its structure and correlate with low density and high density liquid fluctuations.

*This material is based upon work supported by the Department of Energy under award number DE-FG02-09ER16052.
9:00AM F45.00004: Integrating First-Principles Simulations with Electrochemical Experiments: Towards a Realistic Description of Aqueous Interfaces  TUAN ANH PHAM (Presenter), CHENG ZHAN, BRANDON WOOD, TADASHI OGITSU, Lawrence Livermore Natl Lab — Improved understanding of electrochemical interfaces is critical for a wide variety of emerging applications, such as hydrogen production, supercapacitors and water desalination. In this talk, we will discuss how first-principles simulations can be integrated with in-situ experiments to understand physicochemical properties of several representative electrochemical systems. We will present our studies of aqueous solutions at graphitic interfaces, where we show that structure and electrical response of the interfaces is governed by a complex interplay between bias potential, intrinsic electronic properties of the electrode, and specific ion effects-including ion hydration and charge transfer. In addition, we will discuss how a combination of first-principles molecular dynamics simulations, many-body perturbation theory, and X-ray photoelectron spectroscopy can provide insights into the relationship between interfacial structure, electronic properties of semiconductors and their reactivity in aqueous solutions.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344, and is supported by the U.S. DOE, Office of Energy Efficiency and Renewable Energy, Fuel Cell Technologies Office via HydroGEN consortium

9:12AM F45.00005: Stability and reactivity at solid/liquid interfaces studied by ab initio calculations [Invited]  MIRA TODOROVA (Presenter), SU-HYUN YOO, SUDARSAN SURENDRALAL, JOERG NEUGEBAUER, Computational Materials Design, Max-Planck-Institut fuer Eisenforschung — Processes at solid-liquid interfaces are at the heart of many present day technological challenges related to the improvement of battery materials, electro-catalysis, fuel cells, corrosion and others. Obtaining the microscopic information needed to describe and quantify the underlying fundamental mechanisms is equally challenging to experiment and theory. Density functional theory (DFT) calculations are able to resolve processes at the microscopic scale. However, the modelling of electrochemical systems is particularly challenging. The main reason is the presence of different classes of materials and phenomena such as metal electrodes, liquid water, huge electric fields within the same system.

We discuss how by using DFT calculations for polar ZnO(0001) surfaces Pourbaix diagrams can be constructed. These diagrams provide direct insight into the role the aqueous electrolyte plays in shaping surfaces and the high selectivity of solvation effects [Phys. Rev. Lett. 120, 066101 (2018)]. Going beyond the thermodynamic description, we utilize our novel potentiostat design to study reactions at electrochemical solid/liquid interfaces under controlled bias [Phys. Rev. Lett. 120, 246801 (2018)]. Focusing on one of the most corrosive system under wet corrosion, the new approach is shown to solve a problem that puzzled corrosion scientists for more than 150-years: what is the underlying mechanism of the experimentally observed link between H-evolution under anodic conditions and Mg dissolution.
9:48AM F45.00006: First-principles study of the hydrogen-bonding network in water at the biased electrode interface  JUHO LEE (Presenter), YONG-HOON KIM, Korea Adv Inst of Sci & Tech —
A crucial step for the development of next-generation electrochemical devices will be the understanding of the atomic and electronic structures of interfacial waters next to biased electrode surfaces. In this presentation, carrying out first-principles non-equilibrium electronic structure calculation within the multi-space constrained-search density functional theory (MS-DFT) formalism we have recently developed, we study the bias-dependent structural and electronic properties of the hydrogen-bonding network of water molecules at the gold electrode interface. Benchmarking the non-equilibrium force profile of a single water molecule next to the gold electrode obtained from non-equilibrium Green's function (NEGF) calculations, we confirm the practical equivalence between MS-DFT and DFT-NEGF. We also report the advantages of MS-DFT in view of electrochemical device simulations by providing (1) well-defined binding energies and (2) the electrochemical potential profiles. Analyzing the spatial profiles of the electrochemical potentials or quasi-Fermi levels at the gold-water interface at varying bias voltages, we extract several important insights into the nature of hydrogen bond network of liquid water at the biased electrochemical interfaces.

10:00AM F45.00007: Voltage-Dependent Cluster Expansions for Modeling Catalytic Electrochemical Interfaces in Solution Environments*  JAMES GOFF (Presenter), ISMAILA DABO, SUSAN BUTHAINA SINNOTT, Pennsylvania State University — The cluster expansion method provides the framework to represent functions of lattice configurations. We use this method to model energetics of solid-solution interfaces in electrochemical systems. Semi-local density functional theory calculations with implicit solvation are used to obtain effective cluster interactions that include local relaxations and the effects of the solvent. These calculations, in conjunction with electrochemical double layer models, provide the framework for voltage-dependent cluster expansions in a model electrochemical environment. We use these voltage-dependent cluster expansion to model faradaic charging at electrode-electrolyte interfaces, equilibrium configurations of surface alloys, and surface promotion in near-surface alloys. Preliminary voltage-dependent cluster expansion models of skin alloys suggest that amount of catalytically active sites highly sensitive to the applied potential.

*We acknowledge financial support from the U.S. Department of Energy, Office of Science, Basic Energy Sciences, CPIMS Program, under Award No. DE-SC0018646.
We acknowledge support and training provided by the Computational Materials Education and Training (CoMET) NSF Research Traineeship (grant number DGE-1449785).
Multiscale modeling of solvation effects in the Oxygen Evolution Reaction on TiO$_2$  LUCA BURSI (Presenter), NAIWRIT KARMODAK, OLIVIERO ANDREUSSI,
Department of Physics, University of North Texas — Development of sustainable energy generation and storage technologies able to satisfy the needs of modern society represents a major challenge for scientific research. Innovation here essentially rely on hydrogen (H) /oxygen (O) evolution reactions (ER) and /or oxidation of chemical fuels. OER generally represents the bottleneck of (photo)catalytic water splitting, as it requires high overpotentials. This has motivated an impressive search for sustainable high-performance electrocatalysts for OER, which identified TiO$_2$. Recently the microscopic mechanism of OER at TiO$_2$–water interface has been deeply studied. In particular, first principles simulations of rutile TiO$_2$ in explicit water [J. Phys. Chem. C, 123, 18567 (2019)] found the solvent to affect electrostatically the energetics at the interface, rather than to modify the H bond network. Such results pave the way for the use of implicit and hybrid solvation techniques in ab initio simulations of this system to further elucidate the effect of the solvent on OER, and specifically on its rate limiting step. To this aim, we exploit state-of-the-art implicit solvation schemes for condensed matter simulations, as implemented in the Environ plugin[http://www.quantum-environ.org] for Quantum ESPRESSO[http://www.quantum-espresso.org].

Ionic Structure in Dense Electrolytes Confined by Interfaces†  NASIM ANOUSHEH (Presenter), VIKRAM JADHAO, Indiana Univ - Bloomington — Recent surface force measurements have shown that the effective force between mica surfaces does not decay as sharply as predicted by mean-field models when the concentration of the confined electrolytes is high (around 2 M for NaCl). Motivated by these experiments, we use molecular dynamics simulations to extract the ionic structure in aqueous electrolytes confined by two interfaces. Ionic density profiles and contact-region densities are extracted for electrolytes confined between uncharged, charged, and polarizable interfaces at different concentrations with implicit-solvent models. Simulation results show that the net charge density in the contact region near charged surfaces exhibits a distinct trend with increase in interface separation for highly concentrated electrolyte systems (around 2 M for model NaCl) compared to electrolytes at low salt concentration. This behavior is further probed by varying ion sizes, interface charge density, ion valency, and interface polarizability, as well as by computing ion-ion pair correlation functions near the interface. Effects of explicit solvent molecules on the observed ionic structure are also discussed.

†This work is supported by the NSF through Award 1720625.
The Electrokinetic Transport of Multivalent Electrolytes: The Effect of Charge Inversion

ANDRES ROJANO (Presenter), Department of Chemical Engineering, Universidad de Concepcion, JENS HONORE WALTHER, Department of Mechanical Engineering, Technical University of Denmark, HARVEY A ZAMBRANO, Department of Mechanical Engineering, Universidad Tecnica Federico Santa Maria — Devices integrated by nanoconduits hold great potential for clinical and biochemical analysis due to amplified sensibility, faster response and increased portability. In nanoconduits, wherein the electrical double layer may occupy a considerable part of the channel, the hydrodynamics of multivalent electrolytes is highly influenced by interfacial electrokinetic phenomena, such as charge inversion (CI). We conduct atomistic simulations of an electrolyte solution which consists of water as solvent, chlorine as co-ion and different counter-ions, i.e., sodium, magnesium and aluminum. We model Electroosmotic (EOF), Poiseuille (PF) and Couette (CF) flow in silica nanochannels to probe the relation between CI and transport properties. In EOF, we observe that changes induced by CI in the electrokinetic driving force at the diffuse layer, significantly alter the velocity distributions. Moreover, cases of CF and PF flow show that the position of the shear plane is significantly altered by the presence of CI. We find that the nanoconfined electrolytes can be modeled as two immiscible fluids with different transport properties with the shear plane as dividing surface.

*We thank funding from CONICYT scholarship 21181167, computational support from MEK DTU.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F46 GMAG DMP: Pyrochlores I 708 - Jinguang Cheng, Chinese Academy of Sciences - Tag(s): Focus
8:00AM F46.00001: Spherical Neutron Polarimetry and the Phase Diagram of Magnetically Dilute \( \text{Er}_2\text{Ti}_2\text{O}_7 \)

CONNOR BUHARIWALLA (Presenter), Department of Physics & Astronomy, McMaster University, JONATHAN GAUDET, Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University, CISSY SUEN, Department of Physics & Astronomy, McMaster University, NAVID QURESHI, ANNE STUNAULT, Institut Laue-Langevin, TIMOTHY MUNSIE, Department of Physics & Astronomy, McMaster University, HANNA DABKOWSKA, Brockhouse Institute For Materials Research, McMaster University, BRUCE D. GAULIN, Department of Physics & Astronomy, McMaster University —

The ground state of XY pyrochlore antiferromagnet \( \text{Er}_2\text{Ti}_2\text{O}_7 \) has been a rich topic of research due to the selection of a non-coplanar \( k=0 \) magnetically ordered state \( \psi_2 \) through order by disorder. Several proposed mechanisms account for this selection of \( \psi_2 \) over the coplanar \( \psi_3 \), the alternate basis state of the \( \Gamma_5 \) irreducible representation. Recent theory work has proposed that magnetic dilution that will lead to an instability in the ground state selection, resulting in a \( \psi_3 \) ground state for a dilute \( \text{Er}_2\text{Ti}_2\text{O}_7 \). Through systematic substitution of non-magnetic \( \text{Y}^{3+} \) on the \( \text{Er}^{3+} \) site, we have probed the effect of such dilution with samples of 5%, 10%, and 20% \( \text{Y}^{3+} \). While the magnetic structures of \( \psi_2 \) and \( \psi_3 \) are indistinguishable in an unpolarized neutron scattering measurement, the contrast is clear using spherical neutron polarimetry (SNP). In this talk, I will present the results of our SNP study of these 3 diluted samples, following our previous work using inelastic neutron scattering.

8:12AM F46.00002: Magnetic phase competition in the rare-earth pyrochlore \( \text{Er}_2\text{Sn}_2\text{O}_7 \)*

DANIELLE R YAHNE (Presenter), Department of Physics, Colorado State University, LIURUKARA D SANJEEWA, Materials Science and Technology Division, Oak Ridge National Laboratory, JOSEPH KOLIS, Department of Chemistry, Clemson University, LUDOVIC DC JAUBERT, CRNS, LOMA, University of Bordeaux, DARREN PEREIRA, Department of Physics, University of Waterloo, MATTHEW JOHN ENJALRAN, Department of Physics, Southern Connecticut State University, MICHEL J P GINGRAS, Department of Physics, University of Waterloo, KATE ROSS, Department of Physics, Colorado State University — Rare-earth pyrochlore oxides \( (\text{A}_2\text{B}_2\text{O}_7) \) can host a wealth of exotic phenomena due to geometric- and exchange-frustration. \( \text{Er}_2\text{Sn}_2\text{O}_7 \) is especially interesting in this regard as, based on available estimates of the exchange interactions, it lies near a phase boundary in the anisotropic exchange parameter space, between two antiferromagnetic states: the Palmer-Chalker states (where \( \text{Er}_2\text{Sn}_2\text{O}_7 \) orders) and the \( \Gamma_5 \) states. A natural tool to probe such multi-phase competition is the application of an external magnetic field, but until now the absence of single crystals made such approach difficult to analyze. In this talk, we report specific heat measurements on single crystals of \( \text{Er}_2\text{Sn}_2\text{O}_7 \) under fields applied along the three high symmetry directions, \([111]\), \([110]\), and \([100]\). Each field direction provides a distinct phase diagram, but with the shared feature that one (sometimes even two) reentrant lobe(s) appear above a threshold field of 0.2 T. The nature of this reentrance can be understood semi-quantitatively through classical Monte-Carlo simulations and mean field theory, the details of which will be described in a presentation by D. Pereira.

*DE-SC0020071
Rare-earth pyrochlore magnets are known to exhibit a variety of exotic phenomena. The dipolar XY pyrochlore magnets in particular act as playgrounds for effects like order-by-disorder, multiphase competition, and strong quantum fluctuations. $\text{Er}_2\text{Sn}_2\text{O}_7$, a member of the XY pyrochlore family, has recently been synthesized as a single crystal and studied under a magnetic field. The resulting $(H,T)$ phase diagram reveals multiple reentrant lobes for fields applied in the [100], [110], and [111] directions. In this talk, I will discuss our efforts to understand these reentrant phenomena from the theoretical front, drawing from variational mean-field theory, classical Monte Carlo simulations, and classical spin wave analysis. I will argue that the reentrant lobes are related to a complex multiphase competition, in which the changing ground state degeneracy in a field is associated with the apparition of soft mode excitations. We expect our reasoning to be applicable to other rare-earth pyrochlores and frustrated magnets in general, especially for systems with a discrete ground state degeneracy.
High pressure synthesis and characterization of $R_2Pt_2O_7$ pyrochlores

[Invited] JINGUANG CHENG (Presenter), Institute of Physics, Chinese Academy of Sciences — Rare-earth pyrochlore oxides $R_2B_2O_7$ constitute a versatile material platform to study a wide range of magnetic phenomena including order by disorder, geometric frustration, spin ice, and spin freezing. While being non-magnetic, the B-site cations are thought to be able to influence the magnetic properties of these compound primarily through the chemical pressure, which has been well demonstrated in the comparative studies of $R_2B_2O_7$ (B = Ge, Ti, Sn) through varying the radius of the B-site cation. The high-pressure synthesis of $R_2Ge_2O_7$ with the cubic pyrochlore structure is essential for these studies. Recently, we have further extended our research to the $R_2Pt_2O_7$ system, which can only be stabilized under high-pressure conditions. Unlike the previously studied $R_2B_2O_7$ with the B site occupied by either a 3d transition-metal like Ti or a p-block metal such as Ge and Sn, the Pt$^{4+}$ has spatially more extended 5d orbitals and thus enhanced Pt 5d-O 2p hybridizations that might modify the local anisotropic exchange interactions of R3+ ions. Such an effect beyond the steric effect has not been taken into account in previous studies on the geometrically frustrated magnets. Indeed, we found enhanced magnetic ordering temperature in Gd$_2$Pt$_2$O$_7$ due to presence of extra superexchange pathways through the empty Pt-e$_g$ orbitals [1]. We also revealed distinct influences on the anisotropic exchange interactions in the XY pyrochlores Er$_2$Pt$_2$O$_7$ and Yb$_2$Pt$_2$O$_7$ [2]. In addition, we observed unusual behaviors in the classical spin ice Ho$_2$Pt$_2$O$_7$ [3].

References:

*I am grateful for the close collaborations with Y. Q. Cai, Q. Cui, Y. Wan (IOP CAS), Z. L. Dun, H. D. Zhou (Univ. Tennessee), X. Li, J. S. Zhou (Univ. Texas at Austin), and Y. Uwatoko, T. Shibauchi (Univ. Tokyo). This work is supported by the CAS, NSF, and MOST of China.
**9:12AM F46.00005: Single crystal neutron scattering study of the pyrochlore Yb$_2$Ge$_2$O$_7$*\(^*\)**

COLIN SARKIS (Presenter), Colorado State University, JEFFREY RAU, University of Windsor, DUMINDA SANJEEWA, MATTHEW POWELL, JOSEPH KOLIS, Clemson University, JONATHAN J MARBEY, STEPHEN HILL, Florida State University, JOSE RODRIGUEZ-RIVERA, NIST Center for Neutron Scattering, HARIKRISHNAN S NAIR, University of Texas El Paso, MICHEL J P GINGRAS, University of Waterloo, KATE ROSS, Colorado State University — Rare earth pyrochlore oxides have been found to be hosts for a wide breadth of exotic phenomena based on strong frustration. Previous single crystal studies of Yb$_2$Ti$_2$O$_7$ have established that it forms a ferromagnetic (FM) ground state, but lies near a classical phase boundary between FM and antiferromagnetic (AFM) states. Meanwhile, powder neutron scattering studies of Yb$_2$Ge$_2$O$_7$ show it selects the AFM state. Despite this difference, these Yb pyrochlores share the same unusual spin dynamics in zero field. Further experimental progress on Yb$_2$Ge$_2$O$_7$ has been stymied by a lack of large single crystal samples. We report inelastic neutron scattering measurements on single crystals of Yb$_2$Ge$_2$O$_7$ grown by a hydrothermal method. We have used the field-polarized spin waves to determine the exchange parameters for Yb$_2$Ge$_2$O$_7$. The g-tensor was independently determined from electron paramagnetic resonance on a Lu$_{1.98}$Yb$_{0.02}$Ge$_2$O$_7$ sample in order to enable an unambiguous determination of these parameters. Our analysis and theoretical modeling show that Yb$_2$Ge$_2$O$_7$ lies in extreme proximity to the classical phase boundary between the AFM and FM phase, lending strong support to the notion of phase competition as playing a key role in the Yb pyrochlore family.

*DOE:DE-SC0020071

**9:24AM F46.00006: Orientation Dependence of the Magnetic Phase Diagram of Yb$_2$Ti$_2$O$_7$*\(^*\)**

STEFFEN SÄUBERT (Presenter), Colorado State University, ALLEN SCHEIE, Oak Ridge National Laboratory, CHRISTOPHER DUVINAGE, Technical University of Munich, JONAS KINDERVATER, SHU ZHANG, Johns Hopkins University, HITESH CHANGLANI, Florida State University, GUANGYONG XU, NIST Center for Neutron Research, SEYED KOOHPAYEH, OLEG TCHERNYSHYOV, COLLIN LESLIE BROHOLM, Johns Hopkins University, CHRISTIAN PFLEIDERER, Technical University of Munich — We present the orientation dependence of the magnetic phase diagram of stoichiometric Yb$_2$Ti$_2$O$_7$ using four experimental probes: magnetization, heat capacity, susceptibility, and neutron scattering. The magnetic phase diagram for fields along $\langle 110 \rangle$ shows dramatic reentrant character (similar to fields along $\langle 111 \rangle$), whereas for fields along $\langle 100 \rangle$, the upper phase boundary collapses and the system enters a field polarized state for small applied fields. By comparing this data to theoretical models, we show that Yb$_2$Ti$_2$O$_7$ is a cubic ferromagnet that is qualitatively described by Landau theory, but a comparison of upper critical fields show that the system cannot be described only by classical mean-field considerations, more that it is subject to collective or quantum effects.

*DFG (107745057 and 390814868), ERC (291079 and 788031), BMBF (05K16WO6), U.S. DOE (DE-SC0019331), Gordon and Betty Moore foundation (GBMF4532 and GBMF5305), ICAM QuantEmX, NSF-DMR (0821005 and 1508249)
9:36AM F46.00007: Exploring the influence of disorder on magnetic moment fragmentation*
ELI ZOGHLIN (Presenter), JULIAN L SCHMEHR, STEPHEN WILSON, University of California, Santa Barbara — Recent neutron scattering measurements demonstrating concurrent all-in-all-out antiferromagnetic order and pinch-point diffuse scattering in the pyrochlore Nd2Zr2O7 provide compelling evidence for the phenomenon of magnetic moment fragmentation\(^1\). However, the influence of chemical and crystallographic disorder native to the pyrochlore lattice on the formation of this underlying state remains poorly understood. Here we present an experimental exploration of the role of native disorder on the features associated with spin fragmentation in Nd2Zr2O7. Neutron scattering and thermodynamic measurements of crystals with varying defect concentrations, examined by electron microprobe analysis, are studied to resolve the impact of disorder on the ground state of this material.


*We gratefully acknowledge funding from the W.M. Keck Foundation.

9:48AM F46.00008: Magnetization plateaus of the quantum pyrochlore Heisenberg antiferromagnet*
SANTANU PAL (Presenter), Department of Physics, Indian Inst of Tech-Bombay, Powai, Maharashtra, India, SIDDHARTHA LAL, Department of Physical Sciences, IISER Kolkata, Mohanpur, India — We predict magnetization plateaus ground states for S = 1/2 Heisenberg antiferromagnets on pyrochlore lattices by formulating arguments based on gauge and spin-parity transformations. We derive a twist operator appropriate to the pyrochlore lattice, and show that it is equivalent to a large gauge transformation. Invariance under this large gauge transformation indicates the sensitivity of the ground state to changes in boundary conditions. This leads to the formulation of an Oshikawa-Yamanaka-Affleck–like criterion at finite external magnetic field, enabling the prediction of plateaus in the magnetization versus field diagram. We also develop an analysis based on the spin-parity operator, leading to a condition from which identical predictions are obtained of magnetization plateaus ground states. Both analyses are based on the non-local nature of the transformations, and rely only on the symmetries of the Hamiltonian. This suggests that the plateaus ground states can possess properties arising from non-local entanglement between the spins.


*We acknowledge CSIR, Govt. of India and IISER Kolkata for financial support.
Magnetism of classical pyrochlore antiferromagnet Na$_3$Mn(CO$_3$)$_2$Cl*

KAZUHIRO NAWA (Presenter), DAISUKE OKUYAMA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, MAXIM AVDEEV, Australian Nuclear Science and Technology Organisation, HIROYUKI NOJIRI, Institute for Materials Research, Tohoku University, MASAHIRO YOSHIDA, DAICHI UETA, HIDEKI YOSHIZAWA, Institute for Solid State Physics, The University of Tokyo, TAKU SATO, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University — Pyrochlore antiferromagnets have attracted interests in terms of unconventional ground states and spin excitations owing to competing interactions. When its magnetism is dominated by classical spins coupled by Heisenberg interactions, a spin liquid state is expected as its ground state because of infinite degeneracy in the ground state (R. Moessner and J. T. Chalker, Phys. Rev. Lett. 80, 2929 (1998); Phys. Rev. B 58, 12049 (1998)). In this research, we report structural and magnetic properties together with low-temperature neutron diffraction patterns on a new pyrochlore antiferromagnet Na$_3$Mn(CO$_3$)$_2$Cl. The structure of Na$_3$Mn(CO$_3$)$_2$Cl is isotypic with that of the Co-analogue Na$_3$Co(CO$_3$)$_2$Cl, which exhibits all-in-all-out magnetic order below 1.5 K (Z. Fu et al., Phys. Rev. B 87, 214406 (2013)). On the other hand, no magnetic Bragg peak indicating a magnetic order was detected down to 0.05 K in Na$_3$Mn(CO$_3$)$_2$Cl. A high degeneracy near the ground state is suggested by a magnetic entropy estimated from heat capacity experiments and enhancement of diffuse scattering from neutron diffraction experiments.

*This work was supported by a Grant-In-Aid for Scientific Research (No. 17K18744) from MEXT of Japan, and Advanced Material Research Award of Hatano Fundation.

Magnetic properties of distorted pyrochlore lattice Mn$_2$(OD)$_3$X (X = Cl, Br)  
MASATO HAGIHALA (Presenter), KEK, High Energy Accelerator Research Organization, X.G. ZHENG, Saga University, TAKASHI KAMIYAMA, KEK, High Energy Accelerator Research Organization — Atacamite family, of which component is M$_2$(OH)$_3$X (M:3dmetal, X:halogen) forms geometrical frustrated lattice, and behave in an exotic magnetic states; the ground state of clinoatacamite is coexistence of long-range order and strong spin fluctuation[1]. Atacamite(Cu$_2$(OH)$_3$Cl), which is distorted pyrochlore, reported as antiferromagnetic transition at $T_N = 9$ K[2]. Recently, it is reported that atacamite is regarded as $S = 1/2$ sawtooth chains system, and its magnetic order is represented $k = (1/2 \ 0\ 1/2)$ [3,4]. We remark atacamite type compounds Mn$_2$(OH)$_3$X. Both compounds have two successive transitions below $T \sim 3K$ [5]. Our neutron experiment revealed different magnetic orders on these four phases. The ground state of Mn$_2$(OD)$_3$Br is also represented $k = (1/2 \ 0\ 1/2)$, its magnetic structure have two kind of spin configurations on the saw tooth chains. Spin configurations on other three phases are modulated along the $a$ axis. Successive transition and different $k$ vector imply stronger frustration effect than atacamite. [1] X. G. Zheng et al., PRL 95, 057201 (2005). [2] X. G. Zheng et al., PRB 71, 174404 (2005). [3] L. Heinze et al., Physica B 536, 377-378 (2018). [4] L. Heinze et al., arXiv:1904.07820v1. [5] M. Hagihala et al., J. Phys.: Cond. Matt. 19, 145281 (2007).
Magnetometry and transport studies of single crystal pyrochlore iridates*  MATTHEW PEARCE (Presenter), KATHRIN GOETZE, PAUL GODDARD, MARTIN LEES, Department of Physics, University of Warwick, DHARMALINGAM PRABHAKARAN, ANDREW T BOOTHROYD, Department of Physics, University of Oxford, TYCHO SIKKENK, Department of Physics, Utrecht University, ATTILA SZABO, CLAUDIO CASTELNOVO, TCM, University of Cambridge — Magnetic pyrochlore oxides have attracted significant interest due to their geometrically frustrated lattice, which acts to suppress long range magnetic order and leads to a variety of unusual magnetic ground states and exotic excitations.

Some of the most studied pyrochlores are the spin ices $\text{Ho}_2\text{Ti}_2\text{O}_7$ and $\text{Dy}_2\text{Ti}_2\text{O}_7$ – here the rare earth ions are ferromagnetic whilst the Ti is nonmagnetic. Recently, the pyrochlore iridates ($R_2\text{Ir}_2\text{O}_7$, $R =$ rare earth) have risen to prominence. Here, both the rare earth and the Ir are magnetic; the added complexity afforded by the Ir magnetism may be expected to yield a rich variety of physical phenomena. For instance, most of the pyrochlore iridates exhibit a metal to insulator transition which accompanies the ordering of the Ir into an ‘all-in-all-out’ configuration.

Here we report on magnetisation and resistivity measurements on new single crystals of pyrochlore iridates. We present a systematic study of the evolution of these properties with magnetic field, temperature and angle. Supported by Monte Carlo simulations we present our interpretation of the highly anisotropic and hysteretic behaviour observed as well as its wider significance.

*This project has received funding from the European Research Council (grant no. 681260). We also thank the EPSRC.

Magnetisation and monopole density response to applied magnetic fields in rare earth pyrochlore iridates  ATTILA SZABO, TYCHO SIKKENK, CLAUDIO CASTELNOVO (Presenter), Univ of Cambridge, MATTHEW PEARCE, KATHRIN GOETZE, MARTIN LEES, University of Warwick, DHARMALINGAM PRABHAKARAN, ANDREW T BOOTHROYD, University of Oxford, PAUL GODDARD, University of Warwick — We investigate the behaviour of rare earth pyrochlore iridates $\text{Dy}_2\text{Ir}_2\text{O}_7$ and $\text{Ho}_2\text{Ir}_2\text{O}_7$ using dipolar Monte Carlo simulations for the rare earth moments and an effective representation of the Ir moments as local fields [Lefrancois et al, Nat. Comm. 2017]. We study in particular how the magnetisation and defect population respond to externally applied magnetic fields along different crystal directions. We uncover an intriguing interplay between the rare earth moments and the correlations in the underlying Ir moments, and we comment on their possible relevance to experimental results.
Cd$_2$Re$_2$O$_7$ is the first superconductor in pyrochlore oxide family and a prototype compound for spontaneous inversion symmetry breaking with strong spin-orbit coupling. The inversion breaking transition near 200K from centrosymmetric cubic phase to the noncentrosymmetric tetragonal phase. Another structural transition occurs at 120K. However, the distortions are very small and identified controversially in different measurement techniques. Quantum oscillation is very sensitive to the differences of the structures and ideally to study the inversion symmetry breaking from spin splitting Fermi surfaces. In this talk, we will discuss the Fermiology of Cd$_2$Re$_2$O$_7$ by torque magnetometry and compare with the density functional calculations.
In this talk, we will explore the use of permalloy ($\text{Ni}_{80}\text{Fe}_{20}$) thin films in hybrid magnon systems. Permalloy is a classical metallic ferromagnet with well-known magnetic dynamic properties and is easy to grow and integrate into complex devices. In the first part, we demonstrate strong coupling of magnons in a permalloy thin-film device to the microwave photons in a coplanar superconducting resonator\(^6\), via magnetic dipolar interaction. In the second part, we show strong coupling of permalloy magnons to the spatially nonuniform magnon modes of a YIG film via interfacial coupling\(^7\). Besides the interfacial exchange coupling acting as a field-like torque, we also show evidence that spin pumping creates a damping-like coupling torque. This torque leads to an increase in line width for the out-of-phase hybrid mode and a reduction for the in-phase hybrid mode. Our results provide new pathways for implementing on-chip magnonic devices with efficient and coherent information transducers.

*This work was supported by the U.S. DOE, Office of Science, Materials Sciences and Engineering Division and as part of Quantum Materials for Energy Efficient Neuromorphic Computing, an Energy Frontier Research Center funded by the U.S. DOE, Office of Science, as well as AFOSR under grant no. FA9550-19-1-0254.
Strong Interlayer Magnon-Magnon Coupling in Magnetic Hybrid Nanostructures

JILEI CHEN (Presenter), CHUANPU LIU, BeiHang University, TAO LIU, Physics Department, Colorado State University, YANG XIAO, Nanhang University, KE XIA, Beijing Normal University, GERRIT BAUER, Tohoku University, MINGZHONG WU, Physics Department, Colorado State University, HAIMING YU, BeiHang University — Strong couplings between magnons and photons have recently attracted lots of attention due to potential applications in quantum computing by utilizing coherent couplings between spins and superconducting qubits. Here, I will present our recent experimental results on strong interlayer magnon-magnon coupling in an on-chip nanomagnonic device at room temperature [1]. Ferromagnetic nanowire arrays are integrated on a 20-nm-thick yttrium iron garnet (YIG) thin film strip. Large anticrossing gaps up to 1.58 GHz are observed between the ferromagnetic resonance of the nanowires and the in-plane standing spin waves of the YIG film. The coupling strength is tunable by the magnetic configuration, allowing the coherent control of magnonic devices.

Reference:

*We acknowledge the support by NSFC under Grant No. 11674020, No. 61774017, No. 11734004, and No. 21421003, 111 talent program B16001, National Key Research and Development Program of China (Grant No. 2017YFA0303304), U.S. National Science Foundation (EFMA1641989 and DMR-1407962), Japan Society for the Promotion of Science Kakenhi (Japan) Grants-in-Aid for Scientific Research (Grant No. 26103006).
8:48AM F47.00003: Introducing Coherent Time Control to Cavity Magnon Polartion Modes
TIM WOLZ (Presenter), ALEXANDER STEHLI, ANDRE SCHNEIDER, Karlsruhe Institute of Technology, ISABELLA BOVENTER, Institute of Physics, Johannes Gutenberg University Mainz, RAIR MACEDO, James Watt School of Engineering, University of Glasgow, ALEXEY V. USTINOV, Karlsruhe Institute of Technology, MATHIAS KLAUE, Institute of Physics, Johannes Gutenberg University Mainz, MARTIN WEIDES, James Watt School of Engineering, University of Glasgow — By connecting light to magnetism, cavity-magnon-polaritons (CMPs) [1-3] can link quantum computation to spintronics. Consequently, CMP-based information processing devices have thrived over the last years, but have almost exclusively been investigated with single-tone spectroscopy. However, universal computing applications will require a dynamic control of the CMP on demand and within nanoseconds. In this work [4], we perform fast manipulations of the different CMP modes with independent but coherent pulses to the cavity and magnon system. We change the state of the CMP from the energy exchanging beat mode to its normal modes and further demonstrate two fundamental examples of coherent manipulation: First, a dynamic control over the appearance of magnon-Rabi oscillations, i.e., energy exchange, and second, energy extraction by applying an anti-phase drive to the magnon. Our results show a promising approach to control different building blocks for a quantum internet and pave the way for further magnon-based quantum computing research.


9:00AM F47.00004: Nanoscale Detection of Magnon Excitations with Variable Wavevectors Through a Quantum Spin Sensor
ERIC LEE-WONG, University of California, San Diego, RUOLAN XUE, Harvard University, FEIYANG YE, University of California, San Diego, ANDREAS KREISEL, University of Leipzig, TOENO VAN DER SAR, Delft University of Technology, AMIR YACOBY, Harvard University, CHUNHUI DU (Presenter), University of California, San Diego — Control and manipulation of pure spin currents in magnetic insulators has been a central focus of modern spintronic research. Building on the transformative nitrogen vacancy (NV) based quantum sensing platform, we have achieved local detection of a range of spin wave modes in magnetic insulator \( \text{Y}_3\text{Fe}_5\text{O}_{12} \) thin films over a 100-nanometer length scale. Through the multi-magnon scattering process, the excited spin waves generate fluctuating magnetic fields at the NV electron spin resonance frequencies, accelerating the relaxation of the NV spin. By measuring the variation of the emitted photoluminescence of the NV center, the detailed information of the magnon modes can be optically accessed, providing a unique window to reveal the local magnetic properties of the studied materials. Our findings highlight the significant opportunities offered by NV spin quantum sensors in exploring nanoscale spin dynamics of emergent spintronic systems.
9:12AM F47.00005: Spin wave resonance study in a series of etched GaMnAsP films  XINYU LIU (Presenter), Physics, University of Notre Dame, SEUL-KI BAC, SANGHOON LEE, Physics, Korea University, MALGORZATA DOBROWOLSKA, JACEK K. FURDYNA, Physics, University of Notre Dame, HENRYK PUSZKARSKI, PIOTR TOMCZAK, Physics, Adam Mickiewicz University — Although ferromagnetic semiconductor films have already been investigated for the last two decades, some fundamental issues still puzzle the researchers in this field. One of these issues is how the magnetic anisotropy field distributes along the growth direction. In order to resolve this issue in a 108-nm GaMnAsP film, a series of etched samples formed by wet-etching this GaMnAsP film were studied by XRD, SQUID and FMR. The thicknesses of the etched GaMnAsP films were determined by XRD measurements, using the oscillations observed in ω-2θ scans. The XRD peaks from GaMnAsP films are also used to determine the Mn and P contents along the growth direction. Magnetizations of the films are measured by SQUID as a function of field and temperature. FMR measurements were carried out at 4K as function of field orientation, using both out-of-plane and in-plane geometries. A series of spin wave modes are observed when field is applied in the plane of film, as well a critical angle phenomenon is found in specific resonance configurations. The angular dependence of spin wave modes will be analyzed using newly reported spherical surface pinning model in order to map the surface free energy. The results will be summarized as a function of film thickness for all etched samples.

9:24AM F47.00006: Strong angle dependence of auto-oscillating spin wave multi-modes in constricted Py/Pt bilayers  INHEE LEE (Presenter), CHI ZHANG, SIMRANJEET SINGH, BRENDAN MCCULLIAN, P CHRIS HAMMEL, Ohio State Univ - Columbus — Spin-orbit torque driven auto-oscillators (AO) in constricted bilayers can be highly coherent and tunable, even at room temperature. However, the dissipation mechanisms of AO confined by a constriction remain unclear. We have studied the dependence of several AO modes on the angle between the current flow and an in-plane applied magnetic field in a 0.6 μm x 1 μm Py/Pt bilayer. We observe considerable changes in the size, number, and distribution of modes as the angle varies. The spatial profiles of the modes are identified using micromagnetic simulation, and classified into three types: edge, center-like, and their combination. We also characterize the AO modes in terms of resonance frequency, linewidth and power. Beyond a threshold current, the power in the lowest order mode saturates and its linewidth increases. However, this coincides with enhanced excitation of higher order modes such that the power summed over all modes continues to grow with current. We achieve ~ 8 MHz minimum linewidth and ~ 0.5 pW maximum power at 77 K from the lowest order mode at an angle of 65 degree, though below 120 K, the improvement of the mode for the narrower linewidth and the stronger power with decreasing temperature is reduced.
Influence of ferromagnetic films surface properties on spin wave modes

RODRIGO ARIAS (Presenter), IGNACIO ARMIJO, Physics, Universidad de Chile — The frequencies of propagating spin waves in ferromagnetic films may be determined experimentally with some precision, and reflect the surface properties of the films. In particular, if the surface properties break symmetries between both surfaces, there will be frequency non-reciprocity between spin waves that travel in different directions. Furthermore, there is possible shape non-reciprocity of the spin waves even for symmetric films. Thus, in order to relate surface properties to the behavior of spin waves, we study theoretically, within the micro magnetic approximation, spin wave modes under obliquely applied magnetic fields to the film, since in this case the surface properties have a more clear influence in the spin wave properties. For this case the equilibrium magnetization is non-uniform, it deflects close to the surfaces, due to effective surface boundary conditions that model local surface fields. We use the Extinction-Green theorems to determine the spin wave modes, solving numerically differential equations along the transverse direction for the so-called auxiliary functions, and we interpret these numerical results by use of the WKB approximation.

*Fondecyt Project 1170781 (Chile), Basal Program for Centers of Excellence, Grant FB0807 CEDENNA, CONICYT.

Quantitative Study of Spin Wave Chirality in Obliquely Magnetized Magnetic Films

CODY TREVILLIAN (Presenter), VASYL S TYBERKEVYCH, Oakland University — Dipole-dipole interaction in thin magnetic films leads to formation of parity-breaking (i.e., chiral) spin wave (SW) modes, such as, e.g., chiral magnetostatic surface SW (CMSSW) [1] & heterosymmetric SW (HSSW) [2] having a number of unique properties. However, a general theory of the origin of chiral spin wave formation & their chiral properties in obliquely magnetized magnetic films (OMMF) remains absent. Here, we propose a quantitative measure of SW chirality, $C_n = 1 - \left| \langle P \rangle_n \right|$, where $\langle P \rangle_n$ is the expected value of the parity operator for the $n^{th}$ SW mode. Using Kalinikos-Slavin's theory of SW spectrum in OMMF [3], we performed quantitative study of formation of chiral SWs. We show that total parity $\sum_n \langle P \rangle_n$ of all SW modes is approximately conserved, which implies that SW modes acquire chiral properties in pairs through the “parity exchange” mechanism. In particular, we demonstrate formation of strongly chiral modes at odd crossing points of SW spectrum & show that chirality of both CMSSW & HSSW is a result of “parity exchange” between two lowest symmetric & antisymmetric SW modes.

10:00AM F47.00009: Probing phase transition and anisotropy in magnetic insulator based heterostructures employing magnon spin currents  KINGSHUK MALLICK (Presenter), ADITYA A WAGH, Indian Institute of Science - Dept of Physics, ADRIAN IONESCU, CRISPIN H.W. BARNES, Cavendish Laboratory, Physics Department, University of Cambridge, P.S. ANIL KUMAR, Indian Institute of Science - Dept of Physics — Many reports have explored the temperature dependence of Longitudinal Spin Seebeck Effect (LSSE) in insulating magnets. However, there has been a longstanding disparity between theory and experimental evidence with regards to the nature of power law decay of the LSSE while approaching the ferromagnetic phase transition temperature ($T_C$). We investigate bilayers of Pt/La$_2$NiMnO$_6$ (LNMO) and Pt/EuO$_{1-X}$, both predicted to be promising candidates for spintronics. Our findings reveal that the signal near $T_C$ can be fitted to a power law of the form $(T_C-T)^p$. We explain our results based on the magnon-driven thermal spin pumping theory. We comprehensively demonstrate correlation between the critical exponents of LSSE and magnetization for both FMs. Interestingly, the exponent, $p$, remained invariant upon varying the crystallinity in LNMO. In contrast, Spin Hall Magnetoresistance (SMR) measurements on epitaxial LNMO, exhibit distinctly different features. The observed behavior in epitaxial films appears to be dominated by the interface magnetic anisotropy. In addition, we observe SMR and Anisotropic Magnetoresistance (AMR) in Pt/EuO$_{1-X}$ thin films. We deduce possible explanations based on the temperature dependence of EuO$_{1-X}$ bandstructure and spin mixing conductance of the Pt/EuO$_{1-X}$ interface.

10:12AM F47.00010: Tuning entanglement by squeezing magnons in anisotropic magnets*  JI ZOU (Presenter), University of California, Los Angeles, SE KWON KIM, Department of Physics and Astronomy, University of Missouri, YAROSLAV TSERKOVNYAK, University of California, Los Angeles — We theoretically study the entanglement between two arbitrary spins in a magnetic material, where magnons naturally form a general squeezed coherent state, in the presence of an applied magnetic field and axial anisotropies. Employing concurrence as a measure of entanglement, we demonstrate that spins are generally entangled in thermodynamic equilibrium, with the amount of entanglement controlled by the external fields and anisotropies. As a result, the magnetic medium can serve as a resource to store and process quantum information. We, furthermore, show that the entanglement can jump discontinuously when decreasing the transverse magnetic field. This tunable entanglement can be potentially used as an efficient switch in quantum-information processing tasks.

*This work was supported in part by NSF under Grant No.~DMR-1742928 (J.Z. and Y.T.) and by Research Council Grant URC-19-090 of the University of Missouri (S.K.K.).
10:24AM F47.00011: Electron-magnon scattering and magnon generated chiral charge and spin pumping from time-dependent-quantum-transport/classical-micromagnetics approach*  

ABHIN SURESH (Presenter), BRANISLAV NIKOLIC, Univ of Delaware — In this study, we employ recently developed [M. D. Petrovic et. al., Phys. Rev. Appl. 10, 054038 2018] multiscale time-dependent-quantum-transport/classical-micromagnetics formalism (TDNEGF-LLG) to simulate how spin-polarized steady state current of electrons interacts with a magnon modelled as a classical spin wave. We investigate electronic spin and charge currents generated by the excitation of a single frequency spin wave in a one-dimensional finite size magnetic nanowire composed of classical local magnetic moments precessing around the anisotropy axis while the phase of the precession of adjacent moments varies harmonically over the wavelength of spin wave with uniform precession cone angle. We show that spin wave hosted in the middle of two metallic leads pumps chiral electronic spin and charge currents into the leads, which can be flipped by reversing the direction of magnonic spin current carried by the spin wave. When steady spin-polarized electronic charge current is injected from the left lead into the region hosting the spin wave, we observed that outgoing electronic charge and spin currents in the right lead can be reduced or enhanced, depending on the direction of magnonic spin current.

*This work was supported by NSF Grant No. ECCS 1922689.

10:36AM F47.00012: Investigation of the magnon dispersion in Lu$_2$V$_2$O$_7$ and magnon Weyl point*  

SEUNGHWAN DO (Presenter), Materials Science and Technology Division, Oak Ridge National Lab, JEFFREY RAU, Department of Physics, University of Windsor, HASITHA SURIYA ARACHCHIGE, Department of Physics, University of Tennessee, BINOD K. RAI, Materials Science and Technology Division, Oak Ridge National Lab, GABRIELE SALA, VICTOR R. FANELLI, MATTHEW STONE, Neutron Scattering Division, Oak Ridge National Lab, QING HUANG, HAIDONG ZHOU, Department of Physics, University of Tennessee, MARK D LUMSDEN, Neutron Scattering Division, Oak Ridge National Lab, ANDREW D CHRISTIANSON, Materials Science and Technology Division, Oak Ridge National Lab — The ferromagnetic pyrochlore lattice with Dzyaloshinskii-Moriya (DM) interactions has attracted much attention due to predicted Weyl points in the magnon spectrum [1,2]. The pyrochlore Lu$_2$V$_2$O$_7$ has been suggested as a strong candidate to realize the concept [2]; it has a ferromagnetic ground state below $T_C \approx 69.5$ K [3] and the presence of a magnon Hall effect indicates a strong DM interaction [4]. We use inelastic neutron scattering to examine the spin wave excitations in the compound. These measurements enable us to detect sharp magnon dispersions that are well modeled with linear spin wave theory.


*This research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
Spin Seebeck Effect in Helimagnetic Cu₂OSeO₃: Test of Bulk Magnon Spin Current Theory* ARTEM AKOPYAN (Presenter), NARAYAN PRASAI, Physics, Univ of Miami, BENJAMIN TRUMP, GUY G. MARCUS, TYREL MCQUEEN, Chemistry, Johns Hopkins Univ, JOSHUA COHN, Physics, Univ of Miami — Cu₂OSeO₃ exhibits the largest magnon thermal conductivity of any known ferro- or ferrimagnet. Here we report temperature (T) and magnetic field-dependent measurements of magnon thermal conductivity (κₘ) and longitudinal spin Seebeck coefficient (S_LSSE) in 10-nm Pt/Cu₂OSeO₃ heterostructures for 1~K ≤ T ≤ 15~K. Measurements for three different specimens, having spin-mixing conductances that vary by more than an order of magnitude, demonstrate a relationship between κₘ and S_LSSE in good agreement with bulk magnon spin current theory.

*This material is based on work supported by the U.S. DOE, Off. of BES, Div. of Mater. Sci. and Eng., under grant No. DE-SC0008607 (UM). TMM was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. DOE, Off. of Sci., BES under Award No. DE-SC0019331. BAT acknowledges the NSF, Div. of Mater. Res., Sol. St. Chem., CAREER grant No. DMR-1253562. G.G.M. acknowledges generous support from the NSF-GRFP, Grant No. DGE-1232825.

Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F48 DCMP: Superconductivity: General Theory Mile High Ballroom 1A - Khadijeh Najafi, Virginia Tech

How Alfven's theorem explains the Meissner effect JORGE HIRSCH (Presenter), University of California, San Diego — Alfven's theorem states that in a perfectly conducting fluid magnetic field lines move with the fluid without dissipation. When a metal becomes superconducting in the presence of a magnetic field, magnetic field lines move from the interior to the surface (Meissner effect) in a reversible way. This indicates that a perfectly conducting fluid is flowing outward. I explain the nature of this fluid and show that it carries neither charge nor mass, but carries effective mass. This implies that the effective mass of carriers is lowered when a system goes from the normal to the superconducting state, which agrees with the prediction of the unconventional theory of hole superconductivity, with optical and photoemission experiments in some superconducting materials, and with Bardeen's first theory of superconductivity. The 60-year old conventional understanding of the Meissner effect ignores Alfven's theorem and for that reason I argue that it does not provide a valid understanding of real superconductors.
8:12AM F48.00002: Superconductivity induced by fluctuations of momentum-based multipoles
SHUNTARO SUMITA (Presenter), YOUICHI YANASE, Department of Physics, Kyoto University — Recent studies of superconductivity have focused on spin fluctuation, instead of electron-phonon coupling, as an origin of attractive interaction between electrons. On the other hand, a multipole order, which represents electrons' degrees of freedom in strongly spin-orbit coupled systems, is attracting much attention. Therefore, it is helpful for understanding unconventional superconductivity to consider “superconductivity induced by multipole fluctuations,” as an extension of spin-fluctuation-mediated superconductivity. Indeed, previous works have studied superconductivity induced by fluctuations of odd-parity electric multipole orders in isotropic systems.
In this study, we investigate superconductivity induced by fluctuations odd-parity magnetic multipoles, aiming at good understanding of multipole-fluctuation-mediated superconductivity. Furthermore, this study focuses on the effect of crystalline electric fields (CEF) using the classification theory of multipoles, while the previous studies simply assume isotropic systems. As a result, we suggest that a nodal extended s-wave pairing may be favored by an odd-parity magnetic multipole fluctuation under CEF.
*JSPS KAKENHI Grants No. 17J09908

8:24AM F48.00003: Multiple solutions of pairing gap equation in quantum critical metals.
YI-MING WU (Presenter), University of Minnesota, ARTEM G ABANOV, Physics, Texas A&M U, YUXUAN WANG, Physics, U of Florida, ANDREY CHUBUKOV, University of Minnesota — We use Eliashberg theory to analyze superconductivity for a class of quantum-critical models of itinerant fermions interacting with collective massless bosons, with varying scaling dimension γ of a boson (the γ model). A conventional wisdom holds that there is a single $T_c$ for the pairing in a given symmetry channel. We find in this study that at the critical point the situation is different: the linearized gap equation has a cascade of solutions at $T=T_c^{(n)}$. These solutions have the same spatial symmetry, but they are topologically distinct by the number of sign changes as functions of Matsubara frequency. The transition temperatures $T_c^{(n)}$ decrease exponentially with increasing number of nodes $n$, and the largest $T_c^{(0)}$ has no nodes. We further show that below a given $T_c^{(n)}$, the corresponding solution $\Delta(\omega_n)$ of the linearized gap equation grows in magnitude, but maintains the number of sign changes, which in this respect acts as a topological invariant. We discuss how these oscillating solutions evolve with increasing scaling dimension $\gamma$, and how they contribute to destruction of long range superconducting order.
8:36AM F48.00004: The dielectric function method for superconducting materials*
DIETRICH ELST (Presenter), SERGEI N. KLIMIN, JACQUES TEMPERE, Univ of Antwerp — The dielectric function method (DFM), which uses a non-adiabatic approach to calculate the critical temperatures for superconductivity, has been quite successful in describing superconductors at low carrier densities. This semi-phenomenological theory uses the dielectric function of the material to describe the inter-electron interaction and obtains very BCS-like equations for the superconducting gap and the critical temperature. However, DFM uses an interaction of arbitrary form, instead of a constant attraction in a Debye window as is the case for BCS. We investigate the application of DFM to the linear dispersion of single layer graphene. This is done using an interaction potential that uses the Random Phase Approximation dielectric function and thus allows for plasmonic interactions which are most relevant at low carrier doping.

*This research was supported by the joint FWO-FWF project POLOX (Grant No. I 2460-N36) and the Bijzonder Onderzoeksfonds (BOF) of the Research Council of the University of Antwerp.

8:48AM F48.00005: Odd–Parity Spin–Triplet Superconductivity in Antiferromagnetic Metals Lacking Effective Time-Reversal Symmetries*
SEUNG HUN LEE (Presenter), BOHM-JUNG YANG, Seoul Natl Univ — We propose a route to achieve odd-parity spin-triplet superconductivity in metallic collinear antiferromagnets with inversion symmetry. Owing to the existence of hidden antiunitary symmetries, which we call the effective time-reversal symmetries (eTRS), the Fermi surfaces of such systems are generally spin-degenerate. However, by introducing a local inversion symmetry breaking perturbation that also breaks the eTRS, we can lift the degeneracy to obtain spin-polarized Fermi surfaces. In the weak-coupling limit, the spin-polarized Fermi surfaces constrain the electrons to form spin-triplet Cooper pairs with odd-parity. Furthermore, we find that the odd-parity superconducting states host nontrivial band topology. We also solve the finite-size tight-binding models to show the boundary modes appear as a consequence of the bulk topology.

*S.L. was supported by IBSR009-D1. B.-J.Y. was supported by the Institute for Basic Science in Korea (Grant No. IBS-R009-D1) and Basic Science Research Program through the National Research Foundation of Korea (NRF) (Grant No. 0426-20190008). This work was supported in part by the U.S. Army Research Office under Grant Number W911NF18-1-0137.

9:00AM F48.00006: Suppression of superfluidity by dissipation – An application to failed superconductor
KOU MISAKI (Presenter), University of Tokyo, NAOTO NAGAOSA, University of Tokyo, RIKEN CEMS — The ground states of bosons have been classified into superfluid, Mott insulator, and bose glass. Recent experiments in two-dimensional superconductors strongly suggest the existence of the fourth quantum state of Cooper pairs, i.e., bose metal or quantum metal, where the resistivity remains constant at lowest temperature. However, its theoretical understanding remains unsettled. In this talk, we show theoretically that the bosons in the dilute limit subject to dissipation can lose the superfluidity and remain metallic, utilizing the Feynman's picture of superfluidity in the first quantized formulation. This result is relevant to the quantum vortices under an external magnetic field in two-dimensional superconductors with the finite resistivity of the normal core as the source of dissipation.
9:12AM F48.00007: *SP*OT* symmetry and unconventional pairing in non-Hermitian superconductors*  
SUMANTA BANDYOPADHYAY (Presenter), Physics, NORDITA, ALEXANDER V BALATSKY, Physics, NORDITA and University of Connecticut, Storrs, CT — Novel physics with nontrivial topology and nodal structures emerge in the nonhermitian system. In this work, we investigate the role of damping as a mean to induce dynamics in the superconducting system. We find both odd (Berezinskii) and even (BCS) frequency (ω) states emerge as a result of damping in the superconductors. Odd ω pairing emerges as a result of \( SP^*OT^* \) symmetry [1]. To properly introduce Berezinskii classification in the nonhermitian superconductors, this classification should be extended to include particle-hole conjugation (\( C^* \)). \( C^*SP^*OT^* = -1 \). This symmetry constraint allows us to predict new kinds of order parameters in dynamic systems with damping. We have identified the natural occurrence of odd ω superconductivity (OFSc) in the nonhermitian systems such as odd ω s-wave spin-triplet superconducting state. We also propose experimental observables related to OFSc in such a nonhermitian system.


*SB and AVB acknowledge support from VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744) and the European Research Council under the European Unions Seventh Framework ERS-2018-SYG 810451 HERO.

9:24AM F48.00008: Spontaneous Time-Reversal Symmetry Breaking in unconventional Superconductors  
MENG ZENG (Presenter), LUN-HUI HU, CONJUN WU, University of California, San Diego — Time-reversal symmetry plays a crucial role in the study of unconventional superconductivity in strongly correlated systems. When two superconducting order parameters with different pairing symmetries compete, time-reversal symmetry can be spontaneously broken due to a 2\(^{nd}\) order Josephson coupling between the competing order parameters. In this work, we show that time-reversal symmetry breaking transition can occur due to superconducting phase fluctuations before the onset of superconductivity. To illustrate this phenomenon, we employ the Ginzburg-Landau theory, and use an effective two-component XY-model to perform a renormalization group analysis to study superconducting phase fluctuations. In the time-reversal symmetry breaking normal state, neither of the pairing orders develops phase coherence, but their relative phase is pinned at ±π/2.
9:36AM F48.00009: Electromagnetic response of superconductors in the presence of multiple collective modes  RUFUS BOYACK (Presenter), University of Alberta, PEDRO LOPES, University of British Columbia — Collective-mode fluctuations play an essential role in ensuring the electromagnetic response of superfluids is gauge invariant. The contribution of these fluctuations, however, is known to drop out from the Meissner response of uniform superfluids. The same phenomenon is not so established in the context of non-uniform superfluids. To clarify this issue, we revisit how collective modes appear in the Meissner effect. We find that their contributions vanish both in uniform and non-uniform systems, unless an external length scale is present -- as in Fulde-Ferrell or finite sized superfluids. As examples, we consider s- and p-wave superconductors. To facilitate this analysis, we formulate a path-integral matrix methodology for computing the response of fermionic fluids in the presence of multiple collective modes. Closed-form expressions are provided, incorporating effects from phase and amplitude of the superconducting order parameter and electronic density fluctuations. All microscopic symmetries and invariances are manifestly satisfied in this approach, and it can be straightforwardly extended to other scenarios.

9:48AM F48.00010: Calculating the Superconducting Superheating Field within Eilenberger Theory*  ALDEN Pack (Presenter), MARK TRANSTRUM, Brigham Young Univ - Provo — For Type II superconductors in an applied magnetic field, the superconducting Meissner state can persist metastably up to a theoretical maximum, "superheating field", Hsh. Superconducting Resonance Frequency (SRF) cavities are a critical component of particle accelerators for which Hsh represents a fundamental limit to performance. As the accelerator community explores materials for next-generation cavities, such as Nb3Sn, better estimates of Hsh are needed for candidate materials. Previous calculations have used Ginzburg-Landau theory (valid near Tc), however SRF cavities often operate well below the critical temperature. Extensions to Eilenberger theory (valid at all temperatures) in the high-kappa and dirty limits have also been done. Here, we discuss the calculation of Hsh in Eilenberger theory in the clean limit. In addition to an accurate temperature dependence, the clean limit of the Eilenberger theory includes material-specific parameters for the density of states at the Fermi surface. I discuss implications for SRF cavity development.

*This work was supported by the US National Science Foundation under Award OIA-1549132, the Center for Bright Beams.
10:00AM F48.00011: Enhanced Superconductivity in Quasi-periodic Crystals* ZHIJIE FAN (Presenter), GIA-WEI CHERN, Physics, University of Virginia, SHIZENG LIN, Theoretical Division, Los Alamos National Lab — It is ubiquitous that superconductivity emerges in materials with incommensurate structure. Here we study superconductivity in a family of one-dimensional incommensurate system with s-wave pairing interaction. The incommensurate potential changes the characteristics of the electronic wave function either to extended, critical or localized states. Through standard Bogoliubov-de Gennes calculations and analytical analysis utilizing Anderson's idea of pairing the time-reversed exact eigenstates, we find that superconductivity is enhanced when the electronic wave functions are critical. The superconducting transition temperature obeys an unconventional power law relation with respect to the pairing interaction. Consequently, there exists a superconducting dome around the localization transition when the amplitude of the incommensurate potential is tuned, or near the mobility edge when the chemical potential is varied. Our results suggest a way to enhance superconducting transition temperature by introducing an incommensurate potential.

*This work was carried out under the auspices of the U.S. DOE NNSA under contract No. 89233218CNA000001 through the LDRD Program, and was supported by the Center for Nonlinear Studies at LANL.

10:12AM F48.00012: Dynamic Pair-Breaking Current in Superconductors* AHMAD SHEIKHZADA (Presenter), ALEXANDER V GUREVICH, Physics, Old Dominion University — We calculated a dynamic pair-breaking current density $J_d$ and a critical condensate velocity $v_d$ in a thin film superconducting strip or a filament carrying a large-amplitude ac current $J(t) = J_0 \sin \omega t$. Here $J_d(T, \omega)$ and $v_d(T, \omega)$ in a dirty superconductor at $T \approx T_c$ were computed by numerical simulations of the time-dependent Ginzburg-Landau (TDGL) equations, as well as the full time-dependent Usadel and kinetic equations that take into account both a nonequilibrium distribution function of quasiparticles and nonlinear current pairbreaking effects. It is shown that superconductivity is destroyed at $J_0 > J_d$, where the dynamic pairbreaking current density $J_d(T, \omega)$ approaches $\sqrt{2} J_{GL}(T)$ at $\omega \tau > 1$. Here $J_{GL}(T)$ is the GL dc depairing current density and $\tau(T)$ is the energy relaxation time of quasiparticles on phonons. Nonlinear electromagnetic response of a nonequilibrium superconductor and intermodulation at $J < J_d$ were also calculated.

*This work was supported by DOE under grant No. DE-SC0010081.
10:24AM F48.00013: Collective modes in Bogoliubov Fermi surfaces without gapless Goldstone modes*  
JAY SAU (Presenter), BRIAN SWINGLE, Physics, University of Maryland, College Park — We study collective modes of a finite temperature Bogoliubov Fermi surface with no symmetries. The Bogoliubov Fermi surface is assumed to form in a superconductor with Coulomb interactions, so that the plasmon is gapped and there is no low lying Goldstone mode in the system. Despite this we find the existence of a gapless second sound, which is a collective mode of energy and momentum fluctuations that is not related to any Goldstone mode. This is different from previously discussed second sound modes in either superfluids or crystals, where the second sound co-exists with and is related to a spontaneously broken symmetry with a gapless Goldstone mode. Thus these modes are an example of collective modes that are solely related to conservation of energy/momentum.

*JS acknowledges support from the NSF CAREER and Aspen Center for Physics. BS acknowledges support from AFOSR

10:36AM F48.00014: Floquet theory of periodically-driven superconductors*  
DANILO LIARTE (Presenter), JAMES MANISCALCO, MICHELLE KELLEY, NATHAN SITARAMAN, TOMAS ARIAS, MATTHIAS ULF LIEPE, JAMES PATARASP SETHNA, Cornell University — We use Floquet theory to describe dynamics and losses of superconductors under extremely high fields and frequencies. Periodically-driven superconductors at high fields provides an unexplored theoretical territory relevant in modern applications (lower cryogenic costs for particle accelerators), allowing for experimental validation using Superconducting-Radio-Frequency (SRF) cavities. We use the Floquet formalism to solve the Cooper problem in the limit of strong AC fields (in which linear-response analysis does not apply). We also discuss preliminary results combining BCS and Floquet theories to develop an experimentally-verifiable new approach for periodically-driven superconductors that provides explanation and control of dissipation, with relevance for condensed matter physics and the ‘positive Q slope’ of SRF cavities.

*The authors thank the Center for Bright Beams, NSF award PHY-1549132.

F48.00015: Effect of Defects in Superconducting Phase of Twisted Bilayer Graphene  
HUI YANG (Presenter), ZHI-QIANG GAO, FA WANG, Peking Univ — In this work we study the effect of impurity in the superconducting phases of the twisted bilayer graphene (TBG) by analysing bound states induced by the impurity. As a comparison with the superconducting phase, we first consider the impurity effect in the TBG without superconductivity in the scheme of a low energy effective theory. For superconductivity, our basis is a four-band model2 with different superconducting pairing symmetries. Then we construct the effective impurity Hamiltonian and compute the local density of state (DOS). We find that for different kind of pairing symmetries the numbers of bound states are different. These results can in principle be detected in scanning tunnelling microscopy (STM) experiments, and therefore the pairing symmetry may be determined. Finally we consider the multi-impurity effect and compute phase diagrams in terms of effective gap and the strength and density of impurities. We find that in (p + ip)-wave and (d + id)-wave phases superconductivity will be destroyed by impurities with strong strength or concentration.
8:00AM F49.00001: THz emission characteristics from mesa arrays of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ single crystals  
TAKANARI KASHIWAGI (Presenter), TAKAYUKI IMAI, SYUNGO NAKAGAWA, GENKI KUWANO, YUKINO ONO, TOMOYUKI SHIZU, YOUTA KANEKO, SHINJI KUSUNOSE, MAYU NAKAYAMA, JEONGHYUK KIM, MANABU TSUJIMOTO, University of Tsukuba, TAKASHI YAMAMOTO, QuTech Delft University of Technology, HIDETOSHI MINAMI, University of Tsukuba, TAKASHI MOCHIKU, National Institute for Materials Science, HIRONORI NAKAO, Institute of Materials Structure Science, High Energy Accelerator Research Organization, HIROSHI EISAKI, SHIGEYUKI ISHIDA, YASUNORI MAWATARI, National Institute of Advanced Industrial Science and Technology, YUKIO HASEGAWA, The University of Tokyo, RICHARD KLEMM, University of Central Florida, KAZUO KADOWAKI, University of Tsukuba — 

To develop the high power terahertz emission from Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) high-$T_c$ superconducting THz emitters (Bi2212-THz emitters), it is very important to manage self-heating of these devices. We have developed stand-alone mesa structures (SAMs) of Bi2212 single crystals sandwiched by good thermal conducting sapphire substrates to reduce self-heating effects. These thermal managed devices enable us to extend the range of the radiation frequencies up to around 2.4 THz. For applications of THz emitters, 1 mW level of output power and 1 kHz level of radiation linewidth are required. In order to obtain such high performance characteristics from our Bi2212-THz emitters, we have studied not only about thicker SAMs but also arrays of SAMs. The SAMs up to around 8 μm thickness with keeping good shape of mesa structures can be obtained by a wet etching method so far. We made arrays of those SAMs by using the thermal managed device structures. At this moment, we observed about 10 μW level of output power from two arrays of SAMs with the dimensions of 69 × 190 × 4.2~4.4 μm$^3$. The details of the current situation of our Bi2212-THz emitters will be discussed.
8:12AM F49.00002: Mesa sidewall effect on coherent terahertz radiation from Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ intrinsic Josephson junctions* GENKI KUWANO (Presenter), YOUTA KANEKO, KANAE NAGAYAMA, TAKAYUKI IMAI, YUKINO ONO, SHINJI KUSUNOSE, TAKANARI KASHIWAGI, HIDETOSHI MINAMI, KAZUO KADOWAKI, MANABU TSUJIMOTO, University of Tsukuba — Coherent terahertz sources based on the stack of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ intrinsic Josephson junctions (IJJs) have been attracted in the academic and industrial fields. See Ref. [U. Welp et al., Nat. Photonics, vol. 7, p. 702 (2013)] for recent review. In this study, we demonstrate that tapered sidewalls produce a difference in the junction voltages along the stack and thus synchronization among the IJJs fails to occur with distributed oscillation frequencies. Also, our systematic experiment using shielding metal masks reveals that only the ac Josephson current flowing along the sidewall can generate the terahertz waves outside of the mesa. These results suggest that the condition of the sidewall is essentially important to control the radiation characteristics. In this talk, we will present the details of the fabrication process and experimental results and will discuss the role of the mesa sidewalls on the coherent radiation.

*This work was supported by KAKENHI (Grant No. 19H02540) and the Program to Disseminate the Tenure Tracking System at the University of Tsukuba.

8:24AM F49.00003: Electromagnetic field analysis of coherent terahertz radiation emitted from stacks of intrinsic Josephson junctions of BSCCO with microstrip antennas* MANABU TSUJIMOTO (Presenter), YOUTA KANEKO, GENKI KUWANO, KANAE NAGAYAMA, SHINJI KUSUNOSE, TAKAYUKI IMAI, YUKINO ONO, TAKANARI KASHIWAGI, HIDETOSHI MINAMI, KAZUO KADOWAKI, University of Tsukuba — The observation of coherent terahertz radiation from a stack of intrinsic Josephson junctions (IJJs) in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) highlighted the potential of using high-$T_c$ superconductors as compact and convenient terahertz sources. So far, synchronized IJJ mesa arrays were demonstrated to produce the output power up to 0.6 mW [Benseman et al., APL (2013)], which is presently the highest recorded level among all available terahertz sources. To increase the output power further up to milliwatt-level, we need to mitigate impedance mismatch at the boundary between an emitting IJJ stack and a dielectric medium or free space. In this study, we implement the electromagnetic field analysis of the radiation emitted from IJJs stacks with microstrip antennas, which are designed for highly efficient radiation. We established a microfabrication process based on the lift-off technique to pattern the microstrip antenna. In this talk, we will discuss the characteristic radiation behavior associated with the bath and local temperatures and variation in polarization characteristics depending on the bias point.

*This work was supported by KAKENHI (Grants No. 19H02540) and the Program to Disseminate the Tenure Tracking System at the University of Tsukuba.
8:36AM F49.00004: THz emission peak at low voltage bias from stacked intrinsic Josephson junction Bi$_2$Sr$_2$CaCu$_2$O$_8$ terahertz sources*  
KAREN J KIHLSTROM (Presenter), TIMOTHY BENSEMAN, Physics, Queens College CUNY, ALEXEI KOSHELEV, ULRICH WELP, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, KAZUO KADOWAKI, Institute for Materials Science, University of Tsukuba — The extremely anisotropic high-temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_8$ contains stacked 'intrinsic' Josephson junctions with a large superconducting gap energy. Mesa-shaped devices constructed from this material therefore show promise as a source of coherent, continuous-wave radiation in the 'terahertz gap' range. THz emission from these devices has previously been typically observed at frequencies between around 0.4 THz – 2 THz, corresponding to Josephson voltages of between 0.8 mV and 4 mV per intrinsic junction. However, we have recently observed a new type of emission which occurs at bias currents below the retrapping current of the stacked Josephson junctions. This unusual THz emission state is highly reproducible, is metastable over a timescale of hours, and shows systematic temperature dependence. The maximum emitted THz power that can be generated from this mode is comparable to that generated by the more well-established and better-understood THz emission modes in Bi$_2$Sr$_2$CaCu$_2$O$_8$ mesa sources. We will discuss possible mechanisms for the unusual emission mode, together with future directions of related research.

*This research is supported by PSC-CUNY Award 60792-00-48; and by the US Department of Energy, Office of Sciences, Materials Sciences and Engineering Division.

8:48AM F49.00005: Stacked intrinsic Josephson junction Bi$_2$Sr$_2$CaCu$_2$O$_8$ terahertz sources: Design issues for achieving high power output close to $T_c$*  
TIMOTHY BENSEMAN (Presenter), KAREN J KIHLSTROM, Physics, Queens College CUNY, ALEXEI KOSHELEV, ULRICH WELP, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, KAZUO KADOWAKI, Institute for Materials Science, University of Tsukuba — The high-temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_8$ contains stacked 'intrinsic' Josephson junctions, with unrivalled packing density and a high superconducting gap energy. Cuboid 'mesa' devices constructed from this material are consequently a promising technology for coherent, continuous-wave radiation in the 'terahertz gap' range, spanning from approximately 0.3 – 1.5 THz. A key issue for practical applications of such devices is their cryocooling requirements, and it is therefore highly desirable to optimize their performance at temperatures that can be achieved by nitrogen cryogenics. Here we report generation of 0.15 milliwatts of coherent emission power at 0.5 THz, at a bath temperature of 77 Kelvin. This was achieved by exciting the (3, 0) cavity mode of a stack containing 580 junctions, and $T_c$ of 86.5 Kelvin. In order to minimize self-heating, the THz source was mounted on a copper substrate using PbSn solder. We will discuss the choice of mesa dimensions and cavity mode, and implications for the design of devices which are intended to operate close to the material's superconducting critical temperature.

*This research is supported by PSC-CUNY Award 60792-00-48; and by the US Department of Energy, Office of Sciences, Materials Sciences and Engineering Division.
9:00AM F49.00006: Demonstrating phase control in spin-triplet ferromagnetic Josephson junctions* VICTOR AGUILAR (Presenter), REZA LOLOEE, WILLIAM P PRATT, NORMAN BIRGE, Physics and Astronomy, Michigan State University — Ferromagnetic Josephson junctions show promise for application in energy efficient cryogenic memory [1]. Both spin-singlet and spin-triplet supercurrents are being studied by our group for this purpose. Engineering adjacent F layers in a three-layer system to have perpendicular magnetizations allows singlet pairs to convert to spin-aligned triplet pairs. Recent work in our group exploited a synthetic antiferromagnet (SAF) with perpendicular magnetic anisotropy (PMA) as the central layer. These junctions have been shown to exhibit phase control [2] but have a low critical current when compared to singlet junctions. We have shown that removing the SAF while maintaining the PMA increases the critical current by a significant amount. We demonstrate phase-control by fabricating two of these junctions in a SQUID loop, and measuring SQUID oscillations for combinations of the parallel and anti-parallel magnetic states in the two junctions.


*This work was supported by Northrop Grumman Corporation.

9:12AM F49.00007: Ferromagnetic Josephson junctions with perpendicular magnetic anisotropy* NATHAN SATCHELL (Presenter), PHILIPPA SHEPLEY, GAVIN BURNELL, Univ of Leeds — Ferromagnetic Josephson junctions are a strong candidate to become a dissipationless cryogenic memory alternative to dissipative CMOS technologies. In order to build such a memory, the ferromagnetic Josephson junctions must be optimised for both the switching of the ferromagnetic layer and the critical current of the junction. The critical current of the junction decays exponentially with the ferromagnet thickness, making a thin ferromagnet preferable, however typically for in-plane ferromagnets the switching properties worsen as the ferromagnet is thinned. In addition, stray fields from an in-plane ferromagnet add a vector potential in the Josephson junction. To solve these issues, here we explore the use of ferromagnets with perpendicular magnetic anisotropy. We find that, unlike for in-plane ferromagnets, the switching properties of Co in a Nb-Pt-Co($d_{Co}$)-Pt-Nb wedge are optimised for ultra-thin ($\leq$0.6 nm) films. We will also report our progress characterising Josephson junctions with perpendicular Co and CoB ferromagnetic layers.

*This project has received funding from the European Unions Horizon 2020 research and innovation program under Marie Sklodowska-Curie Grant Agreement No. 743791 (SUPERSPIN).
9:24AM F49.00008: High Field Superconductivity and Magnetic Moment Enhancement in Proximity Exchange Coupled GdN/NbN Nano-bridges*  MIRKO ROCCI (Presenter), DHAVALA SURI, Massachusetts Institute of Technology MIT, NORBERT MARCEL NEMES, Fisica de los Materiales, Universidad Complutense de Madrid and ICMM-CSIC, JOSE LUIZ MARTINEZ, MAR GARCIA-HERNANDEZ, Instituto de Ciencia de Materiales de Madrid - CSIC, JAGADEESH MOODERA, Massachusetts Institute of Technology MIT — Proximity effects in ferromagnetic insulator/superconductor (FI/SC) interface have been highly intriguing in terms of fundamental exploration as well as technological relevance [1,2]. We perform detailed investigations on GdN (FI) and NbN (SC) interface via magneto-transport properties of GdN/NbN-based nano-bridges and thin film heterostructures. We observe a clear enhancement of magnetic moment and a drastic increase of coercive field, below the superconducting transition temperature of NbN, which may be attributed to exchange coupled effect between GdN and NbN at the interface. Most interestingly, our nano-bridges exhibit a large magnetic field dependent superconductivity enhancement for fields > 5T similar to the Jaccarino effect [3]. The observed effect is temperature dependent implying a free energy dependence at the interface. Finally, we also discuss the exchange coupled interface effects and their implications in GdN/NbN system.

Ref.:
[2] Y. Zhu et al., Nat. Mat. 16, 195 (2017);

*H2020-MSCA-IF No.796603-EuSuper, ONR(N00014-16-1-2657) and NSF(DMR 1700137).

9:36AM F49.00009: Optimizing supercurrent transmission and magnetic behavior in ferromagnetic Josephson junctions*  SWAPNA SINDHU MISHRA (Presenter), ROBERT M KLAES, REZA LOLOEE, NORMAN BIRGE, Physics and Astronomy, Michigan State University — Josephson junctions with ferromagnetic layers where the ground-state phase difference can be reliably controlled are a potential candidate for applications in cryogenic memory devices, which can greatly reduce the ever-growing energy requirements for large-scale computing. Phase control has been successfully demonstrated with junctions containing a Ni fixed layer and a NiFe free layer[1,2]. However, there are still a number of improvements that can be made to increase the efficiency and reliability of these junctions. We present work on trying to improve the efficiency by using thin layers of Ni “dusting” around the NiFe free layer to further increase the transmission of supercurrent through these junctions. We also present work on improving the switching reliability by replacing the fixed Ni layer with unbalanced Ni SAFs which may have more desirable magnetic properties.


*This research is based upon work supported by Northrop Grumman Corporation.
Three-dimensional (3D) topological semimetals possess unconventional surface and edge states, which play central roles in exotic topological phases. WTe$_2$, as a type-II Weyl semimetal, has 2D Fermi arcs on the (001) surface in the bulk and 1D helical edge states in its monolayer. However, in the intermediate regime between the bulk and monolayer, the edge states have not been resolved owing to its closed band gap which makes the bulk states dominant. Here, we report the signatures of the edge states by superconducting quantum interference measurements in multilayer WTe$_2$ Josephson junctions and we directly map the localized supercurrent. In thick WTe$_2$ (~60 nm), the supercurrent is uniformly distributed on the (001) surface. In thin WTe$_2$ (10 nm), however, the supercurrent becomes confined to the 1D edge modes and its width reaches up to 1.4 μm. Furthermore, an asymmetric Josephson effect, predicted as a unique characteristic of inversion-symmetry-breaking topological systems, is observed in thin WTe$_2$ whereas it is absent in the thick one. The ability to combine superconductivity with these edge states establishes WTe$_2$ as a promising topological system with exotic quantum phases and a rich physics of extra dimensionality and tunability.

An Alternate Scheme to Mode-Lock Quantum Phase Slips. BASTIEN DASSONNEVILLE (Presenter), JOSE AUMENTADO, National Institute of Standards and Technology Boulder — It has been proposed that locking the voltage oscillations of a Quantum Phase Slip Junction (QPSJ) to a microwave source could achieve the transfer of an integer number of elementary charges per microwave cycle. Such a synchronized transfer of charge would correspond to current steps in the current-voltage characteristic of the QPSJ, which could be used to realize a current standard. These proposals focus on realizing a circuit dual to the Josephson voltage standard and therefore require placing a QPSJ close to a resistor whose value is larger than the superconducting quantum of resistance. The observation of current steps for such a circuit is however extremely challenging experimentally, mostly due to the large Joule heating occurring in the resistor. To address this problem, we consider alternative designs that relax the constraint on the resistance and instead rely on the feedback provided by a high-impedance resonator. Through numerical simulations, we demonstrate that mode-locking indeed occurs in such systems and that synchronized charge transfer can be achieved in a resonant environment, without the need for a large resistor. Such a circuit may offer an alternative path toward the realization of a current standard.
10:12AM F49.00012: Exploring parity transitions of Majorana bound states in S-TI-S lateral Josephson junctions

GUANG YUE (Presenter), Department of Physics, University of Illinois at Urbana-Champaign, XIONG YAO, DEEPTI JAIN, JISOO MOON, SEONGSHIK OH, Department of Physics & Astronomy, Rutgers, The State University of New Jersey, ALEXEY BEZRYADIN, DALE J VAN HARLINGEN, Department of Physics, University of Illinois at Urbana-Champaign — It is predicted that S-TI-S lateral Josephson junctions, fabricated by depositing electrodes of a conventional superconductor (S) on the surface of a topological insulator (TI), exhibit Majorana bound states (MBS) at locations in the junction where the phase difference is an odd-multiple of π, i.e. at the cores of the Josephson vortices. There is evidence for this from the lifting of odd nodes in the critical current diffraction patterns and the observation of supercurrent features at magnetic field where the MBS enter the junction. In this talk, we report progress on experiments designed to probe the parity states of MBS pairs and the transitions between them via measurements of the critical current distribution and supercurrent fluctuations. These experiments give information about parity lifetimes and open the door to understand the factors that limit them.

*NSF DMR-1610114 and DMR-1745304

10:24AM F49.00013: Topological Josephson Junctions in Corbino geometry

ANANTHESH SUNDARESH (Presenter), TYLER LINDEMAN, Department of Physics and Astronomy, PURDUE UNIVERSITY, GEOFF C GARDNER, SERGEI GRONIN, Microsoft Quantum Purdue, MICHAEL MANFRA, LEONID ROKHINSON, Department of Physics and Astronomy, PURDUE UNIVERSITY — One-dimensional hybrid semiconductor/superconductor wires and, more recently, long Josephson junctions are the most versatile synthetic topological superconductors where non-abelian excitations can be realized and thoroughly investigated. In both realizations quasiparticle states appear at the physical boundaries, either at the ends of the nanowires or at the edges of the Josephson junction. Signatures of these states have been observed, studied and investigated by several groups with respect to various parameters such as magnetic field, chemical potential and the superconducting phase difference. In this work we report experimental investigation of Josephson junctions in the Corbino geometry fabricated from InAs/Al heterostructures. These devices are in a long junction regime with periodic boundary conditions. Transport studies of these junctions in a normal regime (zero in-plane magnetic field) and in the regime where some regions of the junction are in a topologically non-trivial regime (non-zero in-plane magnetic field) will be presented.

*The project was supported by DOE Basic Energy Sciences award DE-SC0008630.
10:36AM F49.00014: Engineering the spin-orbit interaction in InAs-based quantum wells for superconductor-semiconductor hybrid structures* MICHAEL PRAGER (Presenter), MARTIN SPECKNER, JAY SCHMIDT, DIETER SCHUH, DOMINIQUE BOUGEARD, University of Regensburg — Superconductor (SC)-semiconductor hybrid structures open an access to exotic superconductivity, enabling the creation of Majorana zero modes in appropriate devices. The strength of the spin-orbit interaction (SOI) in the structure represents an important parameter, driving for example the size of the energy gap induced into the SC. InAs-based epitaxial hybrid heterostructures have emerged as a promising candidate for such systems, exploiting the rather large intrinsic SOI of InAs and the epitaxial matching with SCs such as aluminum (Al). In this work, we present a systematic study of two-dimensional electron gases (2DEGs) realized in strongly asymmetric InAs/InGaAs/InAlAs quantum well layouts. We show that the SOI in such 2DEGs is substantially enhanced by engineering the asymmetry through the position of the InAs inset and the doping layer. We characterize the strength of the SOI in the 2DEGs by analyzing SOI-induced features in low temperature magneto transport, such as zero-field spin splitting-induced beating patterns and weak antilocalization, as well as by exploring the energy gap induced into epitaxial superconducting Al.

*We acknowledge funding by the Deutsche Forschungsgemeinschaft via SFB 1277 project A01

10:48AM F49.00015: Anomalously large second Josephson harmonic in quantum well-based junctions AZARIN ZARASSI (Presenter), Univ of Pittsburgh, LUCAS JARJAT, Ecole Normale Superieure, VINCEN VAN DE SANDE, TU Eindhoven, MIHIR PENDHARKAR, JOON SUE LEE, ANTHONY P MCFADDEN, SEAN HARRINGTON, Univ of California, Santa Barbara, SASA GAZIBEGOVIC, GHADA BADAWY, ROY OP HET VELD, TU Eindhoven, MOIRA HOCEVAR, Neel Institute, CNRS, SUSHENG TAN, Univ of Pittsburgh, ERIK BAKKERS, TU Eindhoven, CHRIS J PALMSTROM, Univ of California, Santa Barbara, SERGEY M FROLOV, Univ of Pittsburgh — The current-phase relation (CPR) of a Josephson junction (JJ) contains information about the microscopic mechanisms behind supercurrent. The sinusoidal CPR can successfully describe most JJs made with different materials and synthesis technologies. However, CPR can also deviate from simply sinusoidal form, in particular it can feature higher order sinusoidal terms. We investigate InAs quantum well JJs with epitaxial Al contacts. The distance between Al electrodes is of order 100 nm shorter than the mean free path in the quantum well. We perform diffraction pattern measurements, SQUID measurements and Shapiro step measurements all pointing at a strong intrinsic second order harmonic.
8:00AM F50.00001: Two-dimensional non-Fermi liquids with quenched disorder* PAVEL NOSOV (Presenter), SRINIVAS RAGHU, Stanford Univ — Despite significant theoretical progress, the effect of quenched disorder on non-Fermi liquids with a finite density of fermions interacting with soft order parameter fluctuations near a quantum critical point remains poorly understood. We study the interplay of disorder and interactions in the exactly solvable "matrix large N" non-Fermi liquid model in two spatial dimensions. We investigate the stability of the corresponding strongly interacting fixed point and show that diffusive effects drastically modify the properties of the critical regime and associated critical exponents.

*DOE Office of Basic Energy Sciences, contract DEAC02-76SF00515

8:12AM F50.00002: Pairing Instability on a Luttinger Surface: A Non-Fermi Liquid to Superconductor Transition and its SYK Dual CHANDAN SETTY (Presenter), University of Florida — Instabilities of the Fermi Surface -- contours of poles of the single particle Green function -- such as superconductivity, density waves (CDW, SDW, PDW..) etc are now a commonplace in modern condensed matter physics. In this talk, I will discuss the problem of superconducting instability on a model Luttinger surface, or contours of zeros of the many-body Green function. Unlike a Fermi surface, in the presence of an attractive potential, the model exhibits -- in the strong coupling limit -- a quantum phase transition into a superconducting state. The spectral density of pair fluctuations in the "normal" state of the superconductor has a power-law type van-Hove singularity signalling non-Fermi liquid transport. Crucially, the fluctuation free energy in the non-Fermi liquid resembles well-studied models with gravity duals such as SYK. These results shed light on the role played by order-parameter fluctuations in providing the key missing link between Mottness and strongly coupled toy-models exhibiting gravity duals.

8:24AM F50.00003: Low-energy level spacing and entropy change across SYK non-Fermi liquid to a Fermi Liquid transition for finite-N* SUMILAN BANERJEE (Presenter), SURAJIT BERA, Indian Institute of Science, ARJIT HALDAR, Physics, University of Toronto — We study a quantum phase transition (QPT) between a Sachdev-Ye-Kitaev (SYK) non-Fermi liquid (NFL) and a Fermi liquid in a solvable large-N model where the zero-temperature residual entropy of the NFL vanishes continuously at the QPT in the large-N limit. We show via exact diagonalization that, even at finite-N, the QPT manifests itself in the system-size scaling of low-energy level spacings above the ground state. The evidence of this QPT is also directly visible in the single-particle Greens function and, indirectly, in the thermalization dynamics after a quench. Interestingly, we find that the QPT has little effect on the entanglement entropy in the ground state. We also construct the effective low-energy field theory across the QPT by considering fluctuations around the large-N limit.

*SB is supported by SERB, DST, India and The Infosys Foundation, India through Infosys Young Investigator Award.
8:36AM F50.00004: Phases of the t-J model with random and all-to-all hopping and exchange  
DARSHAN JOSHI (Presenter), CHENYUAN LI, SUBIR SACHDEV, Harvard University — We study a t-J model with both t and J random and all-to-all. This model has been studied earlier [1], and can be mapped to an Anderson impurity coupled to self-consistent fermionic and bosonic baths. We employ renormalization group and large M (for models with SU(M) spin symmetry) analyses, and find evidence for a critical non-Fermi liquid phase at zero temperature and small doping. The critical spin correlations are similar to those in a random magnet [2]. A disordered Fermi liquid phase is expected at large doping. We note connections to the physics of the underdoped cuprates.


8:48AM F50.00005: Fermi-surface Reconstruction in the Repulsive Fermi-Hubbard Model  
IAN OSBORNE (Presenter), NANDINI TRIVEDI, Ohio State Univ Columbus, THEREZA PAIVA, Univ Federale do Rio de Janeiro — One of the fundamental questions about the high temperature cuprate superconductors is the size of the Fermi surface underlying the superconducting state. By analyzing the single particle spectral function for the Fermi Hubbard model as a function of repulsion $U$ and chemical potential $\mu$, we find that the Fermi surface reconstructs from a large Fermi surface enclosing $(1+p)$ holes, matching the Luttinger volume as expected in a Fermi liquid, to a small Fermi surface enclosing only $p$ holes, thereby transitioning into a non-Fermi liquid FL* phase, as the Mott insulator at half filling is approached. We obtain the Fermi surface contour by combining results of: (a) momentum distribution function $n_k = 1/2$, (b) spectral weight $A_k(\omega = 0)$, and (c) retarded Green's function, $G_k^{\text{ret}}(E) = 0$, calculated using determinantal quantum Monte Carlo and analytic continuation methods. We compare our numerical results with experiments on Hall measurements.

9:00AM F50.00006: Probing out-of-time-order correlators using thermofield double states  
ETIENNE LANTAGNE-HURTUBISE (Presenter), STEPHAN PLUGGE, OGUZHAN CAN, MARCEL FRANZ, University of British Columbia — We propose a new family of protocols for measurements of out-of-time order correlators (OTOCs) that do not require backward time evolution. Instead, they rely on ordinary time-ordered measurements performed in the thermofield double (TFD) state, an entangled state formed between two identical copies of a quantum system. In particular, we show how Lyapunov exponents of quantum chaotic systems can be extracted from various time-ordered correlators (including equilibrium Green's functions) in the TFD state. Importantly, TFD states can be realized as ground states of simple Hamiltonians coupling two identical systems, which underlies their usefulness for experimental explorations of quantum chaos. We numerically test our protocols on two coupled SYK models, recently proposed to be dual to an eternal traversable wormhole, and discuss possible realizations of this setup.
Non-Laudau Quantum Phase Transitions and Nearly-Marginal Fermi Liquid

YICHEN XU (Presenter), University of California, Santa Barbara, HAO GENG, Department of Physics, University of Washington, XIAOCHUAN WU, University of California, Santa Barbara, CHAO-MING JIAN, Station Q, Microsoft, CENKE XU, University of California, Santa Barbara — Marginal fermi liquid and quantum critical points (QCP) with strong fractionalization are two exceptional phenomena beyond the classic condensed matter doctrines, which could occur in strongly interacting quantum many-body systems. This work demonstrates that these two phenomena may be tightly connected. To elaborate this connection, we propose a physical mechanism for "nearly-marginal Fermi liquid", namely the fermion self-energy scales as \( \Sigma_f(i\omega) \sim |\omega|^{\alpha} \) with \( \alpha \) close to 1 in a considerable energy window. The nearly-marginal fermi liquid is obtained by coupling an electron fermi surface to unconventional QCPs that are beyond the Landau's paradigm. This mechanism relies on the observation that the anomalous dimension \( \eta \) of the order parameter of these unconventional QCPs can be close to 1, which is significantly larger than conventional Laudau phase transitions. The fact that \( \eta \sim 1 \) justifies a controlled perturbative renormalization group expansion proposed previously. Candidate QCPs that meet this desired condition are proposed.

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Planckian superconductor

YEVHENIIA CHEIPESH, Lorentz Institute for theoretical physics, Leiden University, ANDREI PAVLOV, The Abdus Salam International Centre for Theoretical Physics (ICTP), VINCENZO SCOPELLITI, Lorentz Institute for theoretical physics, Leiden University, JAKUB TWORZYDLO, Institute of Theoretical Physics, University of Warsaw, NIKOLAY GNEZDILOV (Presenter), Physics Department, Yale University — The Planckian relaxation rate \( h/t_p=2\pi k_B T \) sets a characteristic time scale for both equilibration of quantum critical systems and maximal quantum chaos. We show that at the critical coupling between a superconducting dot and the complex Sachdev-Ye-Kitaev model, known to be maximally chaotic, the pairing gap \( \Delta \) behaves as \( \eta h/t_p \) at low temperatures, where \( \eta \) is an order one constant. The lower critical temperature emerges with a further increase of the coupling strength so that the finite \( \Delta \) domain is settled between the two critical temperatures.

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Branching time and Many-body Chaos

YINGFEI GU, Havard, ALEXEI KITAEV, Caltech, HUI ZHAI, Tsinghua University, PENGFEI ZHANG (Presenter), Caltech — Branching time is defined in terms of the retarded kernel to quantify the stringy effects in SYK-like models. In this work, after presenting a weighting trick to calculate the branching time, we prove a bound on the branching time for a large class of systems. We also derive a relation between the branching time, the Lyapunov exponent and the quasiparticle lifetime for weakly coupling models.
9:48AM F50.00010: A cascade of non-Fermi liquid crossovers from an interplay of local and bosonic quantum criticality  
ANDRES FELIPE SCHLIEF RAETHER (Presenter), Max Planck Institute for the Physics of Complex Systems, FRANCISCO MARTIN BLANCO, DEBANJAN CHOWDHURY, Department of Physics, Cornell University — We present examples of multi-orbital electronic lattice models, coupled to bosonic collective modes with modified Sachdev-Ye-Kitaev form of interactions, which become solvable when the number of orbitals and collective modes is taken to be large. At high energies, these models display non-Fermi liquid behavior with local quantum criticality and are described by a strongly coupled electron-boson fluid. As a function of decreasing energy scales, they exhibit a crossover into an incipient heavy Fermi liquid regime, where the interaction between the bosonic mode and the coherent electronic quasiparticles near the Fermi surface leads to Landau damping. When the boson gap is tuned to criticality, the feedback of the damped boson on the electrons leads to a low-temperature non-Fermi liquid with a critical Fermi surface. Our models thus describe a cascade of crossovers from a dynamical critical exponent $z=\infty$ down to $z=3$ in a controlled setting as a function of decreasing energy scales.

10:00AM F50.00011: Bose Metal as a Nematic Phase Glass  
ANTHONY HEGG (Presenter), Shanghai Jiao Tong University, WEI KU, JINNING HOU, Tsung-Dao Lee Institute — A widely accepted microscopic theory for the Bose metal has yet to emerge despite mounting experimental evidence of a metallic phase intervening between the extremes of superfluid and insulator for low-temperature bosons. The reasons for this are two-fold: metallic solutions tend to be highly unstable, and stable solutions tend to utilize the unphysical limit of arbitrarily low particle density. We present a first-of-its-kind stable microscopic theory for the Bose metal with constant particle density in the thermodynamic limit. In this theory, repulsive interactions cause spontaneous symmetry breaking in an otherwise massively degenerate single-particle ground state. The key physics behind the stability of the Bose metal lies in the structure of the phase coherence. In contrast to the typical isotropic long-range order of superfluidity, our 3D theory exhibits long-range nematic phase coherence in each 2D plane while suffering from short range decoherence between planes. The resulting current response cannot maintain phase coherence beyond a finite length scale. Our discovery of a stable low-temperature phase that exhibits metallic conductivity elevates the Bose metal to one of the fundamentally intrinsic bosonic phases of matter alongside that of the superfluid and insulator.
Exploring order-to-order transitions of Dirac fermions in the regime of strong interactions

LUKAS WEBER (Presenter), STEFAN WESSEL, RWTH - Aachen — In recent years, there has been a growing interest in direct and continuous quantum phase transitions between ordered phases that do not conform with the Landau-Ginzburg paradigm. It has since been a challenge to identify models that host such transitions.

One model of interest consists of interacting Dirac fermions coupled to a transverse-field Ising model on the honeycomb lattice. It has been suggested that there is an order-to-order transition between the competing antiferromagnetic (AFM) and Ising ordered phases of this model [1]. However, the quantum Monte Carlo simulations employed were restricted to relatively small system sizes so that finite-size effects remain an issue. In the strongly interacting regime, this system can be described by an effective quantum spin model of coupled Heisenberg and Ising spins.

Within this setting, highly efficient quantum Monte Carlo methods available for spin systems can be used to drastically improve on the precision of the original fermionic estimates. In our simulations, we resolve a narrow coexistence region between the Ising and AFM-ordered phases, in contrast to the direct single transition proposed in Ref. [1].


Work supported by the DFG through FOR 1807 and RTG 1995.

Scale Invariant Entanglement Negativity at the Many-Body Localization Transition

JOHNNIE GRAY, Imperial College London, ABOLFAZL BAYAT, University of Electronic Science and Technology of China, ARIJEET PAL (Presenter), SOUGATO BOSE, Univ Coll London — The exact nature of the many-body localization transition remains an open question. An aspect which has been posited in various studies is the emergence of scale invariance around this point, however the direct observation of this phenomenon is still absent. Here we achieve this by studying the logarithmic negativity and mutual information between disjoint blocks of varying size across the many-body localization transition. The two length scales, block sizes and the distance between them, provide a clear quantitative probe of scale invariance across different length scales. We find that at the transition point, the logarithmic negativity obeys a scale invariant exponential decay with respect to the ratio of block separation to size, whereas the mutual information obeys a polynomial decay. The observed scale invariance of the quantum correlations in a microscopic model opens the direction to probe the fractal structure in critical eigenstates using tensor network techniques and provide constraints on the theory of the many-body localization transition.
10:36AM F50.00014: g=2 nonlinear sigma model revisited  CHAO-JUNG LEE (Presenter), Caltech, MICHAEL C MULLIGAN, Physics and Astronomy, University of California - Riverside — We consider the transport properties of free fermions with gyromagnetic ratio g=2 in the presence of quenched disorder. This system has been shown to be closely related to the mean-field limit of various composite fermion theories [1,2,3]. We derive the nonlinear sigma model that describes the electrical and spin conductivities via the supersymmetric approach [4], and discuss its physical implications for various quantum phase transitions.


Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F51 DCMP: Magnetism and Magnetic Phenomena in 2D Materials Mile High Ballroom 1D - Te-Yu Chien, University of Wyoming

8:00AM F51.00001: Unconventional anomalous Hall effect in Fe₃GeTe₂ and Fe₅GeTe₂*  JUAN MACY (Presenter), YU-CHE CHIU, Physics, Florida State University, ASHLEY WEILAND, GREGORY MCCANDLESS, JULIA CHAN, Chemistry & Biochemistry, University of Texas at Dallas, LUIS BALICAS, National High Magnetic Field Laboratory — Fe₃GeTe₂ and Fe₅GeTe₂ are layered and exfoliable compounds that display what seemingly are ferromagnetic (FM) transitions below T_c ~ 220 and 280 K, respectively. At low fields, both compounds display an anomalous Hall effect (AHE) that scales with the magnetization. For FM materials, this AHE has been described using Berry phase concepts or argued to be topological in nature [1, 2], with a specific scenario [3] proposed for Fe₃GeTe₂. However, measurements of the magnetic torque reveal a second metamagnetic transition observed in both compounds in fields exceeding 10 T. These indicate that neither compound can be considered as a simple collinear ferromagnet [4], in agreement with Ref. [5], and hence that their AHE is not intrinsic. For both compounds, the AHE remains oblivious with respect to the occurrence of these metamagnetic transitions, indicating that an unconventional scenario is required to explain it.


*L.B. acknowledges supported from DOE-BES.
**Gate-tunable magnetism in vanadium-doped tungsten diselenide monolayer**

DINH LOC DUONG (Presenter), Department of Energy Science (DOES), Sungkyunkwan University (SKKU), Korea, SEOK JOON YUN, YOUNG-HEE LEE, Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Korea — Controlling magnetic properties by tuning carrier concentration is a key feature of diluted ferromagnetic semiconductors, giving possibilities for multifunctional spintronic devices. Here, we investigate the gate-modulation of the long-range magnetic order in p-type vanadium-doped WSe$_2$ monolayer by both experiments and simulations. We found that a transition from the long-range ferromagnetic order to the short-range antiferromagnetic order can be tuned by injecting electrons to compensate for the p-doping effect of vanadium by density functional calculations. The magnetic domains observed by magnetic force microscopy are strongly modulated by applying gate biases. Our findings propose the strong coupling between charge and spin order in vanadium-doped WSe$_2$, opening possibilities for using two-dimensional semiconductors for spintronic devices.

*This work was supported by the Institute for Basic Science of Korea (IBS-R011-D1).*

**Proximity effect between graphene and 2D anti-ferromagnetic insulator α-RuCl$_3$**

EDWARD SEIFERT (Presenter), DEVASHISH P GOPALAN, Carnegie Mellon Univ, ZAIYAO FEI, XIAODONG XU, Physics, University of Washington, DAVID MANDRUS, Oak Ridge National Laboratory, BENJAMIN HUNT, Carnegie Mellon Univ — Proximity effects attempting to combine electronic properties of graphene with exotic phenomena in other 2D van der Waals materials have been a central focus of condensed matter research for the past decade. To date, much work has been done studying proximity effects between graphene and ferromagnetic insulators, but little is known experimentally about the coupling between graphene and anti-ferromagnetic insulators. We report transport results from proximity devices consisting of graphene and α-RuCl$_3$, a layered anti-ferromagnetic Mott insulator predicted to host a so-called Kitaev quantum spin liquid. Upon cooling the device, the derivative of resistance with temperature shows a peak-dip feature. Depending on the gate voltage, this feature is seen anywhere from 35-50K, much higher than the Neel temperature of 14K. This could indicate a magnetic phase transition in the heterostructure.

*This work was supported by the Department of Energy under the Early Career Award program, award number #DE-SC0018115*
8:36AM F51.00004: Emergent quantum Hall ground states driven by proximity exchange coupling in 2D material/ferromagnet interfaces*  DHAVALA SURI (Presenter), MASSACHUSETTS INSTITUTE OF TECHNOLOGY, ANDREW SAYDJARI, Harvard University, LINGYI ZHONG, Fudan University, SIDDHARTH OMAR, University of Groningen, ZHONGXUN GUO, Fudan University, MASON GRAY, Boston College, MIRKO ROCCI, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, KENNETH BURCH, Boston College, WENZHONG BAO, Fudan University, BART VAN WEES, University of Groningen, PATRICK A LEE, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, AMIR YACOBY, Harvard University, PENG WEI, University of California Riverside, JAGADEESH MOODERA, MASSACHUSETTS INSTITUTE OF TECHNOLOGY — In hBN/Graphene/EuS layer system we observe phase transitions spanning various quantum Hall regimes from quantum spin Hall edge state to anti-ferromagnetic state via an intermediate canted anti ferromagnetic (CAF) state. This is first demonstration of quantum Hall ferromagnetic ground states driven by proximity coupling with a ferromagnetic insulator (resulting in a huge exchange field) and achieved at a much lower applied magnetic field than any study in the past. The results clearly demonstrate the opening of edge state corresponding to CAF gap, while at much higher fields we observe reentrant insulating phase corresponding to the bulk gap as predicted by theory [1]. We also investigate the effects with WS2/Graphene/EuS stack. This led to interesting ground states emerging as a result of ferromagnet and SOC coupling induced by proximity effects. In this talk we will discuss the details of emergent ground state in 2D material/Ferromagnet interface effects along with future direction.


*CIQM-NSF DMR1231319 NSG-DMR1700137 ONR N00014-16-1-2657

8:48AM F51.00005: Observation of Exchange bias effect in ferro-/antiferromagnetic van der Waals heterostructures*  CHANGGU LEE (Presenter), PAWAN KUMAR SRIVASTAVA, YASIR HASSAN, HYOBIN AHN, SOON-GIL JUNG, YISEHAK GEBREDINGLE, MINWOONG JOE, ABBAS SABBTAIN, BYUNGGIL KANG, TUSON PARK, Sungkyunkwan Univ, JE-GUEN PARK, Seoul National University, KYUNG-JIN LEE, Korea University — Recent discovery of magnetic van der Waals (vdW) materials offers an intriguing possibility for two-dimensional (2D) spintronics. An essential phenomenon for realizing 2D spintronics is the exchange bias effect in ferromagnet (FM)/antiferromagnet (AFM) vdW heterostructures. In a metallic FM /semiconducting AFM vdW heterostructure, we experimentally demonstrate that a finite exchange bias is maintained down to bilayer AFM and it vanishes at monolayer. Moreover, the semiconducting property of AFM allows us to electrically control the exchange bias, providing an energy-efficient knob for spintronic devices.

*This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) (NRF-2016K1A1A2912707, 2016R1A2B4012931, 2016R1A6A3A11934734, 2018R1D1A1B07049669), the Institute for Basic Science (IBS) in Korea (Grant No. IBS-R009-G1), the KISTI grant (KSC-2018-CRE-0119), the Global Frontier Research Center for Advanced Soft Electronics (CASE-2013M3A6A5073173) and by an Institute for Information & Communications Technology Promotion (IITP) grant (B0117-16-1003) funded by the Ministry of Science and ICT of Korea.
9:00AM F51.00006: Edge Effects in Transition Metal Dichalcogenides on Antiferromagnetic Substrates* NATALIA CORTÉS, Departamento de Fisica, Universidad Tecnica Federico Santa Maria, OSCAR AVALOS-OVANDO (Presenter), SERGIO E ULLOA, Department of Physics and Astronomy, Ohio University — We explore proximity-induced antiferromagnetism (AFM) on transition metal dichalcogenides (TMD), focusing on molybdenum ditelluride (MoTe$_2$) ribbons with zigzag and/or armchair edges, deposited on AFM substrates with diverse AFM orders, such as prospective candidates MnO, CoO or MnPX$_3$ (X = S; Se) substrates. We model the heterostructure in real space with a tight-binding model, incorporating the exchange and Rashba fields induced by proximity from the substrate. For the zigzag terminated TMDs, we find augmented Rashba SOC and Rashba type spin splittings for midgap states. For the armchair terminated TMDs, we find propagating pseudohelical edge modes, as well as either gapped or gapless edge modes depending on the ribbon’s width. We also explore the creation of spin polarized currents on these edges. These hybrid structures can serve as building blocks for spintronic devices and provide versatile platforms to further understand proximity effects in diverse materials systems.


*N.C. acknowledges support from Conicyt grant 21160844, DGIIP and the hospitality of Ohio University. S. E. U. and O. A.-O. acknowledge support from NSF DMR-1508325.

9:12AM F51.00007: Partial Flatbands in a Spin-Orbit Coupled Twisted Bilayer Lieb Lattice AVADH SAXENA (Presenter), Los Alamos Natl Lab, SAIKAT BANERJEE, University of Augsburg — Topological classification of band-structure in various solid state materials has become one of the centerpieces of research in modern condensed matter physics. Typically, the specific topological nature of a dispersive band in a lattice system originates from a particular discrete symmetry present in the crystal. In this work, we analyze the topological properties of a partial/complete flatband in an apparently not so well known system -- a bilayer Lieb lattice. We demonstrate the emergence of flatbands with large Chern numbers in the presence of spin-orbit coupling. Our results are then contrasted with the flatbands in bilayer graphene and bilayer kagome lattice. We also consider a multi-layer Lieb lattice with even larger Chern numbers and speculate on the possibility of a superfluid phase in the presence of certain types of interactions.
9:24AM F51.00008: Yttrium-based Janus transition metal chalcogenides: Magnetic layered multiferroics*  PANKAJ KUMAR (Presenter), PRIYANKA MANCHANDA, PRATIBHA DEV, Howard University — The discovery of graphene in 2004 heralded the further discovery of hundreds of other two-dimensional (2D) materials, with a wide range of electronic and optical properties. Till recently, however, it was believed that magnetism cannot exist in 2D materials, in keeping with the Mermin-Wagner Theorem. This changed with the observation of long-ranged magnetism in a few 2D materials, such as CrI$_3$ and Cr$_2$Ge$_2$Te$_6$. This has started an active search for additional magnetic 2D crystals. In this talk, we present our theoretical research on a new class of magnetic 2D materials - Yttrium-based Janus transition metal chalcogenide (TMD) semiconductors. As a prototype of these materials, we studied properties of the YSSe Janus structure. YSSe has a magnetic moment of 1μ$_B$/formula unit (f.u.), and an in-plane magneto-crystalline anisotropy energy of 162 μeV/f.u. Along with broken time reversal symmetry, a YSSe layer also lacks mirror symmetry. Hence, it exhibits ferroelectricity, with a polarization that can be switched under the application of strain, making it a promising candidate material for ultra-compact spintronic and multiferroics-based devices.

*This work is supported by National Science Foundation under grant number DMR-1752840.

9:36AM F51.00009: Enhanced Zeeman splitting in MoS$_2$ monolayers doped with transition metals.  ARINJOY BHATTACHARYA (Presenter), MENGYING BIAN, ARMAN NAJAFI, PEIJIAN WANG, ALIREZA JALOULI, Physics, State Univ of NY - Buffalo, Buffalo, New York, JIEQIONG WANG, MOE Key Laboratory of Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi’an Jiaotong University, China, JIADONG ZHOU, Materials Science and Engineering, Nanyang Technological University, Singapore, SEN YANG, MOE Key Laboratory of Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi’an Jiaotong University, China, ZHENG LIU, Materials Science and Engineering, Nanyang Technological University, Singapore, HAO ZENG, ATHOS PETROU, Physics, State Univ of NY - Buffalo, Buffalo, New York — We developed an approach to dope MoS$_2$ monolayers with controllable concentration of transition metal ions. In this approach, a single phase transition metal-doped MoO$_3$ compound precursor was utilized to deposit ultrathin doped MoO$_3$ film by electron beam evaporation, followed by sulfurization of the precursor oxide layer to achieve monolayer transition metal doped MoS$_2$.

We have used magneto-reflectance spectroscopy to compare the Zeeman splitting of MoS$_2$ monolayers with that of MoS$_2$ doped with transition metals. At T = 7K we find that the A-exciton Zeeman splitting in the doped sample is 23% higher that of the undoped MoS$_2$. The enhancement is attributed to exchange interaction between the spins of carriers and those of the transition metal ions.
9:48AM F51.00010: Optical rotation in thin chiral/twisted materials and the gyrotropic magnetic effect  YANQI WANG (Presenter), University of California, Berkeley, TAKAHIRO MORIMOTO, Applied physics department, University of Tokyo, JOEL MOORE, University of California, Berkeley — The rotation of the plane of polarization of light passing through a non-magnetic material is known as natural optical activity or optical gyrotropy. The behavior of this effect in thin conductors is of current interest. For example, the low frequency limit of gyrotropy in chiral 3D crystals, known as the gyrotropic magnetic effect (GME), is controlled by the orbital magnetic moment of electrons, which has been proposed to be relevant to switching in twisted bilayer graphene. We show that the GME is not limited to bulk materials but also appears for quasi-2d systems with minimal structure incorporated in the third direction. Starting from multi-band Kubo formula, we derive a generic expression for GME current in quasi-2d materials induced by low-frequency light, and provide a Feynman diagrammatic interpretation. The relations between the 2d finite layered formula and 3d bulk formula are also discussed.


*Alexander von Humboldt Foundation, Capes, DPG SFB 1277.
Influence of interface-induced spin-orbit interaction on transport in graphene-on-WSe$_2$ heterostructures* MUHAMMAD ZUBAIR (Presenter), Department of physics, Concordia University, MUHAMMAD TAHIR, Department of physics, Colorado State University, PANAGIOTIS VASILOPOULOS, Department of physics, Concordia University — Proximity effects in graphene/transition-metal dichalcogenides heterostructures are expected to play a major role in the fields of spintronics and valleytronics. We investigate the electronic dispersion of such heterostructures in the presence of a proximity induced spin-orbit interaction (SOI) using a tight-binding (TB) model. The competition between different perturbation terms leads to inverted bands, when graphene is on WSe$_2$, and to topologically trivial band structures when it is placed on MoS$_2$, MoSe$_2$, and WS$_2$. In addition, we study the effect of symmetry breaking terms on ac and dc transport by evaluating the corresponding conductivities within linear response theory. The scattering-dependent diffusive conductivity increases linearly with electron density but weakens as the screening gets stronger. Further, we evaluate the power spectrum and assess its dependence on the spin and valley degrees of freedom and on the scattering which is essential at low frequencies.

*M. Z. and P. V. acknowledge the support of the Concordia University Grant No. VB0038 and Concordia University Graduate Fellowship. The work of M. T. was supported by Colorado State University.

Flavor Quantum Dots and Artificial Quark Model in Transition Metal Dichalcogenides* ZHI-QIANG BAO (Presenter), PATRICK CHEUNG, FAN ZHANG, University of Texas at Dallas — We show that the triply degenerate Q valleys in few-layer transition metal dichalcogenides provide a unique platform for exploring the rare flavor SU(3) symmetry in quantum dot geometry. The single and double dots are reminiscent of the quark model and eightfold way, and their many-body triplets and octets may be regarded as artificial quarks and hadrons. For the artificial quark transistor, each level hosts one central and two side Coulomb peaks of irrational height ratios, and flavor Kondo effects occur at 1/3 and 2/3 fillings with fractional conductance quantization in the unitary limit.

*This theoretical work at UTD is supported by Army Research Office under Grant No. W911NF-18-1-0416 and Natural Science Foundation under Grant No. DMR-1921581 through the DMREF program.
10:36AM F51.00014: Exchange Interaction Between Magnetic Adatoms in Irradiated Graphene* MODI KE (Presenter), MAHMOUD M. ASMAR, WANG KONG TSE, Univ of Alabama - Tuscaloosa — We present a theory for the non-equilibrium RKKY interaction in graphene irradiated by circularly polarized light. A k.p theory of the graphene Floquet Hamiltonian is developed, which provides a successive approximation scheme as the light-matter coupling strength is increased. Based on the Floquet k.p Hamiltonian, we calculate the real-space Floquet Green’s functions and the time-averaged RKKY interaction using Floquet-Keldysh formalism. We find that optical illumination generally suppresses the exchange interaction in undoped graphene, due to a band gap opened at the Dirac point. Results for doped graphene will also be presented.

*This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Early Career Award #DE-SC0019326.

F51.00015: Spin-Induced Optical Anisotropy on van der Waals Antiferromagnet* XINGZHI WANG (Presenter), JUN CAO, HIKARI KITADAI, TIANSHU LI, XI LING, Boston Univ — Two-dimensional (2D) magnetic systems have received growing interest revealing new physics of magnetism in the nanoscale limit. As an important family of van der Waals magnetic materials, metal phosphorus chalcogenides have attracted intense attention due to the intrinsic antiferromagnetism and the electronic bandgap in the visible range. Recently, we observe a strong anisotropy on optical absorption in 2D antiferromagnet, nickel phosphorus trisulfides (NiPS₃), which is induced by its spin structure in the antiferromagnetic phase. The temperature and polarization dependent study indicates the strong correlation between electronic and magnetic structure. A control experiment has been conducted on the other compounds in this family, which further supports our conclusion. Our studies reveal the unique electronic and magnetic properties of NiPS₃, paving the way for potential functionalities and applications of 2D magnetic materials.

*This work is supported by Boston University. X. L acknowledges the membership of the photonics center at Boston University.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F52 DCMP: Surface Chemistry and Photomaterials Mile High Ballroom
1E - Emily Bittle, National Institute of Standards and Technology
8:00AM F52.00001: Work Function Studies of Carbon Nanospikes for Electrochemistry by UPS* ARTHUR BADDORF (Presenter), YANG SONG, DALE K. HENSLEY, ADAM J. RONDINONE, Oak Ridge National Lab — Carbon nanospikes show excellent energy and selectivity for electrochemical conversion of CO$_2$ to ethanol$^1$ and N$_2$ to NH$_3$.$^2$ Reactivity is attributed to physical structure more than composition. A spike geometry concentrates the electric field, promoting local electroreduction of reaction molecules. Using UPS, we have measured the work function of carbon nanospikes transferred to vacuum after extraction from a N$_2$-saturated LiClO$_4$ electrolyte at a range of potentials. The work function exhibits a general decrease with increasing negative emersion potential. The decrease is not 1:1 eV/V to the applied potential, nor is it linear. This may reflect imperfect double layer retention during transfer through air and into vacuum. In most cases, UPS spectra were typical, with an obvious low-energy cutoff. However, for several samples, including the pristine nanospikes, two cutoffs appeared to exist, one suggesting a much lower work function. The nature of the low-energy cutoff and possible connection to the geometry will be discussed.


** A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

8:12AM F52.00002: Structural and Electrical Factors of the Photocatalytic Activity of Bi$_2$WO$_6$ and Bi$_2$MoO$_6$ in Water-Splitting Applications* STEVEN BAKSA (Presenter), Pennsylvania State University, QUINN CAMPBELL, Sandia National Laboratories, ISMAILA DABO, Pennsylvania State University — Artificial photosynthesis is a sustainable technological option to store solar energy through the photocatalytic conversion of carbon dioxide and water into chemical fuels. The main challenges with this photocatalytic process include tuning the band gap of the material to match the solar spectrum and ensuring its stability in aqueous environments. An appealing approach for developing such photocatalysts consists of intercalating functional layers into metal oxides, as is the case for perovskite-derived compounds of the Aurivillius (Bi$_2$A$_{n-1}$B$_n$O$_{3n+3}$) family, which have been shown to be photoactive under visible light. Using density-functional theory, we predict the nanosheet morphology of Bi$_2$WO$_6$ and Bi$_2$MoO$_6$ under applied voltage, and we provide a molecular description of the charged interface under controlled pH and applied voltage. This study offers a molecular interpretation of the competing structural and electrical factors that underlie the facet-dependent photocatalytic activity of layered Bi$_2$A$_{n-1}$B$_n$O$_{3n+3}$ compounds.

* The authors acknowledge support from:
The National Science Foundation under Grant DMR-1654625
The Penn State Computational Materials Education and Training (CoMET) program under Grant DGE-1449785
Density Functional Theory Studies of Protective Interlayer of Graphene for the Back Contact of Copper Zinc Tin Sulphur Thin Film Solar Cell* YAU LUN FELIX CHONG (Presenter), JUNYI ZHU, Chinese Univ of Hong Kong — CZTS(Se) based solar cell is one of the promising candidates in the development of the 3rd generation solar cell absorbers. However, the efficiency of CZTS is insufficient for commercial product. One of the major causes of low performance is poor back contact-absorber interface quality. During annealing process of CZTS, S atom diffuses into Mo back contact layer and form a detrimental secondary phase of MoS₂. Interlayer engineering has been proposed. However, most of the proposed interlayers are based on insulating systems. Here, we propose a new protective material of graphene as an effective diffusion barrier to block any S atom diffusion. Using Climbing Image Nudged Elastic Band Method based on Density Functional Theory calculation to find diffusion barrier and minimum energy path, we can show that the choice of our protective layer can effectively block S atoms diffusion under fabrication and operation environment. We also calculated the band alignment between the proposed protective interlayer and CZTS absorption layer. The results suggest the protective interlayer we proposed will not significantly degrade the performance of the solar cell.

*This work is supported by HKRGC, GRF, with the funding number of 14319416.

The Electromagnetic Enhancement of SERS and the Modified Partition of Optical States in the Strong Matter-Coupling Regime. KRITIKA JAIN (Presenter), MURUGESAN VENKATAPATHI, Indian Institute of Science — Surface enhanced Raman Spectroscopy (SERS) is a powerful optical sensing technique that is based on enhanced Raman signals from molecules in proximity of rough metal surfaces. Experiments¹ have shown unexpected large enhancements in SERS, even up to 10¹⁴. Conventional electromagnetic theory accounts for enhancements only up to 10⁶, and the anomalous enhancements have even been attributed to an unknown chemical origin²,³. We show that when one includes dynamics in fluctuations of an emitter strongly coupled to absorbing matter, such high gains are predicted due to tunneling out of photons from the strongly absorbing metal surface. This modification to the conventional partition of optical states into its radiative and non-radiative parts, is also imperative for emitters proximal to limiting small metal nanoparticles (< 10 nm in dimensions) which are fully absorbing. Some recent experiments have shown such anomalous gains in emission due to these extremely small nanoparticles. This effect can be exploited further in light generation, optical sensing and radiative heat transfer.

8:48AM F52.00005: Protecting high quantum efficiency photocathodes with two dimensional materials for long lifetimes*  GAOXUE WANG, Theoretical Division, T-1, Los Alamos National Laboratory, NATHAN A MOODY, AOT Division, Los Alamos National Laboratory, PING YANG, Theoretical Division, T-1, Los Alamos National Laboratory, ENRIQUE BATISTA (Presenter), Theoretical Division, CNLS, Los Alamos National Laboratory — Since soon after the discovery of the photoelectric effect, the goal of reaching highly efficient photoelectron emission has been a difficult and well sought out goal. Currently, applications such as XFEL and XERL, call for high intensity electron sources that can lead to bright and intense electron and x-ray beams. The intensity of the photoemitted beam, the quantum efficiency of the photocathode, is dominated by the absorption cross section, electron mobility, and surface work function. For practical reasons, the lifetime of the photocathode is important and long-lived photocathodes are very much sought to improve performance. Whereas alkali-based semiconducting photocathodes display much higher QE relative to metal surfaces, their chemical composition makes them very reactive to residual gases even at UHV conditions. We will discuss here approaches for neutralizing such reactivity on the surface not introducing higher barriers to the emitted electrons. A computational study will be presented for screening 2-dimensional coating materials and fundamental principles for the characteristics needed are extracted. We present not only design principles but also candidate materials that should be used for protecting these highly reactive surfaces

*LANL LDRD program

9:00AM F52.00006: Defect mediated self-powered, broad band and ultrafast InGaN based photodetector*  ARUN CHOWDHURY (Presenter), ROHIT PANT, Materials Research Centre, Indian Institute of Science, BASANTA ROUL, Central Research Laboratory, Bharat Electronics, DEEPEndRA KUMAR SINGH, KARUNA KAR NANDA, SALURU BABA KRUPANIDHI, Materials Research Centre, Indian Institute of Science — In this work, Si doped n+-InGaN epilayer has been grown on a 100 nm thick AlN template on an n-type Si (111) substrate to form semiconductor-insulator-semiconductor (SIS) heterostructure by plasma-assisted molecular beam epitaxy (PAMBE). The n+-InGaN/AlN/n-Si (111) device shows excellent self-powered and broad band photo response under UV-Visible (300-800 nm) light illumination and maximum response is observed at 580 nm for low intensity irradiance (0.1 mW/cm²), owing to the intermediate energy states present in InGaN lattice due to nitrogen vacancies. At zero bias, the device exhibits a high responsivity of 9.64 A/W with ultrafast rise and fall times of 19.9 and 21.4 μs, respectively. This is the highest reported responsivity for the InGaN based photodetectors at zero bias to best of our knowledge. Introduction of AlN buffer layer and doping enhance the photoelectrical properties of the device compared to other conventional detectors. This work opens up a new avenue for SIS heterojunction photo detectors with much improved performance as self-powered and broadband detectors over the previously reported values on InGaN.

*Deependra Kumar Singh acknowledges Council of Scientific and Industrial Research, New Delhi for providing senior research fellowship.
9:12AM F52.00007: The Effect of Au Nanoparticles on the Photovoltaic Conversion Efficiency in CdTe/CdS Thin Films*

YUNIS YILMAZ (Presenter), NOELLE SCHILLING, STEPHANE ARSHARUNI, MEHMET ALPER SAHINER, Physics, Seton Hall University — In our last study, we have worked on the effects Ag and Au nanoparticles have on the efficiency of CdS/CdTe thin film solar cells. Both had a positive effect on the efficiency of photovoltaic conversion. Now, we are testing Au nanoparticles on the same cells and plan on comparing the effects of different deposition times, and laser energy on the Au, and how it effects efficiency and Au nanoparticle size. We used PLD (pulsed laser deposition) to create these cells. The laser shoots the target material we want to deposit (CdS,Au,CdTe) turning it into plasma plume that deposits onto ITO (indium tin oxide) coated glass. Varying how long the laser shoots at the Au and at what energy changes the amount of Au deposited and the size and distribution of the particles as well. The more Au in the np junction, the more the increase in the efficiency of the solar cell due to plasmonic resonance effects. However, the efficiency cuts off with after a threshold value for Au deposition. Our last study concluded that we had already passed this saturation point, so now, we are testing lower deposition lengths and energies. The Au embedded cells were characterized by XRD, AFM, SEM/EDX, and a sourcemeter setup.

*This work is supported by NSF Award#: DMI-0420952, TUBITAK-2221Award, & NJSGC (NASA)

9:24AM F52.00008: Development of Molybdenum Nitride Thin-Films on Metal Substrates*

MUHAMMAD SAJID (Presenter), ASIM KHANIYA, WILLIAM KADEN, ABDELKADER KARA, Univ of Central Florida — Molybdenum Nitride exceeds in catalytic activity and product selectivity from industrial grade catalysts for Hydrodenitrogenation (HDN), removal of nitrogen from petroleum feedstocks. δ-MoN is suggested to be more active than bulk γ-Mo_2N phase, but more work is needed to better understand the relation between activity and atomic structure of catalysts. We are using DFT with added vdW effects, to study adsorption of both phases on metal substrates, having minimal lattice mismatch. Through Nudged Elastic Band (NEB) Calculations, reaction pathways and energy barriers of HDN reaction mechanisms of pyridine (simplest N containing aromatic molecule) will to studied. Thin films of catalyst phases will be developed under Ultra-High Vacuum (UHV) and studied via spectroscopic techniques (XPS, LEED, ISS, STM) and fixed or variable temperature mass spectrometry. Predictions from theory will be directly compared and verified with experimental observations. Combination from both theory and experiments will aid us towards reaching to the subtle connection between atomic structure and desired catalytic properties.

*American Chemical Society Petroleum Research Fund, Partial support is from U.S. Department of Energy under Award number DE-SC0007045. Computational resources of NERSC and UCF-Stokes.
DEEPENDRA SINGH (Presenter), ROHIT PANT, ARUN CHOWDHURY, BASANTA ROUL, KARUNA KAR NANDA, SALURU BABA KRUPANIDHI, Indian Institute of Science — Efficient photodetectors require high and fast photo-response as well as low power consumption. In the present work, we have demonstrated MoS$_2$/GaN nanorods/Si based self-powered and most importantly, spectrally distinctive photodetector. GaN nanorods were grown on Si (111) by Volmer-Weber type growth conditions using plasma-assisted molecular beam epitaxy, followed by growth of MoS$_2$ by pulsed laser deposition. HRTEM analysis shows MoS$_2$ has been incorporated on the top and sides of the nanorods, as well as in between them on Si. The device with top-bottom electrodes shows a maximum responsivity of 10.67 A/W at 900 nm in zero bias condition. The response and the recovery times have been estimated to be 30.9 and 33.9 μs, respectively. The spectral response studies also revealed that in the range of infrared wavelength (1000 - 1050 nm), there is an inversion (positive to negative) in the photocurrent. A mechanism based on illumination modulated activation of barriers, and the interaction of MoS$_2$ with GaN and Si has been discussed to explain the observed phenomenon of polarity inversion.

*Deependra Kumar Singh acknowledges Council of Scientific & Industrial Research, New Delhi for providing senior research fellowship.

SU JEONG HEO (Presenter), MEAGAN PAPAC, ANDRIY ZAKUTAYEV, National Renewable Energy Laboratory — Proton-conducting solid oxide electrolysis cell (H-SOEC) is of increasing interest as a result of its promising electrochemical application that efficiently converts electrical energy to chemical energy. However, the poor anode activity towards the water-splitting reaction is still the hindrance of the overall performance of H-SOCEs. In this study, novel perovskite Ba(ZrYPr)O$_3$-δ (BZYP) materials are investigated as the anode for the electrolysis cell to improve its proton-conducting ability. We used high-throughput experimental technique to reveal the chemical and electrical properties of BZYP perovskite and identify their appropriate composition for effective water splitting application. The BZYP combinatorial libraries films are synthesized using combinatorial pulsed laser deposition (PLD) and characterized by spatially resolved techniques for composition, structure, thickness, and electrical properties. Overall, through innovative material discovery and characterization using HTS, an anode with extensively broadened reactive sites will be developed for proton-conducting solid oxide electrolysis cells applications.

*This work was supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE) under the contract number DE-EE0008378.
10:00AM F52.00011: Optical properties and carrier transport in graphene-mesoporous silicon nanocomposites  DÉFI JUNIOR JUBGANG FANDIO (Presenter), Physique, Université de Sherbrooke — Graphene outstanding properties has been used to enhance the performance of various optoelectronic devices, in particular the field of photovoltaics [1]. In this work, we investigate the optical properties and charge carrier transport of mesoporous silicon nanocomposites coated with few—layer graphene. Photoconductivity properties and carrier capture/recombination dynamics of the photocarriers in these films are studied via optical pump-terahertz probe measurements. Our results show influence of carbon deposition temperature on the Si nanocrystallites luminescence bands as well as the appearance of new higher energy emission bands. The carrier recombination dynamics is largely affected by the presence of defects at the Si/graphene interface. The frequency dependent photoconductivity curves are well reproduced by the Drude-Smith model, like that used for studying the properties of a film composed of Si nanoparticles dispersed in an oxide matrix [2]. The relatively high mobility and low carrier recombination time in these nanostructures make them good candidates for THz photoswitch applications.


10:12AM F52.00012: The Role of Metal-Semiconductor Interface in Hybrid Perovskite Devices for High-Performance Solid-State Detectors*  SHREETU SHRESTHA (Presenter), Hsinhan Tsai, Michael YoHo, Fangze Liu, Los Alamos National Laboratory, Yusheng Lei, University of California, San Diego, Jon Baldwin, Sergei Tretiak, Ducta Vo, Wanyi Nie, Los Alamos National Laboratory — Hybrid perovskites have emerged as excellent semiconductors enabling efficient opto-electronic devices. Apart from the intrinsic properties of the semiconductor, interfaces are critical to make a superior device. Here, we use scanning photocurrent microscopy on lateral methylammonium lead triiodide (MAPbI) single crystal devices with commonly used high work function metal and low work function metal contacts to investigate perovskite-metal interfaces. By comparing the spatially resolved photocurrent maps of devices with Au (high work-function metal) to Pb (low work-function metal), we find that a Schottky barrier exists in both cases and the barrier is higher for the Pb/perovskite junction resulting in a lower leakage current. From the decay of the photocurrent profile near the metal contacts, we estimate charge carrier diffusion length to be 9 ± 2 µm. Using this knowledge, we successfully demonstrate a single crystal MAPbI gamma ray detector from which sharp gamma-ray induced pulses are observed. Our study indicates that the interface plays a significant role especially in solid state detector operating at low flux photon counting mode.

*Supported by Laboratory Directed Research Direction Funding from Los Alamos National Laboratory
**10:24AM F52.00013: p-Diamond as a plasmonic material for high frequency applications**

SERGEY RUDIN (Presenter), GREG RUPPER, TONY G. IVANOV, US Army Rsch Lab - Adelphi, MICHAEL S SHUR, Rensselaer Polytechnic Institute — The gate-controlled hole gas at the hydrogenated diamond surface was predicted to have a plasmonic response to a terahertz and sub-terahertz electric field, making p-diamond field effect transistors promising candidates for implementing room temperature plasmonic devices. The predicted performance of diamond plasmonic detectors shows their potential for high temperature, high voltage, and radiation hard applications and for THz communications and spectroscopy. The hole mobilities in our samples allow for a room temperature resonant plasmonic response. It makes possible the realization of p-diamond based emitters in terahertz and sub-terahertz range, using strong current driven plasma instability in gated channels. Toward the optimal design of p-diamond plasmonic devices we simulated the response using the complete set of hydrodynamic equations, including the thermal transport and accounting for effects of viscosity and pressure gradients. In the strong signal regime we find that a shock wave develops in the charge density and drift velocity profiles. Due to high value of the dielectric breakdown field in diamond the diamond plasmonic device can operate in the strong signal regime, when a shock wave propagates in the channel.

**10:36AM F52.00014: Influence of headgroup and chain length on the surface freezing behavior of long chain amphiphiles**

SARANSHU SINGLA (Presenter), AMANDA STEFIN, HE ZHU, ALI N DHINOJWALA, Univ of Akron — Long-chain polar amphiphiles such as alcohols and amines form a finite contact angle on high-energy solid surfaces on account of formation of an oriented monolayer, as opposed to expected complete wetting. Previous experiments with octadecanol (and hexadecanol) suggest that the monolayer formed on alumina displays surface freezing behavior on account of strong headgroup-substrate interactions. However, the data for different headgroups and chain lengths is elusive in literature. In the present study, we investigate the combined effect of headgroup-substrate interactions and chain length on the observed surface freezing behavior using interface-sensitive sum frequency generation spectroscopy (SFG). SFG provides information about ordering of amphiphilic molecules at the sapphire-melt interface along with interaction strength of different headgroups with sapphire. Our study provides insights into the fundamental mechanism of monolayer formation.

*National Science Foundation*
Molecular beam epitaxial growth of high quality BeMgZnO single crystal films for ultraviolet photodetectors

YIFEI FANG (Presenter), Key Laboratory of High Power Laser Materials, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, LONGXING SU, Department of Materials, Sun Yat-Sen University, MIN XU, YIN HANG, Key Laboratory of High Power Laser Materials, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences — High quality ZnO single crystal films and alloy films were prepared on sapphire substrate by molecular beam epitaxy. By studying the influence of growth parameters on quality, components and defect density of the film, repetitive and controllable epitaxial growth conditions were obtained, and the possible positions and effects of doping elements, Be and Mg, in the crystal were further studied. The high quality of film was verified by RHEED and TEM. It is found that with small ionic radius Be doped in the lattice is easy to produce lattice distortion, and has a certain probability of entering the interstitial position. However, Mg atoms have high solid solution in ZnO. Photoconductive, schottky junction and heterojunction UV photodetectors were further prepared and their physical properties were systematically studied. We found that the response speed of the device is greatly slowed down due to the space charge layer caused by O₂ adsorption, and the response time is optimized to a scale of microsecond by Be doping. Heterojunction devices have the advantages of self-drive and ultra-fast response, which can be used as self-powered devices in some unmanned and harsh working environments. This research gives guidance for application of ZnO in semiconductor optoelectronic devices.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F53 DCMP: Transport Properties of 2D Materials

Alexey Lipatov

A hidden quantum phase in two-dimensional WTe₂

SANFENG WU (Presenter), Princeton University — Correlations, spin-orbit coupling and topology are all important in the atomically thin WTe₂ layers. In this talk I will introduce our recent quantum transport studies of two-dimensional WTe₂ where we discover a hidden quantum phase.

*This research was supported by NSF through the Princeton University Materials Research Science and Engineering Center DMR-1420541
8:12AM F53.00002: Anisotropic magnetotransport in few-layer Nb-doped WSe$_2$

HIROYUKI NAKAMURA (Presenter), University of Arkansas, AVAISE MOHAMMED, WILFRIED SIGLE, YI WANG, PETER WOCHNER, Max Planck Institute for Solid State Research, JOHN VILLANOVA, JEB STACY, SALVADOR BARRAZA-LOPEZ, HUGH CHURCHILL, University of Arkansas, PETER VAN AKEN, HIDENORI TAKAGI, Max Planck Institute for Solid State Research — Hole-doped epitaxial WSe$_2$ films with thicknesses of three to six monolayers were grown by a hybrid pulsed-laser deposition, in which metallic alloy targets were laser-ablated under a controlled Se vapor. The Hall effect indicated active Nb-dopant concentrations of 10-50 at%. Scanning transmission electron microscopy revealed that Nb atoms occupy W sites, and 2H- as well as 3R-stacking coexist in the films. A striking anisotropy between magnetoconductance (MC) for in-plane (B // I) and out-of-plane (B ⊥ I) magnetic fields was found, showing a complete absence of weak antilocalization for B ⊥ I, while it restores for B // I at intermediate temperatures. The band structure of 2H-3R Nb:WSe$_2$ obtained by first-principles calculations is shown, based on which a few possible origins of the MC will be discussed.

8:24AM F53.00003: Observation of monolayer-like quantum transport in few-layer MoS$_2$

TIANYI HAN (Presenter), XU HAN, JIANGXIAZI LIN, Physics Department, Hong Kong University of Science and Technology, BENJAMIN A. PIOT, Laboratoire National des Champs Magnétiques Intenses, XIANGBIN CAI, DING PAN, JUNWEI LIU, NING WANG, Physics Department, Hong Kong University of Science and Technology — The conduction band minimum of MoS$_2$ shifts from K valley to Q valley when its thickness increases from monolayer to bulk. Previously, K valley quantum transport has been extensively studied in monolayer MoS$_2$, revealing its intriguing physical properties such as the spin-valley locking effect and the interaction enhanced Zeeman splitting. However, the fabrication of monolayer MoS$_2$ device requires considerable efforts mainly due to the challenges of achieving good electrical contact. Here we report the observation of monolayer-like K valley quantum transport in high quality few-layer MoS$_2$. Well-developed two-fold quantum oscillations are presented, with valley Zeeman splitting and spin polarized Landau levels at high magnetic field. Further, we observe multi K band conduction in the Landau fan diagram, from which the spin-orbit coupling splitting energy is estimated. Our observation offers the possibility of switching from Q valley to K valley transport in few-layer MoS$_2$.

*This work is supported by the Research Grants Council of Hong Kong (Project No. 16300717, C6021-14E, SBI17SC16), HKUST-UoM Seed Fund 2017. We acknowledge the technical support from the Raith-HKUST Nanotechnology Laboratory and the support of the LNCMI-CNRS, member of the European Magnetic Field Laboratory (EMFL).
8:36AM F53.00004: Preferential out-of-plane conduction and quasi-one-dimensional electronic states in layered van der Waals material 1T-TaS$_2$  EDOARDO MARTINO (Presenter), KONSTANTIN SEMENIUK, ALLA ARAKCHEEVA, CARSTEN PUTZKE, PHILIP MOLL, HELMUTH BERGER, Ecole Polytechnique Federale de Lausanne, IVO BATISTIC, University of Zagreb, EDUARD TUTIŠ, Institute of Physics - Zagreb, ANA AKRAP, University of Fribourg, LASZLO FORRO, Ecole Polytechnique Federale de Lausanne — Layered metallic transition-metal dichalcogenides are conventionally seen as two-dimensional conductors, despite a scarcity of systematic studies of the interlayer charge transport. Motivated by the ascending strategy of functionalizing 2D materials by vertical heterostructures we initiated an in-depth study of out-of-plane charge dynamics and emergent properties arising from interlayer coupling. Here, we reveal c-axis-oriented quasi-one-dimensional electronic states in 1T-TaS$_2$, a layered system hosting a plethora of diverse phases, by probing its out-of-plane electrical resistivity using focused-ion-beam-tailored crystals. The in-plane conduction appears non-metallic due to presence of a unique nanoarray of charge density wave (CDW) domains. All the while, the interlayer resistivity has a metallic temperature dependence with the anisotropy close to one, as a result of intertwining of the orbital and CDW orders. The compound is known for what was believed to be a Mott-type localisation below 150 K. Yet with our data, supplemented by ab-initio calculations, we interpret the transition as a Peierls-like instability of the quasi-one-dimensional electronic structure. Our findings present a very unintuitive behaviour in a van der Waals crystal.

8:48AM F53.00005: Band filling and cross quantum capacitance in ion gated semiconducting transition metal dichalcogenide monolayers  HAIJING ZHANG (Presenter), Physics of Quantum Materials, Max Planck Institute for Chemical Physics of Solids, CHRISTOPHE BERTHOD, Department of Quantum Matter Physics, University of Geneva, HELMUTH BERGER, Institut de Physique de la Matiere Complexe, Ecole Polytechnique Federale de Lausanne, THIERRY GIAMARCHI, ALBERTO MORPURGO, Department of Quantum Matter Physics, University of Geneva — Ionic liquid gated field-effect transistors based on semiconducting transition metal dichalcogenides are attracting significant scientific interest, but important aspects of how charge carriers are accumulated in these systems remain elusive. Here we present a thorough analysis of charge accumulation in MoSe$_2$ and WSe$_2$ monolayers. We identify the conditions when the chemical potential enters different valleys in the monolayer band structure (the K and Q valleys in the conduction band and the two spin-split K-valleys in the valence band) and find that an independent electron picture describes the occupation of states well. Unexpectedly, however, the same analysis shows that the total device capacitance cannot be simply described in terms of the series connection of a geometrical capacitance and of a quantum capacitance given by $C_Q = e^2/(d\mu/dn)$, as commonly assumed. This unexpected behavior is attributed to the presence of a cross quantum capacitance, which originates physically from mutual screening of the electric field generated by charges on one plate from charges sitting on the other plate. Our findings therefore reveal an important contribution to the capacitance of physical systems that had been virtually neglected until now.
2e charge transport in a quantum Hall - superconductor junction revealed by shot noise

MANAS SAHU (Presenter), ARUP KUMAR PAUL, JAGANNATH SUTRADHAR, Department of physics, Indian Institute of Science, Bangalore 560012, India, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Material Science, 1-1 Namiki, Tsukuba 305-0044, Japan, SUBROTO MUKERJEE, SUMILAN BANERJEE, ANINDYA DAS, Department of physics, Indian Institute of Science, Bangalore 560012, India — Two remarkable phenomena of condensed matter physics, the quantum Hall (QH) effect and superconductivity, when combined, can give rise to exotic topological excitations and hold great promises for future quantum computation. Andreev reflection (AR) is the underlying phenomena, which determines the quasiparticle dynamics at the QH–superconductor (SC) junction. Even decades after the discoveries of QH and SC, the AR at the QH-SC junction remains elusive. Here we have carried out conductance and shot noise measurements in a graphene QH coupled to a MoRe superconductor. The QH plateaus are observed at 4(N+1/2)e^2/h, which are identical to the conductance plateaus with a normal contact. This observation is consistent with our theoretical calculation of electron-hole mixing due to repetitive AR at QH - SC junction. By measuring shot noise, we observe the Fano factor close to unity when the bias energy is less than the superconducting gap. This is direct evidence of 2e charge transport at QH - SC junction. Above the superconducting gap, the Fano factor almost vanishes, as expected due to regular charge e transport. This work will pave the way for exploration of more exotic systems, such as junction of a fractional QH and a superconductor, by shot noise measurements.

Direct measurement of layer polarizability in a van der Waals ferroelectric semimetal

QINGRUI CAO (Presenter), SERGIO C DE LA BARRERA, VINEETHA BHEEMARASETTY, Department of Physics, Carnegie Mellon University, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, DI XIAO, YANG GAO, BENJAMIN HUNT, Department of Physics, Carnegie Mellon University — A ferroelectric semimetal has coexistence of spontaneous electric polarization and metallicity. A recent study [1] demonstrated bilayer and trilayer 1T'-WTe₂ exhibit an out-of-plane switchable polarization using graphene as an electric-field sensor. However, a direct measurement of its layer polarizability is still lacking. Here, we detect and quantify the ferroelectricity by layer-resolved capacitance measurements [2] in dual-gated bilayer WTe₂, allowing us to control applied electric field and charge density independently. Moreover, we examine the density-dependent polarizability and extract the critical densities above which the polarization becomes weaker. All of our observations, including hysteresis, "near-layer capacitance enhancement", density dependence of the polarization, are consistent with the theoretical predictions based upon an electrostatic model of capacitance derived from a "tilted-Dirac-cone" model of bilayer WTe₂.

9:24AM F53.00008: Electron-phonon scatterings and their roles in vertical charge transport through van der Waals heterostructures  
SU Yong JUNG (Presenter), Korea Research Inst of Standards and Science (KRISS) — Electron–phonon scattering in solid-state systems is a pivotal process in determining many of key physical quantities such as charged carrier mobilities and lattice thermal conductivities. Here, we report electron tunneling measurements with a semiconducting transition metal dichalcogenide, WSe$_2$, as the tunnel medium. In van der Waals (vdW)-coupled vertical heterostructures, inelastic quantum tunnel events activated by turbostratic electron–phonon scatterings constructively establish an adjunct transport channel, which drastically increases its loads in vertical charge flows with increasing tunnel medium thickness. Phonons interacting with the tunnel electrons are layer-number dependent, varying by monolayer vs. bi- and triple-layer WSe$_2$, with an out-of-plane flexural ZA mode as the common excitation. In addition, we find out that second-order electron–phonon scatterings become conspicuous in the multilayered films, involving assorted phonons in the tunnel media and the vDW heterojunctions.

9:36AM F53.00009: Orientation-dependent transport and Goos-Hanchen effect in phorsphorene  
LI RuiGang (Presenter), University of Science and Technology of China, KWOK SUM CHAN, City University of Hong Kong, ZIJING LIN, University of Science and Technology of China — By using the continuum model, we systematically investigate the transport property in the phorsphorene NPN junction. Different devices with different angles between the ribbon and armchair directions are studied. With the increase of this angle from 0°, it is found that the transmission first exhibits the oscillating behavior. Particularly, with the further increase of the angle close to 90°, the transmission goes through a fast drop to zero. We further find that the fast drop arises from the transformation of the transporting carriers from the Dirac quasiparticles into Schrodinger ones, and the angel of this transformation is related to the anisotropy of the effective mass, providing the possibility to shed light on the electronic device design. Furthermore, study of the Goos-Hanchen effect in the phorsphorene NPN junction is also addressed. It is interesting to find that even for the slight change of the angle between the ribbon and armchair directions, remarkable change of the incoming wave pocket is obtained, providing the promising candidate as the wave-pocket-selected filter. Finally, all above properties in NN’N junctions of the bulk phorsphorene are also addressed.
9:48AM F53.00010: Anomalous Coulomb Drag between InAs Nanowire and Graphene Heterostructures  
RICHA MITRA (Presenter), MANAS SAHU, Department of Physics, Indian Institute of Science, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Namiki 1-1, Ibaraki 305-0044, Japan., HADAS SHTRIKMAN, Department of Physics, Weizmann Institute of Technology, Israel, A K SOOD, ANINDYA DAS, Department of Physics, Indian Institute of Science — Correlated charge inhomogeneity breaks the electron-hole symmetry in two-dimensional bilayer heterostructures, responsible for non-zero drag appearing at the charge neutrality point. Although several theories predict this phenomenon, there is no consensus over the actual mechanism responsible for it. Here we report, Coulomb drag in a novel drag system consisting of a two-dimensional (2D) graphene and a one dimensional (1D) InAs nanowire (NW) heterostructures. For monolayer graphene (MLG)-NW heterostructures we observe an unconventional drag resistance peak near the Dirac point due to the correlated inter-layer charge puddles, which decreases monotonically with temperature (∼T⁻²) but increases rapidly with the magnetic field (∼B²). These anomalous responses together with the mismatched thermal conductivities of graphene and NWs establish the energy drag as the responsible mechanism of Coulomb drag in MLG-NW devices. In contrast, for bilayer graphene (BLG)-NW devices the drag voltage reverses sign across the Dirac Point, consistent with momentum drag but remains almost constant with magnetic field and temperature. These Coulomb drag measurements in 2D-1D systems, hitherto not reported before, will pave the future realization of correlated condensate states in novel systems.

10:00AM F53.00011: Gate-defined Quantum Confinement in few-layer Black Phosphorus Transistor*  
JIAWEI YANG (Presenter), SHI CHE, Ohio State Univ - Columbus, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, SEONGPHIL MOON, DMITRY SMIRNOV, national high magnetic field laboratory, MARC W BOCKRATH, RUOYU CHEN, CHUN NING LAU, Ohio State Univ - Columbus — Black phosphorus is a novel two-dimensional(2D) semiconductor which has attracted considerable research interest due to its tunable band gap and high electron mobility. Here we demonstrate quantum confinement defined by split gate in devices based on few-layer black phosphorus. The tunability of split gate can be illustrated by the fact that a device can be tuned off by split gate alone. Quantized conductance is observed when the width of the quantum point contact is varied. In quantum Hall regime, p-p'-p junction formed by tuning split gate are studied. The work opens the door for using black phosphorus as platform for electronic and optoelectronic applications.

*This work is supported by NSF/ECCS 1509958. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490 and the State of Florida. K.W. and T.T. acknowledge support from the Elemental Strategy Initiative conducted by the MEXT, Japan and JSPS KAKENHI Grant Numbers JP26248061, JP15K21722 and JP25106006.
Ultrafast currents in the monolayer of transition metal dichalcogenides

SEYYEDEH AZAR OLIAEI MOTLAGH (Presenter), VADYM APALKOV, MARK I STOCKMAN, Georgia State University — We theoretically predict that in a monolayer of the transition metal dichalcogenide (TMDCs), an applied ultrafast intense optical pulse with the polarization perpendicular to the TMDC's axis of symmetry induces two types of currents: a trivial current, which flows in the direction of the applied pulse and a nontrivial current, which flows in the direction perpendicular to the polarization of the pulse. The applied pulse has a linear polarization with a high amplitude of several Volt per Angstrom and the duration of a few femtoseconds. Our results show that the ultrafast field-driven currents with asymmetric profiles transfer the electrons asymmetrically, which causes the monolayer of TMDC to become electrically polarized. The induced nontrivial current and the net electrical polarization are due to Berry curvature, which is nonzero near the K and K' valleys [1].


On the nature of carrier states around the fermi level at the LAO/STO interface

LIVIU CHIONCEL, TOBIAS STROBL (Presenter), Chair for Theoretical Physics III, Augsburg University, PATRICK SAILER, Chair for Experimental Physics VI, Augsburg University, DANIEL BRAAK, Max Planck Institute for Solid State Research, Stuttgart, THILO KOPP, Chair for Experimental Physics VI, Augsburg University — We propose a minimal tight-binding one-band model for the interface layer of LAO/STO consisting of “effective” carriers (of Ti-dxy character) in random magnetic fields. These fields result from the hybridization of Ti-d(e_g)-bands and oxygen vacancies at the LAO/STO interface and can be seen as local moments (i.e. “effective impurities”) located at the Ti-site. Both the effects of a nonmagnetic on-site potential and the exchange interactions (Zeeman like) between carrier and magnetic impurities are taken into account. We apply the coherent potential approximation in studying this system.

TRR80: From Electronic Correlations to Functionality, Transregional research center of the German Research Foundation (DFG)
Electronic states and transport in graphene-TMD heterostructures

NOHORA HERNÁNDEZ CEPEDA, LILIA MEZA-MONTES (Presenter), Benemerita Universidad Autonoma de Puebla, SERGIO E ULLOA, Department of Physics and Astronomy, Ohio University — The advent of graphene and other monolayer 2D materials has opened the possibility to combine them in stacks that show interesting effects. We study here one interesting example, as the proximity of graphene and transition-metal dichalcogenides (TMD) heterostructures (G-TMD) results on unusual electronic states and transport properties. We employ an effective Hamiltonian that describes the broken inversion symmetry in graphene due to the proximity of the TMD but preserves temporal inversion [1]. The latter symmetry can be broken when an external magnetic field is applied, generating gaps in the band structure and consequent changes in electronic states that we study as function of field direction and magnitude for different TMD systems. We focus on the competition with spin-orbit effects. We also present results on transport properties, calculating the spin-dependent transmission and reflection coefficients of carriers propagating on a graphene sheet decorated with TMD ribbons on top.


Partially supported by CONACyT and VIEP-BUAP, México.

Experimental Quantum Transport Strain Engineering in Graphene

GUOQING WEI (Presenter), ANDREW C MCRAE, LINXIANG HUANG, ALEXANDRE CHAMPAGNE, Department of Physics, Concordia University, Montreal, Canada — We measure ballistic charge conductivity in strained suspended graphene and observe the theoretically predicted [1] strain-induced scalar and vector potentials. To do so, we built an experimental platform for quantum transport strain engineering in 2D materials. This instrumentation permits low temperature (0.3 K- 70 K) transport, 0T - 9T magnetic fields, and a tunable uniaxial strain (up to 3%) which is independent from the gate-tunable charge density. We show slippage-free clamping of high aspect-ratio graphene crystals where atomically ordered edges are unnecessary for quantitative straintronics. We study in detail transport in a graphene channel whose length is 90 nm and width is 600nm. we observe that both the channel and contacts are ballistic. By applying strain, we find the strain-induced scalar potential which shifts the low energy band structure downward by up to 30 meV. We also clearly observe the effect of a gauge vector potential which reversibly suppresses the conductance by up to 13.6%. We next aim to demonstrate total suppression of conductivity [1] and explore straintronics in other 2D materials.

8:00AM F54.00001: Chalker-Coddington network model as a Floquet topological insulator*

VICTOR GURARIE (Presenter), Department of Physics and Center for Theory of Quantum Matter, University of Colorado, Boulder, ANDREW POTTER, Department of Physics, University of Texas at Austin — We re-examine the Chalker-Coddington network model, which was originally introduced to model integer quantum Hall plateau transitions. We point out that the dynamics of this model actually describe a periodically-driven (Floquet) system whose bands have vanishing Chern number throughout the phase diagram. Instead, the topological phase of the network model arises from a non-trivial dynamical Floquet invariant, i.e. the network model describes transitions between trivial and chiral Floquet phases of a distinct topological class from the integer quantum Hall effect. In view of this observation, we re-evaluate the standard arguments given in the past that the quantum Hall plateau transition and the transition in the Chalker-Coddington network model belong to the same universality class.

*This work was supported by NSF DMR-1653007.

8:12AM F54.00002: Quantum Hall Effect in Quasi-One-Dimensional Weak Topological Insulator*

TIANYI XU (Presenter), PATRICK CHEUNG, University of Texas at Dallas, FENGCHENG WU, University of Maryland, College Park, FAN ZHANG, University of Texas at Dallas — Prototypical weak topological insulators (WTI) have been theoretically predicted to be realized in quasi-one-dimensional materials Bi₄X₄ (X = Br, I) [PRL 116, 066801 (2016)] and then experimentally confirmed in ARPES [Nature (London) 566, 518 (2019)]. The unique surface states of such a WTI have two entangled Dirac cones with strong anisotropy. We study theoretically the integer quantum Hall effect of such WTI surface states and show the important roles played by the special geometry, symmetry, topology, and their interplay in Bi₄X₄. We also predict prominent signatures in transport experiments.

*This theoretical work at UTD is supported by Natural Science Foundation under Grant No. DMR-1921581 through the DMREF program and Army Research Office under Grant No. W911NF-18-1-0416.
Non-interacting and interacting Graphene in a strong uniform magnetic field

ANKUR DAS (Presenter), RIBHU KAUL, GANPATHY MURTHY, Univ of Kentucky — We study monolayer graphene in a uniform magnetic field in the absence and presence of interactions. In the non-interacting limit for p/q flux quanta per unit cell, the central two bands have 2q Dirac points in the Brillouin zone in the nearest-neighbor model. These touchings and their locations are guaranteed by chiral symmetry and the lattice symmetries of the honeycomb structure. If we add a staggered potential and a next nearest neighbor hopping we find their competition leads to a topological phase transition. We also study the stability of the Dirac touchings to one-body perturbations that explicitly lowers the symmetry.

In the interacting case, we study the phases in the strong magnetic field limit. We consider on-site Hubbard and nearest-neighbor Heisenberg interactions. In the continuum limit, the theory has been studied before [1]. It has been found that there are four competing phases namely, ferromagnetic, antiferromagnetic, charge density wave, and Kekulé distorted phases. We find phase diagrams for q=3,4,5,6,9,12 where some of the phases found in the continuum limit are co-existent in the lattice limit with some phases not present in the continuum limit.


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US-Israel BSF 2016130

Quantum Hall Effect in Chirality-induced Weyl Semiconductor n-type Tellurene

GANG QIU (Presenter), CHANG NIU, YIXIU WANG, MENGWEI SI, WENZHUO WU, PEIDE (PETER) YE, Purdue Univ — Very recently a new mechanism of generating Weyl nodes were proposed in chiral crystals with strong spin-orbit coupling, which, in sharp contrast to conventional band-inversion-induced Weyl semimetals, can exist in semiconductor systems. Tellurium (Te) is predicted to have these Weyl nodes located at the edge of the conduction band, originated from its DNA-like chiral chain crystal structure. However Te is naturally p-type doped and its conduction band has rarely been studied through transport measurement. In this work we report the first quantum Hall experiment in ALD doped n-type 2D tellurium (dubbed as tellurene) samples with mobility 6,000 cm²/Vs. The chirality-induced Weyl nodes give rise to radial spin texture, and topologically non-trivial π Berry phase was detected in quantum Hall sequences. Additionally, the doping profile forms a wide quantum well with symmetric-antisymmetric energy states leading to an approximate SU(8) isospin symmetry. Our work expands the spectrum of Weyl matters into semiconductor regime for the first time.

*A portion of this work was performed at the NHMFL supported by NSF Cooperative Agreement No. DMR-1644779 and the State of Florida. The synthesis of 2D Te materials is supported by the National Science Foundation under Grant CMMI-1762698.
8:48AM F54.00005: Chiral quasiparticle tunneling between quantum Hall edges in proximity with a superconductor*  
IVAN BORZENETS (Presenter), City Univ of Hong Kong, MING-TSO WEI, ANNE M DRAELOS, ANDREW SEREDINSKI, CHUNG-TING KE, Duke University, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, MICHIHISA YAMAMOTO, SEIGO TARUCHA, RIKEN, FRANCOIS AMET, Appalachian State, GLEB FINKELSTEIN, Duke University — We study a two-terminal graphene Josephson junction with contacts shaped to form a narrow constriction, less than 100 nm in length. The contacts are made from type-II superconducting contacts and able to withstand magnetic fields high enough to reach the quantum Hall regime in graphene. In this regime, the device conductance is determined by edge states, plus the contribution from the constricted region. In particular, the constriction area can support supercurrents up to fields of ∼2.5 T. Additionally, enhanced conductance is observed through a wide range of magnetic fields and gate voltages. This additional conductance and the appearance of supercurrent is attributed to the tunneling between counterpropagating quantum Hall edge states along opposite superconducting contacts. 
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*CityU New Research Initiatives/Infrastructure Support from Central (APRC) No. 9610395, Hong Kong Research Grants Council (ECS) Project No. 9048125, ARO Award No. W911NF16-1-0122, NSF Awards No. ECCS-1610213 and No. DMR-1743907, Department of Energy, under Award No. DE-SC0002765, KAKENHI (Grants No. 38000131 and No. 17H01138).

9:00AM F54.00006: Hall and dissipative viscosity and conductivity in a disordered 2D electron gas  
IGOR BURMISTROV (Presenter), Landau ITP - Chernogolovka, MOSHE GOLDSTEIN, MORDECAI KOT, Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, VLADISLAV KURILOVICH, PAVEL KURILOVICH, Department of Physics, Yale University — Hydrodynamic charge transport is at the center of recent research efforts. Of particular interest is the nondissipative Hall viscosity, which conveys topological information in clean gapped systems. The prevalence of disorder in the real world calls for a study of its effect on viscosity, as well as on its relation with the nonlocal conductivity, the main venue to its experimental measurement. Here we address this question for disordered noninteracting 2D electrons. Analytically, we employ the self-consistent Born approximation, accounting for the modification of the single-particle density of states and the elastic transport time by the Landau quantization. Our results interpolate smoothly between the limiting cases of weak (strong) magnetic field and strong (weak) disorder. In the regime of weak magnetic field we describe the quantum (Shubnikov-de Haas type) oscillations of the viscosity, nonlocal conductivity, and Wen-Zee response. For strong magnetic fields we characterize the effects of the disorder-induced broadening of the Landau levels on the transport coefficients. This is supplemented by numerical calculations for a few filled Landau levels. Our results show that the Hall viscosity and its relation with conductivity are surprisingly robust to disorder.
9:12AM F54.00007: Geometric entanglement in integer quantum Hall states*  LUCIE FOURNIER (Presenter), WILLIAM WITCZAK-KREMPA, Universite de Montreal — We study the structure of entanglement in integer quantum Hall states using the entanglement entropy (EE) as well as the reduced density matrix, through its spectrum and eigenstates. We focus on an important class of spatial regions that have a sharp corner, which leads to an angle-dependent contribution to the EE. We unravel surprising relations by comparing this corner term at different fillings. We further find that the corner term, when properly normalized, has nearly the same angle dependence as conformal theories in 2 spatial dimensions. We also reveal that the low-lying entanglement spectrum and corresponding eigenfunctions describe edge excitations localized at the corner. Finally, we present an outlook for fractional quantum Hall states.

*Discovery Grant from NSERC
Grant from Fondation Courtois
Canada Research Chair
Alexander Graham Bell Canada Graduate Scholarships from NSERC

9:24AM F54.00008: Strong-disorder renormalization group approach to the integer quantum Hall effect  JOÃO GETELINA (Presenter), Sao Carlos Institute of Physics at the University of Sao Paulo; Missouri University of Science and Technology, MARTIN PUSCHMANN, Missouri University of Science and Technology, JOSE A HOYOS, Sao Carlos Institute of Physics at the University of Sao Paulo, THOMAS VOJTA, Missouri University of Science and Technology — The critical behavior of the integer quantum Hall transition has recently reattracted considerable attention [1]. We propose an alternative numerical approach, namely a modified strong-disorder renormalization group (SDRG) method, in order to investigate this transition. The SDRG method is a recursive decimation process which is known to yield exact results for electronic tight-binding models, provided one keeps all links generated under renormalization. In practical applications, the number of kept links is limited. Nonetheless, in a recent study of the Anderson localization transition, it has been shown that one can get reasonable results for the critical exponents by keeping only a relatively small maximum number of links per site [2]. We generalize this method to the integer quantum Hall problem and apply it to both square lattice and long strip geometries.

9:36AM F54.00009: Non-local induced pairing in chiral edge states* ANDREAS MICHELS (Presenter), Physics and Materials Research Science Unit, University of Luxembourg, PATRIK RECHER, Department of Mathematical Physics, TU Braunschweig, BERND H. BRAUNECKER, School of Physics and Astronomy, University of St. Andrews, THOMAS SCHMIDT, Physics and Materials Research Science Unit, University of Luxembourg — A superconductor in contact with a quantum Hall material will induce fundamentally non-local superconducting correlations in the quantum Hall edge state through the proximity effect. Such correlations are often put into models by hand in local approximations, but by building a model without assumed locality we are able predict the strength and non-local spatio-temporal behaviour of the correlation. Accurately modelling this correlation allows us to treat geometries of experimental interest and predict the behavior of interesting effects such as crossed Andreev reflection. This is relevant for several recent experiments, and the treated hybridized state has been proposed as part of a system hosting non-Abelian anyonic zero modes.

*University of Luxembourg and St. Leonard’s fellowship (University of St. Andrews)

9:48AM F54.00010: Reconstruction near the interface of a $\nu=4$ and $\nu=3$ QH systems* AMARTYA SAHA (Presenter), Univ of Kentucky, SUMAN DE, Harish-Chandra research Institute, GANPATHY MURTHY, Univ of Kentucky, SUMATHI RAO, Harish-Chandra research Institute, YUVAL GEFEN, Weizmann Institute of Science — We study the Hartree-Fock ground state near the interface between the $\nu=4$ and $\nu=3$ quantum Hall systems. In this problem we have two tuning parameters, $w$ which is the width of interface in units of $l$ (magnetic length), and $E_c$ which is the strength of coulomb interaction in units of the cyclotron energy. In the bulk, for $2.52 < E_c < 2.94$, the $\nu=3$ state is fully polarised but $\nu=4$ state is a singlet. We have found that in this regime there are two edge phases. Phase 1 has 3 chiral modes, 2 downstream and 1 upstream. In this phase spin is a good quantum number. In Phase 2 we only found 1 chiral mode which is downstream. This phase has a spin rotation and can have a pair of counter propagating neutral modes. We use the time dependent Hartree-Fock method to calculate the collective excitations of these phases.

*G.M. acknowledges support by NSF-DMR 1306897 and US-Israel BSF 2016130, Y.G. further acknowledges support by DFG RO 2247/11-1
10:00AM F54.00011: Spin-1 Photonic Skyrmion in Viscous Quantum Hall Fluids* TODD VAN MECHELEN (Presenter), ZUBIN JACOB, Purdue Univ — We present the fundamental model of a topological electromagnetic phase of matter: viscous Maxwell-Chern-Simons theory. We demonstrate that this is the minimal (exactly solvable) gauge theory with a nontrivial photonic Chern number. The interplay of symmetry and topology is also captured in the Chern number, which is determined by the spin-1 representations of a photonic skyrmion at high-symmetry points in the Brillouin zone. Physically, our predicted electromagnetic phases are connected to a dynamical photonic mass in a viscous quantum Hall fluid. The electromagnetic phase is topologically nontrivial when the Hall viscosity inhibits the total bulk Hall response. Our work bridges the gap between electromagnetic and condensed matter topological physics while also demonstrating the central role of spin-1 quantization in nontrivial photonic phases.

*This research was supported by the Defense Advanced Research Projects Agency (DARPA) Nascent Light-Matter Interactions (NLM) Program and the National Science Foundation (NSF) [Grant No. EFMA-1641101].

10:12AM F54.00012: Excited quantum Hall effect: enantiomorphic flat bands in a Yin-Yang Kagome lattice* YINONG ZHOU (Presenter), GURJYOT SETHI, HANG LIU, University of Utah, ZHENGFEI WANG, University of Science and Technology of China, FENG LIU, University of Utah — Quantum Hall effect (QHE) is one of the most fruitful research topics in condensed-matter physics. Ordinarily, the QHE manifests in a ground state with time-reversal symmetry broken by magnetization to carry a quantized chiral edge conductivity around a two-dimensional insulating bulk. We propose a theoretical concept and model of non-equilibrium excited-state QHE (EQHE) without intrinsic magnetization. It arises from circularly polarized photoexcitation between two enantiomorphic flat bands of opposite chirality, each supporting originally a helical topological insulating state hosted in a Yin-Yang Kagome lattice. The chirality of its edge state can be reversed by the handedness of light, instead of the direction of magnetization as in the conventional quantum (anomalous) Hall effect, offering a simple switching mechanism for quantum devices. Implications and realization of EQHE in real materials are discussed.

*U.S. DOE-BES (Grant No. DE-FG02-04ER46148). DOE-NERSC. CHPC.

10:24AM F54.00013: ferromagnetic transition in chiral metal TONGTONG LIU (Presenter), ZHEN BI, SUNGJOON HONG, LIANG FU, Massachusetts Institute of Technology MIT — This letter studies a spinful 1D chiral electron model with contact interaction and nonlinear dispersion, where an itinerant ferromagnetic phase transition happens at repulsive interaction and an Amperean pairing at attractive interaction, the two phases are symmetrical and connected by a particle-hole transformation. We use bosonization and relate it with the fermion model to study the phase transition criticality and find the spin and charge modes have different dynamical exponent, which leads to a fractional-power time correlation, unlike the Luttinger liquid theory. We also find a similar transition in the quantum Hall edge states, the nonlinear dispersion is replaced with the presence of interaction form factor after projecting to the Landau levels.
10:36AM F54.00014: van der Waals Heterostructures of 3D Topological Insulators and 2D Magnetic Materials* SHUWAN LIU (Presenter), SU KONG CHONG, TAYLOR D. SPARKS, VIKRAM V DESHPANDE, University of Utah — Three dimensional (3D) topological insulator (TI) based van der Waals heterostructures form an excellent platform to study the proximity effect between a TI surface and another layered material, such as a two-dimensional (2D) ferromagnet. Previously we have observed both massless relativistic Dirac fermions and massive (gapped) Dirac fermions in this way for the topological surface state of BiSbTeSe$_2$\textsuperscript{1} and have reported quantum Hall data for these surfaces. However, typical ferromagnets get oxidized easily during the fabrication process. Thus, the induced magnetization in the TI interface is not clean under ambient conditions. To minimize the influence of oxidation, we explore this fabrication inside a glovebox. We will report the performance of such TI based devices in comparison to those built-in ambient conditions and further study the proximity effect in TI-based van der Waals heterostructures.

\textsuperscript{1} Chong S et al 2018 Nano Lett. 18 8047

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F54.00015: Phase transition and anomalous scaling in the quantum Hall transport of topological-insulator Sn-Bi$_{1.1}$Sb$_{0.9}$Te$_2$S devices* FAJI XIE (Presenter), SHUAI ZHANG, FENGQI SONG, Nanjing University — The scaling physics of quantum Hall transport in optimized topological insulators with a plateau precision of $\sim$1/1000 e$^2$/h is considered. Two exponential scaling regimes are observed in temperature-dependent transport dissipation, one of which accords with thermal-activation behavior with a gap of 2.8 meV ($>$20 K), the other being attributed to variable-range hopping (1–20 K). Magnetic-field-driven plateau-to-plateau transition gives scaling relations of $(dR_{xy}/dB)_{\text{max}} \propto T^{-\kappa}$ and $\Delta B^{-1} \propto T^{-\kappa}$ with a consistent exponent of $\kappa \sim 0.2$, which is half the universal value for a conventional two-dimensional electron gas. This is evidence of percolation assisted by quantum tunneling and reveals the dominance of electron-electron interaction of the topological surface states.

*This work was supported by the National Key R&D Program of China (Grant No. 2017YFA0303200), the National Natural Science Foundation of China (Grants No.U1732273, No. U1732159, No. 91622115, No. 11522432, and No. 11574217), the Natural Science Foundation of Jiangsu Province (Grant No. BK20160659), and the Fundamental Research Funds for the Central Universities.

Tuesday, March 3, 2020 8:00 AM - 10:36 AM

Session F55 DCMP: Dirac and Weyl Semimetals: Theory II Mile High Ballroom 2B
8:00AM F55.00001: Non-local annihilation mechanism in momentum space for correlated Weyl fermions.* GIORGIO SANGIOVANNI (Presenter), Universitaet Wuerzburg, Institut fuer Theoretische Physik und Astrophysik and Wuerzburg-Dresden Cluster of Excellence ct.qmat, ADRIANO AMARICCI, LORENZO CRIPPA, Scuola Internazionale Superiore di Studi Avanzati (SISSA), NIKLAS WAGNER, Universitaet Wuerzburg, Institut fuer Theoretische Physik und Astrophysik and Wuerzburg-Dresden Cluster of Excellence ct.qmat, JAN BUDICH, Institute of Theoretical Physics, Technische Universitaet Dresden, MASSIMO CAPONE, Scuola Internazionale Superiore di Studi Avanzati (SISSA) — We discuss the effects of interaction in Weyl semimetals with broken time-reversal symmetry. The spin degeneracy of the gapless Dirac point at the topological quantum phase transition is resolved resulting in two gapless Weyl nodes separated in momentum space. For free fermions, the topological transition requires the two Weyl nodes to annihilate continuously in momentum space. Yet, we show that in presence of a strong local Coulomb repulsion this paradigm breaks down, opening a non-local annihilation channel for the Weyl cones.


* A.A. and M.C. acknowledge support from H2020 Framework Programme, under ERC Advanced Grant No. 692670 “FIRSTORM”. L.C., A.A. and M.C. acknowledge financial support from MIUR PRIN 2015(Prot. 2015C5SEJJ001) and SISSA/CNR project “Superconductivity, Ferroelectricity and Magnetism in badmetals” (Prot. 232/2015). J.C.B. acknowledges financial support from the German Research Foundation (DFG) through the Collaborative Research Centre SFB 1143. G.S. acknowledges financial support by the DFG through SFB 1170 “ToCoTronics” and the Wuerzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter – ct.qmat (EXC2147, project-id 39085490).

8:12AM F55.00002: Quantum Lifshitz criticality of topological semimetals* SHOUVIK SUR (Presenter), ALEXANDER TYNER, PALLAB GOSWAMI, Northwestern University — In the absence of particle-hole symmetry, all clean topological semimetals can be realized in two thermodynamically distinct forms: a power-law, incompressible phase and a compressible phase, respectively possessing zero and constant density of states at the band touching energy. Therefore, the density of states can serve as an order parameter for describing quantum Lifshitz transitions between two thermodynamically distinct but topologically equivalent states of matter. We address the nature of such quantum Lifshitz transitions for different topological semimetals, and show how they can strongly influence thermodynamic, spectroscopic, and transport properties of many quantum materials.

*NSF DMR-1720319
**8:24AM F55.00003: Intrinsic Plasmon damping in Dirac-Fermi liquids**  
PRACHI SHARMA (Presenter), DMITRII MASLOV, University of Florida — A Dirac-Fermi liquid (DFL) — a doped system with Dirac spectrum — is a special and important subclass of non-Galilean-invariant Fermi liquids (FLs), which includes, e.g., monolayer graphene and surface states of three-dimensional topological insulators. The lack of Galilean invariance leads to some interesting features not encountered in conventional Fermi liquids. Namely, the dissipative part of the conductivity of a DFL stays finite at $q \to 0$, whereas for a Galilean-invariant FL it vanishes as $q^2$. We explore the consequences of this fundamental difference for the intrinsic damping of plasmons in DFL. Charge density fluctuation leads to a collective mode, plasmon, in a two-dimensional (2D) system with $q^{1/2}$ dispersion. The imaginary part of charge susceptibility, $\chi''(q, \omega)$, is directly related to the damping rate of the plasmon mode. We obtain the explicit form of $\chi''(q, \omega)$ for DFL, by going beyond the random-phase approximation. We calculate the self-energy, Maki-Thompson, and Aslamazov-Larkin diagrams for a dynamically screened Coulomb potential and find that $\chi''(q, \omega)$ scales as $q^2 \omega$ and the damping rate scales as $q^2$. We show that the same result follows from the Einstein relation between the conductivity and charge susceptibility.

**8:36AM F55.00004: Internodal tunnelling and magnetotransport in Weyl semimetals**  
SERGEY SYZRANOV (Presenter), GRIGORY BEDNIK, University of California, Santa Cruz, KONSTANTIN TIKHONOV, Landau Institute for Theoretical Physics, Karlsruhe Institute of Tehcnology, Skolkovo Institute of Science and Technology — Internodal dynamics of quasiparticles in Weyl semimetals manifests itself in hydrodynamic, transport and thermodynamic phenomena and is essential for potential valleytronic applications of these systems. Charge transfer between the nodes in a Weyl semimetal is often considered as an inelastic process, with the charge carriers quickly thermalising at each node. In an external magnetic field, however, coherent quasiparticle tunnelling between the nodes may lead to a significant modification of the quasiparticle dispersion in a clean Weyl semimetal for certain directions of the magnetic field. In particular, it results in the opening of a gap in the quasiparticle dispersion, whose magnitude depends exponentially on the magnetic field. We study the interplay of such tunnelling with magnetotransport in a Weyl semimetal. We compute microscopically the longitudinal resistivity of a disordered Weyl semimetal with two nodes in a strong magnetic field and demonstrate that it has a strong angular dependence $\rho(\eta) = C_1 + C_2 \cos^2 \eta$, where $\eta$ is the angle between the field and the line connecting the nodes. The first term is determined by the coherent internodal coupling and depends exponentially on the magnetic field, while the second term is independent of this coupling.
8:48AM F55.00005: Low-field anomalous Hall effect in nonmagnetic metals by Wannier interpolation. STEPAN TSIRKIN (Presenter), Department of Physics, University of Zurich, IVO SOUZA, Universidad del País Vasco, San Sebastián — In ferromagnets, the Bloch states acquire a Berry curvature that produces a Hall effect at $B = 0$: the anomalous Hall effect (AHE). In nonmagnetic metals the Hall effect only appears at linear order in $B$. Interestingly, the low-field Hall conductivity of nonmagnetic metals has an anomalous (Berry-curvature) contribution in addition to the ordinary (Lorentz-force) one. In noncentrosymmetric crystals it goes as $\sigma_{\text{AHE}} \propto \int d^3k \Omega_k (m_k \cdot B) f_0'$, where $\Omega_k$ and $m_k$ are the Berry curvature and intrinsic magnetic moment (spin plus orbital) imparted on the Bloch states by the broken inversion symmetry; since $\Omega_k$ and $m_k$ are both odd under time reversal, $k$ and $-k$ contribute equal amounts to $\sigma_{\text{AHE}}$. In centrosymmetric crystals the bands are Kramers degenerate, and the expression for $\sigma_{\text{AHE}}$ involves the trace of the product of $2 \times 2$ matrices describing the Berry curvature and magnetic moment of the degenerate states; in this case $\text{Tr} \Omega_k = \text{Tr} m_k = 0$, but $\text{Tr}(\Omega_k m_k) = \text{Tr}(\Omega_{-k} m_{-k}) \neq 0$. Working in this non-Abelian setting, we develop a Wannier-interpolation scheme to calculate the low-field anomalous Hall conductivity from first principles. As a by-product, we obtain the anomalous $g$ factors of the Bloch states. The low-field AHE is present in all metals, but is more pronounced in Weyl and Dirac semimetals.

9:00AM F55.00006: Ultrafast topological phenomena in Weyl semimetals* FATEMEH NEMATOLLAHI (Presenter), JHIH-SHENG WU, VADYM APALKOV, MARK I STOCKMAN, Georgia State University — For Weyl semimetals, we predict that an intense ultrafast (single-oscillation) circularly polarized optical pulse can induce a large population of the conduction band. The response of Weyl points to an ultrafast laser field is different and so the conduction population is highly textured which we call it topological resonance. The topological resonance is due to the Bloch motion of electrons in the reciprocal space where electron population textures are formed due to non-Abelian Berry curvature.

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4-Department of Energy (DOE); DE-SC0007043
5-University of Central Florida, subcontracted by the Air Force Office of Scientific Research (AFOSR); 24086151 is the subaward number; the Federal Award no. is FA9550-15-1-0037
9:12AM F55.00007: Nodal Chain Semimetal in Geometric Frustrated Acoustic metamaterial*

MENG XIAO (Presenter), Wuhan Univ, XIAO-QI SUN, Physics, Stanford university, SHANHUI FAN, Stanford University — Geometrically frustrated systems and topological semimetals have both attracted much interest and been studied in various systems in recent years. Here we study the interplay between these two systems. We show that a Weyl point can be extended to a chain of degeneracy (a nodal chain) with nonzero charge of Berry flux through geometrical frustration. We propose to realize such a charged nodal chain in an acoustic metamaterial, based on both tight-binding and full-wave numerical simulations. Moreover, we observe a fan-like surface state spectrum, whose dispersion is controlled by the bulk band properties. Our work points to a new class of band degeneracy that carries non-zero Berry flux. The resulting topological metamaterial may be useful for controlling the flow of sound and light.

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9:24AM F55.00008: Quantum distance and anomalous Landau levels of flat bands  JUN-WON RHIM (Presenter), BOHM-JUNG YANG, Seoul Natl Univ — Semiclassical quantization of electronic states under magnetic field, advocated by Onsager, can successfully describe not only the Landau level spectrum but also the geometric responses under magnetic field in metals. Even in graphene with relativistic energy dispersion, for instance, Onsager’s rule correctly described the π-Berry phase as well as the unusual Landau level spectrum of Dirac particles. Here we show that, however, the semiclassical quantization rule completely breaks down for a class of dispersionless flat bands, dubbed the singular flat bands. The singular flat band has a band crossing with another dispersive band enforced by band flatness. In contrast to the conventional isolated flat band which does not respond to external magnetic field, the singular flat band shows anomalous Landau level structures and magnetic responses. We discuss the novel quantum geometric interpretations of them regarding the quantum distance, and how to measure them experimentally.
Superconductivity in interacting Weyl models: A combined auxiliary-field quantum Monte Carlo and mean-field study*  

PETER ROSENBERG (Presenter), NIRAJ ARYAL, EFSTRATIOS MANOUSAKIS, Natl High Magnetic Field Lab — The discovery of superconducting Weyl semimetals has sparked an intense effort to understand the connection between topology and correlations in these materials, specifically, the pairing behavior of emergent Weyl fermions. Here we study a simple 2D Weyl model with attractive interactions using a combination of numerically exact auxiliary-field quantum Monte Carlo calculations and mean-field theory [1]. We focus on the rich pairing behavior that emerges from the interplay of the spin and sublattice degrees of freedom, as well as the bond-density order. Finally, we present preliminary results on a 3D extension of the model, with direct relevance to the case of MoTe$_2$. These high-accuracy results are an important step towards a many-body description of strongly-correlated Weyl materials and topological superconductors.


*This work was supported in part by the U.S. National High Magnetic Field Laboratory, which is funded by NSF DMR-1157490 and the State of Florida.

The optical conductivity of strongly interacting Dirac fermions: a bosonization approach to the Kadanoff-Baym self-consistent resummation  

SEBASTIAN MANTILLA (Presenter), INTI SODEMANN, Max Planck Institute for the Physics of Complex Systems — The optical conductivity of 2D Dirac fermions at low energies is controlled by fundamental constants of nature $\sigma_0 = e^2/16 \hbar$. However, Coulomb interactions produce a non-trivial dependence of the conductivity with the frequency. We use a bosonization approach to implement exactly a self-consistent Kadanoff-Baym resummation of the electron-hole propagator by mapping the momentum space lattice onto a Heisenberg-type model of interacting spins and employ this approach to determine the frequency dependence of the optical conductivity for Coulomb repulsions. We recover the perturbative renormalization group results at small coupling and extend its predictions to strong coupling. We discuss the relevance of our results to Dirac materials such as graphene and 3D topological insulator surface states.
10:00AM F55.00011: SU(3) fermions in a three-band graphene-like model*  SUMIRAN PUJARI (Presenter), Department of Physics, Indian Institute of Technology Bombay, ANKUR DAS, Univ of Kentucky — Two-dimensional graphene is fascinating because of its unique electronic properties. From a fundamental perspective, one among them is the geometric phase structure near the Dirac points in the Brillouin zone, owing to the SU(2) nature of the Dirac cone wave functions. We ask if there are geometric phase structures in two dimensions that go beyond that of a Dirac cone. Here we write down a family of three-band continuum models of noninteracting fermions that have more intricate geometric phase structures. This is connected to the SU(3) nature of the wave functions near threefold degeneracies. We also give a tight-binding free fermion model on a two-dimensional graphene-like lattice where the threefold degeneracies are realized at fine-tuned points. Away from them, we obtain new “three-band” Dirac cone structures with associated nonstandard Landau level quantization, whose organization is strongly affected by the non-SU(2) or beyond-Dirac geometric phase structure of the fine-tuned points.

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International Center for Theoretical Sciences (ICTS) during a visit for participating in the program
The 2nd Asia Pacific Workshop on Quantum Magnetism (Code: ICTS/apfm2018/11)

10:12AM F55.00012: Topological Semimetals with Butterfly-like Four-Point Intersecting Ellipses*  XIAOTING ZHOU (Presenter), HUGO ARAMBERRI, Department of Physics and Astronomy, California State University, Northridge, CHENG-YI HUANG, Institute of Physics, Academia Sinica, Taipei, Taiwan, MAIA G VERGNIORY, Donostia International Physics Center, Donostia-San Sebastian, Spain, HSIN LIO, Institute of Physics, Academia Sinica, Taipei, Taiwan, NICHOLAS KIOUSSIS, Department of Physics and Astronomy, California State University, Northridge — Recent years, the exotic properties of topological semimetals have garnered great attention and efforts in seeking for new topological phases and material realization. In this work, we introduce a new type of nodal line, the butterfly-like four-point-intersecting-ellipses (FPIE) residing in a plane. We identify the criteria for the existence of the FPIE in a time reversal invariant spinless fermion system with negligible spin-orbital coupling (SOC). In addition we demonstrate that its emergence is possible in 7 out of 230 space groups, and identify the locations it would emerge in the Brillouin zone (BZ). Using first-principles band structure calculations, we predict a family of compounds as candidates hosting the FPIE in the Fermi surface (FS) with vanishing SOC.

*The work is supported by NSF-Partnership in Research and Education in Materials (PREM) Grants No. DMR-1828019.
Unconventional Superconductivity and Mott Transition in a Sign-Free Electronic Model*

XIAO YAN XU (Presenter), TARUN GROVER, Department of Physics, University of California at San Diego — It is widely believed that repulsive on-site interactions between electrons can lead to unconventional superconductivity. Further, one expects that proximity of an unconventional superconductor to a Mott transition can lead to a quantum spin-liquid ala resonating valence bond (RVB) picture. Motivated by such folklore, here we construct a sign-problem free model that has unconventional f-wave superconductivity, and a proximate Mott transition to a Neel ordered phase. We present preliminary results on the nature of transition between these two phases, and potential spin-liquid phases in its vicinity. We also show using field-theoretic methods that a direct deconfined quantum critical point is allowed between the superconductor and the Neel phase.

*This project is supported by the National Science Foundation under Grant No. DMR-1752417, and by an Alfred P. Sloan Research Fellowship.

Cyclotron orbit knot and tunable-field quantum Hall effect*

YI ZHANG (Presenter), International Center for Quantum Materials, Peking University — The Bohr-Sommerfeld quantization of the cyclotron orbit in a magnetic field gives rise to discrete Landau levels and a series of fascinating quantum Hall phenomena. Here we consider topologically nontrivial physics from a distinct origin, where the cyclotron orbits take nontrivial knotting structure. We present a scenario of a Weyl semimetal slab, where the Fermi arcs on the opposing surfaces can cross without interfering with each other and form a knot together with the bulk chiral Landau levels. We provide a microscopic lattice model with cyclotron orbits of trefoil-knot geometry and study the corresponding quantum oscillations. Interestingly, unlike the conventional ring-shaped cyclotron orbit, a trefoil knot is self-threading, allowing the magnetic field line along the cyclotron orbit to contribute to the overall Berry phase and therefore altering the external magnetic field for each quantization level. The cyclotron orbit knot offers an arena of the nontrivial knot theory in three spatial dimensions and its subsequent physical consequences.

*Y.Z. acknowledges support from the start-up grant at International Center for Quantum Materials, Peking University, the Bethe fellowship at Cornell University, and the National Science Foundation under Grant No. NSF PHY-1748958.

Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F56 DCMP: Cuprate and Iron Superconductor Normal State Properties Mile High Ballroom 2C - Ming Yi, Rice Univ
8:00AM F56.00001: Fermi surface transformation across the pseudogap critical point in the cuprate Nd-LSCO from thermoelectric measurements  ADRIEN GOURGOUT (Presenter), CLEMENT COLLIGNON, AMIRREZA ATAEI, SVEN BADOUX, GAELE GRISSONNANCHE, MARIE-EVE BOULANGER, FRANCIS LALIBERTE, University of Sherbrooke, JIANSHI ZHOU, University of Texas, QIANLI MA, BRUCE D. GAULIN, McMaster University, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, University of Sherbrooke — In cuprate superconductors, the nature of the pseudogap phase and its interplay with superconductivity are still unclear. Its onset at a doping $p^*$ is characterized by a drop in the carrier density $n$ from $n = 1+p$ above $p^*$ to $n = p$ below $p^*$ [1]. In Nd$_{0.4}$La$_{1.6-x}$Sr$_x$CuO$_4$ (Nd-LSCO), this shows up as a low-temperature upturn in the resistivity $\rho$ and Hall coefficient $R_H$ at dopings below $p^* = 0.23$ [2]. Here we present a series of thermoelectric measurements in Nd-LSCO across $p^*$, in magnetic fields large enough to suppress superconductivity. For a heat current in the CuO$_2$ planes, the Seebeck coefficient $S$ shows a large increase at low temperature below $p^*$, confirming the loss of carrier density. Application of pressure suppresses the low-$T$ upturn in $S/T$, as it did the upturn in $\rho$ and $R_H$ [3]. For a heat current perpendicular to the CuO$_2$ planes, we find that $S$ is isotropic for $p > p^*$, i.e. $S_c/T$ and $S_a/T$ are equal (and positive) in the $T=0$ limit. In sharp contrast, $S_c$ becomes negative at low temperature when $p < p^*$, revealing a profound change in the Fermi surface topology across $p^*$.


8:12AM F56.00002: Spiral magnetic order in high-$T_c$ cuprates - a ground state candidate at high magnetic fields  JOHANNES MITSCHERLING (Presenter), PIETRO MARIA BONETTI, DEMETRIO VILARDI, WALTER METZNER, Max Planck Institute for Solid State Research, Stuttgart, Germany — The normal state beneath the superconducting dome determines the fluctuations that govern the anomalous properties of cuprate superconductors in a wide range of their phase diagram. Recent experiments at very high magnetic fields shed new light on the phenomenology of the high field ground state: A drastic change in the carrier density at the onset of the pseudogap observed in various cuprate compounds, thermodynamic signatures of a quantum critical point at this doping and, very recently, NMR and ultrasound experiments indicated glassy antiferromagnetic order up to the pseudogap onset.

We present incommensurate spiral magnetic order as a potential ground state candidate at high magnetic fields [1,2]. Previous theoretical work suggests that suppression of superconductivity leads to such a ground state [3]. We present quantitative results for magnetic order in the Hubbard model at strong coupling using dynamical mean-field theory [4]. We show that experimental signatures as Fermi arcs, nematicity and the drop in both the DC conductivity and Hall number can be understood within this framework.

8:24AM F56.00003: Thermodynamic evidence of quantum criticality at the pseudogap critical point of cuprate superconductors  CLÉMENT GIROD (Presenter), BASTIEN MICHON, MAUDE LE LIZAIRE, ADRIEN GOURGOUT, SVEN BADOUX, NICOLAS DOIRON-LEYRAUD, FRANCIS LALIBERTE, Universite de Sherbrooke, JOZEPH KAČMARČÍK, Slovak Academy of Sciences, SIMON VERRET, Universite de Sherbrooke, JIANSHI ZHOU, University of Texas at Austin, QIANLI MA, MIRELA DRAGOMIR, HANNAH A. DABKOWSKA, BRUCE D. GAULIN, McMaster University, SUNSENG PYON, TOMOHIRO TAKAYAMA, HIDENORI TAKAGI, University of Tokyo, GUO-QING ZHENG, Okayama University, SHIMPEI ONO, CRIEPI, CHRISTOPHE MARCENAT, Institut Néel, LOUIS TAILLEFER, Universite de Sherbrooke, THIERRY KLEIN, Institut Néel — The emergence of superconductivity in the vicinity of a magnetic quantum critical point (QCP) in heavy-fermion, iron-based, organic and electron-doped cuprate superconductors showcases the important relation between quantum criticality and pairing. In hole-doped cuprates, long-range antiferromagnetic order vanishes with doping well before superconductivity appears. Instead, it is around the critical doping p* where the enigmatic pseudogap phase ends that superconductivity exists. The fact that the electrical resistivity displays a linear temperature dependence at low temperature in all these systems, including hole-doped cuprates [1], is suggestive. Here we provide thermodynamic evidence of a QCP in hole-doped cuprates from low-temperature measurements of the specific heat in magnetic fields up to 35 T, high enough to suppress superconductivity. In LSCO, Eu-LSCO, Nd-LSCO and Bi2201, we observe an electronic specific heat that grows as $C/T \sim \log(1/T)$ at $p \sim p^*$ [2], the classic thermodynamic signature of quantum criticality.


8:36AM F56.00004: Large negative thermal Hall conductivity in cuprate Mott insulators  MARIE-EVE BOULANGER (Presenter), GAEL GRISONNANCHE, MAXIME DION, ETIENNE LEFRANCOIS, Universite de Sherbrooke, RUIXING LIANG, WALTER N HARDY, DOUGLAS A BONN, University of British Colombia, JIANSHI ZHOU, The University of Texas at Austin, LOUIS TAILLEFER, Universite de Sherbrooke — A large negative thermal Hall signal $k_{xy}$ has recently been observed to appear in the pseudogap phase of cuprates [1]. This signal persists to zero doping, in the antiferromagnetic Mott insulator La$_2$CuO$_4$. While it is clearly not due to electrons, this $k_{xy}$ signal could come from magnons, or phonons — or more exotic excitations. To shed light on the underlying mechanism, we measured $k_{xy}$ in two additional cuprate Mott insulators: Nd$_2$CuO$_4$ and Sr$_2$CuO$_2$Cl$_2$. We observe a large negative $k_{xy}$ signal in both materials. Because of the absence of spin canting in either of these materials without apical oxygens, and because of the absence of any change in $k_{xy}$ upon crossing different magnetic states in Nd$_2$CuO$_4$, we infer that magnons are not the heat carriers responsible for $k_{xy}$. The similarity in the temperature dependence of $k_{xy}$ and $k_{xx}$ suggests a phonon scenario. If so, the mechanism whereby the pseudogap phase confers chirality to phonons remains to be elucidated.

8:48AM F56.00005: Deep in the electron-doped cuprate pseudogap regime: a two-particle self-consistent approach with \( \text{GG}_0 \) approximation to the two-dimensional Hubbard model*  
YAN WANG (Presenter), YURI VILK, ANDRE-MARIE TREMBLAY, Universite de Sherbrooke — In cuprate high-\( T_c \) superconductors, the pseudogap (PG) manifests itself at low temperature as a gradual depletion of the density of states at the Fermi level. In electron-doped cuprates, the nonperturbative semianalytical two-particle-self-consistent (TPSC) approach naturally explains the PG as the finite-\( T \) precursor of the antiferromagnetic (AFM) bands of the ordered ground state at \( T=0 \). In contrast to Mott physics, the PG opens in two dimensions at hot spots in momentum space due to scattering off spin-fluctuations when the AFM correlation length becomes longer than the thermal de Broglie wavelength. However, TPSC eventually fails at temperatures deep in the PG regime with exponentially growing AFM correlation length. Here, we extend TPSC with the \( \text{GG}_0 \) approximation to the irreducible particle-hole polarization where one of the propagators \( \text{G} \) is self-consistently dressed by TPSC self-energy. Benchmarking with other controlled numerical methods, we demonstrate that this modified TPSC approach predicts quite accurate one-particle and two-particle properties deep in the PG regime, satisfies various sum rules and consistency relations and joins smoothly with the \( T=0 \) AFM ground state.

*Canada First Research Excellence Fund, NSERC and the Chair in the Theory of Quantum Materials.

9:00AM F56.00006: Disorder effects on the phase diagram of electron-doped cuprates using the two-particle self-consistent approach*  
CHLOE-AMINATA GAUVIN-NDIAYE (Presenter), ANDRE-MARIE TREMBLAY, Institut Quantique, Universite de Sherbrooke — The two-particle self-consistent approach (TPSC) is a highly accurate theoretical method for electronic systems that can be described by the one-band Hubbard model in the weak to intermediate coupling regime. [1] In particular, it can successfully describe the electron-doped cuprates. One of the predictions of TPSC for these materials is that the pseudogap occurs when the antiferromagnetic spin correlation length become larger than the thermal de Broglie wave length. [1,2] This TPSC condition for the pseudogap has been confirmed experimentally in the underdoped regime. However, this analysis fails in the optimal doping regime. [3,4] In this work, we include the effect of impurities and disorder in TPSC using the impurity averaging technique. We then investigate the effect of disorder on the TPSC condition for the pseudogap and on the critical doping for the crossover temperature.


*FRQNT, Canada First Excellence Research Fund, Université de Sherbrooke, NSERC Grant RGPIN-2019-05312, Research Chair in the Theory of Quantum Materials, Compute Canada, Calcul Québec
9:12AM F56.00007: Measured vs. Calculated Phonon Dispersions in the Cuprate HgBa$_2$CuO$_4$*

IRADA AHMADOVA, TYLER STERLING (Presenter), AARON SOKOLIK, ADRIAN MERRITT, University of Colorado, Boulder, DOUGLAS L ABERNATHY, Oak Ridge National Lab, MUN K. CHAN, YANG TANG, GUICHUAN YU, MARTIN GREVEN, University of Minnesota, DMITRY REZNIK, University of Colorado, Boulder — Taking the prototypical high-T$_c$ superconductor HgBa$_2$CuO$_4$ as an example, I will compare ab-initio density-functional-theory (DFT) calculations of the phonon dispersions to inelastic neutron scattering results that exhibit an anomaly in the Cu-O bond stretching branch. We have performed a series of calculations using several codes at different levels of approximation. Our results show good qualitative agreement for all codes, but only one gave a good quantitative agreement (better than 10%). All DFT calculations fail to reproduce the experimentally observed anomalous dispersion of the bond-stretching phonon branch. I will conclude my talk by mentioning other computational methods that may improve the agreement between the calculations and measurement.

*This work was supported by the DOE, Office of Basic Energy Sciences, Office of Science, under Contract No. DE-SC0006939. A portion of this research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

The work at UMN was funded by the Department of Energy through the UMN Center for Quantum Materials under DE-SC-0016371.

9:24AM F56.00008: Nature of the pseudogap in cuprate superconductors*

YOANDRIS VIELZA DE LA CRUZ (Presenter), Department of Physics, Federal University of Pernambuco — The base of the mean-field model that describes the main physical properties of the cuprate superconductors is presented, the single-band Hubbard Hamiltonian of the Mott-states of electrons on CuO-plane. In the present work, the Hamiltonian is diagonalized on a Hartree-Fock base of collinear spins states that leaves fixed the magnetic order on the square sublattices. Adjusted the mean-field in the unit cell to a gap of $\sim$ 2 eV at half-filling and to a maximum value of pseudogap observed of $\sim$ 100 meV, an evaluation of the Hartree-Fock Mott-states in doping with holes and electrons and at the zero absolute temperature is made. It is shown that the mean-field adjust the density of the states at the Fermi level according to the experimental measure. The base of the Hartree-Fock Mott-states prove that the opening of the pseudogap in cuprate superconductors define a phase of low density of states at the Fermi level resulting from Coulomb repulsion on Cu-sites that penalizes two electrons being close to each other. It is also argued that the spontaneous breaking of rotational symmetry in the antiferromagnetic order of the Mott-states leads to the electron pair formation in cuprate superconductors.

*This work was supported by the CNPq project founded by the MCTIC of Brazil.
**9:36AM F56.00009: Criticality vs material inhomogeneity: an analysis of LSCO magnetoresistance data** CHRISTIAN BOYD (Presenter), PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — Recent thin-film LSCO measurements have observed, in addition to the hallmark T-linear resistivity of cuprates near optimal doping, B-linear resistivity in strong magnetic fields. We analyze existing data on this thin-film sample to demonstrate that, contrary to the high-Tc iron superconductors near optimal doping, no single scaling function of temperature and field can describe the magnetoresistance data across all measured temperatures above and below the superconducting Tc. We model the high-temperature data within a classically-disordered system of conducting patches with qualitative accuracy. Interestingly, the breakdown of this model at low temperatures when the mean free path exceeds the lengthscale of disorder happens to correspond with the experimentally observed region where the resistivity changes character to become simultaneously T,B linear.

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*NSF DMR-1919143

**9:48AM F56.00010: What can Density Functional Theory tell us about Pseudogaps?** ROBERT MARKIEWICZ (Presenter), Northeastern University, YUBO ZHANG, Tulane University, CHRISTOPHER LANE, Northeastern University, JAMES FURNESS, Tulane University, MATT MATZELLE, Northeastern University, BERNARDO BARBIELLINI, LUT & Northeastern Universities, JOHN P. PERDEW, Temple University, JIANWEI SUN, Tulane University, ARUN BANSIL, Northeastern University — We have shown recently that advanced exchange-correlation functionals can enable first-principles treatment of the electronic, geometric and magnetic structure of the cuprates and other correlated materials without the need to invoke ad hoc parameters such as the Hubbard U. [1,2] Here, we focus on how in this picture the pseudogap phase in YBaCu3O7 involves a large number of competing magnetic and stripe phases with small energy differences, which can be looked upon as simple antiferromagnets with topological defects, i.e. defects consisting of stacking faults and charged antiphase boundaries or the charged stripes[3,4]. A simple thermodynamic model suggests that the pseudogap consists of fluctuating short-range ordered (SRO) phases, while the strange metal corresponds to defect unbinding. The SRO phases display nematicity and Fermi arcs. Comparisons with experiment will be discussed.

10:00AM F56.00011: Determine the spatial locality of self-energy of LiFeAs*  
MINJAE KIM (Presenter), Department of Physics and Astronomy, Rutgers University, New Brunswick, HU MIAO, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, New Brunswick — Understanding of the electronic correlations is crucial to explain the electronic properties, magnetism, and superconductivity of the iron-based superconductors (FeSCs). An important question is the degree of spatial locality of the electronic correlations. Local correlations is the starting point of dynamical mean-field theory (DMFT), which has been proved to be powerful in understanding spectroscopic properties of the FeSCs [1,2]. However, recent theoretical and experimental reports on one of the FeSCs, LiFeAs, suggested the importance of non local correlations[3,4]. In this presentation, we extract spatially resolved and orbital dependent electronic self-energy of LiFeAs from angle resolved photoemission spectroscopy with density functional theory as a reference frame, and discuss the level of locality in the different orbitals, with the xy orbital being more local than the xz yz. We also discuss how the level of non locality depends on energy.


*This work was supported by Grant No. NSF DMR-1733071.

10:12AM F56.00012: Quasiclassical theory of C4-symmetric magnetic order in disordered iron-based superconductors*  
MAXIM DZERO (Presenter), Kent State Univ - Kent — In some hole-doped iron-based superconductors the magnetic order emerges with underlying C4-symmetry. This magnetic order can be viewed as a state with two ordering vectors with the corresponding magnetizations M1 and M2. In my talk, I will formulate a quasi-classical theory of such a state. Specifically, I will consider a three-band model, which, apart from the magnetic interactions, includes intra- and interband disorder scattering potentials. I will develop the quasiclassical approach for such a model and show how disorder scattering rates enhance the emergence of the C4-symmetric magnetic order.

*NSF-DMR-1506547
Electronic nematicity is the spontaneous breaking of rotational symmetry in a metal, and it has been argued to potentially strengthen superconductivity. It is a key feature of iron-based high-temperature superconductors. In cuprate high-temperature superconductors, a number of experiments have revealed evidence of nematicity, but its origin remains unclear. We measured the in-plane anisotropy of the electrical resistivity $\rho(T)$ and the Seebeck coefficient $S(T)$ in a crystal of the cuprate $\text{YBa}_2\text{Cu}_3\text{O}_y$, at hole concentration $p = 0.12$. By using the same sample and contacts to measure transport along the $a$ axis and the $b$ axis of the orthorhombic crystal structure, by detwining this sample twice, such that its length was first along $a$ and then along $b$, we were able to precisely obtain the intrinsic in-plane anisotropy of these two longitudinal transport coefficients. We find no trace of any additional anisotropy in either $\rho(T)$ or $S(T)$ upon crossing below the pseudogap temperature $T^*$. A large anisotropy appears only at much lower temperature, in tandem with the emergence of charge density wave correlations. We conclude that the pseudogap phase itself is not nematic, and the nematicity in $\text{YBa}_2\text{Cu}_3\text{O}_y$ originates instead from the unidirectional charge order and its precursor correlations.

10:36AM F56.00014: Diverse unconventional density wave states in high-$T_c$ cuprates and other unconventional superconductors HIROSHI KONTANI (Presenter), KOUKI KAWAGUCHI, RINA TAZAI, YOUICHI YAMAKAWA, SEIICHIRO ONARI, Nagoya Univ — We discuss the mechanism of diverse nematic orders in various strongly correlated electron systems, by considering the interference among different fluctuations given by vertex corrections (VCs). We mainly focus on the ferro- and stripe-bond orders in cuprate superconductors and organic superconductor $\kappa$-(BEDT-TTF)$_2X$. The bond order formation is closely related to the pseudogap phenomena in these systems. We also discuss important effects on bond-order fluctuations on the superconductivity and other electronic properties. We also discuss possible time-reversal-symmetry breaking nematic order based on the Hubbard model.

F56.00015: Investigation of the Orbital Moment on the Fe Impurities in Iron-Based Superconductor SHIYU PENG (Presenter), Chinese Academy of Sciences, Institute of Physics, JIANPENG LIU, Physics, The Hong Kong University of Science and Technology, HONGMING WENG, Chinese Academy of Sciences, Institute of Physics, XI DAI, Physics, The Hong Kong University of Science and Technology — Our previous study show that the orbital exchange process induced by large orbital magnetic moment can lead to quantum anomalous vortices, which may further support robust Majorana zero-energy modes together with the topologically nontrivial surface states. In the present study, by applying LDA+Gutzwiller method we have systematically studied the value of the orbital magnetic moment as the function of the height between the Fe impurity and the surface of superconducting Fe(Te,Se). The local Coulomb Interaction between the electrons on the Fe impurities has been treated carefully by the rotational invariant Gutzwiller method with the variational parameters corresponding to the the most generic situation. Our results show the orbital contribution to the magnetic moment is always sizeable in this system and can be strongly affected by the impurity height.
Tuesday, March 3, 2020 8:00 AM - 10:36 AM

Session F57 DMP: Superconductivity In Monolayers Mile High Ballroom 3A - Peide
(Peter) Ye, Purdue Univ - Tag(s): Focus

8:00AM F57.00001: Ultrafast Dynamics in Normal and CDW States of 2H-NbSe$_2^*$  
GORAN KARAPETROV (Presenter), Physics and Materials Science and Engineering, Drexel University, ANTON ANIKIN, Physics, Drexel University, RICHARD D SCHALLER, GARY P WIEDERRECHT, Center for Nanoscale Materials, Argonne National Laboratory — We have performed femtosecond pump-probe reflectivity study of the carrier and lattice dynamics using near-IR pump and white broadband probe at temperatures below and above the charge density wave transition in single crystal NbSe$_2$. The temperature dependence of the frequency of the coherent damped oscillations shows a second order softening when approaching $T_{CDW}$. This mode can be described as a combination of two acoustic phonons, one of which has Kohn anomaly in a broad range of temperatures. We extracted basic characteristics of the soft mode and its anharmonic decay. Global analysis fits from femtosecond to nanosecond scale were applied to describe the relaxation dynamics from the broadband transient reflectivity data.

*This work was supported by the National Science Foundation under Grant No. ECCS-1711015. Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract no. DE-AC02-06CH11357.

8:12AM F57.00002: Two-fold anisotropic superconducting properties of few-layer NbSe$_2^*$  
BRETT HEISCHMIDT, ALEX HAMILL (Presenter), KAN-TING TSAI, DANIEL SHAFFER, XI ZHANG, RAFAEL FERNANDES, KE WANG, VLAD PRIBIAG, University of Minnesota — Transition metal dichalcogenides (TMDs) are a class of layered van der Waals materials that have recently attracted considerable interest due to a wide range of properties in the two-dimensional limit, including superconductivity, topological phases, and spin-valley-locked bands due to strong orbit coupling and inversion-symmetry breaking. Here, we present transport properties of few-layer niobium diselenide (NbSe$_2$), a TMD that exhibits signatures of an unusual Ising superconducting state as its thickness approaches the 2D limit. We perform magneto-transport experiments on high-quality few-layer NbSe$_2$ samples, which are fully encapsulated by hexagonal boron nitride in order to protect the NbSe$_2$ from the deleterious effects of exposure to oxygen and moisture. We find that, despite the three-fold symmetry of the lattice, the magneto-transport exhibits a two-fold in-plane anisotropy for in-plane magnetic fields up to 8 Tesla. This anisotropy is restricted to the temperature region between the $T_c$ onset and $T_c$ offset, and disappears in the normal state. We propose a phenomenological model to explain this unusual observation, discussing its implications to the elucidation of Ising superconductivity.

*This work was supported by NSF DMR-1420013 through the iSuperseed program.
8:24AM F57.00003: Finite-momentum pairing in superconducting monolayer NbSe$_2$ DANIEL SHAFFER (Presenter), University of Minnesota, JIAN KANG, Physics, Florida State University, FIONA BURNELL, RAFAEL FERNANDES, University of Minnesota — The nature of the so-called Ising superconducting state in non-centrosymmetric monolayer transition metal dichalcogenides remains a subject of intense debate. Here, we study the possibility of finite-momentum pairing within a low-energy interacting microscopic electronic model for monolayer 1H-NbSe$_2$. We find that, in the presence of both Rashba and Ising spin-orbit coupling (SOC), a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)-like state is expected to emerge for sufficiently strong in-plane fields. For special orientations of the magnetic field, this FFLO state displays topological Bogolyubov Fermi surfaces or nodes depending on the center-of-mass momentum of the Cooper pairs, protected by a crystalline mirror symmetry. We also show that out of the eight symmetry-allowed interactions involving the low-energy fermions in this model, four of them favor a pair-density wave (PDW) state involving momentum transfer $K$ that may have a helical or chiral character. We investigate the stability and topology of these PDW states and their competition with the uniform superconducting phase in the presence of trigonal warping and mismatch between the $K/K'$ and the $\Gamma$ pockets.

8:36AM F57.00004: Angle dependence of $H_{c2}$ with crossover between the orbital and paramagnetic limits in 2D NbSe$_2$ HIDEKI MATSUOKA (Presenter), MASAKI NAKANO, Univ of Tokyo, TAKASHI SHITAOKOSHI, ISSP, The University of Tokyo, TAKUMI OUCHI, IMR, Tohoku Univ., YUE WANG, YUTA KASHIWABARA, SATOSHI YOSHIDA, KYOKO ISHIZAKA, MASASHI KAWASAKI, Univ of Tokyo, YOSHIMITSU KOHAMA, ISSP, The University of Tokyo, TSUTOMU NOJIMA, IMR, Tohoku Univ., YOSHIHIRO IWASA, Univ of Tokyo — Transition metal dichalcogenides (TMDs) are layered materials of abundant variety, providing emergent two-dimensional (2D) physical phenomena such as 2D superconductivity in few-layer NbSe$_2$. In the previous APS March Meeting, we reported layer-by-layer MBE growth of NbSe$_2$ thin films on insulating sapphire substrates [1], achieving relatively high $T_c$ comparable to that of bulk in the thick-enough regime. With reducing thickness, superconducting properties turned out to exhibit 2D-like behavior, realizing Ising superconductivity with large-area samples. In this presentation, we will present the experimental data on the angle dependence of $H_{c2}$ in a bilayer NbSe$_2$ film measured with a 55 T pulsed magnet at $^3$He temperature. We observed cusp-like angle dependence of $H_{c2}$ around the parallel magnetic fields even far below $T_c$ despite that $H_{c2}$ is purely dominated by the paramagnetic effect in this regime. In order to explain those results, we will propose a generalized Ginzburg-Landau model by taking into account the paramagnetic effect, which well describes the results with a microscopic physical picture. [1] H. Matsuoka et al, APS March Meeting 2018, K35.00009.
8:48AM F57.00005: Superfluid stiffness, optical spectral weight, and $T_c$ bounds in multi-band superconductors*

NISHCHHAL VERMA (Presenter), TAMAGHNA HAZRA, MOHIT RANDERIA, Ohio State Univ - Columbus — Recently we have used the optical sum rule for multi-band systems to bound the superfluid stiffness and derived upper bounds on the superconducting $T_c$ in two dimensions. These bounds were shown [PRX 9, 031049 (2019)] to be particularly important for strongly interacting, narrow band systems, and found to give useful estimates for a variety of systems ranging from cold atoms to twisted bilayer graphene. We explore here various situations where one is forced to include bands far from the chemical potential in order to have localized Wannier functions, simple interactions, or to describe flat bands. Our goal is to compute the low-energy optical spectral weight and obtain tighter bounds on the superfluid stiffness, compared to the full spectral weight that includes all interband transitions. We also gain insight into how band topology impacts optical spectral weight. We will present results for model systems with flat bands, including Lieb and Kagome lattices, and estimate $T_c$ bounds for monolayer FeSe on SrTiO$_3$ and for magic-angle twisted bilayer graphene.

*We acknowledge support from NSF-MRSEC DMR-1420451.
9:00AM F57.00006: Proximity-induced superconducting gap in the quantum spin Hall edge state of monolayer WTe$_2$* [Invited] BENJAMIN HUNT (Presenter), FELIX LÜPKE, DACEN WATERS, SERGIO C DE LA BARRERA, MICHAEL WIDOM, Carnegie Mellon Univ, JIAQIANG YAN, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee, Knoxville, RANDALL M FEENSTRA, Carnegie Mellon Univ — The quantum spin Hall (QSH) state was recently demonstrated in monolayers of the transition metal dichalcogenide 1T'-WTe$_2$ and is characterized by a band gap in the two-dimensional (2D) interior and helical one-dimensional (1D) edge states. Inducing superconductivity in the helical edge states would result in a 1D topological superconductor, a highly sought-after state of matter. In the present study, we use a novel dry-transfer flip technique to place atomically-thin layers of WTe$_2$ on a van der Waals superconductor, NbSe$_2$. Using scanning tunneling microscopy and spectroscopy (STM/STS), we demonstrate atomically clean surfaces and interfaces and the presence of a proximity-induced superconducting gap in the WTe$_2$ for thicknesses from a monolayer up to 7 crystalline layers. At the edge of the WTe$_2$ monolayer, we show that the superconducting gap coexists with the characteristic spectroscopic signature of the QSH edge state. Taken together, these observations provide conclusive evidence for proximity-induced superconductivity in the QSH edge state in WTe$_2$, a crucial step towards realizing 1D topological superconductivity and Majorana bound states in this van der Waals material platform.

*BMH acknowledges primary support from the Department of Energy Early Career program under award number DE-SC0018115; support for some STM work from the National Science Foundation under award number NSF DMR-1809145; and the NSF-MRI program for acquisition of the instrument under NSF DMR-1626099. Crystal growth at Oak Ridge National Laboratory was supported by the Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering; and additional crystal growth at Pennsylvania State University Two-Dimensional Crystal Consortium - Materials Innovation Platform (2DCC-MIP) was supported by NSF DMR-1539916.

9:36AM F57.00007: Local magnetic measurements of few-layer superconducting MoS$_2$* ALEXANDER JARJOUR (Presenter), BRIAN T SCHAEFER, GEORGE M FERGUSON, MENYOUNG LEE, KATJA NOWACK, Cornell University — Under ionic liquid gating, the transition metal dichalcogenide MoS$_2$ exhibits a superconducting dome with a maximum critical temperature of nearly 10 K in few-layer devices gated with an ionic liquid. Here, we report local magnetic measurements combined with electrical transport of this superconducting state as a function of temperature and over a limited range of carrier density. Using a scanning superconducting quantum interference device with an integrated field coil, we measure local diamagnetism at finite frequency. We report progress in extracting quantitative values of the Pearl length and superfluid density from these measurements.

*This work was primarily supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875) and performed in part at the Cornell NanoScale Facility, (NSF NNCI, Grant ECCS-1542081).
9:48AM F57.00008: Superconducting properties of MBE-grown 3R-Ta_{1+x}Se_2 epitaxial thin films YUKI TANAKA (Presenter), HIDEKI MATSUOKA, MASAKI NAKANO, YUE WANG, Department of Applied Physics, The University of Tokyo, SANA SASAKURA, KAYA KOBAYASHI, Okayama University, YOSHIHIRO IWASA, Department of Applied Physics, The University of Tokyo — 2D materials research is one of the hot topics in condensed-matter science, but most studies are performed on nanometer-thick crystals fabricated by mechanical exfoliation. On the other hand, researches based on MBE-grown samples are very much limited in particular for transport studies presumably due to difficulties in making high quality thin films. We have recently established a versatile route to layer-by-layer epitaxial growth of a wide variety of 2D materials and their heterostructures on insulating sapphire substrates by MBE [1,2], opening a door for exploration of emergent transport phenomena even based on hardly-cleavable and/or thermodynamically-metastable compounds. In this presentation, we will report MBE growth of thermodynamically-metastable 3R-Ta_{1+x}Se_2 epitaxial thin films and their superconducting properties, which turned out to be very much different from those of thermodynamically-stable 2H-TaSe_2 in terms of T_c and superconducting anisotropy. [1] M. Nakano et al., Nano Lett. 17, 5595 (2017). [2] Y. Kashiwabara et al., Adv. Funct. Mater. 2019, 1900354 (2019).

*This work was supported by Grants-in-Aid for Scientific Research (Grant Nos. 19H05602, 19H02593, 19H00653, 18K03540, and 15K21732) and A3 Foresight Program from the Japan Society for the Promotion of Science.

10:00AM F57.00009: Type-II Ising superconductivity in two-dimensional materials with spin-orbit coupling CHONG WANG (Presenter), Carnegie Mellon University, BIAO LIAN, Princeton University, XIAOMI GUO, ZETAO ZHANG, JIAHAO MAO, BING-LIN GU, YONG XU, WENHUI DUAN, Tsinghua University — Centrosymmetric materials with spin-degenerate bands are generally considered to be trivial for spintronics and related physics. In two-dimensional (2D) materials with multiple degenerate orbitals, we find that the spin-orbit coupling can induce spin-orbital locking, generate out-of-plane Zeeman-like fields displaying opposite signs for opposing orbitals, and create novel electronic states insensitive to in-plane magnetic field, which thus enables a new type of Ising superconductivity applicable to centrosymmetric materials. Many candidate materials are identified by high-throughput first-principles calculations. Our work enriches the physics and materials of Ising superconductivity, opening new opportunities for future research of 2D materials.
10:12AM F57.00010: Insight into Two-Dimensional Borophene: Five-Center Bond and Phonon-Mediated Superconductivity*  ZHIBIN GAO (Presenter), Department of Physics, National University of Singapore, MENGYANG LI, Institute for Chemical Physics & Department of Chemistry, Graduate School of Science, Xi’an Jiaotong University, JIAN-SHENG WANG, Department of Physics, National University of Singapore — We report a previously unknown monolayer borophene allotrope and we call it super-B with a flat structure based on ab initio calculations. It has good thermal, dynamical, and mechanical stability compared with many other typical borophenes. We find that super-B has a fascinating chemical bond environment consisting of standard sp, sp² hybridizations, and delocalized five-center three-electron π bond, called π(5c-3e), relying on the natural bond orbital analysis. This exceptional distribution of electron orbitals plays a pivotal role in stabilizing the super-B chemically. Moreover, super-B has a critical temperature $T_c$ of 20.8 K at ambient condition. We attribute this high $T_c$ of super-B to the giant anharmonicity of two linear acoustic phonon branches and an unusually low optic phonon mode. These discoveries provide new insight into the chemical nature of low dimensional boron nanostructures and highlight the potential applications of designing flexible devices and high $T_c$ superconductors.


*MOE tier 1 grant R-144-000-402-114.

10:24AM F57.00011: Atomic-layer Rashba superconductor protected by dynamic spin-momentum locking  SHUNSUKE YOSHIZAWA, National Institute for Materials Science, TAKAHIRO KOBAYASHI, YOSHITAKA NAKATA, Chiba University, KOICHIRO YAJI, FUMIO KOMORI, SHIK SHIN, Institute for Solid State Physics, The University of Tokyo, KAZUYUKI SAKAMOTO, Osaka University, TAKASHI UCHIHASHI (Presenter), National Institute for Materials Science — The breaking of the space inversion symmetry at surfaces and interfaces leads to the Rashba-type spin-orbit coupling (SOC) in 2D materials, which can strongly affect superconductivity [1]. In this talk, I will focus on crystalline atomic-layer indium on silicon surfaces with a clear spin-splitting of the Fermi surface and in-plane spin polarizations in the momentum space [2,3]. Our electron transport measurements under ultrahigh vacuum environment reveal that its in-plane critical magnetic field exceeds the Pauli limit by a factor of 3-4 at zero temperature. Through quantitative analysis, we conclude that elastic scattering among spin-momentum-locked electronic states serves as an effective spin-orbit scattering, thereby strongly suppressing the paramagnetic pair-breaking effect [4]. The mechanism is referred to as dynamic spin-momentum locking, which is contrasted to static spin-valley locking in 2D superconductors with Zeeman-type SOC [5].

References
8:00AM F58.00001: Long-Range Correlations in Density Functional Theory [invited] TIM GOULD (Presenter), Queensland Micro- and Nano-technology Centre, Griffith University — Accurate and low-cost reproduction of electron correlations remains one of the most difficult problems in chemical physics. Enormous progress has been made on dealing with short-range correlations. But long-range correlations remain challenging, despite contributing to a range of important quantum chemical problems including dispersion forces [1-2], strong correlations [3-4] and charge transfer excitations [5]. This talk will discuss the origins of key types of long-range correlations in density functional theory, and consider physical, chemical and mathematical perspectives on the problem. It will discuss some low-cost solutions to difficult problems in the field, introduced by the author and others, and will highlight some of the challenges that lie ahead. It will stress the importance of the universal functional in devising new approximations, and how quantum state ensembles can help, even in "mundane" cases.


8:36AM F58.00002: Embedding tools to improve density functionals. ADAM WASSERMAN (Presenter), Chemistry, Purdue University — As is well known, standard approximations to the exchange-correlation (XC) functional often do not yield accurate energies and/or spin-densities when chemical bonds are stretched. We use density embedding theory to examine the behavior of the non-additive contribution to the XC energy and to propose physically-motivated approximations for this contribution as atoms dissociate. We also discuss a recent approach to develop improved approximations for the non-additive non-interacting kinetic energy, and why this is a challenging problem.

*This presentation is based upon work supported by the National Science Foundation under Grant No. 1900301.
8:48AM F58.00003: Kohn-Sham accuracy at a fraction of the cost: Nonlocal subsystem DFT and orbital-free DFT*  MICHELE PAVANELLO (Presenter), Rutgers University, Newark — Subsystem DFT enables first principles simulations to approach realistic time- and length-scales, and most importantly sheds light on the dynamical behavior of complex systems. The accuracy of subsystem DFT is dependent on the quality of the employed nonadditive Kinetic Energy Density Functionals (KEDF). As these are customarily of semilocal character (i.e., they depend locally on the value of the density and its gradient), so far subsystem DFT has only been able to approach weakly interacting subsystems. In this presentation, we employ latest-generation nonlocal KEDF\textsuperscript{1,2} in subsystem DFT\textsuperscript{3} and orbital-free DFT\textsuperscript{4} simulations. Our results are of KS-DFT accuracy while still keeping the computational cost at a fraction of typical KS-DFT algorithms. The developed KEDFs are accurate enough also in the context of orbital-free DFT where we show they are able to approach million-atom semiconductor systems arranged in complex structures featuring Schottky barriers and space-charge regions.

4. X. Shao, W. Mi and M. Pavanello, in preparation.

*NSF CHE-1553993
DOE BES DE-SC0018343

9:00AM F58.00004: Absolutely Localized Multi-reference DFT Embedding  DANIEL GRAHAM (Presenter), XUELAN WEN, Chemistry, University of Minnesota, DHABIH CHULHAI, Chemistry, University of Indianapolis, JASON GOODPASTER, Chemistry, University of Minnesota — While density functional theory (DFT) has been a workhorse for quantum mechanical chemical calculations, current implementations have several deficiencies. Systems which require a multireference description are often poorly described by current DFT methods. Quantum embedding methods provide a strategy for performing localized highly accurate calculations on chemical systems while not incurring high cost computational scaling. Dividing a system into absolutely localized subsystems -- described by only the basis functions of the subsystem atoms -- can significantly reduce computational cost. The Huzinaga projection operator based absolute localization wavefunction embedded in DFT (WF-in-DFT) embedding methods match full system WF energy differences across a diverse test set including multi-reference WF calculations embedded in DFT. We have also studied large metal organic framework (MOF) cluster models, specifically gas adsorption on an Fe-MOF-74 cluster model and can achieve within 0.22 kcal/mol of the full system CASPT2 energy at a fraction of the computational cost. The absolute localization WF-in-DFT method allows for highly accurate calculations on multireference systems beyond the scope of current techniques.
9:12AM F58.00005: Towards an orbital-free kinetic energy density functional for molecular systems*  
OMOLOLU AKIN-OJO (Presenter), ICTP-EAIFR, University of Rwanda — A new kinetic energy density functional (KEDF) for systems composed of many atoms (molecular systems) is proposed. This KEDF contains the full von-Weizsacker KEDF as well as correction terms ("Pauli KEDF") appropriate for describing fermionic systems. Two of these correction terms are investigated: one from approximations based on the kinetic energy of fermions in an infinite well potential and the other from suitable averages of the kinetic energies of atoms. The performance of these new KEDFs will be presented as well as possible routes for further development.

*ICTP East African Institute for Fundamental Research (EAIFR)  
University of Rwanda  
Ministry of Education (MINEDUC), Rwanda

9:24AM F58.00006: Analytic inversion procedure for the exact non-additive kinetic potential functional $V^{nad}$  
MOJDEH BANAFSHEH (Presenter), University of California, Merced & University of Geneva, LEEOR KRONIK, Weizmann Institute of Science, TIM GOULD, Griffith University, DAVID STRUBBE, University of California, Merced, TOMASZ A. WESOLOWSKI, University of Geneva — The non-additive kinetic potential functional $V^{nad}$ is a key issue in density-dependent embedding methods, such as Frozen Density Embedding Theory and Partition-DFT. $V^{nad}$ is a bifunctional of pairs of specific electron densities $\rho_A$ and $\rho_B$. We report here an inversion procedure to generate reference $V^{nad}$ for weakly overlapping $\rho_A$ and $\rho_B$. To obtain the exact $V^{nad}$ we used an analytical inversion procedure that we proposed (M. Banafsheh, T.A. Wesolowski, Int. J. Quant. Chem. 118 (2018): e25410). We discuss the constraints on the choice of electron densities to assure their admissibility. Mathematical challenges of satisfying these constraints will be presented in detail. The potential at small overlap is constructed for various diatomic systems of four electrons at different interatomic distances. These results are compared with the potential obtained using common kinetic functional approximations. $V^{nad}$ is also presented for some diatomic systems including more than 4 electrons in which two electrons are localized with high precision in space and the accuracy of $V^{nad}$ is assured. We are now studying the forward Kohn-Sham problem for some small diatomic systems using the analytically inverted potential and comparing with the standard Kohn-Sham approach.
9:36AM F58.00007: Bond energies of molecules using optimal transport theory for the strictly-correlated-electron (SCE) limit of Density-Functional-Theory*  
KSHITEEJ DESHMUKH (Presenter), KAUSHIK DAYAL, Carnegie Mellon University — **Standard Kohn-Sham DFT starts from a mean-field approximation: the kinetic energy is modeled exactly, while the electron-electron interactions are modeled through a split into a mean-field term, and corrections from the exchange-correlation term. The SCE limit starts from the opposite limit: the electron-electron interactions are assumed to dominate over the kinetic energy, and hence it is a semi-classical limit. It is hence well suited to study strongly-correlated situations, e.g. bond breaking. While the SCE limit includes many-body interactions, it can be identified as a problem from Optimal Transport theory with Coulomb cost function. Hence it can be solved by a nested optimization in its dual (Kantorovich) formulation. We incorporate the Kantorovich solution within the KS-DFT framework and solve it using the finite element method. Bond-energy curve is obtained using this method for hydrogen molecule, and is compared against other exchange-correlation models to show the improved results. We then investigate bond-breaking in ethane and other small molecules using the SCE limit.**

*1) AFOSR MURI

9:48AM F58.00008: How accurate can a metaGGA+vdW functional be simultaneously for chemisorption and physisorption of molecular adsorption on transition metal surfaces?*  
MANISH KOTHAKONDA (Presenter), RUIQI ZHANG, JINLIANG NING, JAMES FURNESS, JIANWEI SUN, Tulane Univ — Understanding molecular adsorption on transition metal surfaces underpins many problems in heterogeneous catalysis. Accurately predicting the adsorption energies has been a challenging task as simultaneously capturing chemical and van der Waals (vdW) bonds in a single functional is difficult. In this work, we combine the semi-local meta-GGA made simple (MGGA_MS) functional with the rvv10 vdW correction [1-3]. We re-parametrize the functional by fitting to the atomization energies of covalently bonded molecules and the Ar2 binding curve. The resulting MGGA_MS + rVV10 is validated against a set of 38 systems including chemisorption and physisorption features with experimental [4] adsorption data.


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DOE under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents.
10:00AM F58.00009: Asymptotic behavior of the exchange-correlation energy density and the Kohn-Sham potential in density functional theory: exact results and strategy for approximations

ELI KRAISLER (Presenter), Hebrew Univ of Jerusalem — Density functional theory (DFT) is nowadays the leading theoretical framework for quantum description of materials from first principles. The predictive power of DFT critically depends on an accurate approximation to the generally unknown exchange-correlation (xc) energy functional. Approximations to the xc functional can be constructed from first principles by satisfying known properties of the exact functional. In this talk I focus on two such exact properties: the asymptotic behavior of the xc energy density per particle, $e_{xc}[n](r)$, and the asymptotic behavior of the Kohn-Sham potential, $v_{xc}[n](r)$, in finite many-electron systems. It is shown that these two properties are independent: fulfillment of one does not guarantee the other. In this process, a new quantity, the xc hole response function, is defined, some of its properties are deduced and its exact exchange part is analytically derived. A strategy for development of advanced approximations for exchange and correlation with a correct asymptotic behavior is suggested [1].


10:12AM F58.00010: Methods of corrections to to GEA approximations of the Pauli potential

JEREMY REDD (Presenter), Physics, Utah Valley University, ANTONIO CANCIO, Physics and Astronomy, Ball State University — In recent years many advances have been made in Orbital-Free Density Functional Theory (OFDFT), which attempts to remove orbitals from the Kohn-Sham DFT approach, either completely, or by approximating the kinetic energy density from meta-GGA exchange correlation functionals. The difficulty in OFKE models is in modeling the Pauli energy, the contribution to the KE of Pauli statistics. One aspect of this problem is correctly producing the OF Pauli potential, the functional derivative of the Pauli KE. Recent mathematical analysis of orbital free kinetic energy models based on Gradient Expansion Approximations (GEA)s, like the Airy gas model, have offered insight in modeling the Pauli potential for neutral atoms. However all of these models suffer from gross inaccuracies in the nuclear cusp region, as well as an unexpected deviation in the core. The exact Pauli potential approaches a constant near the nucleus related eigenvalue of the lowest occupied atomic orbital, but all GEAs become infinitely negative at the singularity. We propose a smooth non-analytic stitching function to correct the error in the near nuclear region for Pauli potential GEAs, and explore the outer core. This is similar to work done by Perdew and Constantin as well as previous work from this group done on KEDs.
10:24 AM F58.00011: Practical Density Functional Theory Beyond the Zero-Sum Limit: M11plus
PRAGYA VERMA, University of Minnesota, BENJAMIN JANESKO (Presenter), Texas Christian Univ, YING WANG, XIAO HE, East China Normal University, GIOVANNI SCALMANI, MICHAEL J. FRISCH, Gaussian, Inc., DONALD G TRUHLAR, University of Minnesota — Conventional approximate DFT functionals are based on what exchange would be a nearly homogeneous electron gas. This model effectively uses like-spin exchange to model opposite-spin correlation, producing a "zero-sum" tradeoff in performance for some classes of problems, including bond energies vs. barrier heights or valence vs. Rydberg excitations. We argue that including new ingredients in a functional can provide beyond-zero-sum broad accuracy. We demonstrate this by adding a new ingredient to the flexible M11 long-range-corrected hybrid meta functional form. The new ingredient is an inexpensive rung-3.5 bound to the exact exchange energy density. The M11 form was reoptimized with these terms, producing a functional called M11plus. Tests for thermochemistry, kinetics, and response properties suggest M11plus is one of the most broadly accurate occupied-orbital-only DFT functionals available to date.

*This work was performed as part of the Nanoporous Materials Genome Center, which is funded by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences under Award DE-FG02-17ER16362. BGJ was supported by NSF DMR-1505343.

10:36 AM F58.00012: Numerical analysis of thermodynamic limit extrapolation power-laws in the uniform electron gas using connectivity-twist-averaged coupled cluster doubles theory
TINA MIHM (Presenter), BINGDI YANG, LAURA WEILER, University of Iowa, ALEXANDRA MCISAAC, Chemistry, MIT, ANDREAS GRUENEIS, Vienna University of Technology, SAI RAMADUGU, JAMES SHEPHERD, University of Iowa — We recently developed a coupled-cluster theory method in the uniform electron gas (UEG) for improving twist averaging in solids [1]. The method finds a special twist angle that gives comparable results to conventional twist averaging at a reduced cost. Here, we apply this new method to calculate the thermodynamic limit energies of the uniform electron gas across a range of densities. The high-density limit is then used to derive general power laws for extrapolation. Time permitting, we will also show preliminary results for real systems using the Vienna ab-initio software package [2][3].


*We thank University of Iowa for their funding.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM
Using magnetic band theory and topological indices obtained from Topological Magnetic Quantum Chemistry (TMQC), we have performed the first high-throughput of about 500 magnetic topological materials and have discovered over 100 magnetic enforced semimetals and topological insulators. This knowledge is crucial for correct ab-initio calculations of the materials' band structure, which we have performed for each of those compounds including complete phase diagrams at different values of Hubbard potential in LDA+U. Using an in-house code for finding the magnetic band representations at high symmetry points, we then feed this data into the topological machinery of TMQC to determined the topological materials, as well as the obstructed atomic limits. We then pick several candidates for showcasing new topological physics and analyze the topological trends in the materials upon varying interactions.
Computational study and discovery of antiferromagnetic topological insulators [Invited] MIKHAIL OTROKOV (Presenter), Materials Physics Center (MPC) — Magnetic topological insulators (MTIs) are narrow gap semiconductor materials that combine non-trivial band topology and magnetic order. Unlike their nonmagnetic counterparts, MTIs may have some of the surfaces gapped due to breaking the time-reversal symmetry, which enables exotic phenomena having potential applications in spintronics. So far, MTIs were only created by means of doping nonmagnetic TIs with 3\textit{d} transition metal atoms however, such an approach leads to strongly inhomogeneous magnetic and electronic properties of these materials, restricting the observation of important effects to very low temperatures. Finding intrinsic MTI, i.e. a stoichiometric well-ordered compound, could be an ideal solution to these problems. Using \textit{ab initio} calculations, we predicted the van der Waals layered compound MnBi\textsubscript{2}Te\textsubscript{4} (MBT) to be the first antiferromagnetic TI (AFMTI) \cite{1,2}. The interlayer AFM ordering makes MBT invariant with respect to the combination of the time-reversal (Θ) and primitive-lattice translation ($T_{1/2}$) symmetries, $S=ΘT_{1/2}$, which gives rise to the $Z_2$ classification of AFM insulators. We find $Z_2=1$ for MnBi\textsubscript{2}Te\textsubscript{4}, which confirms its topologically nontrivial nature. To date, many experimental groups confirmed the AFMTI state in MBT, with the first observation reported in Ref. \cite{1}.

In the 2D limit, MBT is expected to show a unique set of thickness-dependent magnetic and topological transitions, which drive it through FM and (un)compensated AFM phases, as well as quantum anomalous Hall (QAH) and zero plateau QAH states \cite{2}. The latter was predicted to host the axion insulator phase.

The discovery of the first AFMTI opens a new field that focuses on intrinsically magnetic stoichiometric compounds: several MBT-derived MTI-candidates were experimentally synthesized right away, that will be discussed in the talk along with other AFMTI candidates predicted \textit{ab initio}.

\citenum{1} M. Otrokov et al., arXiv:1809.07389.

Computational Search for Magnetic and Non-magnetic 2D Topological Materials using Spin-orbit Spillage KAMAL CHOUDHARY (Presenter), KEVIN GARRITY, FRANCESCA TAVAZZA, Materials Measurement Lab, National Institute of Standards and Technology — Intrinsic two-dimensional materials have a variety of properties that make them attractive for potential topological devices. Using density functional theory-based spin-orbit spillage, Wannier-interpolation, and related techniques, we identify topologically non-trivial intrinsic 2D insulators and semimetals, including both magnetic and non-magnetic materials. Using JARVIS-DFT 2D material dataset we first identify materials with high spin-orbit spillage among 683 materials, resulting in 108 materials with high-spillage values. Then, we use Wannier-interpolation to carry-out Z2, Chern-number, anomalous Hall conductivity, Curie temperature, and edge state calculations. We identify topological insulators and semimetals such as quantum spin-hall insulators (QSHI), quantum anomalous-hall insulators (QAHI), and semimetals. For a subset of predicted QAHI materials, we run GW+SOC and GGA+U calculations. We find that as we introduce many-body effects, only few materials retain non-trivial band-topology, suggesting the importance of high-level DFT methods in predicating 2D topological materials. However, as an initial step, the automated spillage screening and Wannier-approach provides useful predictions for finding new topological materials.
9:00AM F59.00004: Automated Critical Temperature Prediction and High-Throughput Search for Composite Quantum Materials  
NATHAN C. FREY (Presenter), University of Pennsylvania, MATTHEW HORTON, JASON MUNRO, Lawrence Berkeley National Laboratory, VIVEK SHENOY, University of Pennsylvania, KRISTIN PERSSON, Lawrence Berkeley National Laboratory — Composite materials with coexisting quantum phases offer exciting opportunities for solid-state device applications and exploring new physics emerging from the interplay between effects including topology, magnetism, and ferroelectricity. However, both the computational design and experimental realization of magnetic topological materials and multiferroics are confounded by the difficulties inherent to predicting and controlling magnetic behavior, which arises from strong electron correlations. We present a workflow to automate the calculation of exchange parameters and critical temperatures with density functional theory and Monte Carlo simulations. We use our recently developed Python Topological Materials package to screen materials for non-trivial band topology. We then apply this approach to suspected magnetic materials in the Materials Project database. By identifying layered materials, we also accelerate the discovery of van der Waals materials with composite topological quantum phases and multiferroic properties. Our method can be used to screen for thermodynamically stable, robust composite quantum materials for solid-state devices and exploring exotic physics like the quantum anomalous Hall effect and axion electrodynamics.

9:12AM F59.00005: Computational search for magnetic topological materials in Eu compounds*  
LIN-LIN WANG (Presenter), Ames Lab, ROBERT-JAN SLAGER, Department of Physics, Harvard University, HOI CHUN PO, Department of Physics, MIT, ADAM KAMINSKI, Department of Physics and Astronomy, Iowa State University, ASHVIN VISHWANATH, Department of Physics, Harvard University, PAUL C CANFIELD, Department of Physics and Astronomy, Iowa State University — Topological materials are of great interests for both basic research and future technology. Recent developments of symmetry indicators and similar approaches to diagnose band structure topology have resulted in databases of non-magnetic topological materials via high throughput band structure calculations. However, magnetic topological materials have been much less explored. One of the reasons is that the magnetic ground state structures are not readily available like crystallography databases and also different magnetic configurations can be competing in energy. But this also offers the opportunity to use magnetism to control topological properties of materials. Here we have explored Eu compounds using band structure calculations based on density functional theory and found several Eu compounds can host ferromagnetic Weyl, anti-ferromagnetic Dirac as well as anti-ferromagnetic topological insulating states depending on different magnetic configurations.

*This work is supported by the Center for Advancement of Topological Semimetals, an Energy Frontier Research Center funded by the US DOE Basic Energy Sciences, through the Ames Laboratory under Contract No. DE-AC02-07CH11358.
In [Bradlyn et al., *Nature* (2017)], we introduced Topological Quantum Chemistry (TQC) - a real-space predictive theory of band topology and degeneracy constructed from graph theory and atomic orbitals in the 230 time-reversal- ($T$-) symmetric space groups (SGs). TQC subsequently fueled the identification of tens of thousands of topological materials, and the discovery of novel topological insulating (TI) phases, including "higher-order" TIs. However, the 230 SGs only represent a fraction of the 1651 Shubnikov SGs, which characterize the symmetries of both magnetic and non-magnetic crystals. In this talk, we extend TQC to the magnetic Shubnikov SGs (MSGs), forming the complete theory of Magnetic Topological Quantum Chemistry (MTQC). Using MTQC, we construct a complete classification of the magnetic atomic limits [i.e., magnetic Elementary Band Representations (MEBRs)]. Through the MEBRs, we also obtain the little-group corepresentations of the MSGs, complete eigenvalue indicators for strong and fragile magnetic TIs and semimetals, and all possible mean-field band connectivities in crystals with lattice-commensurate magnetism. We introduce new tools on the Bilbao Crystallographic Server for accessing this information, and discuss magnetic topological materials identified using MTQC.

We perform a comprehensive study of band degeneracies protected by 3D magnetic space groups in the bands of magnons and of electrons, and obtain all new classes of degeneracies (nodes) that cannot appear in non-magnetic materials. The new nodes protected by magnetic space groups are unified and classified using the group cohomology of the corresponding point group. We propose a method to find if the effective theory of any new degeneracy has linear dispersion in all three directions, and use the method to identify all linear-dispersing nodes of four or higher degeneracy.
9:48AM F59.00008: Searching for Double Dirac Fermions*  
TANYA BERRY (Presenter), Johns Hopkins University, RAFAL WAWRZYNCKAZ, JOHANNES GOOTH, CLAUDIA FELSER, Chemical Physics of Solids, Max Planck Institute, TYREL MCQUEEN, Johns Hopkins University — The field of topological materials is developing rapidly, exhibiting new physical phenomena and inviting potential applications in the emerging fields of quantum computing and sensing. Normally, the maximal degeneracy of states in any electronic system is six. Topological considerations predict that in certain materials the double group cross product of two irreducible representations (irreps.) or the cross product of one irrep. on itself can yield eight states that are degenerate in energy at a high symmetry point in reciprocal space. Materials including CuBi$_2$O$_4$ and PdBi$_2$O$_4$ have been previously predicted to be such 8-fold fermion or double Dirac systems on the basis of their symmetries. However, their insulating behavior hinders photoemission and transport characterizations, which are crucial for unambiguous identification. Here we present a strategy for designing real materials with 8-fold fermions based on chemical principles and provide an update on experimental detection of this novel topological state.

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331.

10:00AM F59.00009: Axion coupling in the hybrid Wannier representation*  
NICODEMOS VARNAVA (Presenter), Physics and Astronomy, Rutgers University, IVO SOUZA, Centro de Fisica de Materiales, Universidad del Pais Vasco (UPV/EHU), DAVID VANDERBILT, Physics and Astronomy, Rutgers University — One of the most important quantized responses of 3D topological insulators (TIs) is due to the axion coupling \( \theta \). Strong TIs, axion insulators, and the topological magnetoelectric effect owe their robustness to the quantization of the axion coupling (the axion \( \mathbb{Z}_2 \) index). Time reversal was the first quantizing symmetry to be recognized, but recently a plethora of magnetic symmetries were found to have the same effect. After we enumerate all the quantizing symmetries, we explore how the nature of these symmetries affects the topological properties of the system. One tool that has proven especially useful in that respect is the hybrid Wannier (HW) representation. In this representation the quantizing symmetries can be divided into three distinct classes. By analyzing each of them in turn, we are able to explain whether the connectedness of the HW band structure in a topological phase is robust or fragile. Furthermore, we clarify the correspondence between the connectedness of the HW band structure and the appearance of either topologically protected metallic surfaces or insulating surfaces with half-quantized anomalous Hall response. We corroborate our results with various tight-binding models.

*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331
**10:12AM F59.00010: Domain-wall states in Chern insulator with in-plane ferromagnetism**

YAFEI REN (Presenter), TAO HOU, ZHENHUA QIAO, Department of Physics, University of Science and Technology of China (USTC) — Topological phase is global and beyond the Landau paradigm of phases described by local order parameters. In this work, we report the electronic and transport properties of in-gap domain-wall states between domains with the same topology but different local magnetic orders, which lie in plane. We consider a buckled honeycomb lattice model that can host Chern insulating phase from in-plane magnetization with azimuthal angle \( \varphi_0 \), which breaks the three-fold rotation symmetry of original lattice. The topological phase remains the same at different \( \varphi_p = \varphi_0 + 2\pi p/3 \) (\( p=0-2 \)). Along the domain wall, we find one-dimensional in-gap states whose electronic dispersion depends on the magnetic structure and domain wall width despite the same Chern number at different domains. At a symmetric \( Y \)-shape junction formed by three regions of different \( \varphi_p \), we find counter-intuitive chiral current partition law that is tunable by electrical means. In a network by combining \( Y \)-shape junction to form a honeycomb, we find that the in-gap states form nearly flat Bloch bands with different topological Chern numbers providing a intriguing platform to investigate many-body effects.

*National Key R & D Program, NNSFC

**10:24AM F59.00011: Half-integer quantization of Hall conductance in semi-magnetic topological insulator**

MASATAKA MOGI (Presenter), YOSHIHIRO OKAMURA, Univ of Tokyo, MINORU KAWAMURA, RYUTARO YOSHIMI, RIKEN CEMS, KENJI YASUDA, Univ of Tokyo, ATSUSHI TSUKAZAKI, Tohoku University, KEI TAKAHASHI, RIKEN CEMS, TAKAHIRO MORIMOTO, Univ of Tokyo, NAOTO NAGAOSA, RIKEN CEMS, MASASHI KAWASAKI, YOUTAROU TAKAHASHI, Univ of Tokyo, YOSHINORI TOKURA, RIKEN CEMS — The emergence of two-dimensional (2D) Dirac fermions in condensed matter systems, such as graphene and three-dimensional (3D) topological insulators, has greatly deepened quantum Hall physics. The anomalous integer quantization of Hall conductance as observed in graphene is understood by the half-integer topological number of each Dirac cone. However, the Dirac cones always appear in pairs in such 2D lattices, hiding the half-integer number from experimental observations. The 3D topological insulators, on the other hand, can possess a single Dirac cone in each top and bottom surface, serving as an ideal system to explore the half-integer quantization phenomena. Here, we will report the observation of half quantized Hall conductance in ‘semi-magnetic’ topological insulator films, where one of the surfaces is gapped by magnetic doping whereas the opposite one remains non-magnetic and gapless. Using time-domain terahertz magneto-optical spectroscopy as well as electrical transport, we observed half quantized Faraday and Kerr rotations and half quantized Hall conductivity at zero fields. This result provides experimental evidence for the predicted fractional quantized state in 3D topological insulators.

*This research was supported by JST CREST (no. JPMJCR16F1) and JSPS (no. 17J03179).
10:36AM F59.00012: Antiferromagnetism and spin density waves in Dirac semimetals
GRIGORY BEDNIK (Presenter), University of California, Santa Cruz — We perform mean-field study of possible magnetic instabilities in Dirac semimetals. We find that Dirac electrons naturally host antiferromagnetic or spin density wave ground states, though their specific configurations may vary depending on specific model, as well as chemical potential and temperature. We also discuss paramagnetic susceptibility in Dirac semimetals. In the cases, when Dirac electrons do not have orbital momentum, the magnetic properties may be $\mu$ and $T$ independent.

*NSERC of Canada

10:48AM F59.00013: Intrinsic magnetic topological insulator $\text{MnBi}_2\text{Te}_4$
JIAHENG LI (Presenter), DUAN WENHUI, YONG XU, Department of Physics, Tsinghua University — The interplay of magnetism and topology offers great opportunities to explore variant emerging topological quantum phenomena. Here we will present that van der Waals layered $\text{MnBi}_2\text{Te}_4$-related materials intrinsically host nontrivial band topology, which possess A-type antiferromagnetism characterized by ferromagnetic intralayer and antiferromagnetic interlayer coupling. Extremely rich 2D and 3D topological quantum states emerge in $\text{MnBi}_2\text{Te}_4$, including 3D antiferromagnetic topological insulator with the long-sought topological axion states on the surface, the simple magnetic Weyl semimetal with one pair of Weyl points, as well as intrinsic axion insulators and QAH insulators in even- and odd-layer films, respectively [1]. Furthermore, we will show a series of magnetically controllable topological quantum phase transitions in the material [2]. Relevant experimental progresses will also be introduced [3-5].


Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F60 DMP: Topological Materials: Magnetism and Hybrid Structures
Mile High Ballroom 4A - Jisoo Moon, US Naval Research Laboratory - Tag(s): Focus
WENBO WANG (Presenter), University of California, Santa Barbara — Quantum anomalous Hall effect (QAHE), which is related to the momentum-space Berry phase, was experimentally realized in Cr-doped (Bi,Sb)$_2$Te$_3$ (BST) and V-doped BST thin films. The full quantization of anomalous Hall effect (AHE) in these two systems requires extremely low temperature (<50mK) [1][2]. Magnetic inhomogeneity has been proposed as one of the main reasons that limit the temperature for the realization of QAHE. In the first part, we will present direct visualization of long-range ferromagnetism in the Cr,V co-doped BST films, by using the MFM and in-situ transport measurement[3]. The magnetization reversal process reveals typical ferromagnetic domain behavior, i.e. domain nucleation and domain wall propagation. In the second part, we will discuss topological Hall effect (THE), a real-space Berry phase effect that originates from the non-coplanar spin textures[4]. Intrinsic THE was revealed at different temperatures in the magnetic topological insulator heterostructure Sb$_2$Te$_3$/V-doped Sb$_2$Te$_3$, after a back-gate voltage was applied to zero the AHE. The high-temperature THE persists above the Curie temperature, which originates from the spin chirality fluctuations[5]. At temperatures well below the Curie temperature, THE emerges around the coercive fields, when the ferromagnetic bubble domains form. The low-temperature THE likely results from the static topological charges at the chiral domain walls.


*This work is supported by DOE BES under award # DE-SC0018153
8:36AM F60.00002: Magneto-transport in Pb\textsubscript{x}Sn\textsubscript{1-x}Se Quantum Well*  

JIASHU WANG (Presenter), XINYU LIU, LOGAN S RINEY, JACEK K. FURDYNA, BADIH A ASSAF, University of Notre Dame — Pb\textsubscript{x}Sn\textsubscript{1-x}Se (0.16<x<0.4) is a narrow gap semiconductor that exhibits a topological phase transition to a topological crystalline insulator (TCI) when the concentration of Sn increases. It is a valley degenerate topological system that can exhibit exotic quantum Hall effects and strong coupling between the crystal and electronic structures. Here we investigated the transport properties of PbEuSe/Pb\textsubscript{x}Sn\textsubscript{1-x}Se/PbEuSe quantum wells, of which the thickness is 30 and 50nm and x=0.3. By doping Bismuth during the growth, we can efficiently tune the carrier type from p type to n type with carrier densities as low as 1E18cm\textsuperscript{-3} and high mobility (>10000cm\textsuperscript{2}/ (Vs)). We found out that the sample showed linear magnetoresistance starting at relatively low field (<1T). The slope of ΔR/R\textsubscript{0} is proportional to the mobility. We applied several model to explain this phenomenon. Further process like gating is also used to investigate the mechanism. With high mobility and low carrier density in the quantum well, it will be a great platform to study 2D quantum phenomenon in the landau quantized regime.

*Jiashu Wang and Badih A. Assaf acknowledge ND-Nano for funding support.

8:48AM F60.00003: Magnetotransport properties in antimony single crystals*  

PAUL C. W. CHU (Presenter), ZHENG WU, LIANGZI DENG, MELISSA GOOCH, TREVOR BONTKE, Texas Center for Superconductivity and Physics Department at the Univ of Houston — The magnetoresistance of antimony single crystals has been measured with the measuring current perpendicular and parallel to the magnetic field, respectively. Extremely large positive transverse magnetoresistance (TMR) up to 1,000,000% was obtained in a magnetic field of 7 T. Field dependence of TMR followed the power law MR ∝ H\textsuperscript{2α} in all measured temperatures from 2 K to 300 K. The extremely large TMR is attributed to the well compensated electron and hole carriers with high mobility. A very pronounced negative longitudinal magnetoresistance (LMR) at high field and a valley at zero field was observed. The general behavior appears to be consistent with the chiral magneto effect predicted in quantum solids. Moreover, a very unusual negative potential from voltage leads was detected by IV curve, dc, and ac resistance measurements at high magnetic field. This observation cannot be understood in terms of available theories and may be related to some exotic topological characteristics predicted for antimony.

*The work performed at TcSUH is supported by US Air Force Office of Scientific Research Grant FA9550-15-1-0236, the T. L. L. Temple Foundation, the John J. and Rebecca Moores Endowment, and the State of Texas through the Texas Center for Superconductivity at UH.
**9:00AM F60.00004: Thickness Dependence of Electronic Properties of Topological Antiferromagnet MnBi$_2$Te$_4$ Films**  
YIFAN ZHAO (Presenter), GUANG WANG, LINGJIE ZHOU, Pennsylvania State University, DMITRY OVCHINNIKOV, University of Washington, FEI WANG, LING ZHANG, HEMIAN YI, BAITAO ZHANG, MOSES HUNG-WAI CHAN, Pennsylvania State University, XIAODONG XU, University of Washington, CUI-ZU CHANG, Pennsylvania State University — The prerequisite for the realization of the quantum anomalous Hall (QAH) state is an interplay between topology and magnetism. More recently, MnBi$_2$Te$_4$ was experimentally demonstrated to be a material in which the topological and magnetic states intrinsically coexist. The QAH and axion insulator states were predicted in thin films of MnBi$_2$Te$_4$ when the number of layers is odd and even, respectively. Here, we synthesized MnBi$_2$Te$_4$ thin films with thicknesses down to one layer using molecular beam epitaxy (MBE) and systematically studied the thickness dependence of electronic properties. Both Hall and Magneto-Optical Kerr Effect measurements show a clear ferromagnetic hysteresis in the one-layer sample. For films thicker than one layer, similar to the exfoliated MnBi$_2$Te$_4$ devices, the samples show a small ferromagnetic hysteresis loop at the low magnetic field and spin flop transitions at the high magnetic field. We also found the Hall resistance under zero magnetic field displays an odd/even oscillation, i.e., the samples with odd (even) layers exhibit an anomalous Hall (AH) hysteresis loop with a negative (positive) sign. 
*This work is supported by ARO (W911NF1810198), DOE (DE-SC0019064), and Alfred P. Sloan Research Fellowship.

**9:12AM F60.00005: Discovery of a quantum topological kagome magnet by vector magnetic field-based STM**  
JIAXIN YIN (Presenter), Physics, Princeton University, WENLONG MA, School of Physics, Peking University, SONGTIAN SONIA ZHANG, TYLER COCHRAN, Physics, Princeton University, XITONG XU, School of Physics, Peking University, NANA SHUMIYA, BIAO LIAN, ZHIDA SONG, Physics, Princeton University, KUN JIANG, Physics, Boston College, TAY-RONG CHANG, Physics, National Cheng Kung University, TITUS NEUPERT, Physics, University of Zurich, ZIQIANG WANG, Physics, Boston College, NAN YAO, Physics, Princeton University, SHUANG JIA, School of Physics, Peking University, ZAHID HASAN, Physics, Princeton University — Kagome magnets have been known to exhibit rich topologically based vector magnetic field responses, including giant and anisotropic spin-orbit tunability (J.-X. Yin et al. Nature 562, 91-95 (2018)) and negative flatband magnetism (J.-X. Yin et al. Nature Physics 15, 443-448 (2019)). Here we use the same vector magnetic field-based STM technique combined with Berry curvature sensitive transport to discover a new quantum topological kagome magnet. We observe striking Landau quantization of the kagome lattice, dissipationless chiral edge state, and quantum-limit Hall response. These combined results point to the realization of a high-temperature quantum topological kagome magnet.

*Experimental and theoretical work at Princeton University was supported by the Gordon and Betty Moore Foundation (GBMF4547/ Hasan) and the United States Department of Energy (US DOE) under the Basic Energy Sciences program (grant number DOE/BES DE-FG-02-05ER46200). The work in Peking University was supported by the National Natural Science Foundation of China No. U1832214, No.11774007, the National Key R&D Program of China (2018YFA0305601) and the strategic Priority Research Program of Chinese Academy of Sciences (XDB28000000).
9:24AM F60.00006: Quantum oscillations in thin films of antiferromagnetic kagome metal FeSn

MINYONG HAN (Presenter), HISASHI INOUE, Massachusetts Institute of Technology MIT, MUN K. CHAN, National High Magnetic Field Laboratory, LANL, DAVID E GRAF, National High Magnetic Field Laboratory, Florida State University, LINDA YE, TAKEHITO SUZUKI, JOSEPH G CHECKELSKY, Massachusetts Institute of Technology MIT — FeSn is an antiferromagnetic metal, consisting of two-dimensional layers of corner-sharing triangles of Fe, separated by honeycomb Sn spacer layers. This geometrical arrangement of Fe atoms, known as the kagome lattice, is predicted to give rise to Dirac fermions and topological flat bands. Recent photoemission and quantum oscillation studies on FeSn bulk single crystals have experimentally confirmed the existence of these features in their electronic structures [1]. Here we report the quantum oscillation studies on thin films of FeSn. The observed oscillation frequency reproduces the previous measurements on FeSn bulk single crystals. Temperature and field-angle dependent oscillation frequencies respectively reveal the scattering timescale and morphology of the observed Fermi pocket. The realization of high quality FeSn thin films offers a promising platform to explore the interplay of magnetism and electronic topology via quantum confinement or electrostatic gating [2].

References:

9:36AM F60.00007: Dirac-Surface-State-Modulated Bilinear Magnetoresistance in Topological Insulators*

FEI WANG (Presenter), LING ZHANG, ZIQIAO WANG, YIFAN ZHAO, RUN XIAO, GUANG WANG, HEMIAN YI, LINGJIE ZHOU, RUOXI ZHANG, BAITAO ZHANG, MOSES HUNG-WAI CHAN, NITIN SAMARTH, QI LI, Department of Physics, Pennsylvania State University, WEIWEI ZHAO, School of Materials Science and Engineering, Harbin Institute of Technology, CUI-ZU CHANG, Department of Physics, Pennsylvania State University — Topological insulators (TIs) are a class of quantum materials in which the interior is insulating but electrons can travel through the two-dimensional (2D) conducting surfaces known as Dirac surface states. The Dirac surface states harbor a helical spin texture and thus provide a good platform for potential spintronic applications. Prior experiments have shown that the helical spin texture of the Dirac surface states can be resolved using bilinear magnetoresistance (BMR) measurements. The observation of BMR in previous studies was attributed to the presence of the hexagonally warped Fermi surface at the Dirac surface state in samples with heavy doping. Here, we fabricated a series of (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$ samples with different $x$ and systematically studied their BMR. When the chemical potential is near the Dirac point and the warping effect of the Dirac surface state disappears, the BMR reaches a maximum rather than vanishes. This observation is further confirmed in a dual-gate-tuned device. Our work indicates that BMR has more complex origins than the warping effect of the Dirac surface state alone.

*This work is supported by DOE (# DE-SC0019064), the Alfred P. Sloan Research Fellowship, and NSF 2DCC-MIP (DMR-1539916).
Dirac Band Engineering of Topological Insulator/Graphene Hybrid Structures*  
GUANG WANG (Presenter), Department of Physics, National University of Defense Technology, YIFAN ZHAO, Department of Physics, The Pennsylvania State University, HUIXIA FU, Department of Condensed Matter Physics, Weizmann Institute of Science, ZENGLE HUANG, Department of Physics and Astronomy, Rutgers University, FEI WANG, HEMIAN YI, TIMOTHY PILLSBURY, LINGJIE ZHOU, Department of Physics, The Pennsylvania State University, CHENGYE DONG, JOSHUA ROBINSON, Department of Materials Science and Engineering, The Pennsylvania State University, NITIN SAMARTH, Department of Physics, The Pennsylvania State University, WEIDA WU, Department of Physics and Astronomy, Rutgers University, BINGHAI YAN, Department of Condensed Matter Physics, Weizmann Institute of Science, CUI-ZU CHANG, Department of Physics, The Pennsylvania State University — Dirac materials such as graphene and topological insulators (TI) have attracted much attention because of their unique electrical properties. Stacking these two Dirac materials to form a heterostructure provides a platform for the exploration of the interesting physics of coupled Dirac fermions. We recently used molecular beam epitaxy to fabricate the (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$/graphene hybrid structures and systematically studied the electronic band structures as a function of $x$ and thickness. Because the ratio between the lattice constants of Sb$_2$Te$_3$ and graphene is $\sqrt{3}$, the Dirac cone of graphene can be folded to the $\Gamma$ point of the Brillouin zone of Sb$_2$Te$_3$. The coexistence of two different Dirac low-energy states is indeed observed in angle-resolved photoemission spectroscopy measurements. This phenomenon is further demonstrated by scanning tunneling microscopy results and first-principles calculations. Our work is of great importance for understanding the interplay of Dirac fermions across the TI/graphene interface and paves a new way to study band engineering in Dirac materials.

*This work is supported by the NSF-CAREER award (DMR-1847811) and NSF-2DCC-MIP (DMR-1539916).

Topological Properties of SnSe/EuS and SnTe/CaTe Heterostructures  
SHUYANG YANG (Presenter), CHUNZHI WU, NOA MAROM, Carnegie Mellon University — We use density functional theory (DFT) to study epitaxial interfaces of the topological crystalline insulators SnSe and SnTe with the ferromagnetic semiconductor EuS and the nonmagnetic semiconductor CaTe, respectively. We consider both surface slab models and periodic "sandwich" heterostructures. We find that a gapped surface state arises in the SnSe/EuS interface due to the magnetic proximity effect. By comparison, the gapless topological surface state at the interface of SnTe/CaTe is unperturbed.
Synthesis of hybrid oxide/chalcogenide interfaces to explore topological crystalline insulator properties

STEPHEN D ALBRIGHT (Presenter), Department of Physics, Center for Research on Interface Structures and Phenomena, Yale University, KE ZOU, Department of Physics & Astronomy, Stewart Blusson Quantum Matter Institute, The University of British Columbia, SHUHANG PAN, Department of Physics, Center for Research on Interface Structures and Phenomena, Yale University, FREDERICK J WALKER, CHARLES H AHN, Department of Applied Physics, Center for Research on Interface Structures and Phenomena, Yale University — The class of topological crystalline insulators (TCIs), including SnTe, provides new opportunities to explore topological behaviors. Surface carriers in TCIs experience the same spin-momentum locking as conventional topological insulators, but are protected by crystalline symmetry, which makes possible controlling topological states in SnTe through electric field gating. This work presents growth of SnTe thin enough to achieve topological state control on a substrate, SrTiO$_3$, easily integrated into field-effect devices. We grow SnTe films by co-sublimation-deposition, where a high-quality thick film is controllably thinned by elevating the substrate temperature in constant flux. X-ray diffraction and atomic force microscopy confirm SnTe films grown by this process are uniform down to 7 nm. Carrier density over a range of film thickness, extracted from Hall measurements, reveals surface-dominated transport in SnTe films less than 16 nm. Weak antilocalization (WAL) behavior observed in magnetotransport is consistent with topological conduction through these surface states, and we fit WAL to theory to extract details of the topological transport. The growth method presented here opens up future opportunities to design heterostructures to further explore topological behavior.
10:24AM F60.00011: Modular Arithmetic with Nodal Lines: Drumhead Surface States in ZrSiTe*  LUKAS MUECHLER (Presenter), Center for Computational Quantum Physics, Flatiron Institute, ANDREAS TOPP, Max Planck Institute for Solid State Research, RAQUEL QUEIROZ, Department of Condensed Matter Physics, Weizmann Institute of Science, MAXIM KRIVENKOV, ANDREI VARYKHALOV, Helmholtz-Zentrum Berlin fuer Materialien und Energie, JENNIFER CANO, Department of Physics and Astronomy, Stony Brook University, CHRISTIAN R AST, Max Planck Institute for Solid State Research, LESLIE SCHOOP, Department of Chemistry, Princeton University — We study the electronic structure of the nodal line semimetal ZrSiTe both experimentally and theoretically. We find two different surface states in ZrSiTe - topological drumhead surface states and trivial floating band surface states, which can be easily distinguished in ARPES experiments. Using the spectra of Wilson loops, we show that a non-trivial Berry phase that exist in a confined region within the Brillouin Zone gives rise to the topological drumhead-type surface states. The \( Z_2 \) structure of the Berry phase induces a \( Z_2 \) 'modular arithmetic' of the surface states, allowing surface states deriving from different nodal lines to hybridize and gap out, which can be probed by a set of Wilson loops. Our findings are confirmed by \textit{ab-initio} calculations and angle-resolved photoemission experiments, which are in excellent agreement with each other and the topological analysis.
Ref: arXiv:1909.02154

*Supported by NSF through the Princeton Center for Complex Materials, a Materials Research Science and Engineering Center DMR-1420541 and DFG proposal no. SCHO 1730/1-1 and Max Planck Society. We thank HZB for the allocation of synchrotron radiation beamtime. The Flatiron Institute is a division of the Simons Foundation.

10:36AM F60.00012: NMR investigation of topological quantum material ZrTe\textsubscript{5}*  YEFAN TIAN (Presenter), NADER GHASSEMI, JOSEPH HANSBRO ROSS, Department of Physics and Astronomy, Texas A&M University — In this work, we performed \(^{125}\text{Te}\) NMR measurements on the topological quantum material ZrTe\textsubscript{5}. The measured spin-lattice relaxation rates (1/\( T_1 \)) can be well-explained by a theoretical model for Dirac electron systems, which reveals that the topological characteristic of ZrTe\textsubscript{5} is \( T \)-dependent. Combined with DFT calculations, the topological transition ordering can be confirmed from weak topological state to strong topological state with temperature increasing, the reverse of what has been proposed. The \( T \)-dependence of Dirac band gap can be derived from NMR results, demonstrating a gapless Dirac semimetal state occurring at a Lifshitz transition temperature, \( T_c = 85 \) K in our crystals. We also show that the changes in NMR shift at the Lifshitz transition provide direct evidence of band inversion when the topological phase transition occurs.

*This work was supported by the Robert A. Welch Foundation, Grant No. A-1526.
Recent work has shown evidence of ferromagnetic order at room temperature in epitaxial single layer VSe$_2$, providing promising opportunities for emergent properties particularly when integrated with other 2D materials. In this work, we report the results of the heteroepitaxial growth of VSe$_2$ on epitaxial graphene/6H-SiC(0001) and topological insulator Bi$_2$Se$_3$. Using in situ scanning tunneling microscopy, we find markedly different growth behaviors on these two substrates. On top of graphene, hexagonal VSe$_2$ islands first nucleate randomly within the terraces, and then coalesce to form single layer VSe$_2$ upon further growth. In contrast, the epitaxial Bi$_2$Se$_3$(111) substrate surface exhibits spirals with atomically smooth terraces up to 50 nm in width. Here, the VSe$_2$ epilayer preferentially nucleates at the Bi$_2$Se$_3$ spiral step edges forming a distinct lateral Bi$_2$Se$_3$-VSe$_2$ heterojunctions. This growth mode of VSe$_2$ on Bi$_2$Se$_3$ provides unique opportunities to explore one-dimensional topological-magnetic heterostructures whose structural and electronic properties will be discussed at the meeting.

Tuesday, March 3, 2020 8:00 AM - 10:36 AM

Session F61 DMP DCMP DCOMP: Fe-Based Superconductors - Inhomogeneous Order Parameter  Mile High Ballroom 4B - Elena Gati, Ames Lab - Tag(s): Focus
8:00AM F61.00001: A strongly inhomogeneous superfluid in an iron-based superconductor*

[Invited] MILAN ALLAN (Presenter), Leiden University — Although the possibility of spatial variations in the superfluid of unconventional, strongly correlated superconductors has been suggested, it is not known whether such inhomogeneities—if they exist—are driven by disorder, strong scattering or other factors. In this seminar, I will present our recent atomic-resolution Josephson scanning tunneling microscopy study that reveal a strongly inhomogeneous superfluid in an iron-based superconductor. By simultaneously measuring the topographic and electronic properties, we find that the inhomogeneity in the order parameter is not caused by structural disorder or strong inter-pocket scattering, and does not correlate with variations in the energy of the Cooper pair-breaking gap. Instead, we see a clear spatial correlation between the order parameter and the quasiparticle strength, defined as the height of the coherence peak, on a local scale. This result places iron-based superconductors on equal footing with copper oxide superconductors, where a similar relation has been observed on the macroscopic scale. When repeated at different temperatures, our technique could further help elucidate what local and global mechanisms limit the critical temperature in unconventional superconductors. Time permitting, I will further discuss our recent atomic-scale noise spectroscopy studies in conventional and unconventional superconductors [2,3].


*We acknowledge funding from a ERC Starting Grant and NWO.

8:36AM F61.00002: Superconducting Fluctuations and Pairing Enhancement in Ultra-Thin FeSe/SrTiO3

BRENDAN FAETH (Presenter), Cornell University, SHUOLONG YANG, University of Chicago, JASON KAWASAKI, Materials Science, University of Wisconsin-Madison, JOCIENNE NELSON, PRAMITA MISHRA, Cornell University, CHEN LI, Cal Tech, DARRELL SCHLOM, KYLE M SHEN, Cornell University — A central challenge in understanding the Tc enhancement mechanism in FeSe/SrTiO3 monolayer films has been to decouple the myriad effects that the underlying substrate imposes on the superconductivity. Alkali surface-dosed multilayer films provide a natural comparison where the heavily electron-doped superconducting layer is constrained to the film-vacuum interface, analogous to the monolayer FeSe/STO interface but lacking any STO phonon contribution. To better understand the influence of the STO phonon contribution, we systematically explore the evolution of superconductivity as measured unambiguously by in situ electrical resistivity under varied conditions of film thickness, surface doping concentration, and substrate interface condition. In contrast to observations from spectroscopic probes which indicate a substantial enhancement in the pairing Tc, we observe only modest discrepancies in the zero-resistance temperature for surface doped layers in comparison to monolayer films. We demonstrate that this behavior is due to the shared influence of 2D fluctuation effects which act to suppress the resistive transition well below the cooper pair formation temperature, and discuss the implications of our results on the broader understanding of the FeSe/STO enhancement phenomenology.
8:48AM F61.00003: Nonlocal Correlations in Iron Pnictides and Chalcogenides

KRISTOFER BJORNSON (Presenter), Niels Bohr Institute, SHINIBALI BHATTACHARYYA, University of Florida, KARIM ZANTOUT, Goethe-Universität Frankfurt, ANDREAS KREISEL, Universität Leipzig, ROSER VALENTI, Goethe-Universität Frankfurt, BRIAN M ANDERSEN, Niels Bohr Institute, PETER HIRSCHFELD, University of Florida — Deviations of low-energy electronic structure of iron-based superconductors from density functional theory predictions have been parameterized in terms of band-dependent mass renormalizations and energy shifts. Theoretically, these have typically been described either in terms of a local self-energy within the framework of Dynamical Mean Field Theory, or in terms of nonlocal effects due to interband scattering. By calculating the renormalized bandstructure in both random phase approximation and the two-particle self-consistent approximation, we show that correlations in pnictide systems like LaFeAsO and LiFeAs can be described rather well by nonlocal correlations. In particular, Fermi pocket shrinkage as seen in experiment occurs along the paradigm of interband scattering scenario. We also show agreement with experimentally observed non-local scattering lifetime data for LiFeAs. Next, we compare with the canonical iron chalcogenide system FeSe in its bulk tetragonal phase, and show that band renormalizations are completely inconsistent with this picture. We discuss possible reasons for this discrepancy.

9:00AM F61.00004: Tunable impurity states in the unconventional superconductor FeTe$_{0.55}$Se$_{0.45}$

DAMIANOS CHATZOPOULOS (Presenter), DOOHEE CHO, KOEN M BASTIAANS, Leiden University, GENDA GU, Brookhaven National Laboratory, MILAN P. ALLAN, Leiden University — When a single impurity interacts with an unconventional superconductor, localized bound states appear inside its superconducting gap. Interestingly, these states can be used as a tool to bring insight into the electronic states of the material at stake. In this study, we use a low temperature scanning tunneling microscope operating at ultra-high vacuum, to find impurity states in the iron-based unconventional superconductor FeTe$_{0.55}$Se$_{0.45}$ ($T_c$=14.5 K). In order to enhance the energy resolution, a superconducting tip (Pb-coated) was employed. We find that the energy of the states shifts spatially and can be tuned by changing the distance between the sample and our scanning probe at the impurity site. In this talk I will discuss possible mechanisms that can lead to this dispersive behavior of the impurity energy state in space.

*Leiden University, NWO, NanoFront, ERC
9:12AM F61.00005: k\textsubscript{z} selective scattering within Quasiparticle Interference measurements of FeSe\textsuperscript{*} LUKE RHODES (Presenter), Royal Holloway Univ of London, MATTHEW D. WATSON, University of St Andrews, TIMUR KIM, Diamond Light Source, MATTHIAS ESCHRIG, University of Greifswald — Quasiparticle interference (QPI) provides a wealth of information relating to the electronic structure of a material. However, it is often assumed that this information is constrained to two-dimensional electronic states. Here, we show that this is not necessarily the case. For FeSe, a system dominated by surface defects, we show that it is actually all electronic states with negligible group velocity in the \textit{z}-axis that are contained within the experimental data. By using a three-dimensional tight-binding model of FeSe, fit to photoemission measurements, we directly reproduce the experimental QPI scattering dispersion, within a T-matrix formalism, by including both \(k_z = 0\) and \(k_z = \pi\) electronic states. This result unifies both tunnelling and photoemission based experiments on FeSe and highlights the importance of \(k_z\) within surface-sensitive measurements of QPI.


\*LCR is funded by an 1851 Early Career Research Fellowship.

9:24AM F61.00006: STM studies on FeSe\textsubscript{x}Te\textsubscript{1-x} thin films grown on Bi\textsubscript{2}Te\textsubscript{3} single crystal\textsuperscript{†}

GUANNAN CHEN (Presenter), LIN JIAO, JORGE OLIVARES RODRIGUEZ, ANUVA AISHWARYA, University of Illinois at Urbana-Champaign, LIANYANG DONG, STEPHEN WILSON, Materials Department, University of California, Santa Barbara, VIDYA MADHAVAN, University of Illinois at Urbana-Champaign — The iron-based superconductor FeSe\textsubscript{x}Te\textsubscript{1-x} has attracted intensive interest for the fundamental understanding of unconventional superconductivity. Here we report nanoscale studies on FeSe\textsubscript{x}Te\textsubscript{1-x} films on Bi\textsubscript{2}Te\textsubscript{3} single crystal. Three different kinds of heterostructures: fully embedded monolayer; half-embedded monolayer; and top monolayer were studied systematically using Scanning Tunneling Microscopy/Spectroscopy (STM/STS). The studies show different superconducting behaviors for the three different monolayers. In the half-embedded monolayer, we find an identical statistical distribution of superconducting gaps with similar gap size values to the ones in the bulk. Furthermore, on Bi\textsubscript{2}Te\textsubscript{3} surface, a proximitized gap is observed with a uniform distribution. If time permits, we will present our measurements of Fourier transform quasiparticle interference (QPI) for studying the order parameter.

\*The work was supported by the Gordon and Betty Moore Foundation’s EPIQS Initiative through Grant GBMF4860 and NSF-DMREF program through Grants 1629382 and 1629068.
Visualization of impurity-induced magnetism in FeSe using scanning tunneling microscopy

SANG YONG SONG (Presenter), JUNGPIL SEO, Daegu Gyeongbuk Institute of Science and Technology — High temperature superconductivity (HTSC) is typically found in the vicinity of the magnetic ordering. As the magnetic ordering is reduced by various means including chemical doping, intercalation and applying pressure, spin fluctuations (SF) emerge which are believed to mediate the Cooper pairing between electrons. Therefore, understanding of emergence of magnetism in HTSC is one of the fundamental keys to reveal the secret of the unconventional superconductivity. For most iron-based superconductors, the parent state of materials shows stripe antiferromagnetic (AFM) ordering which breaks the C4 symmetry of the lattice. However, such long range magnetism is absent in FeSe which has been one of mysteries in iron-based superconductors. Recently, theories suggest FeSe is close to the magnetic quantum critical point and thus weak impurities could induce local magnetism in FeSe. Here, we show the local magnetism is directly induced by impurities of FeSe using scanning tunneling microscopy (STM). More interestingly, the induced magnetism was consistent with the (pi,0) magnetic ordering, showing that this material falls into the category of Hund's metal in which orbital selectivity plays an important role.

High-field superconducting phase in FeSe investigated by spectroscopic-imaging scanning tunneling microscopy

TETSUO HANAGURI (Presenter), TADASHI MACHIDA, RIKEN CEMS, YUKI SATO, SHIGERU KASAHARA, Dept. Phys., Kyoto Univ., TAKASADA SHIBAUCHI, Dept. Adv. Mat. Sci., Univ. Tokyo, YUJI MATSUDA, Dept. Phys., Kyoto Univ. — The iron-based superconductor FeSe is characterized by its small Fermi energy that is only several times larger than the superconducting gap amplitude. In such a situation, so-called Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state with periodic nodal planes in the order parameter is expected near the upper critical field at low temperatures. In FeSe, magnetic-field dependence of thermal conductivity exhibits a cusp-like anomaly below the upper critical field, which is argued as a signature of the transition from the low-field normal vortex state to the high-field FFLO state [1]. We performed high-field spectroscopic-imaging scanning tunneling microscopy at an ultra-low temperature below 90 mK to investigate the change in the electronic state across the phase boundary. We found that the vortex image diminishes at about 14 T where the thermal conductivity shows a cusp. This result suggests that the nodal plane is pinned at the surface, if the high-field phase is an FFLO state. [1] S. Kasahara et al., Proc. Natl. Acad. Sci. U.S.A. 111, 16309 (2014).

*This work was supported by the JSPS KAKENHI (No. JP19H05824).
10:00AM F61.00009: Probing antiferromagnetic order of iron-based superconductors through the surface*  ZHUOZHI GE (Presenter), QIANG ZOU, MINGMING FU, SHIVANI RAJPUT, Center for Nanophase Materials Sciences, Oak Ridge National Lab, LIURUKARA D SANJEEWA, ATHENA S. SEFAT, Materials Science & Technology Division, Oak Ridge National Laboratory, LIAN LI, Department of Physics and Astronomy, West Virginia University, ZHENG GAI, Center for Nanophase Materials Sciences, Oak Ridge National Lab — Understanding the surface structural and electronic properties of iron-based superconductors (FeSCs) is of great significance, as it can reveal the bulk superconducting properties. Previous study reveals a state near 0.2eV below Fermi level on √2×√2 or 2×1 reconstructed surface of Ba(Fe1-xCox)2As2, which is identified as a surface state by ARPES and DFT calculations. This state has also been observed on the surfaces of other 122 FeSCs with different doping levels, alkaline earth metal elements, and surface reconstructions. Its common presence suggests an origin other than simple surface state. Here, we systematically investigated low-temperature cleaved parent and slightly doped BaFe2As2 superconductors by scanning tunneling microscopy/spectroscopy (STM/S). We observed the same state on all √2×√2, 2×1 and even mixed surfaces. However, it vanishes when heating the sample above the Neel temperature (TN), and recovers after cooling down below TN, suggesting it is related to the bulk antiferromagnetic order.

*This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility. Z.Ge, L.S. and A.S.’s research are supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

10:12AM F61.00010: Investigation of the FeSe/SrTiO3 interface using Atom Probe Tomography*  SAMANTHA O’SULLIVAN (Presenter), RUIZHE KANG, CHRISTIAN MATT, JASON HOFFMAN, JENNIFER E. HOFFMAN, Harvard University — Monolayer FeSe on SrTiO3 (FeSe/STO) is a high temperature superconductor with Tc above 100 K. Although scanning tunneling microscopy (STM) imaging has characterized its surface in detail, the content and behavior in the FeSe/STO interface remains unclear. Characterizing the interface is important to gain further understanding on the mechanism for the unexpected high-temperature superconductivity in this system. Techniques such as scanning transmission electron microscopy (STEM) have been used to demonstrate that the interface structure is correlated with the material’s superconducting properties, however much remains unclear about the specific composition and behavior of the interface. Here we characterize the interface using atom probe tomography (APT), which reveals the structural and chemical properties of the FeSe/STO interface and provides insight into the origin of the material’s superconductivity.

*This work supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4536, the STC Center for Integrated Quantum Materials, NSF Grant DMR-1231319, and Office of Naval Research, Grant N00014-18-1-2691.
10:24AM F61.00011: Imaging Nematic Transitions in Iron-Pnictide Superconductors with a Quantum Gas*  
FAN YANG, STEPHEN TAYLOR (Presenter), STEPHEN D EDKINS, JOHANNA PALMSTROM, IAN FISHER, BENJAMIN L LEV, Stanford Univ — The SQCRAMscope is a recently realized Scanning Quantum CRyogenic Atom Microscope that utilizes an atomic Bose-Einstein condensate to measure magnetic fields emanating from solid-state samples. Here, we combine the SQCRAMscope with an in situ microscope that measures optical birefringence near the surface of a sample to study iron-pnictide superconductors, where the relationship between electronic and structural symmetry-breaking resulting in a nematic phase is under debate. We conduct simultaneous and spatially resolved measurements of both bulk and surface manifestations of nematicity via transport and structural deformation channels, respectively. By performing the first local measurement of emergent resistivity anisotropy in iron pnictides, we observe a spatially inhomogeneous increase in the temperature at which optical birefringence appears near the surface over that at which anisotropic local transport appears within the bulk. This is consistent with the existence of a higher-temperature surface nematic transition, albeit one that emerges inhomogeneously. More broadly, these measurements demonstrate the SQCRAMscope's ability to reveal important insights into the physics of complex quantum materials.

*Supported in part by ONR and DOE.

F61.00012: Manipulating superconductivity of monolayer FeSe on graphene/SiC(0001) surface  
WAN-TONG HUANG, HAICHENG LIN, CHENG ZHENG, YUGUO YIN, XINQIANG CAI, SHUAI-HUA JI (Presenter), XI CHEN, Tsinghua University — Compared with those of bulk FeSe, the sizes of electron and hole pockets become smaller in monolayer FeSe because the absence of inter-layer coupling tends to narrow the energy band and decrease the overlap between electron and hole pockets in energy. For FeSe monolayer grown on graphene/SiC(0001) surface, we find the Fermi energy is in the range of a few meV. In addition, we demonstrate an approach to tuning the Fermi energy by the thickness of graphene layers. At the base temperature of STM, the film grown on trilayer graphene becomes superconducting with Δ=0.62meV. In contrast, no signature of superconductivity has been detected in the dI/dV spectra of FeSe monolayer on bilayer graphene. The FeSe monolayer on graphene/SiC(0001) has the potential to study the intriguing physics where the Fermi energy, the superconducting gap and the Zeeman energy in magnetic field are in the same order of magnitude.

Tuesday, March 3, 2020 8:00 AM - 10:48 AM

Session F62 DMP: Nanostructures and Metamaterials IV  
Igal Brener, Sandia National Laboratories
8:00AM F62.00001: Engineering quantum light emission from color-centers in atomically thin crystals with phase gradient metasurfaces. PANKAJ JHA (Presenter), GHAZALEH KAFAIE SHIRMANESH, HAMIDREZA AKBARI, MEIR GRAJOWER, BENJAMIN VEST, HARRY ATWATER, Caltech — Single-photon sources are elementary building blocks for photonic quantum technologies. However, progress in photonic quantum technologies has been constrained due to a lack of suitable materials with desired optical properties and the challenges in achieving coherent light-matter interaction at the quantum level. Here, we report a new approach for building chip-scale quantum hardware with color-centers in wide bandgap materials, such as hexagonal boron nitride (hBN), interfaced with planar arrays of classical nanoantennas, also known as metasurfaces. We investigated both exfoliated and chemical vapor grown hBN samples at room temperature. We performed photon-photon correlation measurements to isolate centers with single-photon emission characteristics and designed a phase gradient metasurface such that the emission from these color-centers can be efficiently extracted as well as redirected along a preferred direction. Our approach of interfacing these bright emitters with photonic metasurfaces and manipulating their emission characteristics would enable new opportunities for on-chip quantum photonics.

8:12AM F62.00002: Modeling NV charge stability in nanodiamonds with DFT CLAIRE MEARA (Presenter), PATRICK BRIDDON, MARK RAYSON, JONATHAN GOSS, Univ of Newcastle — The nitrogen-vacancy (NV) defect in diamond is a controllable quantum system with strong fluorescence. When placed in nanodiamonds it provides nanoscale magnetometry and single biological cell tracking[1]. NV must be stable and negatively charged close to the nanodiamond surface. However, NV charge-state fluctuations near surfaces result in intermittent fluorescence; this effect is highly correlated with surface type and structures[2]. Electron affinity has been posited as a cause, but contradictions exist and underlying mechanisms still need to be fully understood. Recent work shows NV charge alternates with pH[3], suggesting acceptor levels from surface radicals play a role. Using DFT the electronic structure of NVs in nanodiamonds is studied for different, commonly observed terminations, adsorbates and surface radicals. A measure of charge stability is defined and an underlying cause for observed charge instability for certain terminations is proposed. Routes to manipulating NV surfaces to provide stable NV- in nanodiamonds is discussed, thereby allowing more reliable spatiotemporal nanosensors.

1. J. C. Arnault (Ed.) William Andrew, Ch. 17 (2017)
Epsilon-near-zero modes in transdimensional planar plasmonic nanostructures*  IGOR BONDAREV (Presenter), HAMZE MOUSAVI, Math & Physics Dept, North Carolina Central Univ, VLADIMIR SHALAEV, ECE & Birck Nanotechnology Center, Purdue University — Transdimensional (TD) materials are ultrathin planar nanostructures composed of a precisely controlled finite number of monolayers[1]. Plasmonic TD materials offer advances such as controlled light confinement and thickness-controlled light-matter coupling that can further develop the fields of nanophotonics and metamaterials. We use quantum electrodynamics and the confinement-induced nonlocal dielectric response model based on the Keldysh-Rytova electron interaction potential to study the epsilon-near-zero modes (ENZ) of plasmonic films in the TD regime[2]. New remarkable effects are revealed. They are the plasmon mode degeneracy lifting and the dipole emitter coupling to the ENZ modes split. The latter leads to the thickness-controlled spontaneous decay with up to three-orders-of-magnitude increased rates. Knowledge of these features is advantageous both for the fundamental understanding of the electromagnetic properties and for the development of the new design principles of efficient photonic nanodevices with desired characteristics that are built on ultrathin metallic TD films. -- [1]A.Boltasseva & V.M.Shalaev, ACS Photonics 6, 1 (2019); [2]I.V.Bondarev, H.Mousavi, & V.M.Shalaev, arXiv1908.00640.

*NSF DMR-1830874 (I.V.B.), DOE DE-SC0007117 (H.M), DOE DE-SC0017717 (V.M.S.)

Plasmon Assisted Coherent Random Lasing*  DIPENDRA S KHATRI (Presenter), JIYANG CHEN, University of Memphis, YING LI, University of Nebraska-Lincoln, ELYAHB ALLIE KWIZERA, XIAOHUA HUANG, University of Memphis, CHRISTOS ARGYROPOULOS, University of Nebraska-Lincoln, THANG HOANG, University of Memphis — Random lasing occurs as the result of a coherent optical feedback from multiple scattering centers. Here, we demonstrate that plasmonic gold nanostars, through their small tips, are efficient light scattering centers which assist very narrow bandwidth and highly amplified coherent random lasing at a low lasing threshold. First, by embedding plasmonic gold nanostars in a rhodamine 6G dye gain medium, we observed a series of very narrow random lasing peaks with full-width at half-maximum (FWHM) ~0.8 nm. By contrast, free rhodamine 6G dye exhibited only a single lasing peak with FWHM of 6 nm. The lasing threshold for the dye with gold nanostars was two times smaller than that for a free dye. Further, by coating the tip of a single-mode fiber with these nanostars, we demonstrated the collection of the random lasing signal through the fiber that can easily be guided and analyzed. Time-resolved measurements showed a significant increase in the emission rate at above the lasing threshold, indicating a stimulated emission process.

*This work was supported by National Science Foundation (DMR-1709612) and The Fedex Institute of Technology at the University of Memphis.
8:48AM F62.00005: Photoluminescence quantum efficiency of nanowire quantum dots on silicon substrates  JIARONG CUI (Presenter), YIFEI WANG, HO VINH, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — Nanowire quantum dots grown on silicon substrates provide promising technologies for integrating advanced photonic technologies on a silicon microelectronics. In this research our GaAsP nanowires contain GaAs quantum dot in the middle of the nanowires. We report the photoluminescence quantum efficiency as well as the thermal quenching mechanism of nanowire quantum dots prepared by vapor–liquid–solid method. We have performed high resolution spectroscopy, quantum yield, power dependence, and temperature dependence measurements of photoluminescence intensity from nanowire quantum dots. The data provide a picture of the quantum efficiency, thermal quenching processes and activation energy levels of nanowire quantum dots. The results provide an important step in the realization of nanowire quantum dots for photonic devices on silicon platform.

9:00AM F62.00006: Environmentally friendly core-shell quantum dots for light-emitting devices: A computational study*  MARIAMI RUSISHVILI (Presenter), University of Chicago, STEFAN WIPPERMANN, Max-Planck-Institute for Iron Research GmbH, DMITRI TALAPIN, GIULIA GALLI, University of Chicago — Semiconductor quantum dots (QDs) have been successfully used as light emitters in a variety of applications [1]. CdSe QDs exhibit the best performance in terms of tunable colors in the visible range and luminescence quantum yield. However, they contain a toxic heavy metal and the search for environmentally friendly nanostructured semiconductors is an active field of research. Recently InP based QDs have emerged as a promising alternative [2] to CdSe, although they exhibit broader emission spectra, possibly due to the sensitivity of their electronic structure to small morphological changes. Here we report on a first principle computational study of the structural and opto-electronic properties of InP/Zn(S/Se) core shell QDs. We used DFT with semi-local and hybrid functionals and the QuantumEspresso package (https://www.quantum-espresso.org/). We show that composition and interface morphology are key to achieve narrow emission lines, and we discuss the interplay between quantum confinement and strain in determining the electronic properties of these systems.


*This work was supported by DOE/BES.
9:12AM F62.00007: Engineering thermochromic properties with plasmonics, quantum dots, and 2D materials. DONGHEON HA (Presenter), EVGHENI STRELCOV, IREAP, University of Maryland, STEVEN BLANKENSHIP, National Institute of Standards and Technology, AMIT AGRAWAL, IREAP, University of Maryland, ANDREI KOLMAKOV, NIKOLAI ZHITENEV, National Institute of Standards and Technology — For temperature-sensing applications, it is desirable to obtain strong thermochromic response in visible spectral range. We experimentally evaluate possible enhancements of sensitive thermochromic materials based on vanadium oxide (VO\textsubscript{x}) by nanophotonic engineering. First, we compare various growth methods, including a deposition and annealing of thin films and an electrochemical growth of single crystals. Second, we perform macro- and microscale temperature-dependent optical measurements of materials with different composition. Then, we demonstrate an enhanced thermochromic behavior by the application of plasmonic and quantum materials. With periodic gold hemispherical structures atop VO\textsubscript{2} crystals, the optical contrast at the VO\textsubscript{2} phase transition from semiconductor to metal is increased by \(\approx 15\)\% at visible/near-infrared wavelengths. The enhancement is due to the localized surface plasmon resonances of gold particles and can be described within the Maxwell-Garnett effective medium theory. We also discuss other approaches, including the coupling of two dimensional materials and colloidal quantum dots, to further tailor temperature-dependent optical response of thermochromic materials. Finally, we introduce possible applications focusing on nanoscale temperature sensing.

9:24AM F62.00008: Surface functionalization of nanoparticles for fabrication of size-tunable and electrochemically actuable nanostructured shell assembly* MARK BARTOLO (Presenter), Materials and Biomaterials Science and Engineering, University of California, Merced, RYAN BRISBIN, RYAN BAXTER, Chemistry and Chemical Biology, University of California Merced, SAYANTANI GHOSH, Physics, University of California Merced — Surface modification of quantum dots (QDs) is one of the most versatile methods of customizing their optical and electronic properties. Our goal is to leverage surface functionalization of CdSe/ZnS QDs for optimal directed assembly to be utilized in biological and biomedical cargo delivery systems. We have developed nano-assembled micro-shell structures composed of gold nanoparticles functionalized with custom-designed ligands\textsuperscript{1} which allowed plasmonic actuation. Here, we focus on Bis(Imino)Pyradine (BIP) ligands which have improved thermal stability, optical properties, and biocompatibility of the shell structures, while allowing cargo release via electrochemical stimulation. In addition, the versatility of the BIP ligands have made it possible for us to tune the shell diameter from 200 nm to 1 micron, which vastly broadens the field of applications. In this study we present a systematic characterization of the QD surface chemistry to observe and understand correlations between QD diameter, ligand size and shell size.


*This research was supported by NSF CREST grant no. HRD-1547848
9:36AM F62.00009: Transition to strong coupling regime for quantum emitters near a plasmonic nanostructures  
TIGRAN SHAHBAZYAN (Presenter), Jackson State Univ — We present a model for exciton-plasmon coupling based on energy exchange mechanism between quantum emitters (QE) and localized surface plasmons in metal-dielectric structures. Plasmonic correlations between QEs give rise to a collective state exchanging its energy cooperatively with a resonant plasmon mode. By defining carefully the plasmon mode volume for a QE ensemble, we obtain a relation between the QE-plasmon coupling and the cooperative energy transfer rate that is expressed in terms of local fields. For a single QE near a sharp metal tip, we find analytically the enhancement factor for the QE-plasmon coupling relative to the QE coupling to a cavity mode. For QEs distributed in an extended region enclosing a plasmonic structure, we find that the ensemble QE-plasmon coupling saturates to a universal value independent on system size and shape, consistent with the experiment.

9:48AM F62.00010: Tip-controlled Strong Coupling with Infrared Polaritonic Heterostructures  
SAMUEL C. JOHNSON (Presenter), University of Colorado Boulder, NISHANT NOOKALA, Department of Electrical & Computer Engineering, The University of Texas at Austin, MIKHAIL A. BELKIN, Walter Schottky Institute and ECE Department, Technical University of Munich, MARKUS B. RASCHKE, University of Colorado Boulder — Infrared polaritonic metasurfaces based on a multi-quantum-well intersubband transition coupled to a gold antenna heterostructure exhibit record-high nonlinear optical responses and optical power limiting behavior. However, these structures are limited to passive performance depending on fabrication parameters. Here, we use infrared scattering scanning near-field optical microscopy to image single antenna quantum well heterostructures, and to actively tune quantum-well saturation, coupling strength, and quantum path interference through manipulation of the nanocavity mode volume through tip-sample distance control. Further, the AFM tip as a coupled antenna resonator is used to enhance far-field coupling to control photon emission, field orientation, and nanoscopic field heterogeneity. Previous picosecond laser far-field optical power limiting and pump-probe characterization is extended with near-field spectroscopy, using femtosecond laser, picosecond laser, and synchrotron infrared light sources.
10:00AM F62.00011: Active Tuning of Phonons and Surface-Phonon Polariton Resonances
ADAM DUNKELBERGER (Presenter), CHASE ELLIS, DANIEL RATCHFORD, ALEXANDER GILES, D. SCOTT KATZER, United States Naval Research Laboratory, ANDREA GRAFTON, VANESSA BRESLIN, ELIZABETH RYLAND, NRC RAP Postdoctoral Fellow, MIJIN KIM, KeyW Corp, CHUL SOO KIM, IGOR VURGAFTMAN, JOSEPH G TISCHLER, JEFFREY OWRUTSKY, United States Naval Research Laboratory, JOSHUA D CALDWELL, Vanderbilt University — The infrared spectra of many polar semiconductors are dominated by highly reflective reststrahlen bands that occur between the transverse and longitudinal optical phonons. Through the LOPC effect, free carriers shift the reststrahlen band to higher frequencies. We have previously shown that photoinjected carriers transiently and reversibly modify the infrared reflectivity of bulk SiC. Within the reststrahlen band, SiC and InP nanostructures can exhibit surface-phonon polariton resonances. Here we report, for the first time, active tuning of SiC and InP surface-phonon polariton resonances via carrier photoinjection, achieving better modulation depths than active tuning in plasmonic systems. In SiC, ultraviolet excitation with femtosecond laser pulses induces $>10$ cm$^{-1}$ shifts in the transverse dipole resonance (width = 7 cm$^{-1}$). Time-resolved infrared reflection spectroscopy reveals that the photoinduced shifts decay in tens of ps, depending on the initial carrier density. Our results suggest that spatial redistribution of photoexcited carriers dominates the time dependence of the active tuning. We also report, for the first time, direct time-resolved infrared spectroscopy of the LO mode of GaN, made experimentally accessible through the Berreman effect.

10:12AM F62.00012: Excitation of non-radiating anapoles in dielectric nanospheres*
UTTAM MANNA (Presenter), Illinois State University, JOHN A. PARKER, University of Chicago, HIROSHI SUGIMOTO, Kobe University, BRIGHTON COE, DANIEL EGGENA, Illinois State University, MINORU FUJII, Kobe University, NORBERT F. SCHERER, University of Chicago, STEPHEN K GRAY, Argonne National Laboratory — Nonradiating anapoles are superposition of internal modes that can act as an energy reservoir by reducing the far-field scattering. We report experimental excitation of the electrodynamic anapole mode in isotropic silicon nanospheres at the optical frequencies using radially polarized beam illumination. The superposition of equal and out-of-phase amplitudes of the Cartesian electric and toroidal dipoles produces a pronounced dip in the scattering spectra with the scattering intensity almost reaching zero – a signature of anapole excitation. The total scattering intensity associated with the anapole excitation is found to be more than 10 times weaker, and the internal energy is found to be 6 times greater for illumination with radially vs. linearly polarized beams. Our approach provides a simple, straightforward alternative path to realize electrodynamic anapole mode at the optical frequencies.

*This material is based upon work supported by the National Science Foundation (NSF) under Grant No. ECCS-1809410. H.S. and M. F. acknowledge KAKENHI grant numbers 18K14092 and 18KK0141.
Tailoring the chiro-optical response of Si-Ag/Au chiral heterostructure thin films fabricated by glancing angle deposition technique

UFUK KILIC (Presenter), MATHEW HILFIKER, Electrical and Computer Engineering Department, University of Nebraska - Lincoln, RENE FEDER, The Fraunhofer Institute for Microstructure of Materials and Systems (IMWS), RAFAL KORLACKI, EVA SCHUBERT, CHRISTOS ARGYROPOULOS, MATHIAS SCHUBERT, Electrical and Computer Engineering Department, University of Nebraska - Lincoln — Chiro-optical response of subwavelength scale nanostructures have been the subject of many research projects such as bio-sensors, topological insulators, and photonic integrated circuit designs. [1] In this study, by using glancing angle deposition technique, subsequent and repeated depositions of silicon(Si) and gold(Au)/silver(Ag) lead to nanometer-dimension sub-chiral segments, and thus, we successfully fabricated spatially coherent, highly porous, super lattice type chiral heterostructure (CHS) thin films. We incorporated the transmission mode Mueller matrix spectroscopic ellipsometry technique with finite element modeling environment in order to investigate the chiro-optical properties of this new type plasmonic metamaterials. Interestingly, Au/Ag sub-chiral segments in CHS result in the emergence of multiple plasmonic modes which can be tunable depending on the Au/Ag-Si ratio in a single turn. Unlike the other studies [2,3] which employs periodic nanostructures made up of single type material, we observed extraordinary optical activity in our fabricated CHS thin films.

References:
10:36AM F62.00014: STM Characterization of hBN-Decoupled Covalent Organic Frameworks* DANIEL RIZZO (Presenter), University of California, Berkeley, QINGQING DAI, Georgia Institute of Technology, CHRISTOPHER BRONNER, GREGORY VEBER, University of California, Berkeley, BRIAN J SMITH, Bucknell University, MICHIO MATSUMOTO, Northwestern University, SIMIL THOMAS, Georgia Institute of Technology, GIANG DUC NGUYEN, PATRICK R FORRESTER, WILLIAM ZHAO, JAKOB H JORGENSEN, University of California, Berkeley, WILLIAM DICHTEL, Northwestern University, FELIX FISCHER, University of California, Berkeley, HONG LI, JEAN-LUC E BREDAS, Georgia Institute of Technology, MICHAEL F CROMMIE, University of California, Berkeley — Covalent organic frameworks (COFs) are crystalline molecular networks with potential applications in filtration, organic electronics, energy storage, and catalysis. Recent advances in COF synthesis have permitted the growth and characterization of COFs that exhibit different symmetries and that use a wide range of molecular building blocks. Despite this progress, there have only been a limited number of experimental demonstrations of the electronic structure-function relationship for COFs, particularly in the 2D limit. One experimental challenge is how to separate the intrinsic COF electronic structure from the influence of metallic growth substrates. In order to accomplish this, we have introduced an atomic insulating film of hBN between a COF and an underlying metallic substrate to act as a decoupling layer. Using scanning tunneling microscopy and spectroscopy we are able to obtain more detailed spectral information on hBN-decoupled COFs compared to those grown directly on a metallic substrate. First-principles DFT and tight-binding calculations confirm that hBN-decoupled COFs possess spectral features that reflect the COF's Kagome lattice symmetry.

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DOE BES no. DEAC02-05CH11231
DOD High Performance Computing Modernization Program

F62.00015: Strain Effect on Silicene Quantum Dot Embedded in Silicane* BI-RU WU (Presenter), Chang Gung Univ — A new design for silicene quantum dots (SiQDs) embedded in silicane probably makes magnetism and band gap of the SiQD being controllable by hydrogen. In this paper, the strain effect for the embedded SiQD in silicane was investigated by a first-principles method. The homogeneous strain and two types of uniaxial strains are considered. As expected, the band gap can be tuned by strains and the behavior of the band gap are distinct while applied with different strain types. However, the magnetism is still determined by the size and shape of the SiQD. Strain cannot alter the magnetism of the embedded SiQD. The variation of band gap of various shapes of embedded SiQD also have different behaviors under strains.

*This work was supported by the Ministry of Science and Technology of Taiwan (ROC) under grant numbers MOST 108-2112-M-182-002.
8:00AM F63.00001: Temperature and Phase Dependence of Carrier Diffusion in Single Crystal MAPbI₃ Perovskite Microstructures* LUKE MCCLINTOCK (Presenter), RUI XIAO, YASEN HOU, HENRY TRAVAGLINI, University of California, Davis, DAVID ABRAMOVITCH, University of California, Berkeley, LIANG TAN, Lawrence Berkeley National Laboratory, DONG YU, University of California, Davis — Understanding and improving carrier transport in photovoltaic materials is crucial to developing high quality solar energy harvesting devices. Here, we have investigated carrier diffusion lengths in single crystal methylammonium lead iodide (MAPbI₃) microstructures via scanning photocurrent microscopy. Carrier diffusion lengths were found to increase abruptly once below the transition temperature from the tetragonal to the orthorhombic phase and reached 200 ± 50 μm at 80 K. Enormous mobility values of 3 x 10⁴ cm² / V s were extracted at 80 K using these long diffusion lengths in combination with transient photocurrent lifetime measurements. We attributed the increased diffusion lengths to the emergence of an excitonic nature to the transport in the orthorhombic phase. Our findings provide significant fundamental insights on the temperature and phase-dependent charge transport properties of halide perovskites.

*This work was supported by the U.S. National Science Foundation Grant DMR-1710737 and the UC Laboratory Fees research program.

8:12AM F63.00002: Quantifying exciton heterogeneities in mixed-phase organometal halide multiple quantum wells via Stark spectroscopy studies ERIC AMERLING (Presenter), SANGITA BANIYA, Chemistry, University of Utah, EVAN LAFALCE, Physics, University of Utah, STEVE BLAIR, Electrical Engineering, University of Utah, ZEEV VALY VARDENY, Physics, University of Utah, LUISA WHITTAKER-BROOKS, Chemistry, University of Utah — Solution processable organic-inorganic hybrid perovskite (OIHP) quantum wells naturally self-assemble through weak van der Waals forces. In this study, we investigated the structural and optoelectronic properties of \((\text{C}_4\text{H}_9\text{NH}_3)_{2}(\text{CH}_3\text{NH}_3)_{n-1}\text{Pb}_{n}\text{I}_{3n+1}\), varying \(n\) from 1 to 4. Through conventional structural characterization, the thin films showcase high-quality phase purity. However, while investigating the optoelectronic properties, it was clear that these van der Waals heterostructures consist of multiple quantum well thicknesses coexisting within a single thin film. We utilized modulation spectroscopy, electroabsorption, and Liptay theory analysis to deconvolute the different excitonic features arising from different quantum well thicknesses (n). Rather than merely identifying what quantum well heterostructures are present within a thin film, this novel method of analysis provides powerful insight into the exact exciton composition in the thin film and can be utilized to analyze the optoelectronic properties of many other mixed-phase quantum well heterostructures beyond those formed by OIHPs.
8:24AM F63.00003: Angle-Resolved Time-Resolved Microwave Conductivity  SHIRSO PRATIM CHATTOPADHYAY (Presenter), Materials Science, Oregon State University, JOHN LABRAM, Electrical Engineering and Computer Science, Oregon State University — The contactless electronic characterization technique time resolved microwave conductivity (TRMC) provides a very convenient way of quickly evaluating carrier mobilities and lifetimes for a variety of semiconducting materials. However, the technique has one notable limitation in that it can conventionally only be used to resolve carrier mobilities in the plane of substrate (lateral mobility).

Here we present a novel approach for resolving charge carrier mobilities in different planes within a sample. Using a range of 3D-printed samples holders, where the sample is held at various angles relative to the incident light, we are able to resolve the mobility in the plane of the sample and out of the plane of the sample. Because charges generally travel in the direction perpendicular to the substrate in solar cells, identifying carrier mobility in this direction is particularly valuable. We studied the archetypical hybrid halide perovskite compound, methylammonium lead iodide. Our results show that for films prepared using our solution-processing route, mobilities in-plane are significantly higher than those out-of-plane.

8:36AM F63.00004: Peculiar Defects Behavior in Charge Recombination of Metal Halide Perovskites  WEIBIN CHU (Presenter), Univ of Southern California, WISSAM A SAIDI, Univ of Pittsburgh, JIN ZHAO, Univ of Science and Technology of China, OLEG PREZHD0, Univ of Southern California — Defects are inevitably introduced in the near room-temperature and solution-based growth of metal halide perovskites (MHPs) thin films for solar cell devices. However, the astonishing improvements in the efficiency of the corresponding solar cells indicate that MHPs have a strong defect tolerance. Motivated by the recent experimental demonstration of a new state-of-art β phase CsPbI$_3$ with a stable and impressive efficiency reaching 18.4% at ambient conditions, we investigate the non-radiative recombination processes in CsPbI$_3$ using ab initio non-adiabatic molecular dynamics within real-time time-dependent Kohn-Sham formalism and surface-hopping framework. Regardless of their nature, we find that the native defects in CsPbI$_3$ do not accelerate the charge recombination process. We show that the strong tolerance of electron-hole recombination against defects is explained due to the combination of having low-frequency lattice phonons and weakly overlapping electron and hole states. The deep-level defect becomes tolerant owing to the strong covalency, which contrary to predictions from SRH theory in previous work. Considering similar results found in MAPbI$_3$, we propose that the strong defect tolerance is general to the metal halide perovskites.
8:48AM F63.00005: Small Urbach energies in halide perovskites due to anharmonicity and short-range correlated disorder  
CHRISTIAN GEHRMANN (Presenter), DAVID A. EGGER,  
Department of Physics, TU Munich — Halide perovskites (HaPs), a class of up-and-coming solar absorber materials, feature small Urbach energies and sharp optical absorption edges. These characteristics render the fabrication of efficient HaP based solar-cell devices possible. But they also indicate a low amount of disorder, which is seemingly in contrast with the complex nuclear dynamics and structural effects known for HaPs. Here, we present our findings on spatial correlations in the disorder potential induced for electronic states due to nuclear dynamics in several HaPs. Our theoretical results are based on density functional theory (DFT) calculations and DFT-based molecular dynamics [1]. With this approach, anharmonicity in the nuclear dynamics is accounted for up to all orders in the Taylor expansion of the crystal potential. We find that correlations in the disorder potential are dynamically shortened. The mechanism responsible for this shortening is found to be the nuclear motion of A-site and X-site ions. We conclude that sharp optical absorption edges and small Urbach energies in HaPs are possible due to the dynamical shortening of correlations in the disorder potential.


9:00AM F63.00006: The evolution of ultrafast carrier dynamics in situ perovskite solar cells*  
EXIAN LIU (Presenter), Physics & Astronomy, Clemson University, JINHUI TONG, National Renewable Energy Laboratory, KANISHKA KOBBEKADUWA, PAN P ADHIKARI, Physics & Astronomy, Clemson University, KAI ZHU, National Renewable Energy Laboratory, JIANBO GAO, Physics & Astronomy, Clemson University — Photoelectric performances of perovskite solar cells (PSC), such as photovoltage, short-circuit current density, fill factor and power-conversation-efficiency are determined by the charge carrier dynamics, especially the early-stage processes including charge generation, recombination and interface transfer. These photophysics dynamics, which are within pico- to nano-second timescale, directly relate to the PSC working mechanism. However, the study on the ultrafast photophysics dynamics in situ PSC is still in infancy although considerable works were performed on the performance improvement at steady-state condition. 
Aim to elucidate ultrafast carrier dynamics in-situ PSC, in this talk, we present the carrier dynamics in-situ organic–inorganic halide perovskite solar cells utilizing ultrafast photocurrent spectroscopy with sub-40 picosecond time. We study the evolution of ultrafast carrier dynamics in situ perovskite solar cells, in term of the evolution of open-circuit voltage, short-circuit current, and fill factor, in addition to addressing the desirable fundamental questions including carrier lifetime, mobility, trap density, and carrier transport mechanisms.

*Clemson University
9:12AM F63.00007: Defects in polymorphous cubic halide perovskites: coexistence of shallow and deep vacancy transition levels*  
GUSTAVO DALPIAN (Presenter), Univ Federal do ABC, XINGANG ZHAO, ALEX ZUNGER, University of Colorado Boulder — Halide perovskites are usually said to be defect tolerant materials suggesting a possible explanation for being good solar compounds. Molecular dynamics (MD) simulations of Cohen et al revealed that the orbital energy of the Br-vacancy in CsPbBr\(_3\) resides deep in the gap (i.e., not defect tolerant) and can considerably fluctuate on the time scale of the MD trajectories. Recently, it was pointed out that the static structure of cubic halide perovskites involves a distribution of different local environments such as tilting and atomic displacements, being a polymorphous network [Zhao, X., Dalpian, G. M., Wang, Z. & Zunger, A. *The polymorphous nature of cubic halide perovskites.* arXiv:1905.09141 (2019)]. We have studied anion vacancies in different, inequivalent lattice sites in the polymorphous network of CsSnI\(_3\), CsPbI\(_3\), MaPbI\(_3\), and CsPbBr\(_3\), finding that all except CsPbBr\(_3\) have shallow transition levels whereas the latter has a bimodal distribution with some deep levels (mostly shallow). We show how these results correlate with the local geometric deformations of the various sites in the polymorphous network.

*Supported by NSF-DMREF, No. 1921949 and FAPESP.

9:24AM F63.00008: Hot Carrier Dynamics in Bulk and 2D Perovskites*  
SHASHI SOURABH (Presenter), VINCENT R. WHITESIDE, HAMIDREZA ESMAIELPOUR, BRANDON DURANT, Department of Physics and Astronomy, University of Oklahoma, GILES E. EPERON, MATTHEW C BEARD, National Renewable Energy Laboratory, IAN R SELLERS, Department of Physics and Astronomy, University of Oklahoma — A comparison of the effect of carrier-carrier and carrier-phonon interactions in 2D (BA)\(_2\)PbI\(_4\) Ruddlesden-Popper (n=1) and conventional bulk MAPbI\(_3\) perovskite thin films is presented. It is shown that the nature and strength of the exciton binding energy strongly mediate the nature of their interaction with phonons. Specifically, more strongly coupled excitons manifest themselves in the formation of small polarons that interact with lattice via the emission of LO-phonon replicas, while weakly bound (or free) excitons interact with phonons to form large polarons resulting in large LO-phonon broadening and strong carrier-phonon scattering. These results suggest that the unusual hot carrier thermalization observed in the perovskites is dominated by the strength and nature of the exciton-phonon interaction and subtelty different from more conventional semiconductors. To support this hypothesis, comparisons of the hot carrier dynamics and electron-phonon interaction in a number of stable and well-studied perovskites are also presented.

*Support is acknowledged through the Department of Energy ESPCoR program and the Office of Basic Energy Research, Materials Science and Energy Division under Award No.# DE-SC0019384
Unravelling free carrier and exciton dynamics in hybrid organic-inorganic perovskites using transient absorption spectroscopy  
CHANG QING (Presenter), DAMING ZHAO, Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Tech Univ, HONGWEI HU, YENG MING LAM, School of Materials Science and Engineering, Nanyang Tech Univ, EE MIN CHIA, Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Tech Univ — Mixed-cation lead mixed-halide perovskites have been shown to good photostability, thermal stability and high power conversion efficiency, proving to be good candidates as energy harvesting materials [1]. Transient absorption spectroscopy is a powerful tool to study the response of free carriers and excitons upon photoexcitation in the perovskites [2]. Here, we excite FA_{0.85}Cs_{0.15}PbI_{2.9}Br_{0.1} thin films with bandgap and above-bandgap pump pulses, and probe the sample with white light. Our results show that, compared to resonant excitation, shorter-wavelength excitation generates more free carriers, and by increasing the pump fluence, bandgap renormalization and hot-phonon bottleneck can be achieved.

References  

Observation of large negative thermo-optic coefficients in lead halide perovskites*  
TAKETO HANDA (Presenter), HIROKAZU TAHARA, YOSHIHIKO KANEMITSU, Institute for Chemical Research, Kyoto University — Lead halide perovskites are a new class of semiconductor materials for photonic devices [1]. Despite intensive research in the last decade, some of their fundamental physical properties still remain unclear. Here, we report that the halide perovskite CH₃NH₃PbCl₃ shows a large negative thermo-optic coefficient, i.e., a distinct decrease of the refractive index upon temperature rise [2]. We demonstrate that this unique response provides new photonic applications [2,3]. Furthermore, the negative thermo-optic property indicates unusual thermally-induced changes in the electronic states. We investigated the origin of the negative coefficient through the temperature dependence of the absorption spectra of a CH₃NH₃PbCl₃ thin film. With increasing temperature, a slight blueshift in the absorption peak energy was observed. Our analysis suggests that both the absorption blueshift and large thermal expansion contribute to the large negative thermo-optic coefficients of halide perovskites.

References  

*Part of this work was supported by JST-CREST (JPMJCR16N3) and KAKENHI (17J09650).
10:00AM F63.00011: Breaking the Defect Bottleneck in Halide Perovskite Semiconductors

[Invited] ARON WALSH (Presenter), National Renewable Energy Laboratory — The physical properties of semiconducting solids depend on the imperfections they contain[1]. Defects come in a few flavours: conductivity-promoting defects create free carriers that enable electronics; killer defects (deep centres) trigger recombination; and charge scattering defects reduce mobility. Our understanding of halide perovskites is limited in comparison to inorganic semiconductors. I will discuss recent progress, from theory and experiment, to identify, characterise and control point defects and defect processes in this family of compounds. I will cover charge compensation mechanisms [2], carrier trapping phenomena[3], the effect of grain boundaries[4], and how this understanding can be applied to engineer defect populations and distributions. The use of `defect tolerance` as a metric to develop and screen post-perovskite materials will be critically addressed.


10:36AM F63.00012: Electrohydrodynamically Assisted Deposition of organo-metallic hybrid perovskite thin films for Photovoltaics applications*

ALBERT DIBENEDETTO (Presenter), WILLIAM DELMAS, SAYANTANI GHOSH, University of California, Merced — The creation of lightweight and high efficiency photovoltaic devices is challenging, especially for deployment under extreme conditions, such as in outer space. Deposition techniques like drop casting or spin coating produce nonuniform films and are only useful under the influence of gravity. We have developed an alternative technique to prepare thin films via electrohydrodynamically (EHD) assisted deposition. Using Marangoni flow, this process allows precursors of different vapor pressures to be guided (via an applied electric field) onto a substrate in order to self-organize and produce uniform thin films while minimizing the amount of waste solution. In this talk, we will present different perovskite solar cell prototypes with different space qualified substrates that were prepared via EHD assisted deposition. To compare each prototype, we use characterization using photoluminescence (PL), spectroscopy, scanning electron microscopy (SEM), and atomic force microscopy (AFM). As a final goal, we aim to develop and optimize perovskite solar cell prototypes from inks of high wettability and space qualified substrates.

*This grant was supported by NASA grant no. NNX15AQ01.
Two-dimensional (2D) perovskite solar cells that boast of high stability and high efficiency have attracted significant attention. A systematically static and dynamic structure investigation is carried out to show the details of 2D morphology evolution. A dual additive approach is applied, in which the synergic efforts of alkali metal cation and polar solvent lead to high quality 2D perovskite thin film with well orientation. The novel structure can induce high quality 2D slab growth as well as reduce internal and surface defects, thus resulting in a high device efficiency of 13.65%. Steady-state and transient absorption spectra reveal the carrier transporting from low n to high n species of different kinetics. An \([\text{PbI}_6]^{4-}\) octagon coalescence transformation mechanism coupled with metal and organic cations wrapped is proposed, which then subjects to solvent vapor annealing to recrystallize and reorient 2D perovskite slabs to form an ideal structure to give rise to the improvement of device efficiency and stability.
Advances in computing charge carrier dynamics in oxides from first principles* [Invited] JIN-JIAN ZHOU (Presenter), MARCO BERNARDI, Department of Applied Physics and Materials Science, California Institute of Technology — Advances in first-principles calculations enable accurate predictions of charge carrier mobility and scattering mechanisms in materials. However, many oxides remain an open problem for these methods since they exhibit soft phonon modes due to structural phase transitions and electron-phonon interactions strong enough to form polarons. The presence of polarons and soft modes makes first-principles calculations of charge transport highly challenging even in non-correlated oxides.

This talk will discuss new approaches for treating electron-phonon coupling due to soft phonon modes, as well as a cumulant diagram-resummation approach for rigorously computing the carrier mobility in the large polaron regime. We apply these approaches to cubic SrTiO$_3$ perovskite as a paradigmatic case and analyze in detail soft mode and polaron contributions to charge transport.

Our advances allow us to accurately predict the temperature dependence [1] and absolute value [2] of the mobility in SrTiO$_3$, while providing long-sought microscopic details about the scattering mechanisms, bandstructure renormalization and beyond-quasiparticle features in the spectral function due to the strong electron-phonon coupling. Efforts to extend these calculations to a range of oxides and future application of these approaches to interfaces and heterostructures will be discussed.


*This work was supported by the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award Number DE-SC0004993.
Superconducting split-gate quantum point contacts in ionic liquid-gated SrTiO₃

EVGENY MIKHEEV (Presenter), ILAN ROSEN, DAVID GOLDHABER-GORDON, Stanford Univ — SrTiO₃ is one of few materials to exhibit superconductivity at carrier densities low enough to be manipulated electrostatically. In this work, we demonstrate electrostatically defined superconducting devices that combine global ionic liquid gating of the leads with local dielectric split gates. This design enables patterning of a 2D electron system with sub-100 nm features without the need for mesa etching. When tuned into a normal state, these devices behave as ballistic quantum point contacts, with conductance quantization near pinch-off. Quantization is in increments of e²/h, even at zero magnetic field, suggesting spontaneous spin-polarization. When the device leads are tuned to be superconducting, the weak link can be gated through a sequence of transport regimes: pinch-off, coulomb blockade, superconducting tunnel junction, and SNS or SS'S Josephson junction. We demonstrate that the local constriction can be tuned into a regime where its critical field exceeds that of its superconducting leads. This offers promise of exploring the microscopic physics of underdoped SrTiO₃, where two-dimensional superconductivity is usually suppressed by the lack of macroscopic coherence.

*This research was funded by the Air Force Office of Scientific Research through grant no. FA9550-16-1-0126

Probing the superconductivity of ferroelectric SrTiO₃ films

TIMO SCHUMANN (Presenter), LUCA GALLETTI, KAVEH AHADI, HANBYEOL JEONG, SUSANNE STEMMER, University of California, Santa Barbara — We report on the superconducting characteristics of doped 180-nm-thick SrTiO₃ films, grown by molecular beam epitaxy on (001) LSAT substrates. The epitaxial compressive strain induced by the substrate stabilizes a ferroelectric phase in the SrTiO₃ for carrier concentrations ranging from 5×10¹⁹ – 1.5×10²⁰ cm⁻³ [1,2]. A systematic study of the critical temperature and critical field as a function of the carrier density and type of doping atom reveal deviations from those expected for a single-band BCS superconductor. In particular, the critical temperature and critical field show qualitative different evolutions, with the latter exceeding the Pauli limit for certain values. We discuss the role of the band structure and inversion symmetry breaking.

9:00AM F64.00004: Superconductivity and Antiferrodistortive Phase Transition in Sr\textsubscript{1-x} Nd\textsubscript{x} TiO\textsubscript{3} Films  
JIN YUE (Presenter), Department of Chemical Engineering and Materials Science, University of Minnesota, YILIKAL ZAYINO, MARIA NAVARRO GASTIASORO, School of Physics and Astronomy, University of Minnesota, EYLON PERSKY, ALEX HANUKOV, Department of Physics and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat Gan, Israel, TRISTAN TRUTTMANN, Department of Chemical Engineering and Materials Science, University of Minnesota, BEENA KALISKY, Department of Physics and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat Gan, Israel, RAFAEL FERNANDES, VLAD PRIBIAG, School of Physics and Astronomy, University of Minnesota, BHARAT JALAN, Department of Chemical Engineering and Materials Science, University of Minnesota — Despite over 60 years of extensive research, the study of superconductivity, ferroelectricity and antiferrodistortive phase transition in SrTiO\textsubscript{3} remains puzzling yet intriguing. Through intrinsic defect management, we achieved for the first time electron density as low as 3 \times 10^{17} \text{ cm}^{-3} in Sr\textsubscript{1-x} Nd\textsubscript{x} TiO\textsubscript{3} films with the corresponding mobility exceeding 42000 \text{ cm}^{2}/\text{vs} at 1.8 K. By systematically varying the carrier density over three orders of magnitude, we present an important role of intra- vs. inter-band scattering on the superconducting transition temperature \( T_c \) across the Lifshitz transition. Significantly, we show a sizable effect of the antiferrodistortive phase transition on the normal state transport properties around 110 K. Finally, we discuss the role of dopant concentration, strain and dimensionality on the interplay between antiferrodistortive phase transition, incipient ferroelectricity, and normal and superconducting transport behavior in epitaxial Sr\textsubscript{1-x}Nd\textsubscript{x}TiO\textsubscript{3} thin films grown by hybrid molecular beam epitaxy approach.

9:12AM F64.00005: Ferroelectric Control of Normal and Superconducting States in Oxide Interface by Intrinsic and Extrinsic Bias  
GAL TUVIA (Presenter), Tel Aviv University, YIFTACH FRENKEL, physics, Bar Ilan University, PRASANNA KUMAR ROUT, Delft University of Technology, ITAI SILBER, Tel Aviv University, BEENA KALISKY, physics, Bar Ilan University, YORAM DAGAN, Tel Aviv University — We deposit the polar oxide LaAlO\textsubscript{3} on Ca doped SrTiO\textsubscript{3} with various Ca concentrations. The latter becomes ferroelectric below 30K. The resulting interface is conducting with a critical thickness of 3 unit cells of LaAlO\textsubscript{3}. A large increase in the interface resistance is observed as the temperature is decreased below the ferroelectric transition with a strong hysteretic behavior as a function of gate voltage. Below \( T_c \) 300mK the sample becomes superconducting with a clear hysteresis in \( T_c \) with respect to the applied gate voltage. We use scanning SQUID to image the current flow patterns and follow them as a function of gate voltage. We find that the polar LaAlO\textsubscript{3} induces an effective gate bias even when cooling down at zero applied electric field. This effective gate bias has a three-fold effect: it pins the ferroelectric domains near the interface, it reduces the carrier density and confines the current flow. We suggest this effective gate bias as a way to control the initial state of a ferroelectric material. The hysteresis observed both in the normal state and in the superconducting one can lead to a multifaceted controllable memory device.
Nonlinear transport in gate-induced 2D Rashba superconductor SrTiO$_3$

YUKI ITAHASHI (Presenter), TOSHIYA IDEUE, The Univ. of Tokyo, Tokyo, Japan., YU SAITO, University of California at Santa Barbara, Santa Barbara, USA., SUNAO SHIMIZU, Central Research Institute of Electric Power Industry, Yokosuka, Japan., TAKUMI OUCHI, TSUTOMU NOJIMA, Tohoku Univ., Sendai, Japan., YOSHIHIRO IWASA, The Univ. of Tokyo, Tokyo, Japan. — A polar conductor with Rashba spin-orbit coupling is a potential material platform for exotic quantum transport and spintronic functionalities [1,2]. One of their inherent properties is the nonreciprocal transport, where the magnetoresistance becomes inequivalent between the rightward and leftward current directions, because of the breaking of both spatial inversion and time reversal symmetries. Such a rectification effect reflecting polar symmetry has been studied at the interface or bulk polar semiconductor [3,4]. However, the mechanism of the nonreciprocity in a polar superconductor remains elusive.

To elucidate the noncentrosymmetric nature of the Rashba superconductor, we have investigated the nonreciprocal transport in gated SrTiO$_3$, which is known as a 2D Rashba superconductor. We found the gigantic enhancement in the nonlinear resistance in the amplitude and phase fluctuation regions. Also, we discuss the possible origins of nonreciprocity in the 2D Rashba superconductor, such as paraconductivity with a parity mixing in the Cooper pairs and rectified vortex-antivortex motions.

Fingerprints of interface superconductivity in ferroelectric tunnel junctions

FERNANDO GALLEGO (Presenter), 2D Foundry, Instituto de Ciencia de Materiales de Madrid, VICTOR ROUCO, Física de Materiales, Universidad Complutense de Madrid, MARIONA CABERO, Centro Nacional de Microscopía electrónica, Universidad Complutense de Madrid, DAVID SANCHEZ MANZANO, JAVIER TORNOS, Física de Materiales, Universidad Complutense de Madrid, RALPH EL HAGE, KEVIN SEURRE, Unité Mixtée de physique, CNRS, FABIAN ANDRES CUELLAR, ALBERTO RIVERA-CALZADA, ZOUHAIR SEFRIOUI, Física de Materiales, Universidad Complutense de Madrid, FEDERICO MOMPEAN, MAR GARCIA-HERNANDEZ, 2D Foundry, Instituto de Ciencia de Materiales de Madrid, JOSE MARIA GONZALEZ-CALBET, Centro Nacional de Microscopía electrónica, Universidad Complutense de Madrid, JAVIER VILLEGAS, Unité Mixtée de physique, CNRS, CARLOS LEON, JACOBO SANTAMARIA, Física de Materiales, Universidad Complutense de Madrid — Ferroelectric tunnel junctions open the possibility of controlling the tunneling current with the ferroelectric state of the barrier. We have studied ferroelectric tunnel junctions with La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) bottom electrode, a ferroelectric (FE) BaTiO$_3$ barrier and La$_{0.84}$Sr$_{0.16}$CuO$_3$-$\delta$ (LSCO) top electrode. LSCO is a cuprate capable of hosting large densities of oxygen vacancies (OV), yet superconductivity has never been observed. Coupled switching of oxygen vacancies and the ferroelectric polarization may produce drastic changes of the doping of the interface yielding unexpected electronic phases. We have found that the removal of OV from the cuprate interface has a strong hole doping effect of the material. We have observed the emergence of a new gap in the tunneling differential conductance curves which scales with temperature as a superconducting gap, strongly suggesting the nucleation of a superconducting phase at the interface. Switching the ferroelectric polarization of the barrier with an external electric field enables turning the superconducting gap on and off suggesting the possibility of the field effect control of the interface superconductivity.

*National project: Interface devices with tunable electronic structure and spin Memristors MAT2014-52405-C2-2-R
In Situ, Monolayer Control over the 2D Electron Gas on SrTiO$_3$*  

XI YAN (Presenter), FRIEDERIKE WROBEL, Materials Science Division, Argonne National Laboratory, Lemont, IL, 60439, USA, HAWOONG HONG, Advanced Photon Source, Argonne National Laboratory, Lemont, IL, 60439, USA, JIRONG SUN, Beijing National Laboratory for Condensed Matter & Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People’s Republic of China, JESSICA L MCCLESNEY, HUA ZHOU, Advanced Photon Source, Argonne National Laboratory, Lemont, IL, 60439, USA, DILLON FONG, Materials Science Division, Argonne National Laboratory, Lemont, IL, 60439, USA — SrTiO$_3$ (001) is the principal material in the field of oxide electronics, due to both its properties and the fact that the composition of its surface can be controlled, leading to TiO$_2$ surface termination. Employing in situ synchrotron X-ray methods during growth by molecular beam epitaxy (MBE) and angle-resolved photoemission spectroscopy (ARPES), we discover the existence of a 2D electron gas (2DEG) at the as-prepared, TiO$_2$-terminated SrTiO$_3$ (001) surface. Interestingly, the 2DEG appears correlated with the presence of a TiO$_2$ double layer [S. Cook et al., Sci. Adv. 5, eaav0764 (2019).], as deposition of single layer of SrO leads to island formation and complete elimination of the 2DEG. The subsequent growth of a TiO$_2$ monolayer leads to smoothing and return of the 2DEG. We will provide an atomic-level description of the evolving surface and how it relates to the surface electronic structure.

*Work supported by the Department of Energy, Office of Science, Basic Energy Sciences under contract no. DE-AC02-06CH11357.
A combined experimental and first principles study of small hole polarons in YTiO$_3$ thin films*

IFLAH LARAIB (Presenter), Materials Science and Engineering, University of Delaware, JIN YUE, Chemical Engineering and Materials Science, University of Minnesota, NICHOLAS F QUACKENBUSH, Materials Measurement Science Division, Materials Measurement Laboratory, National Institute of Standards and Technology, BHARAT JALAN, Chemical Engineering and Materials Science, University of Minnesota, ANDERSON JANOTTI, Materials Science and Engineering, University of Delaware — Rare-earth titanate YTiO$_3$ is a Mott insulator whose electronic structure description has been quite challenging to density functional theory (DFT) calculations within standard (semi)local approximations to the exchange-correlation term. The reported onset of optical absorption in YTiO$_3$ is $\sim$0.6 eV while the calculated Mott-Hubbard gap using hybrid DFT is $\sim$2 eV. Combining experiments on hybrid molecular beam epitaxy (MBE) grown YTiO$_3$ heterostructures with DFT calculations we investigated the electronic and transport properties of YTiO$_3$. We test the performance of the meta-GGA SCAN functional in the description of the electronic structure of YTiO$_3$, comparing the results of hybrid functional and photoemission measurements. We also study the formation, stability and migration of small hole polarons in YTiO$_3$, and compare our findings with the measurements of the Seebeck coefficient and temperature-dependent resistivity. We also carry out a detailed analysis of the effects of the TiO$_6$ octahedral tilt and rotations, and lattice distortions on the Mott-Hubbard gap.

*Theory work was supported by the National Science Foundation Early Career Award Grant No. DMR-1652994. Experimental work supported by the DOE Center for Quantum Materials, University of Minnesota.

Controlling spin-polarized carriers at the SrTiO$_3$/EuO interface via the ferroelectric field effect

WENTE LI (Presenter), ALEXANDER DEMKOV, University of Texas at Austin — Using first principle calculations, we investigate the magneto-electric field effect at the SrTiO$_3$/EuO interface in the BaTiO$_3$/SrTiO$_3$/EuO heterostructure. The spontaneous polarization in tetragonal BaTiO$_3$ is demonstrated to control the movement of the two-dimensional electron gas in SrTiO$_3$ across the interface with ferromagnetic EuO as well as induce spin polarized two-dimensional hole gas and influence the electronic structure at this interface. We also investigate the effect of oxygen vacancy in SrTiO$_3$ near the SrTiO$_3$/EuO interface. To investigate the ferroelectric polarization morphology, we use the phenomenological Landau-Khalatnikov model and compare it with the results of first principle calculations.
10:24AM F64.00011: Anomalous Transverse Resistance at the Interface of (111) (La$_{0.3}$Sr$_{0.7}$)(Al$_{0.65}$Ta$_{0.35}$)O$_3$ /SrTiO$_3$ Heterostructures* PATRICK KRANTZ (Presenter), VENKAT CHANDRASEKHAR, Northwestern University, ZHEN HUANG, KUN HAN, ARIANDO ARIANDO, THIRUMALAI VENKATESAN, Department of Physics, National University of Singapore — A variety of interesting physical phenomenon have been found to live at the interface between complex oxide layers. Significant work has been done to characterize the electrical transport properties of the two dimensional conducting gases present in systems like LaAlO$_3$ (LAO)/ SrTiO$_3$ (STO). Recently, (La$_{0.3}$Sr$_{0.7}$)(Al$_{0.65}$Ta$_{0.35}$)O$_3$ (LSAT) /STO has been investigated due to improved lattice matching when compared to LAO/STO, and interesting effects due to strong spin orbit interactions$^{1,2}$. Here we report an anomalous transverse resistance observed in Hall bars at the interface of (111) oriented LSAT/STO. This effect does not track with low field Hall coefficient, nor longitudinal resistance over temperatures from 4 K to 70 K. We discuss these findings in the context of similar effects seen in La$_{2-x}$Sr$_x$CuO$_4$ (LSCO)/STO and LAO/STO systems$^{3,4}$.


*US DOE Grant No. DE-FG02-06ER46346

10:36AM F64.00012: Synthesis of epitaxial ferrimagnetic NiCo$_2$O$_4$ thin films on SrTiO$_3$ and Sr$_3$Al$_2$O$_6$ buffered SrTiO$_3$ substrates* QIUCHEN WU (Presenter), LE ZHANG, YIFEI HAO, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln — The inverse spinel NiCo$_2$O$_4$ (NCO) is ferrimagnetic with high Curie temperature ($T_C$) and spin polarization. It is of high research interest to integrate it with other functional oxides, while many of them have the perovskite structure. We investigated the effects of a perovskite substrate on the magnetotransport properties of NCO by depositing 30 nm NCO thin films on SrTiO$_3$ (STO) and Sr$_3$Al$_2$O$_6$ (SAO) buffered STO substrates using off-axis RF magnetron sputtering. Both types of samples exhibit insulating behavior below 300 K, and the films on SAO buffered STO shows more than 10 times higher resistivity at 300 K. We estimated the $T_C$ from the magnetoresistance hysteresis. These samples show $T_C$ of up to 150 K, well below that for films deposited on MgAl$_2$O$_4$ substrates (above 300 K). The reduced $T_C$ can be attributed to a high density of anti-phase boundaries due to the structural mismatch between NCO and STO. We also discuss the possibility of suspending the NCO thin films by water etching the SAO buffer layer.

*This work was supported by NSF through Grant No. DMR-1710461, Nebraska MRSEC Grant No. DMR-1420645, and Nebraska Center for Energy Sciences Research.
10:48AM F64.00013: Deal-Grove-like thermal oxidation of Si (001) buried under a thin layer of SrTiO$_3$*

WEI GUO (Presenter), AGHAM POSADAS, ALEXANDER DEMKOV, University of Texas at Austin — Dry oxidation of Si (001) beneath a thin epitaxial SrTiO$_3$ layer has been studied using furnace annealing in flowing oxygen. A 10-nm layer of SrTiO$_3$ is epitaxially grown on Si with no SiO$_2$ interlayer. For such a structure, an annealing temperature of 800°C was found to be the limiting temperature to prevent silicate formation and disruption of the interface structure. The effect of annealing time on thickness of the SiO$_2$ layer was investigated. *In situ* x-ray photoelectron spectroscopy (XPS) and reflection-high-energy electron diffraction (RHEED) were used to ensure that the quality of SrTiO$_3$ is unchanged after the annealing process. The experimental annealing data is compared with a theoretical oxygen diffusion model based on those due to Deal, Grove and Massoud. The model fits the experimental data well, indicating that oxygen diffusion through the SrTiO$_3$ layer is not the limiting factor. One can therefore readily control the thickness of the SiO$_2$ interlayer by simply controlling the annealing time in flowing oxygen.

*This research was partially supported by the National Science Foundation through the Center for Dynamics and Control of Materials: an NSF MRSEC under Cooperative Agreement No. DMR-1720595 and by the Air Force Office of Scientific Research under Grant FA9550-18-1-0053.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F65 DMP: Defects and Dopants in Bulk Materials II Mile High Ballroom

4F - Jinkyoung Yoo

8:00AM F65.00001: High-Q Nanophotonic Resonators on Diamond Membranes using Atomic Layer Deposition TiO2*

AMY BUTCHER (Presenter), XINGHAN GUO, ROBERT SHREINER, KAI HAO, ALEXANDER A HIGH, University of Chicago — Nanophotonic resonators are critical elements in solid state quantum networks, as they enable individual optical photons to interact with quantum spin states. In diamond, current techniques to fabricate these devices often introduce significant surface roughness and lattice strain, which limit performance and scalability. Using atomic layer deposition of TiO2, we developed a nanophotonic fabrication platform that avoids substrate etching while retaining the potential for high-cooperativity interfacing with color centers in thin diamond membranes. The resulting devices are exceptionally smooth and can be built on arbitrary substrates. In this work, we fabricated ring resonators and 1D photonic crystal cavities with quality factors exceeding $10^4$ and demonstrated our platform’s potential for quantum networking applications on diamond.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1746045.
8:12AM F65.00002: Single crystal diamond membranes for quantum networking and sensing*  
XINGHAN GUO (Presenter), Pritzker School of Molecular Engineering, University of Chicago, NAZAR DELEGAN, Center for Molecular Engineering and Materials Science Science Division, Argonne National Laboratory, AMY BUTCHER, DAVID AWSCHALOM, Pritzker School of Molecular Engineering, University of Chicago, JOSEPH P HEREMANS, Center for Molecular Engineering and Materials Science Science Division, Argonne National Laboratory, ALEXANDER A HIGH, Pritzker School of Molecular Engineering, University of Chicago — Atomic defects in single crystal diamond, such as nitrogen vacancy centers and silicon vacancy centers, are promising qubit candidates for quantum communication and quantum sensing applications. However, it is difficult to fully utilize their advantages in bulk diamond due to its high refractive index and limited nanofabrication methods. Therefore, to allow better integration flexibility of color centers while maintaining their coherence properties, we developed a process to create high quality, atomically smooth, large-scale single crystal diamond membranes that can be placed on any carrying wafers. Herein we will present the fabrication steps in detail, including He\(^+\) implantation, CVD overgrowth, electrochemical etching, flipping, transfer, and backside etching. Additionally, recent progress related to the integration of these diamond membranes will be demonstrated, namely, photonic cavity integration and creation of group IV and nitrogen vacancy defect centers, which would be beneficial in multi-qubit network, hybridized quantum systems, and quantum sensing.

*This work is partially supported by DARPA. The Diamond CVD growth at Argonne National Lab is supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

8:24AM F65.00003: Single-shot readout of \(^{171}\text{Yb}:\text{YVO}\) ions embedded in a nanophotonic cavity*  
JONATHAN KINDEM (Presenter), ANDREI RUSKUC, JOHN G BARTHOLOMEW, JAKE ROCHMAN, YAN QI HUAN, ANDREI FARAON, Caltech — Solid-state emitters coupled to photonic resonators are an attractive platform for building quantum light-matter interfaces required for scalable quantum networks. Rare-earth ions (REIs) in solids offer a promising system for such interfaces due to their long optical and spin coherence times at cryogenic temperatures, but harnessing these properties at the single ion level has proven to be challenging due to the inherently weak coupling of REIs with light. Here we present the initialization, coherent manipulation, and readout of individual ytterbium-171 ions embedded in a nanophotonic cavity fabricated directly in the yttrium orthovanadate (YVO) host crystal. These ions possess coupled electron-nuclear spin states that are first-order insensitive to magnetic field fluctuations, which allows for optical linewidths less than 1 MHz and spin coherence times greater than 30 ms. We show that Purcell enhancement in the nanophotonic cavity increases the optical emission rate by a factor of 120 and improves the cyclicity of the cavity-coupled optical transitions, which enables efficient initialization and conditional single-shot readout of the hyperfine spin state with fidelity greater than 95%.

*The authors gratefully acknowledge funding from the NSF, IQIM, and AFOSR.
8:36AM F65.00004: Spin dynamics of 171Yb:YVO ions embedded in a nanophotonic cavity*
ANDREI RUSKUC (Presenter), JONATHAN KINDEM, JOHN G BARTHOLOMEW, JAKE ROCHMAN, YAN QI HUAN, ANDREI FARAON, Caltech — Optically addressable spin qubits in solid state hosts are a promising platform for developing scalable quantum networks. We present results on a possible architecture based on single 171 Yb ions doped into yttrium orthovanadate. By coupling these ions to nanophotonic cavities we leverage the Purcell regime of cavity QED to enhance the weak, highly coherent optical transitions typically associated with rare earth ions thereby enabling detection and readout. This talk focuses on ground state spin dynamics. At zero field, the combination of electron and nuclear spin 1/2 leads to a clock transition that is first-order insensitive to magnetic field fluctuations. Ramsey coherence times are limited by interactions with slowly fluctuating lattice spins via second-order perturbations to the Yb ion Hamiltonian. By applying CPMG dynamical decoupling sequences we can extend the spin coherence time to 30ms at temperatures up to 1.2K. Furthermore, we investigate spin lifetimes (T1) in the ground state manifold and find that these are limited by magnetic dipole-dipole interactions with other Yb ions. We also discuss the prospects of working with this platform at high magnetic field and demonstrating remote spin-spin entanglement.

*The authors acknowledge funding from the NSF, IQIM and AFOSR MURI.

8:48AM F65.00005: An in-situ single photon source detection platform for deterministic nanometer resolution ion implantation*
MICHAEL TITZE (Presenter), KULTURANSINGH HOOGHAN, Sandia National Laboratories, HAN HTOON, Los Alamos National Laboratory, EDWARD S BIELEJEC, Sandia National Laboratories — Single photon sources (SPS) are of interest for usages from metrology to the basis of quantum communication, computation and sensing. SPS based on color centers in SiC and other wide band gap semiconductors such as hBN, diamond, etc. require the control over both the positioning as well as the number of optically active color centers. We have developed focused ion beam implantation using our nanoImplanter (nI) which allows spatial control to <50 nm and implantation down to single impurity atoms using counted ion implantation. However, the typical conversion efficiency from implanted impurity atom to optically active color center can range from <3% to >80% depending on the material and the implantation energy. For these low efficiency processes an in-situ technique to identity the creation of SPS is required. To this end we have designed an in-situ photoluminescence (PL) setup integrated into the nI allowing for detection of single photon emission during ion implantation. Using this PL setup in conjunction with a Hanbury Brown Twiss interferometer allows us to deterministically create and measure single color centers in a range of materials systems with nanometer resolution.

*SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525; SAND2019-12446A
9:00AM F65.00006: Introduction of spin centers in single crystals of \( \text{Ba}_2\text{CaWO}_{6-\delta} \) - MEKHO

Sinha (Presenter), Johns Hopkins University, Tyler J. Pearson, Chemistry, Northwestern University, Allen Scheie, Timothy Reeder, Hector K. Vivanco, Johns Hopkins University, Danna Freedman, Chemistry, Northwestern University, William Adam Phelan, Tyrel McQueen, Johns Hopkins University — Electronic spins are ideal qubit candidates both for their modularity and their ease of manipulation with microwave radiation. While fundamentally, \( T_2 \), the spin-spin relaxation time, represents the functional operating time of a qubit, \( T_1 \), the spin-lattice relaxation time, is ultimately the most restrictive parameter, as \( T_1 \) represents the theoretical upper limit to \( T_2 \). Design approaches to maximize \( T_1 \) remain an open question. We report the coherence properties of \( W^{5+} \) spin centers in \( \text{Ba}_2\text{CaWO}_{6-\delta} \) generated by oxygen vacancies. We characterized these defects by measuring the \( T_1 \) and \( T_2 \) times from \( T = 5 \) to 150 K. Correlation of the \( T_1 \) lifetimes obtained from pulse EPR with phonon modes obtained from the heat capacity data quantifies the contribution of respective phonon modes to the spin-phonon coupling in the system. These results demonstrate that systematic defect generation in double perovskite structures can generate viable paramagnetic point centers for quantum applications.

*This work was funded by PARADIM, a National Science Foundation Materials Innovation Platform (NSF DMR-1539918). TMM acknowledges the David and Lucile Packard Foundation. TJP acknowledges an NSF Graduate Research Fellowship (DGE-1324585). AS acknowledges the Gordon and Betty Moore foundation, EPIQS, GBMF4532.


Alexander Crook (Presenter), Christopher Anderson, Department of Physics, University of Chicago, Kevin Miao, Alexandre Bourassa, Pritzker School of Molecular Engineering, University of Chicago, Hope Lee, Department of Physics, University of Chicago, Sam L Bayliss, Pritzker School of Molecular Engineering, University of Chicago, David O Bracher, Xingyu Zhang, Department of Physics, Harvard University, Hiroshi Abe, Takeshi Oshima, National Institutes for Quantum and Radiological Science and Technology (QST), Evelyn L Hu, Department of Physics, Harvard University, David Awschalom, Pritzker School of Molecular Engineering, University of Chicago — Silicon carbide (SiC) has recently been developed as a platform for optically addressable spin defects in the form of the neutral divacancy, most notably in the 4H polytype [1-3]. Here we present the Purcell enhancement of a single divacancy coupled to a photonic crystal cavity. We use a combination of nanolithographic techniques and a dopant-selective photoelectrochemical etch to produce suspended cavities with quality factors exceeding 5000. This corresponds to a Purcell factor of \( \sim 50 \) for a divacancy within the cavity mode and results in an increased photoluminescence into the zero-phonon line (ZPL) when on resonance with the cavity, as well as a shortened excited state lifetime. Additionally, we observe coherent control of the divacancy ground state spin inside of the cavity nanostructure. This system represents a major advance towards applications for the scalability of long-distance entanglement protocols using SiC that require the interference of indistinguishable photons from spatially separated single qubits.

*This work is supported by AFOSR, ARO, NDSEG, NSF, and UChicago MRSEC.
9:24AM F65.00008: Engineering Light-Hole Quantum States in an Optically Active Group IV Low Dimensional System  ANIS ATTIAOUI (Presenter), SIMONE ASSALI, OUSSAMA MOUTANABBIR, Ecole Polytechnique de Montreal — Hole spins have attracted a great deal of attention because of their reduced coupling to the nuclear spin bath. However, most of experimental investigations on 2D gas systems have so far focused on heavy-hole states (HH). This is attributed to the nature of the heterostructure currently exploited, where compressive strain lifts the valence band degeneracy and leaves HH states energetically well above the light-hole (LH) states. However, the ability to exploit LH states will be a powerful paradigm beneficial for quantum information technologies, as the orbital angular momentum of LH states makes them more powerful and versatile. To harness these largely unexplored advantages of LH states, we present a new low-dimensional system consisting of highly-strained Ge quantum well (QW) grown on silicon wafers using GeSn as barriers. To quantify the effect of the LH confinement as well as the LH-HH mixing, several spectroscopic techniques were used to identify the LH confined states in the Ge well. The obtained heterostructure shows optical transitions that can be modulated in the midinfrared range. This ability to engineer quantum structure where LH is the ground state in an optically active group IV platform lays the groundwork for a new class of Si-compatible quantum technologies.

9:36AM F65.00009: First-principles theory of highly correlated electronic states in semiconductor spin qubits*  HE MA (Presenter), University of Chicago, MARCO GOVONI, Argonne National Lab, GIULIA GALLI, University of Chicago — Point defects in wide-gap semiconductors are promising platforms for quantum sensing applications and quantum networks. We present a quantum embedding theory to describe highly correlated electronic states of point defects that are not addressable by conventional density functional theory. We describe the implementation of the method, built on the coupling of the Qbox (www.qboxcode.org/) and WEST (http://www.west-code.org) codes [1], and we demonstrate its accuracy and efficiency for the nitrogen-vacancy center in diamond and several other defects in diamond and SiC.


*Supported by the Midwest Integrated Center for Computational Materials (MICCoM) as part of the Computational Materials Sciences Program funded by DOE/BES
9:48AM F65.00010: Electrically driven optical interferometry with spins in SiC* KEVIN MIAO (Presenter), ALEXANDRE BOURASSA, CHRISTOPHER ANDERSON, SAMUEL J WHITELEY, ALEXANDER CROOK, SAM L BAYLISS, GARY WOLFOWICZ, Pritzker School of Molecular Engineering, University of Chicago, GERGÖ THIERING, PÉTER UDVARHELYI, VIKTOR IVADY, Wigner Research Centre for Physics, Hungarian Academy of Sciences, HIROSHI ABE, TAKESHI OHSHIMA, National Institutes for Quantum and Radiological Science and Technology, ADAM GALI, Wigner Research Centre for Physics, Hungarian Academy of Sciences, DAVID AWSCHALOM, Pritzker School of Molecular Engineering, University of Chicago — Interfacing solid-state defect electron spins to other quantum systems is an ongoing challenge. The ground-state spin's weak coupling to its environment bestows excellent coherence properties [1], but also limits desired drive fields. The excited-state orbitals of these electrons, however, can exhibit stronger coupling to phononic and electric fields [2]. Here, we demonstrate electrically driven coherent quantum interference in the optical transition of single, basally oriented divacancies (VV) in commercially available 4H silicon carbide [3]. By applying microwave frequency electric fields, we coherently drive the VV's excited-state orbitals and induce Landau-Zener-Stückelberg interference fringes in the resonant optical absorption spectrum. Additionally, we find remarkably coherent optical and spin subsystems enabled by the basal VV's symmetry. These properties establish VVs as strong candidates for quantum communication and hybrid system applications, where simultaneous control over optical and spin degrees of freedom is paramount.


*This work is supported by AFOSR, ARO, DARPA, NDSEG, NSF, and UChicago MRSEC.

10:00AM F65.00011: Controlling Number of Dopants per Site in Si:P Quantum Devices JONATHAN WYRICK (Presenter), XIQIAO WANG, RANJIT KASHID, PRADEEP NAMBOODIRI, FAN FEI, RICHARD SILVER, National Institute of Standards and Technology — STM-based fabrication of atomically precise Si:P structures has been demonstrated as a promising platform for the realization of dopant-based qubit quantum computing. There is a growing broader interest in applying this technique to other quantum systems in Si, for example artificial lattices to engineer band structure, as well as arrays of atoms acting as tunable Hubbard simulators. We present results from a single-atom transistor and few-atom cluster transistors demonstrating the effect that the number of dopants per site has on the energy spectrum of these devices, with the important implication that for many applications of interest it will be necessary to control this parameter with absolute precision. We detail our efforts using STM-based feedback-controlled techniques to engineer placement and number of dopants per site with the goal of reducing the fabrication uncertainty of dopants per site to zero.
10:12AM F65.00012: Tracking interfacial disorder in SiGe qubit material* LUIS FABIAN PEN (Presenter), JUSTIN C KOEPKE, EZRA BUSSMANN, Sandia National Laboratories — Theory predicts quantum dot electrons interact with interface atomic-scale disorder, perturbing energetics, creating new potentially useful states, and adding complexity that could dictate viability of some future qubit technologies. Although profoundly impactful, the predictions are challenging to test, since relevant structures are difficult to measure and correlate with qubit behavior. We've measured atomic step disorder at Si/SiGe interfaces using scanning tunneling microscopy coupled to an epitaxial growth tool. We report a counterintuitive evolution of roughness and step spatial correlations during growth. The results are meaningful toward elucidating structure-function relationships in SiGe QDs.

*This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or U.S. Government.

10:24AM F65.00013: Device development and characterization of Er doped epitaxial Y2O3 on Silicon platform* MANISH KUMAR SINGH (Presenter), University of Chicago, ABHINAV PRAKASH, GARY WOLFOWICZ, Argonne National Lab, YIZHONG HUANG, CHRISTINA WICKER, University of Chicago, ALAN DIBOS, JIANGUO WEN, TIJANA RAJH, Argonne National Lab, DAVID AWSCHALOM, TIAN ZHONG, SUPRATIK GUHA, University of Chicago — Spin-optical interface in rare-earth ions enables storage of optical quantum information in the long-lived nuclear spin levels. Er3+ has an optical excitation that matches the telecom transmission wavelength, making it technologically attractive. Further, very narrow transition linewidths and high spectral stability in Er3+ has been demonstrated when embedded in a crystalline host making it an ideal candidate for solid state quantum memory. Using molecular beam epitaxy (MBE), we demonstrate the growth and characterization of high quality single crystal thin films of Er:Y2O3 on Si 111 and Si 100. Photoluminescence (PL) and EPR show substitution of Er at Y sites. PL linewidths of 7.9 GHz and 6 GHz for the 1536 nm transition are obtained at 4 K and 7 mK, respectively. We will discuss the role of the microstructure, buffer layers, isotopic purity (Er 167), and Er3+ proximity to the interfaces on the optical linewidths. Finally, we report the optical transition lifetime, optical and spin coherence lifetimes on the devices fabricated on this platform. Q values for microdisk resonators and loss (db/cm) in optical waveguides will also be presented.

*Part of the work was funded by EFRC funds through the Department of Energy
Coherent driving of quantum spins via electrically controlled nonlinear magnetization precessions in quantum-classical spin hybrids* AVINASH RUSTAGI (Presenter), Purdue Univ, SHIVAM KAJALE, Indian Institute of Technology Bombay, PRAMEY UPADHYAYA, Purdue Univ — Coherent drives that are spatially local and at the same time add minimal decoherence when manipulating quantum spins, are of significant interest for quantum technology applications. Spin-spin interactions in quantum impurity spin [like Nitrogen vacancy (NV) center]-nanomagnet hybrids provide a platform where spintronic tools controlling nanomagnet dynamics, can be leveraged to coherently drive the quantum spin. However, decoupling coherent and incoherent dynamics is required for attaining large quality factors. Here, we propose to utilize a novel dynamics regime where electrically controlled nonlinear magnetization precessions of a nanomagnet [Nature materials 11, 39 (2012)] can be used to drive the quantum spin to arbitrary quantum states over the Bloch sphere. We demonstrate that the coherent and incoherent dynamics are decoupled in this regime, thereby showing that such quantum-classical spin hybrids can serve as a coherent drive that is local, electrically-controlled, and decoupled from incoherent dynamics.

*We acknowledge NSF grants DMR-1838513 and ECCS 1810494.
Spin triplet superconductivity was recently discovered at temperatures below 1.6 K in the correlated electron compound UTe$_2$ (1), with remarkably anisotropic and large upper critical field values, exceeding 35 T. Although it shares many characteristics with the ferromagnetic spin-triplet superconductors, UTe$_2$ does not order magnetically; instead, it exhibits properties of a quantum critical ferromagnet. The attendant strong magnetic fluctuations likely play an important role in establishing the superconducting pairing and protecting it against the typical destabilizing effects of high magnetic fields. Accumulating evidence supports the notion of a spin-triplet, nodal order parameter. Moreover, an unprecedented reentrant superconducting phase has been identified in UTe$_2$ at even higher magnetic fields, between 40 T and 65 T (2).

References:
(1) Science 365, 684 (2019)
(2) Nature Physics (2019), https://doi.org/10.1038/s41567-019-0670-x
Manipulation of time reversal symmetry breaking superconductivity in Sr$_2$RuO$_4$ by uniaxial strain* [Invited] HANS-HENNING KLAUSS (Presenter), VADIM GRINENKO, SHREENANDA GHOSH, RAJIB SARKAR, FELIX BRÜCKNER, Faculty of Physics, TU Dresden, Germany, JEAN-CHRISTOPHE ORAIN, ARTEM NIKITIN, DEBARCHAN DAS, ZURAB GUGUCHIA, Paul-Scherrer-Institut, Villigen, Switzerland, JOONBUM PARK, Los Alamos National Laboratory, MARK E BARBER, MPI CPfS, Dresden, Germany, NAOKI KIKUGAWA, 5National Institute for Material Science, Japan, JAKE BOBOWSKI, Department of Physics, Kyoto University, Japan, DMITRY SOKOLOV, MPI CPfS, Dresden, Germany, HUBERTUS LUETKENS, Paul-Scherrer-Institut, Villigen, Switzerland, YOSHITERU MAENO, Department of Physics, Kyoto University, Japan, ANDREW MACKENZIE, CLIFFORD W. HICKS, MPI CPfS, Dresden, Germany — Although the normal-state electronic structure of Sr$_2$RuO$_4$ is known with exceptional precision, even after two decades of research, the symmetry of it's certainly unconventional superconducting state is currently under strong debate, e.g. the long time favoured spin-triplet $p_x + ip_y$ state is ruled out by recent NMR experiments [1]. However, in general time-reversal-symmetry breaking (TRSB) superconductivity indicates complex two-component order parameters. Probing Sr$_2$RuO$_4$ under uniaxial offers the possibility to lift the degeneracy between such components [2]. One key prediction for Sr$_2$RuO$_4$, a splitting of the superconducting and TRSB transitions under uniaxial stress has not been observed so far. Here, we report results of muon spin relaxation (μSR) measurements on Sr$_2$RuO$_4$ placed under uniaxial stress. We observed a large stress-induced splitting between the onset temperatures of superconductivity and TRSB. Moreover, at high stress beyond the van Hove singularity [2], the TRSB phase is suppressed and a long-range ordered magnetic spin density wave phase is observed with an approx. 50 times stronger internal field. We will discuss the uniaxial strain dependent electronic phase diagram and its implications for the symmetry of the superconducting order parameter in Sr$_2$RuO$_4$.


*This work was supported by DFG (GR 4667, GRK 1621, and SFB 1143).
**9:12AM F66.00003: Knight Shift and Leading Superconducting Instability From Spin Fluctuations in Sr$_2$RuO$_4$** [Invited]  
ASTRID RØMER (Presenter), Niels Bohr Institute, University of Copenhagen, ILYA EREMIN, Institut für Theoretische Physik III, Ruhr-Universität Bochum, PETER HIRSCHFELD, Department of Physics, University of Florida, BRIAN M ANDERSEN, Niels Bohr Institute, University of Copenhagen — The chiral triplet pairing scenario proposed for Sr$_2$RuO$_4$ has been challenged by recent nuclear magnetic resonance (NMR) studies [A. Pustogow et al., arXiv:1904.00047 and K. Ishida et al., arXiv:1907.12236]. We perform a detailed theoretical study of spin-fluctuation mediated superconductivity guided by the spin-fluctuation spectrum measured from neutron scattering of this compound. Nodal even-parity solutions as well as odd-parity states with spins aligned predominantly out of the RuO$_2$ planes are found, both of which are compatible with the new data. The usual odd-parity state with spins primarily in the plane, the chiral $k_x+ik_y$, is difficult to stabilize and in contradiction to both NMR and neutron experiments. The presence of nodes in the spectral gap appears as a common feature for both even- and odd parity gaps. A surprising near-degeneracy of the nodal s' and d$_{x^2-y^2}$-wave solutions suggests the possibility of a near-nodal time-reversal symmetry broken s' +id$_{x^2-y^2}$-wave pair state. Finally we discuss local signatures of such a state near nonmagnetic disorder, as well as the possibility of induced SDW in vicinity of impurities and under strain.

*The Carlsberg Foundation

**9:48AM F66.00004: Interplay of heavy fermion quantum criticality and unconventional superconductivity** [Invited]  
FRANK STEGLICH (Presenter), OLIVER STOCKERT, JULIA ARNDT, HIRALE S. JEEVAN, Max Planck Institute for Chemical Physics of Solids, CORNELIUS KRELLNER, Goethe University Frankfurt, HUIQIU YUAN, MICHAEL SMIDMAN, Center for Correlated Matter, Zhejiang University, ERWIN SCHUBERTH, MARC TIPPMANN, LUCIA STEINKE, Walther Meissner Institute, TU Munich, QIMIAO SI, Rice University, EMILIAN NICA, Arizona State University, RONG YU, Renmin University of China — According to the ‘Quantum Critical Paradigm’, antiferromagnetic (AF) quantum critical points (QCPs) in pristine heavy fermion metals cause emergent unconventional superconductivity (SC). This will be demonstrated for both CeCu$_2$Si$_2$ (CCS) and YbRh$_2$Si$_2$ (YRS) [M. Smidman et al., Phil. Mag. 98, 2930 (2018)]. CCS exhibits a 3D spin-density-wave QCP and was considered a d-wave superconductor until recently, when its specific heat was found to follow an exponential temperature dependence at low temperatures [S. Kittaka et al., Phys. Rev. Lett. 112, 067002 (2014)]. Based on atomic - substitution, neutron - scattering and penetration - depth results we show that CCS cannot be an (isotropic/anisotropic) s-wave superconductor but is best described by a model for a fully gapped two-band d-wave superconductor [G. M. Pang et al., Proc. Natl. Acad. Sci. USA 115, 5343 (2018); E. N. Nica et al., npj Quantum Materials 2, 24 (2017)]. YRS exhibits a magnetic-field induced partial-Mott AF QCP. For this material, no SC had been detected above 10 mK. However, magnetic and specific-heat measurements performed to about 1 mK revealed HF, i.e., unconventional, SC to develop at $T_c = 2$ mK. This is ascribed to a competition between nuclear-dominated AF hybrid order and the primary AF order of the 4f-electron spins by which the system is pushed towards its QCP [E. Schuberth et al., Science 351, 485 (2016)]. Our observations support the relevance of the Quantum Critical Paradigm, regardless of the microscopic origin of the AF instability.
Pairing Tendencies, Orbital Selective Mott Phases, and Magnetic Block States in Multiorbital Models for Iron-Based Ladders and Chains* [Invited] ELBIO DAGOTTO (Presenter), University of Tennessee, Knoxville, and Oak Ridge National Laboratory — The discovery of superconductivity at high pressure in iron-based two-leg ladder 123 materials [1] established a new playground to better understand pairing tendencies in iron superconductors. Similarly as in Cu-oxide ladders, computational calculations using correlated electronic models can be performed with good accuracy in quasi-1D systems. Here, I will review our recent results for multiorbital Hubbard models varying the Hubbard and Hund couplings, and the electronic density. Clear indications of pair formation are found in lightly-doped ladders [2] and chains [3], and robust spin-singlet pair-pair correlations develop in those chains [3] (as in Cu-based ladders, we assume pressure leads to doping of the iron network [4]). An explanation for spin-singlet pairing based on an "orbital resonant valence bond" state is discussed for chains [5]. The magnetic properties in ladders and chains are also unexpectedly rich. An "orbital selective Mott phase" dominates in a wide range of parameters. In this regime, magnetic ``block" states emerge, such as up-up-down-down patterns. We calculated the dynamical spin structure factor, finding a mixture of acoustic and optical modes [6] as in neutron experiments. Even more extended block states were recently discovered [7,8]. This complex behavior unveiled in models for 1D iron superconductors when studied accurately suggests that the physics of these materials could be far richer than anticipated.

[4] Y. Zhang et al., PRB 95, 115154 (2017); PRB 97, 045119 (2018)
[8] J. Herbruch et al., submitted

*Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Tuesday, March 3, 2020 8:00 AM - 11:00 AM

Session F67 DCMP: Broken Symmetries and Electron Pairing in Magic-Angle Flat Bands Four Seasons 2-3 - Pablo Jarillo-Herrero, Massachusetts Institute of Technology MIT - Tag(s): Invited
8:00AM F67.00001: Superconductors, Orbital Magnets, and Correlated States in Magic Angle Bilayer Graphene

[Invited] DMITRI EFETOV (Presenter), ICFO-The Institute of Photonic Sciences —

Superconductivity often occurs close to broken-symmetry parent states and is especially common in doped magnetic insulators. When twisted close to a magic relative orientation angle near 1 degree, bilayer graphene has flat moire superlattice minibands that have emerged as a rich and highly tunable source of strong correlation physics, notably the appearance of superconductivity close to interaction-induced insulating states. Here we report on the fabrication of bilayer graphene devices with exceptionally uniform twist angles. We show that the reduction in twist angle disorder reveals insulating states at all integer occupancies of the four-fold spin/valley degenerate flat conduction and valence bands, i.e. at moire band filling factors \( \nu = 0, \pm 1, \pm 2, \pm 3 \), and superconductivity below critical temperatures as high as 3 K close to -2 filling. We also observe three new superconducting domes at much lower temperatures close to the \( \nu = 0 \) and \( \nu = \pm 1 \) insulating states. Interestingly, at \( \nu = \pm 1 \) we find states with non-zero Chern numbers. For \( \nu = -1 \) the insulating state exhibits a sharp hysteretic resistance enhancement when a perpendicular magnetic field above 3.6 tesla is applied, consistent with a field driven phase transition. Our study shows that symmetry-broken states, interaction driven insulators, and superconducting domes are common across the entire moire flat bands, including near charge neutrality.

*D.K.E. acknowledges support from the Ministry of Economy and Competitiveness of Spain through the “Severo Ochoa” program for Centres of Excellence in R&D (SE5-0522), Fundació Privada Cellex, Fundació Privada Mir-Puig, the Generalitat de Catalunya through the CERCA program, the H2020 Programme under grant agreement n° 820378, Project: 2D-SIPC and the La Caixa Foundation.
8:36AM F67.00002: Competing Orders, Nematicity and Novel Josephson Effects in Magic-Angle Graphene Superlattices [Invited] YUAN CAO (Presenter), Massachusetts Institute of Technology MIT — The emergence of two-dimensional materials have provided physicists with unprecedented way of studying the motion of electrons in a superconductor. Although superconductivity itself has been studied for more than a century, the recent advances of “twistronics” research in graphene superlattices brings fundamentally new physics into the picture [1,2]. In this talk I will present that demonstrate some peculiar aspects of magic-angle twisted bilayer graphene (MATBG) which has recently been discovered to exhibit correlated insulating phase and unconventional superconductivity. In an in-plane magnetic field, MATBG exhibits a highly anisotropic critical magnetic field within the sample plane that strongly suggests nematicity in the order parameter of the superconductivity. Furthermore, the phase diagrams of some MATBG samples show a distinctive kink in Tc in the ‘underdoped’ region which is reminiscent of quantum critical point behavior in some cuprates such as YBa$_2$Cu$_3$O$_{6+\delta}$[3]. These observations signify the similarity between MATBG and established strongly-correlated systems, and might provide key insight into the underlying mechanism that is responsible for the emergence of 2D unconventional superconductivity. In a second experiment, we performed transport experiments on versatile gate-defined planar junction devices made from MATBG. Our results show that using this device geometry, all-graphene Josephson junctions can be realized by electrostatic gating with configurable tunneling barrier type and strength. Furthermore, we find peculiar Fraunhofer pattern in a magnetic field that exemplifies the intrinsic low dimensionality of the superconducting phase. These results pioneer in novel superconducting devices based on twisted bilayer graphene and might be utilized in future magnetic field sensing applications.


9:12AM F67.00003: Engineering Correlation and Topology in Two-Dimensional Moire Superlattices [Invited] FENG WANG (Presenter), University of California, Berkeley and MSD, LBNL — Van der Waals heterostructures of atomically thin crystals offer an exciting new platform to design novel electronic and optical properties. In this talk, I will describe how to engineer correlated and topological physics using moire superlattice in two dimensional heterostructures. I will show that we can realize and control extremely rich condensed matter physics, ranging from correlated Mott insulator and superconductivity to ferromagnetism and topological Chern insulator, in a single device featuring the ABC trilayer graphene and boron nitride moire superlattices.
9:48AM F67.00004: Strong coupling phases of partially filled twisted bilayer graphene
narrow bands.* [Invited] OSKAR VAFEK (Presenter), Florida State Univ, JIAN KANG, Soochow University, Suzhou, China — States favored by Coulomb interactions projected onto the basis of the four narrow bands of the “magic angle” twisted bilayer graphene will be presented. Due to the unusual shape and symmetry of the Wannier orbitals [1], the resulting strong coupling problem is qualitatively different from the much studied (topologically) trivial narrow band i.e. a solid in an atomic limit. Instead, a dramatically new form of the interaction Hamiltonian is obtained [2]. It contains terms beyond the usual Hubbard term, leading to different strong coupling phases as in the atomic limit. Specifically, the usual anti-ferromagnetic super-exchange mechanism fails and turns ferromagnetic with an approximate spin-valley SU(4) symmetry.
Results of DMRG and variational trial state calculations will also be presented.


*NSF Grant No. DMR-1916958 and NSF Grant No. DMR-1157490

10:24AM F67.00005: Correlated insulating states and broken symmetries in magic angle
twisted bilayer graphene* [Invited] MING XIE (Presenter), University of Texas at Austin, PAWEL POTASZ, Wroclaw University of Technology, ALLAN MACDONALD, University of Texas at Austin — Magic angle twisted bilayer graphene exhibits insulating and superconducting behaviors when its low energy flat bands are partially filled[1]. Insulating states have been seen near all integer band filling factors, which strongly suggests that they are associated with states that break spin/valley flavor but not translational symmetries. I will first present our understanding of the nature of the insulating states[1] based partially on self-consistent Hartree-Fock (SCHF) calculations, which show that the insulating states can be understood qualitatively in terms of broken symmetries that gap the continuum model’s Dirac points as the twist angle is approached[2] from above and the Dirac velocities approach zero. Remote conduction and valence bands play an important quantitative role. Screening of Coulomb interactions due to the response of the metallic gates weakens Coulomb interactions, and can among other effects enlarge the stability region of superconducting states. Away from integer filling the bilayer system is metallic. I will argue on the basis of recent experiments that spin/valley flavor symmetries are often broken even in metallic and superconducting states and extend our SCHF calculations to metallic cases in an effort to shed light on electronic properties in the metallic regime. I will also discuss our recent effort using exact diagonalization method calculations based on a continuum-model defined low energy Hilbert space, which confirm some of the main results obtained using SCHF and point to some limitations. The exact diagonalization calculations suggest that Coulomb interaction alone are not enough to yield Cooper pairing, and that phonon induced effect attractive interactions have to be included in order to have a Cooper instability.


*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award# DE-SC0019481.
8:00AM F68.00001: Statistical Mechanics and Phase Transitions of Semiflexible Polymers*

[Invited] KURT BINDER (Presenter), Johannes-Gutenberg Univ — By large scale computer simulations theoretical concepts on semiflexible polymers are tested. When the chain stiffness varies, crossover scaling of the polymer radius occurs in bulk dilute solutions. For contour lengths $L$ exceeding the persistence length $l$, gaussian coils occur only in $d=3$ dimensions: in $d=2$ coil swelling due to excluded volume begins for $L > l$. The initial decay length of orientational correlations in $d=2$ is twice as large as in $d=3$; but adsorbed chains do not behave strictly two-dimensional, perpendicular excursions occur on a lateral scale of the deflection length, and a gradual crossover of the decay length of orientational correlations is found. The adsorption threshold scales with the minus $1/3$ power of $l$. In concentrated lyotropic solutions, nematic order occurs; the transition depends on both ratios $L/l$ and $D/l$ ($D =$ chain thickness). The effect of deflection length fluctuations on nematic order is elucidated, and the transition to smectic order is studied.

*Support by the Deutsche Forschungsgemeinschaft and the Alexander von Humboldt foundation is acknowledged.

8:36AM F68.00002: Cartilage-inspired superlubricious hydrogels*

[Invited] JACOB KLEIN (Presenter), Weizmann Institute of Science — The uniquely-efficient lubrication of articular cartilage up to high physiological pressures in the major joints (hips and knees) has been attributed to surface boundary layers of macromolecules complexed with phosphatidylcholine (PC) lipids, where the exposed highly hydrated phosphocholine groups massively reduce friction via the hydration lubrication mechanism. We have emulated nature by constructing hydrogels exposing similar PC-based boundary layers at their surfaces, and by incorporating such PC lipids in the hydrogel bulk we achieve self-maintaining lubricant layers which permanently reduce the friction and wear of the hydrogels by up to a 100-fold or more, down to the superlubrication level (coefficient of friction < 0.01) at contact stresses up to many MPa. Such hydrogels hold promise in a wide range of biomedical applications.

(I thank my co-workers on this study: Weifeng Lin, Monika Kluzek, Noa Iuster, Eyal Shimony, Nir Kampf and particularly Ronit Goldberg)

*We thank the European Research Council (ERC AdG Cartilube), the McCutchen Foundation, the Israel Science Foundation-National Science Foundation China (Grant 2577/17), the Israel Ministry of Science and Technology (Grant 713272) and the Weizmann-EPFL Collaboration Program funded by the Rothschild Caesarea Foundation, for support of this work., and Michael Urbakh for comments on the ms. The electron microscopy studies were conducted at the Irving and Cherna Moskowitz Center for Nano and Bio-Nano Imaging at the Weizmann Institute of Science.
9:12AM F68.00003: Some Thoughts On Polyelectrolyte Persistence Length [Invited]  PHILIP PINCUS (Presenter), University of California, Santa Barbara — Electrically charged, intrinsically flexible polymers in low ionic strength aqueous solutions are known to be stretched in order to reduce the Coulomb self-energy. As the solution ionic strength increases with added salt, Debye screening weakens the repulsion between distant parts of the chain and the polymer is envisioned as a semi-flexible chain with a persistence length that is governed by the Debye screening length. However for nearly fifty years, the dependence of this electrostatic persistence length on ionic strength has been controversial. This presentation will discuss recent experiments and theoretical thoughts that might contribute to unraveling this dilemma.

9:48AM F68.00004: Conformational properties and phase behavior of polymers in ionic liquids* [Invited]  ARUN YETHIRAJ (Presenter), University of Wisconsin - Madison — Ionic liquids have generated considerable excitement for their varied potential applications and their interesting physical properties. The viability of ionic liquids (ILs) in materials applications is limited by their lack of mechanical integrity, which may be provided by mixing them with a polymeric material. Recent experiments on polymers in ILs have unearthed a wealth of interesting phenomena that raise fundamental questions. This talk focuses on computational studies of PEO in imidazolium ILs. We develop a physically motivated first principles force field for PEO and [BMIM][BF_4]; this force field is in quantitative agreement with experiment with no adjustable parameters. Based on the same quantum calculations we develop a hierarchy of united atom models with decreasing resolution and increasing computational efficiency. Microsecond simulations are required to obtain converged properties of the polymer, which displays a combination of ring-like and extended conformations. The simulations show the existence of a lower critical solution temperature which arises from conformational restrictions on the polymer molecules at low temperatures.

*This work was supported by US Department of Energy, Basic Energy Sciences through grant DE-SC0017877.
In the first part, we compare two prominent types of transitions on bare substrates: One is the adsorption transition of a loop (a chain with two ends bound to an attractive substrate) driven by an attraction parameter $\varepsilon$, and the other is the loop-stretch transition in a chain with one end attached to a repulsive substrate, driven by an external end-force $F$ applied to the free end. Close to the transition points, both the static and the dynamic behavior of chains with different length are very well described by a scaling Ansatz with the scaling parameters $(\varepsilon-\varepsilon_c)N^{\phi}$ (adsorption transition) and $(F-F_c)N^{\nu}$ (loop-stretch transition), respectively, where $\phi$ is the crossover exponent of the adsorption transition, and $\nu$ the Flory exponent. Explicit crossover functions are based on an Ansatz for the analytical form of the order parameter distributions at the respective transition points. The transition between the adsorbed state and the stretched state is first order. Nevertheless, the characteristic relaxation time is found to grow according to a power law as the transition point is approached. We present a dynamic effective interface model which reproduces these observations an provides an excellent quantitative description of the simulation data.

In the second part, we discuss the adsorption transition of a single adsorption-active polymer embedded in a polymer brush. This transition is first order and can serve as a basis for the design of a polymer-based sensor or switch with sharp switching transition and fast response time. We discuss in particular the influence of polydispersity in the brush, and show how it can be used to tune the characteristics of the switch, i.e., the sharpness of the transition and the response time.

*DFG grant Schm 985/13, TRR 146 (Project C1)
8:00AM F70.00001: Enhanced deep water acoustic range estimation based on ocean General Circulation Models*  
PETER WEICHMAN (Presenter), BAE Systems — Improved acoustic range estimation supports ocean climate monitoring, ocean model improvement, and underwater navigation, and is limited by the availability of accurate models of ocean sound speed variability. I will describe efforts to test the limits of currently available GCM data to accurately estimate absolute range based on data collected during the PhilSea10 experiment using 510 km source-receiver separation. The methods compare observed acoustic records with synthetic records computed through the GCM ocean sound speed model. The most reliable ranging methods, emphasizing the most reproducible parts of the data records, are able to achieve 20 m or better accuracy. The principles underlying these methods are transportable and are expected to provide reliable range estimates in a broad range of deep-water settings. Generalization to ocean regions with stronger, less well characterized dynamics, is a major challenge, requiring new sources of data to constrain the models.

*The Philippine Sea experiments were supported by the Ocean Acoustics Program at the Office of Naval Research under APL-UW grants N00014-08-1-0843, N00014-08-1-0797, N00014-13-1-0009, N00014-15-1-2233 and N00014-18-1-2213, and Scripps Institution of Oceanography grant No. N00014-08-1-0840.

8:12AM F70.00002: Physics-based Inverse Design of Elastic Rods with Deep Neural Network  
LONGHUI QIN (Presenter), WEICHENG HUANG, MOHAMMAD KHALID JAWED, University of California, Los Angeles — Rod-like structures, such as DNA, climbing plants, and cables, pervade the nature and our daily life, which usually assume a deformed shape based on the competition between elastic (stretching, bending, twisting) and external (e.g. gravity) forces. We take a combination of physics-based and machine learning-driven approach to tackle the problem of obtaining the undeformed shape, given the deformed configuration under gravity. Conventional methods typically couple a numerical simulation of the elastic rods with optimization subroutines. We focus on rapidly solving the inverse problem in real-time using the Discrete Elastic Rods (DER) algorithm to simulate the forward problem and deep neural networks (DNNs) to store a large number of solutions. However, problems involving very long rods cannot be stored in DNNs due to the requirement of vast training dataset and insufficient precision in complex regression problems. We overcome this issue by decomposing a large rod into a series of smaller parts; the solution involving the smaller parts are stored in DNNs. Using the balance of forces and moments at the joints between two smaller parts, these smaller solutions are combined together to construct the larger solution.
Synthesizing arbitrary lattice models using a single degenerate cavity*
ZHENGWEI ZHOU (Presenter), SU WANG, XIANG-F A ZHOU, GUANG-CAN GUO, University of Science and Technology of China, HAN PU, Department of Physics and Astronomy, Rice University — We propose a general method to simulate arbitrary lattice models by manipulating optical synthetic dimension in a single degenerate main cavity. Such a cavity supports a large number of degenerate optical modes with different angular momenta. Couplings between different optical modes can be readily controlled. These features allow us to simulate lattice models that are not convenient to realize using other systems, particularly models in high dimensions and with complicated hopping amplitudes. As a concrete example, we demonstrate how to construct two topological lattice models: the two-dimensional Haldane model and a four-dimensional time-reversal invariant model. For the latter case, we show how topological properties can be detected from the outputs of the cavity, where the second Chern number can be extracted. In the presence of open boundaries, the chirality of the Weyl edge modes can also be detected using the input-output formalism of the cavity modes.

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The effect of mass fluctuations on Dirac materials sensors for dark matter*
BART OLSTHOORN (Presenter), ALEXANDER BALATSKY, NORDITA — Dirac materials with a non-zero mass term can form a small energy gap that is typically orders of magnitude smaller than accessible with semiconductors. This energy range provides the sensitivity to search for light (i.e. sub-MeV) dark matter while still blocking out the background noise. We study the effect of disorder through a discrete and continuous random mass-term, which both lead to tails (e.g. Lifshitz tails) in the density of states. The presence of disorder puts stringent constraints on the sensor material properties.

*Support from VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744), the European Research Council under the European Unions Seventh Framework ERS-2018-SYG 810451 HERO, and the Knut and Alice Wallenberg Foundation.
Magnetic proximity and nonreciprocal current switching in a monolayer WTe$_2$ helical edge

WENJIN ZHAO (Presenter), ZAIYAO FEI, TIANCHENG SONG, HAN KYOU CHOI, TAUNO A PALOMAKI, BOSONG SUN, PAUL MALINOWSKI, University of Washington, MICHAEL MCGUIRE, Oak Ridge National Lab, JIUN-HAW CHU, XIAODONG XU, DAVID COBDEN, University of Washington — The introduction of magnetic order into topological band structure gives rise to new phenomena such as proximity effect and nonreciprocal magnetoelectric effects. We couple the helical edges states in a 2D topological insulator, monolayer WTe$_2$, to a 2D layered antiferromagnet, CrI$_3$. We find that the edge conductance is sensitive to the magnetization state of the CrI$_3$, and the coupling can be understood in terms of an exchange field from the nearest and next-nearest CrI$_3$ layers that produces a gap in the helical edge state. We also find that the nonlinear edge conductance depends on the magnetization of the nearest CrI$_3$ layer relative to the current direction. At low temperatures this produces an extraordinarily large nonreciprocal current that is switched by changing the antiferromagnetic state of the CrI$_3$.

Far-field thermal radiation at the optical topological transition

SANJAY DEBNATH (Presenter), EVGENII NARIMANOV, Purdue Univ — We develop theoretical description of far-field thermal emission near optical topological transitions (OTTs). OTTs originate from a transformation in the topology of the phase space in the medium which results in drastic changes in the photonic density of states. In this work, we show that the unique evolution of this transition leads to a characteristic signature in the far-zone thermal emission. In particular, we find (APL 115, 151906 (2019)) a strong asymmetric pattern of reduced emission near the transition from type-I hyperbolic to dielectric responses present in both naturally available and composite media. The existence of the asymmetric feature should be experimentally observable and can be used as a tool to detect the OTT between type-I hyperbolic and dielectric electromagnetic responses.

*We acknowledge the National Science Foundation(1629276-DMR), and Gordon and Betty Moore Foundation.
9:12AM F70.00007: A bizarre state of confined He-3* VALERIY DOLMATOV (Presenter), Univ of North Alabama — Atoms under various types of external confinements have been scrutinized by theorists for many years now. Here, we focus on a He-3 atom whose 1s^2 shell is known to undergo a tiny hyperfine spin-splitting: 1s^2 → 1s↑1s↓. We treat the spin-split He-3 within the known spin-polarized Hartree-Fock approximation which we modify by the incorporation of a spin-dependent adjustable parameter to model the hyperfine splitting. We place He-3 inside a spherical potential box of a height U_0, width Δ (U_0 = 5 Ry, Δ = 5 a.u., as a case study), and an adjustable inner radius R_0. The resultant atomic potential becomes a double-well potential with the inner and outer wells being separated by about 5 a.u. We model the pressure on He-3 by narrowing the inner radius R_0. We find that, at R_0 ≤ 0.85 a.u., the 1s↓-electron migrates into an outer well. The 1s↑-electron remains in the inner well as long as R_0 > 0.4 a.u. We, thus, unravel a possibility of creating a bizarre state of He-3 with the much different orbital radii and energies of the 1s↑- and 1s↓ electrons. At R_0's ≤ 0.4 a.u. both electrons reside in the outer well, far away from the nucleus, and He-3 turns into a novel type of a low-n (n = 1) and low-l (l = 0) "Rydberg" atom.

*A travel grant from the CAS Research Committee at UNA is acknowledged.

9:24AM F70.00008: Benchmark calculations of the doublet S-states of the singly charged carbon ion* SERGIY BUBIN (Presenter), ISTVAN HORNЯYAK, Nazarbayev University, LUDWIK ADAMOWICZ, University of Arizona — We report accurate variational calculations of the five lowest doublet S-states of the C^+ ion. The wave functions of the six-particle system (five electrons and nucleus) have been expanded in terms of 16000 all-particle explicitly correlated Gaussians whose nonlinear variational parameters were subject to extensive optimization. The motion of the finite-mass nucleus has been explicitly included in the Hamiltonian, while relativistic corrections to the energy levels have been computed in the framework of the perturbation theory. Lowest-order quantum electrodynamics (QED) corrections have also been estimated. The results obtained for the energy levels have enabled the determination of transition frequencies with sub-wavenumber accuracy.

*This work has been supported by the Ministry of Education and Science of Kazakhstan (grant No. BR05236454), Nazarbayev University (faculty development grant No. 090118FD5345), and the National Science Foundation (grant No. 1856702).
Compact tunable plasma muon accelerator for ultrashort micron-scale muon pair beams

AAKASH SAHAI (Presenter), University of Colorado, Denver, VLADIMIR D SHILTSEV, Accelerator Research, Fermilab, TOSHIKI TAJIMA, Physics, University of California, Irvine — Experimentally accessible schemes of compact plasma muon acceleration are introduced and modeled using a novel technique of controlled post-processing of cascade showers. These schemes use propagating structures in plasma, driven as wakefields of femtosecond-scale high-intensity laser or dense particle beams, to capture muons of a divergent cascade shower of: (a) hadronic type from proton-nucleon or photo-production reactions or, (b) electromagnetic type. Apart from the direct trapping and acceleration of particles of a raw shower in a plasma wakefield, a conditioning stage is proposed to selectively focus only one of the charge states. Not only is the high gradient of plasma acceleration structures well suited for rapid acceleration to extend the lifetime of short-lived muons but their inherent spatiotemporal scales also make possible production of unprecedented ultrashort, micron-scale muon beams. Compact muon acceleration schemes hold the promise to open up new avenues for applications.

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Reinforcement Learning and the Cost of Observation

RORY COLES (Presenter), University of Ontario Institute of Technology, COLIN BELLINGER, ISAAC TAMBLYN, National Research Council of Canada — Reinforcement learning has recently been used for practical application in both physics and chemistry laboratories. When conducting experiments in these environments, measurements can often be expensive, either due to the resources used or the time that is taken. Due to this, measurements are typically taken intermittently or when exploring new conditions. If we were to use reinforcement learning to optimise a laboratory experiment, it would ideally act in a similar manner. Therefore, it would need to act without perfect information and balance the cost of observation with the need for new data.

In this work, we show how an agent can build an internal hypothesis of its environment, using experience from past measurements, that it can then act on. The measurements it will obtain come from various sensors that each have an associated cost. The informativeness will vary given the current state, so the agent needs to determine the most valuable information to sample. We also demonstrate how the agent's behaviour changes when certain measurements are limited by cost.

* We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC).
A modified reference approach implemented in Python (MRAIP) to obtain CO\textsubscript{2} emissions in any region\textsuperscript{*}  
HYCIENTH ABOH (Presenter), Department of Physics, Nigerian Army University, Biu, Nigeria, GODFREY EJIROGHENE AKPOJOTOR, MERRIOUS OFOMOLA, Department of Physics, Delta State University, Abraka — There is a general consensus that good quality estimates of CO\textsubscript{2} emissions from fuel combustion are essential for the construction of inventories since they have direct link between fuel use and emission which is key to strategizing how to reduce these emissions. In the study here, we develop a modified reference approach implemented in Python (MRAIP) to obtain the CO\textsubscript{2} emissions in any location such as a country, region, state or town once its apparent consumptions can be determined. The simplicity of the MRAIP is that it can be used to estimate the amount of CO\textsubscript{2} that is emitted in n-litres of fuel combustion with limited additional effort and data requirements. Therefore, it can be used to obtain both small and large scale inventories even with QPython in Android smartphones. The MRAIP was demonstrated to obtain both states and national CO\textsubscript{2} emission inventories in Nigeria from 2000 to 2019. Further, we discuss simple ways to include other major CO\textsubscript{2} emitters which varies from one location to another such as coal/peat, natural gas, deforestation, cement, and even the minor petroleum products as well as bunker fuel which are not included in the MRAIP.

\textsuperscript{*}We appreciate the authorities of the Nigeria National Petroleum Corporation for the availability of the data used in this study.

**Tuesday, March 3, 2020 10:00 AM - 5:00 PM**

**Session F71 APS: Graduate School Fair 2020 II** Exhibit Hall C/D - Tag(s): Careers, Education, Undergrad Friendly

10:00AM F71.00001: Graduate School Fair 2020 — Graduate schools are invited to distribute literature and meet with students about their graduate programs. Each participating school will receive a small table with signage in the undergraduate student lounge. Both powered and unpowered options are available.

**Tuesday, March 3, 2020 11:15 AM - 2:15 PM**

**Session G01 DAMOP DCMP: Topological States in AMO Systems I** 103 - Zhexuan Gong - Tag(s): Focus
Disorder and topology have many deep connections, and can have a rich combined influence on the transport properties of quantum particles. Some of the most useful and intriguing properties of topological systems relate to the robustness of their edge states with respect to weak disorder. Rich phenomena are expected to occur as strong disorder is added to such systems, relating to the global unwinding of the non-local topological order. Surprisingly, it has even been predicted that the addition of disorder can induce topological order in otherwise topologically trivial materials. Despite these deep and rich connections, the difficulty of creating controlled disorder in real materials has prevented the exploration of disorder-driven changes in topology in experiments. Here we describe how a type of synthetic lattice can be engineered for dilute atomic gases at ultracold temperatures, allowing us to mimic the physics of disordered topological materials. We describe two types of topological transitions driven by the addition of disorder to one-dimensional atomic wires. The first is the breakdown of a nontrivial band topology by the addition of strong disorder, relating to a random-singlet topological transition. The second is a counter-intuitive "order by disorder" transition in which nontrivial topology arises due to disorder, relating to the observation of the topological Anderson insulator phase predicted nearly a decade ago. We discuss extensions to this result, including prospects for exploring disordered topological materials in higher dimensions.

In collaboration with Eric J. Meier - University of Illinois at Urbana; Fangzhao Alex An - University of Illinois at Urbana; Alexandre Dauphin - Barcelona Institute of Science and Technology, Complesso Universitario di Monte Sant'Angelo; Pietro Massignan - Barcelona Institute of Science and Technology, Universitat Politècnica de Catalunya; Taylor L. Hughes - University of Illinois at Urbana.
Recent experiments have placed cold atoms into optical lattices in the presence of synthetic fields. This talk will review studies of Hubbard-Hofstadter models in regimes revealing topological phases of ultracold fermions arising from the interplay of inter-particle interactions and synthetic fields in kagome and square optical lattices. Focusing on one regime in particular, attractive interactions in a square optical lattice, we find that attractive s-wave interactions lead to a higher-order topological superfluid [1]. Higher-order topological superconductors hosting Majorana-Kramers pairs as corner modes have recently been proposed in solids. Here, we show that such Majorana-Kramers pairs can be realized using a conventional s-wave superfluid in an optical lattice but with a soliton. The Majorana-Kramers pairs emerge at the “corners” defined by the intersections of line solitons and the one-dimensional edges of the system. Our scheme sets the stage for observing possible higher-order topological superfluidity with conventional s-wave superfluids of cold atoms.


*We acknowledge support from ARO (W911NF-16-1-0182, W911NF-17-1-0128), NSF (DMR-1414683), and AFOSR (FA9550-18-1-0505, FA9550-16-1-0387).

12:03PM G01.00003: Topological Phase Transitions in Finite-size Systems Across Boundary Conditions*  

Systems driven unitarily across different topological phases seem to exhibit contrary behaviors depending on their boundary conditions [1] and the commensurability of system sizes [2]. In particular, a “no-go” theorem forbidding the change of the Chern number exists for periodic boundary systems. Here we first demonstrate the scaling of dynamical phase transition points in driven periodic boundary systems for different turn-on speeds and incommensurate system sizes, which consist of a Landau-Zener governed regime and an adiabatic following regime. Similar regimes are also identified in the case of open boundary systems, proving that these boundary conditions agree in the thermodynamic limit. Finally, we show that with slow turn-ons the dc Hall response of a driven fermi sea starting from a trivial state does acquire a non-trivial value in a finite-size system, even when the “no-go” theorem applies.


*The computations were done at the Institute for CyberScience at Penn State.
**12:15PM G01.00004: Tenfold way for quadratic Lindbladians**

SIMON LIEU (Presenter), MAX MCGINLEY, NIGEL COOPER, University of Cambridge — We uncover a topological classification applicable to open fermionic systems governed by a general class of Lindblad master equations. These ‘quadratic Lindbladians’ can be captured by a non-Hermitian single-particle matrix which describes internal dynamics as well as system-environment coupling. We show that this matrix must belong to one of ten non-Hermitian Bernard-LeClair symmetry classes which reduce to the Altland-Zirnbauer classes in the closed limit. The Lindblad spectrum admits a topological classification, which we show results in gapless edge excitations with finite lifetimes. Unlike previous studies of purely Hamiltonian or purely dissipative evolution, these topological edge modes are unconnected to the form of the steady state. We provide one-dimensional examples where the addition of dissipators can either preserve or destroy the closed classification of a model, highlighting the sensitivity of topological properties to details of the system-environment coupling.

*This work was supported by the EPSRC and by a Simons Investigator Award.

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**12:27PM G01.00005: Lattice gauge theories and string dynamics in Rydberg atom quantum simulators**

FEDERICA MARIA SURACE (Presenter), PAOLO PIETRO MAZZA, GIULIANO GIUDICI, ALESSIO LEROSE, ANDREA GAMBASSI, SISSA, MARCELLO DALMONTE, ICTP — Lattice gauge theories are at the basis of our understanding of fundamental interactions and quantum simulations are one of the most promising paths to go beyond the exponential complexity of this quantum many body problem. We show that Rydberg atom setups represent an ideal platform for the investigation of equilibrium and non-equilibrium properties of lattice gauge theories, by proving their equivalence to abelian (and possibly non abelian) gauge theories on the lattice. Building on this correspondence, we show that the recently observed anomalously slow dynamics corresponds to a string-inversion mechanism, reminiscent of the string-breaking typically observed in gauge theories.

*This work is partly supported by the ERC under grant number758329 (AGEnTh), and has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 817482.

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**12:39PM G01.00006: Exact quantum many-body scar states intrinsic to periodically driven system in the Rydberg-blockaded atom chain**

SHO SUGIURA (Presenter), Harvard University, TOMOTAKA KUWAHARA, RIKEN, KEIJI SAITO, Keio University — In a periodically driven many-body system, any quantum state usually ends up an infinite temperature state. This is called the Floquet energy eigenstate thermalization hypothesis (Floquet ETH). Here we discuss the violation of the Floquet ETH with realistic Hamiltonians. Our periodically driven model is based on the PXP type interaction, which is demonstrated in a recent experiment in the Rydberg atoms chain by Harvard group. By showing explicit expressions of the wave functions, we exactly prove the existence of the many-body scar states, which show non-thermal behavior, while other states obey the Floquet ETH. In addition, we systematically engineer various periodically-driven Hamiltonians having Floquet many-body scar states.
12:51PM G01.00007: Exact quantum many-body scar states in the two-dimensional PXP model and their dynamical signatures  CHENG-JU LIN (Presenter), Perimeter Inst for Theo Phys, VLADIMIR CALVERA, Physics, Stanford University, TIMOTHY HSIEH, Perimeter Inst for Theo Phys — The two-dimensional PXP model is an effective model describing the dynamics of a two-dimensional Rydberg atom array in the nearest-neighbor blockade regime. We discover exponentially many exact quantum many-body scar states in the two-dimensional PXP model. These exact scar states have valence bond solid order, therefore breaking the lattice translation symmetry, despite being at effectively infinite temperature. As a manifestation of these scar states, we propose a quench experiment starting from a charge-density-wave initial state, resulting in strong oscillations in the total Rydberg-excitation number. Another signature is long-lived valence bond solid order of the scar states after a quench into a weakly perturbed model.

1:03PM G01.00008: Fragmented Hilbert Spaces and Slow Dynamics in Quantum Dimer Models*  JOHANNES FELDMEIER (Presenter), FRANK POLLMANN, MICHAEL KNAP, Tech Univ Muenchen — The presence of dynamical constraints can have severe impacts on the non-equilibrium dynamics of closed quantum systems, leading to slow or even non-ergodic behavior at finite energy densities. One mechanism for the occurrence of such features is a fragmentation of the Hilbert space structure in systems of fractons, consisting of particles with reduced mobility [1]. Within this context, we investigate the connectivity of configuration spaces resulting from the hard core constraint in close-packed dimer models. On the square lattice, we uncover the emergence of effectively immobile defects within a staggered background, whose dynamics is impeded up to high orders in perturbation theory. This fracton-like structure of the low energy Hilbert space is shown to give rise to glassy behavior for states at low temperatures [2]. We further discuss extensions to different lattices and dimensions that allow for the explicit construction of large sets of conserved quantities, leading to slow dynamics and localized modes for typical states also at high energies.


*We acknowledge support from the DFG grant No. KN 1254/1-1 and DFG TRR80 (Project F8).
**1:15PM G01.00009: Thermalization and its Breakdown for a Large Nonlinear Spin**

SHANE KELLY (Presenter), Los Alamos National Laboratory, SHAN-WEN TSAI, Physics and Astronomy, University of California Riverside, EDDY M.E. TIMMERMANS, Los Alamos National Laboratory — By developing a semi-classical analysis based on the Eigenstate Thermalization Hypothesis, we determine the long time behavior of a large spin evolving with a nonlinear Hamiltonian. Despite integrable classical dynamics, we find the Eigenstate Thermalization Hypothesis is satisfied in the majority of eigenstates and thermalization is generic. The exception is a novel mechanism for the breakdown of thermalization based on an unstable fixed point in the classical dynamics. Using the semi-classical analysis we derive how the equilibrium values of observables encode properties of the initial state. We conclude with a discussion of relevant experiments and the potential generality of this mechanism for the breakdown of thermalization.

Arxiv 1910.03138

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**1:27PM G01.00010: CPT invariant topological phase in non-Hermitian spin-1/2 quantum systems**

TANMOY DAS (Presenter), Indian Institute of Science, ANANYA GHATAK, Institute of Physics, University of Amsterdam — Non-Hermitian system has recently found its place in laboratories, raising the hope to obtain unconventional and uncharted physical properties. Over the last two to three years, we have made several contributions to time-dependent theory for parity (P), time-reversal (T) invariant non-Hermitian Hamiltonians; delineating its conservation laws, CPT gauge invariance, and new term in the Berry phase. I will talk about a realizable spinful non-Hermitian system exhibiting the non-Abelian Berry phase and supersymmetric edge states.

Ananya Ghatak, Tanmoy Das. arXiv:1907.07333
1:39PM G01.00011: Topological insulator-superconductor phase transition in a non-Hermitian spin chain  
YUNMEI LI (Presenter), XIWANG LUO, JUNPENG HOU, CHUANWEI ZHANG, University of Texas at Dallas — Non-Hermitian systems can host nontrivial topological phases with the topological characterization distinct from Hermitian systems. Here we consider a 1D XY spin model with non-Hermitian out-of-plane magnetic field, which is periodically modulated. For isotropic XY interaction, the system corresponds to a topological insulator (TI) with pseudo-anti-Hermiticity, which supports edge states characterized by the quantized Zak phase. The anisotropy of XY interaction gives rise to superconducting pairing, and the system experiences a transition from TI to topological superconducting (TSC) as the anisotropy increases. The transition point, where the system undergoes a band touch at E=0, can be tuned by the modulation phases and amplitudes of the non-Hermitian field. The TSC phase supports Majorana edge modes, protected by the chiral symmetry. The model can be experimentally simulated with trapped ions. Our work provides a method to investigate the interplay between non-Hermiticity and superconducting interaction and paves the way for exploring various topological insulators and superconductors in non-Hermitian systems.

1:51PM G01.00012: Non-adiabatic topological energy pumps with three incommensurate frequencies  
RONGCHUN GE (Presenter), University of Texas at Dallas, FREDERIK NATHAN, Niels Bohr Institute, TAKAHIRO MORIMOTO, University of Tokyo, SNIR GAZIT, The Hebrew university of Jerusalem, MARK RUDNER, Niels Bohr Institute, MICHAEL KOLODRUBETZ, University of Texas at Dallas — Recent developments have shown topological energy pumping in quantum systems driven with either one or two incommensurate frequencies near their adiabatic limit. In this talk, we generalize such multichromatic Floquet techniques to study the topological properties of one-dimensional systems driven by two non-adiabatic drives and two-level systems driven by three incommensurate drives. We find a well-quantized, topologically non-trivial plateau, given by the topology of the micromotion. As the ratios among the frequencies is increased, the photonic modes become delocalized before a topological transition is reached. At fixed ratio of the frequencies, changing the magnitude of the frequencies gives transitions from topologically trivial to non-trivial and back to trivial again in the large frequency limit. We will also discuss plausible experimental possibilities to observe these novel topological effects.
2:03PM G01.00013: Quadrupole Topological Photonic Crystals* LI HE (Presenter), ZACHARIAH M ADDISON, EUGENE JOHN MELE, BO ZHEN, University of Pennsylvania — Quadrupole topological phases, exhibiting protected boundary states that are themselves topological insulators of lower dimensions, have recently been of great interest. Extensions of these ideas from current tight binding models to continuum theories for realistic materials require the identification of quantized invariants describing the bulk quadrupole order. Here we identify the analog of quadrupole order in Maxwell’s equations for a photonic crystal (PhC). Unlike prior studies relying on threaded flux, our quadrupole moment is quantized purely by crystalline symmetries. Furthermore, through the bulk-edge correspondence of Wannier bands, we reveal the boundary manifestations of nontrivial quadrupole phases as quantized polarizations at edges and bound states at corners. Finally, we relate the nontrivial corner states to the emergent phenomena of quantized fractional corner charges and a filling anomaly.

*This work was partly supported by the NSF through the University of Pennsylvania MRSEC DMR-1720530 and grant DMR-1838412. L.H. was supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0133. B.Z. was supported by the Army Research Office under award contract W911NF-19-1- 0087.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G02 DAMOP: Hybrid AMO/condensed matter quantum systems 105

11:15AM G02.00001: Controlling the motion of levitated particles by coherent scattering ONDREJ CERNOTIK (Presenter), RADIM FILIP, Palacky Univ — Levitated particles are a promising platform for cavity optomechanics owing to lack of clamping losses allowing, in principle, generation of nonclassical mechanical states and high-precision sensing of external forces. One important tool for controlling the particle motion, which has remained largely unexplored, is the trapping field itself. Recently, a crucial step in understanding its capabilities has been made by using coherent scattering of tweezer photons into a cavity mode to cool the motion of a levitated particle. Here, we build on these results and show that coherent scattering, accompanied by amplitude modulation of the trapping beam, can be used for more general control of particle motion. We show how this mechanism (leading to modulation of the mechanical potential, which is impossible with clamped mechanical resonators) can be used to generate strong mechanical one- and two-mode squeezing both in the transient and steady-state regimes. We also discuss how to use these techniques for efficient readout of the mechanical motion similar, in spirit, to two-tone, backaction-evading readout. With straightforward extensions of our ideas to all three motional modes of levitated particles, our results pave the way to full quantum control of particle motion.
11:27AM G02.00002: Dynamical multistability in a quantum-dot laser* MATTIA MANTOVANI (Presenter), Universität Konstanz, ANDREW D. ARMOUR, University of Nottingham, WOLFGANG BELZIG, GIANLUCA RASTELLI, Universität Konstanz — Quantum dots coupled to microwave cavities or nanomechanical resonators allow to investigate novel regimes of electron-phonon and electron-photon interactions, because of their highly tailorable properties. Here, we consider a hybrid implementation of a single-atom laser [1], where a quantum dot with two spin-split levels is coupled to a harmonic resonator and is embedded between two ferromagnetic contacts with opposite polarization. A spin-polarized current driven through the dot brings the resonator in a highly-excited lasing state. We show that the high efficiency of this pumping mechanism breaks the rotating-wave approximation (RWA) usually employed for the laser, without any need of ultrastrong spin-resonator coupling. Remarkably, the oscillator displays a rich multistable regime characterized by a multi-peaked Fock distribution. Multistability can be detected by monitoring the current in time, as it switches between distinct current levels corresponding to different states of oscillation [2].


*Work supported by German Excellence Initiative through Zukunftskolleg and Deutsche Forschungsgemeinschaft through SFB 767.

11:39AM G02.00003: Quantum state preparation for coupled period tripling oscillators* NIELS LOERCH (Presenter), University of Basel, YAXING ZHANG, Yale University, CHRISTOPH BRUDER, University of Basel, MARK DYKMAN, Michigan State University — We investigate the quantum transition to a correlated state of coupled oscillators in the regime where they display period tripling in response to a drive at triple the eigenfrequency. Correlations are formed between the discrete oscillation phases of individual oscillators. The evolution toward the ordered state is accompanied by the transient breaking of the symmetry between seemingly equivalent configurations. We attribute this to the nontrivial geometric phase that characterizes period tripling. We also show that the Wigner distribution of a single damped quantum oscillator can display a minimum at the classically stable zero-amplitude state.

*CB and NL acknowledge financial support by the Swiss SNSF and the NCCR Quantum Science and Technology. MID's research was supported in part by the National Science Foundation (Grant No. DMR-1806473) and the Moore Scholarship from Cal- tech. Y.Z. was supported by the National Science Foundation (DMR-1609326).
11:51AM G02.00004: Steering sound with light*  
TIRTH SHAH (Presenter), Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, HENGJING REN, Applied Physics and Material Science, Caltech, CHRISTIAN BRENDEL, Max Planck Institute for the Science of Light, HANNES PFEIFER, Institute For Applied Physics, University of Bonn, VITTORIO PIANO, Max Planck Institute for the Science of Light, OSKAR PAINTER, Applied Physics and Material Science, Caltech, FLORIAN MARQUARDT, Max Planck Institute for the Science of Light — Phononic circuits have been emerging as a growing field of research for applications in optical signal processing, sensing and emerging quantum technologies. We describe the design of a micron-scale on-chip patterned silicon device supporting i) helical transport of phonons along the interface of two topologically distinct domains, ii) photonic crystal optical cavities as a means of excitation and read-out of these mechanical vibrations via optomechanical parametric coupling. Our unique design can be characterized as a multi-scale optomechanical crystal, and we will describe possibilities to test its operation in experimental devices.

*Tirth Shah acknowledges support from the European Union’s Horizon 2020 Programme for Research and Innovation under grant agreement No. 722923 (Marie Curie ETN - OMT).

12:03PM G02.00005: Efficient photon excitation readout for individual erbium ions in silicon  
GUANGCHONG HU (Presenter), GABRIELE DE BOO, CHUNMING YIN, CQC2T, School of Physics, UNSW, MATTHEW J. SELLARS, CQC2T, RSPE, Australian National University, SVEN ROGGE, CQC2T, School of Physics, UNSW — Here we would report the charge detection mechanism of a single erbium ion in a silicon transistor by pulsed light. Erbium atoms were implanted in a silicon transistor and then the device was cooled down to 4K[1]. In the continuous wavelength scan, we saw a binary signal when the erbium ion was on resonance. Based on this feature, instead of using continuous wavelength scan, we utilised Dark-OnRes-Dark-Reset pulse sequences to excite the erbium ion. We found a 30MHz wide line width while the line width was 120MHz via continuous wavelength scan. We would also give a upper bound for the optical lifetime of 13/2 excited state, which is around 20us, limited by the bandwidth of our setup.

12:15PM G02.00006: Study of Erbium-doped yttrium orthovanadate crystal for the microwave to optical transduction* TIAN XIE (Presenter), JAKE ROCHMAN, JOHN G BARTHOLOMEW, ANDREI RUSKUC, JONATHAN KINDEM, IOANA CRAICIU, ANDREI FARAON, Caltech — Quantum transduction between the microwave and optical domain is essential for connecting superconducting quantum platforms in a quantum network. Ensembles of rare-earth ions (REIs) coupled to both optical and microwave cavities offer a promising architecture for achieving this conversion because of their collective and coherent properties in the microwave and optical domains. The critical properties of the REI ensemble needed for high transduction efficiency are the optical and microwave transition dipole moments and the optical and spin inhomogeneities. Erbium ions are of particular interest because they have transitions at telecom wavelengths which allows for the compatibility with optical fiber telecommunication networks. Here, we report the bulk properties of Erbium-doped yttrium orthovanadate (Er:YVO) including the Zeeman splitting, optical absorption spectra, oscillator strength, and spin inhomogeneity. We also demonstrate proof of concept microwave to optical conversion with a loop gap microwave resonator. The measured strong dipole moment and narrow inhomogeneities point to the Er:YVO as a promising material for quantum transduction.

*The authors acknowledge support from the ONR Young Investigator Award and ARO/LPS CQTS.

12:27PM G02.00007: INAS QUANTUM DOTS AND SURFACE ACOUSTIC WAVE CAVITIES FOR QUANTUM TRANSDUCTION TRAVIS AUTRY (Presenter), SAMUEL BERWEGER, National Institute of Standards and Technology Boulder, LUCAS R SLETTEN, JILA, University of Colorado, RICHARD MIRIN, PAVEL KABOS, National Institute of Standards and Technology Boulder, KONRAD LEHNERT, JILA, University of Colorado, KEVIN SILVERMAN, National Institute of Standards and Technology Boulder — Quantum information technology based on superconducting microwave technology is progressing rapidly and is now widely adopted by large corporations and small startup firms. These components operate at ~20mK temperatures. An emerging problem is the transfer of quantum information out of and into the cryostat. Recently, hybrid quantum devices involving SAW cavities and superconducting qubits have been successfully integrated [1]. We present progress on a new type of transducer involving an InAs quantum dot and coupled to surface acoustic wave cavity (SAWc). In a SAWc, phonons will parametrically modify the resonance frequency of a QD via strain [2]. In this work, we demonstrate progress in developing state-of-the-art, stable SAWc operating at ~ 3.4GHz. We demonstrate a reduction in the SAWc mode volume by using focusing SAW mirrors. These devices are characterized using near-field microwave measurements of SAWc cavity-modes demonstrating high-quality focusing phononic wavefronts. Finally, we discuss reducing bulk scattering, theoretical coupling rates and discuss efficient photon extraction.

References
Tunable Microwave Resonators Composed of Stoichiometric Titanium Nitride and Multilayer Titanium Nitride/Titanium

**DAVID S WISBEY, JACOB BREWSTER** (Presenter), Saint Louis University, **MICHAEL R. VISSERS, JIANSONG GAO**, National Institute of Standards and Technology Boulder — Low-temperature high-Q frequency tunable microwave resonators were fabricated and measured. Two different types of material were fabricated and tested: Titanium nitride/titanium (TiN/Ti) multilayers and stoichiometric titanium nitride (sTiN). The multilayer resonators had a tunable resonant frequency and still maintained a high internal quality factor at temperatures around 50 mK. Multilayer TiN/Ti resonators had a $T_c$ of 1.5K and sTiN resonators had a $T_c$ of 4.5K. Biasing was accomplished using lithographically etched lines and an external power supply. The frequency tunability, as before [1], was achieved by injecting a DC through a current-directing circuit into the nonlinear inductor whose kinetic inductance is current dependent. We were able to achieve a frequency tunability of up to 20MHz, or .5 % fractional frequency shift, while maintaining a base temperature of less than 50 mK, without measurable heating of the device. Different lengths and widths of bias lines were compared to determine the effect on the microwave resonators. We were able to achieve an internal quality factor of $Q_i > 250,000$ for certain designs.


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Potential applications of solid-state laser cooling in silica glass

**ESMAEIL MOBINI** (Presenter), **MOSTAFA PEYSOKHAN, ARASH MAFI**, University of New Mexico — Solid-state laser cooling (SSLC) can remove heat from materials via anti-Stokes fluorescence cooling. Since the first observation of SSLC in ZBLAN glass in 1995 by R. Epstein et al., a variety of materials have been successfully cooled. Among the materials, Yb-doped crystals have gained more attention than others due to their higher ion solubility that could lead to high cooling efficiency. However, over the past two decades, the laser cooling of silica glass as the most widely used optical material has been void of success. This lack of success has led many to question the possibility of SSLC in silica. Recently, we have observed the SSLC in Yb-doped silica glass that potentially opens up new applications from radiation-balancing in fiber amplifiers to spot-cooling in silicon photonics. Here, we first investigate all the parameters that govern the SSLC in the materials and will show that SSLC in pure silica glass is achievable, and second, revisit some of our results on the SSLC of Yb-doped silica. Finally, we investigate the minimum temperature that an ultra-pure Yb-doped silica glass can achieve.


*AFOSR MURI: FA9550-16-1-0362
1:03PM G02.00010: Strain activated hBN color centers in photonic and plasmonic systems*

NICHOLAS PROSCIA (Presenter), ROBERT COLLISON, CARLOS MERILES, VINOD M MENON, The City College of New York — A photonic-chip-based source of quantum light is highly desirable for long range quantum commutation. One promising material system for this is the Van der Waals material hexagonal Boron Nitride (hBN) which hosts room temperature single photon emitters in its bulk and 2d limit. The ultra-thin nature of hBN allows for the ability to conform and integrate with other material systems and offers a way to control its the electronic and optical properties through strain and electro-magnetic nearfields. Here we demonstrate a deterministic coupling method by activation of such emitters via strain applied by mechanical bending at precise locations. We use the topography of the photonic element structure to induce the bending and strain engineer heightened defect emission within the field mode of two micro and nano-photonic elements, e.g. Si$_3$N$_4$ microdisk (MD) cavities and surface lattice resonances (SLRs) of plasmonic Ag pillar array. We subsequently show coupling of the hBN defect emission to these cavity structure and find this method to be a promising step towards more accessible quantum states of light for study in on-chip devices.

*The NSF CREST IDEALS center, NSF MRSEC program (DMR-1420634) and the NSF EFRI 2-DARE program (EFMA -1542863), CUNY ASRC NanoFabrication Facility.

1:15PM G02.00011: Absolute quantum efficiency measurement of single photon emitters in hexagonal Boron Nitride

NIKO NIKOLAY (Presenter), Department of Physics, Humboldt University of Berlin, NOAH MENDELSOHN, School of Mathematical and Physical Sciences, University of Technology Sydney, ERSAN ÖZELCI, BERND SONTHEIMER, FLORIAN BÖHM, GÜNTER KEWES, Department of Physics, Humboldt University of Berlin, MILOS TOTH, IGOR AHARONOVICH, School of Mathematical and Physical Sciences, University of Technology Sydney, OLIVER BENSON, Department of Physics, Humboldt University of Berlin — Single photon emitters in two-dimensional hexagonal boron nitride (hBN) have been intensively studied for several years, since their outstanding properties could qualify this material system as promising candidates for future sources of quantum states of light [1]. However, the atomic origin and some important basic properties of these defects are yet unknown. One of them is the quantum efficiency (QE) with respect to the ratio of radiative and non-radiative rate. We have performed an absolute measurement using the Drexhage method, which is free of incomplete excitation saturation, indirect excitation paths and the detection efficiency of the setup. Instead, it relies on lifetime measurements alongside a controlled change in local density of states achieved by a precise mirror placement using an atomic force microscope. In this contribution, we will report on the mentioned method, the experimental results on two emitter families with different QEs (with the highest QE found approaching 87(7) %) [2], the discovery of part of the underlying level system, specifically the absolute de-excitation rates, and the effects on the expected maximum photon count rate.

1:27PM G02.00012: Quantum Correlations in the Stokes-anti-Stokes Raman Scattering: Photonic Cooper Pairs*  
FILOMENO AGUIAR JÚNIOR (Presenter), Physics, Federal University of Minas Gerais (MG) - Brazil - UFMG, ANDRE L SARAIVA, MARCELO FRANÇA SANTOS, BELITA KOILLER, Physics, Federal University of Rio de Janeiro (RJ) - Brazil - UFRJ, REINALDO DE MELO E SOUZA, Physics, Federal University Fluminense (RJ) - Brazil - UFF, ARTHUR PATROCÍNIO PEN, Physics, Federal University of Minas Gerais (MG) - Brazil - UFMG, RAINA ARMOND DA SILVA, Physics, Federal University of Uberlândia (MG) - Brazil - UFU, CARLOS HENRIQUE MONKEN, ADO JORIO, Physics, Federal University of Minas Gerais (MG) - Brazil - UFMG — The production of correlated Stokes (S) and anti-Stokes (aS) photons (SaS process) mediated by real phonon is well known in the literature. However, in recent work we demonstrated that Photons can interact with each other in condensed matter through the same mechanism that forms Cooper pairs in superconductors—the exchange of virtual phonons [Phys. Rev. Lett. 119, 193603 (2017)]. We investigate the energy, momentum and production rate of correlated Stokes–anti-Stokes (SaS) photons in diamond and we show the rate of correlated SaS production depends on the energy shifts of the pair, which in the BCS theory determines whether there should be an attractive or repulsive interaction. With this view, we only observe correlated SaS in the case of attractive interactions [PRB 99, 100503 (2019)]. We also observe that the SaS photons crosses the sample following the same path as the noninteracting laser. Finally, we investigate the polarization of correlated SaS photons, demonstrating that they have mainly the same polarization of the excitation laser. By pump-probe experiments we measure the decay rate of the SaS pair production, evidencing the fundamental difference between the real and virtual phonon exchange processes.

*CAPES, CNPq, FINEP, FAPERJ

1:39PM G02.00013: Controlling van der Waals Phenomena at the interface of Atomic and Two-Dimensional Dirac Quantum Matter*  
AADITYA DIMRI (Presenter), JOSEPH TURNER, ADRIAN DEL MAESTRO, VALERI KOTOV, Univ of Vermont — We discuss how the presence of two-dimensional (2D) materials, such as graphene, can significantly affect two intrinsically quantum phenomena that have traditionally served as probes of the fundamental van der Waals (VDW) interaction. First, we show theoretically that Quantum Reflection (QR) of slow atoms off attractive VDW potential tails (due to interactions with 2D materials) is very strongly dependent on material characteristics (such as band structure, doping and screening level, etc). Secondly, we analyze manifestations of such 2D effects for many atoms forming a confined Bose-Einstein condensate (BEC) placed near 2D materials, which in turn makes the BEC frequency sensitive to the interface. In both cases we find that relatively small 2D material changes (either by external factors such as strain or doping, or by using gapped 2D materials instead of graphene) can have a profound effect on the above phenomena. In particular, Quantum Reflection at a given energy can experience a significant enhancement or supression (relative to conventionally used bulk materials) making 2D quantum materials an attractive playground for the study of many-body phenomena at the interface of atomic and solid state physics.

*This work received support under NASA grant number 80NSSC19M0143.
1:51PM G02.00014: Magneto-electric Rectification: A New Universal Second-order Nonlinearity*  
MINH T TRINH (Presenter), GREGORY SMAIL, DASEUL YANG, JINSANG KIM, STEPHEN COLBY RAND, Univ of Michigan - Ann Arbor — Ultrafast magneto-electric (M-E) interactions have attracted a great deal of attention because they potentially enable novel ultrafast all-optical switching, sensing technology, and terahertz emission. Most M-E effects have been observed in multiferroic materials or in metamaterials. Very interestingly, it has been reported recently that magnetic properties of homogeneous dielectric media can be controlled by optical nonlinearities driven jointly by electric and magnetic field components of light. Through the action of optical torque at the atomic scale, magneto-electric (M-E) interactions drive the bound electrons to move in curved trajectories even under non-relativistic conditions, breaking temporal and spatial inversion symmetry. As a result, several unforeseen physical phenomena take place, such as longitudinally polarized second harmonic radiation, induced transverse magnetization at the optical frequency, and forward optical rectification. Interestingly, no special crystal symmetry is necessary for M-E rectification. In this work, we report the first observation of the transient forward magneto-electric rectification in a pentacene thin-film using an electric-field-induced second harmonic generation (EFISH) technique.

*This research was supported by AFOSR.

2:03PM G02.00015: Theory of Magneto-electric Dynamics in Charge Separation*  
GREGORY SMAIL (Presenter), MINH T TRINH, STEPHEN COLBY RAND, Center for Dynamic Magneto-Optics, Univ of Michigan - Ann Arbor — A time dependent theory of magneto-electric nonlinearities at the molecular level is presented, with an emphasis on rectification. Magneto-electric nonlinearities are interactions that involve both the electric and magnetic fields of light. Recent experimental evidence indicates that these interactions are mediated by the transfer of orbital angular momentum to molecular rotations through the action of optical torque at low intensities. By including torque dynamics in an otherwise classical electron oscillator model, a quantitative model of the interactions can be developed to include temporal evolution. The solutions to the equations of motion clearly show the role of both a parametric resonance and torque dynamics in driving the magneto-electric nonlinearities. Simulations are directly compared to experimental measurements of magneto-electric rectification to examine the accuracy of the model.

*This research was supported by the Air Force Office for Scientific Research (AFOSR).

Tuesday, March 3, 2020 11:15 AM - 1:39 PM

Session G03 GSCCM DMP: Materials in Extremes: Carbon and Related Materials at Extreme Conditions  
107 - Nir Goldman, Lawrence Livermore Natl Lab
11:15AM G03.00001: Detonation-induced transformation of graphite to hexagonal diamond.* ELISSAIOS STAVROU (Presenter), MICHAEL BAGGE-HANSEN, JOSHUA A HAMMONS, WILLIAM L SHAW, WILL BASSETT, SORIN BASTEA, LISA LAUDERBACH, RALPH HODGIN, NICHOLAS PEREZ-MARTY, MATT NELMS, MATTHEW P KROONBLAWD, BRAD STEELE, SARANSH SINGH, Lawrence Livermore Natl Lab, NICHOLAS SINCLAIR, YUELIN LI, PINAKI DAS, ADAM SCHUMAN, Dynamic Compression Sector (DCS), Washington State University, KAMEL FEZZAA, ALEX DERIY, Advanced Photon Source, Argonne National Laboratory, THOMAS BUNT, LARA LEININGER, TREvor M WILLEY, Lawrence Livermore Natl Lab — The structural evolution of graphite under elevated thermodynamic conditions has been the subject of intense research interest. Early studies, back in 90s, clearly indicate the shock-induced transformation of graphite to a phase with much higher density, presumably a sp$^3$ allotrope, above 20 GPa. However, only recently the capability of in-situ X-ray diffraction under shock conditions allowed the structural characterization of the relevant phases. Here we explore the structural evolution of highly oriented pyrolytic graphite (HOPG) under detonation-induced shock conditions using in situ synchrotron X-ray diffraction in the ns time scale. We observe the formation of hexagonal diamond (lonsdaleite) at pressures above 50 GPa, in qualitative agreement with recent gas gun experiments. Moreover, we observe an extended pressure stability of the initial HOPG crystal structure up to ~50 GPa, in contrast with previous shock and static compression results.

*This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344. We gratefully acknowledge the LLNL LDRD program for funding support of this project under 18-SI-004.

11:27AM G03.00002: Kinetics of carbon clustering in detonation of high explosives: Particle growth along hydrodynamic streamlines KIRILL VELIZHANIN (Presenter), Los Alamos Natl Lab — Chemical reactions in detonation of carbon-rich high explosives yield solid carbon as a major constituent of the products. Efforts to theoretically describe the kinetics of carbon clustering go back to the seminal paper by Shaw and Johnson, where it was modeled as a diffusion-limited irreversible coagulation of smaller clusters into larger ones. In this talk, we will discuss recent direct experimental observations of carbon cluster growth in detonation of high explosives, based on time-resolved small-angle X-ray scattering (TR-SAXS). We will focus on comparison of these results with calculations based on (i) realistic hydrodynamic modeling of detonation of PBX 9502 high explosive, (ii) the Shaw-Johnson model of carbon particulate growth along the streamline obtained from the hydrodynamic simulations, and (iii) accurate simulations of the TR-SAXS signal. We demonstrate that this three-step simulation approach agrees well with the recent experimental results. The implications of this agreement on our present understanding of in-detonation carbon clustering processes will be discussed.
11:39AM G03.00003: Morphological evaluation of nanophase carbons recovered from deflagrated vs. detonated PBX 9502  MILLICENT FIRESTONE (Presenter), SOKHNA DIOUF, SUZANNE M.L. SHEEHE, Los Alamos Natl Laboratory — Understanding the correlation between detonation conditions and nanophase carbon formation is important for achieving greater accuracy in predicting high explosive performance. To advance our understanding, and ultimately improve our ability to accurately predict the nanophase carbon products, requires knowledge of the operable carbon framework reactions and nascent particle assembly mechanisms ensuing behind the shock front. The detonation chemical reaction zone (CRZ) is temporally short (ns) and spatially small (100’s microns), making it difficult to directly probe. Further complicating direct interrogation is the high optical opacity. Deflagration, however, is less extreme characterized by a larger dimensional reaction zone (mm) that is temporally longer (ms). Furthermore, deflagration produces lower opacity at pressures in the MPa range. Thus, deflagration offers a means for carrying out direct spectroscopic monitoring of the generated and evolving carbon products as a function of HE chemical composition. In this presentation, the morphology of nanophase carbons recovered from the detonation and deflagration soot derived from PBX 9502 is characterized. The data is interpreted in the context of emission spectra recorded in the deflagrating flame.

11:51AM G03.00004: Probing metastability of carbon at high pressures by predictive first-principles simulations  ASHLEY WILLIAMS (Presenter), KIEN NGUYEN-CONG, JONATHAN T WILLMAN, IVAN OLEYNIK, University of South Florida — In spite of extensive experimental and theoretical efforts, the behavior of carbon at extreme conditions is not completely understood. Previous hydrostatic studies demonstrate the stability of diamond and the absence of any other phase of carbon at pressures up to 1 TPa. However, new metastable phases might appear upon uniaxial compression generated by shock waves. We explore unknown metastable phases of carbon under both hydrostatic and uniaxial compressions up to 5 TPa using first-principles crystal structure prediction methods. It is predicted that several new metastable phases appear to survive upon decompression to ambient conditions. The experimental validation of these predictions will open up a new avenue in synthesizing new metastable carbon materials.
12:03PM G03.00005: Bottom up molecular doping approach to synthesizing HPHT color centers in nanostructured diamond*  
ABBIE GANAS (Presenter), MATTHEW J CRANE, RYAN BECK, University of Washington, ALESSIO PETRONE, Dipartimento di Scienze Chimiche, Università di Napoli Federico II, YUE HUANG, University of Washington, RHONDA MICHELE STROUD, United States Naval Research Laboratory, XIAOSONG LI, PETER J. PAUZAUSKIE, University of Washington — Diamond nanocrystals are advantageous for a myriad of biological and technological applications because its optical color centers are tunable between the ultraviolet and near-infrared (NIR) spectral regions. Our work describes a molecular approach to dope diamond nanocrystals with silicon heteroatoms at extreme temperature (>1800K) and pressure (>15 GPa) conditions using argon as a near-hydrostatic pressure medium. Tetraethylorthosilicate (TEOS) molecules chemically dope an amorphous carbon aerogel during nanodiamond synthesis within a laser-heated diamond anvil cell. Pressure-dependent photoluminescence is used in tandem with ab initio quantum cluster calculations to measure the pressure dependence of the SiV- centers’ zero phonon line (λ ~ 738 nm, 0.9 meV / GPa). Aberration-corrected scanning transmission electron microscopy images heteroatoms on the surfaces and also the interiors of diamond nanocrystals. Scanning transmission x-ray absorption microscopy (STXM) measurements, along with electron energy loss spectroscopy and ab initio quantum cluster calculations, suggest a partial graphitic surface reconstruction of the diamond nanocrystals.

*The authors acknowledge primary support for this work from the National Science Foundation (CAREER Award #1555007, MRSEC).

12:15PM G03.00006: Facile diamond synthesis from lower diamondoids  
SULGIYE PARK, IWINETIM I ABATE, Stanford University, JIN LIU, Center for High Pressure Science and Technology Advanced Research, CHENXU WANG, Stanford University, JEREMY DAHL, ROBERT CARLSON, SLAC - Natl Accelerator Lab, YANG LIUXIANG, Center for High Pressure Science and Technology Advanced Research, VITALI PRAKAPENKA, ERAN GREENBERG, Center for Advanced Radiation Sources, THOMAS DEVEREAUX, Stanford University, CHUNJING JIA, SLAC - Natl Accelerator Lab, RODNEY C. EWING, WENDY MAO, Stanford University, YU LIN (Presenter), SLAC - Natl Accelerator Lab — Carbon-based nanomaterials have exceptional properties that make them attractive for a variety of technological applications. In this talk, I discuss the use of diamondoids (diamond-like hydrocarbons) as promising precursors for laser-induced high-pressure, high-temperature diamond synthesis. The lowest pressure and temperature (P-T) conditions that yielded diamond were 12 GPa (at ~2000 K) and 900 K (at ~20 GPa), respectively. This represents a significantly reduced transformation barrier compared with diamond synthesis from conventional (hydro)carbon allotropes. At 20 GPa, diamondoid-to-diamond conversion occurs rapidly within < 19 us, forming diamond in a range of sizes ~tens of nm to ~4 um crystals, depending on the synthesis conditions. Molecular dynamics simulations indicate that once dehydrogenated, the remaining diamondoid carbon cages reconstruct themselves into diamond-like structures at high P-T. The surprisingly low P-T regime necessary to grow diamond from diamondoids is attributed to the similarities in the structure and bonding of diamondoids and bulk diamond. This study is the first successful mapping of the P-T conditions and onset timing of the diamondoid-to-diamond conversion and elucidates the physical and chemical factors that facilitate diamond synthesis.
First-principles phase diagram of carbon at extreme conditions

KIEN NGUYEN-CONG (Presenter), University of South Florida, ANATOLY BELONOSHKO, Royal Institute of Technology, IVAN OLEYNIK, University of South Florida — The accurate phase diagram of carbon at extreme temperatures and pressures is of paramount importance for design of inertial confinement fusion capsules where diamond is used as an ablator material. In spite of intensive experimental and theoretical efforts, there still exist outstanding problems including disagreement between theoretical predictions and experiment. We present results of first-principles molecular dynamics simulations of thermodynamic properties of carbon at high temperatures and pressures, which are performed with the goal of constructing an accurate phase diagram of carbon. To address the issue of accuracy and reliability, a relatively large number of atoms is used for calculation of melting transitions (melt curve) as a function of pressure using two-phase method. We specifically focus on important region of high pressure, high temperature phase diagram where melt line of diamond exhibits a negative slope, while intersecting the melt line of high-pressure bc8 phase at diamond-bc8-liquid triple point.

Color center qubit formation by local electronic excitation

THOMAS SCHENKEL (Presenter), ARUN PERSAUD, QING JI, SVEN STEINKE, JIANHUI BIN, STEPAN BULANOV, Lawrence Berkeley National Laboratory — Color centers e. g. in diamond are promising qubit candidates. Efforts to find color centers with desired properties, e. g. emission in the telecom bands and long coherence times, are limited by the parameter space in which materials can be processed. Recently, color center formation with fs-laser pulses and using swift heavy ions have been reported. Intense pulses of local excitation can drive materials very far from equilibrium followed by rapid quenching. This extends the parameter range where novel color centers can be formed. We report on mechanisms underlying NV-center formation with swift heavy ions, our search for rare-earth color centers in diamond and new capabilities that we are developing for color center formation far from equilibrium using intense, local pulses of ions and lasers [1-3].

References

*Acknowledgments
The work was supported by and LDRD at LBNL and by the U.S. DOE Office of Science Offices of HEP and FES (including through LaserNetUS) under Contract No. DE-AC02-05CH11231. J. H. Bin acknowledges financial support from the Alexander von Humboldt Foundation.
12:51PM G03.00009: Probing the strain field and structural variation in shock-produced amorphous silicon by scanning nano-probe electron diffraction  SHITENG ZHAO (Presenter), University of California Berkeley, ERIC N HAHN, UC San Diego, BRUCE ALLEN REMINGTON, Lawrence Livermore National Laboratory, COLIN OPHUS, BENJAMIN H SAVITZKY, Lawrence Berkeley National Laboratory, CHRISTOPHER WEHRENBERG, Lawrence Livermore National Laboratory, MARC A MEYERS, UC San Diego, ANDREW M MINOR, University of California Berkeley — Shock-induced amorphization can occur when crystalline solids are uniaxially strained in an extremely short time scale. This phenomenon also opens a new door for prototyping the exotic amorphous structures when the conventional methods failed. Taking silicon as an example, we have recovered its amorphous phase from laser shock compression experiments and illustrated the formation mechanisms by both experiments and simulations. However, one missing information is whether the amorphous silicon produced by shock wave is fully relaxed, i.e. are they structurally different than the amorphous structure produced by other techniques such as chemical vapor deposition. We use a newly developed scanning nano-probe electron diffraction technique to tackle this question. A nanometer-sized electron probe is focused onto and rastering over the electron-transparent sample and simultaneously, convergent beam electron diffraction patterns at each pixel are collected, which can be used to compute strain distribution of the region of interest. The strain field in the vicinity of the amorphous band and the radial distribution function within the amorphous domain will be discussed. A tremendous amount of structural variation can be found even within the amorphous domain.

1:03PM G03.00010: Computer Simulations and Experimental Studies on Transition Metal Borides to 390 GPa*  YOGESH VOHRA (Presenter), KALEB BURRAGE, CHRISTOPHER PERREAULT, GOPI K SAMUDRALA, CHIA-MIN LIN, CHENG-CHIEN CHEN, Physics, Univ of Alabama - Birmingham, NENAD VELISAVLJEVIC, HPCAT, Argonne National Laboratory — The attainment of near TPa static pressure in the laboratory has led to a renewed interest in phase transformations and shear strength measurements of incompressible transition metals rhenium (Re), osmium (Os), and their superhard diborides (ReB₂ and OsB₂) We have compressed hexagonal ReB₂, OsB₂, and Os₂B₃ to multi-megabar pressures using Focused Ion Beam machined toroidal diamond anvils. The phase transformations and equation of state were studied using micro-beam angle-dispersive x-ray diffraction at HPCAT beamline 16-BM-D. The platinum pressure marker was employed to the highest pressure of 390 GPa. First-principles simulations based on density functional theory (DFT) were utilized to model ReB₂ and OsB₂ under external pressure. The ambient-pressure lattice parameters computed by the projector augmented-wave method with generalized gradient approximation agree well with the experiment within 1% of error. We will present a comparison of experimental shear strength and equation of state with the elastic constants from DFT calculations up to the highest pressure under study.

* Supported by NSF DMR Grant No. DMR-1904164. HPCAT operations are supported by DOE-NNSA.
1:15PM G03.00011: Thermal stability of silicon carbide  YUEJIAN WANG (Presenter), Physics, Oakland University — A large volume cubic anvil press integrated with synchrotron energy-dispersive X-ray diffraction was employed to study the yielding behavior of powdered beta SiC under high pressure and high-temperature conditions up to 7.4 GPa and 1400°C. During the compression and thereafter heating, x-ray pattern was collected at each pressure-temperature point, and then via assessing the peak width of the X-ray diffraction pattern, the strains/stresses developed inside the sample under varied pressure-temperature conditions was calculated. From the constitutive response of the sample as a function of pressure and temperature, we did not observe the yielding occurrence in SiC at cold compression. In contrast, high temperature induces a yielding at 1100°C with a constant loading pressure ~7.4 GPa. By the comparison, we found that this material is the most stable material, among the other three strong materials (diamond, moissanite, and alfa silicon nitride), in terms of the yielding under high pressure and temperature conditions. Along with its much higher pressure and temperature requirements for phase transition and decomposition, SiC is a competent material to be used in the harshly extreme working environment, such as deep drilling, high-speed cutting, and aerospace engineering.

1:27PM G03.00012: On the strain-rate dependence of dynamic tensile strength in single and nanocrystalline SiC*  WANGHUI LI (Presenter), South China Univ of Tech, ERIC N HAHN, Los Alamos National Laboratory, XIAOHU YAO, South China Univ of Tech, TIMOTHY GERMANN, BIAO FENG, Los Alamos National Laboratory, XIAOQING ZHANG, South China Univ of Tech — The strain-rate dependence of dynamic tensile strength in single and nanocrystalline SiC is investigated via large scale molecular dynamic simulations. A quasi-isentropic loading method is used to evaluate the strain rate to over six-order from \(10^7\) to \(10^{12}\) s\(^{-1}\). SiC with [001] orientation exhibits a perfectly reversible deformation twinning mechanism that enables a high tensile strength, while [110] and [111] crystals contain irreversible defects after unloading that results in a significant decrease in strength. Octahedral cleavage along \{111\} family planes is found to occur only in [001] SiC within \(10^9\) s\(^{-1}\) of the strain rate due to its covalent bond. A power model can be fit basing on the tensile strengths at extremely high strain rate regime which yields a good prediction of strengths at plate-impact experimental strain rates.

*This work was supported by China Scholarship Council (CSC) and National Postdoctoral Innovation Talent Support Program (L1190540). The simulations were run using Los Alamos National Laboratory Institutional Computing Resources. Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396.
G03.00013: High pressure forms of aqueous carbon* NORE STOLTE, ZIXIN CHEN, DING PAN
(Presenter), Hong Kong University of Science and Technology — The chemistry of carbon in aqueous fluids at extreme pressure and temperature conditions is of great importance to Earth's deep carbon cycle. A major obstacle to understanding deep carbon transport is the lack of knowledge of carbon reactions in water at the extreme conditions found in Earth's deep interior. Here, by applying first-principles molecular dynamics simulations, we predicted a few interesting and important carbon reactions in supercritical water, which are dramatically different from what we know at close to ambient conditions. We found that carbonic acid can be the most abundant carbon species in aqueous CO$_2$ solutions at $\sim 10$ GPa and 1000 K. In CO$_2$-rich solutions, significant proton transfer between carbonic acid molecules and bicarbonate ions may enhance the conductivity of solutions. In less oxidized solutions, the reactions of carbon monoxide may participate in the diamond formation.

*The work is supported by the Croucher Foundation through the Croucher Innovation Award and the Sloan Foundation through the Deep Carbon Observatory.

Tuesday, March 3, 2020 11:15 AM - 1:51 PM

Session G04 DCP DSOFT DPOLY DLS: Coherent Nonlinear Optical Microscopy II 109 - Adrian Pegoraro, Univ of Ottawa - Tag(s): Focus

11:15AM G04.00001: Nonlinear Pump-Probe Microscopy Improves Early Detection of Metastatic Melanoma [Invited] WARREN WARREN (Presenter), DAVID GRASS, MARTIN C FISCHER, XIAOMENG JIA, Duke University — More people die from melanoma after a Stage I diagnosis (localized) than after a Stage IV diagnosis (distant metastatic disease), because the tools available to clinicians do not readily identify which early-stage cancers will be aggressive. We pursue an alternative approach, complementary to conventional histopathology, based on ultrafast pump-probe microscopy. Melanocytes, the neoplastic cells in melanoma, produce a brown to black colored pigment melanin. Analysis of the electronic and vibrational dynamics of melanin with ultrashort laser pulses reveal information like type (pheo, DHI or DHICA eumelanin) and state of aggregation, for example. We use these insights to evaluate primary tumor biopsies with the goal to distinguish between localized melanoma (without metastases) and melanoma that developed metastatic disease. In this talk we focus on our efforts of translating pump-probe microscopy into clinics and our current status on detection of metastatic disease of melanoma.
11:51AM G04.00002: Visualizing molecular structure and function in soft matter using coherent Raman imaging* [Invited] SAPUN PAREKH (Presenter), University of Texas at Austin —
Structure-function relationships define the how molecular processes give rise to macroscopic observables. In this talk, I will present an overview of our recent work using nonlinear vibrational spectroscopic imaging to reveal unique structural-function relationships in polymeric soft matter systems. We have used this imaging technology to map protein structure in fibrin biopolymer networks (that lie at the heart of blood coagulation) and demonstrated that fibrin biopolymers change structure in a spatially heterogeneous manner when exposed to tensile, but not shear, loads. This result hints at a unique self-regulating mechanism via a direct biophysical feedback loop in a physiological context. In another project measuring real-time water transport, we have shown that under-coordinated microscopic water transport and macroscopic proton transport are related in nano-structured polymer fuel cell membranes. From these data, we have proposed a strategy to boost efficiency in fuel cell membrane materials.

*Deutsche Forschungsgemeinschaft
Human Frontier in Science Program
Welch Foundation

12:27PM G04.00003: Correlating Multiphoton-Absorption-Induced Luminescence (MAIL) with Morphology in Noble-Metal Nanostructures* ANNA GRAFOV (Presenter), XIAOYING LIN, Farah Dawood, John T Fourkas, University of Maryland, College Park — The optical properties of nanostructured noble metals differ drastically from those of their bulk counterparts due to surface plasmon (SP) resonance. When incident light couples with the SPs of a noble-metal nanoparticle, it gives rise to strong, localized electromagnetic field enhancement. In particular, surfaces with high curvature experience especially strong field enhancement. Silver and gold SP absorption cross sections lie in the visible region, which make nanostructures of these metals ideal for studying optical phenomena. Multiphoton-absorption-induced luminescence (MAIL) is a nonlinear optical phenomenon that involves ultrafast pulses of light impinging on a nanostructured surface. The SP field enhancement allows for more efficient multiphoton absorption, and highly-efficient, broadband luminescence over the visible spectrum is produced as a result. We examine how the morphologies of noble-metal nanostructures correlate with their MAIL signals. Specifically, we focus on silver nanodendrites, synthesized from galvanic displacement reactions, and gold nanorings and nanotriangles, grown through colloidal synthesis. The absorption order, intensities, and spatial distribution of MAIL signals are examined for different morphologies.

*NSF Grant CMM-11449309
12:39PM G04.00004: Stimulated Raman scattering spectroscopic optical coherence tomography* [Invited] FRANCISCO ROBLES (Presenter), Georgia Inst of Tech — Stimulated Raman scattering (SRS) enables fast, high-resolution imaging of chemical constituents important to biological structures and functional processes in a label-free manner. While this technology has shown remarkable potential, acquisition of SRS signals remains largely limited to point scanning at a few Raman bands. To overcome this limitation, we take advantage of the fact that SRS is a coherent process and can thus be integrated into a single platform with spectroscopic optical coherence tomography (SOCT). SOCT is an extension of OCT that leverages the broadband nature of low-coherent light sources, along with advanced digital signal processing methods, to simultaneously obtain three-dimensional spatial and spectral information, but SOCT has very limited endogenous molecular targets. Thus, the combined approach, termed SRS-SOCT, overcomes limitations of both individual methods and achieves fast, volumetric, and highly sensitive label-free molecular imaging. Here we will present a theoretical framework for SRS-SOCT, discuss its advantages and limitations, and show experimental results from excised tissues.

*Funding Sources: National Cancer Institute (NCI) (R21CA223853); Burroughs Wellcome Fund (BWF) (CASI BWF1014540).

1:15PM G04.00005: Spectroscopic Fourier-Transform Coherent Raman Microscopy [Invited] MARCUS CICERONE (Presenter), XAVIER AUDIER, WEI-WEN CHEN, RONIT SHARON-FRILLING, Georgia Inst of Tech — Spectroscopic coherent Raman imaging (CRI) methods allow label-free, chemically specific imaging of materials and biological systems, and are opening up many exciting possibilities for understanding phenomena in these systems. I will briefly introduce spectroscopic CRI, specifically broadband coherent anti-Stokes Raman scattering (BCARS), discussing key features required to make these methods practical, current impediments to improvements in speed and sensitivity, and new approaches we are taking to overcome these impediments. I will also present BCARS imaging results that have provided physical insights into biological processes on cellular and organism levels.

Tuesday, March 3, 2020 11:15 AM - 1:27 PM

Session G05 DCP DAMOP DCMP DPOLY: Electronic-Vibrational Coupling in Light Harvesting II. Excitons, Polarons, Perovskites, and Non-Adiabatic Dynamics 111 - David Jonas, University of Colorado, Boulder - Tag(s): Focus
Excitons and polarons play a critical role in the electronic properties of organic molecular aggregates as well as conjugated polymers and aggregates thereof. For many conjugated organic molecules neutral excitations (excitons) and charged excitations (polarons) are coupled strongly to nuclear degrees of freedom involving the symmetric vinyl-stretching mode (i.e. the aromatic-quinoidal vibration when conjugated rings are present). In this talk the photophysical properties of excitons and polarons in conjugated organic materials are compared and contrasted within the framework of a theory based on the Holstein Hamiltonian, which treats local electron-vibrational coupling exactly. Applications are made to excitons in perylene diimide crystals [1] and dopant-induced positively-charged polarons (holes) in poly(3-hexylthiophene) films. [2,3] It is shown how simple optical probes like steady-state absorption and photoluminescence can be used to extract the exciton and polaron coherence lengths, quantities which are important for understanding energy and charge transport.


*This work was supported by the National Science Foundation (DMREF, 1533954).
The spectral line-shape of the mid-IR absorption spectrum provides valuable information about the “hole” polaron coherence length in doped and undoped conjugated polymer films. Using a theory based on the Holstein Hamiltonian for mobile holes in P3HT, the IR line-shape is successfully reproduced for several recently measured spectra recorded in doped and undoped films, confirming the association of an enhanced peak ratio (A/B) with extended polaron coherence. Emphasis is placed on the origin of components polarized along the intra- and inter-chain directions and their dependence on the spatial distribution of disorder and the position of the dopant relative to the π-stack. The model has been further adapted to treat donor-acceptor copolymers.

References:

*NSF DMREF 1533954
12:03PM G05.00003: Correlating Structure and Function in Two-Dimensional Organic-Inorganic Hybrid Perovskites [Invited] Cherie Kagan (Presenter), Daniel Straus, Sebastian Hurtado Parra, Qinghua Zhao, James Makato Kikkawa, University of Pennsylvania — Two-dimensional, organic-inorganic hybrid perovskites (2DHPs) are stoichiometric compounds composed of alternating sheets of corner-sharing, metal-halide octahedra and organoammonium cationic layers. We study 2DHPs containing single lead iodide layers separated by intervening substituted, phenethylammonium cations with the chemical structure \((\text{x-PEA})_2\text{PbI}_4\), where \(\text{x}=\text{F}, \text{Cl}, \text{Br}, \text{or CH}_3\). These 2DHPs form type-I heterojunctions in which excitons and carriers are confined to the lead halide layers and strong quantum and dielectric confinement effects establish exciton binding energies that exceed 150 meV. We use powder and single-crystal x-ray diffraction studies, in combination with variable-temperature, steady-state and time-resolved absorption and photoluminescence (PL) measurements to uncover the correlation between their structure and photophysical properties. 15 K spectra of unsubstituted \((\text{PEA})_2\text{PbI}_4\) show splitting of the excitonic absorption and PL into regularly spaced resonances every 40-46 meV. In addition, anti-Stokes hot exciton PL is observed at the same energy as optical absorption resonances. Substitution on the organic cations, for example in the para position, increases the length of the organic cation and therefore the interlayer spacing, but leaves the cross-sectional area for the organic cation unchanged and results in structurally similar metal halide frameworks. As the length of the cation increases in the 2DHP, the absorption spectra broaden and blueshift, but the PL spectra remain invariant. We show that the excitonic structure is consistent with strong electron-phonon coupling and slow vibrational relaxation originating from the softness of the metal halide framework and the organic cations.

12:39PM G05.00004: Investigating how biological membrane parameters influence the ring opening of Provitamin D Danielle Sofferman (Presenter), Roseanne J Sension, Univ of Michigan - Ann Arbor — Ultrafast photochemical transformations of 7-Dehydrocholesterol (DHC, Provitamin D\(_3\)), DHC-Acetate and Ergosterol (Ergo, Provitamin D\(_2\)) to previtamin (D\(_3\), D\(_3\)-acetate and D\(_2\)) occurs upon a ring-opening reaction in the excited state where a Cyclohexadiene (CHD) chromophore embedded within the molecules opens to form a previtamin D species. In isotropic environments, the ring opening reaction occurs within 1-2ps therefore it is necessary to use ultrafast techniques such as transient absorption to capture the kinetics. However, in the lipid bilayer this reaction is slowed to 11ps. Here we are studying DHC and its analogs in lipid bilayers as a simple model for biologically relevant skin membrane models. To investigate the 6 fold slow down, the ring opening of DHC will be discussed in terms of lipid properties such as Van der Waals interactions, Hydrogen Bonding and membrane ridgidity.
Superradiance of two-dimensional molecular aggregates* [Invited] ALEX EISFELD (Presenter), Max Planck Institute for the Physics of Complex Systems — Assemblies of molecules (so-called molecular aggregates) have become versatile quantum systems with applications in photography, opto-electronics, solar cells, and photo-biology. The remarkable properties of these aggregates stem from the strong transition dipole-dipole interaction between the individual molecules which leads to eigenstates with excitation shared coherently by a large number of molecules. As a consequence the aggregate possesses strikingly different optical properties compared to the individual molecules.

In this talk I will discuss the superradiant emission of organic molecules arranged on dielectric surfaces. A particular focus is on the relation between the temperature dependence and the underlying eigenfunctions of the aggregate [1]. Knowledge about these eigenfunctions is not only important to understand the optical properties but also for the transfer characteristics of the aggregates. Optical spectroscopy, in principle, allows one to infer information on these eigenstates and about the interactions between the molecules. However, traditional optical techniques using an electromagnetic field which is uniform over the relevant size of the aggregate cannot access most of the excited states because of selection rules. We demonstrate that by using localized fields and machine learning techniques one can obtain information about these otherwise inaccessible states. As an example, we discuss in detail the case of local excitation via radiation from the apex of a metallic tip, which allows also scanning across the aggregate. The resulting spatially resolved spectra provide extensive information on the eigenenergies and wave functions [2,3].


*Grant No EI 872/5-1 (Heisenberg fellowship) from the German Research Foundation (DFG)

A resonant confinement of polariton under strong photon-exciton coupling is predicted to exist within the microcavity of the crystals own natural boundaries. Moreover, the radiative energy of a localized exciton falls into the spectrum of the confinement.

The spontaneous emission of an excited pigment would undergo a two-step process. It should first decay to an excitonic polariton trapped by the cavity resonance. The captive intermediate could then funnel the energy directly to doped acceptors, leading to the observed over 90% transfer efficiency at less than 1/1000 acceptor-donor ratio.

The proposed mechanism is supported by parameter-free analyses entirely based on experiment data. Our finding may imply possible polariton-mediated pathways for energy transfers in biological photosynthesis.

*This work was supported in part by the National Natural Science Foundation of China No. 16Z103060007 (P.A.).
11:15AM G06.00001: Breaking Down Barriers to Science and Physics Communication in China - Do Veritasium YouTube Videos Translate?  
HANYU ZHANG (Presenter), Applied and Engineering Physics, Cornell University, DEREK MULLER, Veritasium — Educational content on YouTube has seen incredible growth and gotten significant traction. Physics-focused YouTube channels are no exception. From the earliest days of education on YouTube, Veritasium [1,2], an educational physics YouTube channel now with over 6 million subscribers and 650+ million views, has educated and engaged the general public about physics.

However, due to political barriers, Veritasium and other YouTube channels are blocked in China. This energy barrier, although significant, is not insurmountable. Veritasium has recently become one of the first YouTube channels to fully overcome the language, cultural, and political barriers and step into China. With close to 50 thousand subscribers and 2 million views on a Chinese platform, Veritasium has demonstrated that accessible physics education content can also go viral in China. This realization leads to an opportunity for anyone interested in making an impact in physics education to do so anytime anywhere with simple code and existing content.

[1] YouTube channel: youtube.com/veritasium  

11:27AM G06.00002: Physics to Environmental Science: Solution Seeker of today’s world  
LIBIA HAZRA (Presenter), N. SRINIVAS, Gandhi Institute of Technology and Management — In this talk I share my journey as a solution-seeker to restore the natural state of our environment as I move from an agriculture-based society into studying physics and then switching into environmental science to help develop a sustainable environment and a culture of high-yielding organic farming. As I prepare to work on using satellite images to help benefit agriculture, ecotoxicology, environmental chemistry, and controlling salt-water intrusion, I realize at every step that application of Physics concepts is quite an integral part of Environmental science. I will discuss how my background in Physics, Maths and Chemistry gives me strength to better understand the current topics in environmental science as I aspire to apply my natural aptitude for instruments and experiments to estimate the pollutants in our air, water, land and food and want to invent and implement feasible solution to better the health of all living being and mother earth.
For students with environmental mind-set (future environmentalists), I strongly suggest for a thorough foundation in Physics, Maths, Chemistry and Computer Science to be better equipped in tackling the towering task that an environmentalist have to do.
**11:39AM G06.00003: Share your research at FunSize Physics**  
SHIREEN ADENWALLA (Presenter), JOCELYN BOSLEY, University of Nebraska - Lincoln, LEIGH M SMITH, Physics, University of Cincinnati — www.funsizephysics.com is a colorful, user-friendly website created in Spring 2016 with the express purpose of showcasing exciting new developments in condensed matter physics to a broad audience of non-experts. The research descriptions are written by the researchers themselves, serving as an efficient, low bar broader impact activity in a PI's portfolio. Google Analytics allows researchers to quantify the impact of their contributions, tracking the number of views, stars, thumbs up and viewing time. We have optimized the existing website to make it more user-friendly and made a short video advertising the website. In addition, by making the website a convenient place in which to collaborate and discuss a variety of outreach efforts, it serves as a resource for NSF PIs to develop best practices for outreach activities to K-12 students and the general public. We invite contributions from students, post-docs and faculty-share your beautiful, ground breaking science with a wider audience, discuss the advantages and disadvantages of your outreach activities-make it yours!

*Funded by NSF-DMR-1725823*

**11:51AM G06.00004: Physics outreach as teaching and service-learning experience for students**  
TATIANA ERUKHIMOVA (Presenter), Texas A&M University — We will present the results of an innovative program at Texas A&M University that aims to add hands-on, teamwork, and outreach components to the learning and research experiences of undergraduate and graduate students. In this program, undergraduates taking introductory physics classes work throughout the school year in small teams led by physics graduate students on design and fabrication of exciting physics demonstration experiments: from a giant Galilean cannon to liquid sand pool, Texas-sized Tesla coil, superconducting train, and supersonic gun. Student teams demonstrate their experiments at high-profile outreach events such as the Texas A&M Physics & Engineering Festival, Physics Shows, Just Add Science, and Game Day Physics. They film their experiments in 2-3 min video clips posted at realphysicslive.com. The demonstrations are also used in regular physics classes at Texas A&M.

**Tuesday, March 3, 2020 11:15 AM - 2:03 PM**

**Session G07 FED: Topics in Physics Education**  
102 - Gerald Feldman, George Washington Univ - Tag(s): Education, Undergrad Friendly
Group Exam as an Instructional Technique to Promote Consistency Checking in Student Reasoning

ALISTAIR MCINERNY (Presenter), LIOUDMILA KRYJEVSKAIA, Physics, North Dakota State University — Many students tend to provide intuitively appealing (but incorrect) responses to some physics questions despite demonstrating (on similar questions) the formal knowledge necessary to reason correctly. While these inconsistencies are typically persistent even in active learning environments, we believe that adding a group component to the exam may engage students sufficiently to resolve these instances of inconsistent reasoning. In our study, students were given opportunities to revisit their answers to questions known to elicit strong intuitively appealing (but incorrect) responses in a collaborative group component of an exam immediately following a traditional individual component. Students discussed their responses with group members but were required to submit their own answers and reasoning. In this presentation, we will examine the effectiveness of a collaborative group exam approach in addressing and resolving inconsistencies in student reasoning and will compare the effectiveness of this approach to a more traditional peer instruction technique.

This material is based upon work supported by the National Science Foundation under Grants Nos. DUE-1821390, DUE-1821123, DUE-1821400, DUE-1821511, DUE-1821561, DUE-1431940, DUE-1431541, DUE-1431857, DUE-1432052, and DUE-1432765.

Developing the First Two Years of an Undergraduate Physics Program - A Ten-Year Study

EFFROSYNI SEITARIDOU (Presenter), Physics and Astronomy, Oxford College of Emory University — Oxford College (OC) is an undergraduate division of Emory University focused on the liberal arts education of 950 first- and second-year students. After their second year, the students move to Emory College (EC) to complete the remainder of their undergraduate education. Between 2008-2010, OC contributed only 5 physics majors to the graduating classes at EC. To expand student interest in first- and second-year physics courses and increase its contribution to the number of physics majors OC applied many strategies, including those recommended by the National Task Force of the American Association of Physics Teachers [1]. The strategies focused on creating a rigorous curriculum and an environment and evaluation process to meet the students’ individual needs. Among the outcomes were that between 2010-2019 the physics faculty grew from one to three, the enrollment of women in a sophomore-level course increased from 17% to 38%-50%, and OC’s contributions to the total number of EC’s physics majors increased to 19 in years 2017-2019. An additional 13 students are estimated to graduate in 2020 alone. This presentation will provide an overview of the applied strategies and their outcomes.

11:39AM G07.00003: “Not Required,” “No Required Minimum,” and “Optional” General and Physics GRE Requirements: The Impact on Prospective Graduate Students* LINDSAY OWENS (Presenter), BENJAMIN M ZWICKL, CASEY MILLER, Rochester Institute of Technology — When applicants search for graduate schools, they research multiple aspects of the programs and reflect on how well they envision themselves fitting into each program. Graduate program’s reported Physics and General GRE requirements, recommended minimum scores, and previous cohort score averages influence students’ decisions about where to apply. In recent years, the test-optional language of No Required Minimum and GRE Optional requirements has muddied the waters for prospective applicants, particularly for women. In this qualitative study, 54 graduate students (25-F; 27-M; 2-DND) from 23 different graduate programs were asked how they decided where to (and not to) apply to graduate school. All students felt welcome to apply to graduate programs whose admissions requirements stated GRE Not Required or Do Not Send. However, women were far less likely than men to apply to graduate programs that stated No Required Minimum or GRE Optional language on their admission requirements webpage. This talk will highlight (1) how students interpreted these phrases, (2) how such phrases influenced students’ self-reflection about fit, and (3) how these factors influenced their decision on where to apply to graduate school.

*Supported by NSF-1633275

11:51AM G07.00004: Solid State Physics across the Undergraduate Curriculum ANDRA PETREAN (Presenter), Austin College — Solid state physics encompasses a variety of physics phenomena, including modern ones such as high temperature superconductivity and nanotechnology. Despite its appeal, teaching it at undergraduate level can present challenges, as students may not have the necessary physics background until late in their undergraduate studies. Faculty at small physics departments often need to teach a range of courses, spanning from courses for the physics majors to service courses for the larger student body, and hence they may not be able to offer solid state physics as an elective. In this context, I will present the approach I took at Austin College, a small liberal arts school, in incorporating solid state physics in our curriculum, from our first-year course to capstone projects. I have used theoretical, experimental, lecture-based and project-based approaches. The topics included superconductivity through synthesis and characterization of high temperature superconductors, and nanotechnology through synthesis of carbon nanotubes and deposition and characterization of thin films at nanoscale.

12:03PM G07.00005: New Methods for the Advanced Lab RUDI MICHALAK (Presenter), Univ of Wyoming — The advanced lab lives at the awkward intersection of irrelevance and capstone course. I contend that it has a big part to play in the future of physics education and that it can be instrumental in turning undergraduate majors into professional physicists and astronomers. Tools that can be developed and which can convince lower and higher administration to invest into costly equipment include: Embedding of lab goals into institutional goals, assessment, and career outcomes. Cultivating critical thinking and presentation skills. Creating belonging and rapport that appeals to minorities. Reinvigorating tired out majors into this-is-what-I-came-here-for mindsets.
12:15PM G07.00006: A Single-axis Tunneling Microscope for Undergraduate Labs  RANDY LINDGREN, JOSHUA VEAZEY  (Presenter), Grand Valley State University —
I will discuss the conception and development of a low-cost z-axis tunneling microscope (ZTM) for learning about quantum mechanics and electronic structure in undergraduate labs. Inspired by the scanning tunneling microscope, this device cuts costs and complexity for the undergraduate lab setting by limiting tip control to the tip-sample separation. To further reduce cost, an off-the-shelf ceramic capacitor (MLCC) is used as the piezo actuator [1]. Students can observe the exponential dependence of the tunneling current on barrier width ($I-z$), as well as the local electronic density of states ($I-V$) for many samples under ambient conditions.

12:27PM G07.00007: The Tolman-Stewart Experiment – A Modern Interpretation  JOSHUA SCHMIDT  (Presenter), MATTHEW C. SULLIVAN, Ithaca Coll — The Tolman-Stewart Experiment, published in 1916 by Richard C. Tolman and T. Dale Stewart, proved that the charge carriers in a conductor were identical to the electrons previously discovered in cathode rays and beta rays. The concept of free electrons in a conductor is still an essential building block of electrodynamics, and the Tolman-Stewart experiment demonstrates this in a fundamental way. Our interpretation of this experiment makes use of modern circuitry and computer control to better adapt the experiment for an advanced undergraduate lab course. We spin a coil of copper or aluminum wire up to sufficiently high speeds and brake it suddenly. This stops the nuclei, but the free electrons keep moving, creating a short-lived current pulse. This current pulse is amplified, converted to a voltage, and recorded using a simple circuit and data acquisition system. Modern rotational encoders accurately determine the rotational speed. Our results confirm that the charge carriers inside both copper (negative charge carriers via the Hall Effect) and aluminum (positive charge carriers via the Hall Effect) are electrons. This interpretation brings a canonical experiment to the advanced lab for the first time and yields compelling proof of the identity of charge carriers in a conductor.
12:39PM G07.00008: Statistical differences in over 1000 Student Lab Reports and 9000 Lab TA comments using new Experimental Design Pedagogy*  DAVID MCKENNA, ABIGAIL MECHTENBERG (Presenter), University of Notre Dame — At a rate of 700+ students/year implementation of this experimental design (ED) pedagogy, 4.5 years of data was collected. This ED pedagogy moves the lab culture from cookbook labs into inquiry-based deviations, and towards a research-based final project. Three ED thought spheres scaffold all labs into cookbook-based pattern recognition: measurements (M), calculations (C), and variations (V). Three ED connection pathways teach students how, when and why scientists critically think about doing science (regression versus derivation approaches) using 3 interconnected stages Design, Data, and Analysis. With Google Classroom, Lab TAs wrote feedback comments as well as the rubric-based grades for student lab reports in one term alone. We analyzed all comments in terms of total words, tone, complexity, and probing level. It was hypothesized that the tone of Lab TA comments were correlated to student evaluations; however, it was complexity, word count, and probing level of comments which were correlated to student evaluations (and final exam scores). We discuss future research into the differences between Teaching/Learning pair types: Judging Teacher and Obedient Student (Active-Reactive) versus the Socratic Teacher and Constructive Student (Reactive-Active).

*Physics ND Seed Funding

12:51PM G07.00009: The Wolfram Language: A general tool for science education  JASON MARTINEZ (Presenter), Wolfram Research — The Wolfram Language (WL) provides a wide range of scientific data, tools, and algorithms for students of all levels. The WL includes an extensive knowledge base on subjects from the properties of subatomic particles to the details of orbits to the changing magnetic field of the earth. Students can engage with the WL in a wide range of formats. They can start out with simple natural language queries on Wolfram|Alpha, getting guidance on solving complex equations using its step by step functionality. Through the Wolfram Demonstrations Project, they can find thousands of dynamic examples for a wide range of physics concepts. In Wolfram|Alpha Notebook Edition students turn their natural language queries into actual code as well as make use of the Wolfram Function Repository which expands the WL with specialized independently submitted functions. Using the WL fully students can manipulate formulas with explicit units and physical quantities, propagate uncertainty in their calculations, compute eigenvalue and vectors, use advanced tools to solve ODEs and PDEs, analyze results using statistical models, create dynamic and insightful visualizations, employ machine learning algorithms, and utilize a wide range of other computational tools.
**1:03PM G07.00010: Relating to Students via Simulation of Cutting Edge Experimental Physics (Virtual RIXS)**  
TODD HOLDEN (Presenter), Physics, Queensborough Community College of CUNY — In contrast to other fields, it is difficult to satisfactorily explain the work of a modern day research physicist to an undergraduate physics major, even after the sophomore year. This is in large part because quantum mechanics is abstract, difficult, and counterintuitive. As part of a pilot project to address these issues, we present a PhET-based spectroscopy simulator (viewable at https://heldentodd.github.io/phetsims/RIXS-simulator/RIXS-simulator_en.html) and some related pedagogical materials for formal and informal education. Currently the simulator is geared toward exploring discoveries enabled by the recent advances in resonant inelastic x-ray scattering (RIXS). This allows us to introduce ideas in advanced materials physics (electronic properties) to second year physics students as part of their mainstream curriculum, as well as to give students a better idea of modern physics research. Emphasis has been placed on developing basic concepts such as energy, momentum, electric fields, and elementary quantum physics. Student and instructor reaction to this project will be discussed, along with future education and dissemination projects aimed at both higher and lower level students.

**1:15PM G07.00011: Controlled Studies of Stereoscopic Virtual Reality in Freshman STEM Classes**  
JONATHAN BROWN (Presenter), CHRISTOPHER D PORTER, JOSEPH R SMITH, CHRIS ORBAN, Ohio State Univ - Columbus — Stereoscopic virtual reality (VR) driven by smartphones is a relatively new tool for teaching concepts that rely on detailed three-dimensional visuospatial skills. VR has long been a topic of education research, and smartphone-driven VR significantly reduces the barrier to entry for both students and instructors and can be implemented for all students at once in the classroom. However, best practices for effective VR implementation are needed. To this end, we implemented VR interventions for freshmen physics, math, and engineering classes at OSU. In the physics course, our electrostatics VR module covered vector fields. Initially, we compared VR to traditional media, and in a follow-up study, we found that training in VR can have a small but significant effect on learning gains during a VR treatment. In a multivariate calculus course, students chose between various media for viewing content. In the engineering visuospatial thinking course, we found small gains when comparing modules with and without VR treatments. Overall, we find that VR is an effective tool for increasing student engagement, but that learning gains, when present, do not seem to depend on medium. Instead, a key factor is that students have a choice to use media that they are comfortable with.
1:27PM G07.00012: Virtual Reality Simulations for Solid State Physics Education  JAMILEH BEIK MOHAMMADI (Presenter), JOHN SEEFELDT, Loyola University New Orleans — Solid-state physics is considered hard to grasp since it requires a strong background in math and quantum mechanics. Even with a solid knowledge of math and quantum mechanics, it is still challenging to visualize the three dimensional and even complicated two-dimensional structures. In the meantime, the spatial visualization of crystals is critical to understand the symmetries of a physical system.

We have utilized virtual reality simulations to improve the students' spatial visualization ability and help them to have a more interactive learning experience in a solid-state physics context. In this talk, I will present on the details of how virtual reality simulations are used as a virtual lab [1] to build different types of crystals and associate the lattice structure with the physical properties such as magnetic and electronic properties of solids.


1:39PM G07.00013: Teaching Women's History in Physics  BETH PARKS (Presenter), Physics and Astronomy, Colgate University — Much effort has been expended to uncover contributions by women in physics and publicize examples of female physicists to students, largely to help female students see themselves in physics. However, the physicists who formulated the ideas taught in college courses were almost all men, and women's absence from these important roles will be noted by students. If we don’t acknowledge and address their absence, then female students won't feel fully supported in their decision to become physicists, since they'll see women only in less influential roles. We need to discuss the social context in which these most influential physicists worked. Since the necessary combination of educational opportunities, family support, social acceptance, financial means, and employment opportunities were available to a much smaller fraction of women than men, it's no surprise that a small fraction of discoveries were made by women. This talk will present a brief sampling of history, looking at the opportunities of three important male physicists—James Clerk Maxwell, Robert Millikan, and Albert Einstein—and comparing them to their female peers. Instructors might use a few minutes of class time to discuss this disparity, and simultaneously open the door to discussions of current social conditions.
Students in physics classes have the skills and background to add high-quality content to Wikipedia while gaining depth of knowledge about the subject and taking ownership of their learning experience. Since 2014, university students in physics and engineering classes have added over 400,000 words to Wikipedia articles using tools and support provided by Wiki Education, a nonprofit organization dedicated to improving Wikipedia's quality, equity, and reach. These articles were viewed over 7.5 million times in the semesters in which the students were active.

We will discuss our experience running assignments (Vershinin) and the overall impact of the program (Ramjohn). Attendees will gain insight into the benefits of trying this assignment in their courses, and will leave with information about getting started.

Tuesday, March 3, 2020 11:15 AM - 1:15 PM

Session G10 GIMS: Detectors, Sensors, and Transducers 108 - Roger Proksch, Asylum Research

11:15AM G10.00001: Semiconductor Particle Detector based on Work Function Modulation*

ELAINE RHOADES (Presenter), WILLIAM HUNT, AARON GREEN, Georgia Inst of Tech — A novel type of solid state particle detector has been designed and investigated. The essential design is a bandgap reference circuit with a Schottky diode comprised of gallium nitride, a semiconducting piezoelectric material, designed to output the Schottky barrier height. As a semiconductor, this material exhibits an electrical response to high-energy particle impingement through the creation of electron-hole pairs. It also exhibits an additional and very unique type of response to lattice vibrations induced in the crystal lattice by momentum transfer from the incident particle. These acoustic waves create mechanical strain which induces an in-phase signal via the piezoelectric effect, which subsequently modulates the effective barrier height of the Schottky diode. This talk presents functional demonstration of a prototype circuit and transient responses to neutron irradiation.

*This material is partially based upon work supported by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists, Office of Science Graduate Student Research (SCGSR) program. The SCGSR program is administered by the Oak Ridge Institute for Science and Education (ORISE) for the DOE. ORISE is managed by ORAU under contract number DE-SC0014664.
11:27AM G10.0002: Characterization of Micro-Magnets on Mechanical Oscillators, and Other Sensors Using Fiber-Optic Interferometry*  
PETER W. KAMPSCHROEDER (Presenter), SIERRA M CASTEN, NIMISHA RAMPRASAD, ALLEN C. WEN, SCOTT S. WILLIAMS, JOHN T. MARKERT, Department of Physics, The University of Texas at Austin — We report the design, construction, and use of a fiber-optic interferometer system with variable applied dc and ac magnetic fields and magnetic field gradients for the characterization of micro-magnets on oscillators. The system has measured calibrated displacements to determine resonant frequencies (~1–800 kHz), quality factors (~100–8000), amplitudes, and spring constants (~0.01 N/m) of resonances. Thermal-noise-driven data determined spring constants. The driven response to ac magnetic field gradients (amplitudes ~0.4–40 x10⁻⁴ T/m) provided direct measurement of magnetic moments. E.g., for a ~45±5-µm-diameter permalloy sphere, we measure a magnetic moment of 2.8±0.1 x10⁻⁸ J/T, in agreement with the expected saturation moment of 3.1±0.6 x10⁻⁸ J/T. Characterization of these micro-magnets supports our nuclear magnetic resonance force microscopy (NMRFM) studies. In addition to NMRFM, other ongoing work involving fiber-optic interferometry includes its use in integrated, narrow (~0.2–2 mm Φ) oscillator-fiber sensors for placement in thin channels (e.g., for fast, local quench detection) and its use in a fast-response pressure sensor for operation under extreme (jet/rocket engine) conditions.

*Support from University of Texas, College of Natural Sciences Freshman Research Initiative.

11:39AM G10.00003: Secondary Electron Count Imaging in a Scanning Electron Microscope*  
AKSHAY AGARWAL (Presenter), JOHN SIMONAITIS, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, VIVEK GOYAL, Department of Electrical and Computer Engineering, Boston University, KARL BERGGREN, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology — We have implemented secondary electron (SE) count imaging on a Zeiss LEO 1525 scanning electron microscope (SEM). We established the signal level of single SEs using two methods – image histograms and oscilloscope outcoupling. In both methods, we imaged a uniform sample of aluminum at low beam currents (< 5 pA) and pixel dwell times between 500 ns and 7 µs using both the in-chamber and in-lens SE detectors. In the first method, histograms of the sample images showed distinct peaks corresponding to the number of SEs emitted from each pixel. We used these peaks to establish the single SE signal level and calculated the detective quantum efficiency of our detectors. In the second method, we outcoupled the signal from our SE detectors to a 2 GHz oscilloscope. The output signal trace showed a sequence of pulses of mean duration 180 ns, corresponding to single SEs. Histograms of the total area of the output signal matched the image histograms for the same pixel dwell time. Finally, we synchronized data capture on the oscilloscope with the SEM scan signal to generate SE count images, which showed an improved signal-to-noise ratio compared to conventional images.

*We acknowledge funding from the Gordon and Betty Moore Foundation and the U.S. NSF under Grants 1422034 and 1815896.
11:51 AM G10.00004: Bio-Inspired MEMS Direction Finding Underwater Acoustic Sensor Operating in Neutral-Buoyant Configuration* LELAND MCCARTY (Presenter), JAEHYUN PARK, FABIO ALVES, GAMANI KARUNASIRI, The Naval Postgraduate School — MEMS acoustic sensors were developed based on the mechanically coupled auditory structure of the *Ormia Ochracea* fly in order to enhance underwater directional sound-sensing technologies. MEMS directional acoustic sensors consist of two wings connected by a bridge in the middle. The entire mechanical structure is connected to a substrate using two torsional legs. The mechanical vibrations under sound excitation is transduced to an electrical signal using interdigitated comb finger capacitors attached to the edges of the wings. This presentation covers the design, fabrication, and characterization of *Ormia*-based MEMS directional acoustic sensor operated underwater as an inertial sensor. The sensors were designed using FE modeling tools and fabricated using commercially available MEMSCap SOIMUMPS processes. Characterization was performed in air and underwater, showing the predicted frequency and directional responses. For underwater operation, the sensors were housed in a near-neutral-buoyant, hermetically sealed enclosure. Results indicate that the MEMS acoustic sensor’s microphone characteristics are preserved when operated as accelerometers, and they have a great potential to be used for underwater applications in a neutral-buoyant configuration.

*Supported by ONR.

12:03 PM G10.00005: New system for high sensitivity study of magnetoelectric effects* ALI SIRUSI, MARC LEWKOWITZ (Presenter), JOHNNY ADAMS, RUYANG SUN, NEIL SULLIVAN, Department of Physics and The Center for Molecular Magnetic and Quantum Materials, University of Florida — We report a novel experimental technique for studying magnetoelectric couplings in matter using a tunnel diode to power a specially designed coil cell. The system can detect small changes in frequency of 0.5 ppm, allowing precise measurement of magnetic susceptibility induced by an applied electric field. This system operates over a temperature range from 1.8 K to 100 K, while maintaining the tunnel diode at superfluid helium temperature. The aim of this device is to study magnetoelectric couplings in molecular magnets and spin crossover systems.

*This work was supported as part of the Center for Molecular Magnetic Quantum Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0019330.
12:15PM G10.00006: Performance of superconducting nanowire single photon detectors in strong magnetic fields

TOMAS POLAKOVIC (Presenter), Physics Division, Argonne Natl Lab,
VOLODYMYR YEFREMENKO, High Energy Physics Division, Argonne Natl Lab, JOHN PEARSON, Materials Science Division, Argonne Natl Lab, WHITNEY ARMSTRONG, ZEIN-EDDINE MEZIANI, KAWTAR HAFIDI, Physics Division, Argonne Natl Lab, GORAN KARAPETROV, Department of Physics & Department of Materials Science and Engineering, Drexel University, VALENTYN NOVOSAD, Materials Science Division & Physics Division, Argonne Natl Lab — Superconducting nanowire single photon detectors (SNSPD) have found applications in many fields, including nanophotonics, quantum communication and computing. There is potential in applications in high energy physics, but operation in high magnetic fields is required.

We study the performance of SNSPDs in high magnetic fields by implementing superconducting type-II materials with high upper critical fields and critical currents. Using the recently developed ion-beam assisted sputtering method[1], we fabricate Niobium Nitride SNSPDs on non-epitaxial substrates using a two-step process, and perform optoelectronic characterization across a wide range of magnetic fields. We demonstrate performance with zero dark counts and saturated internal quantum efficiency in fields of up to 8 T for visible wavelength photons with no need for changes to the common meander geometry[2].


*This work was supported by the U. S. Department of Energy (DOE), Office of Science, Offices of Nuclear Physics, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract # DE-AC02-06CH11357.
A portion of this work was conducted at the Center for Nanoscale Materials, a U.S. Department of Energy, Office of Science (DOE-OS) user facility.

12:27PM G10.00007: High Sensitivity Photodetector Based on Graphene-Germanium Quantum Dot

YIFEI WANG (Presenter), HO VINH, PRASHANT PRADHAN, DANIEL SEITZ, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech, MICHAEL P. COONEY, NASA Langley Research Center, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — Graphene has shown great potential for realizing optoelectronic devices, especially for photodetectors. Here, we experimentally demonstrate a fabrication of photodetector based on graphene-germanium quantum dots that can detect a broadband spectrum from visible to infrared region. The device, based on graphene-germanium quantum dots, demonstrates an improved responsivity and response time. Characteristically, the fabricated photodetector shows a responsivity of 1,500 A/W at room temperature and a fast photoresponse time in the order microseconds. The results address key challenges for broadband photodetectors in the visible to infrared region, and also are promising for the development of graphene-based optoelectronic applications.

*Supported by the Earth Science Technology Office (ESTO), NASA
Advanced thermal readout techniques for ac voltage metrology

JOSEPH HAGMANN (Presenter), NIKOLAI KLIMOV, JASON M UNDERWOOD, STEFAN CULAR, National Institute of Standards and Technology — One of the most accurate methods for quantifying ac voltage amplitude to compare the rms amplitude of an ac waveform to an equivalent dc voltage using a device called a multi-junction thermal converter (MJTC). The MJTC produces a dc output voltage in response to the temperature rise from Joule heating due to electrical power dissipation in a resistive heater. The uncertainty of an MJTC measurement is about 1 µV/V (1 ppm) for voltages in the range of 0.5 V to 10 V and frequencies in the range of 40 Hz to 20 kHz. Conventionally, the rise in temperature due to Joule heating is measured on the MJTC by an array of thermocouples. Although well-established, this type of readout suffers is made challenging by the relatively large resistance (~10kΩ) of the thermocouple array, and the low (several mV) thermovoltage. Here, we present our research into alternative measurement techniques based on physical phenomena such as infrared emission, superconductivity, and photonics in order to achieve improved stability and sensitivity and to extend the voltage and frequency range in which the measurement is accurate, bridging fundamental research with the engineering problems of harnessing useful physics to achieve advanced measurement technology.

Measurement of Alzheimer’s Enzymes at Physiological Concentrations with Solid-State Dual-Gate 2D-MoS2 Transistors

SON LE (Presenter), NIST & Theiss Research, NICHOLAS B. GUROS, National Institute of Standards and Technology, NIRANJANA AMIN, HARISH C PANT, National Institutes of Health, ARVIND BALIJEPALLI, CURT RICHTER, National Institute of Standards and Technology —

We have developed sensors based on ionic liquid gated field-effect transistors (FETs) operating at the quantum capacitance limit that allow ultrasensitive pH measurements for biophysics applications [1]. To improve the durability and accessibility of the devices for the broader biological research community, we have recently developed a solid-state version of these high-performance devices and applied it to measure the activity of enzymes relevant to Alzheimer’s disease. The FETs are fabricated with a single-monolayer of the 2D transition metal dichalcogenide MoS2 and are top-gated with a high-k dielectric gate oxide. The asymmetric capacitive coupling between the high- k top-gate and the back-gate dielectric (substrate oxide) enables amplification of a voltage applied to the top gate by up to a factor of 8. We leveraged the high performance of the devices to enable pH measurements with sensitivities that exceed the Nernst value of 59 mV/pH at room temperature. The improved sensitivity allows the detection of pH changes as small as 0.004. We demonstrate that this enhanced sensitivity facilitates the measurement of activity and kinetics of enzyme-catalyzed phosphorylation of substrate proteins at physiological concentrations.

1:03PM G10.00010: Twin slot antenna coupled graphene THz heterodyne mixer*  
JAYAPRAKASH POOJALI (Presenter), FRANCOIS JOINT, ASHRAF ALI, KEVIN DANIELS, THOMAS E. MURPHY, HOWARD DREW, University of Maryland, College Park — The unique hot electron properties of graphene make it an ideal platform for terahertz (THz) heterodyne mixers. However, prior graphene-based heterodyne mixers are designed to operate at cryogenic temperatures and show poor performance above 4 K. In this work, we describe the design of a room temperature graphene based heterodyne mixer optimized to work in the THz spectral range of interest to space based astronomy. The proposed mixer is coupled to a twin slot antenna and a coplanar waveguide transmission line with an impedance matching network. Numerical simulation predicts that the coupling efficiency of the incoming radiation to the graphene mixer is over 90% at 1 THz. The mixer has a predicted intermediate frequency bandwidth of 100 GHz with 90% coupling efficiency. Further, the proposed optimized antenna can match graphene device impedances from 70 Ω – 250 Ω by optimizing the slot width of the antenna. Epitaxial grown quasi-free-standing graphene on silicon carbide substrate was used and it is integrated with a silicon lens. We are currently characterizing the IF mixing bandwidth of our heterodyne mixer at various temperatures and plan to calibrate its sensitivity.

*Supported by: NASA, # 80NSSC18K0933

Tuesday, March 3, 2020 11:15 AM - 1:15 PM

Session G15 DFD DSOFT: Active Colloids I 210/212 - Arvind Gopinath, University of California, Merced

11:15AM G15.00001: Active Microrheology, Hall Effect, and Jamming in Active Chiral Fluids
CYNTHIA REICHHARDT (Presenter), CHARLES REICHHARDT, Los Alamos Natl Lab — We examine the motion of a probe particle driven through an active chiral fluid composed of circularly swimming disks. We find that the probe particle travels in both the longitudinal direction, parallel to the driving force, and in the transverse direction, perpendicular to the driving force, giving rise to a Hall angle. Under constant driving force, we show that the probe particle velocity in both the longitudinal and transverse directions exhibits nonmonotonic behavior as a function of the activity of the circle swimmers. The Hall angle is maximized when a resonance occurs between the frequency of the chiral disks and the motion of the probe particle. As the density of the chiral fluid increases, the Hall angle gradually decreases before reaching zero when the system enters a jammed state. We show that the onset of jamming depends on the chiral particle swimming frequency, with a fluid state appearing at low frequencies and a jammed solid occurring at high frequencies.
11:51AM G15.00002: Hydrodynamic Spin Lattices* PEDRO J SAENZ (Presenter), UNC Chapel Hill, GIUSEPPE PUCCI, Institut de Physique de Rennes, SAM E TURTON, RUBEN R. ROSALES, JORN DUNKEL, JOHN W M BUSH, MIT — In this talk, we introduce hydrodynamic spin lattices (HSLs) of walking droplets as a new class of highly tunable active spin analog systems. Millimetric liquid droplets can walk across the surface of a vibrating fluid bath, self-propelled through a resonant interaction with their own guiding wave fields. A walking droplet, or walker, may be trapped by a submerged circular well at the bottom of the fluid bath, leading to a clockwise or counterclockwise angular motion centered at the well. When a collection of such wells is arranged in a 1D or 2D lattice geometry, a thin fluid layer between wells enables wave-mediated interactions between neighboring walkers. For sufficiently strong pair-coupling, wave interactions between neighboring droplets may induce local spin flips leading to ferromagnetic or antiferromagnetic order. Transitions between these two forms of magnetic order can be induced through variations in non-equilibrium driving, lattice geometry and Coriolis forces mimicking an external magnetic field. Our experimental results agree with theoretical predictions from a generalized Kuramoto model, establishing HSLs as a generic paradigm for active phase oscillator dynamics with complex particle-wave coupling.

*NSF CMMI-1727565

12:03PM G15.00003: Emergence of multi-vortex states in swarms of active magnetic rollers* KOOHEE HAN (Presenter), Materials Science Division, Argonne National Laboratory, GAŠPER KOKOT, Northwestern Argonne Institute of Science and Engineering, ANDREAS GLATZ, ALEXEY SNEZHKO, Materials Science Division, Argonne National Laboratory — Active matter represents an emergent class of out-of-equilibrium dissipative systems demonstrating complex self-organization, collective behavior, and tunable functionalities. In both artificial and biological active systems, the vortex phase is of great interest because of its spontaneous emergence from a translational motion of elementary units and its ability to maintain the emergent dynamic structures. However, the generation of long-lived multi-vortex states without geometrical confinement has been challenging. We report that flocking magnetic rollers driven by a vertical a.c. magnetic field [1,2] can form long-lived multi-vortex states in an unconfined environment. We reveal that the absence of confining boundaries allows the emergence of multiple vortices with a wide distribution of vortex size and angular speed. In addition, these vortices exhibit equal probability distribution of clockwise or counterclockwise rotation with characteristic opposite chiralities of nearest neighboring vortices.


*The research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.
12:15PM G15.00004: Controlled Self-Assembly of Vortex in Ensembles of Active Magnetic Rollers*  
ANDREY SOKOLOV (Presenter), GAŠPER KOKOT, ALEXEY SNEZHKO, Argonne National Laboratory — Magnetically driven colloids, an example of active matter, are able to demonstrate complex collective behavior and self-organize into coherent dynamic patterns via short- and long-range interactions. Here we present a method for guided self-assembly of ferromagnetic rolling particles energized by a uniform AC magnetic field into a stationary vortex via magnetic interaction with an additional strongly localized magnetic field. By tuning the parameters of the additional field we effectively control vortex dimensions, internal order, and a number of entrapped rollers. We find that vortex self-organization is assisted by field-induced magnetic steering and controlled by a phase shift between alternating magnetic fields. The presented method for assisted self-organization of rolling colloids into a vortex with on-demand characteristics suggests a new paradigm for active matter control and may lead to the development of new approaches for microscopic transport in active particles systems.

*This work was supported by the US DOE, Office of Basic Energy Sciences, Division of Materials Science And Engineering, under contract No. DE AC02-06CH11357

12:27PM G15.00005: Self-phoretic helical colloids  
WILLIAM USPAL (Presenter), RUBEN POEHNL, Mechanical Engineering, University of Hawai‘i at Manoa — Chemically active colloids self-propel by catalyzing the decomposition of molecular "fuel" available in the surrounding solution. If the various molecular species involved in the reaction have distinct interactions with the colloid surface, and if the colloid has some intrinsic asymmetry in its surface chemistry or geometry, there will be phoretic flows in an interfacial layer surrounding the particle, leading to directed motion. Most studies of chemically active colloids have focused on spherical, axisymmetric “Janus” particles, which (in the bulk, and in absence of fluctuations) simply move in a straight line. For particles with complex (non-spherical and non-axisymmetric) geometry, the dynamics can be much richer. Here, we consider chemically active helices and helix-sphere dimers. Via numerical calculations and slender body theory, we study how the translational and rotational velocities of the particle depend on geometry and the distribution of catalytic activity over the particle surface. Significantly, we find that both tangential and circumferential concentration gradients contribute to the particle velocity, and that the relative importance of these effects, which can be tuned by varying the particle geometry, determines the topology of the surrounding flow field.
Microorganisms exhibit autonomous locomotion through complex media and can react to changes in their environment. *Leptospira* bacteria, for example, swim towards regions of high viscosity [1]. This ability of bacteria and living cells to adapt their motion in response to external stimuli is called taxis [2]. While different kinds of taxis have been studied, most notably chemotaxis, the mechanism behind viscotaxis was not investigated until recently. Liebchen et al. found that swimmers with nonuniaxial body shapes swim up viscosity gradients due to the generation of asymmetric viscous torques acting on different parts of the swimmer [3]. We are testing these theoretical predictions using artificial microswimmers created by 3D printing based on two-photon lithography that gives us access to virtually any shape. We have started with the fabrication of trimers on the micrometre scale, the simplest form of a nonuniaxial body shape, but we are also exploring the motion of other nonuniaxial swimmers such as starships.


To develop active nanomaterials that can instantly respond to external stimuli with designed mechanical motions is an important step towards the realization of nanorobots. Herein, we present our finding of a versatile working mechanism that allows instantaneous change of alignment direction and speed of semiconductor nanowires in an external electric field with simple visible-light exposure. The light induced alignment switch can be cycled over hundreds of times and programmed to express words in Morse code. With theoretical analysis and simulation, the working principle can be attributed to the optically tuned real-part (in-phase) electrical polarization of a semiconductor nanowire in aqueous suspension. The manipulation principle is exploited to create a new type of microscale stepper motor that can readily switch between in-phase and out-phase modes, and agilely operate independent of neighboring motors with patterned light. This work could inspire the development of new types of micro/nanomachines with individual and reconfigurable maneuverability for many applications.

*We are grateful for the support of NSF via the CAREER Award (grant no. CMMI 1150767 and intern supplement) and research grant (EECS-1710922) and Welch Foundation (grant no. F-1734).
1:03PM G15.00008: Bulk Viscosity of Dilute Gases using Nonequilibrium Molecular Dynamics Simulations  BHANUDAY SHARMA (Presenter), RAKESH KUMAR, Department of Aerospace Engineering, Indian Institute of Technology Kanpur, India — Recent studies have reported that bulk viscosity, $\mu_b$, may play an important role in several fluid mechanical phenomena including fluid instabilities, turbulence, and hypersonic flows. However, accurate estimation of $\mu_b$ is a challenging task and relies on indirect techniques like acoustic spectroscopy, Rayleigh-Brillouin scattering, and Green-Kubo method. These techniques have several limitations. In the present work, a new method is proposed for the estimation of the bulk viscosity of dilute gases using nonequilibrium molecular dynamics simulations. In this method, the fluid is expanded or compressed with a known expansion/compression rate ($\nabla \cdot v$), where $v$ is the velocity of the fluid. During this volume change process, mechanical ($p_{\text{mech}}$) and thermodynamic pressures ($p_{\text{thermo}}$) are estimated using instantaneous translational and total kinetic energy, respectively. The $\mu_b$ is then obtained by the relation: $\mu_b = (p_{\text{thermo}} - p_{\text{mech}}) / \nabla \cdot v$. The proposed method is applied to estimate the $\mu_b$ of dilute nitrogen gas. The results are compared with available experimental data and a good agreement is observed. Effects of temperature, pressure, rate and direction (i.e., expansion or compression) of volume change, and humidity on $\mu_b$ are reported. (Sharma, B., & Kumar, R., Phys. Rev. E 100, 013309)

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G16 DQI: DQI Invited Session: Experimental Advances in Quantum Sensors and Sensing 201 - Kater Murch, Washington University, St. Louis - Tag(s): Invited, Undergrad Friendly

11:15AM G16.00001: Quantum metrology methods for dark matter searches* [Invited]  KONRAD LEHNERT (Presenter), JILA and Physics, University of Colorado, Boulder — Can emerging quantum technologies speed up the search for dark matter? For the case of ultralight dark matter particles with rest mass energies of an meV or less, they can. In particular, laboratory searches for such hypothetical particles attempt to sense a persistent, oscillatory, and classical dark matter signal acting on a quantum harmonic oscillator. Not only can emerging quantum technologies measure the oscillator's motion at the quantum limit, but they can also circumvent that quantum noise in an inference of the classical signal. I will describe the particular case of axionic dark matter, in which superconducting quantum circuits can be used to search for dark matter at a rate exceeding the quantum-limited value.

*This work was supported by the National Science Foundation, under Grants No. PHY-1607223 and No. PHY-1734006 and the Deparment of Energy QuantISED project.


1:03PM G16.00004: Morgan W Mitchell Invited Talk [Invited] —
11:15AM G17.00001: RuleSet-based Operation of the Quantum Internet* [Invited] RODNEY VAN METER (Presenter), Keio Univ — The challenges in building a Quantum Internet extend far beyond having a physical layer that can create entanglement across a distance. Quantum Internet nodes must share management of distributed tomography, errors, entanglement swapping, multiplexing of resources, selection of routes, and more to support application-requested actions for distributed cryptographic functions, quantum sensor networks, and distributed quantum computation. RuleSet-based operation allows for single-point but any-location decisions on policy for a connection and distributed, real-time selection of actions consistent with those policies. Only such an architecture will provide the full flexibility needed to support inter-technology, inter-organizational communications on a long-lived, multi-generational Quantum Internet.

*This material is based upon work supported by the Air Force Office of Scientific Research under award number FA2386-19-1-4038.

11:51AM G17.00002: Resource-efficient quantum communication using all-photonic graph states generated from quantum emitters* PAUL HILAIRE (Presenter), EDWIN BARNES, SOPHIA ECONOMOU, Virginia Tech — The emergence of quantum communication technologies shows great promise for applications ranging from the secure transmission of secret messages to distributed quantum computing. Due to fiber losses, long-distance quantum communication requires the use of quantum repeaters, for which there exist quantum memory-based schemes and all photonic schemes. While all-photonic approaches based on graph states generated from linear optics avoid coherence time issues associated with memories, they outperform repeaterless protocols only at the expense of a significant overhead in resources. Here, we consider using quantum emitters to produce the graph states and show how the resource/performance trade-off can be optimized to yield a protocol that outperforms both repeaterless and memory-based schemes. Our results should pave the way towards the practical implementation of both resource-efficient and fast long-distance quantum communication.

*This research was supported by NSF (GrantNo. 1741656).
12:03PM G17.00003: Stable Polarization Entanglement based Quantum Key Distribution over Metropolitan Fibre network* YICHENG SHI (Presenter), MOE THAR SOE, HOU SHUN POH, JAMES ANTHONY GRIEVE, CHRISTIAN KURTSIEFER, ALEXANDER LING, Centre for Quantum Technologies, National University of Singapore — We demonstrate a Quantum key distribution (QKD) system implemented with polarisation-entangled photons over telecom fibre network. The photon pairs are generated at telecom O-band with one side propagating through 10 km of deployed fibre. Drift of polarisation state over fibre is compensated using liquid crystal variable retarders to minimize the Quantum Bit Error Rate (QBER). This ensures stable, continuous QKD operation with an average QBER of 6.4% and a final key rate of 109 bits/s.

*This research is supported by the National Research Foundation, Prime Ministers Office, Singapore under its Corporate Laboratory@University Scheme, National University of Singapore, and Singapore Telecommunications Ltd.

12:15PM G17.00004: Experimental Study of an Elementary Cryogenic Microwave Quantum Network* PAUL MAGNARD, PHILIPP KURPIERS, JANIS LÜTOLF, FABIAN MARXER, SIMON STORZ (Presenter), JOSUA SCHÄR, ANDREAS WALLRAFF, ETH Zurich — Scaling up quantum computers can follow two routes in parallel: increasing the computing power of single processors, and connecting multiple processors into quantum networks using chip-to-chip deterministic quantum protocols. In both cases, modularity is a key concept. Similarly, the space available at cryogenic temperatures and cooling power needed for superconducting quantum processors can be scaled-up in a modular way by connecting dilution refrigerators into cryogenic networks. In this talk, we present an experimental study of essential elements of a cryogenic quantum network. Based on a modular design, we realize a proof-of-concept, cryogenic link between two network nodes. We thoroughly analyze the thermal properties of the link elements and extrapolate to distance scales which appear attainable in the presented approach. We also report progress toward transferring quantum information between nodes of the network.

*This work is supported by the European Research Council (ERC) through the "Superconducting Quantum Networks" (SuperQuNet) project, by the National Centre of Competence in Research "Quantum Science and Technology" (NCCR QSIT), a research instrument of the Swiss National Science Foundation (SNSF), and by ETH Zurich.
12:27PM G17.00005: Rapid transfer of a qubit state into a microwave pulse using a notch Purcell filter*  
YOSHIKI SUNADA (Presenter), The University of Tokyo, SHINGO KONO, RIKEN, JESPER ILVES, SHUHEI TAMATE, YUTAKA TABUCHI, YASUNOBU NAKAMURA, The University of Tokyo — Modules in a distributed quantum computer need to communicate rapidly and coherently with each other. A recent implementation [1] involves transferring the quantum state between a superconducting qubit and an itinerant microwave pulse. To realize high-speed communication with this scheme, the qubit has to be coupled to a waveguide via a low-Q resonator. However, this increases the energy decay rate of the qubit through the Purcell effect. To break this trade-off, a Purcell filter with a high extinction ratio is required. Here, we use a notch filter to demonstrate the rapid transfer of a qubit state into a microwave pulse. The Purcell decay is suppressed by the destructive interference between multiple decay paths through a multi-mode resonator. This is realized in a simple device with one port and one coaxial transmission line resonator [2]. We report our progress on analyzing the filter performance and the fidelity of the state transfer.


*This work is partly supported by MEXT Q-LEAP (JPMXS0118068682), JST ERATO (JPMJER1601), JSPS KAKENHI (26220601), and UTokyo XPS.

12:39PM G17.00006: A genuine quantum router for microwave photons  
ZHILING WANG (Presenter), ZENGHUI BAO, YUKAI WU, HONGYI ZHANG, YIPU SONG, LUMING DUAN, Tsinghua University — A quantum router uses a control qubit to direct the signal qubit to a certain address, which could take a quantum superposition depending on the quantum state of the control qubit. As the elementary building block of a quantum network and a quantum random access memory, the development of a quantum router may accelerate many research fields like quantum entanglement distribution and quantum machine learning. In recent years, many attempts have been made to realize a quantum router in the optical domain. In this talk, I will introduce our experiments of realizing a genuine quantum router in the microwave domain based on superconducting circuit quantum electrodynamics system and demonstrate the coherent routing of a microwave quantum state with high fidelity using a transmon qubit.
12:51PM G17.00007: Quantum communication networks with superconducting qubits*
YOUPENG ZHONG (Presenter), AUDREY BIENFAIT, HUNG-SHEN CHANG, MING-HAN CHOU, CHRISTOPHER R CONNER, University of Chicago, ETIENNE DUMUR, Argonne National Laboratory; University of Chicago, JOEL GREBEL, RHYS G POVEY, DAVID I SCHUSTER, University of Chicago, ANDREW CLELAND, Argonne National Laboratory; University of Chicago — Deterministic state transfer and remote entanglement with microwave photons has recently been demonstrated using different superconducting circuit approaches. More recently, a qubit-to-qubit transfer fidelity greater than 94% has been achieved in Ref. [1]. This experiment used gmon tunable couplers to control the coupling of the qubits to a 0.78 m long transmission line, achieving few nanosecond tuning speed and large tuning range, thereby allowing for the violation of Bell's inequality in a superconducting quantum communication architecture. In this talk, we examine the scalability of this architecture, and explore more complex quantum communication network designs and protocols.


*This work is supported by AFOSR MURI (FA9550-15-1-0029), UChicago MRSEC (NSF DMR-1420709), DOE, UChicago PNF via SHyNE (NNCI NSF -1542205), ARL (W911NF-15-2-0058), and ANL.

1:03PM G17.00008: Unidirectional emitter and receiver of an itinerant microwave photon in an open waveguide*
NICOLAS GHEERAERT, RCAST, The University of Tokyo, SHINGO KONO (Presenter), CEMS, RIKEN, YASUNOBU NAKAMURA, RCAST, The University of Tokyo — Quantum networks based on itinerant microwave photons can be an alternative approach toward a large-scale superconducting quantum computing. Recently, there have been several implementations of quantum state transfer between two localized superconducting qubits. Toward more complex networking, the control of the propagation direction of itinerant photons, such as routing, switching or circulating, is demanded. Here, we theoretically demonstrate unidirectional emission and absorption of an itinerant microwave photon in an open waveguide using a unit consisting of two superconducting qubits that are parametrically coupled to the waveguide via transfer resonators a quarter-wavelength apart. Upon preparing an appropriate entangled state of the two qubits, a photon is then unidirectionally and deterministically emitted to the open waveguide, as a result of the destructive interference — on the right or left of the device — of the radiation emitted from each qubit in both directions. We also show that this two-qubit system is able to deterministically receive a photon arriving from either direction of the waveguide, which cannot be realized with a single qubit.

*This work is partly supported by JSPS KAKENHI (18F18799), JST ERATO (JPMJER1601), and MEXT Q-LEAP (JPMXS0118068682).
Modular networks present a compelling approach to constructing complex quantum machines, but rapid and faithful communication between modules remains a challenge. Reliance on lossy elements such as circulators, hybrids, and connectors have prevented previous demonstrations from taking advantage of the high intrinsic quality of superconducting transmission line links between modules. Here we present an all-superconducting demountable coaxial link which supports low-loss standing-wave modes. We use one of these modes as a quantum bus, coupling two 3D cavity bosonic qubits in separate modules with parametric conversion, and construct a beamsplitter-type transformation between the two cavity modes. This talk will discuss how this flexible operation can be used for bidirectional state transfer and entanglement generation between modules.

*The U.S. Army Research Office (ARO) grant number W911NF-18-1-0212
The U.S. Army Research Office (ARO) – MURI grant number W911NF-16-10349

We use a quantum bus to transfer qubits and generate entanglement across a two-node network. Crucially, both of these operations can be made less sensitive to loss in the bus by encoding information with multiple photons and detecting loss errors. We transfer a bosonic qubit, tracking loss events to preserve the quantum information, achieving an error rate as low as that in a single-photon encoding. Further, we generate entanglement with two-photon interference and postselect against errors with local parity measurements, producing a Bell state with a high success probability and half the error of single photon case. These results provide several approaches for high-fidelity gates in a quantum network.

*This work is supported by U.S. Army Research Office (ARO) grant number W911NF-18-1-0212 and ARO MURI grant number W911NF-16-10349.
Josephson-Photonics Devices as a Source of Entangled Microwave Photons

SIMON DAMBACH (Presenter), School of Physics and Astronomy, University of Nottingham, AMBROISE PEUGEOT, SPEC (UMR 3680 CEA-CNRS), CEA Paris-Saclay, JUHA LEPPÄKANGAS, Physikalisches Institut, Karlsruhe Institute of Technology, BJÖRN KUBALA, Institute for Complex Quantum Systems, Ulm University, MARC WESTIG, GERBOLD MÉNARD, YURI MUKHARSKY, CARLES ALTIMIRAS, PATRICE ROCHE, PHILIPPE JOYEZ, DENIS VION, DANIEL ESTEVE, FABIEN PORTIER, SPEC (UMR 3680 CEA-CNRS), CEA Paris-Saclay, JOACHIM ANKERHOLD, Institute for Complex Quantum Systems, Ulm University — The realization and characterization of efficient sources of entangled microwave photons is of paramount importance for many future applications of quantum technology. Josephson-photonics devices are very promising candidates for this task since they allow one to create a broad range of different entangled states in a surprisingly simple and robust way. These devices consist of a dc-voltage–biased Josephson junction which is placed in series to several microwave cavities. Steady states with multifaceted entanglement properties are reached here naturally due to the interplay of multiphoton creation processes by the Josephson current and subsequent individual photon leakage from the cavities. In this talk, we present a detailed theoretical study of the bipartite entanglement between photon pairs in the output transmission lines. Numerical simulations, taking into account low-frequency fluctuations of the bias voltage and the finite bandwidth of microwave signal detectors, show excellent agreement with recent experimental data.

*This research work is funded by the Center for Integrated Quantum Science and Technology (IQST), the German Research Foundation (DFG) through Grant No. AN336/11-1, the Carl Zeiss Foundation, and the German Academic Exchange Service (DAAD).
**1:51PM G17.00012: Superconducting Qubits for Robust Remote Entanglement via Adiabatic State Transfer**

HUNG-SHEN CHANG (Presenter), YOUPENG ZHONG, AUDREY BIENFAIT, MING-HAN CHOU, CHRISTOPHER R CONNER, University of Chicago; ETIENNE DUMUR, University of Chicago; Argonne National Laboratory, JOEL GREBEL, University of Chicago, GREGORY PEAIRS, University of California, Santa Barbara; University of Chicago, RHYS G POVEY, University of Chicago, KEVIN SATZINGER, University of California, Santa Barbara; University of Chicago, ANDREW CLELAND, University of Chicago; Argonne National Laboratory — Efficient quantum communication between remote quantum nodes relies on high fidelity quantum state transfer and entanglement generation. Loss in the communication channel connecting the quantum nodes can significantly limit the efficiency of these processes. One proposed method to overcome channel loss is to use adiabatic protocols to transfer quantum states without populating the lossy communication channel. Here we construct and operate a superconducting system to test such methods, using two superconducting qubits connected by a 0.73 m long transmission channel, where the channel loss can be externally varied over two orders of magnitude (as measured by the Q of the resonant channel modes). We demonstrate that in the limit of low loss, an adiabatic passage method performs as well as previously demonstrated relay method [1], while in the presence of strong loss, the adiabatic passage achieves states transfer and entanglement fidelities more than a factor of two larger than the relay method.


*This work is supported by AFOSR MURI (FA9550-15-1-0029), UChicago MRSEC (NSF DMR-1420709), DOE, UChicago PNF via SHyNE (NCCI NSF -1542205), ARL (W911NF-15-2-0058), and ANL.

**Tuesday, March 3, 2020 11:15 AM - 2:15 PM**

**Session G18 GSNP: Quantum Biology: Beyond Photosynthesis** 205 - Clarice Aiello, University of California, Los Angeles - Tag(s): Invited
11:15AM G18.00001: Quantum Biology: From Theoretical Principles to Methods of Verification* [Invited] MARTIN PLENIO (Presenter), Institute of Theoretical Physic and Center for QuantumBioSciences, Ulm University — With the improvement of experimental technique, recent years has seen the emergence of the field of quantum biology that unfolds at the interface of the quantum and the life sciences. This field examines several broad lines of development. First, it aims to explore the possible role of quantum dynamics in fundamental processes of life and has led theory to the discovery of a range of underlying principles that may support such processes, notably, the highly non-trivial interplay of quantum coherence and environmental noise. Secondly, the need for experimental verification of such phenomena provides new impetus to the development of quantum technologies that enable the observation of biological phenomena in hitherto unachieved detail making use for example of ultrafast laser spectroscopy but potentially also quantum sensors such as the NV-center in diamond. Thirdly, biological systems themselves may enable the realisation of new sensor functionalities that make use of the newly discovered theoretical principles such as the interplay of quantum coherent dynamics and noise. In this talk I will present key aspects of these three lines of development.

*This work was supported by the European Research Council Synergy grant BioQ (Grant No. 319130), the EU H2020 Quantum TechnologyFlagship project ASTERIQS (Grant No. 820394), the EUH2020 Project Hyperdiamond (Grant No. 667192) and the BMBF via NanoSpin and DiaPol.

11:51AM G18.00002: New horizons in quantum biology: Plasmon, exciton, and phonon correlations in complex biomolecular systems [Invited] PHILIP KURIAN (Presenter), Howard University — The emergence of supramolecular complexes, biological polymers, and hybrid quantum information processing assemblies from fundamental constituents and interactions involves a delicate interplay between forces of disorder (chaos) and order (logos). Quantum behaviors including electron dispersion, superradiance, and optical-to-phonon transduction have risen to the surface of our nano-, meso-, and macro-scopic perception within the open systems of biology. Extended, many-body van der Waals effects are implicated in the uncanny ability of certain enzymes to synchronize catalysis, and ultraviolet photoexcitations in large (L >> λ), highly symmetrical aggregates reveal collective, cooperative, and coherent properties that are within observational reach (few-picosecond) of ultrafast spectroscopy experiments. Intriguingly, the aqueous environment--matrix of life--challenges purely Brownian descriptions and conspires with biomatter in the precise spatiotemporal orchestration of diverse processes within the living organism. The tantalizing possibility that such ubiquitous quantum phenomena in biology can be exploited in vivo would herald a new era for diagnostic and therapeutic applications in medicine, particularly in complex neurodegenerative diseases without clear biochemical targets.
The electron's spin and chirality, the source for quantum effects in biology* [Invited] RON NAAMAN (Presenter), Weizmann Institute of Science — While the charge of the electron is known to play a major role in biological processes, and charge transfer was investigated extensively, it is usually assumed that the electron's spin does not play any important role. We found that chiral organic molecules can act as spin filters in electron transfer. The new effect, termed Chiral Induced Spin Selectivity (CISS), was found, among others, in biomolecules and in bio-systems.

In nature, very important molecules like proteins and sugars, are chiral. Chiral molecules lack mirror symmetry and they appear in two forms, enantiomers, that are not imposable on each other. Interestingly, all chiral molecules in nature appear basically in one enantiomeric form, while the other form is missing.

The issue of the origin of homo chirality in nature is under extensive debate. Independent on its origin, the question is “why evolution preserves chirality?” Another related question is why electron transfer in Biology occurs through proteins, that are bad conductors, and not through conjugated molecules for example. In other word, an important question is if the chirality in biomolecule serves specific functions that cannot be fulfilled with achiral molecules.

Based on the CISS effect, it will be shown that indeed chirality is essential for many functions in biology and this “topological” property is used by nature at physiological relevant temperatures.

*John Templeton Foundation
Minerva Foundation
VW Foundation
Israel Science Foundation

Proton and electron tunneling effects in enzymes [Invited] ADAM OFFENBACHER (Presenter), East Carolina University — Accumulating evidence supports the quantum mechanical treatment of both electron and proton transfer associated with homolytic C-H bond cleavage reactions catalyzed by natural enzymes. These reactions are quantified and characterized by inflated kinetic isotope effects corresponding to the primary bond cleaved and the corresponding differential enthalpic barrier for the transfer of hydrogen and its heavy isotopes. Herein, select examples will be presented that demonstrate the quantum behavior in enzyme catalysis and highlight how these kinetic tools can be applied to resolve the origins of enzyme reactions.
Quantum-Based magnetic sensing: How can birds detect 10 nT magnetic fields? [Invited] THORSTEN RITZ (Presenter), University of California, Irvine — Migratory birds and other animals can navigate thousands of miles to find their destinations. In this they are aided by a “sixth sense”, i.e. the ability to detect the geomagnetic field. Growing evidence indicates that the threshold of the biological magnetic sensor is on the order of 10 nT. This poses a major challenge for physicists since no mechanism can currently explain how such sensitivity can be realized in a concrete biomolecular system. Light-induced radical-pair reactions can be sensitive to earth-strength magnetic fields and thus may form the basis for the long-sought after magnetic sensors. If this hypothesis was proven, it would be a dramatic demonstration of the use of coherent quantum mechanics to establish biological functionality. We will review the current theoretical questions regarding this mechanism, such as how to design a particularly sensitive receptor system, the role of noise, symmetries and dealing with decoherence before turning to experimental evidence for this hypothesis. We will present a roadmap of key steps that will ultimately enable us to prove or disprove the now nearly twenty year old suggestion that cryptochromes may be the magnetoreceptor molecule and the even older suggestion of a radical-pair mechanism underlying magnetic sensing.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G19 DPOLY: Revealing the Microscopic Dynamics Driving Nonlinear Polymer Flows

11:15AM G19.00001: Self-Healing Recovery and Dynamics of Associating Polymers under Uniaxial Extension [Invited] NICOLAS ALVAREZ (Presenter), ZACHARY R HINTON, Drexel Univ — Associating polymers are a desirable class of materials with intrinsic abilities to self-heal without the need for additional components or added stimulus. While experimental and theoretical measurements of recovery exist in the literature, quantifying recovery in terms of fundamental rheological parameters is often difficult. In this work we use filament stretching uniaxial extension to probe the recovery of unentangled and entangled hydrogen bonding polymers. Using a novel methodology, we confirm the role of process timescales such as the time before and after recovery on both the transient rheology and ultimate recovery of associating polymers. Furthermore, we show the importance of architecture and molecular timescales of the network on recovery. We find that while strongly associating groups provide improved mechanical strength, they often delay the process of recovery. Additionally, we show that the presence of entanglements has a complex role on recovery, introducing the flow timescale as an additional parameter. With this work, we develop a framework that is both useful for evaluation of self-healing soft materials and for design of novel self-healing polymers.
11:51AM G19.00002: Decoding the viscoelastic response of monodisperse and bidisperse linear polymers under uniaxial extension [Invited]  EVELYN VAN RUYNBEKE (Presenter), CELINE HANNECART, ALEXIS ANDRE, TAISSIR SHAHID, Bio and Soft Matter, IMCN, Université catholique de Louvain — Predicting the linear viscoelastic properties of linear polymers has reached a quantitative level, based on mesoscopic approaches such as slip-link models or the Doi-Edwards tube-model theory combined with established relaxation mechanisms such as reptation, contour length fluctuations and constraint release. A consistent molecular picture could be proposed for describing the linear regime, which allows explaining the different experimental data based on the same framework. In particular, in case of polymer chains diluted in an oligomer matrix, the universality of linear viscoelastic response of polymers has been demonstrated with different chemical structures and concentrations: as long as the chains contain the same number of entanglements, their normalized viscoelastic properties will be the same.

On the contrary, it was shown recently that the universality between polymer melts and solutions breaks down under nonlinear elongational flows: while polymer melts exhibit a monotonic extension-thinning behavior for all applied strain rates, polymer solutions with the same number of entanglements exhibit an initial thinning behavior followed by a strong extension-hardening, which occurs at rates comparable to the reciprocal Rouse time of the chains. As a result, molecular theories for linear flows cannot be extended to nonlinear flows without further considerations.

In the present work, we explore the elongation properties of systematic sets of polymer blends and oligomer solutions in order to understand the molecular origin of this non-universality and the absence of extension thickening for polymer melts. This allows us to show the importance of analyzing separately flow-induced and time-induced relaxation processes in order to reunify the behavior of polymer melts and solutions. We then show how these mechanisms can be taken into account in tube-based models, towards a general picture to describe the viscoelastic properties of entangled polymers under elongation flow.

12:27PM G19.00003: Evidence of Flow-Induced Crystallization in Material Extrusion Additive Manufacturing [Invited]  ANTHONY KOTULA (Presenter), National Institute of Standards and Technology — Material extrusion additive manufacturing processes force molten polymer through a printer nozzle at high (>100 s⁻¹) shear rates prior to cooling and crystallization. This can lead to flow-induced crystallization in common polymer processing techniques, but the magnitude of this effect is unknown for additive manufacturing. Here, we will show the effect of the material extrusion on the morphology of poly(lactic acid), a common semicrystalline polymer used in material extrusion. The talk will encompass materials characterization (rheology and crystallization kinetics) relevant to printing, process line temperature measurements, and polarized optical microscopy techniques to characterize the final microstructure, which we compare with continuum modeling. Although no crystalline domains are seen in the as-printed part, a post-print annealing process reveals spherulitic domains with sizes that dramatically decrease near the weld line. Our results show that residual chain stretch from the extrusion and deposition process enhances the nucleation rate in the weld regions between extruded layers. The higher nucleation density in these regions is not obvious in the as-printed part but is revealed only through the annealing process, which is captured in the model.
Many industrial processes elongate polymer liquids at rates much faster than the molecular chain's characteristic relaxation times. These nonlinear extensional flows can strongly deform microscopic polymer conformations and drive dynamic transitions that produce large changes in polymer viscosity. Understanding how flow depends upon and drives such changes in polymer microstructure is essential for improving established and emerging fabrication methods like fiber spinning and 3D printing. However, most microscopic understanding of these nonlinear flows has been drawn from indirect techniques that infer molecular dynamics from macroscopic rheology. This has begun to change with the recent development of new experimental and numerical simulation techniques that allow researchers to control, sustain, and microscopically probe polymer dynamics during strong extension. Here, I’ll present molecular simulations for linear, star, and ring polymer melts and blends deformed in uniaxial extensional flow. In all three cases, coarse-grained molecular dynamics simulations reproduce the nonlinear rheology observed in extensional flow experiments, and also reveal the microscopic dynamics driving observed nonlinear trends. For some architectures, simple theoretical arguments can directly relate the elongated conformations of molecules to the nonlinear viscosity. In other cases, simulations show how extensional flows can drive polymers to topologically self-assemble or micro-phase separate in ways not seen in equilibrium. These new, far from equilibrium behaviors could provide new routes for controlling polymer microstructure during processing.

*TOC acknowledges the Harry S. Truman Fellowship. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science.
Polymer Scission in Contraction Flows* [Invited]  
PETER OLMSTED (Presenter), Georgetown University, SANDEEP GARREPALLY, FRANCOIS LEQUEUX, ESPCI, STEPHANE JOUENNE, Total SA — Polymer scission has been studied for many years! It has numerous practical implications in areas such as drug injection, spraying and printing, and oilfield harvesting. When injected through a contraction flow, high molecular weight polymer solutions exhibit a sharp increase of apparent viscosity due to chain stretching during fluid extension. This stretching can induce polymer scission, which then decreases the extensional viscosity. We revisit this old problem using specially-designed microfluidic hyperbolic contraction flows. We study the pressure-flux relation for high molecular weight polymer solutions passing through the contraction, and find that the ratio of the pressure drop to that of the (Newtonian) solvent has a maximum due to the competition between polymer extension and degradation (scission). From the dependence of the pressure maximum on flow rate and molecular weights we can quantify the decrease in equivalent molecular weight due scission in the contraction. We find a geometry-dependent quasi-universal relation between the flow rates at which the maximum occurs for successive passage in a given contraction, which appears to be independent of molecular weight, concentration, solvent quality and viscosity, and can be used to predict degradation under successive passes. I will discuss what we can learn about the the details of the scission kinetics in flow from these observations.

*Funding provide by Total, ESPCI, and Georgetown University (Joseph Semmes Ives endowment).

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G20 GDS: Data Science II: Machine Learning 301 - Brian Barnes, US Army
Rsch Lab - Aberdeen
11:15AM G20.00001: Addressing the Elephant in the Room: Uncertainties in Physical Predictions From Machine-Learned Force Fields  STEFAN CHMIELA (Presenter), HUZIEL SAUCEDA, KLAUS-ROBERT MÜLLER, Tech Univ Berlin, ALEXANDRE TKATCHENKO, University of Luxembourg — Learning molecular force-fields (FF) has played a leading role in the path towards reliable molecular dynamics simulations in biology, chemistry, and materials science[1,2]. However, simulation's predictive power is only as good as the underlying interatomic potential. Although it is common practice to evaluate the reliability of trained FF models based on typical error measures, this only quantifies the error on the database given a set of training points. The relevant question to ask is how well a learned FF reproduce the actual physical properties a system. Here, we present an analysis of the uncertainties in properties derived from learned-FFs, such as vibrational spectrum and thermodynamics. A clear correlation is found between learning errors and the derived properties' uncertainty. The robustness of the symmetric gradient-domain machine learning (sGDML) framework[1] against such problem is evinced by its fast uncertainty minimization with the training set size. These results will serve as reference for the developing of robust and predictive learned physical models.


11:27AM G20.00002: Understanding key challenges in digitizing and contextualizing experimental results  HA-KYUNG KWON (Presenter), CHIRRANJEEVI GOPAL, BRIAN D STOREY, Toyota Research Institute, SANTIAGO CAICEDO, JARED KIRSCHNER, EPAM-Continuum — Recent advances in automated, high-throughput experimentation have enabled scientists to leverage machine learning methods and structured data in screening large parameter spaces. These approaches could be even more effective if supplemented by data collected in traditional experimental labs, where samples are handed off between collaborators at multiple processing and characterization steps. In these settings, unstructured experimental observations recorded in physical lab notebooks can provide context for data and metadata collected from a variety of instruments. Despite a number of electronic lab notebook products available in market, digitization of experimental notes remains a challenge due to low levels of adoption by researchers. In this talk, we present our findings from user research conducted in three different academic labs, on researchers' behaviors and needs throughout the experimental process. We discuss methods based on human-centered design to guide the development of an easily adoptable solution that seeks to 1) integrate experimental notes into data-driven software platforms, 2) contextualize experimental data obtained from multiple sources, and 3) enhance knowledge transfer between collaborators, thereby accelerating scientific discovery in experimental labs.
11:39AM G20.00003: Using Machine Learning to Reduce Low-Q Disorder in Quasiparticle Interference Maps*  
AIDAN WITECK (Presenter), YU LIU, JENNIFER E. HOFFMAN, Physics, Harvard University — Scanning tunneling microscopy (STM) is a commonly used technique to examine a material on the atomic scale. Quasiparticle interference (QPI) extends its ability to resolve the band structure of materials in the reciprocal space by imaging the scattering patterns of impurities in the real space. Those scattering patterns are normally analyzed with the Fourier transform. However, the Fourier transform suffers from low-q noise arising from correlations between impurity centers, drastically decreasing band resolution in low-q regions. Here we present a novel algorithm that uses Fourier filtering and machine learning to reduce low-q noise. We validate this method using both simulated QPI data and real QPI data from various materials. Our method reduces low-q disorder without the introduction of artifacts, allowing us to more clearly examine the low-q band structure.

*STM work was supported by DOE EFRC, Center for the Advancement of Topological Semimetals, award SC-19-488.

11:51AM G20.00004: CdTe nanoparticles as temperature sensors via machine learning of optical properties  
JOHN COLTON (Presenter), JAMES W ERIKSON, CHARLES LEWIS, CARRIE E MCCLURE, DEREK SANCHEZ, TROY MUNRO, Brigham Young Univ - Provo — We have investigated using CdTe nanoparticles as non-invasive temperature sensors. Optical photoluminescence (PL) spectra and time-resolved photoluminescence (TRPL) were measured as functions of temperature and used as inputs to an artificial neural network (ANN) for purposes of machine learning. Two regimes were studied: low temperature, data taken from 10-320 K in steps of 10 K; and high temperature, data taken from 325-346 K in steps of 1 K. Five data sets were withheld for validation from the low temperature data; four from the high temperature. We used preprocessing techniques of min-max normalization and (for the low temperature regime) interpolation to generate additional training samples. Best results for both regimes were obtained using a seven layer fully connected ANN architecture. Hyperparameters varied to optimize the network include number and size of layers (including convolutional layers), batch normalization, activation functions, learning rates, and dividing the PL and TRPL data into separate input branches. Using a typical 80-20 training/testing split, the low temperature (high temperature) network was able to be trained to 0.1 K (1.0 K) training error and 0.3 K (2.5 K) testing error, which results in an error on the withheld validation data of 3.4 K (5.5 K).

NICHOLAS MARCELLA (Presenter), ANATOLY I FRENKEL, State Univ of NY - Stony Brook — The energy dependent X-ray absorption coefficient encodes the electronic and real space structure of select element species within a material. We have found that the neural network (NN) is capable of modeling this relationship in X-ray absorption near edge (XANES) and extended fine structure (EXAFS), resulting in a powerful analytic tool. To date, our NN-assisted analysis methods have been used to investigate the structure and dynamics of nanoparticles and oxide clusters as small at 4 atoms. The availability of large amounts of reliable training data, in terms of both labeling and quality, is key to an accurate NN model. For XANES and EXAFS, a database of such is not experimentally obtainable, so we must use ab initio spectroscopy codes to create a theoretical database. Because theoretical training data only approximates real observations (due to theoretical limitations, and experimental considerations such as noise, resolution, and glitching), many local minima emerge when optimizing for accurate experimental predictions. We will discuss how, by probing various local minima during training, with a set of labeled experimental data, we can find a NN which generalizes theoretical features for use in experimental predictions.

12:15PM G20.00006: Machine learning on the electron-phonon spectral function and the superconductor gap function

MING-CHIEN HSU (Presenter), WAN-JU LI, TING-KUO LEE, SHIN-MING HUANG, Physics, Natl Sun Yat Sen Univ — The phonon mediated superconductor can be described well by the Eliashberg equation. Once the electron-phonon spectral function is known either ab initially or estimated from experiments, the superconductor properties such as the gap function and the wave function renormalization can be solved self-consistently from the Eliashberg equation. However, it is important to investigate in a reverse way by inferring the possible original spectral function from known superconductor properties. The mapping can be learned by using the machine learning technique. We generate various spectral functions with numerous peaks and different shapes and solve their gap functions self consistently. With these data, the relation between each pair of the gap function and the corresponding spectral function can be learned by the machine. The functions are learned and recognized in terms of the basis function found by the neural network. The loss function will be hugely reduced each time when the neuron successfully learns a basis function. We find that in general, the neural network is very efficient to learn the correspondence between the electron-phonon spectral function with the superconductor functions mentioned.
**12:27PM G20.00007: Characteristic space of XRD patterns in machine-learning**  KEISHU UCHIMURA (Presenter), Japan Adv Inst of Sci and Tech, MASAO YANO, HIROYUKI KIMOTO, TOYOTA MOTOR CORPORATION, KENTA HONGO, Research Center for Advanced Computing Infrastructure, JAIST, RYO MAEZONO, Japan Adv Inst of Sci and Tech — X-ray diffraction (XRD) is a commonly used analytical technique to identify crystal structures. Recent advances in automatic measuring techniques enable one to obtain thousands of XRD patterns within a day. Basically, however, their analysis is done by comparing measured patterns with reference ones, which relies on experts' knowledge and great efforts. Even using a computational implement of the Rietveld refinement, characterization of some XRD patterns would take a few hours (or more) even for experts. Thus, automation/acceleration of the XRD analysis is really desired for managing high throughput XRD patterns. In this study we adopted an unsupervised machine learning technique, auto-encoder, to analyze XRD patterns. Vectorizing XRD patterns to make feature vectors, the encoder itself maps the high-dimensional vectors onto low-dimensional (say, 2-dim.) ones. It was found that XRD patterns get into groups of different compositions in the reduced feature space. We thus concluded that our scheme can capture slight difference in lattice constant caused by atomic substitutions in magnetic alloys without any prior knowledge.

**12:39PM G20.00008: Using machine learning to understand mutations***  MARTHA VILLAGRAN (Presenter), NIKOLAOS MITSAKOS, JOHN MILLER, RICARDO AZEVEDO, Univ of Houston — A single harmful base substitution in a DNA sequence can, on occasion, cause a devastating fatal disease. Determining why this happens for some mutations, but not for others, is critical to developing effective treatments and poses a central challenge to modern medicine. Mitochondrial DNA (mtDNA) is especially vulnerable, mutating about 100 times faster than the nuclear genome. Uncovering how DNA's electronic fingerprint influences its mutation spectrum is of critical importance to genetics and evolutionary biology. At the same time, machine learning, with the added capabilities of deep architectures that saw tremendous advances recently, provides a framework that allows recognizing patterns in data, even when these patterns are governed by very complex interlinked properties. We are investigating the capability of machine learning, with a focus on deep learning architectures, for detecting and predicting potential mutation locations in mtDNA. We demonstrate that these models can learn to discriminate between locations on the DNA where mutations can occur versus stable locations, to the extent that these situations are effectively represented in the available data.

*State of Texas through Texas Center for Superconductivity, University of Houston Health Research Institute and NIH.*
BRIAN BARNES (Presenter), BETSY M RICE, ANDREW E SIFAIN, CCDC Army Research Laboratory — We present advances in accurate, rapid prediction of detonation pressure, detonation velocity, heat of formation, density, and melting point of energetic molecules. Molecules evaluated are CHNO-containing organic molecules drawn from public datasets and known explosives. These models may be integrated into a larger effort for high-throughput virtual screening or rapid pre-screening of molecules before any hazardous synthesis is attempted. Our research evaluates a message-passing neural network (MPNN) model with representation learned from 2D structure trained on a large body of data generated by physics-driven (quantum mechanically derived) models, and also a thermodynamic fingerprint representation used to train a gradient-boosted decision tree method on a smaller body of experimental data. The utility of each representation and statistical model is discussed. The Python workflow for each analysis is discussed. This data-driven approach is shown to provide advances in speed and accuracy for energetic material property prediction. A brief introduction to energetic materials and detonation physics is provided for non-experts.

1:03PM G20.00010: Simulation of atmospheric turbulence with generative machine learning models  
ARTURO RODRIGUEZ (Presenter), CARLOS R CUELLAR, LUIS FERNANDO RODRIGUEZ, ARMANDO GARCIA, JOSE TERRAZAS, University of Texas, El Paso, VM KRUSHNARAO KOTTEDA, The University of Wyoming, RAO GUDIMETLA, Air Force Research Lab, VINOD KUMAR, JORGE MUNOZ, University of Texas, El Paso — The Large Eddy Simulation (LES) modeling of turbulence effects are computationally expensive even when not all scales are resolved, especially in the presence of deep turbulence effects in the atmosphere. Machine learning techniques provide a novel way to propagate the effects from inner- to outer-scale in atmospheric turbulence spectrum and to accelerate its characterization on long-distance laser propagation. We simulated the turbulent flow of atmospheric air in an idealized box with a temperature difference between the lower and upper surfaces of 10 degrees Celsius with the LES method. The volume was voxelized and several quantities such as the velocity and the pressure were obtained at regularly-spaced grid points. These values were binned and converted into symbols that were concatenated along the length of the box to create a ‘text’ that was used to train a long short-term memory (LSTM) neural network and a naïve Bayes model. LSTMs are used in speech recognition and handwriting recognition tasks and naïve Bayes is used extensively in text categorization. The trained LSTM and the naïve Bayes models were used to generate instances of turbulent-like flows.
1:15PM G20.00011: Identification of informative acoustic features in the transition from non-violent to violent crowd behavior  KATRINA PEDERSEN (Presenter), BROOKS A BUTLER, SEAN WARNICK, KENT L GEE, MARK TRANSTRUM, Brigham Young Univ - Provo — Human crowds can exhibit a variety of collective behaviors. Here, we explore the transition from peaceful to violent behavior in human crowds using acoustic data. Predicting when a crowd will transition from a peaceful to a violent state has many potential applications, such as peace-keeping and security. Relative to video, acoustic data is easier to obtain and is less affected by lighting conditions, such during night or in dark areas. We apply machine learning methods to a data set that includes both video and audio recordings of violent and non-violent crowds. Previous results showed that audio data was only marginally less effective than video alone for classifying violent/non-violent scenes. In this work, I conduct a feature-importance study to identify which acoustic metrics are most informative for correctly classifying peaceful and violent crowds.

1:27PM G20.00012: "Robust Speaker Identification System Under Adverse Conditions"  SWATI PRASAD (Presenter), Electronics and Communication Engineering, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India — When only a speech utterance is given, finding out the person who spoke the given speech utterance from a group of reference speakers is referred to as Speaker Identification. It is also known as biometric based on voice. Its success has great potential to bring a paradigm shift in the way we communicate with the machine. It will facilitate in the easier and secure communication between Man and Machine using speech. It will particularly benefit the elderly members of the society. Factors like voice disguising, emotional state of the person, background noise and throat diseases create a mismatch between the training and the test speech data, referred to as Mismatched Problem. It decreases the speaker identification accuracy and needs to be addressed. To make the speaker identification system robust against these mismatched conditions, we have developed speech frame selection methods for feature extraction. It captures the characteristics of the speech signal efficiently from the time-domain signal. For modeling the speaker, the machine learning technique, Gaussian Mixture Model with 64 components is utilized. It has shown good performance under voice disguise and environmental noise conditions. Future work will test its performance for emotional and diseased speech.
1:39PM G20.00013: Hyperbolic non-metric multidimensional scaling reveals intrinsic geometric structure in high-dimensional data  
YUANSHENG ZHOU (Presenter), University of California, San Diego, TATYANA OLEGIVNA SHARPEE, Salk Institute — Modern datasets characterize objects with respect to many variables and assign distances between objects based on a Euclidean metric. However, recent results suggest that for data produced by underlying hierarchical tree-like networks a hyperbolic metric might be more appropriate than a Euclidean one. We develop non-metric multidimensional scaling (MDS) in hyperbolic space to perform hyperbolic embedding of points. Using simulations we show that hyperbolic MDS, combined with Euclidean MDS, can be used to detect intrinsic geometry of data. Applying hyperbolic MDS to human gene expression data, we find that the samples taken from local clusters have Euclidean structure, but samples taken broadly from the whole population show hyperbolic metric, which indicates that the human gene expression space is locally Euclidean but globally hyperbolic. Further we quantify the hyperbolic radii of cells from other diverse biological systems including different mouse organs, finding that mouse brain and embryonic stem cells are also hyperbolic while organs like mouse lung, kidney and placenta are Euclidean. Our method provides a quantitative approach to detecting hidden geometric structures and quantifying cell hierarchies of diverse biological systems.

1:51PM G20.00014: Data Augmentation and Pre-training for Template-Based Retrosynthetic Prediction  
MIKE FORTUNATO (Presenter), CONNOR COLEY, Department of Chemical Engineering, Massachusetts Institute of Technology, BRIAN BARNES, Detonation Science and Modeling Branch, CCDC Army Research Laboratory, KLAVS JENSEN, Department of Chemical Engineering, Massachusetts Institute of Technology — A key step in computer-aided synthesis planning (CASP) is the prioritization of candidate molecular transformations for retrosynthetic analysis. Recent methods obtaining state-of-the-art accuracy have used machine learning (ML) models as recommendation engines to rank reaction templates extracted from databases of recorded reactions. However, data scarcity limits the ability for ML models to recommend rare, often highly desired, transformations. In this work we discuss the augmentation of open-access reaction databases with synthetically generated molecular transformations to teach neural networks generalized template applicability. We use this as a pre-training strategy, which is followed by fine tuning of the model parameters using true, recorded reactions, in order to increase the diversity of suggested retrosynthetic transformations. While previous methods have focused on learning a one-to-one-mapping from featurized molecular inputs to a single template transformation, pre-training with general template applicability allows these new models to learn a one-to-many mapping to multiple templates. The implications of performing data augmentation and pre-training on different sized datasets is discussed, as well as the changes in performance for rare reaction templates.
2:03PM G20.00015: Neural network-assisted analysis of X-ray absorption spectra of metal oxide clusters*  
YANG LIU (Presenter), NICHOLAS MARCELLA, ANATOLY I FRENKEL, Stony Brook University — It is challenging to understand the reactivity from structure perspective for the supported metal oxide clusters. Many operando characterization techniques for solving such challenge are limited due to the low-metal loading and high temperature condition. Because of the sensitivity of X-ray absorption near edge (XANES) to the local structure, we demonstrated that XANES can be analyzed and provide structural information combing with supervised machine learning method. In this work, we apply the neural network method to the analysis of grazing incidence XANES spectra of size-selective Cu oxide clusters on flat support, measured in operando condition. The convolution neural network was trained to build the correlation between the XANES and structural descriptors (Cu-Cu coordination numbers). Our result indicates that we can distinguish between different structural motifs of Cu oxide cluster during the reaction conditions and invert the experimental XANES to obtain structure parameters which helps the understanding of the structure-properties relation of the catalysts.

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Horizon, Award/Contract Number 2020

Tuesday, March 3, 2020 11:15 AM - 2:03 PM

Session G21 GERA: Perovskites and Chalcopyrites for Energy Applications

11:15AM G21.00001: Chemical trends of absolute volume deformation potentials of all-inorganic ABX₃ halide perovskites  
SHANSHAN WANG (Presenter), MENG LIN HUANG, SHIYOU CHEN, East China Normal University — The absolute volume deformation potential (AVDP) is an important physical quantity that describes the energy level shift under pressure, which, however, has not been investigated for halide perovskites. We systematically calculate the valence band maximum (VBM) and conduction band minimum (CBM) AVDPs of all-inorganic ABX₃-type perovskites (where A = K, Rb, Cs; B = Ge, Sn, Pb; X = Cl, Br, I) in cubic structure using ab-initio calculation methods. Although it was shown that spin-orbit coupling played an important role in the band structure calculation of ABX₃ perovskite, we prove that it has negligible effect on AVDP calculation. We show that the AVDPs of VBM are all negative and large, indicating the energy level will shift down when the volume increases, while AVDPs of CBM are mostly positive and small. There are clear trends in the calculated AVDPs of both VBM and CBM which will be discussed. Our results suggest that strain is an effective way to adjust the energy level of valence band edge in ABX₃, which may be of great significance to design optoelectronic devices.
11:27AM G21.00002: Relative stability of perovskite and non-perovskite phases of inorganic trihalogeno germanates.*  WALTER LAMBRECHT (Presenter), SANTOSH KUMAR RADHA, Case Western Reserve University — One of the main problems of halide perovskites is the existence of competing non-perovskite phases. Here we focus on (Cs,Rb)GeX₃ compounds which exist either in a rhombohedrally distorted ferroelectric perovskite phase exhibiting cornersharing octahedra or a monoclinic and various orthorhombic phases with edge-sharing octahedra. We show that the GeX₃ tetrahedral building blocks are arranged antiferroelectrically (AFE) in the monoclinic phase and ferroelectrically (FE) in the perovskite phase. The electrostatic dipole interaction favors the AFE arrangement but the additional bond formation favors the perovskite. A spin model and first-principles calculations explain why the Rb based compounds prefer the monoclinic and Cs compounds prefer the perovskite form. Similar phases exist for CsSnX₃. The different structural arrangement is accompanied by a large change in band structure with a much larger gap and flat bands in the monoclinic form, which is unsuitable for photovoltaic applications. This new insight in the stability of these phases suggests the use of an electric field to control the phase transition.

*Supported by DOE-BES DE-SC0008933

11:39AM G21.00003: Contrasting GGA and hybrid functionals description of dynamic properties of CsPbI₃  ALI KACHMAR (Presenter), MARCELO CARIGNANO, QEERI, Hamad Bin Khalifa University — Caesium lead iodide perovskite exhibit similar structural properties than methylammonium (MA) lead iodide, in particular with respect to the inorganic cage. Both systems show anharmonic behavior in the halide dynamics. Having Cs instead of MA as the cation allows for a study based on expensive hybrid functionals. Considering that most of the reported first principles molecular dynamics simulations were performed using GGA functionals, it becomes pertinent to question what are the corresponding results when the forces are accounted for using the more accurate hybrid functionals. In this work we present a comparison between PBE and HSE functionals for the anharmonicity of the halide atoms at high temperature. Our study is based on first principles molecular dynamics simulations on large 444 supercells and trajectories extending up to 40 ps.
Carrier Dynamics and Recombination in Low-Dimensional Halide Perovskites: Role of Structural Fluctuations*  
DIBYAJYOTI GHOSH (Presenter), AMANDA NEUKIRCH, SERGEI TRETIAK, Los Alamos National Laboratory — Low-dimensional halide perovskites have demonstrated promising luminescence properties for light-emitting diodes due to their high radiative recombination rate.\cite{1} However, the lack of a complete understanding of the structure-property relationship hinders the systematic design of these materials to enhance their luminescence efficiency. Combining state-of-the-art nonadiabatic molecular dynamics and time-domain density functional theory, we explore the substantial effects of structural fluctuations on the excited state dynamics and carrier recombination in these perovskites. Here, I will demonstrate how structurally rigid perovskites experience weaker electron-phonon interactions, resulting in suppressed non-radiative carrier recombination and enhanced photoluminescence quantum yield (PLQY).\cite{2,3} Our work revealed that stacking of the spacer cations, and halogen composition of the inorganic layers substantially tune the PLQY of these materials. Based on these understanding, we further propose a combination of suitable spacer cations and inorganic layer compositions to improve the PLQY of low-dimensional halide perovskites.

Ref.  
1. Smith et al., Chem. Rev. 2019, 119, 3104  
2. Ghosh et al. Under preparation, 2019  
3. Leveillee et al. Submitted to Nano Lett. 2019

Tailoring structural transitions in layered 2D perovskites using light  
WENBIN LI (Presenter), HAO ZHANG, Applied Physics, Rice Univ, SIRAJ SIDHIK, Chemical and Biomolecular Engineering, Rice Univ, MERCOURI KANATZIDIS, Chemistry, Northwestern Univ, JACKY EVEN, Physics, Institut national des sciences appliquées de Rennes, JEAN-CHRISTOPHE BLANCON, ADITYA MOHITE, Chemical and Biomolecular Engineering, Rice Univ — Organic-inorganic (hybrid) perovskite have recently emerged as a new semiconductor platform for next generation optoelectronics devices. These perovskite solids feature weak bonds between their organic and inorganic building blocks, which results in an intrinsic softness and dynamics disorder of the lattice and an acute sensitivity to external stimuli. For example, our group demonstrated that continuous sunlight illumination leads to a uniform expansion of the perovskite lattice, which impact the optoelectronic properties of the three-dimensional perovskites. In particular, this effect is beneficial as it helps cure electronics impurities and lowers energetic barriers near the surface/interface. Here, we present comprehensive in-situ light induced structural dynamics to layered two-dimensional (2D) hybrid perovskites. We correlate the changes in the structure of the 2D perovskite to modification of both the physical properties and the figures of merit in solar cells. We propose a new microscopic model to explain the evolution of the structure and optoelectronic properties under an external stimulus. These results demonstrate that structural characterization of hybrid perovskite under external perturbation is key in unraveling the fundamental physics of these materials.
12:15PM G21.00006: Optimization of recombination region within inorganic perovskite light emitting diodes  
LINDSEY GRAY (Presenter), XIAOHENG YAN, Wake Forest Univ, XIANG ZHANG, Jilin University, DAVID CARROLL, Wake Forest Univ — Recent advances in metal halide perovskite-based LEDs have included high brightness, extended lifetimes, and excellent color saturation in comparison with other thin film light sources such as OLEDs. We have shown that many of these properties can be traced to nanoscale sub-phase formation within the larger perovskite matrix, which leads to exciton self-trapping. However, since such phase formation modifies carrier mobility, a significant challenge in per-LEDs is optimizing device design such that the driving voltage, sensitive of recombination zone formation and position within the emitting layer, is overcome. In this work we examine the use of various organic layers, such as poly-TPD, in barrier formation and recombination zone stability. We show that interface preparation between the perovskite and transport layers can play a major role in barrier formation. Focusing on the correlation of brightness and efficiency with device structure modification, we demonstrate that optimized carrier balance can allow for maintained efficiency over a wide range of driving voltages and brightnesses.

RAMESH KUMAR (Presenter), JITENDRA KUMAR, PRIYA SRIVASTAVA, MONOJIT BAG, Indian Inst of Technology Roorkee — Owing to the exceptional optoelectronic properties, Hybrid halide perovskites (HHPs) have attracted great attention leading to the variegated application in optoelectronic devices. Study of carrier kinetics in perovskite solar cells using Impedance Spectroscopy (IS) has been the topic of research since the last few years. But, research in Perovskite LEDs (PeLEDs) is still sparse. Here, we have studied the charge carrier kinetics of PeLEDs using IS at different applied bias. The electrical equivalent circuit of the device was modelled and the variation of different parameters with applied bias was studied. We have observed the bias dependent transition of capacitance from positive to negative at low frequency. The inflection point along with the magnitude of this negative capacitance depends significantly on the morphology of the perovskite film. We have also observed anomalous capacitive behaviour for the first time at high frequency due to the interplay between electronic and ionic charge transport. We have proposed a possible model responsible for anomalous capacitive behaviour and its correlation with active layer morphology in PeLEDs.

References
12:39PM G21.00008: Identifying electronic descriptors to predict work functions of perovskite electrodes* YIHUANG XIONG (Presenter), WEINAN CHEN, WENBO GUO, HUA WEI, ISMAILA DABO, Pennsylvania State University — The ability to predict work functions of semiconductor electrodes is critical to the development of photocatalytic and electrocatalytic systems. Understanding the compositional and structural dependence of the interfacial electronic structure of semiconductors could enable us to screen and select appropriate functional materials for electronic applications. We address this problem with a focus on perovskite oxides (ABO$_3$) in the metastable cubic phase by enumerating the possible compositions for A- and B-site cations. We analyze the computed work functions by means of statistical learning using elemental and bulk chemical descriptors. The resulting descriptor-based model not only delivers accurate predictions of computed work functions using a limited number of features, but also allows us to interpret the complex correlations between electronic levels and surface structure across a vast chemical space.

*The authors acknowledge financial support from the National Science Foundation under Grant No. DMREF-1729338. The computational work was performed using high performance computing resources from the Penn State Institute of CyberScience.

12:51PM G21.00009: Modeling the dynamics of interacting defects, charge carriers, and excitons in perovskite solar cells BARBARA SANBORN (Presenter), Whitman College, ABDUL SHAIK, DRAGICA VASILESKA, Arizona State University — This talk presents calculations based on a theoretical model that includes the dynamics of excitons, free charge carriers, and electrically active defects, to study the stability of perovskite solar cells. Previously, the PVRD-FASP tool was developed and released for public use (www.pvrdfasp.com) to model metastability and reliability issues of solar cells. In the model, charge carriers and electrically active defect centers are treated on an equal footing, as both obey the same reaction-kinetic equations: the continuity, drift-diffusion, and the Poisson equations. The rate terms in these equations are highly non-linear and require solution of a system of stiff partial differential equations. To efficiently solve such systems, a reaction solver based on the forward Euler method implicit in time with a Newton step was proposed and implemented. The Jacobian for the Newton step was analytically calculated. The PVRD-FASP tool was used successfully to study the role of Cu migration in CdTe solar cells. In current work, the theoretical model of the tool is expanded to include the dynamics of excitons. The expanded solver is used to study the stability of perovskite solar cells in the presence of light-induced formation and annihilation of defects acting as carrier trap states.
1:03PM G21.00010: The interplay of bulk and interfacial dynamics in methylammonium lead triiodide perovskite solar cells revealed via current noise spectroscopy*  
KEVIN DAVENPORT (Presenter), MARK HAYWARD, ANDREY ROGACHEV, University of Utah — Hybrid organic-inorganic perovskite solar cells are one of the most promising emerging technologies capable of competing with silicon devices, chief among them those based on methylammonium lead triiodide (MAPbI$_3$). Fundamental understanding of electrical transport and degradation processes in these devices, however, is important for commercial realization. We have performed cross-correlated current noise spectroscopy on a series of MAPbI$_3$ devices. Under illumination, we find near-full-scale shot noise (Fano factor $F \sim 1$), indicating the dominance of a single element in the device stack. We further observe generation-recombination noise which emerges with illumination and increasing device thickness. This signal is attributed to radiative bimolecular recombination. Finally, we observe a $1/\alpha$ flicker noise ($\alpha \sim 1.4$) which deviates from the expected $I^2$ dependence. This indicates the superposition of canonical resistance fluctuations and a current and/or light-driven source, likely the migration of halide ions through the bulk.

*This work was supported by NSF CAREER Grant No. 0955484 and NSF Grant No. DMR 1611421.

1:15PM G21.00011: Understanding the role of Sn substitution and Pb vacancy in FAPbBr$_3$ perovskites: A hybrid functional study  
MANJARI JAIN (Presenter), SASWATA BHATTACHARYA, Physics, Indian Institute of Technology Delhi — Hybrid inorganic-organic perovskites (HIOPs) solar cells have attracted intense attention because of its high carrier lifetime, long diffusion length and low manufacturing cost. Formamidinium Lead Bromide (FAPbBr$_3$), a HIOPs is immensely promising class of material for photovoltaic application. However, due to presence of hazardous Pb, its application to real life is hindered. Therefore, its our profound interest to understand if substitution of adatoms (e.g. Sn, Ge) or creation of Pb-vacancy [Vc] or doing the same simultaneously will be effective considering its efficiency in solar cell devices.

We address here the role of Sn substitution and Pb-Vc in regulating stability using state-of-the-art hybrid density functional theory. The explicit role of spin orbit coupling (SOC) and electron self interaction error are discussed. We find while SOC has significant role in regulating electronic bands, it doesn't affect the relative hierarchy of thermodynamic stability of different configurations of FAPb$_{(1-x-y)}$Sn$_x$Vc$_y$Br$_3$. However inclusion of electron self interaction error is absolutely important to estimate formation energy of configurations correctly. The Spectroscopic Limited Maximum Efficiency (SLME) is compared of the most stable defected system with respect to the pristine FAPbBr$_3$. 
1:27PM G21.00012: Absence of large valence band Rashba splitting in metal halide perovskites  
OLIVER RADER (Presenter), MARYAM SAJEDI, MAXIM KRIVENKOV, DMITRY MARCHENKO, ANDREI VARYKHALOV, JAIME SÁNCHEZ-BARRIGA, Helmholtz-Zentrum Berlin, ANOOP CHANDRAN, IRENE AGUILERA, Forschungszentrum Jülich — Organic and inorganic lead halide perovskites share the same properties of high efficiency in energy conversion and high spin-orbit interaction. For both, a large Rashba effect has been invoked to be responsible for the high efficiency by prohibiting direct recombination. In the valence band of methylammonium lead bromide a static Rashba effect has been reported by angle-resolved photoemission (ARPES) and circular dichroism with giant values of 0.7 to 1.1 eV nm [1]. We present precise ARPES band dispersion measurements of methylammonium lead bromide and cesium lead bromide to show that a Rashba effect of the reported size does not exist. Moreover, we use spin-resolved ARPES to confirm the conclusions. We also observe a large circular dichroism effect and demonstrate that this effect does not imply any measurable spin polarization and Rashba effect. Our results exclude a static Rashba effect in the valence band as origin of the high efficiency of metal halide perovskites.  

1:39PM G21.00013: Simulations of the electronic stopping power in perovskites*  
MARIO BORUNDA (Presenter), Oklahoma State University-Stillwater — Electronic stopping power describes the energy transfer rate to electrons in material during ion irradiation. We use time-dependent density functional theory to calculate electronic stopping power in triple-cation perovskites (formamidinium, methylammonium, and cesium). These materials have some of the highest power conversion efficiencies for perovskite-based photovoltaics. From simulations we can estimate the stopping process of ions and this would have implications for the use of photovoltaic devices for space missions.  

*This material is based upon work supported by the National Aeronautics and Space Administration under Agreement No 80NSSC19M0140 issued through NASA Oklahoma EPSCoR.
1:51PM G21.00014: Role of Cu deficient layer in chalcopyrite based solar cells  ABHISHEK SHARAN (Presenter), Univ of Delaware, JOEL VARLEY, Lawrence Livermore National Laboratory, ANDERSON JANOTTI, Univ of Delaware — Chalcopyrites are a demonstrated material platform for realizing efficient thin-film photovoltaics, with the most well-known Cu(In,Ga)Se$_2$ (CIGS) based solar cells exceeding 23%. The presence a Cu-poor phase layer between the absorber and buffer layers in CIGS solar cells is known to enhance device performance, however, the overall properties and role of very thin layer remain poorly understood. Using first principles calculations based on density functional theory with screened hybrid functionals, we explore the electronic structure and stability of a series ordered vacancy compounds (or OVCs) as a model for the Cu-poor phase layer. We calculate band offsets between the OVCs and defect-free chalcopyrite Cu and Ag based compounds (ABX$_2$ where A = Cu, Ag; B = In, Ga, Al and X = S, Se). Using AB$_3$X$_5$ and AB$_5$X$_8$ stoichiometries as model OVC systems, we report on the variation of the band gap with A/B ratio and discuss the trends in other Cu and Ag-based chalcopyrites beyond CuInSe$_2$. We additionally perform device-level simulations to understand the implications of formation of OVCs, finding that valence band offsets of OVCs are favorable for hole transport, while the conduction band offsets of chalcopyrites beyond CuInSe$_2$-based absorbers may be detrimental to device performance.

Tuesday, March 3, 2020 11:15 AM - 1:39 PM

Session G22 DBIO DSOFT: Biopolymers: Nucleic Acids and Structural 303 - Ralf Bundschuh, Ohio State Univ - Columbus

11:15AM G22.00001: Autonomous synthesis and assembly of a ribosomal subunit on a chip  MICHAEL LEVY (Presenter), REUVEN FALKOVICH, SHIRLEY S. DAUBE, ROY H. BAR-ZIV, Weizmann Institute of Science — Ribosome biogenesis is an efficient and complex assembly process that has not been reconstructed outside a living cell so far, yet is the most critical step for establishing a self-replicating artificial cell.

We recreated the biogenesis of Escherichia coli's small ribosomal subunit by synthesizing and capturing all its ribosomal proteins and RNA on a chip. Surface confinement provided favorable conditions for autonomous step-wise assembly of new subunits, spatially segregated from original intact ribosomes. Our real-time fluorescence measurements revealed hierarchal assembly, cooperative interactions, unstable intermediates, and specific binding to large ribosomal subunits.

Using only synthetic genes, our methodology is a crucial step towards creation of a self-replicating artificial cell and a general strategy for the mechanistic investigation of diverse multi-component macromolecular machines.
The formation of filopodia bridge and intercellular nanotube: A Critical rule of torque and restorative force.*  O-CHUL LEE (Presenter), MINHYEOK CHANG, JAEHO OH, JONG-BONG LEE, JAE-HYUNG JEON, Pohang Univ of Sci & Tech — In mammalian cells, a network of intercellular membrane nanotubes enables long-distance communication which is an intercellular transfer of cytoplasmic molecules and even organelles and viruses. The main component in filopodia which constitutes membrane intercellular nanotubes is consists of bundled actin filamentous. Also, several studies have confirmed the dynamic behavior of the filopodia which are undergoing restorative force by myosin II and torque by myosin V. Using a fluorescence imaging method, we have found that filopodia grown from two adjacent cells form the helical structure resulting. To understand the mechanism of forming the intercellular nanotube, we model a filopodium as a bundle of wormlike chains whose net persistence length is consistent with the value measured by our optical tweezers experiment. In this study, we quantitatively investigate the conformation, stability, and dynamics of the filopodia in comparison with the experiment by using the Langevin dynamics simulation. From the simulation results, we propose a region of a magnitude of tension and torque applied to the filopodia to form the nanotube.

*Department of physics, Pohang university of science and technology

A novel coarse-grained energy functions for RNA folding*  DONG ZHANG (Presenter), SHI-JIE CHEN, Univ of Missouri - Columbia — Coarse-grained models combined with effective sampling techniques are now poised to address a wide range of problems in biological systems. An accurate coarse-grained force field is crucial for quantitative modeling of structure, dynamics, and function. We recently developed a novel approach to extract RNA coarse-grained energy functions from the structural database. The key ingredient of the approach is to stepwise build the correlations between the different interactions and the inherent chain connectivity and excluded volume interactions through an iterative construction of the reference states. The novel approach allows us to extract energy functions from the inverse Boltzmann law. The validity of this approach is supported by the close agreement between the simulated distributions for all the structural parameters and those observed from the experimental structure database. Benchmark tests on tertiary structure folding and 3D structure predictions show comparable or much improved predictions than existing coarse-grained models. This novel method for the treatment of many-body correlation effects can be easily transferred to other computational biology problems.

*This research was supported by NIH grants GM063732 and GM117059.
Non-ergodic transport and conformational dynamics of DNA in biomimetic cytoskeleton networks*  

JONATHAN GARAMELLA (Presenter), GINA AGUIRRE, Univ of San Diego, KATHRYN REGAN, Biomedical Engineering, Boston University, RYAN J. MCGORTY, RAE M ROBERTSON-ANDERSON, Univ of San Diego — Macromolecular crowding is an increasingly relevant biophysical phenomenon that affects drug delivery, protein function, and intracellular transport. Of particular interest is the influence that cytoskeletal filaments have on the transport and conformational dynamics of large DNA molecules. Here, we use single-molecule conformational tracking (SMCT) to elucidate the transport properties and conformational dynamics of linear and relaxed circular (ring) DNA in in vitro composite networks of actin and microtubules with variable types of crosslinking. Specifically, we investigate the impact of crosslinking actin to actin, microtubules to microtubules, and actin to microtubules. While both linear and ring DNA undergo anomalous subdiffusion in all networks, the transport properties are heavily influenced by DNA topology. Linear DNA chains are compacted and display a single mode of subdiffusion, while ring DNA polymers are swollen and exhibit biphasic subdiffusion suggestive of transient threading by the biomimetic cytoskeleton. These results are bolstered by non-Gaussian van Hove distributions and non-ergodic behavior of both DNAs, with the transport of ring DNA molecules becoming less ergodic than their linear counterparts at longer times.

*NIH Award #R15GM123420
NSF-CBET-1603925

Single nucleotide polymorphisms affect RNA-protein interactions at a distance through modulation of RNA secondary structures*  

RALF BUNDSCHUH (Presenter), ELAN SHATOFF, Department of Physics, Ohio State University — RNA-protein interactions play an important role in regulating gene expression. Since RNA-protein interactions are affected by RNA secondary structure, single nucleotide polymorphisms in the vicinity of protein binding sites can affect these interactions. This provides a mechanism for single nucleotide polymorphisms outside coding regions and outside the actual protein binding sites to convey a phenotype. Here, we use a modified version of the Vienna RNA folding package and PAR-CLIP data for HuR (ELAVL1) in humans to characterize the genome-wide effect of single nucleotide polymorphisms on HuR binding and show that they can have a many-fold effect on the affinity of HuR binding to RNA transcripts from tens of bases away. We also find that the effect of single nucleotide polymorphisms on protein binding appears to be under selection, with the minor alleles tending to make it harder for a protein to bind.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1719316.
12:15PM G22.00006: COARSE-GRAINED MODELING OF DNA PLECTONEME FORMATION IN THE PRESENCE OF BASE-PAIR MISMATCHES  PARTH RAKESH DESAI (Presenter), SIDDHARTHA DAS, University of Maryland, College Park, KEIR C NEUMAN, National Institutes of Health — Defects in double stranded DNA can arise from mismatched base pairs. In vivo, these must be rapidly repaired since they affect a variety of cell processes. Here we use molecular dynamics to study the effect of mismatched bps on DNA supercoiling. Magnetic tweezers-based studies of DNA supercoiling have shown that in DNA harboring a single mismatch, the plectoneme always localizes at the mismatch. These studies were conducted at relatively high salt concentrations (>0.5M). Theoretical studies have predicted that under physiological salt concentrations of ~0.2M, plectoneme localization becomes probabilistic. However, both approaches are currently limited to positively supercoiled DNA. We develop a simulation framework using the oxDNA model to study the effect of mismatches on both positively and negatively supercoiled DNA. We find that for a positively supercoiled DNA, the oxDNA framework can reproduce the experimentally observed plectoneme pinning at high force and high salt concentrations. Under physiological salt concentrations (0.2M), we find that the plectoneme localization at the mismatch becomes probabilistic. The utility of the simulation approach is highlighted by the ability to quantify the effect of mismatches on the motion of plectonemes along the DNA molecule.

12:27PM G22.00007: A quantitative model of temperature actuated DNA origami nanocaliper constructs*  KYLE CROCKER (Presenter), Department of Physics, The Ohio State University, JOSHUA JOHNSON, Interdisciplinary Biophysics Graduate Program, The Ohio State University, CARLOS E CASTRO, Department of Mechanical and Aerospace Engineering, The Ohio State University, RALF BUNDSCHUH, Department of Physics, The Ohio State University — Manipulation of temperature can be used to actuate gold nanoparticle incorporated into DNA origami nanocalipers. We develop a physical model of this system that uses partition function analysis of the interaction between the nanocaliper and nanoparticle to predict the probability that the nanocaliper is open at a given temperature. The model agrees well with experimental data, and the comparison between model and experiment reveals surprising insights into the nanocaliper-nanoparticle system. For instance, geometric constraints on the system are suggested. Additionally, the model predicts experimental conditions that allow the actuation temperature of the nanocaliper to be tuned over a wide range of temperatures from 20°C to 60°C. This combination of physical insight and predictive potential is likely to inform future designs that integrate nanoparticles into dynamic DNA origami structures. Furthermore, our modeling approach could be expanded to consider the incorporation, stability, and actuation of other types of functional elements or actuation mechanisms integrated into nucleic acid devices.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1719316, as well as the Department of Energy grant DE-SC0017270.
**12:39PM G22.00008: A dynamic model of DNA Supercoiling**  BIAO WAN (Presenter), JIN YU, XINLIANG XU, Beijing Computational Science Res Ctr — The dynamics of DNA supercoiling is important for many biological functions of DNA, such as gene expression regulation. In this investigation we first studied DNA supercoiling generation through a Brownian dynamics simulation of DNA, which is modeled as a discrete worm-like chain. Two well-separated time scales are observed: mechanical balance along the DNA can be regarded as instantaneous (10^{-3}−10^{-2} ms) when compared to the global configuration change of the DNA supercoil structure (>10^0 ms). Based on this time separation, we developed a new model where the fast mechanical balancing dynamics are coarse grained. While the numerical simulation of DNA supercoil dynamics based on this model can be shown to fully reproduce DNA dynamical behavior above millisecond time scale, the computational efficiency is greatly improved. In our example of a DNA segment of 6000 base pairs, simulation based on the new model is times faster than the original Brownian dynamics simulations, making numerical study of DNA dynamics at biologically relevant time scales (e.g. 1−10 sec) possible.

**12:51PM G22.00009: Real-Time Tracking and Quantification of Transposable Element Activity***  DAVNEET KAUR (Presenter), Physics, University of Illinois at Urbana-Champaign, GLORIA LEE, University of San Diego, NICHOLAS SHERER, ELLIOT URRIOLA, Physics, University of Illinois at Urbana-Champaign, HNEIL KIM, University of California, Berkeley, CHI XUE, Physics, University of Illinois at Urbana-Champaign, K. MICHAEL MARTINI, Emory College, NIGEL GOLDENFELD, Physics, University of Illinois at Urbana-Champaign, THOMAS E KUHLMAN, Physics, University of California, Riverside — Transposable elements (TEs), or jumping genes, are DNA sequences that can change their position in a genome using a cut-and-paste or copy-and-paste mechanism. They are fundamental building blocks of all genomes, accounting for large fractions of genomic masses, and may have played a major role in the emergence of genetic diversity and function. Even so, many open questions remain regarding their differential abundance among organisms, the functions of their individual proteins, rates of protein activity and transposition and the effects of TEs on their hosts. To address these unanswered questions, we have constructed and released inducible TEs in bacteria to quantify their rates of activity and physiological effects on their hosts. To quantify dynamics, we've designed fluorescent visualization and quantification techniques to make real time high resolution observations of protein expression and transposition events as they occur in living cells. We show that we can obtain a deeper understanding of the roles of TEs and their individual proteins through our analysis.

*This work was supported by startup funds from the University of California, Riverside, the NSF Center for the Physics of Living Cells, the Alfred P. Sloan Foundation, and the NASA Astrobiology Institute.
1:03PM G22.00010: Simulating the Polarization Effects of Gas-Phase Nucleic Acids*  
CHRISTOPHER MYERS (Presenter), Physics, University At Albany, ALAN CHEN, Chemistry, University At Albany —  
Molecular dynamics (MD) simulations coupled with ion mobility spectrometry (IMS), a gas-phase extension to mass spectrometry that further filters analytes by conformation, allows researchers to perform three dimensional structural elucidation of nucleic acids. As opposed to neutral liquid phase MD simulations where electrostatic interactions are considered to be relatively weak and short ranged, highly charged, gas phase IMS simulations require a stronger description of Coulomb and polarization effects. In the work presented here, we explore the dynamical properties an appropriately tuned electrostatic force field for gas phase nucleic acids should replicate. Based off of density functional theory calculations of small oligonucleotides, we examine how one could adjust the partial charges throughout an MD simulation to more accurately replicate Coulomb interactions for charged and protonated nucleic acids.  
*This work is funded by NSF grant number MCB1651877.

1:15PM G22.00011: Existence of the B-Form DNA helix in nanoDNA liquid crystals and its variation due to aggregate assembly*  
GREGORY SMITH (Presenter), University of Colorado, Boulder, TOMMASO FRACCIA, ESPCI Paris, Intitut Pierre-Gilles de Gennes, MIKHAIL ZHERNENKOV, NSLS-II, Brookhaven National Laboratory, TOMMASO BELLINI, University of Milan, NOEL ANTHONY CLARK, University of Colorado, Boulder —  
We show using diffraction of a synchrotron X-ray microbeam that liquid crystalline aggregates of 12mer nanoDNA, such as the Drew-Dickerson Dodecamer (DD), demonstrate a B-form DNA double helix with a comparable degree of order to that seen in longer DNA, such as the calf-thymus DNA used by Rosalind Franklin to produce the historic Photo 51. This finding is significant because it shows that B-form helical order persists in liquid crystals of DD even though the backbone of the column contains a double-strand break at every twelfth position and the DD segments are not part of a full structured crystal. The coherence of the B-form helix is influenced by the mode of aggregate self-assembly, where aggregates assembled by a base-paired sticky-end produce much longer helical correlation lengths than those formed by hydrophobic blunt-ends. Finally, we found that aggregates of blunt-end 4mer oligomers shorter than half of a single B-form helical turn no longer display the B-form helical diffraction pattern but order with a different structure. This study gives fundamental insight into the extent to which the classical DNA helix is affected by discontinuity in the polymer backbone.  
*Funding provided by NSF MRSEC Grant DMR-1420736 and NSF Biomaterials Grant DMR-1611272.
It is known that several kinds of paper (including the common copy paper) increase in thickness when stretched. Previously, we examined several commercially available papers and found this behavior in some of them. We also devised, utilizing a few other reports, a mechanistic explanation for the origin of this auxetic response. In this research, we apply our understanding of this mechanism to construct auxetic paper handsheets. Key structural parameters of a nonwoven cellulose fiber network in paper – fiber length, sheet thickness and crosslinking density, that were previously predicted to affect the magnitude and sign of Poisson’s ratio, were altered to produce a range of handsheets. It was found that longer fibers, crosslinking density, extent of refining, and sheet thickness significantly affect the magnitude of auxetic response in paper.

*Paper Science and Engineering Fellowship to Prateek Verma.
ACE/SLOAN retirement transition legacy award to Anselm C Griffin.

Tuesday, March 3, 2020 11:15 AM - 1:51 PM

Session G23 DBIO GSNP: Evolutionary and Ecological Dynamics I:
Population Ecology 304 - Jeffrey Gore, Massachusetts Institute of Technology MIT - Tag(s): Focus

11:15AM G23.00001: The price of a shortcut [Invited] WENYING SHOU (Presenter), Basic Sciences, Fred Hutch Cancer Research Center — I will discuss the importance of quantitative mathematical modeling in biology. I will also experiment with a different presentation style where scientific work is described through story-telling. My talk will be accessible to specialists who study physical biology and to general audience with little knowledge of biology. I also hope to get feedback from the audience on how well this style worked for them.
11:51AM G23.00002: Long-term Nutrient Cycling in a Materially Closed Ecosystem  

LUIS DE JESÚS ASTACIO (Presenter), ZEQIAN LI, KAUMUDI PRABHAKARA, SEPPE KUEHN, Physics, University of Illinois at Urbana-Champaign — Closed Microbial Ecosystems (CES) are hermetically sealed microbial communities that support self-sustaining nutrient cycles using only light as an input. CESs have been proposed as controlled model systems to understand the principles governing ecosystem organization and persistence. However, we do not yet understand how the nutrient cycling capabilities of a CES depend on its community structure and composition. To address this question, we present a new method for making precision measurements of carbon cycling in CES using low-cost piezoresistive pressure sensors. With these devices, we quantify carbon cycling rates in a set of CESs over periods of months. Our data show that previously studied synthetic CES comprised of model organisms exhibit declining carbon cycling rates on long-timescales. We go on to self-assemble CESs using the phototrophic alga *Chlamydomonas reinhardtii* combined with complex, soil-derived, bacterial communities. We find that these CESs persistently cycle carbon on timescales of many weeks. Also, we characterize the limiting nutrients in these CESs as well as their community-level metabolic capabilities. Finally, we use next-generation sequencing to characterize the taxonomic and metagenomic composition of these persistent microbial biospheres.

12:03PM G23.00003: Growth and form control population dynamics of cellular aggregates*

ALEXANDER GOLDEN (Presenter), KIRILL S KOROLEV, Physics, Boston University — While the colony morphology reflects the interplay of biophysical processes such as nutrient diffusion, motility, and growth. How these processes control genetic correlations within the population remains an open question. To understand how growth morphology influences evolutionary dynamics, we have developed a numerical model of two-dimensional colonies in which microbes grow by consuming a diffusible nutrient and have a density-dependent motility. We show that this model can reproduce a diverse family of shapes observed in the experiments. Many of these morphologies exhibit a qualitatively different pattern of genetic drift compared to microbial colonies with a moderately rough front, which have been the focus of previous work. We report the scaling exponents for both morphological and genetic quantities for each of the growth regime. Most importantly, we show the consequences of the transition from pulled to pushed expansions in two-dimensional models with nutrient diffusion.

*Simons Foundation Grants #409704, Research Corporation for Science Advancement through Cottrell Scholar Award #24010, Scialog grant #26119, Moore foundation grant #6790.08
12:15PM G23.00004: Synergistic effects of nitrogen and phosphorous on the growth of algal cells revealed by a microfluidic platform*  
FANGCHEN LIU (Presenter), MOHAMMAD YAZDANI, NICOLE GOULDING WAGNER, BETH A. AHNER, MINGMING WU, Cornell University — A sudden growth of photosynthetic algal cells causes Harmful Algal Bloom (HAB), depleting water resources and disrupting the balance of aqua ecosystems. HAB is an emerging environmental problem exacerbated by climate change and population growth. Despite the urgency of the problem, there still lacks a systematic understanding of the environmental conditions (physical, chemical, and biological) under which HABs occur. In this presentation, we studied the growth of a model algal strain, *Chlamydomonas reinhardtii*, under a dual concentration gradient of nitrogen (N) and phosphorous (P) and found that N and P synergistically promoted algal cell growth. Interestingly, no discernible response was observed under single nutrient gradient. We also demonstrated the potential application of the newly developed microfluidic platform that integrated the array microhabitat format with dual gradient generation, enabling fast screening of environmental factors for algal growth studies. Future investigations will include the dynamics of bacterial community under controlled environmental condition.

*This work was supported by the USDA NIFA, AFRI project [2016-08830], the Academic Venture Fund from Cornell ACSF, the NY State Hatch fund, and performed in part at CNF, supported by NSF Grant NNCI-1542081.

12:27PM G23.00005: Dynamics of prey-predator: effect of cooperative interaction and inertial forces*  
DIPANJAN CHAKRABORTY (Presenter), RUMI DE, IISER Kolkata — A swarm of preys when attacked by a predator is known to rely on their cooperative interactions to escape. We present a simple theoretical model to investigate the effect of cooperative interactions on the survival chances of a prey group while chased by a predator. Our study shows that very short-range or very long-range interactions are not beneficial for preys to escape. However, in the intermediate range of interaction, an optimality criterion can be established where the survival probability of the prey group is maximum. We further explore the effect of inertial forces on the survival chances and escape trajectories of the prey group. Interestingly, we observe a transition from non-survival to survival of the prey group as a function of increasing predator mass. Our analysis also shows that prey group size and predator strength have an immense effect on this survival regime.

12:39PM G23.00006: Representing spatially extended ecological oscillators by kinetic Ising models with memory*  VAHINI REDDY NAREDDY (Presenter), University of Massachusetts Amherst, JONATHAN MACHTA, University of Massachusetts Amherst, Santa Fe Institute, KAREN ABBOTT, Case Western Reserve University, SHADISADAT ESMAEILI, University of California at Davis, ALAN HASTINGS, University of California at Davis, Santa Fe Institute — Synchronous behavior in spatially-extended ecological systems can be modeled by noisy, coupled oscillators. If the individual oscillators are in a two-cycle regime, the transition to synchrony as a function of noise strength and coupling strength has been shown to be in the Ising universality class [1]. On the other hand, a nearest neighbor Ising model may not provide an accurate description of non-universal properties. In this talk we will discuss the question of accurately representing a system of coupled, noisy two-cycle oscillators by an Ising model. We show that an accurate representation requires a kinetic Ising model with a self-interaction (memory) term. Even if this kinetic Ising model with memory includes only nearest-neighbor couplings in the dynamics, its equilibrium states are described by a Hamiltonian with more distant neighbor coupling and multi-spin terms. Using maximum likelihood methods we are able to infer an accurate kinetic Ising representation of synthetic data from a noisy lattice map system. We also discuss applications to field data in ecology.


*This work is supported in part by NSF grant DMS-1840221

12:51PM G23.00007: Ocean currents promote rare species diversity in protists  PAULA VILLA MARTIN (Presenter), ALES BUCEK, TOM BOURGUIGNON, SIMONE PIGOLOTTI, Okinawa Inst of Sci & Tech — Oceans host communities of plankton composed of a huge number of rare species that, as estimated in metagenomic studies, decay as a steep power law of their abundance. We propose that the way oceanic currents limit protists dispersal is a key factor of such biodiversity pattern. We introduce a spatially explicit coalescence model able to reconstruct species ancestry and diversity in the presence of currents. Our model predicts a steep power law decay of the species abundance distribution and a steep increase of the number of observed species with sample size. Metagenomic studies of planktonic protist communities show excellent agreement with our results.
1:03PM G23.00008: Spatial segregation as a necessity for beneficial gene loss in cross-feeding bacterial communities: a kinetic perspective on the Black Queen Hypothesis
MARIO DI SALVO (Presenter), SIMA SETAYESHGAR, JAMES MCKINLAY, Indiana Univ - Bloomington —
Cross-feeding communities are common across diverse environments, such as soil, water, and host microbiomes. The Black Queen Hypothesis (BQH) [1] asserts that some metabolic functions are leaky and thus provide a public resource within a community. The public resource allows some community members to lose genes for the production of that resource as long as at least one member continues to produce the resource. Nitrogen fixation as a process that leaks ammonium is used as an example to explain why only certain prokaryotes encode nitrogenase. We explore the emergence of mutualistic cross-feeding in bacterial cocultures in the context of the BQH. We pair a slow-growing nitrogen-fixing cooperator with fast-growing fermentative partners that can either also fix nitrogen gas or require the product, ammonium. We demonstrate that spatial heterogeneity is necessary for the emergence of a partner strain that loses nitrogen-fixation.


1:15PM G23.00009: Localization transitions in age-structured populations
TAKASHI NOZOE (Presenter), EDO KUSSELL, Biology, New York University —
We discuss age-structured population models that exhibit a range of collective phenomena including phase transitions and population-level oscillations. We present an analysis that predicts the lineage properties of single cells, and demonstrate how the optimal lineage in a population undergoes a qualitative change in its statistical properties as model parameters are varied past a localization transition point that is analytically computed. We observe aging dynamics of the population in the localized phase, and illustrate connections with other problems in evolutionary dynamics.

1:27PM G23.00010: Formation of Phage Lysis Patterns and Implications on Co-Propagation of Phages and Motile Host Bacteria
JING CHEN (Presenter), Virginia Tech —
Coexistence of bacteriophages, or phages, and their host bacteria plays an important role in maintaining the microbial communities. In natural environments with limited nutrients, motile bacteria can actively migrate towards locations of richer resources. Although phages are not motile themselves, they can infect motile bacterial hosts and spread in space via the hosts. Therefore, in a migrating microbial community coexistence of bacteria and phages implies their co-propagation in space. Here, we combine an experimental approach and mathematical modeling to explore how phages and their motile host bacteria coexist and co-propagate. When lytic phages encountered motile host bacteria in our experiments, a sector-shaped lysis zone formed. Our mathematical model indicates that local nutrient depletion and the resulting inhibition of proliferation and motility of bacteria and phages are the key to formation of the lysis pattern. The model further reveals the straight radial boundaries in the pattern as a tell-tale sign for coexistence and co-propagation of bacteria and phages. Emergence of such a pattern, albeit insensitive to extrinsic factors, requires a balance between the intrinsic physiology of phages and bacteria, which likely results from co-evolution of phages and bacteria.
1:39PM G23.00011: Spatial competition of toxin-secreting strains of yeast  ANDREA GIOMETTO (Presenter), ANDREW MURRAY, DAVID R. NELSON, Harvard University — Antagonistic interactions are widespread among microbes and can affect the structure and composition of microbial communities. Theoretical models of well-mixed population genetics with antagonistic interactions predict that a stronger competitor can invade a weaker one only if its initial population is larger than a critical inoculum size. In spatially-extended populations, the invasion of one competitor by another can be mapped to a nucleation problem and the invasion is predicted to be successful only above a critical nucleation size. To test these predictions, we have genetically engineered two strains of the baker's yeast *Saccharomyces cerevisiae* to release two different toxins, whose production rates we can vary independently. These strains allowed us to study how antagonistic interactions affect the population dynamics and population genetics of spatially-structured populations at different levels of toxin production, i.e. at different relative strengths of the two competitors. We show that, both in spatially-structured and in well-mixed populations, a toxin-producing strain can displace another toxin-producing strain only if the initial inoculum is larger than a critical threshold, even if the invader strain enjoys a selective advantage.

Tuesday, March 3, 2020 11:15 AM - 2:03 PM

Session G24 GSNP DBIO: Noise-Driven Dynamics in Far-From-Equilibrium Systems II 401 - Jeffrey Weiss, University of Colorado, Boulder

11:15AM G24.00001: Minimal Model for Intermittent Dynamics and "Turbulence" in Many-Body Systems*  GURAM GOGIA (Presenter), WENTAO YU, JUSTIN BURTON, Emory University — Complex systems are known to exhibit emergent properties that are missing on the constituent level. One particular property shared by many seemingly unrelated complex systems is intermittent switching between distinct dynamical states. Inspired by our previous experimental findings [1], here we present computational results for a particle-based system that exhibits intermittent switching between two distinct phases. The emergent dynamics are a direct consequence of coupling between structural disorder arising from particle polydispersity, inertial dynamics, and external forcing. Modelling the orthogonal mechanical energies of the system using ODEs with both noise and coupling terms based on kinetic arguments surprisingly results into predator-prey-like interactions. Such equations have recently been employed to describe intermittent turbulence in a pipe flow [2]. The only non-dimensional number derived from our equations resembles the Reynolds number in fluid flow and accurately predicts where intermittent dynamics are manifested.


*NSF, DMR-1455086
**11:27AM G24.00002: Stochastic transitions between phase-locked steady states in RF-irradiated graphene Josephson junctions**  
* TREVYN LARSON (Presenter), LINGFEI ZHAO, ETHAN ARNAULT, Physics, Duke University, MING-TSO WEI, Physics, University of Maryland, ANDREW SEREDINSKI, Physics, Duke University, HENGMING LI, Physics, Appalachian State University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, FRANCOIS AMET, Physics, Appalachian State University, GLEB FINKELSTEIN, Physics, Duke University — We investigate the Shapiro steps in a graphene-based Josephson junction with large gap MoRe leads. A wide variety of patterns are obtained, depending on the carrier density, temperature, RF frequency, and magnetic field. A particularly interesting regime of intermediate driving power is identified, in which the zero voltage state becomes unstable even at zero bias, and the junction spontaneously develops a voltage $V = \pm hf/2e$, which could persist for a several hours. We study the switching time between the $\pm hf/2e$ states as a function of applied power and temperature, and find a novel non-monotonic regime, in which the switching time between these attractors demonstrates a pronounced minimum at intermediate temperatures.

*Measurements conducted by T.L. and E.A were supported by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under Award No. DE-SC0002765. M-T.W. and A.S. performed lithographic fabrication and characterization of the samples with the support of NSF awards ECCS-1610213 and DMR-1743907. L.Z. and G.F. were supported by ARO Award W911NF16-1-0122. H.L. and F.A. acknowledge the ARO Award W911NF-16-1-0132.

BERNARDO SPAGNOLO (Presenter), Physics and Chemistry, Univ of Palermo — The noise-driven dynamics of three far-from-equilibrium systems are investigated: (i) transient dynamics in unstable potential and in Josephson junctions with Lévy noise; (ii) escape from a quantum dissipative metastable state in the presence of an external driving; (iii) the switching dynamics in a stochastic model of memristor.

We obtain: (i) exact analytical results of the residence time in the presence of Lévy flights in unstable potential profile, and noise enhanced stability phenomenon is observed in the system investigated and in JJs. (ii) a nonmonotonic behavior of the escape time versus the system-bath coupling, the temperature, and the frequency of the driving. The quantum noise enhanced stability phenomenon is observed in the system investigated. (iii) the nonstationary distribution and relaxation time of the stochastic model of memristors, which shows a nonmonotonic dependence, with a maximum, on the intensity of fluctuations.

**References**

11:51AM G24.00004: Anomalous Phase Dynamics of Driven Graphene Josephson Junctions
SANDESH KALANTRE (Presenter), FAN YU, MING-TSO WEI, University of Maryland, College Park, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science 1-1 Namiki, Tsukuba, 305-0044, Japan, MIGUEL HERNANDEZ-RIVERA, FRANCOIS AMET, Department of Physics and Astronomy, Appalachian State University, Boone, NC, USA, JAMES WILLIAMS, University of Maryland, College Park — Josephson junctions with weak-links of exotic materials allow the elucidation of the Josephson effect in previously unexplored regimes. In this work, we report on DC and AC Josephson effect of high-mobility, hexagonal boron nitride encapsulated graphene Josephson junctions. We measure phase-locked Shapiro steps on the application of RF radiation. The shape of resistive transitions between the steps is anomalous in the form of extended nodes. Moreover, an unexpected bistability between ±1 steps is observed with switching times on the order of seconds. A critical scaling of a bistable state with DC current and RF power is measured directly from the switching time, allowing for a comparison to numerical simulations. We show such intermittent chaotic behavior is a consequence of the nonlinear dynamics of underdamped junctions and has a sensitive dependence on the current-phase relation. We numerically investigate the switching time scaling as a consequence of the interplay between noise level and basin structure of the solutions. This work draws connections between nonlinear phenomena in dynamical systems and their implications for ongoing condensed matter experiments exploring topology and exotic physics.

12:03PM G24.00005: A theoretical model for ionic transport in a viscosity gradient*
DEREK STEIN (Presenter), BENJAMIN N WIENER, Physics, Brown University — We recently discovered that imposing a viscosity gradient across a nanofluidic channel made of glass causes ionic current to flow. The current is evidently carried by positively charged counterions in the electric double layers near the channel walls drifting toward the lower viscosity side. We present an explanation based on the Maxwell-Stefan (MS) theory of diffusion. Within the MS theory, transport of a given species is driven by a gradient in its chemical potential, and that driving force is balanced by a friction force with every other molecular species. Relating the MS theory to our nanofluidic experiments, we consider a fluid comprising a viscous fluid, a thin fluid, and counterions. The viscous and thin components of the mixture flow in opposite directions inside the channel, and as they do, each one exerts a frictional force on the counterions. There is a net motion of those counterions in the direction of decreasing viscosity because the drag coefficient with the viscous component is larger than the coefficient with the thinner component. There is also no mystery where the energy to drive the current comes from: It comes from the free energy of mixing of the viscous and thin fluids.

*This work was supported by NSF award #1904511.
12:15PM G24.00006: Pulling cargo increases the precision of molecular motor progress
AIDAN IVAR BROWN, Physics, University of California, San Diego, DAVID SIVAK (Presenter), Physics, Simon Fraser University — Biomolecular motors use free energy to drive a variety of cellular tasks, including the transport of cargo, such as vesicles and organelles. We find that the widely used "constant-force" approximation for the effect of cargo on motor dynamics leads to a much larger variance of motor step number compared to explicitly modeling diffusive cargo, suggesting the constant-force approximation may be misapplied in some cases. We also find that, with cargo, motor progress is significantly more precise than suggested by a recent result. For cargo with a low relative diffusivity, the dynamics of continuous cargo motion—rather than discrete motor steps—dominate, leading to a new, more permissive bound on the precision of motor progress which is independent of the number of stages per motor cycle.

DANIEL SEARA (Presenter), BENJAMIN B MACHTA, MICHAEL MURRELL, Yale University — Due to the lack of symmetries and variational principles, non-equilibrium systems have been difficult to treat theoretically. Recent work has focused on measuring entropy production rates as a measure of a system's distance from equilibrium, but little connection has been made between entropy production and the complex, spatiotemporal dynamics that arise at different time and length-scales in driven systems. We present a generic method for estimating entropy production rates from stochastic time series data for both random variables and fields while providing insight into the dissipative processes underlying their dynamics. Our method provides insight into the relationship between pattern formation and dissipation in mesoscopic, driven reaction-diffusion systems. Importantly, this technique does not depend at all on the underlying system and can be used with data in any number of spatial dimensions.

12:39PM G24.00008: Learning the Non-Equilibrium Dynamics of Brownian Movies
FEDERICO GNESOTTO, GRZEGORZ GRADZIUK, Ludwig Maximilian University of Munich, PIERRE RONCERAY, Princeton University, CHASE BROEDERSZ (Presenter), Ludwig Maximilian University of Munich — Soft living systems such as cytoskeletal networks, membranes, and tissues are driven out of thermodynamic equilibrium by internal enzymatic activity. Measuring and characterizing the non-equilibrium properties in these systems is a major challenge, owing to the large number of interacting degrees of freedom. Typically, the experimental characterizations of such systems rely on tracking the trajectories of embedded or endogenous probes. However, it is not clear how to select appropriate tracer probes and how this choice affects the resulting characterization; in general, it is unknown a priori which degrees of freedom are most informative about non-equilibrium activity in the system. In this talk, we present a new approach that does not rely on the tracking of probes in the system. Instead, we directly learn the non-equilibrium dynamics from a Brownian movie of a fluctuating soft assembly, yielding force fields and entropy production rates. Our approach is based on a principled analysis that reduces the dimensionality of the system by identifying the most dissipative components. We will discuss how this approach performs in different scenarios inspired by cytoskeletal networks.
12:51PM G24.00009: Spectral decomposition of irreversibility reveals structure of nonequilibrium activity in biological systems  ALEXANDRU BACANU (Presenter), JAMES F PELLETIER, YOON JUNG, Massachusetts Institute of Technology MIT, JORDAN HOROWITZ, University of Michigan, NIKTA FAKHRI, Massachusetts Institute of Technology MIT — Biological systems, such as cytoskeletal networks, exhibit stochastic mechanical fluctuations on mesoscopic scales which can violate detailed balance. The spatiotemporal structure of nonequilibrium activity on these scales remains unexplored, due to a lack of methods able to reliably quantify irreversibility. To probe activity in both space and time, we image spatially extended single-walled carbon nanotubes (SWNTs) embedded in actin-intact Xenopus cytoplasmic extract. Using normal mode decomposition of filament shape fluctuations, we infer the structure of the actomyosin-driven mechanical fluctuations. Metrics for irreversibility based on normal mode correlation functions quantify the spatiotemporal extent of nonequilibrium activity. To estimate the noise floor of our analysis, we compare our results to the fluctuations of SWNTs in an equilibrium, entangled F-actin gel. By altering network architecture and generating chemostatted ATP reservoirs, we probe the response of nonequilibrium activity to distinct perturbations. Our analysis quantifies the spatiotemporal structure of irreversibility on mesoscopic scales and shows it is affected by network mechanics and its coupling to the ATP chemical reservoir.

1:03PM G24.00010: Noisy driven oscillators: Adaptive drives break the fluctuation-dissipation theorem  JANAKI SHETH (Presenter), ALEX LEVINE, DOLORES BOZOVIC, Physics, UCLA — The steady-state dynamics of complex nonlinear systems include limit cycles in which the dynamic variables trace a closed path in phase space. Biological systems are replete with examples of such driven oscillators in a diverse range of systems including circadian rhythms, neuronal central pattern generators, and the active mechanics of hearing. These biological systems are inherently noisy, and they are typically controlled by active feedback. We explore the fluctuations and response functions of intrinsically noisy limit-cycle oscillators starting with models of stereocilium dynamics in the inner ear. We show that one can obtain a generalized fluctuations-dissipation theorem (GFDT) for the system in a reference frame comoving with the mean dynamical state moving about the limit cycle. However, in the presence of adaptive drives where there is feedback so that the energy input driving the oscillator depends on the state of the system, as in the driven stereocilium, even these generalized fluctuation theorems fail. We further explore the essential role of these feedback mechanisms in breaking GFDTs in noisy driven systems using a combination of simple computational models, analytical calculations, and stereocilium dynamics data.
1:15PM G24.00011: A generalized theory of interactions for complex multiscale stochastic systems with thermodynamic irreversibility*  SANTIAGO NÚÑEZ-CORRALES (Presenter), ERIC JAKOBSSON, University of Illinois at Urbana-Champaign — Understanding nonlinear, hierarchically structured complex systems through the discovery and application of statistical mechanics principles remains a significant challenge. Considering thermodynamic irreversibility is simultaneously essential and often intractable in these cases. Additionally, the presence and filtering of noise across scales often translates into stochastic differential equations for the dynamics, a theoretically and computationally onerous task. We present ongoing work towards a novel mathematical physics development that aims to capture statistical mechanical properties of complex multiscale stochastic systems driven by irreversible thermodynamics, a generalized theory of interactions (GToI) with a purely relational view in which interactions are fundamental entities, while objects and laws are derived. We show how these can be instantiated into concrete theories of interaction (CToIs) capable of capturing key ensemble properties. We exemplify its application to unveiling the underlying complexity of gases and discuss some aspects of its relation to differential models, including relevant computational considerations.

*Illinois Informatics Program, University of Illinois at Urbana-Champaign, ACM SIGHPC/Intel Computational and Data Science Fellows program (2017).

1:27PM G24.00012: Non-equilibrium response of a strongly coupled rotary motor  EMMA LATHOUWERS (Presenter), JOSEPH N. E. LUCERO, DAVID SIVAK, Physics, Simon Fraser Univ — Living systems at the molecular scale are complex (composed of many constituents with strong and heterogeneous interactions), far from equilibrium, and subject to strong fluctuations. This poses significant challenges to efficient, precise, and rapid free energy transduction, yet nature has evolved numerous molecular machines that do just this. Using a simple model of FoF1-ATP synthase (the primary motor for ATP synthesis), we investigate the interplay between non-equilibrium driving forces, natural equilibrium fluctuations, and interactions between the strongly coupled subsystems of this ingenious rotary machine. Additionally, we consider the resulting design principles for effective free energy transduction. Most notably, while one would naively assume that tight coupling between subsystems is preferred, we find that the output power is maximized at intermediate-strength coupling, which permits lubrication by stochastic fluctuations with only minimal slippage.
**1:39PM G24.00013: Stochastic Dynamics and Selection in the One Dimensional Stabilized Kuramoto-Sivashinsky Equation**  
SALONI SAXENA (Presenter), JOHN MICHAEL KOSTERLITZ, Brown University — Many spatially extended nonlinear systems are known to exhibit coarsening - starting from an initial uniform (disordered) state, ordered structures appear, the size of which increases with time. We study coarsening dynamics in the stabilized Kuramoto-Sivashinsky (SKS) equation in one dimension, with and without noise. The SKS equation is used to describe the growth of crystal surfaces, in particular the motion of terrace edges in step-flow growth [1]. The key feature of this equation is that it displays a bifurcation from a uniform steady state to a band of periodic states, depending on the control parameter. Coarsening is studied by analyzing the time evolution of the structure function for a range of control parameter values, starting from a uniform initial state. We find that the width of the structure function decays as a power law with time during an intermediate time regime, until a narrow peak centered at a given wave number is obtained. This is consistent with the emergence of an ordered (periodic) state which grows in spatial extent. We calculate the decay exponents and discuss the influence of the noise amplitude on the values of the exponents. We also make connections with wave number selection.


**1:51PM G24.00014: Maxwell's demons with finite size and response time**  
NATHANIEL RUPPRECHT, DERVIS VURAL (Presenter), University of Notre Dame — Nearly all theoretical analyses of Maxwell's demon focus on its energetic and entropic costs of operation. Here, we focus on its rate of operation. In our model, a demon's rate limitation stems from its finite response time and gate area. We determine the rate limits of mass and energy transfer, as well as entropic reduction for four such demons: those that select particles according to (1) direction, (2) energy, (3) number, and (4) entropy. Last, we determine the optimal gate size for a demon with small, finite response time, and compare our predictions with molecular dynamics simulations with both ideal and nonideal gasses.


**Tuesday, March 3, 2020 11:15 AM - 2:15 PM**

**Session G25 GSNP: Mechanical Metamaterials III / Physics of Liquids I**

402 - Sung Kang, Johns Hopkins University - Tag(s): Focus
11:15AM G25.00001: Inflatable Kirigami Structures*  LISHUAI JIN (Presenter), ANTONIO ELIA FORTE, BOLEI DENG, School of Engineering and Applied Sciences, Harvard University, AHMAD RAFSANJANI, Department of materials, ETH Zürich, KATIA BERTOLDI, School of Engineering and Applied Sciences, Harvard University — Kirigami inspired metamaterials have shown increasing potential in science and engineering due to their ability to achieve large deformations and morphology changes. Here, by embedding a thin kirigami shell into a soft silicon rubber, we present a novel, programmable and inflatable kirigami structure that can deform into a desired shape or trajectory at a given pressure. Moreover, we can easily assemble different actuators together to obtain very complex deformations via a modular design. Sequencing can also be achieved by introducing pressure drops in between the different modules, and feeding a pressure profile as a single input to the actuators. This could potentially benefit future designs for climbing robots and robotic arms, where disposing of multiple outputs given a single input is often necessary. Our study provides a simple, yet powerful strategy to design unprecedented kirigami balloons that will enrich the functionalities of inflatable structures.

*The research was supported by the NSF Grant DMR-1420570 and Army Research Office Grant W911NF-17-1-0147.

11:27AM G25.00002: Capillarity-driven Transformation of Microscopic Cellular Structures  BOLEI DENG (Presenter), SHUCONG LI, KATIA BERTOLDI, JOANNA AIZENBERG, Harvard University — Cellular structures are attracting increasing interest because of their unique mechanical, thermal, electrical, and acoustic properties, which largely depend on their size, shape and topology. As such, systems with tunable functionality can be constructed by tuning the geometry of the structures. Here we report a capillarity-driven transformation on 2D onsite microcellular structures that enables us to change their topology on demand and reversibly. To trigger such transformation both the cellular structure and the material have to be carefully designed, as it requires the formation of capillary menisci upon solvent evaporation at the unit-cell scale as well as the softening and stiffening of the material at the molecular scale. Finally, we show that our strategy can be applied to realize surface with tunable properties including adhesion, friction, hardness, and particle trapping.
Multiscale frequency conversion through input-independent dynamics of bistable lattices*  
MYUNGWON HWANG (Presenter), ANDRES F. ARRIETA, Mechanical Engineering, Purdue university — In this study, we extend the input-independent dynamics to higher-dimensional metastructures. A metabeam is constructed by integrating a bistable lattice along a beam-like outer frame. We obtain frequency response diagrams showing output frequency spectra for each input frequency and observe nonlinear out-of-plane behavior as long as transition waves are triggered along the in-plane bistable lattice direction. Similar to the observations in its one-dimensional counterpart, the transverse output frequencies remain coherent around a single dominant frequency regardless of the input frequency that triggers the transition waves. This result shows transfer of energy between two different length scales – localized in-plane waves and global out-of-plane deflections – and implies that such metabeams display efficient multiscale frequency conversion. Also identified is two qualitatively different routes to frequency conversion depending on the discreteness of the bistable lattice, enabling a greater design freedom. Furthermore, the unit cell design can be easily tuned to alter the metabeam properties, especially in terms of the operating frequency range and output frequency, allowing for a broad range of engineering applications.

This work was supported by NSF under Grant No. CMMI-1935137.

Tunable vibro-acoustic metamaterials  
OSAMA BILAL, Univ of Connecticut - Storrs, DAVID BALLAGI (Presenter), LUKAS ULRICH, Mechanical Engineering, ETH Zurich, CHIARA DARAIO, Mechanical and Civil Engineering, California Institute of Technology — Phononic crystals and acoustic metamaterials are architected lattices designed to control the propagation of acoustic or elastic waves. In these materials, the dispersion properties and the energy transfer are controlled by selecting the geometry of the lattices and their constitutive material properties. Most designs, however, only affect one mode of energy propagation, transmitted either as acoustic airborne sound or as elastic structural vibrations. Here, we present a design methodology to attenuate both acoustic and elastic waves simultaneously in all polarizations. We experimentally realize a three-dimensional load-bearing architected lattice, composed of a single material, that responds in a broadband frequency range in all directions and polarizations for airborne sound and elastic vibrations simultaneously. In addition, we show how we can tune the vibro-acoustic response of the metamaterial through external stimuli.
MICHAEL CZAJKOWSKI (Presenter), Georgia Inst of Tech, CORENTIN COULAIS, Institute of Physics, Univ. Amsterdam, MARTIN VAN HECKE, Institute of Physics, Univ. Leiden, ZEB ROCKLIN, Georgia Inst of Tech — Maximally Auxetic behavior, where Poisson’s ratio is the most negative, has been explored and identified in 2D perforated elastic sheets in which rigid square elements are connected at the corners by comparatively flexible elastic “hinges”. While these metamaterials are designed to emulate a uniform zero-energy motion of the free hinge material (mechanism), experiments have revealed qualitatively different non-uniform mechanical response. To understand this, we utilize a coarse graining approach, combined with highly detailed finite element simulations and experiments, to reveal that the perforated elastic sheet mechanics is controlled by a novel set of soft modes that correspond precisely to the well-studied planar Conformal Maps. We exploit this very convenient result to demonstrate new and highly accurate methods of analytically solving for linear and non-linear deformations of real materials. This includes a powerful holographic approach, in which large non-linear deformations may be predictably controlled by simple actuation at the boundary. Finally, we introduce a more general methodology for identifying and controlling the soft modes associated with a broad class of 2D mechanisms including the Miura and Eggbox origami patterns.

PAVEL GALICH (Presenter), EDWIN THOMAS, Rice Univ — Alternating a lossy with a near-lossless material within a structure can lead to remarkable asymmetry in wave propagation. The field of passive (without control of gain and loss by external stimuli) non-Hermitian acoustics is quickly emerging. Here, we propose a simple system comprised of a single pair of lossless (metallic) and lossy (polymeric) resonators in the form of circular ~0.1 mm thin sheets – that demonstrates close to 100% asymmetry in the acoustic reflection coefficient, while at the same time the transmission coefficients are identical. Experimental measurements and theoretical modeling over a wide range of audible frequencies (reflection and transmission coefficients from 1 kHz up to 6.3 kHz) reveal a nearly ideal sonic unidirectional reflector. Such asymmetric acoustic properties are valuable, for example, for concealing objects from sonars, while allowing communication.

12:27PM G25.00007: A universal identity for the Poisson ratios of oblique Miura-ori  
HUSSEIN NASSAR (Presenter), Univ of Missouri - Columbia, ARTHUR LEBÉE, École des Ponts - ParisTech, LAURENT MONASSE, INRIA — Certain origami and origami-like tessellations, such as the Miura-ori and the eggbox pattern, remarkably exhibit equal and opposite in-plane and out-of-plane Poisson ratios. In this talk, we propose and prove a generalization of this identity to all tessellations that can be obtained as the translation surface of one zigzag along another. These include in particular the entire family of oblique, i.e., non-orthotropic, Miura-ori. The proof is based on a perturbative scheme and makes some typical assumptions of rigid folding kinematics; it remains valid for small and large deformations whether the underlying tessellation is symmetrical, developable, flat-foldable, or not.

12:39PM G25.00008: BREAK  —
**12:51PM G25.00009: Toward a microscopic understanding of the dynamics of simple glass-forming liquids**  
* [Invited]  
PATRICK CHARBONNEAU (Presenter), Duke University — The dynamical arrest predicted by mode-coupling theory and the entropy crisis at the random first-order transition are both exact descriptions of simple glass-forming liquids, albeit only in abstract, infinite-dimensional systems. What survives of these features and what other processes come into play in three-dimensional glass formers are questions that remain largely unanswered. In this talk, I present our recent advances toward a microscopic understanding of the finite-dimensional echo of the infinite-dimensional transitions, and of some of the activated processes that affect the dynamical slowdown of simple yet realistic glass formers.

*Simons Foundation Grant No. 454937

**1:27PM G25.00010: Unifying the percolation and mean-field description of the random Lorentz gas**  
PATRICK CHARBONNEAU, Department of Chemistry, Duke University, ERIC CORWIN, Department of Physics, University of Oregon, YI HU (Presenter), Department of Chemistry, Duke University, HARUKUNI IKEDA, FRANCESCO ZAMPONI, Laboratoire de Physique, Ecole Normale Superieure — The random Lorentz gas (RLG) is a minimal off-lattice model of transport in porous media. It is also a minimal model of structural glasses. The exact mean-field, infinite-dimensional limit solution of the RLG indeed predicts a discontinuous dynamical caging transition akin to that of simple liquid glass formers. The RLG, however, is also in the percolation universality class, in which the dynamical caging transition is continuous. These two descriptions are thus fundamentally contradictory. To resolve this paradox, we study the caging regime of the RLG as a function of dimension. We find that the static cage size quantitatively matches the mean-field predictions, and that the percolation transition and the (finite-dimensional echo of the) dynamical transition are clearly distinguishable in all dimensions. As dimension increases, however, the system dynamics grows increasingly controlled by the dynamical transition. In fact, the escape time from the dynamical cage grows exponentially quickly with d, thus resolving the paradox. More significantly, cage escape events are similar to hopping processes, which had mostly eluded theoretical description in standard supercooled liquids.

*This research is supported by a grant from the Simons Foundation (#454937, Patrick Charbonneau).
1:39PM G25.00011: Unveiling the connection between liquid water and its amorphous/glass states  FAUSTO MARTELLI (Presenter), IBM Research UK — Water is unique in many ways. One of the most remarkable peculiarities of water is its polyamorphism, i.e., its capability to acquire more than one amorphous state. The very nature of amorphous ices is still highly debated, but even less is known about their connection to the liquid state. The possibility of a continuous thermodynamic link between the supercooled liquid(s) and the amorphous ices is highly debated. On the other hand, probing such connection is a challenging task, mostly because of the lack of theoretical and/or experimental tools able to account for the high degeneracy of local configurations in statistically isotropic materials.

In this work, we bypass these difficulties by proposing a new strategy that explores structural similarity between the different disordered configurations. We combine GPU-accelerated molecular dynamics simulations with a neural network approach that allows us to clarify the connections between equilibrium liquid water and its amorphous/glass states. Moreover, our results also confirm that liquid water can be interpreted as a two state system, an hypothesis that was always considered at the theoretical level and that is at the heart of water anomalies.

1:51PM G25.00012: Dynamical theory predicted correlation between activated relaxation and thermodynamics in glass-forming liquids  BAICHENG MEI (Presenter), YUXING ZHOU, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — The microscopic Elastically Collective Nonlinear Langevin Equation (ECNLE) theory of glassy dynamics, in conjunction with an a priori mapping of thermal liquids to an effective hard sphere fluid, captures the structural relaxation time of nonpolar molecular liquids over 14 decades. We re-visit this theory for monodisperse hard spheres using the modified-Verlet integral equation theory closure as equilibrium input. Comparison with simulation shows the equation-of-state, static correlation lengths, radial distribution function, and structure factor are remarkably well captured up to very high volume fractions. Numerical ECNLE theory calculations then reveal that the logarithm of the alpha time scales behaves as an inverse power law of the dimensionless compressibility which is a thermodynamic property that quantifies the amplitude of long wavelength density fluctuations. The scaling is linear (cubic) in the low (high) barrier regime, establishing an operational link between glassy relaxation and thermodynamics. The predicted connection is directly tested using solely experimental data, and is well verified for molecular liquids. By introducing one adjustable parameter to capture the low to high barrier crossover, experimental data over 14 decades can be linearized.
How does the character of the Sastry transition depend on the range of interatomic interactions? CAITLIN GISH (Presenter), KAI NAN, ROBERT HOY, Univ of South Florida — The mean pressure $<P_{IS}(\rho)>$ within the inherent structures (IS) of liquids maintained at density $\rho$ and temperature $T >> T_{melt}$ is minimized at the “Sastry” density $\rho_S$. For $\rho < \rho_S$ ($\rho > \rho_S$), these IS are typically cavitated (homogenous). Using molecular dynamics simulations of Mie liquids [$U_n(r) = \varepsilon(r^{2n} - 2r^n)$ with $4 \leq n \leq 12$], we determine how the character of the transition between cavitated and homogeneous IS depends on the range of the interatomic pair potential. We find three principal results: (i) As $n$ increases with $T$ held fixed, $\rho_S$ approaches and then exceeds the crystallization density $\rho_X$; (ii) as a consequence, the portion of systems’ phase diagrams (in terms of $P$ and $T$) where systems are liquids with predominantly cavitated IS decreases with increasing $n$; (iii) For $\rho > \rho_S$, the pair correlation functions $g(r)$ of the liquids’ IS are nearly conformal, i.e. the $g(r)$ for different $n$ nearly map to a common reduced pair correlation function $G(\rho^{1/3}r) = \rho^{-1/3}g(r)$. We discuss the implications of these results for condensation and cavitation of simple atomic liquids.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G26 DBIO: Morphogenesis, Tissues, and Cancer 403 - Zi Chen, Dartmouth Coll

Investigation into the dynamics of lipid membrane remodeling
ABHIMANYU SHARMA (Presenter), Physics & Astronomy, University of Utah, HENRY NGUYEN, NATHANIEL TALLEDGE, Biochemistry & Biophysics, University of California San Francisco, JOHN MCCULLOUGH, Biochemistry, University of Utah, FRANK MOSS III, Biochemistry & Biophysics, University of California San Francisco, JANET IWASA, Biochemistry, University of Utah, MICHAEL VERSHININ, Physics & Astronomy, University of Utah, WESLEY SUNDQUIST, Biochemistry, University of Utah, ADAM FROST, Biochemistry & Biophysics, University of California San Francisco — Lipid membranes play a key role in biology, enclosing entire living cells, as well as intracellular compartments. Cellular processes such as endocytosis, virus budding, and cytokinesis involve changes in membrane shape and connectivity. Membrane remodeling is essential, common, and tightly regulated. A variety of pathways, including the endosomal sorting complexes required for transport (ESCRT) machinery are involved in locally changing membrane curvature (both invagination and evagination), tabulation, and scission. However, the mechanics of many of these remodeling events are still poorly understood. We have used an in vitro GUV system, and investigated the details of membrane reshaping under local mechanical load and in several ESCRT protein backgrounds. We will discuss our results, which demonstrate how protein-based regulation can help remodel bilayer membranes.
**11:27AM G26.00002: Investigating cell shape changes during organogenesis using a 3D vertex model**

PAULA SANEMATSU (Presenter), Department of Physics, Syracuse University, GONCA ERDEMCI-TANDOGAN, Institute of Biomaterials and Biomedical Engineering, University of Toronto, MATTHIAS MERKEL, Alan Turing Centre for Living Systems and Centre de Physique Théorique, Aix-Marseille University, JEFFREY D. AMACK, Department of Cell and Developmental Biology, State University of New York, Upstate Medical University, M. LISA MANNING, Department of Physics, Syracuse University

— Left-right (LR) asymmetry present in internal organs of vertebrates initiates during embryonic development with observable changes to individual cell shapes which are vital to the creation of functional organs. However, the mechanisms that drive cell shape changes remain poorly understood. Kupffer's vesicle (KV) is a transient organ in the Zebrafish embryo that acts as the LR organizer. As the KV moves through the surrounding tissue during development, KV cells change shape along the anterior-posterior (AP) axis, a necessary process for subsequent LR asymmetry[1]. Erdemci-Tandogan et al.[2] used a 2D vertex model and experimental data to show that surrounding tissue rheology and KV cell motility could drive KV cell shape changes. Since the KV is inherently 3D, and that 2D and 3D drag forces can be very different, we extend that work by studying drag forces on the KV in a 3D model. We show that cell shape changes along the AP axis do occur in 3D due to drag forces. By implementing particle-image-velocimetry (PIV) analysis, we quantitatively compare simulation and experimental data of the flow of surrounding cells past the KV as it develops.

1. Dasgupta et al., eLife 2018;7:e30963.
2. Erdemci-Tandogan et al., Biophys. J. 115, 2018

*This work was supported by NIH grant R01GM117598.


SAMIRA ANBARI (Presenter), JAVIER BUCETA FERNANDEZ, Chemical and Biomolecular Engineering, Lehigh Univ — Within the topic of morphogenesis, tissue elongation is a necessary process in all metazoans to shape their body plans which is not fully understood. For example, in the particular case of the limb, it has been shown that tissue elongation cannot be explained by either a localized proliferation of cells or their oriented divisions and, surprisingly, the tissue elongates perpendicular to the direction along which cell grow. Here we propose a mechanism of tissue elongation that couples the mechanical properties of cells with the concept of positional information to modulate the former in a location-dependent manner. To illustrate our proposal, we use morphogen gradient thresholds as well as Turing patterning system as the mean used by cells to “know” their relative positions within a primordium. Our numerical simulations are based on the vertex model system and we show that if the cell-cell adhesion is modulated as a function of the location of cells within a primordium, an auto-catalytic cell intercalation process develops and the tissue elongates. Moreover, our results reveal that cells grow perpendicular to the elongation direction as experimentally reported. Altogether, our results shed light on the tissue elongation problem and pave the way to better understand morphogenesis.
11:51AM G26.00004: Morphogenesis and fractal dimension of bacterial pellicles  BOYANG QIN (Presenter), NED WINGREEN, BONNIE BASSLER, HOWARD A STONE, Princeton University — Bacteria cells can self-organize into structured communities at phase boundaries, known as biofilms. At liquid-liquid and liquid-air interfaces, these soft, living materials of cells and extracellular polysaccharides – called pellicles – confer survival advantages and protection against environmental insults to the community. These benefits are not attainable by individual planktonic cells. The mechanics driving pellicle formation and morphology are not understood. Here, using a home-made adaptive stereoscope instrument and fluorescent microscopy, we identify a series of mechanical and architectural transitions in *Vibrio cholerae* pellicles at a liquid-oil interface. There are three distinct stages: emergence of founding colonies, onset of primary and secondary wrinkling instabilities, and a fractal-order increase in complexity. We show that although cells in a pellicle share a habitat, founder colonies remain monoclonal, hence the community maintains spatial and genetic heterogeneity.

12:03PM G26.00005: Learning about human development from clinical IVF data  BRIAN LEAHY (Presenter), HELEN YANG, WON-DONG JANG, Harvard University, DALIT BEN-YOSEF, Lis Maternity Hospital, VINOTHAN MANOHARAN, DANIEL NEEDLEMAN, Harvard University — The early human embryo is the physicist’s dream for studying development. Between fertilization and implantation in the uterus, mammalian embryos undergo a global reorganization (compaction) followed by a symmetry-breaking differentiation (blastocyst formation), with no external direction from the mother. But for ethical reasons, we cannot do experiments with human embryos. So how can we understand human development without experiments? Here, we examine tens of thousands of videos of human embryos recorded during routine clinical IVF procedures. We use those videos to explore the natural variability in mammalian preimplantation embryo development, and we leverage this variability to identify critical factors in early development.
Emergence of helical growth and morphogenesis in fungal cells from cell wall dynamics*

SHANKAR LALITHA SRIDHAR (Presenter), GUILLAUME LOSTEC, Mechanical Engineering, University of Colorado, Boulder, JOSEPH K.E. ORTEGA, Mechanical Engineering (Emeritus), University of Colorado Denver, FRANCK J. VERNEREY, Mechanical Engineering, University of Colorado, Boulder — Walled cells such as plants, algae and fungi achieve expansive growth using turgor pressure that helps mediate irreversible wall deformation and regulates their shape and volume. The architecture of the cell wall plays a crucial role in this process where a network of microfibrils and tethers (complex polysaccharides and proteins) dynamically mediate the network topology via continuous detachment and reattachment events. The growth of Phycomyces blakesleeanus, a wiry single-celled sporangiophore that typically grows longitudinally, is particularly intriguing as it also rotates (clockwise from top) indicating helical growth. There is no apparent functional purpose for this rotation which has led to speculation that it is a direct consequence of wall architecture, and specifically a microfibril re-orientation mechanism. Interestingly, in piloboloid mutants longitudinal growth is combined with radial growth to produce a rotation inversion, i.e. anti-clockwise rotation. In this talk, we will present a novel approach based in statistical mechanics to model the organization and dynamics of microfibrils and tethers in the cell wall of to help explain this phenomenon.

*We gratefully acknowledge the support of the National Science Foundation under CAREER award 1350090.

Understanding cell contact constriction in epithelial morphogenesis through data driven reverse-time inference

NICOLAS LENNER (Presenter), Max Planck Institute for Dynamics and Self-Organization, DEQING KONG, Faculty of Medizin, University of Göttingen, STEPHAN EULE, Max Planck Institute for Dynamics and Self-Organization, JÖRG GROSSHANS, Faculty of Medizin, University of Göttingen, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — Tissue elongation via convergent extension mediated by cell intercalation is a frequent mechanism in the development of metazoans. During Drosophila germband extension cell intercalation is achieved by acto-myosin driven junction shrinkage of neighboring cells, its resolution into a vertex of four neighboring cells, and subsequent junction formation in orthogonal direction. Despite tremendous progress in the understanding of the molecular underpinnings involved in this process called a T1 transition, a quantitatively tested mechanism that predicts the dynamics of individual cell-junctions is still not available. We here show how our mathematically novel approach of reverse time ensemble inference allows to infer the process of junction shrinkage in reverse time, starting from the endpoint of the dynamic, i.e. the 4-vertex. We apply our inference scheme to ~1000 T1 transitions and systematically rule out model classes of increasing complexity using all accessible ensemble statistics. We find visco-elastic like dynamics, infer the onset of each individual junction collapse and link the inferred junctional dynamics to the simultaneously recorded myosin dynamics.
12:39PM G26.00008: Experiments and modeling of “irreversible” brain torsion in early chick embryos*  ZI CHEN (Presenter), HAO ZHANG, GUANGCHAO WAN, Thayer School of Engineering, Dartmouth College, WEI ZENG, University of Virginia, HANNAH GROVER, SHICHENG HUANG, Thayer School of Engineering, Dartmouth College — The rightward torsion of the chick embryonic brain tube is one of the earliest organ-level left-right asymmetry developmental events, often associated with birth defects such as situs inversus, but the biomechanics of this process remains incompletely understood. Previous works showed that vitelline membrane (VM) exerts a force on the brain that drives the torsion, and surface tension (ST) can replace the mechanical role of VM. However, our experiments showed when ST was removed the torsion does not fully reverse suggesting other overlooked mechanical factors. Here, we use a combination of experiments and modeling to reveal that the deformation during the early brain torsion can be path and stage dependent. With optical coherence tomography imaging, we tracked the twisting and untwisting in a step-wise manner. A computational model is employed to help interpret the findings, in particular the path-dependent, "irreversible" shape evolution. Results show that the body forces such as gravity and buoyancy also play an important role during this left-right asymmetric morphogenesis process, thus revealing the hidden mechanical factors in the normal and abnormal development of early embryos.

*Branco Weiss-Society in Science fellowship, Dartmouth startup fund.

12:51PM G26.00009: Dynamics of a single cell fate decision*  SIMON FREEDMAN (Presenter), KRISTIN JOHNSON, CAROLE LABONNE, MADHAV MANI, Northwestern University — As an animal develops from a fertilized egg into a complex multicellular organism, its cells change from being pluripotent to lineage restricted. These state changes are often driven by morphogens, molecules that launch signalling cascades that affect DNA transcription and modify a cell's protein makeup. While morphogens and cell fates have been extensively identified, the process through which a morphogen changes a cell's fate is not well understood. To elucidate these dynamics, we performed bulk RNA sequencing at multiple time points during a single cell fate decision in which pluripotent Xenopus laevis (African frog) cells differentiate to one of two fates: neural progenitor and epidermis. We found that the geometric structure of both transitions include linear temporal trends that correspond with development toward a neural fate, and that epidermal fated cells exhibit a second, non-linear temporal trend that corresponds with BMP activation. Our analyses enabled us to predict a point-of-no-return for the epidermal fate, which we experimentally verified. Our work highlights the importance of examining intermediate developmental times to discern fate specification, and sheds light on distinguishing the internal and external forces that drive embryonic development.

*NSF-Simons CQuB
1:03PM G26.00010: Binary establishment and maintenance of discrete cell fates in development  JIAXI ZHAO (Presenter), Department of Physics, University of California, Berkeley, JACQUES BOTHMA, MATTHEW NORSTAD, HERNAN G. GARCIA, Department of Molecular and Cell Biology, University of California, Berkeley — During embryonic development, cells must ultimately adopt discrete fates. Positive autoregulation has been proposed as a general mechanism for establishing and maintaining these discrete cell-fate decisions. Here, we quantitatively dissect the role of autoregulation and bistability in establishing binary cellular fates in the fruit fly Drosophila melanogaster. Specifically, we apply recently developed single-cell live imaging techniques to quantify transcriptional and protein dynamics of the Drosophila pair-rule gene fushi tarazu as cells decide whether to commit to the expression of the gene.

1:15PM G26.00011: A variational principle for power dissipation in low frequency conduction in biological tissues.  FRANCISCO SOLIS (Presenter), School of Mathematical and Natural Sciences, Arizona State University, VIKRAM JADHAO, Intelligent Systems Engineering, Indiana University Bloomington — Propagation of low-frequency electrical signals in biological tissues appears naturally in neural and cardiac physiological systems. These signals can also be externally applied to tissues as part of experimental probes or therapeutic tools. Models for propagation of these signals usually consider tissues as purely conductive materials. In large systems such as whole bodies or organs, these models consider the systems as composed of finite domains of homogeneous regions with distinct conductivities. The electric fields in these model systems exhibiting piecewise-uniform conductivity obey equations similar to those of electrostatics in polarizable media, but with boundary conditions set by current conservation. In this presentation we show that the electric fields can be obtained via a variational principle based on the minimization of dissipated power. In addition to providing a conceptual framework to the problem, this principle allows the construction of approximate solutions. It can also be used to establish bounds on the spectrum of the integral and differential operators that appear naturally in these problems.

1:27PM G26.00012: A biophysical model uncovers the size distribution of migrating cell clusters across cancer types  FEDERICO BOCCI (Presenter), Center for Theoretical Biological Physics, Rice University, MOHIT KUMAR JOLLY, Indian Institute of Technology, JOSE N ONUCHIC, Center for Theoretical Biological Physics, Rice University — Migration from the primary tumor is a crucial step in the metastatic cascade. Cells with various degrees of adhesion and motility migrate into the bloodstream as single circulating tumor cells (CTCs) or multi-cellular CTC clusters. The frequency and size distributions of these clusters have been recently measured, but the underlying mechanisms enabling these different modes of migration remain poorly understood. We present a biophysical model that couples intra-tumoral heterogeneity enabled by the epithelial-mesenchymal transition (EMT) with cell migration to explain the modes of individual and collective cancer cell migration. This reduced physical model undergoes a transition from individual migration to collective cell migration and robustly recapitulates CTC cluster fractions and size distributions observed experimentally across several cancer types, thus suggesting the existence of common features in the mechanisms underlying cancer cell migration. Overall, this biophysical model provides a platform to continue to bridge the gap between the molecular and biophysical regulation of cancer cell migration, and highlights that a complete EMT might not be required for metastasis.
1:39PM G26.00013: Spatial Distribution of Immune Cells in Tumors*  

JULIANA C. WORTMAN (Presenter), Department of Physics and Astronomy, University of California, Irvine, TING-FANG HE, SHAWN SOLOMON, ROBERT ZHANG, ANTHONY ROSARIO, ROGER WANG, TRAVIS Y. TU, Department of Immuno-Oncology, City of Hope Comprehensive Cancer Center, DANIEL SCHMOLZE, Department of Pathology, City of Hope Comprehensive Cancer Center, YUAN YUAN, SUSAN E. YOST, Department of Medical Oncology and Therapeutics Research, City of Hope Comprehensive Cancer Center, XUEFEI LI, HERBERT LEVINE, Department of Bioengineering, Rice University, GURINDER ATWAL, Cold Spring Harbor Laboratory, PETER P. LEE, Department of Immuno-Oncology, City of Hope Comprehensive Cancer Center, CLARE YU, Department of Physics and Astronomy, University of California, Irvine — The goal of immunotherapy is to enhance the ability of the immune system to kill cancer cells. Immunotherapy is more effective and, in general, the prognosis is better, when more immune cells infiltrate the tumor. We describe various techniques we have developed to explore the question of whether the spatial distribution rather than just the density of immune cells in the tumor is important in forecasting whether cancer recurs. We apply our approach to immune cells in images of tumor tissue taken from (triple negative) breast cancer patients. We find that there is a distinct difference in the spatial distribution of immune cells between good clinical outcome (no recurrence of cancer within at least 5 years of diagnosis) and poor clinical outcome (recurrence within 3 years of diagnosis).

*This work was supported by Stand Up To Cancer, The V Foundation, and the Breast Cancer Research Foundation. The work of CCY and JCW was also supported in part by the Cure Breast Cancer Foundation.

1:51PM G26.00014: Computationally tractable mechanistic model of inhomogeneous -- anisotropic drug diffusion and tumor ablation  

ERDI KARA (Presenter), AMINUR RAHMAN, EUGENIO AULISA, Mathematics and Statistics, Texas Tech Univ, SOUPARNO GHOSH, Statistics, University of Nebraska–Lincoln — In this work, we study the effect of drug distribution on tumor cell death when the drug is internally injected in the tumorous tissue. We derive a full 3-dimensional inhomogeneous – anisotropic diffusion model. To capture the anisotropic nature of the diffusion process in the model, we use an MRI data of a 35-year old patient diagnosed with Glioblastoma multiform (GBM) which is the most common and most aggressive primary brain tumor. After preprocessing the data with a medical image processing software, we employ finite element method in MPI-based parallel setting to numerically simulate the full model and produce dose-response curves. We then illustrate the apoptosis (cell death) fractions in the tumor region over the course of simulation and proposed several ways to improve the drug efficacy. Our model also allows us to visually examine the toxicity. Since the model is built directly on the top of a patient-specific data, we hope that this study will contribute to the individualized cancer treatment efforts from a computational bio-mechanics viewpoint.
A possible role for epigenetic feedback regulation in the dynamics of the epithelial-mesenchymal transition (EMT)\footnote{This research is supported by Physics Frontiers Center NSF Grant PHY-1427654 (WJ and HL); NSF Grant PHY-1605817 (WJ, AD, SM and HL); NIH,R01CA200970 (SM) and 2R01CA155243-06A1 (AD and SM). MKJ is supported by Ramanujan Fellowship awarded by SERB, DST, Government of India (SB/S2/ Rjn-049/2018).}

WEN JIA (Presenter), Rice Univ, ABHIJEET DESHMUKH, SENDURAI A MANI, MD Anderson Cancer Center, MOHIT KUMAR JOLLY, Indian Institute of Science, HERBERT LEVINE, Rice Univ — Epithelial-mesenchymal transition (EMT) plays an important role in cancer metastasis and drug resistance, and involves epigenetic remodeling. However, how epigenetic changes affecting the dynamical traits such as plasticity or memory are not fully understood. Here, we analyzed the effects of epigenetic feedback on EMT through integrating this feedback on various aspects of the miR-200/ZEB loop – a core circuit regulating EMT. Epigenetic feedback on self-activation of ZEB has minor effects in population distribution and transition times, but epigenetic feedback on the inhibition of miR-200 by ZEB can largely stabilize the mesenchymal state, thus making the process irreversible. Follow-up preliminary experiments show that when EMT is induced in epithelial cells, a certain percentage of cells can stay in mesenchymal state after the inducing signal is removed. This percentage depends on the extent of induction of EMT, thus well recapitulating our model-based predictions.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G27 FIAP: Electronic Structure: Thermodynamic & Optical Properties

11:15AM G27.00001: Carrier Lifetime and Mobility in GaAsNBi Alloys\footnote{We gratefully acknowledge support from the National Science Foundation (Grant Nos. DMR 1410282, DMR 1810280 and DMR 0959341)}

BRENNAN ARNOLD, JAMES HEYMAN (Presenter), Physics, Macalester Coll, ANDRA CHEN, JARED MITCHELL, RACHEL GOLDMAN, Materials Science Engineering, University of Michigan — III-V alloys incorporating Nitrogen and Bismuth are of significant interest for optoelectronic applications in the near- and mid-infrared. We report measurements of the photoconductivity lifetime and photocarrier mobility in a series of GaAs\(_{1-x-y}\)N\(_x\)Bi\(_y\) samples grown on GaAs by MBE. We find short conductivity lifetimes of order 3ps to 5ps and carrier mobilities of order 30 to 80cm\(^2\)/Vs. Time-resolved photoconductivity was obtained from optical pump, THz probe measurements, and steps were taken to avoid the influence of the GaAs substrate: A tunable optical pump permitted excitation below the GaAs bandgap, and transient THz reflection was used as a surface-specific probe of the conductivity. The short carrier lifetime and low carrier mobility likely arises due to rapid carrier trapping in these materials.
11:27AM G27.00002: Study of \( \beta\text{-Ga}_2\text{O}_3 \) Photoluminescence with Above Bandgap Laser Excitation

JEFFREY LAPP (Presenter), DINESH T THAPA, Univ of Idaho, JESSE HUSO, Klar Scientific, AMRAH CANUL, Univ of Idaho, MATTHEW MCCLUSKEY, Washington State University, LEAH BERGMAN, Univ of Idaho — \( \beta\text{-Ga}_2\text{O}_3 \) is being considered as a next generation ultra-wide bandgap semiconductor with promising UV device applications. \( \beta\text{-Ga}_2\text{O}_3 \) films were grown via RF sputtering and photoluminescence (PL) was performed using 5.1 eV laser excitation, which is above the predicted bandgap of \( \sim 4.9\text{eV} \). Weak UV PL was detected at 4.85eV and 4.20eV. The near band edge (NBE) PL at 4.85eV is consistent with subsequent transmission measurements of the films that showed a bandedge value of 4.85eV. Due to the strong trapping affinity of holes in \( \text{Ga}_2\text{O}_3 \) previously predicted by theory, observation of NBE PL at 4.85eV PL has been deemed unlikely. We speculate that the laser intensity employed in our experiments was sufficient to create a small density of free holes enabling NBE in \( \text{Ga}_2\text{O}_3 \). The 4.20eV PL emission exhibits peak shifts up to \( \sim 100\text{meV} \) under different annealing environments. Strong UV emissions were also observed at 3.14eV and 3.56eV, which have been attributed to donor-acceptor recombination and self-trapped holes, respectively. Emission due to self-trapped holes was not detected when sub-bandgap laser excitation of 3.8eV was utilized.

*This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering, Award No. DE-FG02-07ER46386

11:39AM G27.00003: Optical properties of GaN/Er:GaN/GaN core-cladding planar waveguides

YAQIONG YAN (Presenter), ZHENYU SUN, TREY BRENDBAN SMITH, WEIPING ZHAO, JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech University — Erbium doped GaN (Er:GaN) is a promising candidate as a gain medium for high energy lasers (HELs) operating at the “retina-safe” spectral region around 1.5 \( \mu\text{m} \) due to outstanding thermal, mechanical and optical properties of GaN host. Compared to YAG, GaN has a much higher thermal conductivity of \( k \approx 253 \text{ W/m*K} \) and a smaller thermal expansion coefficient of \( \alpha \approx 3.53 \times 10^{-6} \text{ °C}^{-1} \) and the potential to significantly outperform YAG based HELs. We report here the successful fabrication and optical characterization of GaN/Er:GaN/GaN core-cladding planar waveguides (PWGs). Optical confinement in the core layer has been investigated. The measured optical loss coefficients of Er:GaN PWGs at 1.54 \( \mu\text{m} \) have been measured and are respectively 1.0 \( \text{cm}^{-1} \) for the transverse electric (TE) and 1.2 \( \text{cm}^{-1} \) for the transverse magnetic (TM) modes. Approaches to further reduce the optical loss and optimal configuration for resonantly pump GaN/Er:GaN/GaN PWGs for achieving amplification near 1.5 \( \mu\text{m} \) have been identified.

*The work is supported by the Directed Energy – Joint Transition Office Multidisciplinary Research Initiative program (grant #N00014-17-1-2531). H. X. Jiang and J. Y. Lin would also like to acknowledge the support of Whitacre Endowed Chairs by the AT & T Foundation.
**11:51AM G27.00004: Optical properties of indium tin oxide thin-films at high temperature**

JIWOONG KIM (Presenter), Department of Physics, Pusan National University, SUJAN SHRESTHA, MARYAM SOURI, JOHN G CONNELL, Department of Physics and Astronomy, University of Kentucky, SUNGYUN PARK, Department of Physics, Pusan National University, AMBROSE SEO, Department of Physics and Astronomy, University of Kentucky — Indium tin oxide (ITO) is one of the most widely used transparent conductors. However, its high-temperature optical properties, which are important for device applications in extreme conditions such as space missions, have not been studied. We have investigated the optical properties of ITO thin-films up to 800 °C using *in situ* optical spectroscopic ellipsometry equipped within a vacuum chamber. The amorphous ITO films show an abrupt change of optical constants at 300 °C due to crystallization. Above 400 °C, the bandgap energy of the ITO thin-film decreases with increasing temperature, implying that electron-phonon interaction broadens the interband optical transitions. The reduction of bandgap energies due to electron-phonon interaction is also observed in epitaxial ITO thin-films. Nevertheless, both amorphous and epitaxial ITO thin-films remain optically transparent even at high temperatures up to 800 °C. In addition, background gas environments reversibly alter the bandgap energies of the epitaxial ITO thin-films, suggesting that the diffusion of oxygen vacancies occurs vigorously.

*This work was supported by National Science Foundation grant DMR-1454200 for sample synthesis and characterizations. J. Kim acknowledges the support of NRF-Korea (2015H1A2A1034200).*

**12:03PM G27.00005: On the Thermo-Optical Interactions at the Band-Edge in ZnO Thin Films**

AMRAH CANUL (Presenter), DINESH T THAPA, JEFFREY LAPP, Univ of Idaho, GRANT NORTON, Washington State University, LEAH BERGMAN, Univ of Idaho — The study of the band edge in UV-Vis absorption spectra has impacted fundamental understanding of semiconductor physics as well as advances in technological application. An analytical approach based on the derivative of the absorption spectra was used to explore the nature of the near band edge (NBE) of ZnO thin films grown via the sputtering technique. It was found that the NBE is composed of a Gaussian where the width and peak position were employed to model the electron-phonon (e-p) interaction and defect characteristics of the film. These characteristics were studied via transmission experiments in the temperature range of 77 K to 532 K. The as-grown film was found to exhibit a very weak e-p coupling relative to the static contribution of defects. Upon successive controlled annealing of the ZnO film, up to 800 °C, the defect component diminished and the phonon contribution became dominant. X-ray diffraction and imaging studies agree with these results. The defects in the ZnO films are discussed in terms of structural inhomogeneities and Zn interstitials which are prevalent in ZnO films grown via sputtering.

*This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering, Award No. DE-FG02-07ER46386.*
12:15PM G27.00006: Comparison of ZnO Nanoparticles Synthesized by Microwave-assisted and Precipitation Method*  RUSIRI RATHNASEKARA (Presenter), HARI PARAMESWAR, Univ of Tulsa — In this work, Zinc Oxide (ZnO) Nanoparticles were synthesized using precipitation and microwave methods with different pH values (8, 9, and 10). Structural properties were studied by means of Transmission Electron Microscopy (TEM), X-ray Diffraction Spectroscopy (XRD), Impedance Spectroscopy, and Optical Spectroscopy. TEM images revealed that the morphology of nanoparticles increased from 8 nm to 16 nm synthesized by precipitation method while the diameter increased from 9 nm to 15 nm in microwave assisted method. The XRD confirmed the wurtzite structure in all samples with no secondary phases. Optical properties were studied by means of Photoluminescence (PL) and absorption measurement. Band gap of nanoparticles were also calculated and found to decrease from 3.25 eV to 3.18 eV in ZnO particles prepared by the precipitation method, whereas bandgap decreases from 3.21 eV to 3.19 eV in the microwave method. Electrical transport properties of nanoparticles were analyzed by impedance spectroscopy using Cole-Cole plot technique. From Impedance spectra, we observe that resistance and capacitance of nanoparticles depend on the size of nanoparticles synthesized by both precipitation and microwave method.

*Oklahoma NASA EPSCoR (Grant Number-NNX15AM75A)

12:27PM G27.00007: Realizing GaN/Er:GaN/GaN core-cladding planar waveguide gain medium via hydride vapor phase epitaxy*  ZHENYU SUN (Presenter), YAQIONG YAN, TREY BRENDAN SMITH, WEIPING ZHAO, JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech Univ — Erbium doped gallium nitride (Er:GaN) bulk crystals have been identified as a promising optical gain material for solid-state high energy lasers (HELs) operating at the 1.5 mm “retina-safe” spectral region. A highly desired design of HEL gain medium is the core-cladding planar waveguide (PWG) structure, capable of providing excellent heat dissipation and optical confinement. We report the realization of a GaN/Er:GaN/GaN core-cladding PWG structure grown by hydride vapor phase epitaxy (HVPE) and processed by mechanical and chemical-mechanical polishing. An Er doping concentration of [Er] = 3 × 10^{19} \text{ atoms/cm}^3 has been confirmed in the core layer via secondary ion mass spectrometry measurements. The structure emitted strong 1.54 \mu m emission under 980 nm resonant excitation. It was shown that a 96% optical confinement can be achieved in the Er:GaN core layer with a core thickness of 50 \mu m and [Er] = 3 \times 10^{19} \text{ atoms/cm}^3. This work paves the way and marks an important progress towards the practical application of Er:GaN gain medium for “retina-safe” HELs.

*The work is supported by the Directed Energy – Joint Transition Office MRI program and ONR (grant # N00014-17-1-2531). H. X. Jiang and J. Y. Lin would like to acknowledge the support of Whitacre Endowed Chairs by the AT & T Foundation.
12:39PM G27.00008: Two-photon absorption spectroscopy and anisotropy of bulk zincblende and diamond symmetry semiconductors and quantum dots*  BRANDON FUREY (Presenter), University of Texas at Austin, RODRIGO MISAEL BARBA-BARBA, ALAN BERNAL, Centro de Investigaciones en Optica, TUSHTI SHAH, BRIAN KORGEL, University of Texas at Austin, RAMON CARRILES, BERNARDO MENDOZA SANTOYO, Centro de Investigaciones en Optica, MICHAEL C DOWNER, University of Texas at Austin — Si quantum dots (SiQD) are potential candidates for biologically-inert theranostic applications. Excitation in the red-near infrared (NIR) by two-photon absorption (2PA) is useful for confocal microscopy and therapy techniques. We studied the spectroscopic response and size-dependence of 2PA in colloidal ligand-passivated SiQDs in the red-NIR by indirect two-photon induced photoluminescence (2PIP) and direct pump-probe modulation spectroscopy (PPMS). We are developing a model to explain the spectra for the nanocrystalline response from ab initio calculations using length gauge theory for bulk Si. We measured the 2PA spectra and anisotropies of bulk Si, GaAs, and GaP in the range 650-2000 nm using PPMS in the femtosecond excitation regime to further verify these calculations.

*Robert Welch Foundation Grants F-1038 and F-1464
Laboratorio de Optica Ultrarrapida en CIO, Mexico
National Science Foundation Grant CHE-1308813

12:51PM G27.00009: Scanning Photocurrent Measurements of Degenerately Doped Si*  MAARTEN DE HAAN (Presenter), TIANHAN LIU, XI WANG, HANWEI GAO, PENG XIONG, Florida State Univ — Scanning photocurrent microscopy (SPCM) has shown much promise as a means for direct and efficient measurements of carrier lifetime and diffusion in novel semiconductors including topological insulators. High spatial resolution and electrical sensitivity in these setups has made detection of properties such as diffusion length routine. Degenerately doped Si with a surface oxide are often used as back-gating substrates for thin films or flakes of the materials. However, the high photocurrent of the silicon often complicates the elucidation of the same photo responses in thin films/flakes. Here, we present SPCM measurements of a degenerately doped silicon substrate. After buffered HF etching of the surface oxide, Cr/Au electrodes were defined via thermal evaporation through a shadow mask, resulting in a device of 25 μm channel width between two back-to-back Schottky contacts. An elevated photocurrent was measured in the regions near the electrodes at zero bias voltage, indicating a diffusion current. The experiment has shown the structure as a viable platform for SPCM measurements of thin topological insulators under continuous backgate tuning.

*Work supported by NSF grant DMR-1905843
Temperature dependence of the indirect-gap photoluminescence from Ge

JOSE MENENDEZ, CHRISTIAN POWELEIT, SEAN TILTON (Presenter), Arizona State Univ — Few experimental reports have been published to date on the temperature dependence of the photoluminescence (PL) from Ge, and no attempts have been made to model the spectra using the standard Van Rosbroeck-Schockley equation that relates absorption to spontaneous emission. This anomaly can be traced back to the fact that the standard textbook expressions for indirect absorption are not applicable to Ge due to the proximity of the direct and indirect gaps. If such expressions are used to compute the PL, not even a peak is predicted.

We report here a PL study of high-quality Ge samples at temperatures $10 \, \text{K} \leq T \leq 300 \, \text{K}$. The spectra display a rich structure with a rapidly changing lineshape as a function of $T$. We show that when the more realistic theory of LA-phonon assisted absorption from Ref. 1 is used to compute the PL, peaks at about the right energy are predicted. However, the agreement between theory and experiment requires the additional incorporation of “forbidden” channels involving LO and TA phonons. Analytical expressions for the absorption assisted by these phonons are derived, and the resulting expressions are combined to predict a PL spectrum in very good agreement with experiment.


First-principles calculation of Jerk current in polar and nonpolar semiconductors

BERNARDO MENDOZA SANTOYO, Centro de Investigaciones en Optica, A.C., BENJAMIN FREGOSO, SUMAN PANDAY (Presenter), Kent State Univ - Kent — The bulk photovoltaic effect is the archetypical example of nontrivial carrier dynamics in illuminated insulators lacking a center of inversion. The injection current (also known as ballistic current or circular photogalvanic effect), a component of the bulk photovoltaic effect, could play an important role in optoelectronic applications, e.g. solar cells or as a probe of the topology of materials. The Jerk current is a generalization of the injection current to third order in the electric fields [1]. We present a first-principles calculation of the Jerk current spectrum in prototypical semiconductors Si, CdSe, GaAs and novel two-dimensional ferroelectric monolayer GeSe, GeS, SnS and SnSe. We show that, similar to the injection current, the jerk current is a sensitive probe of the geometry of the Bloch wave specially in reduced dimensions. Experimental ramifications are also discussed.


*CONACYT Proyecto A1-S-9410 (MBS) and NERSC-DOE DE-AC02-05CH11231 (SRP,BMF)
1:27PM G27.00012: Exploration of Free Carrier Relaxation Dynamics in Bulk Gallium Arsenide
ADAM HALAOUI (Presenter), GEOFFREY DIEDERICH, MARK SIEMENS, Univ of Denver — Multidimensional coherent spectroscopy (MDCS) is an ultrafast spectroscopic measurement that spreads coherent information across multiple dimensions, disentangling congested spectral features. Both coherent and incoherent transport processes, as well as their dynamics, can be easily separated and measured with MDCS. These attributes make MDCS ideal for studying complex material behaviors such as carrier-carrier scattering and exciton formation in semiconductors.

Here, we present MDCS spectra of bulk gallium arsenide (GaAs) showing strain-induced separation of the heavy-hole and light-hole exciton states\(^1\), exciton formation from free carriers across a broad energy distribution, and relaxation from GaAs quantum wells in the same sample. The spectra clearly show the Sommerfeld enhancement of the free carrier absorption at long times, while early times show a transient feature related to the fast relaxation of states near the band-edge. We suspect that this transient feature is caused by correlated free carrier pairs or higher-lying excitonic states that form a quasi-continuum near the band edge.


*We acknowledge the financial support of the National Science Foundation

1:39PM G27.00013: Evaluation of BaTiS\(_3\) for Thermoelectric Applications by Using First Principles Theory
TULA PAUDEL (Presenter), EVGENY Y TSYMBAL, University of Nebraska - Lincoln — BaTiS\(_3\) is a semiconductor with a band gap of about 0.5 eV and very strong transport anisotropy for both electron and hole conduction. The conduction band minimum is very dispersive with a small effective mass and large mobility because of split-off \(dz^2\) band contribution. The optical phonons are relatively soft, and the ground state non-centrosymmetric phase is favorable by just about 1 mev/fu over the centrosymmetric phase, indicating possibility of phase intermixing and reduced thermal conductivity at finite temperatures. Electrons can be doped easily for instance by an external dopant La. The possibility of large electrical conductivity with a tunable thermal conductivity by external doping and phase intermixing makes this compound excellent candidate for thermoelectric applications. By using the first principles density functional theory and linearized Boltzmann transport theory, we calculate electrical conductivity, thermal conductivity and the Seebeck coefficient and report reasonable thermoelectric figure of merit, ZT, of about 0.4 at 800K for n-type BaTiS\(_3\). Additional possibility to enhance the figure of merit by doping, phase intermixing and band engineering is discussed.
1:51PM G27.00014: First Principles Study of Electronic, Magnetic and Thermoelectric Properties of Perovskite BaTbO$_3$

DHURBA JAISHI (Presenter), Central Department of Physics, Tribhuvan University, DINESH KUMAR YADAV, Condensed Matter Physics Research Center, Butwal-11, Rupandehi, Nepal, MADHAV PRASAD GHIMIRE, Central Department of Physics, Tribhuvan University — Perovskite material have been on focus for many applications in spintronic device due to their novel properties such as ferroelectric, metal-insulator-transition, half-metallicity, non-trivial topological properties, etc. Recently these materials are found to show interesting thermoelectric properties which are expected to lead to new devices to harvest waste heat into efficient energy. In this work, we have investigated the electronic, magnetic, and thermoelectric properties of BaTbO$_3$ using the density functional formalism. The structure are fully relaxed and the value of the calculated lattice constant is 4.29 Å, in good agreement with the experimental values. The magnetic ground state of BaTbO$_3$ is found to be G-type antiferromagnet, with a band gap of 1.68 eV with an on-site Coulomb interaction of 4 eV for Tb atoms. Transport properties is computed using the BoltzTrap code. The calculated figure of merit (ZT) is 0.97 at 800 K, which indicates the suitability of BaTbO$_3$ as an efficient thermoelectric material.

2:03PM G27.00015: NMR and Mössbauer study of p-type half-Heusler thermoelectrics

YEFAN TIAN, RUI LI (Presenter), FARIT VAGIZOV, NADER GHASSEMI, Department of Physics and Astronomy, Texas A&M University, WUYANG REN, HANGTIAN ZHU, ZHIFENG REN, Department of Physics, University of Houston, JOSEPH HANSBRO ROSS, Department of Physics and Astronomy, Texas A&M University — To investigate the local behavior of defects and mixed compositions in NbFeSb-based semiconductors, for improved thermoelectric efficiency, we have performed $^{93}$Nb and $^{121}$Sb NMR, as well as Mössbauer measurements, on pure NbFeSb and a series of p-type Ti-substituted (Nb,Ti)FeSb samples with different substitution levels. A small but consistently increasing paramagnetic defect density is observed with the increase of Ti substitution level revealing the existence of additional Ti-induced paramagnetic defects. NMR line shapes show a clear difference between effect of intrinsic and extrinsic defects in NbFeSb. The NMR shifts can be well understood by a model combining a Knight shift and composition-dependent chemical shift. The results indicate a nearly rigid-band behavior for the valence band with a small enhancement of effective mass vs substitution. For pure NbFeSb samples, the Mössbauer spectra include an additional T-dependent singlet. The increase of its area can be explained based on carriers activated into a shallow acceptor-like defect level above the valence band, consistent with the defect activation results obtained with NMR. In samples with Ti substitution, the Mössbauer spectra are consistent with a random neighbor distribution, indicating no preferential local ordering.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G28 FIAP GIMS: Infrared Sensing and Imaging 405-407 - Carola Emminger, New Mexico State Univ - Tag(s): Industry, Invited
GeSn alloys with dilute Sn concentrations around the near-infrared indirect to direct transition have been thoroughly investigated in recent years. However, the GeSn alloy system, in much the same way as the HgCdTe alloy, is expected to have a continuum of band gaps that reach a value of zero. Covering this IR spectral range requires much higher Sn concentrations, which are not obviously attainable given the thermodynamic metastability of the Ge-Sn system. Sporadic reports of such alloys have appeared in the literature, but in most cases the samples were unsuitable for band gap determinations.

In this presentation we discuss recent work\(^1\) characterizing the band gap and electronic structure of GeSn alloys which Sn concentrations as high as 33\%. These materials have direct band gaps approaching 0.15 eV (~ 8 μm), thus reaching well into the mid-IR spectral range. The high-quality GeSn films required for optical characterization were grown directly on Si substrates by CVD reactions of polygermanes and stannanes at temperatures between 240-290°C. The structural properties of the films are similar to those of their dilute counterparts, in spite of the fact that the fraction of Sn-Sn bonds is expected to be significant. For example, we find that the lattice parameter of the alloys still follows Vegard's law, as reported for lower Sn concentrations.

Ellipsometric measurements of the complex dielectric function make it possible to determine the band gap by modeling the absorption edge. Our model includes excitonic, band filling (Burstein-Moss), and non-parabolicity effects. We find that the compositional dependence of the band gap cannot be described by a simple quadratic polynomial, as is the case in many alloy systems. The implications of this finding for the ability of the GeSn system to cover the 8-12 μm mid-IR window will be discussed in detail.


*Supported by AFOSR Grants FA9550-17-1-0314 and FA8650-18-C-1152.
11:51AM G28.00002: Antimonides T2SLS Infrared Focal Plane Arrays for Space Remote Sensing Applications* [Invited] SARATH GUNAPALA (Presenter), NASA Jet Propulsion Laboratory — Ga-free type-II strained layer superlattice (T2SLS) mid-wave infrared (MWIR) and long-wave infrared (LWIR) barrier infrared detector (BIRD) such as nBn and xBn focal plane arrays (FPAs) could easily operate at higher operating temperature (i.e. compared to InSb and quantum well infrared photodetectors (QWIP) and FPAs) due to the strong suppression of G-R dark current due to SRH processes as explained earlier. We have successfully fabricated MWIR HOT-BIRD FPA and integrated with a dewar cooler assembly for the CubeSat Infrared Atmospheric Sounder (CIRAS) 6U CubeSat. We have also successfully fabricated LWIR BIRD FPA for the Hyperspectral Thermal Imager (HyTI) 6U CubeSat and it will be integrated with a dewar cooler assembly as well. These antimonides based T2SLS BIRDs outperform existing thermal infrared detectors such as QWIPs and InSb. Another 20-30K higher operating temperature advantage can be achieved when we further improve the performance by hybridizing the T2SLS LWIR BIRD detector array to the high-dynamic range in-pixel digital ROICs. Based on III-V compound semiconductors, the T2SL BIRDs offer a breakthrough solution for the realization of low cost (high yield), highperformance FPAs with excellent uniformity and pixel-to-pixel operability. Therefore, T2SLS MWIR and LWIR BIRD FPA technology is very attractive to Earth and planetary remote sensing instruments.

*The research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration (80NM0018D004).

12:27PM G28.00003: Low-cost infrared imaging technology development at the Air Force Research Laboratory* [Invited] ARNOLD KIEFER (Presenter), CHARLES REYNER, JOSHUA DURAN, BRUCE CLAFLIN, GAMIINI ARIYAWANSA, JARRETT VELLA, Sensors Directorate, Air Force Research Laboratory — Infrared imaging technology has numerous commercial, military, and scientific applications. As performance requirements increase, so do the costs of fabricating and operating infrared imaging systems. While many high-performance applications can be met using the very well-developed mercury cadmium telluride material system, the overall manufacturing and operational costs of the imaging system as a whole can be prohibitively expensive. The Air Force Research Laboratory (AFRL) is actively exploring various technologies using different materials and device physics to achieve adequate performance for the given application at significantly lower costs. A sample of different technologies will be reviewed with an emphasis on fundamental science and basic research needs.

*AFOSR
Photonics for Mobile Handset through Automotive 3D Sensing Consumer Applications [Invited]  BRANDON COLLINGS (Presenter), Lumentum — Machine learning and predictive algorithms are increasingly providing new opportunities for technology to directly participate in our interaction with the physical world around us. A crucial element of this interaction is the detailed digital characterization of that physical environment as an input to these algorithms. While digital visible light cameras have advanced dramatically, optical sensor systems able to add accurate depth measurements to 2D images within practical consumer environments are being developed to enable new consumer applications. Primary examples of these sensor driven applications include biometric authentication on mobile phone handsets and LIDAR scene mapping for autonomous vehicles. This presentation will provide an overview of the architectures of these 3D sensor systems, their underlying enabling photonic technologies, including VCSEL arrays, narrow linewidth semiconductor lasers, MEMS and optomechanical packaging, and how such complex technological solutions are being successfully brought to the consumer market.

Mid-Wave Infrared Resonant Cavity Detectors [Invited]  GARY W WICKS (Presenter), University of Rochester — The dominant issue confronted by designers and users of mid-wave infrared (MWIR) detectors is their large dark current and its noise-producing fluctuations. MWIR dark current is more than a million times that of short-wave (telecom) IR detectors. Several decades of work on dark current reduction via attention to material quality and epitaxial structure are nearing maturity. Significant improvements in dark current require new approaches. Our approach reduces dark current by reducing the volume of the detector’s absorber layer. A thin absorber layer is located inside an optical cavity formed by two mirrors – the so-called Resonant Cavity Detector (RCD). Optical absorption of the thin layer is typically ~1%, which would produce unacceptably small quantum efficiency (QE) in a single-pass detector. In an RCD, the light passes through the thin absorber many times (~50-100) as it re-circulates within the optical cavity, which produces good QE, and also low dark current. RCDs with QE~50% have achieved nearly 10× reduction in dark current and we expect to eventually reduce dark current by 100×. The RCD approach also affects frequency bandwidth (speed) and spectral bandwidth. RCDs absorbers are ~100× thinner than conventional detectors, which reduces minority carrier transit time, thus the frequency bandwidth is expected to increase to > 10 GHz. The spectral bandwidth, Δ, of RCDs is greatly reduced due to interference of the recirculating light with itself. RCDs with Δ ~ 20 nm have been produced, and Δ ~ 3 nm seems feasible. The narrow Δ and low dark current makes RCDs ideal for narrow band applications, such as detection of lasers or sensing spectrally sharp absorption features of gases. The RCD’s spectral response can be tuned 50-100 nm with detector temperature or the light’s angle of incidence. Finally, we discuss the tolerance on the epitaxial growth, which is significantly tighter for RCDs (1% layer thickness control) than for conventional MWIR detectors.

Tuesday, March 3, 2020 11:15 AM - 1:51 PM

Session G29 DSOFT GSNP: Emergent Mechanics of Active, Robotic, and Living Materials I 501 - Corentin Coulais, Univ of Amsterdam - Tag(s): Focus
11:15AM G29.00001: Transmission hysteresis and edge modes in bounded space-time composites [Invited] HUSSEIN NASSAR (Presenter), Univ of Missouri - Columbia — The vibrational frequency response of bounded composites, e.g., metamaterials and sonic crystals, is often understood thanks to band diagrams established in the absence of boundaries. Introducing a pump wave that modulates in time the properties of the composite challenges the correspondence between the vibrations picture and the waves picture. The talk revisits this correspondence in the context of the nonreciprocal acoustics of space-time composites. Specifically, we establish in the weak coupling regime how the hybridization of total bandgaps into pairs of one-way bandgaps triggers nonreciprocal hysteresis transmission loops in the space-frequency domain and alters, qualitatively and quantitatively, the vibrational frequency response in the presence of reflecting boundaries. The theoretical analysis is assessed numerically and exploited to shed new light on previously obtained experimental data. Last, extrapolating our study to the strong coupling regime, transmission hysteresis is shown to explain the emergence of topological vibrational modes with one-way edge-bulk and bulk-edge transitions.

11:51AM G29.00002: Motion via Bistability in Viscous Fluids* MOHAMED ZANATY (Presenter), Harvard University, WILLIAM ZUNKER, University of Minnesota-Twin Cities, JOCHEN MUELLER, KATIA BERTOLDI, Harvard University — We study the behavior of bistable beams in viscous media and their application to aquatic locomotion. Specifically, we exploit asymmetric actuation of bistable beams, which leads to a nonreciprocal deformation path. As an example, we use double pinned axially compressed bistable beams. We actuate the beam asymmetrically by imposing an angular position on one of the beam extremities.

Using a combination of numerical simulations and experiments, we find that when the beam is surrounded by a viscous fluid, the position of the stable states is not impacted. However, a higher moment is needed to deform the beam compared to air. Importantly, the beam motion non-reciprocity results in thrust in the axial direction, and, therefore, propulsion. The thrust increases with increasing beam compression.

*M.Z. acknowledges the financial support provided by the Swiss National Science Foundation under grant number P2ELP2_184497
12:03PM G29.00003: Non-reciprocal solitons in robotic materials  MARTIN BRANDENBOURGER (Presenter), HANS DEKKER, CORENTIN COULAIS, Institute of Physics, University of Amsterdam — The recent development of robotic materials, which are assemblies of building blocks integrating sensors and actuators, enables the implementation of non-conservative interactions within mechanical systems. This opens the way to the emergence of unique large scale mechanical properties.

Here, we use this new platform to generate soliton waves that indefinitely propagate in only one direction.

We show that these waves emerge from a smart balance between mechanical non-linearities and linear non-reciprocal interactions, namely, which preferably transmit motion in one direction. Using experiments, theoretical models and simulations, we rationalize the conditions of existence of these solitons and demonstrate that they exist even in the presence of friction. These results establish new ways to reliably transport mechanical energy.

12:15PM G29.00004: Topological locomotion  KATIA BERTOLDI (Presenter), BOLEI DENG, MOHAMED ZANATY, Harvard University — We investigate how the propagation of the topological domain walls through a metamaterial based on the squares rotating mechanism can be harnessed to generate locomotion. First, we add internal elastic constraints to transform the system into a bi-stable system, with the two energy minima being the two symmetry-related rotated phases. Such metamaterial supports topological solitons that take the deformed metamaterial from one static equilibrium position to another one. Remarkably, our results indicate that by combining the propagation of such finite-width topological solitons with angle-dependent friction (that can be easily realized by putting the system on wheels) we can realize a crawler.

12:27PM G29.00005: Topology by activity in non-Hermitian mechanical metamaterials  COLIN SCHEIBNER (Presenter), WILLIAM THOMAS MARK IRVINE, VINCENZO VITELLI, University of Chicago — A simple view of an active solid is a network of masses interacting via non-conservative bonds. We examine 2D topological lattices equipped with non-reciprocal active bonds that inherit two key properties from their passive counterparts: their interactions conserve linear momentum and depend only on the relative positions of the masses. We characterize the flow of Berry curvature and exceptional points in the resulting non-Hermitian band structure as activity is tuned from the passive limit to the brink of instability. Along this flow, we find a discrete onset of topologically charged bands whose activity threshold can be controlled via zero-mode deformations of the underlying lattice. Simulations and analytical calculations reveal the emergence of persistent edge modes influenced by the interplay of a topologically protected penetration depth and an effective quality factor derived from non-Hermitian gain and loss. Our work sheds light on non-Hermitian band theory and the design of active metamaterials that conserve linear momentum.
**12:39PM G29.00006: The topology of nonlinear mechanical systems**  
PO-WEI LO (Presenter), MICHAEL J LAWLER, Cornell University, CHRISTIAN SANTANGELO, University of Massachusetts Amherst, BRYAN G CHEN, Leiden University, KRISHANU ROYCHOWDHURY, Stockholm University, CHAO-MING JIAN, University of California, Santa Barbara — Following the pioneering work of Kane and Lubensky (and others), commendable advancements have been made in the field of topological mechanics. The majority of the work, however, concerns the topology of linear zero modes primarily engaging the framework of linear response theory (often drawing parallels to electronic responses in topological insulators). We, in the present work, attempt an extension to accommodate nonlinear effects that are more natural to occur in realistic mechanical systems and feature topologically protected zero modes. Invoking the tools of differential geometry, we present an exact theory to demonstrate this topology. Our theory (inspired by topological quantum field theory), remarkably, predicts the existence of a $Z$-type topological invariant which arises only from the nonlinearities and does not demand any symmetry imposition (unlike the linear zero modes). We further include example systems to illustrate the physics.

**12:51PM G29.00007: Mechanical metamaterial inspired by biological tissues**  
XINZHI LI (Presenter), DAPENG BI, Northeastern University — We introduce an amorphous mechanical metamaterial inspired by how cells pack in biological tissues. The spatial heterogeneity in the local stiffness of these materials has been recently shown to impact the mechanics of confluent biological tissues and cancer tumors (Li et al Phys. Rev. Lett. 123, 058101 (2019)). Here we use this bio-inspired model as a design template and show that this heterogeneity can give rise to amorphous cellular solids with large, tunable phononic bandgaps. Unlike in phononic crystals, the band gaps here are directionally isotropic due to their complete lack of positional order. The size of the bandgap can be tuned by a combination of local stiffness heterogeneity and the local elasticity modulus. Finally, we also investigated the possibility of introducing a topological nature in the mechanical response using a hexagonal lattice version of the same model. By tuning the local elasticity moduli, we demonstrate the emergence of a pseudo-spin state and as well chiral mechanical response. This constitutes a mechanical analogue of the quantum spin Hall effect.
1:03PM G29.00008: Modeling tunable acoustic transport in driven graphene nanoresonator arrays

PRAGALV KARKI (Presenter), DAVID MILLER, ANDREW D BLAIKIE, BRITTANY CARTER, BENJAMIN J ALEMAN, JAYSON PAULOSE, Univ of Oregon — Arrays of graphene nanoelectromechanical resonators show promise as a platform for precise, programmable manipulation of acoustic waves at the nanoscale. Besides harboring technologically relevant resonant frequencies and high quality factor, graphene resonators display a remarkable tunability of the local membrane tension through electrostatic back-gating or laser heating, which can be used to modulate vibrational properties. Motivated by experiments, we present a theoretical and computational study of the acoustic properties of coupled graphene resonators with dynamical spatiotemporal modulation of the tension. Starting from the theory of thin elastic plates, we develop a reduced description of the collective modes arising from the coupling of the fundamental modes on individual resonators and evaluate the effects of externally driven changes in tension on wave propagation. We will also describe early efforts at calibrating and testing the model against experimental measurements of coupled resonator acoustic modes. Our results pave the way towards designing driven graphene nanoelectromechanical resonator arrays with a manifestly out-of-equilibrium acoustic response.

1:15PM G29.00009: Transitions from conservative to non-conservative regimes in optical binding of colloidal matter.*

DOMINIQUE DAVENPORT (Presenter), DUSTIN KLECKNER, University of California, Merced — We study light generated inter-particle interactions known as optical binding. These forces are mediated by the particle light scattering making it uniquely responsive to simple changes in the parameter space. For instance, we find that many colloidal particles placed in a weakly focused laser beam can self-assemble into higher-order and multi-leveled structures which can be tuned with simple alterations. We share experimental results which conclude a dramatic change in assembly patterns by changing particle index of refraction; namely, a switch between a conservative pair-wise regime to highly non-conservative many-body regime.

*Hellman Fellows Fund

1:27PM G29.00010: What kinds of forces does optical binding produce?*

DUSTIN KLECKNER (Presenter), DOMINIQUE DAVENPORT, University of California, Merced — Optical binding is an attractive tool for controlling colloidal forces because it offers a highly tunable method of producing inter-particle forces without chemical modifications. Previous studies of optically bound particles have tended to focus on small numbers of particles in relatively static configurations. By contrast, our experimental studies of many wavelength sized particles exhibit novel dynamics which are indicative of driven, non-conservative forces. I will discuss how these forces arise, and how they might be controlled to study colloidal dynamics in novel regimes.

*This work was supported by a grant from the Hellman Fellows Fund.
1:39PM G29.00011: The odd flows of a colloidal chiral fluid* EPHRAIM BILILIGN (Presenter), VISHAL H SONI, University of Chicago, SOFIA MAGKIRIADOU, École Polytechnique Fédérale de Lausanne (EPFL), STEFANO SACANNA, New York University, DENIS BARTOLO, École Normale Supérieure de Lyon, MICHAEL JOHN SHELLEY, New York University, WILLIAM THOMAS MARK IRVINE, University of Chicago — We report the assembly of a chiral fluid composed of millions of spinning colloidal magnets. By activating the fluid at the single unit level, we observe macroscopic flows with no counterpart in conventional fluids. Odd viscous stresses drive the propagation of unidirectional free-surface waves damped by odd (or Hall) viscosity. Further, the competition between odd stress and cohesive forces results in intermittent bulk flows, blurring the distinction between solid and liquid.

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Tuesday, March 3, 2020 11:15 AM - 2:03 PM

Session G30 DSOFT DPOLY DBIO: Self-Limiting Assemblies III: Soft Assemblies and In and Out of Equilibrium 502 - Gregory Grason, Univ of Mass - Amherst

11:15AM G30.00001: Pitch-balanced helical motifs in tightly packed lamellar structures EFI EFRATI (Presenter), Weizmann Institute of Science — Many biological and manmade lamellar structures form minimal surfaces due to surface area or bending energy minimization (or both). Recently, the endoplasmic reticulum sheets were shown to contain both right and left-handed helical motifs at equal amounts. In this talk, I will show that the lamellar structures that house photosynthesis in some plants, the thylakoid, also display right and left-handed motifs. The oppositely handed motifs, unlike those of the endoplasmic reticulum, differ in pitch and diameter, yet the stoichiometry is such that pitch is balanced between the differently handed motifs. We argue that the optimal packing of helical motifs in lamellar structures requires global pitch balance. We support this by a new constructive recipe that allows us to generate exact minimal surfaces with any arrangement of helical motifs.
11:27AM G30.00002: Colloidal membrane thickness sets critical surface area for vesicle formation*  JOANNA ROBASZEWSKI (Presenter), Brandeis University, LEROY JIA, THOMAS R POWERS, ROBERT ALAN PELCOVITS, Brown University, ZVONIMIR DOGIC, University of California, Santa Barbara — The malleable size and shape of biological membranes allow them to act in a wide range of cellular functions. Vesicles in particular have different uses, from transport to compartmentalization, depending on their size and shape. However, the rapidity with which bio-membranes bend and change structure on the nanoscale makes studying the physics that drive these changes difficult. We use colloidal membranes as experimental models to study the forces governing vesicle formation. Due to the larger length and time scales present in our colloidal system, we directly observe membranes undergoing lateral growth and then bending into vesicles. Both theory and experiment indicate that the size of the final vesicle structure depends on the thickness of the membrane. By tuning the thickness of our colloidal membranes, we can set the critical surface area at which a flat sheet will transition into a vesicle. Our system therefore allows for direct probing of vesicle formation physics, measurement of physical properties, and control over membrane curvature and structure size.

*This work was supported by NSF-MRSEC-DMR-1420382, NSF-CMMI-1634552, and NIH-T32EB009419

11:39AM G30.00003: How Curvature and Tension Direct Morphology and Interactions of Solid Membrane Domains in Fluid Vesicles*  MARIA SANTORE (Presenter), WEIYUE XIN, HAO WAN, Univ of Mass - Amherst — Multi-phospholipid giant unilamellar vesicles containing at least one high melting lipid (such as DPPC) exhibit the coexistence of fluid and solid membrane domains. To the extent that the inner and outer leaflets of the membrane are matched in composition and molecular number, symmetry dictates flat solid domains. The curvature imposed we show that at sufficiently high tensions, the curvature imposed by global vesicle shape influences the growth of solid domains, producing deviations from hexagon domain shape to include edge instabilities that appear as flowers. At high tensions domains appear to fracture. At lower tensions, exclusion of curvature into the fluid membrane region produces reversible interactions between solid domains that give rise to aggregation or long range order, depending on the relative sizes of vesicle domains, curvature, and excess membrane area. These behaviors are demonstrated in a model experimental vesicle system.

*US Department of Energy
**11:51AM G30.00004: Collapse and folding of flexible colloidal polymers**  
ANGUS MCMULLEN, JASNA BRUJIC (Presenter), Physics, New York University — The self-assembly of colloids can yield novel materials with unusual optical or mechanical properties. Unlike periodically repeating structures, here we introduce a new paradigm of self-assembly in which flexible colloidal polymers find a ‘fold’, similar to the way polypeptides fold into proteins. We have previously shown how emulsion droplets decorated with DNA sticky ends self-assemble into freely-jointed polymers. Here, we demonstrate the addition of secondary, switchable interactions along the length of a self-assembled polymer. These interactions are triggered by a temperature quench, whose rate governs the folding pathways from the extended to the collapsed states. The folding time scales with the length of the chain, in agreement with the increase in entropy. Using the simplest form of sequence control, we show that labeling alternating particles with secondary interactions eliminates some folding pathways visited when all droplets along the chain interact, narrowing the ensemble of folded configurations. This result opens up the prospect of programmable sequence design to achieve a unique stable structure, as the Anfinsen’s dogma for protein folding proposes. This work was supported by the NSF MRSEC Program (DMR-0820341).

**12:03PM G30.00005: Dissolving a DNA liquid through competition**  
GABRIELLE ABRAHAM (Presenter), OMAR SALEH, University of California, Santa Barbara — Coacervation plays a key role in spatial and temporal organization within the cell. Short nucleic acids are one mechanism that has been shown to control the intracellular dense liquids (e.g., introducing or removing short nucleic acids causes changes in the properties and appearance of droplets.) Here, we employ a model DNA liquid system and quantify the dissolution by short nucleic acids. Previous work has confirmed that this system is similar to intracellular droplets in terms of physical properties and spatial control (i.e., specific molecules are enriched or depleted in the droplet phase). The liquid is comprised of DNA in the shape of a 4-armed nanostar with each arm ending in a palindromic sequence that allows nanostars to interact and condense into droplets. By incorporating a toe-hold sequence on the nanostar, short hairpins are able to outcompete the nanostars for interaction sites causing the droplets to dissolve. Using confocal microscopy, we track DNA liquid break-up and compare the rate of decay to hairpin-nanostar interaction strength, concentration of the hairpin, and toe-hold location. This work will give insight into the different mechanisms that drive coacervate dissolution.
12:15PM G30.00006: Theory and simulation of reaction diffusion models of self-limiting droplet formation*  TREVOR GRANDPRE (Presenter), Physics, University of California, Berkeley, DAVID T. LIMMER, Chemistry, University of California, Berkeley — Liquid droplets are a generic feature of biological systems. Within the cell, liquidlike substructures form that contain Cajal bodies, germ granules, and centrosomes. In the absence of surfactants or long ranged interactions, the thermodynamically stable phase separated state of a liquid will always be that which minimizes the surface area of the droplet resulting in macroscopic domains. For this reason, it remains unclear how cells mitigate the formation of such large scale structure. We discuss ways in which macroscopic domains can be avoided by slow coarsening dynamics accompanying gelation or active processes that modulate Ostwald ripening. Theory and computer simulations are used to understand the mechanisms of droplet formation and dynamics. Implications for T-cell signaling pathways are also discussed.

*U.S. Department of Energy, Office of Basic Energy Sciences through Award Number DE-SC0019375

12:27PM G30.00007: Nonequilibrium Variational Control Forces for Self-Limited Colloidal Assembly*  AVISHEK DAS (Presenter), DAVID T. LIMMER, University of California, Berkeley — Materials with tunable functionalities can be synthesized bottom-up by controlled self-assembly of colloidal particles. Design principles that are rooted in thermodynamic principles and optimize specific interactions are often thwarted by kinetic limitations and confined to compact surface energy minimizing structures. We discuss a variational principle for the optimization of interparticle and nonequilibrium driving forces, which lead to robust assembly of self-limited clusters. Molecular dynamics simulations and a novel optimization strategy are used to solve for these optimal control forces. Our results expand the design space outside thermal equilibrium and provide new principles for tuning the dynamics of self-limited assembly in colloidal systems.

*This work was supported by the UC Berkeley College of Chemistry and the U.S. Department of Energy, Office of Basic Energy Sciences through Award Number DE-SC0019375.
12:39PM G30.00008: Kinetic entrapment: a mechanism for periodic one-dimensional growth  THOMAS WITTEN (Presenter), James Franck Institute, University of Chicago, MARTIN Lenz, LPTMS, CNRS, Université de Paris Sud — Globular proteins and other irregularly-shaped but identical molecular objects often self-assemble into fibers such as sickle-cell hemoglobin fibers. Such fibers are typically one-dimensional aggregates of fixed width, indefinitely long length and strong periodic order. A recent numerical study [Lenz, Witten 2017] gave strong evidence that such one dimensional fibers arise generically when a) the constituents are identical, b) their shape is asymmetric, so that they do not tile space, c) they aggregate irreversibly under the influence of a short-range attraction, and d) the energetic cost of distorting the constituents into bonding configurations is comparable to the attachment energy gained by this bonding. Here we propose a common kinetic mechanism in which the next growth site is a generic, deterministic function of the current aggregate configuration. We take the growth function to depend only on a local neighborhood of the previous growth site. A small bias favoring convex regions causes the growth site to revisit a given neighborhood of the deposit sufficiently often that the sequence of neighborhoods and growth sites reliably falls into a fixed, repeating cycle. This self entrapment does not occur when the bias parameter is halved.

12:51PM G30.00009: Pattern recognition through molecular self-assembly*  CONSTANTINE G EVANS, Maynooth University, JACKSON O'BRIEN (Presenter), University of Chicago, ERIK WINFREE, California Institute of Technology, ARVIND MURUGAN, University of Chicago — The functional role of many weak promiscuous interactions among molecules in biology is not clear and is often assumed to be deleterious. Here, we exploit promiscuous interactions to engineer an experimental system of 917 single-stranded DNA molecules capable of associative pattern recognition on the high dimensional concentration patterns of these molecular assembly components. Such pattern recognition is achieved by exploiting a process of competitive nucleation between different polymorphic DNA structures that are predominantly made of the same molecules but co-localized in different combinations. We test the system with numerous concentration patterns and confirmed nucleation-based pattern recognition through Atomic Force Microscopy (AFM) and fluorescence measurements. We discuss how this system, in conjunction with additional enzymatic components (e.g. DNA ligase), can potentially learn the promiscuous interactions needed to perform unsupervised clustering of concentration patterns.

*NSF-MRSEC 1420709
1:03PM G30.00010: Strain-Adaptive Self-Assembled Networks of Linear-Bottlebrush-Linear Copolymers* HEI LIANG (Presenter), ZILU WANG, ANDREY DOBRYNIN, Univ of Akron — We study the strain-adaptive behavior of the self-assembled networks of linear-bottlebrush-linear (LBL) triblock copolymers using a combination of analytical calculations and molecular dynamics simulations. Interactions between immiscible blocks result in microphase separation and formation of soft and strain-adaptive composite networks. Such unique network properties are manifestations of the architectural asymmetry of two blocks: (i) flexible linear chains that aggregate into domains and (ii) bottlebrush strands that form a soft matrix. The mechanical response of the networks is a two-stage process, which starts with the extension of the bottlebrush network strands (elastic regime) followed by the pulling out of the linear chains from L-domains (yielding regime). The two-stage network deformation process is incorporated into a unifying model of strain-adaptive network deformation. The model predictions are confirmed by molecular dynamics simulations of uniaxial deformation of self-assembled LBL copolymer networks and by experimental results for copolymers consisting of poly(dimethyl siloxane) bottlebrush block and two poly(methyl methacrylate) linear chain blocks with different compositions and block lengths.

*NSF DMR-1535412, DMR-1921923

1:15PM G30.00011: Self-directed Self-assembly of Block Copolymers HEJIN HUANG (Presenter), ALFREDO ALEXANDER-KATZ, Materials Science and Engineering, Massachusetts Institute of Technology MIT — Directed self-assembly (DSA) of block copolymers (BCP) provides a powerful tool to fabricate complex thin film structures at small length scale. Despite its success in fabricating various 2D patterns, fabrication of complex 3D nanostructures remains a challenge. Here, we introduce a novel method, which enables self-directed self-assembly of 3D tailored nanostructures. Dissipative particle dynamics (DPD) is employed, which demonstrates that uniform multilayer nanostructures could be obtained through stacking two different block copolymers alternatively. By introducing graphoepitaxy or chemoepitaxy to the first layer and performing multilayer stacking, information propagates upwards. Different complex bilayer and trilayer structures have been achieved through carefully choosing the BCP used in each stacking layer. We will show several examples of the complex uniform multilayer structures.
Identification of a Frank–Kasper Z phase from shape amphiphile self-assembly

STEPHEN CHENG (Presenter), MINGJUN HUANG, South China University of Technology, South China Advanced Institute for Soft Matter Science and Technology, ZEBIN SU, Univ of Akron —

Frank–Kasper phases, a family of ordered structures formed from particles with spherical motifs, are found in a host of materials, such as metal alloys, inorganic colloids and various types of soft matter. All the experimentally observed Frank–Kasper phases can be constructed from the basic units of three fundamental structures called the A15, C15 and Z phases. The Z phase, typically observed in metal alloys, is associated with a relatively large volume ratio between its constituents, and this constraint inhibits its formation in most self-assembled single-component soft-matter systems. We have assembled a series of nano-sized shape amphiphiles that comprise a triphenylene core and six polyhedral oligomeric silsesquioxane cages grafted onto it through linkers to give a variety of unconventional structures, which include the Z phase.

*This work was supported by National Science Foundation (DMR-1408872 to S.Z.D.C.) and the Program for Guangdong introducing Innovative and Entrepreneurial Teams (no. 2016ZT06C322). This research used resources of the Advanced Photon Source under contract no. DE-AC02-06CH11357.

Theory of Complex Spherical Packing Phases in Surfactant Systems

JIAYU XIE (Presenter), CHI TO LAI, ANCHANG SHI, McMaster Univ — The emergence and stability of complex spherical phases from a vast number of soft matter systems have been attracting tremendous attention recently. In particular, recent experiments have demonstrated the formation of Frank-Kasper and Laves phases (A15, σ, C14 and C15) in surfactant systems. Specifically, it has been shown that micelles self-assembled from amphiphilic molecules in water could pack and form these complex spherical packing phases in the presence of hydrocarbon molecules. Theoretically, we model the surfactant molecules by short diblock copolymers composed of a hydrophilic head and a hydrophobic tail. The phase behaviour of the model system is examined by using self-consistent field theory applied to a model system of short diblock copolymers and homopolymers. Our results indicate that the complex spherical packing phases could become stable for a set of model parameters corresponding to surfactant systems. Phase diagrams containing a large number of complex phases are constructed. The theoretical results demonstrate that the emergence and stability of complex spherical packing phases could be regulated by surfactant composition and concentration, thus shedding light to the understanding of the formation mechanisms of complex phases in soft matter systems.

*NSERC
1:51PM G30.00014: Predictive Modeling of Dendrimer Directed Nanoparticle Self-Assembly*

THI VO (Presenter), Chemical Engineering, University of Michigan - Ann Arbor, KATHERINE ELBERT, Chemistry, University of Pennsylvania, NADIA KROOK, Materials Science and Engineering, University of Pennsylvania, WILLIAM E ZYGMUNT, Chemical Engineering, University of Michigan - Ann Arbor, JUNGMI PARK, Chemistry, University of Pennsylvania, KEVIN YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory, RUSSELL COMPOSTO, Materials Science and Engineering, University of Pennsylvania, SHARON C GLOTZER, Chemical Engineering, University of Michigan - Ann Arbor, CHRISTOPHER B MURRAY, Chemistry, University of Pennsylvania — Traditional methods in nanocrystal self-assembly often rely on linear ligands isotropically grafted onto spherical cores. More recently, there has been a shift towards utilizing cores of varying shapes to expand on the current library of accessible morphologies. However, predictive simulations and designed experiments combining both the effect of ligand architecture as well as their anisotropic grafting onto nonspherical cores for self-assembly are still in their infancy. Here, we present a combined experimental and theoretical study in which a series of dendrimer ligands are used to direct the assembly of nanoplates into 2D and 3D geometries. We show that dendrimer ligands can be used to tune the degree of corona anisotropy about the nanoplates that then drives the formation of an off-set, layer-by-layer nanoplate architecture observed experimentally in 3D films. Our findings show that ligand architecture serves as a handle for layer specific, fine-tuning of self-assembly and provide a systematic approach to theoretically predict morphology purely from experimental design parameters.

*Office of Naval Research Multidisciplinary University Research Initiative Award
National Science Foundation
K.C.E: NSF GRFP
W.E.Z: NDSEG

Tuesday, March 3, 2020 11:15 AM - 2:03 PM

Session G31 DSOFT: Colloids 503 - Andrew Hollingsworth, New York Univ NYU
Shape and Interaction Decoupling for Colloidal Pre-Assembly

Lucia Baldauf, University of Amsterdam, Erin Teich, University of Michigan, Greg Van Anders (Presenter), Queen's University, Peter Schall, University of Amsterdam, Laura Rossi, Delft University of Technology — Creating materials with a structural hierarchy that is independently controllable at a range of scales requires breaking naturally occurring hierarchies. Breaking natural hierarchies is possible if building block attributes can be decoupled from the structure of pre-assembled, mesoscale building blocks that form the next level in the structural hierarchy. Here, we show that pre-assembled colloidal structures achieving geometric and interaction decoupling can be prepared in emulsions of silica superballs, which are cubic-like particles with rounded edges. We show that, for clusters of up to nine particles, colloidal superballs pack consistently like spheres, despite the presence of shape anisotropy and facets in the cubic-like particles. We compare our results with clusters prepared with magnetic superballs and find good qualitative agreement, suggesting that the cluster geometries are solely determined by the shape of the constituent particles. Our findings demonstrate that highly shape-anisotropic building blocks, under suitable conditions, can be pre-assembled into structures that are not found in bulk, thereby achieving a decoupling that can be further exploited for hierarchical materials development.

Topological states of hard rods in extreme annular confinement*

René Wittmann (Presenter), HHU Düsseldorf, Louis Brian Georges Cortes, Dirk Aarts, University of Oxford, Hartmut Löwen, HHU Düsseldorf — Hard particles are a standard model for colloidal systems and can be effectively studied within classical density functional theory (DFT). Fundamental mixed measure theory (FMMT) allows to predict the phase behavior of a hard-body fluid solely from the shape of individual particles.

Recent experimental advances allow for the synthesis of colloids with a nearly hard interaction that can be analyzed on the single-particle level. Slices of a system of such silica rods confined in a three-dimensional chamber under gravity can be considered a quasi-two-dimensional fluid that exhibits typical liquid-crystal behavior in confinement.

Applying FMMT to hard discorectangles in two dimensions, we map out a full phase diagram. Then we focus on a smectic fluid in extreme complex confinement, where the optimal bulk layer spacing competes with the extrinsic geometric and topological constraints. As a result, we characterize a variety of topologically different states in an annular geometry, also observed in particle-resolved experiments with silica rods. By further comparing the free energy of the different states, naturally provided by our DFT, we map out a topological phase diagram, indicating the stable topology depending on the details of the annular confinement.

*Funding by the DFG: LO 418/20-2
11:39AM G31.00003: Do cavities matter? Suppression of crystallization in hollow microgel solutions  ANDREA SCOTTI (Presenter), RWTH - Aachen University, ALAN DENTON, North Dakota State University, MONIA BRUGNONI, RWTH - Aachen University, RALF SCHWEINS, ILL Institut Laue-Langevin, WALTER RICHTERING, RWTH - Aachen University — Microgels are crosslinked polymeric networks in the colloidal domain that exhibit phase behavior comparable to soft spheres. Solutions of microgels have been widely used as model systems to study self-assembly of condensed matter and complex fluids. Here we study the phase behavior of hollow microgels, characterized by a solvent-filled cavity in their center. Surprisingly, the phase behavior of these microgels, which lack a dense polymeric core, does not show crystal formation. The absence of crystals is independent of both the softness of the network and the size of the cavity. By means of small-angle neutron and X-ray scattering, both the form factors and the interparticle separations of hollow microgels are measured in overcrowded environments, revealing a complex interplay between interpenetration and deswelling. We confirm these findings by Monte Carlo simulations of microgel solutions modeled by the Flory-Rehner single-particle free energy and the Hertz pair potential.

11:51AM G31.00004: Buckling of 2D complex plasma crystals  ALEXANDRA ZAMPETAKI (Presenter), ALEXEI IVLEV, Max-Planck Institute for Extraterrestrial Physics, HARTMUT LOEWEN, University of Dusseldorf — Complex plasmas (or dusty plasmas) consist of microsized dust particles and a weakly ionized gas and as such they are often regarded as the "plasma state of soft matter". Apart from their particularly strong coupling, such systems exhibit also other surprising properties, such as a non-Hamiltonian behavior, due to the emergent plasma wakes. In this talk I will present some very recent theoretical results about the ways in which the existence of plasma wakes affects the structure of complex plasma crystals under a harmonic confinement. The main focus thereof will be on the buckling transition from a 2D monolayer to bilayer or triple-layer complex plasma crystals, taking place as the confinement frequency is decreased. Such structural transitions provide further insight to the underexplored properties of systems with effective non-reciprocal interactions occurring often in non-equilibrium soft matter.

12:03PM G31.00005: Tuning Interactions between Charged Structured Colloids and Hydrophobic Salts for the Production of Pickering Emulsifiers  DOUGLAS SCOTT (Presenter), ROBERT K PRUD'HOMME, RODNEY PRIESTLEY, Chemical & Biological Engineering, Princeton University — Pickering emulsifiers have been demonstrated as advantageous alternatives to traditional small molecule surfactants, owing to their high interfacial adsorption energy and mechanical functionality. However, translating these advantages on an industrial scale requires continuous fabrication processes. Flash nanoprecipitation (FNP) has been demonstrated as a scalable process for the production of nanocolloids with a rich library of morphologies including homogeneous, core-shell, and Janus structures, the last of which presents an opportunity for generating amphiphilic Pickering emulsifiers. In this work, the FNP of homopolymers with ionomer analogs is presented as a route for the tunable expression of charge groups on distinct hemispheres of Janus particles. Utilizing this enhanced surface charge, the interaction between colloids and hydrophobic salts is studied, showing non-monotonic trends in size stability. Lastly, the surface activity of various colloid-salt combinations is demonstrated via the formation of highly stable Pickering emulsions.
12:15PM G31.00006: Bayesian inference of particle size distributions from dynamic light scattering* THY DOAN MAI LE (Presenter), JEROME FUNG, Ithaca College — Autocorrelation functions from dynamic light scattering experiments have previously been analyzed either by performing least-squares fits to determine the mean and variance of the particle size distribution, or by using constrained regularization techniques to infer the size distribution. We present open-source tools for performing Bayesian inference of particle size distributions while rigorously incorporating smoothness and non-negativity constraints on the inferred distributions. We successfully apply these tools to simulated autocorrelation functions at multiple scattering angles. We intend to release these tools for use by the soft condensed matter and biophysics communities in the near future.

*This project was funded by the Charles A. Dana Internship fund and the School of Humanities & Sciences' Summer Scholars program at Ithaca College.

12:27PM G31.00007: Confinement of colloidal smectic phases* LOUIS BRIAN GEORGES CORTES (Presenter), Cornell University, RENÉ WITTMANN, Heinrich Heine University Düsseldorf, ROEL P. A. DULLENS, University of Oxford, HARTMUT LÖWEN, Heinrich Heine University Düsseldorf, DIRK AARTS, University of Oxford — We report on the confinement of colloidal liquid crystals in three dimensional chambers. We exploit silica rods’ relatively large density difference with respect to the dispersing solvent to study isotropic, nematic and smectic phases confined into a single chamber. Combining laser scanning confocal microscopy and soft-lithography techniques enables us to characterize the configurations down to the single particle level. We focus on the smectic phase observed in direct vicinity of the bottom wall. We first consider chambers with square footprint finding occurrences of the smectic bridge state, characterized by two parallel disclination lines, in good agreement with simulation of 2-dimensional hard rods. We then examine the case of topologically different annular chambers. By progressively varying the confinement from a disk to a thin annulus we induce a transition from the smectic bridge state, formerly found in square, to the smectic ring state with distinctive edge dislocations. The results are compared to very recent density functional theory calculations.

*This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement No 641839.
12:39PM G31.00008: Molecular dynamics simulations resolve the encapsulation of testosterone propionate by both solid and liquid lipid nanoparticles  DEMI PINK (Presenter), Physics, Kings College London, JAYNE LAWRENCE, Division of Pharmacy & Optometry, University of Manchester, CHRISTIAN D. LORENZ, Physics, Kings College London — Solid lipid nanoparticles (SLNs) have a crystalline lipid core which is stabilised in solution by interfacial surfactants. They are considered favourable candidates for future drug delivery vehicles as they are capable of storing and release bioactive molecules. Following our successful study on the self-assembly of the SLN and our characterisation of the resulting structure, we have expanded our work to investigate the formation of triolein-based liquid lipid nanoparticles (LLNs) stabilised by the Brij O10 surfactant. LLNs are, like SLNs, of interest for their potential applications in drug delivery and so a thorough understanding of their structure is vital in the development and optimisation of drug delivery formulations. In this work we have characterised the structure and formation of LLNs by means of small angle neutron scattering and atomistic molecular dynamics simulations. We have also characterised and compared the processes involved in the encapsulation and localisation of a steroidal drug, testosterone propionate, for both the SLN and the LLN. By comparing the two nanostructures and the localisation of the drug within them we have shed light on the relationship between a nanoparticle’s internal structure and its role in drug delivery.

12:51PM G31.00009: Dynamics and contact microstructure of rough colloids*  SHRAVAN PRADEEP (Presenter), LILIAN C HSIAO, North Carolina State University — Colloidal particles with hard-sphere interactions have been used to study crystallization and glassy dynamics. Here we synthesize smooth and rough poly(methyl methacrylate) colloids and disperse them in an index-matched solvent, squalene, at volume fractions (Φ) ranging from dilute (Φ=0.1) to random close packing (RCP). We use confocal microscopy to obtain 3D image-stacks of the colloidal suspensions and process them to obtain particle centroids with subpixel precision. We estimate the contact numbers for smooth and rough colloids at RCP to be 6 and 4 respectively, as predicted by simulations of frictional granules. In both the systems, scaling of the form <z>~Φ^a was observed, where parameter 'a' varies with surface roughness. We hypothesize that the power law variations are related to the phase behaviors and associated dynamics (mean-squared displacement) of these particles at various Φ. We believe our approach to connect the contact microstructure to dynamics in suspensions will enable better understanding of the effect of surface anisotropy on colloidal crystallization, rheological phenomena, and osmotic pressure of suspensions.

*Authors acknowledge funding from National Science Foundation (CBET-1804462), ACS Petroleum Research Fund (#59208-DNI9) and NC State CBE Startup Grant.
1:03PM G31.00010: Liquid crystal-mediated growth and assembly of polymer colloids*
XIAOSHUANG WEI (Presenter), LAURA BRADLEY, Univ of Mass - Amherst — Templating the director field of liquid crystals (LCs) has been shown to organize colloids into a variety of ordered assemblies, including chain-like structures and hexagonal lattices. Most systems produce LC-mediated assemblies by pre-mixing colloids in host mesogens or by depositing colloids at LC interfaces. In our work, we demonstrate simultaneous growth and assembly of polymer colloids at LC-air interfaces. The polymer colloids are produced by polymerization of acrylate monomer mixed in non-reactive liquid crystal mesogens. Colloids spontaneously form ordered assemblies at the LC-air interface. Systematic experiments varying the reaction time were conducted to monitor the nucleation, growth, and assembly. Simultaneous colloid growth and assembly in LCs can open new opportunities to utilize LC-templated polymerization for the preparation of large-scale assemblies or continuous network structures.

*This work is supported by an NSF CAREER Award (#1845631).

1:15PM G31.00011: Holographic Perfusion Porosimetry of Individual Colloidal Particles*
DAVID G GRIER (Presenter), Department of Physics, New York University, MARY ANN ODETE, FOOK C CHEONG, ANNEMARIE WINTERS, Spheryx, Inc., JESSE J ELLIOTT, Department of Physics, University of Chicago, LAURA A PHILIPS, Spheryx, Inc. — The in-line hologram of a micrometer-scale colloidal sphere can be analyzed with the Lorenz-Mie theory of light scattering to obtain precise measurements of the sphere's diameter and refractive index. The same technique also can be used to characterize porous and irregularly shaped colloidal particles provided that the extracted parameters are interpreted with effective-medium theory to represent the properties of an equivalent effective sphere. We demonstrate through experiments on mesoporous silica spheres, protein aggregates and nanoparticle agglomerates that the effective-sphere model consistently accounts for the influence of the medium on the particle's measured effective refractive index. This dependence yields information on the particles' structure and composition that cannot be obtained in other ways, including their porosity, the polydispersity of their porosity, and the size distribution and connectivity of their pores.

*This work was supported by the National Science Foundation under Award Number IPP-1631815, and by the National Center For Advancing Translational Sciences of the National Institutes of Health under Award Number R44TR001590. Additional support was provided by the MRSEC program of the National Science Foundation under award number DMR-1420073.
1:27PM G31.00012: Controlling the flexible polymer - hard colloid duality of temperature-responsive microgels at interfaces by the adsorption pathway*  MARIE FRIEDERIKE SCHULTE (Presenter), ANDREA SCOTTI, STEFFEN BOCHENEK, MONIA BRUGNONI, WALTER RICHTERING, RWTH - Aachen — We study the effect of the adsorption pathway on the morphology and temperature-induced collapse of PNIPAM microgels at the solid/liquid interface by means of atomic force microscopy (AFM). Two samples with extreme differences in softness are probed: i) regularly 5 mol% BIS, and ii) ultra-low cross-linked microgels (ULC). ULC microgels are strongly deformed when being deposited either by spin-coating or by Langmuir-Blodgett technique from an oil-water interface. After rehydration, the ULC microgels cannot collapse as entire objects instead small globules are formed. Such a strong deformation can be avoided by in-situ adsorption to the substrate. Then, the ULC microgels exhibit half-ellipsoidal shapes with a smooth surface similar to more cross-linked microgels. Due to the extreme softness of ULC microgels, they can be selectively trapped either in a more particle-like or in a more polymer-like behavior. Coatings with strongly different topographies and properties can be prepared by one and the same ultra-low cross-linked microgel.

*The Deutsche Forschungsgemeinschaft (DFG) is acknowledged for financial support within the Sonderforschungsbereich SFB 985 “Functional Microgels and Microgel Systems”

1:39PM G31.00013: Localization to delocalization transitions in size asymmetric mixtures of colloidal particles with grafted chains*  HECTOR MANUEL LOPEZ RIOS (Presenter), ALI EHLEN, MONICA OLVERA DE LA CRUZ, Northwestern University — We study binary systems of polymer-grafted colloidal particles, in which the diameter of one species is substantially larger than the other. It has recently been shown [1] that, in these systems, the larger colloids order to form a lattice while the smaller ones may form a sublattice or delocalize within the interstitial space, depending on system parameters. We develop a simplified molecular dynamics model to study these colloidal systems and the nature of the delocalization of the smaller species under varied conditions. Using this model, we explore phase transitions between different lattice and sublattice types as a function of temperature.


*We acknowledge and thank the computational support of the Sherman Fairchild Foundation.
Two Coupled Mechanisms Produce Fickian, yet non-Gaussian Diffusion in Heterogeneous Media

INDRANI CHAKRABORTY (Presenter), YAEL ROICHMAN, School of Chemistry, School of Physics & Astronomy, Tel Aviv University — In several biological and soft matter systems, Fickian yet non-Gaussian diffusion has been observed, where the mean square displacement remains linear in nature, but the displacement distribution is non-Gaussian. The underlying reasons behind this strange behavior still remain speculative. Here, we perform a set of controlled experiments that quantitatively explore the effect of spatial heterogeneities on the appearance of non-Gaussianity in Fickian diffusion. Specifically, we study the diffusion of fluorescent colloidal particles in a matrix of lithographically fabricated micropillar arrays having a range of structural configurations: from completely ordered to completely random. Structural randomness and density are found to be the two most decisive factors in making diffusion non-Gaussian. We show that non-Gaussianity emerges as a direct consequence of two coupled physical mechanisms that produce a superstatistical behavior of the ensemble in a structurally heterogeneous environment. The two mechanisms identified here are relevant for many systems of crowded heterogeneous environments where non-Gaussian diffusion is frequently observed, for example in biological systems, polymers, gels and porous materials.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G32 DPOLY DSOFT DBIO: Responsive Polymers, Soft Materials, and Hybrids III

Ordering hard-sphere particle suspensions by medium crystallization: Effect of size and interaction strength* VIANNEY GIMENEZ-PINTO (Presenter), Department of Science, Technology and Mathematics, Lincoln University, Missouri — While microstructure in soft materials is usually given by the self-assembly of their constituting building blocks, colloidal assembly can also be obtained via templating a morphology in a disordered suspension of particles by solidification of the melt. This sweep-templating process is applicable in different soft matter systems with a variety of characteristic length scales, including particle suspensions in water, liquid crystal materials, and polymer melts. Here, I numerically investigate the effect of particle-size and solvent-size in the process of solidification templating by implementing a simple coarse-grain model for the kinetics of hard-sphere particles at the melt/crystal interface. Results show that the threshold speed for solidification templating trails a power-form as size changes. Furthermore, this work analyzes and reports the effect of particle-crystal interaction strength in combination with size effects. This scaling study from a numerical perspective sets a starting point for the development of hybrid soft materials via structural templating, allowing solidification-driven particle ordering in different systems with length-scales that range from a few tens of nanometers to microns and centimeters.

*Work funded by NSF DMR-1408323
11:27AM G32.00002: Exploring Solution Behavior of Fully Rigid “Block Copolymers” with Sphere-Rod Molecular Architecture* JIANCHENG LUO (Presenter), TONG LIU, STEPHEN CHENG, TIANBO LIU, Univ of Akron — The rich solution behavior of block copolymers, especially self-assembly of amphiphilic block copolymers in solution, have been extensively explored in past decades. While the traditional block copolymers often involve flexible chains, some novel “copolymers” containing rigid components might also demonstrate interesting self-assembly behavior. Here, we explore solution behavior of fully rigid “block copolymers” hybrid macromolecules based on spherical polyoxometalates and rod-like oligofluorenes. We report here that rigid macromolecules can achieve continuous curvature change and consequently form unexcepted multilayer vesicular structures. The highly uniform, multilayered vesicles have complete onion-like structure from most inner to outer layers with fixed interlayer distance, and the vesicle size/layer number can be accurately controlled by solution conditions including temperature, solvent composition, and salt concentration. Additionally, reversible response of vesicle size/layer number is observed by simplify changing the solution temperature. The effects of rod length and molecular architecture will also be discussed.

*NSF (CHE1904397), the Pearl River Talent Recruitment Program of Guangdong Province (no.2016ZT06C322), National Natural Science Foundation of China (U1832220).

11:39AM G32.00003: Stimuli-responsive phase behavior of block copolymers in ionic liquids CLAIRE SEITZINGER (Presenter), CECILIA C HALL, TIMOTHY LODGE, University of Minnesota — Block copolymers microphase separate into well-defined ordered morphologies as a function of temperature and composition. However, not all applications are amenable to changes in temperature or composition, but still require transitions between disorder and order, or between different ordered symmetries. We explore the light-mediated phase behavior of a diblock copolymer, poly(methyl methacrylate)-b-poly(benzyl methacrylate-s-4-phenylazophenyl methacrylate), in a selective ionic liquid solvent, 1-alkyl-3-methyl imidazolium bis(trifluoromethylsulfonyl)imide. By adjusting the length of the alkyl chain on the imidazolium group, we can control the phase transition temperatures (order-disorder and order-order transitions). In this system, the solubility of the 4-phenylazophenyl methacrylate-containing block in the ionic liquid is altered by irradiation with UV light. The phase behavior is monitored by small amplitude oscillatory shear rheology under either UV or visible light, and the ordered phases identified by small angle X-ray scattering. Understanding the phase behavior of this model system allows us to work towards inducing morphology changes in a contactless manner.
11:51AM G32.00004: Exploring the Limits of Actuation Force Output of Stretch-based Deformation of Liquid Crystalline Elastomers*  JOSELLE MCCRAKEN (Presenter), KELSEY M LYNCH, TIMOTHY J WHITE, University of Colorado, Boulder — Liquid crystal elastomer (LCE) films are amenable to surface-enforced alignment.[1] Physical limits of surface-enforced alignment constrain the thickness of LCEs aligned by this approach to a maximum of 50 µm.[2] The force output of stretch-based deformation of topologically patterned LCEs is enhanced with thickness, which we have previously accessed using a lamination approach for actuator fabrication.[3] This contribution details our exploration of the boundaries of achieving high force actuation from these soft materials. We describe several facile approaches for accessing thick LCE actuators (>30x a standard film), including the preparation of devices with interlaid compliant electrodes that allow rapid electrothermal deformation in the multi-laminate LCEs.


*DARPA-SHRIMP

12:03PM G32.00005: Electro-responsive Ionic Liquid Crystal Elastomers*  CHENRUN FENG (Presenter), Advanced Materials and Liquid Crystal Institute, Kent State University, CHATHURANGA PRAGEETH RAJAPAKSHA, VIKASH KAPHLE, BJORN LUSSEM, Department of Physics, Kent State University, THEIN KYU, Department of Polymer Engineering, University of Akron, ANTAL ISTVAN JAKLI, Advanced Materials and Liquid Crystal Institute, Kent State University — We will describe the preparation, physical properties and electric bending actuation of a new class of active materials - ionic liquid crystal elastomers (iLCEs). It is demonstrated that iLCEs can be actuated by low frequency AC or DC voltages of less than 1 V. The bending strains of the not optimized first iLCEs are already comparable to the well-developed ionic electroactive polymers (iEAPs). Additionally, iLCEs exhibit several novel and superior features, such as the alignment that increases the performance of actuation, the possibility of pre-programed actuation pattern at the level of cross-linking process, and dual (thermal and electric) actuations in hybrid samples. Since liquid crystal elastomers are also sensitive to magnetic fields, and can also be light sensitive, iLCEs have far-reaching potentials toward multi-responsive actuations that may have so far unmatched properties in soft robotics, sensing and biomedical applications.

*This work was financially supported by NSF DMR-1307674 and DMR-1502543.
Soft dielectric elastomers have aroused considerable interest in both research and industrial communities. Applications of elastomers include artificial muscle actuators, adaptive optics and energy harvesting. The basics of electro-elasticity have been highlighted by Toupin(1). We have modelled the behaviour of a soft deformable dielectric body under the combined effect of mechanical loading and electric field through non-linear finite element analysis. These materials are capable of large voltage-induced deformation, but achieving it in practice poses serious challenge due to electromechanical instability and electric breakdown. Our work is based on ideal dielectric elastomers. We precisely point out the extent of harnessing voltage-induced deformation in case of a soft cylindrical actuator and the suitable applications where such precise control is required. Additional results show an effective way of utilising the “snap through” phenomena in such actuators. The computations are carried out in Abaqus Software in conjunction with user-subroutine UEL in order to invoke the coupling effect in our problem. 

References:

Biomaterials find wide use in many branches of medicine and engineering. Success examples are hard biomaterials like titanium used in dentistry and prosthetics. Soft biomaterials, however, haven’t replicated these successes in repairing soft tissues. The reason is simple yet fundamental: existing soft biomaterials cannot match or integrate with soft tissues mechanically; they are often vulnerable to rupture and difficult to adhere on soft tissues, especially when interfacing with dynamic tissues such as skin and beating heart; their functionality is passive and limited. This talk will present new strategies and material systems to overcome these material constraints. A series of bioinspired hydrogel adhesives will be presented. One can be tougher than articular cartilage and achieve unprecedented adhesion performance on a variety of soft wet tissues, even under exposure of blood and dynamic movements [1]. The other can respond to the skin temperature, actively contract and heal skin wound effectively [2]. A mechanistic investigation with theoretical and computational mechanics approaches will be shown. This talk will also show how to realize spatiotemporal control of tissue adhesion on demand through controlling the surface and structure of the adhesive, and via external stimuli like ultrasound. This talk will highlight how to leverage a variety of physical, chemical and mechanical cues to finely tune the interactions between tissues and biomaterials to promote tissue repair and regeneration.

References

*This work was supported by the Natural Sciences and Engineering Research Council of Canada, Canada Foundation for Innovation, and New Frontiers in Research Fund.
Flexoionic effect of Ionic Liquid Crystal Elastomers

CHATHURANGA PRAGEETH RAJAPAKSHA (Presenter), Department of Physics, Kent State University, CHENRUN FENG, Liquid Crystal Institute, Kent State University, CAMILO PIEDRAHITA, HAMAD ALBEHAIJAN, Department of Polymer Engineering, University of Akron, VIKASH KAPHLE, PUSHPA PAUDEL, BJORN LUSSEM, Department of Physics, Kent State University, THEIN KYU, Department of Polymer Engineering, University of Akron, ANTAL ISTVAN JAKLI, Department of Physics, Kent State University — Flexoelectricity (strain gradient induced electricity) has potential of a wide variety of applications such as strain sensors and micropower generators. Our present study was motivated by the novel phenomenon of mechanoelectrical conversion (flexoionic effect) of ionic electroactive polymers [1 ] and a new class of active material – ionic liquid crystal elastomers (iLCEs) [2]. Here we report the flexoionic effect of iLCEs. Highly ionic conductive iLCEs are prepared using M1 (4-(6-Acryloxy-hex-1-yl-oxy) phenyl-4-(hexyloxy) benzoate), M2 (1,4-Bis-[4-(6-acryloyloxyhexyloxy) benzoyloxy]-2-methylbenzene), ionic liquid (1-Hexyl-3-methylimidazolium hexafluorophosphate) and the photo initiator. The effect of alignment (planar, homeotropic and hybrid) and ionic liquid concentration at the function of bending amplitude are studied on the mechanoelectrical conversion.

Reference

Statistical field theory model for Liquid Crystal Elastomers

PRATIK KHANDAGALE (Presenter), KAUSHIK DAYAL, CARMEL MAJIDI, Carnegie Mellon Univ — Liquid Crystal Elastomers (LCEs) are composed of relatively stiff liquid crystal molecules connected with flexible polymeric chains. LCEs show fast reversible shape change with temperature because of nematic-isotropic phase transition of the liquid crystals. Thus, LCEs have promising applications as thermally active soft actuators, shape memory material and artificial muscles.

Existing models for LCE response are typically based on continuum mesoscale approaches such as phase field methods. While these models provide macroscopic predictive capability once material constants are calibrated, they are unable to predict mesoscale structure and response. In particular, these methods are unable to provide insight into the behavior of LCE composites composed of active components such as liquid metals or carbon nanotubes.

We develop a statistical mechanics-based field theoretic model for LCE response to enable us to probe these questions. The polymer chain elasticity is entropic while the liquid crystalline free energy is based on the Maier-Saupe mean field theory for liquid crystals. The model is solved numerically using a finite element approach. We extend this to the many-chain setting and examine the effects of temperature, geometry and loading conditions.
1:27PM G32.00010: Branching out and back: Reconfigurable nematic drops driven by molecular heterogeneity*  
WEI-SHAO WEI (Presenter), Department of Physics and Astronomy & LRSM, University of Pennsylvania, YU XIA, Department of Materials Science and Engineering, University of Pennsylvania, SOPHIE A ETTINGER, Department of Physics and Astronomy & LRSM, University of Pennsylvania, YUCHEN WANG, SHU YANG, Department of Materials Science and Engineering, University of Pennsylvania, ARJUN G YODH, Department of Physics and Astronomy & LRSM, University of Pennsylvania — Traditionally, polydispersity in matter is often avoided, since it tends to impede self-assembly and state transformation. Here we report reconfigurable nematic liquid crystal oligomer drops, which reveal, surprisingly, that molecular heterogeneity facilitates equilibrium transitions among dramatically different morphological structures, via spatial segregation. Specifically, fine-tuning the temperature and oligomer chain length distribution alters the balance between interfacial tension and liquid crystal elasticity, driving spontaneous formation of roughened spheres, flowers, and highly branched filamentous networks with uniform and controllable diameters. This feature provides potential connections to surface patterning in biological world, such as pollen grains. Further, we employ the achieved structures to template assembly of plasmonic nanoparticles, as well as helical coils with chiral dopant. With the capabilities of being produced reversibly and permanently locked into liquid crystal elastomers, the demonstrated simple rules thus offer new routes for programmed spatio-temporal networks.

*This work is supported by NSF DMR16-07378, PENN MRSEC DMR-1720530, and NASA Grant 80NSSC19K0348 and NNX13AL27G.

1:39PM G32.00011: Imaging crack propagation in tough model gels by ultrasound elastography*  
HEIVA LE BLAY (Presenter), THOMAS DEFFIEUX, MICKAEL TANTER, ALBA MARCELLAN, ESPCI Paris — Assessing biomechanical properties of soft tissues by ultrasound imaging is still a challenge to help physicians to characterize pathologies. Benefiting from the recent progress in the field, the idea is to develop a novel, non-invasive tool with a high time-resolution to understand crack propagation processes in synthetic model gels. This approach offers new insights into soft matter fracture. This project focuses on the use of shear wave elastography for a local elasticity mapping at the vicinity of an advancing crack. Model polymer networks with well-controlled mechanical responses are synthetized following the protocol of Rose et al.[1]. By addition of silica nanoparticles (NPs), these gels combine a covalent polymer network (elasticity) with physical interactions by adsorption of polymer onto silica NPs (viscoelasticity) [2]. The gels are characterized in a wide range of frequencies in tensile mode (small strain rates) coupled with high frequency shear wave spectroscopy described by Deffieux et al.[3].


*The authors thank the program UpToParis.
1:51PM G32.00012: Photoisomerization in a Glassy Matrix: Predicting a Broad Distribution of Dynamics with Machine Learning
KENNETH SALERNO (Presenter), TIMOTHY W SIRK, US Army Res Dev & Eng Command, JUAN DE PABLO, Pritzker School of Molecular Engineering, University of Chicago —

The response of azo-containing molecules undergoing a trans → cis photoisomerization transition has been primarily studied through simulation and experiment in solution or vacuum. The response of these photoactive molecules in glassy solids, where barriers to motion are significantly higher, is poorly characterized. Results from molecular dynamics simulations show that the dynamics of photoactivated molecules in glassy solids depends critically on local density features. A characteristic power-law wait time for photoisomerization occurs in samples for densities that vary with photoactive molecule and glass-matrix material. Dynamic behavior is driven by difficult-to-identify local density features, which suggests an opportunity for a machine-learning approach. We apply methods from structural analysis of an ideal disordered solid [1] to an all-atom molecular system for the first time, predicting a propensity to isomerize as an analog to “softness.” Our results not only demonstrate that simple machine learning methods can be applied to complex, all-atom molecular systems, but also highlight predictive features of local environments far beyond simple scalar quantities or visually identified features.


2:03PM G32.00013: Response of Polymer Conformations to Crowded Environments
KURT VANDONSELAAR (Presenter), MATTHEW KURTTI, ALAN DENTON, North Dakota State Univ —

Quantifying the effects of macromolecular crowding on conformations of polymers is important for understanding the structure and function of macromolecules in cellular environments, e.g., biochemical reactions between biopolymers. To efficiently study conformations of crowded polymers in good solvents, we adopt a coarse-grained model of a polymer as a penetrable ellipsoid whose size and shape fluctuate according to the statistics of a self-avoiding walk [1]. We model the crowders as spherical particles that interact via Lennard-Jones or Yukawa pair potentials with hard cores that can penetrate the polymer at a cost in entropy predicted by polymer field theory. To compute the polymer shape distribution, radius of gyration, and asphericity, we perform Monte Carlo simulations, including trial displacements and trial changes in polymer conformation. By varying interactions between crowders, we find that with increasing strength of attraction, the polymer geometric properties settle towards their uncrowded limits as a result of clustering of the crowders. These results may offer insight into reaction rates and functions of folded proteins within cells.


Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G33 DPOLY DSOFT GSNP: Polymer Nanocomposites: Structure and Property
505 - Shiwang Cheng, Michigan State Univ - Tag(s): Focus
11:15AM G33.00001: Silicone-Iron Oxide Nanocomposite Encapsulants for Common Mode Noise Reduction in Switching Power Electronics*  HAYDEN CARLTON (Presenter), REECE WHITT, AMOL DESHPANDE, SARAH MYANE, NOAH AKEY, DAVID HUITINK, Univ of Arkansas-Fayetteville — The use of polymer encapsulants continues to permeate the electronics industry as a way to improve the reliability of packaging solutions, and the incorporation of nanomaterials presents an area of potential advancement. Management of electromagnetic noise represents a design challenge in power electronics that can be aided through the use of nanoparticle-enhanced encapsulants. Aluminum heat sinks often create common mode noise from AC disturbances generated by switching power supplies. Mitigation of this noise in modern electronics results in large increases in device efficiency; nanoparticles which have an intrinsic susceptibility to electromagnetic fields could add another dimension to encapsulant functionality by improving noise shielding. In the study presented herein, iron oxide nanoparticles were incorporated into a silicone rubber matrix to create an electromagnetically-susceptible nanocomposite in an effort to reduce common mode noise. After applying the nanocomposites to a prototype heat sink, a noticeable reduction in common mode noise was observed with just a relatively small amount of nanomaterial. Introducing this simple concept to modern designs will aid in improving noise management in power electronics devices.

*We would like to acknowledge funding from POETS-ERC.

11:27AM G33.00002: Flexible Textured Nanocomposite for Energy Harvesting Applications  VINEY GHAI (Presenter), HARPREEET SINGH, PRABHAT K AGNIHOTRI, Mechanical Engineering, Indian Institute of Technology Ropar — The present study provides a method for designing and fabricating a multifunctional flexible absorber (flexorb) that can be used as a coating material for ultra-high absorption applications. Untextured nanocomposite (UNC) is synthesized by reinforcing 1 wt. % of nanofillers [carbon nanotubes (CNTs), zinc oxide nanorods and iron nanoparticles] in polydimethylsiloxane (PDMS). Homogeneous mixture of these nanoparticles led to an ultra-high absorption ≥ 96 % from 300-2000 nm. Subsequently, texturing on the surface of UNC, enhance the absorption ≥ 99 % in entire UV-Vis-NIR wavelength range. This increase in absorption is due to the multiple scattering of incident beam along with the surface texture. In addition to this CNTs reinforced in flexorb provides better impedance matching which results in lower reflection losses from flexorb/air interface. Moreover, the textured nanocomposite exhibited a better tensile, tear, shear and peel-off strength than pure PDMS and UNC. The flexorb has an advantage of flexibility which ensures that it can be deformed in variety of shapes without any damage or creasing failure. Such a ultra-black textured nanocomposite may find many applications such as suppression of stray light in telescopes, thermal imaging sensors, spectroscopy and energy harvesting.
11:39AM G33.00003: Nanoparticle Assembly Modulated by Biobased Polymers and Its Coating Application* EMILY OLSON, YIFAN LI, FANG-YI LIN, ANA MILLER, FEI LIU, AYUNA TSYRENOVA, GREG CURTZWILER, KEITH VORST, ERIC COCHRAN, SHAN JIANG (Presenter), Iowa State University — We study how nanoparticles assemble in a dried film containing biobased polymers. Different nanoparticles were dispersed with hydroxyethyl cellulose (HEC) and hydroxyethyl starch (HES). It was discovered that polymer morphology has a profound influence on the assembly structures of nanocomposite. In addition, an unexpected highly fractal network structure assembled by nanoparticles were formed in HEC matrix with different types of nanoparticles. Electron microscopy and small X-ray scattering offer the detailed analysis of the structures. Based on these results, we further developed a biobased waterborne coating system to effectively block the UV radiation while maintaining the transparency using ZnO nanoparticles. Our new coating materials can lead to coating films ~ 100 times thinner than the previously reported coating systems of similar UV-blocking performance. The same concept can be applied to other polymer nanocomposite systems. The study opens the opportunity of utilizing more sustainable biobased materials for high-value functional coating applications.

*We thank NSF I/UCRC The Center for Bioplastics and Biocomposites (CB²), polymer and food protection consortium, USDA NIFA grant no. 2019-67013-29016 and NSF-DMR-1626315.

11:51AM G33.00004: Coarse-grained molecular dynamics simulations on mechanical properties of polymer composites for bulk heterojunction solar cells YUTA YOSHIMOTO (Presenter), SOU SUGIYAMA, TOSHIHIRO KANEKO, SHU TAKAGI, IKUYA KINEFUCHI, Univ of Tokyo — We investigate mechanical properties of polymer composites of poly(3-hexylthiophene) (P3HT) and fullerene C_{60} using coarse-grained molecular dynamics (CGMD) simulations, where the P3HT monomer unit and C_{60} are represented by three CG beads and a single CG bead. Pure P3HTs with the degrees of polymerization (DPs) of 50, 100, and 150 exhibit almost identical tensile moduli, while the tensile strength increases with the DP. We quantify an increase in the number of molecular chain entanglements resulting from increasing DP, which in turn enhances the tensile strength. Meanwhile, the decomposition of molecular interactions contributing to stress indicates that the tensile modulus is primarily determined by non-bonded potentials and bond length potentials, almost independent of the chain entanglements. Furthermore, the addition of C_{60} leads to higher tensile modulus and hence more brittle behavior of the composite in accordance with experiments. We find that an increase in C_{60} mass fraction further inhibits molecular chain entanglements, leading to a significant reduction of the tensile strength. Meanwhile, an increase in the tensile modulus mainly originates from an increase in non-bonded interactions associated with C_{60}. 
12:03PM G33.00005: Nanoparticle Templating of Ultrathin and High Density 6 nm Pore Arrays* GRAYSON JACKSON (Presenter), University of Chicago, XIAO-MIN LIN, Argonne National Laboratory, HEINRICH M. JAEGER, University of Chicago — Active layers for next-generation water filtration membranes require large area and uniform arrays of nanometer-sized pores. We demonstrate an alignment-free method to transform freely suspended nanoparticle (NP) monolayer sheets into mechanically robust, high density 6 nm pore arrays using electron beam irradiation and subsequent wet chemical etching. As the secondary electrons responsible for ligand crosslinking originate from the NPs themselves, our substrate-free approach benefits from a variable crosslink density throughout the ~10 nm film thickness. We apply this general strategy to two NP systems—gold NPs with alkanethiol ligands and Fe₃O₄ NPs coated with oleic acid—to fabricate nanostructured polymer films with either thiol or carboxylate pore chemical functionalities.

*We acknowledge support from the Office of Naval Research under grant ONR N00014-17-1-2342.

12:15PM G33.00006: Gas Transport of Self-assembled Polymer Nanocomposites with Binary Nanoparticle Size* SOPHIA CHAN (Presenter), MAYANK JHALARIA, ANDREW JIMENEZ, SEBASTIAN T RUSSELL, Chemical Engineering, Columbia University, BRIAN C BENICEWICZ, Chemistry and Biochemistry, University of South Carolina, SANAT KUMAR, Chemical Engineering, Columbia University — Covalently grafting organic (hydrophobic) polymer chains to inorganic (hydrophilic) nanoparticles is a facile means of addressing their inherent immiscibility. We have previously shown that membranes comprised of such grafted nanoparticles (GNPs) exhibit remarkable increases in gas permeabilities relative to that of the neat polymer. Here, we go beyond these previous works and combine GNPs of two different core sizes (14 nm and 50 nm) to probe the role of NP size polydispersity on NP structuring and therefore properties. Structurally, we find that the GNPs form self-assembled structures that fill space. We present the self-assembled morphologies and measured gas transport properties of these polymer nanocomposites with binary core sizes.

*NSF
12:27PM G33.00007: Polymer Composites of Two-Dimensional Layered Materials for Structural Applications*
SEHMUS OZDEN (Presenter), 1) Princeton Institute for the Science and Technology of Materials; 2) Department of Chemical and Biological Engineering; 3) Department of Mechanical and Aerospace Engineering, NIKITA S. DUTTA, KATELYN RANDAZZO, CRAIG ARNOLD, RODNEY PRIESTLEY, Princeton University — Polymer composites of two-dimensional (2D) layered nanostructures such as graphene, graphene oxide (GO) and h-BN have promising potential in future technologies. However, although it has been more than a decade polymer composites of 2D-layered materials have been investigated, still fundamental challenges remain for practical applications. Currently, poor load transfer, good interfacial engineering and dispersion of layered materials in polymer matrix remain as a big challenge that needs to be overcome for the commercialization of these materials. 2D-layered materials offer significant advantages for developing thermally stable with robust mechanical properties, high electrical and thermal conductivities toward building ultra-lightweight multifunctional composites. Here, we report the development of highly porous, ultralight-weight and flexible polymer composite of 2D-layered structures for high temperature environmental applications. Physical, chemical and interfacial interactions of various polymer and 2D-layered structures will be discussed with the support of fully atomistic reactive molecular dynamics simulations that discloses unusual interface interactions between polymer matrix and 2D-layered structures.

*Princeton Center For Complex Materials Post-Doctoral Fellowship

12:39PM G33.00008: Mesostructured Metal Superconductors via Block Copolymer Nanocomposites: Quantum Metamaterials from Soft Matter*
RANDAL THEDFORD (Presenter), SOL MICHAEL GRUNER, ULRICH WIESNER, Cornell University — Three-dimensionally mesostructured superconductors have unique properties compared to thin film or bulk analogues, but their investigation has been limited by the lack of facile synthesis methods. Though largely unexplored in this application, block copolymers (BCPs) can serve as structure-directing agents to tune material architectures and, by extension, properties over scales on the order of characteristic lengths in superconductors (10s of nm). Hybrid BCP-inorganic self-assembly provides a route to mesostructured NbN superconductors, but complex materials chemistry prevents comparison with bulk equivalents. In recent work we demonstrate a versatile approach to mesoscale ordered metal superconductors via self-assembly of BCP nanocomposites. Results indicate quantum metamaterials behavior, with evidence that properties such as the transition temperature, coherence length, and critical field change substantially in a 3D periodic mesostructure (e.g., the bicontinuous double gyroid). Future work will investigate emergent phenomena such as angle-dependent magnetization behavior, and expansion of our technique to other metals could lead to novel photonic, electronic, and/or catalytic properties.

*R.P.T. supported by NSF GRFP (DGE-1650441)
12:51PM G33.00009: Experiments and Simulations of Nanoplate String Assembly in Lamellar Diblock Copolymer*  RUSSELL COMPOSTO (Presenter), NADIA KROOK, CHRISTIAN TABEDZKI, University of Pennsylvania, KEVIN YAGER, Brookhaven National Laboratory, KATHERINE ELBERT, CHRISTOPHER B MURRAY, ROBERT RIGGLEMAN, University of Pennsylvania — Within poly(styrene-b-methyl methacrylate) (PS-b-PMMA) block copolymer (BCP) lamellae, oriented nanoplates grafted with polyethylene glycol assemble into aligned strings at small interparticle separations. These assemblies are studied using X-ray scattering, electron microscopy, and hybrid particle/self-consistent field theory (hSCFT) simulations. The insertion of a nanoplate in a BCP microdomain is expected to produce a local domain bulge as the PS/PMMA interface distorts to optimize conformational chain entropy. 2D simulations of the equilibrium BCP structure show bulge formation around the nanoplates. As a function of particle separation, the potential of mean force (PMF) reveals a global minimum corresponding to an interparticle spacing of 7.0 nm, in good agreement with experimentals, 6.42 nm. The PMF calculation exhibits an activation barrier due to the high curvature penalty between two nanoplates at a separation of 21.7 nm. Ultimately, nanoplate strings form to optimize free energy contributions from interfacial area and chain stretching. The effect of BCP molecular weight on the PMF will also be presented.


1:03PM G33.00010: Molecular engineering of graft and matrix polymers for tuning grafted particle dispersion in polymer nanocomposites: A theory and simulation study*  ARJITA KULSHRESHTHA (Presenter), ARTHI JAYARAMAN, Univ of Delaware — In polymer nanocomposites (PNCs) comprised of grafted nanoparticles in a polymer matrix, tailoring the graft and matrix polymers is a way to tune the effective inter-particle interactions and morphology. In this talk we present our work using molecular simulations and theory showing how increasingly attractive graft-matrix interactions affect the interpenetration of matrix and graft chains (termed as grafted layer wetting) and the dispersion/aggregation of grafted particles in the matrix. Past work by our group on similar systems has shown that wetting/dewetting and dispersion/aggregation are two distinct phase transitions, former a continuous one and the latter a first-order transition as a function of graft-matrix interactions. In this work we find that as the graft-matrix attraction increases, the graft chains extend and matrix chains increasingly wet the grafted layer, leading to larger and harder grafted particles compared to analogous PNCs with athermal graft-matrix interactions. Simultaneously, the PNC structure changes from an aggregated/dispersed morphology dictated by the entropic limit to a dispersed morphology due to favorable weak graft-matrix attraction, and finally, to a correlated fluid of hard grafted particles at stronger graft-matrix attraction.

*DOE #DE-SC0017753
1:15PM G33.00011: Polymer grafted nanoparticles on Polymer Films: Entropic and Enthalpic effects on strcture and dynamics*  JAYDEEP BASU (Presenter), NIMMI DAS ANTHUPARAMBIL, APARNA SWAIN, Indian Institute of Science — Nanoparticle based ultra-thin membranes have been shown to have remarkable mechanical properties while also possessing novel electrical, optical or magnetic properties, which could be controlled by tailoring properties at the level of individual nanoparticles. Here we report thermal stability and the corresponding microscopic dynamics of polymer supported ultra-thin membranes comprising of self-assembled, ordered grains of polymer grafted nanoparticles having tunable mechanical properties. The initially ordered membranes show distinct pathways for temperature induced disordering depending on membrane flexibility as well as on interfacial entropic and enthalpic interactions with the underlying polymer thin film. We also observe contrasting temperature dependence of microscopic dynamics of these membranes depending on whether the graft polymer-substrate polymer interactions are predominantly entropic or enthalpic in nature. Our results suggest that apart from their varied applications, the soft nanoparticle-polymer hybrid membranes are a playground for rich physics involving subtle entropic and enthalpic effects along with the nanoparticles softness, which eventually determine their thermo-mechanical stability

*Department of Science & Technology, India (Nanomission).

1:27PM G33.00012: Gradient-Based Explicit Theoretical Framework for Simulation of Block Copolymer-Nanoparticle Co-assembly  DANIIL BOCHKOV (Presenter), FREDERIC GIBOU, University of California, Santa Barbara — The co-assembly of dispersed nanoparticles in block copolymers is a promising avenue for creating ordered structures at the nanoscale and materials with unique properties. Consequently, the theoretical understanding of this phenomenon is of great interest. In this talk, we present a novel theoretical framework for the simulation of the block copolymer-nanoparticle co-assembly. In this approach, we explicitly keep track of each particle in a sharp fashion while describing the polymer material using the Self-Consistent Field Theory. We consider particles of arbitrary shapes and allow the particle's surface affinity for different polymer components to be variable in space. The relaxation of block copolymer-nanoparticle mixtures to (meta) stable configurations is performed using a gradient-type approach based on the analytically derived expression for the virtual work of nanoparticles or, in other words, the full derivative of the system's energy with respect to the particles's orientations and positions. We provide several benchmark examples to demonstrate the capabilities of the proposed framework.
1:39PM G33.00013: Relating Entanglements and Toughness in Model Polymer-Grafted Nanoparticles  [Invited]  LISA HALL (Presenter), Ohio State Univ - Columbus — Polymer-grafted nanoparticles (PGNs) are a means to create precisely structured inorganic-organic hybrid materials. The graft length and graft density are key parameters that control interparticle spacing and other structural and mechanical properties. To guide materials design, we use coarse-grained molecular dynamics (MD) simulations to relate these parameters to structure, entanglements, and mechanical properties. We consider moderate to high graft density PGNs, which do not have large bare surface regions and are stable in the melt state in a hexagonally packed monolayer on a smooth attractive surface. As intuitively expected, grafts on adjacent PGNs are more interpenetrated in lower graft density systems. We define the interparticle entanglements (involving grafts originating from two different particles) and analyze these using both a topological and a time averaging method. We find that lower graft density (increased interpenetration) leads to increased interparticle entanglements per chain and increased toughness in both the melt and glassy state. The relationship between entanglement type and location and toughness will also be discussed.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G34 DPOLY DBIO DCOMP: Machine Learning and Data in Polymer Physics II  506 - Tyler Martin, National Institute of Standards and Technology - Tag(s): Focus

11:15AM G34.00001: Machine Learning and Data in Polymer Physics Research - Interpretation of Experiments, Model Development, and Enhanced Sampling  [Invited]  JUAN DE PABLO (Presenter), University of Chicago — Advances in molecular modeling algorithms, optimization strategies, and machine learning techniques, are ushering a new era of materials science and engineering in which computational tools are routinely used to probe, design, and interrogate matter and functional materials systems. The way in which problems and questions are formulated is rapidly changing, and it is important to rethink the role of research scientists and engineers in the context of these advances. In this presentation I will illustrate some of these ideas by relying on a variety of examples taken from polymer physics. In the first, I will discuss the coupling of experiments and molecular models, and how that coupling can be used to extract additional information from experiments that would otherwise be difficult to generate. In the second I will present models of biological systems – DNA and chromatin - that use machine learning to integrate experimental and computational information form a wide range of sources, and explain how the resulting information can be used to address important questions in epigenetics. In the third, I will discuss how machine learning can be used to design polymer structures or architectures for specific target properties.
11:51AM G34.00002: Neural Network Accelerated Self-Consistent Field Theory  HEJIN HUANG, Materials Science and Engineering, Massachusetts Institute of Technology MIT, KARIM GADELRAH, Bosch USA, ALFREDO ALEXANDER-KATZ (Presenter), Materials Science and Engineering, Massachusetts Institute of Technology MIT — Self-consistent field theory (SCFT) has demonstrated excellent capabilities in predicting self-assembled structures of block copolymers (BCP) at equilibrium. This method has been widely implemented in BCP self-assembly to understand its assembly process. Although SCFT gives accurate results, it is a relatively time-consuming method: SCFT involves solving differential equation numerically in matrix form at each time step and normally takes thousands of steps to reach the final structure at equilibrium, which makes it difficult to be applied to large 3D systems. In this work, we train a neural network (NN) to predict the evolving field during SCFT free energy minimization. After training the NN, we implement a hybrid algorithm combining SCFT with the trained NN. This NN-SCFT model helps to shorten the SCFT simulation time significantly (approximately x10 speedup), with convergence being achieved in all different cases (different volume ratio, and the chemical incompatibility between blocks). The NN-SCFT hybrid system, thus, provides a powerful tool for further exploration of larger BCP directed self-assembly systems and inverse self-assembly.

12:03PM G34.00003: Neural network for phase diagrams of polymer-containing liquid mixtures*  ISSEI NAKAMURA (Presenter), Physics, Michigan Technological Univ — We develop deep neural networks (DNNs) that consider the phase separation of polymeric liquids. In this talk, we discuss our new hidden layer that is constructed through coarse-grained mean-field theory and the scaling laws in polymer physics. This characteristic hidden layer enables us to perform the learning process efficiently with relatively small numbers of artificial neurons and hidden layers and provides the DNNs with reasonable predictive power. To demonstrate the efficacy of our DNNs, we will discuss the phase diagrams of polymer solutions, and the salt-free and salt-doped diblock copolymer melts. Moreover, we will show the predictive power of the DNNs by considering some experiments for the lithium salt-doped diblock copolymers such as PEO-b-PS.

*This work was supported by the Research Excellence Fund of Michigan Technological University.
Predicting the glass transition behaviors of polymers via integration of molecular simulations, theory, and machine learning

WENJIE XIA (Presenter), AMIRHADI ALESADI, North Dakota State Univ — Understanding and predicting the glass transition behavior of glass-forming polymers are of critical importance from both physical and practical standpoints. The substantial change in polymer relaxation and dynamics upon cooling causes major change in most physical properties, including mechanical modulus, density, specific heat, damping characteristics, dielectric properties of a polymer. The cheminformatics-based approach based on machine learning (ML) algorithms is often applied to draw the quantitative relationships between key molecular parameters/descriptors and properties of polymers. In this work, we develop an innovative framework by integrating cheminformatics and coarse-grained molecular dynamics (MD) simulations to predict the glass transition temperature of diverse sets of hundred polymers. Moreover, the use of generalized entropy theory in conjunction with ML uncovers the critical roles of key molecular parameters (i.e., cohesive interactions, chain stiffness, and branching) in influencing the glass transition temperature as well as other characteristic temperatures associated with glass formation of polymers.

Extracting molecular mechanisms of shear-thinning of liquids at high strain rates using machine learning*

VIKRAM JADHAO (Presenter), JCS KADUPITIYA, Intelligent Systems Engineering, Indiana Univ - Bloomington — Recent nonequilibrium molecular dynamics simulations have shown that shear-thinning of molecular liquids such as squalane at high strain rates (over 10^5 per second) exhibit a transition from a low-Newtonian-viscosity regime described well by power-law models to a high-Newtonian-viscosity regime where the flow properties are consistent with thermally-activated flow models. This talk explores the use of machine learning to probe the molecular origins of this rheological transition. Molecular trajectory data from simulations of small-molecular liquids sheared over a broad range of pressures and rates are used to design a 3D feature matrix. Using this matrix as input, several linear and nonlinear dimension reduction techniques are used to reduce the dimensionality of the feature space. We find that t-distributed stochastic neighbor embedding (t-SNE) can rapidly and effectively cluster trajectory data enabling the identification of molecular features (sets of atom pairs) diagnostic of the evolution in molecular order. Subsequent calculations of the order parameter and its linking with macroscopic rheological properties enable the determination of the amount of shear-thinning that comes from the evolution in order.

*This work is supported by Indiana University startup funds.
12:39PM G34.00006: Hybrid machine learning/materials science modeling for semi-crystalline polymer during film fabrication process  JIAN YANG (Presenter), TERESA KARJALA, JONATHAN MENDENHALL, VALERIY GINZBURG, RAJEN PATEL, FAWZI HAMAD, ELVA LUGO, PAVAN VALAVALA, The Dow Chemical Company — For semi-crystalline polymer like polyethylene (PE), it is well known that PE film physical properties is heavily dependent on the morphology of both the crystalline phase and amorphous chains, which can be largely influence by the film processing conditions. A clear understanding of the relationships of polymer molecular fingerprint, formulation, fabrication conditions and physical properties is important for future materials design, which can be traced back to polymerization process. However, this is generally considered to be a very complicated problem due to the large parameter space. In this report, we developed a new hybrid approach to combine the power of machine learning and fundamental materials science to characterize semi-crystalline PE, develop structure-property relationship and study the effect of fabrication conditions on physical properties during blown film fabrication process and to inform the design of new polymer structures.

12:51PM G34.00007: Developing Databases for Polymer Informatics  ROSELYNE TCHOUA, DePaul University, ZHI HONG, University of Chicago, DEBRA AUDUS (Presenter), National Institute of Standards and Technology, SHRAYESH PATEL, LOGAN WARD, KYLE CHARD, JUAN DE PABLO, IAN FOSTER, University of Chicago — One significant barrier to the adoption of polymer informatics is a lack of large FAIR (Findable, Accessible, Interoperable, Reusable) databases. In an effort to overcome this barrier, we developed pipelines to harness the vast quantities of valuable experimental polymer data trapped in the literature. In our first effort, we developed the largest Flory-Huggins chi parameter database using crowdsourcing and found that the burden to review papers could be lessened by training a classifier to identify promising articles. To further reduce human input, we turned to natural language processing software coupled with specially designed software modules to extract glass transition temperatures with minimal human input; ultimately, we extracted over 250 glass transition temperatures. All of the resulting data is freely available at the Polymer Property Predictor and Database website (http://pppdb.uchicago.edu). During this process, we found that identification of the polymer names within the literature was a key problem as polymers are referred to by common names, sample names, labels, etc. and subsequently explored named entity recognition to tackle this problem. To further extend our databases, we are working on allowing them to accept user submitted data.
As a powerful example of how machine learning (ML) algorithms can streamline discovery from experimental data, scientists at the LBNL Advanced Light Source have employed Convolutional Neural Networks (CNN) [1, 2] to enable lattice structure classification using diffraction patterns, and Gaussian process regression to construct surrogate models and error functions based on the limited experimental data. Diffraction patterns have come from Grazing Incidence Small Angle X-ray Scattering (GISAXS), a surface sensitive technique with increasingly usage growth in probing complex morphologies, such as conductive polymers. GISAXS allows electron density correlation analyses at surfaces by combining features from small-angle X-ray scattering and diffuse X-ray reflectivity. Resulting scattering patterns work as signatures, which depend on the size, shape, and arrangement of the nano-structured components. We will illustrate some of the advantages of using ML methods over traditional ways of searching for configurations in large materials databases. We will also discuss scaling analysis to high-throughput data to enable quick selection of materials, and benefits of autonomous experiments [3], faster experimental sessions and accelerated scientific discovery from materials science samples.

1:39PM G34.00009: Parameter Estimation for Spatio-Temporal Models using Bayesian Optimisation and Gaussian Processes* NIGEL CLARKE (Presenter), Department of Physics and Astronomy, University of Sheffield, JOAO CABRAL, Department of Chemical Engineering, Imperial College, RICHARD WILKINSON, School of Mathematics and Statistics, University of Sheffield, WIL WARD, Department of Physics and Astronomy, University of Sheffield, SEBASTIAN PONT, Department of Chemical Engineering, Imperial College — With many physical models having only numerical solutions, it can be challenging to fit predictions to data. We show how accurate joint estimation of parameters can be achieved efficiently with Bayesian optimization and Gaussian processes, even for spatio-temporal models, using the Cahn-Hilliard equation of phase separation as an exemplar.

To find globally optimal parameters, we represent the distance between the results of simulation and some observed outcome using a loss function. Instead of a computationally expensive grid-based search for the minimum loss, we adopt a Bayesian optimisation approach placing a Gaussian process over the loss, representing the function as an infinite-dimensional normal distribution that can be used to estimate it over its entire input space, with quantified uncertainty. The GP can be trained using a small number of evaluations, and a suggestion for the next test-point can be obtained automatically. New evaluations are used to update the GP estimation. Bayesian optimisation has the ability to localise regions where minima occur within a small number of iterations. The intrinsic incorporation of uncertainty allows for an effective trade-off between this exploitation and exploration of the wider input space.

*EPSRC EP/S014985/1

1:51PM G34.00010: Evolutionary couplings detect side-chain interactions in protein structures* ADAM J. HOCKENBERRY, CLAUS WILKE (Presenter), University of Texas at Austin — Patterns of amino acid covariation in large protein sequence alignments can inform the prediction of de novo protein structures, binding interfaces, and mutational effects. While algorithms that detect these so-called evolutionary couplings between residues have proven useful for practical applications, less is known about how and why these methods perform so well, and what insights into biological processes can be gained from their application. Here, we show that evolutionary coupling analyses are significantly more likely to identify structural contacts between side-chain atoms than between backbone atoms. We use both simulations and empirical analyses to highlight that purely backbone-based definitions of true residue–residue contacts may underestimate the accuracy of evolutionary coupling algorithms by as much as 40% and that a commonly used reference point (Cβ atoms) underestimates the accuracy by 10–15%. These findings show that co-evolutionary outcomes differ according to which atoms participate in residue–residue interactions and suggest that accounting for different interaction types may lead to further improvements to contact-prediction methods.

*This work was funded by NSF Cooperative Agreement no. DBI-0939454 and NIH grant R01 GM088344.
2:03PM G34.00011: Tracking Accelerated Aging of Cross-Linked Polyethylene Pipes by Applying Machine Learning Concepts to Infrared Spectra  MELANIE HILES, JOSEPH D’AMICO (Presenter), BENJAMIN MORLING, FATEMEH ABBASI, MICHAEL GROSSUTTI, JOHN DUTCHER, Univ of Guelph — Cross-linked polyethylene (PEX) pipes are promising replacements for metal or concrete pipes used for water, gas and sewage transport. Characterizing changes to the polymer and additive compounds with in-service use is paramount to predicting pipe failure. Infrared (IR) microscopy combines the chemical specificity of IR spectroscopy with the high spatial resolution of light microscopy, and we have used this technique to track variations in the degree of crystallinity and additive concentration across the wall thickness of PEX pipes. We have shown that principal component analysis of IR absorbance peaks can be used to differentiate and classify different pipe formulations [1]. We have used this methodology to characterize changes to pipes that have been subjected to accelerated aging involving heating in water and air, and exposure to ultraviolet radiation. This has allowed us to identify and track IR peaks that are most relevant to pipe degradation. We have used these results, together with machine learning techniques, to identify and classify different modes of pipe degradation.


Tuesday, March 3, 2020 11:15 AM - 1:39 PM

Session G35 DPOLY: Padden Award Symposium

11:15AM G35.00001: Photo-induced Melting of Semi-Crystalline Polymers via Azobenzene Isomerization*  ALEXA KUENSTLER (Presenter), RYAN HAYWARD, University of of Massachusetts - Amherst — Incorporation of photo-isomerizable molecules into macromolecular systems is a powerful method to harness Angstrom-level geometry changes induced by light to drive macroscopic shape changes and force generation. The most commonly explored material platforms exploit azobenzene isomerization-driven disordering of nematic polymer networks. While these materials generally perform better than isotropic networks due to cooperative nanoscale organization, higher ordering of azo-molecules into crystalline lattices presents a potential route to further enhance photogenerated work output. To this end, we have explored semi-crystalline azo polymers as a means to enhance ordering while preserving the processability inherent to polymer systems. We show that upon UV light exposure these materials undergo an isothermal melting of crystalline lamellae due to trans-cis isomerization, and that crystalline order can be restored upon re-isomerization back to the trans state. Interestingly, this process is found to be strongly suppressed at temperatures sufficiently far below the melting point. Finally, using shear alignment, we demonstrate the fabrication of well-aligned crosslinked fibers wherein reversible and directional crystallization can be harnessed for photoactuation.

*ONR N00014-18-1- 2624
11:27AM G35.00002: Materials by design for hairy nanoparticle assemblies*  NITIN HANSOGE (Presenter), SINAN KETEN, Northwestern University — A computational framework that combines machine learning and coarse-grained molecular dynamics (CGMD) simulations to tailor the mechanical properties of hairy nanoparticle assemblies (aHNP) is proposed. CGMD informed metamodel on PMMA-grafted nanocellulose assemblies revealed the necessity of having relatively low grafting density, high molecular weight, and high nanoparticle loading on achieving Pareto optimality. Utilizing theoretical scaling relationships derived from Daoud–Cotton theory, we identified the critical length scale \(N_{cr}\) governing Pareto optimality, originating based on conformational transition from concentrated to semi-dilute brush regime. We verified this finding by expanding our analysis to other common polymers, and quantified the role of polymer chemistry, backbone rigidity and side-group size of a polymer on the chain conformations and \(N_{cr}\). Remarkably, normalization of the monomer radial distribution curves using \(N_{cr}\) and other key molecular parameters collapsed the curves for 110 distinct model aHNP systems to a universal curve governing the chain conformations in aHNPs. The novel modeling framework along with the new physical insights into the confinement and interface effects in aHNPs pave the way for superior designs of aHNPs.

*PECASE, Award #N00014163175

11:39AM G35.00003: Multiscale Polymer and Nanoparticle Dynamics in Attractive Polymer Nanocomposite Melts  ERIC BAILEY (Presenter), RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — The addition of nanoparticles (NPs) to a polymer matrix, forming a polymer nanocomposite (PNC), has been used to extend and control macroscopic material properties. Many macroscopic properties are dictated by microscopic dynamic processes, including the dynamics of the polymer segments, chains, and NPs, which remain poorly understood in PNCs. This work experimentally explores the hierarchy of dynamics in model PNC melts with poly(2-vinylpyridine) and attractive NP-polymer interactions. In PNCs with 26-nm diameter NPs, we show that a bound polymer layer forms in solution and persists to the melt state. Using various techniques, we report that segmental relaxations near the NP interface are slower than in neat polymer and lead to polymer chain desorption that is \(~10^4\) times slower than bulk diffusion. Interestingly, when the NP size is commensurate with the polymer segments (~2 nm), the dynamics are quite different. For example, polymer segments are slowed homogeneously, slow chain diffusion is quantitatively described by increased segmental friction, and the NPs diffuse anomalously fast. Overall, these results highlight the complex and synergistic effects of NPs and polymers in PNCs and provide insights to help design functional PNCs for a variety of applications.
Polymers under Extreme Nanoconfinement

HAONAN WANG (Presenter), YIWEI QIANG, JYO LYN HOR, AHMAD ARABI SHAMSABADI, University of Pennsylvania, PRANTIK MAZUMDER, Sullivan Park, Corning Incorporated, DAIEWSHON LEE, ZAHRA FAKHRAAI, University of Pennsylvania — Polymers under nanoconfinement can show significantly deviated properties from bulk. Capillary Rise Infiltration (CaRI) can produce extreme polymer confinement by infiltrating the polymer into densely-packed nanoparticle (NP) films. Here, we use CaRI films to study physical and chemical properties of polymers under extreme nanoconfinement, including glass transition temperature ($T_g$), fragility, and thermal degradation. Polystyrene(PS)/SiO$_2$ and Poly(2-vinylpyridine)(P2VP)/SiO$_2$ CaRI films were used as the model systems with weak and strong interfacial interactions. The degree of confinement was tuned by using polymers with different molecular weights and NPs with different sizes (forming pores with 3-30 nm average size). We show that $T_g$ can increase by ~57 K for PS and ~100 K for P2VP confined in 3 nm pores. Furthermore, P2VP in CaRI films shows broader glass transition width but slightly lower fragility than bulk, indicating the gradient of dynamics in the pores. The thermal stability of both polymers are significantly enhanced in CaRI films with less char formation. The details of the process shows that the activation energy of PS degradation can increase by ~50 kJ/mol under nanoconfinement.

*We acknowledge Corning and NSF (DMR-1720530) for the funding of this study.

Deformation response of a two-dimensional polymer

BEATRICE SOH (Presenter), PATRICK DOYLE, Massachusetts Institute of Technology MIT — Kinetoplast DNA is the mitochondrial DNA of trypanosomes and related parasites. A kinetoplast is a complex two-dimensional network of topologically interlinked circular DNA. There has been much interest in studying the kinetoplast from a microbiology point of view, but little is known about the material properties of the network structure. The stretching response of a one-dimensional linear polymer has been studied extensively using single-molecule experiments. In this work, we probe experimentally the deformation response of the kinetoplast as a model two-dimensional polymer. We subject kinetoplasts to planar elongational fields in microfluidic channels and study the dynamics of kinetoplasts under a constant strain rate, as well as the relaxation dynamics of kinetoplasts.
12:15PM G35.00006: Decoupling the role of entanglements and mobility in the mechanics of ultrathin polymer glasses

R. KONANE BAY (Presenter), ALFRED J CROSBY, Polymer Science and Engineering, University of Massachusetts Amherst — As polymer glasses are processed into ultrathin films, neighboring polymer chains become less entangled, and surface-bound chains with altered states of mobility play an increasingly important role. Such changes in physical properties have long been studied, but changes in mechanical strength and deformation processes have remained difficult to quantify. We have developed a method to directly measure the uniaxial stress-strain response of ultrathin glassy polymer films of both liquid supported and freestanding films. In our work, we quantify the influence of thickness (10nm - 360nm), and molecular weight (61kDa - 2135kDa) on the deformation and failure response of ultrathin polystyrene films. We observe a molecular weight independent thickness-transition in strain localization and elastic modulus, and a molecular weight dependent decrease in maximum stress. We associate the changes in strain localization and elastic modulus to the surface mobile layer, and we form a model to capture the role of the average molecule size and the number of entanglements per chain on the decrease in maximum stress. These results provide new fundamental insights into how polymer behavior is altered due to changes in the entanglements and mobility in a polymer network upon confinement.

*NSF DMR-1608614

12:27PM G35.00007: Influence of Polymer Polarity on Ion Transport in Polymer Electrolytes

BILL WHEATLE (Presenter), NATHANIEL A LYND, VENKATRAGHAVAN GANESAN, University of Texas at Austin — Polymer electrolytes are materials that could improve the safety and performance of lithium-ion and -metal batteries. Despite their promising attributes, such as high shear modulus and electrochemical stability, they tend to have sluggish ionic transport. Several properties have been shown to improve ionic transport, including host segmental dynamics. Recently, we showed that host polymer polarity, measured by the dielectric constant, is also an influencing factor in ionic transport. We found that higher polarity polymers more effectively break up ionic aggregates, which reduces correlated ionic motion. However, our study focused on polymers with a narrow dielectric constant range (~3–7), which prohibited a general understanding of the extent to which improving polarity could improve ionic transport.

In this work, we turn to a coarse-grained simulation model with which we explore a wide range of polymer polarities and simultaneously explore the influence of polymer molecular weight and salt concentration. We show that ionic transport maximizes at intermediate polarity due to a competition between reduced ionic aggregation and slowed polymer dynamics. We demonstrate that ionic transport only couples to molecular weight and salt concentration once a threshold polarity is exceeded.
**12:39PM G35.00008: Solvation-Site and Dielectric Control of Ion Conduction in Polymer Electrolytes**

NICOLE MICHENFELDER-SCHAUSER (Presenter), DOUGLAS GRZETIC, GLENN H FREDRICKSON, RAM SESHADRI, RACHEL A SEGALMAN, University of California, Santa Barbara — Solid polymer electrolytes have the promise of improving safety and performance in energy storage devices. Metal cation-containing polymers provide a path to effective electrolytes, with dynamic metal-ligand interactions allowing mechanical properties and ionic conductivity to be widely and separately tuned. A modular synthetic platform based on thiol-ene click chemistry is presented that allows polymers to be post-functionalized with a variety of metal-binding ligands. This well-controlled model system has enabled the study of factors known or suspected to influence ionic conductivity, including segmental dynamics, dielectric constant, solvation site density, and ligand identity. Design rules based on this model platform have been developed by combining experimental results with field-theory-based simulations. The results underscore that low dielectric constant is not necessarily detrimental to ionic conductivity, especially in systems where the resulting ion aggregates form percolating domains.

*This work is supported by the NSF MRSEC at UC Santa Barbara (DMR 1720256, IRG-2).

**12:51PM G35.00009: Self-assembly of Salt-Doped Ternary Polymer Blends**

SHUYI XIE (Presenter), TIMOTHY LODGE, University of Minnesota — Ternary polymer blends comprising A and B homopolymers and an A-B block copolymer can self-assemble into various microstructures, depending on the polymer composition, chain architecture and temperature. When doped with salt, such blends are promising for applications such as lithium ion batteries due to the tunable morphology. The addition of lithium bis(trifluoromethane)sulfonamide (LiTFSI) to a polymer blend system containing low molar mass poly(ethylene oxide) (PEO) and polystyrene (PS) homopolymers, and a PS–PEO block copolymer (SEO) induces either macroscopic or microscopic phase separation. Blends with different total homopolymer compositions (fH) and volume ratios of PEO and PS homopolymer (fPEO/fPS) at specific temperatures are investigated. In some regions of the phase prism, addition of salt recovers the microphase separated structures of conventional ternary blends, and in particular creates a wide bicontinuous microemulsion (BμE) channel. With still higher fH, a surprising C15 Laves phase is found. This work will help understand the self-assembly of ion-containing A/B/A-B ternary polymer blends and guide the experimental design of polyelectrolyte systems with tunable nanostructures.

1:03PM G35.00010: SANS Partial Structure Factor Analysis for Determining Protein-Polymer Interactions in Semidilute Solution* HELEN YAO (Presenter), AARON HUANG, BRADLEY OLSEN, Massachusetts Institute of Technology MIT — Protein-polymer interactions play a crucial role in many processes, including protein crystallization, biofouling, and self-assembly of protein-polymer bioconjugates. However, it is often difficult to measure these interactions in multicomponent systems, especially in semidilute solutions. Here, contrast-variation small-angle neutron scattering (CV-SANS) was used to quantify the interactions between three water-soluble polymers (PNIPAM, POEGA, and PDMAPS) and a model protein mCherry. CV-SANS enables decomposition of SANS intensities into partial structure factors that describe polymer-polymer, protein-protein, and polymer-protein interactions. The three polymers span various chemistries and properties, with PNIPAM and POEGA being non-ionic polymers with different hydrogen-bonding capabilities and PDMAPS being a zwitterionic polymer. PNIPAM/mCherry interactions were repulsive and dominated by depletion forces. In contrast, POEGA/mCherry interactions are attractive, with polymer enrichment at the protein surface. PDMAPS/mCherry interactions are more complex, with both depletion and electrostatic contributions. CV-SANS thus represents a powerful method to separate, quantify, and reveal the nature of interactions in multicomponent systems.

*This work is funded by DOE Award DE-SC0007106

1:15PM G35.00011: Self-regulating metal cross-linked hydrogels via competition SETH CAZZELL (Presenter), NIELS HOLTEN-ANDERSEN, Massachusetts Institute of Technology MIT — Polymer networks with dynamic cross-links have generated widespread interest as tunable and responsive viscoelastic materials. However, narrow stoichiometric limits in cross-link compositions are typically imposed in the assembly of these materials to prevent excess free cross-linker from dissolving the resulting polymer networks. Using both computational and experimental methods, we demonstrate how the presence of molecular competition allows for vast expansion of the previously limited range of cross-linker concentrations that result in robust network assembly. Specifically, we use metal-coordinate cross-linked gels to verify that stoichiometric excessive metal ion cross-linker concentrations can still result in robust gelation when in the presence of free ion competing ligands, and we offer a theoretical framework to describe the coupled dynamic equilibria that result in this effect. We believe the insights presented here can be generally applied to advance engineering of the broadening class of polymer materials with dynamic cross-links.
1:27PM G35.00012: Deciphering Low-Temperature Dielectric Relaxation of a Series of Amorphous Polymers  DANIEL WILCOX (Presenter), GRIGORI MEDVEDEV, HOSUP SONG, JAMES M CARUTHERS, BRYAN BOUDOURIS, Purdue Univ — In contrast to the crystalline solid and gaseous phases, the physics behind the behavior of liquids and amorphous solids remains a significant challenge. Current descriptions of relaxation behavior in these materials are highly empirical, either utilizing fitting functions with tenuous physical significance, or fitting to a spectrum of Debye relaxation processes, where typical procedures implicitly make the unphysical assumption that the spectral density with respect to the characteristic times is constant and unvarying with temperature. Recently, we have found that the relaxation behavior of a moderately cross-linked epoxy resin is well described by a relaxation spectrum where the spectral strengths of individual components are constant while the spectral density is non-uniform and varies with temperature. The sub-Tg γ-relaxation is well described by a constant strength spectrum spanning over roughly 12 orders of magnitude in the frequency domain. In this work we use this newly developed approach to study the γ-relaxation of a series of epoxy resins with differing crosslink densities. From this, we develop maps showing the temperature dependence of the relaxation spectra, with which we aim to pinpoint the effect of crosslinking on the relaxation behavior of these materials.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G36 DBIO: Delbruck Prize Session 601/603 - Phil Nelson, University of Pennsylvania - Tag(s): Invited

11:15AM G36.00001: Synthetic Biology: Physical Biology by Design [invited]  JAMES COLLINS (Presenter), Massachusetts Institute of Technology MIT — Synthetic biology is bringing together physicists and biologists to model, design and construct biological circuits out of proteins, genes and other bits of DNA, and to use these circuits to rewire and reprogram organisms. These re-engineered organisms are going to change our lives in the coming years, leading to cheaper drugs, rapid diagnostic tests, and synthetic probiotics to treat infections and a range of complex diseases. In this talk, we highlight recent efforts to create synthetic gene networks and programmable cells, and discuss a variety of synthetic biology applications in biotechnology and biomedicine.
11:51AM G36.00002: Physical principles from evolutionary synthetic biology* [Invited]  GABOR BALAZSI (Presenter), State Univ of NY - Stony Brook — Synthetic biology designs and builds artificial biological systems, using principles from engineering, mathematics and physics. Just like engineering was crucial for many traditional physics discoveries over the past centuries, synthetic biology can advance biological physics by providing sensors, switches, oscillators, control knobs and other tools for quantitatively monitoring and perturbing living cells. Moreover, synthetic biological devices can serve as simple model systems to elucidate complex biophysical processes. For example, synthetic biological devices evolve along with the cells that carry them, providing new opportunities to investigate cellular and molecular evolution. I will present examples of how evolving synthetic gene circuits can provide deeper understanding of evolutionary processes, specifically of gene networks mediating the adaptation of cell populations.

*This research is supported by NIH/NIGMS MIRA grant R35 GM122561 and by the Laufer Center for Physical and Quantitative Biology.

12:27PM G36.00003: Synthetic Biology: Building to learn so that we might learn to build [Invited]  JEFF HASTY (Presenter), Univ. California San Diego — Synthetic Biology can be broadly parsed into the “top-down creation” of entire genomes and the “bottom-up engineering” of relatively small genetic circuits. A defining component of the gene circuit approach is the development of theory that can serve as the foundation for a new type of cellular engineering. This talk will be anchored by my quest to build genetic oscillators in cells, with a particular focus on the utility of mathematical modeling in determining general design principles. I'll first describe the design and construction of an intracellular circuit that cycles over a wide range of environmental conditions (http://biodynamics.ucsd.edu/Intracellular.mov). The large space of observed oscillatory behavior drove a revision of model equations that revealed unanticipated coupling of the clock to native cellular processes. More generally, the necessity of the model revision led to our ongoing exploration of biochemical networks that act as queues that can be balanced at a type of critical point. In terms of engineering, the clock was not of the Swiss variety; the period and amplitude exhibited large intracellular variability. However, viewed through the lens of dynamical systems theory, the noisy oscillator provided a benchmark for the development of general synchronization strategies that can restore determinism. This led to three studies describing (i) how quorum sensing can be used to couple clocks between cells (biodynamics.ucsd.edu/Intercellular.mov), (ii) how redox signaling can combine with quorum sensing to couple colonies at centimeter length scales (biodynamics.ucsd.edu/Intercolony.mov), and (iii) how intra- and inter-cellular dynamics can be rapidly coupled and used to encode information (biodynamics.ucsd.edu/Multiplexing.mp4). I'll conclude with a brief description of current applications that have arisen from our progress in traversing the scales from mathematical design in single cells to observable dynamics at the macroscopic level.
1:03PM G36.00004: Context dependence of biological circuits: Predictive models and engineering solutions [Invited] DOMITILLA DEL VECCHIO (Presenter), Massachusetts Institute of Technology MIT — Engineering biology has tremendous potential to impact a number of applications, from energy, to environment, to health. As the sophistication of engineered biological circuits increases, the ability to predict system behavior becomes more limited. In fact, while a system’s component may be well characterized in isolation, the salient properties of this component often change in surprising ways once it interacts with other components in the cell. This context-dependence of biological circuits makes it difficult to perform rational design and often leads to lengthy, combinatorial, design procedures where each component is re-designed \textit{ad hoc} when other parts are added to a system. In this talk, I will review some causes of context-dependence. I will then focus on problems of resource loading and describe a design-oriented mathematical model that accounts for it. I will introduce a general engineering framework, grounded on control theoretic concepts, that can serve as a basis for creating devices that mitigate context-dependence. Example devices will be introduced that mitigate context-dependence due to resource loading in both bacterial and mammalian genetic circuits. These solutions support rational and modular design of sophisticated genetic circuits and can serve for engineering biological circuits that are more reliable and predictable.

1:39PM G36.00005: Universality in Cardiac Dynamics* [Invited] LEON GLASS (Presenter), McGill Univ — Cardiac dynamics displays universal features that stem from similarities in the underlying molecules and structures in the hearts of different species. But the universality can also be considered from the context of nonlinear dynamics. Nonlinear dynamical processes of wave initiation, wave propagation and wave collision prevail over diverse organisms and experimental preparations. Concepts such as period-doubling bifurcations, Cantor sets, and circle maps arise naturally. Application of these concepts provides a physical perspective to the classification of cardiac arrhythmias by cardiologists. Determining the factors that facilitate or impede the persistence of cardiac arrhythmias offer potential directions for improving therapy. I will illustrate these ideas with examples derived from theory, experiment and clinical data with emphasis on paroxysmal rhythms that start and stop suddenly. I will mention several different cardiac arrhythmias including "palpitations", heart block, atrial fibrillation, ventricular tachycardia. The talk may be personally relevant if you (or a close friend or relative) have experienced one of these common arrhythmias.

*NSERC and the Canadian Heart and Stroke Foundation

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G37 DCMP: Disorder-Driven Transitions in Dirac Materials and Related Systems 605 - Leo Radzihovsky, University of Colorado, Boulder - Tag(s): Invited
11:15AM G37.00001: High-dimensional disorder-driven phenomena in nodal semimetals and systems with long-range hopping [Invited] SERGEY SYZRANOV (Presenter), University of California, Santa Cruz — Systems of non-interacting electrons are believed widely to exhibit only one type of disorder-driven transitions: the Anderson localisation transition. It has been suggested, however, that systems with the power-law quasiparticle dispersion $k^\alpha$ in high dimensions $d>2\alpha$, exemplified by 3D Weyl and Dirac semimetals, may exhibit transitions in a different universality class, as well as unconventional energy-level statistics, Lifshitz tails and ballistic-transport properties. In this talk, I will review existing results on the non-Anderson transitions and other unconventional disorder-driven phenomena in nodal semimetals and related systems (quantum kicked rotors, arrays of ultracold ions, 1D and 2D plasmonic systems, etc.). Also, I will demonstrate that the field theories of disordered nodal semimetals with $\alpha<d$ can be mapped exactly onto those of systems with long-range hopping of quasiparticles, where hopping decays with distance $r$ slower than $1/r^d$ (trapped ultracold ions, spins in solids, nitrogen defects in diamonds, etc.). This duality allows to describe the properties of each of these two classes of systems using the results established for the other class and, in particular, establishes the existence of unconventional disorder-driven transitions in systems with long-range hopping.

11:51AM G37.00002: Disordered Weyl Semimetals: From Lattice Models to the Continuum [Invited] JED PIXLEY (Presenter), Rutgers University, New Brunswick — We will discuss numerical studies of disordered Weyl semimetals focusing on the effects of rare regions at low energy. We will review our work on lattice models of Weyl semimetals which demonstrates the existence of rare region induced non-perturbative eigenstates, an exponentially small but non-zero density of states at the Weyl node, an exponentially large quasiparticle lifetime, and an avoided quantum critical point. We will then present our recent study of a single Weyl cone in the presence of short-range disorder. To numerically handle the continuum we represent the Hamiltonian in a "mixed" way between real and momentum space so that we are able to invoke fast Fourier transforms to take advantage of efficient numerical routines (such as Lanczos and the kernel polynomial method) that rely on sparse matrix-vector multiplications. As a result, we can reach sufficiently large system sizes that are comparable to our lattice model calculations. We will report results on the nature of rare regions and the density of states as a function of the strength of disorder and the ultra violet cut off, as well as compare and contrast single-node and multi-node results. In all of the cases studied, we will demonstrate that the putative semimetal to diffusive transition is rounded into a cross over.

1:03PM G37.00004: Nodal points of Weyl semimetals survive the presence of moderate disorder [Invited] MICHAEL BUCHHOLD (Presenter), Caltech, SEBASTIAN DIEHL, ALEX ALTLAND, University of Cologne — This talk addresses the physics of individual three-dimensional Weyl nodes subject to a moderate concentration of disorder. Previous analysis indicates the presence of a quantum phase transition below which disorder becomes irrelevant and the integrity of sharp nodal points of vanishing spectral density is preserved in this system. This statement appears to be at variance with the inevitable presence of statistically rare fluctuations which cannot be considered as weak and must have strong influence on the system's spectrum, no matter how small the average concentration. We here reconcile the two pictures by demonstrating that rare fluctuation potentials in the Weyl system generate a peculiar type of resonances which carry spectral density in any neighborhood of zero energy, but never at zero. In this way, the vanishing of the DoS for weak disorder survives the inclusion of rare events. We demonstrate this feature by considering three different models of disorder, each emphasizing specific aspects of the problem: a simplistic box potential model, a model with Gaussian distributed disorder, and one with a finite number of s-wave scatterers.

1:39PM G37.00005: Spectrum-wide quantum criticality at the surface of class AIII topological phases: An "energy stack" of integer quantum Hall plateau transitions* [Invited] BJOERN SBIERSKI (Presenter), University of California, Berkeley, JONAS KARCHER, Karlsruhe Institute of Technology, MATTHEW S. FOSTER, Department of Physics and Astronomy and Rice Center for Quantum Materials, Rice University — In the absence of spin-orbit coupling, the conventional dogma of Anderson localization asserts that all states localize in two dimensions, with a glaring exception: the quantum Hall plateau transition (QHPT). In that case, the localization length diverges and interference-induced quantum-critical spatial fluctuations appear at all length scales. Normally QHPT states occur only at isolated energies; accessing them therefore requires fine-tuning of the electron density or magnetic field. In this paper we show that QHPT states can be realized throughout an energy continuum, i.e. as an "energy stack" of critical states wherein each state in the stack exhibits QHPT phenomenology. The stacking occurs without fine-tuning at the surface of a class AIII topological phase, where it is protected by U(1) and (anomalous) chiral or time-reversal symmetries. Spectrum-wide criticality is diagnosed by comparing numerics to universal results for the longitudinal Landauer conductance and wave function multifractality at the QHPT. Results are obtained from an effective 2D surface field theory and from a bulk 3D lattice model. We demonstrate that the stacking of quantum-critical QHPT states is a robust phenomenon that occurs for AIII topological phases with both odd and even winding numbers. The latter conclusion may have important implications for the still poorly-understood logarithmic conformal field theory believed to describe the QHPT.

*This research was supported by NSF CAREER Grant No. DMR-1552327 (MSF), the KHYS research travel grant (JFK) and the German National Academy of Sciences Leopoldina through grant LPDS 2018-12 (BS).

Tuesday, March 3, 2020 11:15 AM - 2:15 PM
11:15AM G38.00001: Towards Effective, Inclusive Mentorship* [Invited]  THE COMMITTEE ON EFFECTIVE MENTORING IN STEMM, MARIA LUND DAHLBERG (Presenter), The Board on Higher Education and Workforce, The National Academies of Sciences, Engineering, and Medicine — Mentorship has always served an essential role in the process of turning students into science, technology, engineering, mathematics, and medicine (STEMM) professionals. Yet despite the central role that mentorship plays in STEMM culture, mentorship rarely receives the focused attention, evaluation, and recognition of other aspects of the professional development process like teaching and research. There is, however, well-document evidence, theories, and practical implementation strategies that you can use to develop intentional, inclusive, effective mentoring relationships. This talk will review some of the key findings and recommendations from the National Academies consensus study report on The Science of Effective Mentorship in STEMM [1] and the accompanying online guide [2]. It will provide insights into the elements and stages of mentorship and review possible tools to use in your mentoring relationships. It will discuss some principles of institutional culture change and how they relate to supporting a culture of effective, inclusive mentorship.


*This activity was supported by contracts between the National Academy of Sciences and Howard Hughes Medical Institute (#52008818), Alfred P. Sloan Foundation (#G-2017-9885), Burroughs Wellcome Fund (#1017761), and by a grant from the Gulf Research Program of the National Academies of Sciences, Engineering, and Medicine under award number 3-Nov2017-01.
11:51AM G38.00002: Challenges Facing Women in Physics* [Invited] ANNE MARIE PORTER (Presenter), American Institute of Physics — Although the number of women has increased over time, women continue to be underrepresented in the physics field. According to 2018 survey data from the Statistical Research Center at the American Institute of Physics (AIP), women earned 22% of physics bachelor’s degrees, 20% of physics doctoral degrees, and were 19% of faculty members employed in physics departments. Our survey findings also showed that women experience more challenges during their physics career. Based on results from the 2011 PhD Plus 10 survey of mid-career physicists, women earned a significantly lower salary than men, and women more often reported that gender bias and family obligations were barriers during their career. We found that similar challenges were shared by women in physics around the world. The 2018 Global Survey on Gender Gaps in the Sciences surveyed physicists in 159 unique countries, and women were significantly more likely to report negative relationships with their graduate advisors, slower career progression, and experiences with gender discrimination and sexual harassment. These findings can be used to better understand and improve the experiences of women in the physics community.

*The 2018 Global Survey on Gender Gaps in the Sciences was funded by the International Council for Science (ICSU).

12:27PM G38.00003: Mental health challenges for early career physicists [Invited] ANDREA WELSH (Presenter), Georgia Inst of Tech — In the past few years, more studies about poor mental health in academia have been conducted and found that PhD students are almost 3 times as likely to develop mental health problems than then general population. While studies have not been conducted yet on postdoctoral researchers, anecdotal evidence has shown similar concern about mental health on blogs such as Chronically Academic, and others. Topics often linked with poor mental health are work-life balance, job demands, long work hours, supervisor’s leadership, and financial concerns. Many of these stressors are often exacerbated for those with an underrepresented identity with the addition of factors such as stereotype threat, imposter syndrome, or microaggressions. I will discuss the challenges that lead to poor mental health for early career physicists as well as some possible solutions that can be implemented by individuals and the community.

1:03PM G38.00004: Physics abroad, physics at home: a trans perspective on building supportive physics communities [Invited] SAVANNAH GARMON (Presenter), Osaka Prefecture Univ — I will discuss some of my experiences as a trans woman and research physicist who transitioned during her career, which will serve as a backdrop to an exploration of ideas on building stronger and more supportive physics communities, especially for early-career folks. This will include some ideas on better support for postdocs, who may be vulnerable to experiences of isolation and other issues. I will also discuss some outcomes and recommendations from the 2016 report by the APS ad hoc committee on LGBT issues in physics.

1:39PM G38.00005: Monica J Plisch Invited Talk [Invited] —

Tuesday, March 3, 2020 11:15 AM - 2:15 PM
11:15AM G39.00001: Reproducibility, precision and accuracy in $GW$ calculations [Invited]
MICHEL VAN SETTEN (Presenter), IMEC — For many years, computational limits have forced $GW$ calculations to employ approximations without the possibility to systematically evaluate their validity. In such a situation, the search for accuracy and precision can become very challenging, up to the point where one risks sacrificing precision for the sake of accuracy. With increased computational resources, this situation is changing but performing fully converged none approximated $GW$ for solids is still a big challenge. For finite size systems, however, calculations can be more tractable.

In this contribution I summarize the results of the $GW100$ project. The $GW100$ set is a benchmark set of the ionization potentials and electron affinities of 100 molecules computed using the $GW$ method using different independent $GW$ codes and different $GW$ methodologies. The quasi-particle energies of the HOMO and LUMO orbitals are calculated for the $GW100$ set at various levels of approximations. The use of different codes allows for a quantitative comparison of the type of basis set (plane wave or local orbital), handling of unoccupied states, the treatment of core and valence electrons (all electron or pseudopotentials), the treatment of the frequency dependence of the self-energy (full frequency or more approximate plasmon-pole models), and the algorithm for solving the quasi-particle equation.

At present 12 different codes have contributed to the project resulting in over 80 data sets. At $G0W0@PBE$ level very tightly converged results obtained with very different codes, including fully analytic $GW$, answer the question on precision. A comparison of seven different levels of self-consistency in $GW$ to reference values calculated at CCSD(T) level of theory answers the question on accuracy.
11:51AM G39.00002: Solving the Bethe-Salpeter Equation on a Subspace: Approximations and Consequences for Band-Edge and Core-Level Excitons in Quasi Low-dimensional Materials*  DIANA QIU (Presenter), Yale University, FELIPE H. DA JORNADA, Materials Science, Stanford University, STEVEN LOUIE, Physics, University of California, Berkeley and Lawrence Berkeley National Lab — It is known that environment can dramatically renormalize the quasiparticle energy gap and exciton binding energies in quasi low-dimensional materials, but the effect of environmental screening on the energy splitting of the spin-singlet and spin-triplet exciton states is less explored. The renormalization of the exciton binding energy arises from additional environmental screening of the attractive direct Coulomb term in the kernel of the Bethe-Salpeter equation (BSE). The repulsive exchange interaction responsible for the singlet-triplet slitting is in principle unscreened, though it has been argued that in practical calculations using a subspace of the full Hilbert space the exchange interaction should be modified and effectively screened by states outside of the chosen subspace, the “S” approximation. We explore the accuracy of the S approximation for different systems, including molecules, heterostructures and core level excitations. We show, additionally, that the S approximation is actually exact in the limit of small exciton binding energies provided that a screening consistent with the Tamm-Dancoff approximation is employed.

*This work was supported by C2SEPEM, which is funded by the U.S. DOE, Office of Science, Basic Energy Sciences, under Contract No. DE-AC02-05CH11231.

12:03PM G39.00003: Pyrene-Stabilized Acenes as Intermolecular Singlet Fission Candidates: Importance of Exciton Wave-Function Convergence  XINGYU ALFRED LIU (Presenter), RITHWIK TOM, XIAOPENG WANG, Carnegie Mellon University, BOHDAN SCHATSCHNEIDER, Cal-Poly Pomona, NOA MAROM, Carnegie Mellon University — Singlet fission (SF) is the conversion of a singlet exciton into two triplet excitons. SF could increase the efficiency of organic solar cells by harvesting two carriers from one photon. Polyacene crystals, such as tetracene and pentacene, have shown outstanding SF performance. However, their instability prevents them from being utilized in SF-based photovoltaic devices. In search of practical SF chromophores, we use many-body perturbation theory with the GW approximation and Bethe-Salpeter equation to study the excitonic properties of pyrene-stabilized acenes. We propose a criterion to determine the convergence of exciton wave-functions with respect to the fine k-point grid used in the BerkeleyGW code. An open-source Python code is presented to perform exciton wave-function convergence checks and streamline the double-Bader analysis of exciton character. We find that the singlet excitons in pyrene-stabilized acenes have a higher degree of charge transfer character than in the corresponding acenes. The pyrene-fused tetracene and pentacene derivatives exhibit comparable excitation energies to their corresponding acenes, making them potential SF candidates. The pyrene-stabilized anthracene derivative is considered as a possible candidate for triplet-triplet annihilation (TTA).
12:15PM G39.00004: An energetics perspective on why there are so few triplet-triplet annihilation emitters  XIAOPENG WANG, RITHWIK TOM, XINGYU ALFRED LIU, NOA MAROM (Presenter), Carnegie Mellon University — The efficiency of organic solar cells may be increased by utilizing photons with energies below the band gap of the absorber. This may be enabled by upconversion of low energy photons into high energy photons via triplet-triplet annihilation (TTA). The quantum yield of TTA is often low due to competing processes. The singlet pathway where a high-energy photon is emitted has a 1/9 probability according to the Clebsch-Gordon rules. The quintet pathway is typically too high in energy to be accessible, leaving the triplet pathway as the main competing process. Using many-body perturbation theory in the GW approximation and the Bethe–Salpeter equation, we calculate the energy release in both the singlet and triplet pathways in 61 chromophores of different chemical families. We find that in most cases the triplet pathway is open and has a larger energy release than the singlet pathway. Thus, the energetics perspective explains why there are so few TTA emitters and their low quantum yields.

12:27PM G39.00005: Analysis of Excitons in Stacked Perylene Diimide Derivatives*  KASIDET JING TRERAYAPIWAT (Presenter), Department of Chemistry, Boston University, ALIYA MUKAZHANOVA, Division of Materials Science and Engineering, Boston University, SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University — π-stacked organic molecules are tunable light-absorbing materials that are promising for many optoelectronic applications; thus, it is necessary to understand how both inter- and intra-molecular interactions influence optical excitations. We use first-principles time-dependent density functional theory (TDDFT) to study the nature of these interactions in functionalized perylene diimide oligomers stacked on a DNA-like backbone. Taking a Franck-Condon Herzburg-Teller approach to vibronic coupling, and sampling of ground state vibrations via molecular dynamics, we obtain an ensemble of excited-states that may occur. By analyzing ~100 dimer and trimer structures, we elucidate the parameters that correlate with the nature of the excited-state. Charge transfer (CT) character analysis shows that the degree of CT-like character in a bright state correlates with the strength of electronic transition and with its inter-molecular vibrations. Furthermore, we determine that displacement and rotation between monomers leads to reordering of direct excitations. Such a finding is important for technologies such as singlet fission photovoltaics where the CT excitation character is directly related to performance.

*The authors acknowledge financial support from NSF (DMR-1610031, DMR-1847774).
First-principles $G_0W_0$ calculations for ferrocene, anthracene and porphyrin* MASOUD MANSOURI (Presenter), Centro de Física de Materiales-MPC (CSIC-UPV/EHU), PETER KOVAL, Donostia International Physics Center (DIPC), DANIEL SANCHEZ-PORTAL, Centro de Física de Materiales-MPC (CSIC-UPV/EHU) — Hedin's GW approximation is well-known as a powerful method in the material science community because of its high quality and relatively low computational cost. In this study, we evaluate the performance of the $G_0W_0$ approximation for the charged quasi-particle excitation energies of three gas-phase molecules of interest for organic electronics, including ferrocene, porphyrin and anthracene. Moreover, we assess the undesired starting-point dependence in this method by benchmarking the ionization energies obtained from $G_0W_0$ on top of the spin-resolved Hartree-Fock and Kohn-Sham methods. The merit of dynamic effective GW self-energy leads to significant improvement of ionization energies compared to mean-field calculations and deviations less than 0.4 eV as compared to experiment. The calculations are carried out by the use of numerical atomic orbitals and contour deformation technique along with an iterative procedure to deal with the energy dependency of GW self-energy and full matrix elements of the dynamically screened Coulomb interaction.

Authors acknowledge support from Spanish MINECO Grants MAT2016-78293-C6-4-R and RTC-2016-5681-7 (SIESTA-PRO).

Exciton temperature dependence dictated by localization in organic semiconductors* ANTONIOS ALVERTIS (Presenter), RICHARD H. FRIEND, AKSHAY RAO, Univ of Cambridge, ALEX W. CHIN, Sorbonne University, BARTOMEU MONSERRAT, Univ of Cambridge — The response of organic semiconductors in optoelectronic devices is dominated by room temperature excitons. However, exciton calculations of organic crystals at finite temperature can be challenging, due to the need to combine the effects of exciton-phonon coupling and thermal expansion. Here we overcome this challenge by employing a combination of Green's function methods for the electronic structure, and non-perturbative finite difference methods for the interaction with the lattice. We apply our methodology to the acene series of molecular crystals and find that different localization ranges of excitons lead to different responses to exciton-phonon coupling and thermal expansion. As a result, the energies of singlet and triplet excitons have different temperature dependencies, as do the singlet energies between the different materials. We expect that the combination of exciton-phonon coupling and thermal expansion, together with their interplay with the exciton localization range, provides a general mechanism for understanding the temperature dependence of exciton energies in molecular crystals.

EPSRC grant EP/L015552/1, Simons Foundation grant 601946. B.M. acknowledges Robinson College, Cambridge and the Cambridge Philosophical Society for a Henslow Research Fellowship.
**1:03PM G39.00008: Probing energy transfer design principles in photosynthetic light harvesting systems with predictive electronic structure calculations**  
CAROLINE MCKEON (Presenter), SAMIA M HAMED, University of California, Berkeley, CHENCHEN SONG, Lawrence Berkeley National Laboratory, JEFFREY B NEATON, University of California, Berkeley — A thorough theoretical understanding of photosynthetic light-harvesting systems is critical to our ability to mimic their unparalleled energy transduction efficiency in synthetic contexts. Here, we present a workflow for calculating optical absorption spectra of chromophore monomers and dimers within the Franck-Condon approximation, using classical molecular dynamics simulations, and time-dependent density functional theory. We apply our approach to Sulforhodamine B (SRB) and AlexaFluor488 chromophore monomers and dimers and compare our results with complementary experimental absorption spectra. We discuss how conformation, the presence of counter-ions, solvation models, and choice of functional influence the predicted absorption spectra. We discuss progress towards identifying key factors in the high quantum efficiencies found exclusively in natural photosynthetic systems. This work is supported by the Department of Energy.

*This work is supported by the Department of Energy and computational resources are provided by the Molecular Graphics Facility at University of California, Berkeley.

**1:15PM G39.00009: Exciton coherence times and diffusion constants in molecular crystals from exciton-phonon coupling with an ab initio GW-BSE approach**  
JONAH HABER (Presenter), Physics, University of California, Berkeley, FELIPE DA JORNADA, Materials Science and Engineering, Stanford University, SIVAN REFAELY-ABRAMSON, Department of Materials and Interfaces, Weizmann Institute of Science, GABRIEL ANTONIUS, Département de Chimie, Biochimie et Physique, Université du Québec à Trois-Rivières, Trois-Rivières, STEVEN LOUIE, JEFFREY B NEATON, Physics, University of California, Berkeley — Predictive theories of exciton dynamics are of growing importance as increasingly complex materials, with strong electron-hole interactions, are used in device physics applications. For instance, in organic photovoltaics, an important part of energy conversion processes involves the diffusion of a photo-excited exciton to donor-acceptor interfaces where charge separation can occur. To quantitatively understand exciton dynamics, a microscopic theory of exciton-phonon interactions is required. Here, we describe an ab initio framework for computing exciton-phonon matrix elements, using density functional perturbation theory in conjunction with many-body perturbation theory within the GW plus Bethe-Salpeter equation (BSE) approach. We apply this formalism to crystalline tetracene, a prototypical organic semiconductor with strong electron-hole interactions. We compare and contrast how low-lying spin singlet and triplet excitons couple to the phonon field. We perturbatively compute phonon-limited exciton coherence times throughout the Brillouin zone and report exciton diffusion constants, evaluated using the relaxation time approximation. In all cases, we compare with experimental measurements, where available.

*This work is supported by the DOE; computational resources at NERSC.*
**1:27PM G39.00010: Effects of dynamical lattice screening on excitonic and optical properties of polar compounds**

JOSHUA LEVEILLEE (Presenter), XIAO ZHANG, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — The Bethe-Salpeter equation (BSE) framework is very common for predicting optical and excitonic properties in materials. Typically, only high-frequency electronic dielectric screening is considered in the screened electron-hole Coulomb interaction. In materials hosting polar phonon modes that induce macroscopic electric fields, there is an additional dynamical lattice screening effect. To describe this contribution, we use the Shindo approximation and the Fröhlich model to predict exciton binding energies in NaCl, MgO, AlN, and GaN. Dynamical lattice screening exerts a small influence on the excitonic properties of the high band gap materials NaCl and MgO. In AlN, the predicted exciton binding energy reduces from 145 to 112 meV. In GaN, dynamical lattice screening drastically reduces the exciton binding energy from 52 to 30 meV, in good agreement with experiments. The optical spectra for all compounds are predicted to be in good agreement with experimental spectra under the inclusion of effective dynamical lattice screening, and we find that it is a critical contributor to the screened electron-hole interaction in polar materials with low exciton binding energies and high longitudinal optical phonon frequencies.

*Funding from National Science Foundation (NSF) DMR1555153


TOMMASO FRANCESE (Presenter), University of Chicago, FRANCOIS GYGI, University of California Davis, GIULIA GALLI, University of Chicago — Thermally activated delayed fluorescence compounds (TADFs) are a class of purely organic light emitting diodes\[1\] based on reverse intersystem crossing processes. Despite the successful synthesis of blue/green TADF compounds, the search for efficient orange-red fluorescent TADFs remains an open problem. NAI-DMAC\[2\] \([C_{37}H_{32}N_2O_2]\) is one of the few orange-red light emitters with an external quantum efficiency of ~ 30%. Here we present a first principle study of NAI-DMAC both in the dilute and solid state limit. We carried out First-Principles Molecular Dynamics simulations with the Qbox code (http://qboxcode.org) at different temperatures and computed ground to excited state transitions by employing range-separated hybrid functionals\[3\], as well as the SCAN functional\[4\]. We present results for the energy difference between singlet and triplet excited states (\(\Delta E_{ST}\)), and we discuss how \(\Delta E_{ST}\) is related to structural differences in the ground and excited states, in particular to the dihedral angle between the donor and acceptor moieties.


*MURI Project (N00014-19-1-2453)*
1:51PM G39.00012: Predictive and Tractable GW Approach for Energy Level Alignment at Organic-Inorganic Interfaces with Significant Charge Transfer*  
NICHOLAS LIN QUAN CHENG (Presenter), FENGYUAN XUAN, SU YING QUEK, Natl Univ of Singapore — The energy level alignment (ELA) at organic-inorganic interfaces is critical for determining charge injection barriers in organic and molecular electronic devices. Many-body perturbation theory in the GW approximation enables the quantitative prediction of ELA in many systems, but can be computationally challenging for large interfaces. We have recently developed an approach [1] to perform GW calculations on large interface systems, which involves the expansion of the polarizability (chi) matrix from a unit cell to the supercell, the addition of chi from the two subsystems, and the use of wavefunctions from the Full interface to compute the self-energies. This XAF-GW method has been shown to work even in the presence of interface hybridization to form bonding and antibonding orbitals. Here, we show that the XAF-GW method fails in some cases with significant interface charge transfer. We modify the XAF-GW approach to specifically account for charge transfer effects, and obtain good agreement between the modified XAF-GW method and a regular full GW calculation for F4TCNQ on bilayer graphene. We further discuss the application of our new approach to other experimentally relevant systems.


*This work is funded by grant MOE2016-T2-2-132.

2:03PM G39.00013: Electronic structure of semiconductor nanoparticles from stochastic evaluation of imaginary-time path integral: nonrelativistic U(1) lattice gauge theory in the Kohn-Sham basis  
ANDREI KRYJEVSKI (Presenter), North Dakota State Univ — In the Kohn-Sham orbital basis imaginary-time path integral for electrons in a semiconductor nanoparticle has a mild fermion sign problem and is, therefore, amenable to evaluation by the standard stochastic methods. Utilizing output from the density functional theory simulations with Perdew, Burke and Ernzerhof exchange-correlation functional we compute imaginary-time electron propagators in several silicon hydrogen-passivated nanocrystals, such as Si_{35}H_{36}, Si_{87}H_{76} and Si_{147}H_{100}, and extract energies of low-lying electron and hole levels. Our quasiparticle gap predictions agree with the results of recent G\textsubscript{0}W\textsubscript{0} calculations from M. Govoni, G. Galli, “Large Scale GW Calculations”, J. Chem. Theory Comp., 11 (2015).

Tuesday, March 3, 2020 11:15 AM - 2:03 PM

Session G40 DCOMP DMP: Matter in Extreme Environments I: Advanced Experiments 705 - Xiaoyu Wang - Tag(s): Focus
Despite being the subject of numerous shock compression studies, the behavior of silicon under dynamic loading is vigorously debated [1-4]. The few studies that combine shock compression and X-ray diffraction have exclusively focused on "normal" X-ray geometry whereby X-rays are collected along the shock propagation direction, consequently sampling numerous strain states at once, and hence greatly complicating both phase identification and studies of phase transition kinetics.[5] Here, we present a novel setup to perform in situ X-ray diffraction studies perpendicular to the shock propagation direction at the Matter in Extreme Conditions end station at Linac Coherent Light Source, SLAC. Combining the extremely bright, micro-focused X-ray beam available at the LCLS with a nanosecond laser driver, we unambiguously characterize of the complex multi-wave shock response in silicon for the first time. We further combine this platform with simultaneous imaging with diffraction from shock compressed germanium.

Reference
[3] Colburn et al., JAP, 43, 5007 (1972)

*E.E.M and A.S. acknowledge funding from the Volkswagen Foundation. J.S.W. is grateful for support from EPSRC under grant EP/J017256/1. This work is supported by the French Agence Nationale de la Recherche (ANR) with the ANR IRONFEL 12-PDOC-0011. Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515. The MEC instrument is supported by the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under contract No. SF00515.
11:51AM G40.00002: Laser shock induced insulator-metal transition in quasi-one dimensional single-component radical

YONG HU (Presenter), SHENQIANG REN, State Univ of NY - Buffalo — Laser shock is a relatively new surface treatment for high pressure study[1]. The shock waves can create over one hundred GPa transient shock pressure[2]. Here we found the laser shock induced revisable insulator-metal transition in single-component radical, K-TCNQ[3], where the effect of antiferromagnetic spin ordering causes insulating behavior. The manipulation of spin exchange interaction with external laser shock wave, electric field and magnetic field is accompanied by insulator to metal transition, gigantic magnetoelectric and magneto capacitance effects. One dimensional systems therefore provide a new area to search for conducting magnetoelectric media.


*Work at the University at Buffalo (S.R.) was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Award DE-SC0018631 (Physical properties of molecular electronic crystals). The U.S. Army Research Office supports S.R. under Award W911NF-18-2-0202 (Self-assembly of organic crystals).

12:03PM G40.00003: Overview of High Pressure Collaborative Access Team (HPCAT) facility at the Advanced Photon Source at Argonne National Laboratory

NENAD VELISAVLJEVIC (Presenter), Lawrence Livermore Natl Lab, MADDURY SOMAYAZULU, HPCAT, APS, X-ray Science Division Argonne National Laboratory — HPCAT is a dedicated facility for high pressure research and is located within the Advanced Photon Source. Goal of HPCAT is to develop and implement synchrotron-based x-ray techniques that are coupled with diamond anvil cell, portable large volume press, and other platforms for studying materials at extreme pressure-temperature conditions.

Comprised of four simultaneously operational beamlines, HPCAT is the largest dedicated high-pressure synchrotron-based facility in the world and provides broad range of cutting-edge x-ray techniques, as well as complementary high-pressure support equipment. Over the years numerous high-pressure x-ray diffraction, spectroscopy, and imaging techniques have been developed and established for high pressure research through a robust national laboratory and university partnership, and broad general user operation.

Currently, HPCAT has two insertion device beamlines, one for diffraction and the other for spectroscopy, and two bending magnet beamlines, one for general purpose and the other for white-beam application. Our presentation will provide overview of HPCAT and recent experimental techniques being developed.

*HPCAT operations are supported by DOE-NNSA's Office of Experimental Sciences.
12:15PM G40.00004: Crystal Structure and Reflectivity of Laser Ramp-Compressed Sodium*

[Invited] DANAE POLSIN (Presenter), XUCHEN GONG, LINDA CRANDALL, MARGARET F HUFF, THOMAS BOEHLY, GILBERT W COLLINS, JAMES R RYGG, University of Rochester, JON HENRY EGGERT, AMY JENEI, MARIUS MILLOT, Lawrence Livermore National Laboratory, MALCOLM I McMAHON, University of Edinburgh — Extreme compression can alter the free-electron behavior of “simple” metals such as sodium. At pressures exceeding 200 GPa, Na was observed to become transparent to visible light under static compression. First-principles calculations suggest this is caused by a transformation to an electride phase where electrons are localized in interstitial positions. Laser-driven ramp compression is used to compress Na into an unexplored pressure regime to investigate the crystalline structure, reflectivity, and melting behavior. X-ray diffraction is used to constrain the crystalline structure and detect melting. Optical reflectivity measurements at 532 nm are used to detect a transition to the observed insulating electride phase. We show the highest-pressure solid x-ray diffraction and reflectivity data on Na to date. The results indicate the Na phase diagram is more complicated than predicted by zero-temperature DFT.

*This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856.

12:51PM G40.00005: Neutron Scattering Research on Quantum Materials under Pressure*

ANTONIO DOS SANTOS (Presenter), Oak Ridge National Lab — Quantum Materials are characterized by an extreme sensitivity to weak external perturbations (H, E, P). Among these, pressure is unique in that, even in a moderate range, it induces structural changes energetically equivalent to thousands of K. In addition, samples subjected to pressure do not suffer from chemical segregation or disorder, characteristic of chemical manipulation. In this context, neutron scattering, with its ability to inspect simultaneously the lattice and spin degrees of freedom, while not depositing any energy, is uniquely suitable for the study of quantum systems. Instruments at modern neutron sources, such as the spallation neutron source, are now fitted with custom made pressure devices, that extend the realm of the possible in neutron scattering of the quantum world. Indeed, the range of pressure, temperature and field available, allow faster measurements on smaller samples. Here we will present the current suite of instrumentation available to research of quantum materials at the SNS, including new developments in instrumentation and pressure devices. These advances will be illustrated with science examples that benefited from these new capabilities.

**1:03PM G40.00006: Magnetic Structure of the High-Pressure Phases of Holmium**

CHRISTOPHER PERREAULT (Presenter), YOGESH VOHRA, Department of Physics, Univ of Alabama - Birmingham, ANTONIO MOREIRA DOS SANTOS, JAMIE MOLAISON, Neutron Scattering Division, Oak Ridge National Laboratory — The magnetic phases in rare earth metals are well established under ambient pressure conditions, however, little is known about the magnetic ordering in their corresponding high pressure crystalline modifications. Holmium (Ho) was studied in a large-volume diamond anvil cell at the Spallation Neutron Source to 20 GPa and 10 K. The ambient pressure hexagonal close packed phase (hcp) of holmium shows two magnetic transitions below 10 GPa one to Antiferromagnetic (AFM) incommensurate phase and another to a Ferromagnetic (FM) phase. At pressures above 10 GPa, Ho transforms to the alpha-Samarium (α-Sm) phase which shows only one transition marked by appearance of a magnetic peak at 3 Å below 20 K that is more intense than the nuclear peaks. This magnetic order remains even when pressure is increased past 19 GPa where the sample again transforms, this time to the double hexagonal close packed (dhcp) phase. The magnetic ordering temperature increases with pressure from below 20 K at 15 GPa to around 25 K at 20 GPa. The magnetic phase diagram of Ho is presented to 20 GPa and 10 K.

*Supported by DOE Award DE-NA-0003916. A portion of this research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.*

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**1:15PM G40.00007: Lattice Dynamics of Highly Porous Materials**  
MATTHEW RYDER (Presenter), Oak Ridge National Lab — Highly porous materials such as MOFs, COFs and HOFs have been shown to have promising electronic and dielectric properties. However, high levels of porosity often couple with low structural stability. Therefore, the collective lattice dynamics reveal a diversity of valuable information relating to the structural flexibility and the mechanistic origins of anomalous mechanical phenomena. Spectroscopic techniques such as inelastic neutron scattering (INS), in conjunction with DFT, are used to study the phonon mode dynamics, including those related to gate opening and breathing, trampoline-like mechanisms and molecular rotors reminiscent of negative thermal expansion (NTE), and buckling of 2D layers. The work has also revealed the effect of external stimuli (pressure and temperature) and shown stimuli-induced phase transitions and amorphization.

8. CrystEngComm, 18, 4303 (2016)  
Mechanochemical activation by high-energy milling has become a widely used method for solid state synthesis, and alternative to high-temperature processes. It has been successfully used for synthesis of crystalline and amorphous alloys, intermetallic compounds, metastable phases, nanomaterials and metal-ceramic composites. Mechanochemical synthesis utilizes high-energy impact phenomena to initiate chemical reactions or structural phase transitions. The peak impact pressures which the individual sample particles experience vary depending on the type of mill, milling speed, as well as size, shape and density of the attritor components, but can reach 20 GPa, while the temperature typically remains below 100°C. Remarkably, this is achieved with significant sample quantities (grams), over a short period of time, and very inexpensively. Whereas mechanisms and kinetics of solid-state reactions induced by temperature or static pressure are fairly well understood, transformations of materials under continuous impact in a milling assembly remain largely unexplored and are based almost exclusively on ex situ studies. During the mechanical activation particles undergo heavy deformation and experience significant strains. This results in formation of a variety of crystal defects such as dislocations, vacancies, stacking faults and increased number of particle boundaries, making the milled material energetically less stable. An on-going project at the PX² synchrotron beamline will adapt the in situ real-time X-ray diffraction monitoring of structural and chemical changes during the milling process. This presentation will also introduce a new project to develop more economical mechanochemical paths towards synthesis of the cubic phase of boron nitride.

*Funding from ONR MI/HBC program and COMPRES under NSF Cooperative Agreement EAR-1661511 is gratefully acknowledged.

Tuesday, March 3, 2020 11:15 AM - 2:03 PM

Session G41 GMAG: Magnetic Characterization and Imaging 707 - Cosmin Radu, Lake Shore Cryotronics (United States) - Tag(s): Focus
11:15AM G41.00001: Optical characterization of in-plain spin texture in 10-nm-scale Neel-type magnetic domain wall

DONGHA KIM (Presenter), KAB-JIN KIM, MIN-KYO SEO, KAIST — We present that dark-field longitudinal magneto-optical Kerr effect (MOKE) microscopy can visualize the in-plain spin texture of the subwavelength-scale Neel-type magnetic domain wall. Conventional MOKE microscopy has never resolved the spin texture at the nanoscale due to not only the optical diffraction limit but also extremely small magneto-optic (MO) susceptibility. The dark-field illumination isolates the MOKE signal of the domain wall from those of the magnetic domains effectively with a high signal-to-background ratio. Also, we employed a perfect optical absorption multilayer to vanish the non-MO signals dramatically and boost the measurement efficiency. We examined the Neel-type magnetic domain wall of the Pt/Co/Pt/Ta film and measured its MO scattering width to be ~9.14 pm, experimentally. The intensity of the longitudinal MOKE signal from the domain wall depends on the orientation of in-plane magnetization relative to the azimuthal angle of incidence. Angle-dependent, precise measurement of the longitudinal MOKE scattering enables us to identify spatial magnetization distribution along the 10-nm-scale magnetic domain wall. We expect our work will offer a new possibility in research on complex in-plane spin textures such as vertical Bloch lines and skyrmions.

11:27AM G41.00002: Microsphere-assisted super-resolution magneto-optic imaging

MICHAEL VOGEL (Presenter), Argonne Natl Lab, ARTHUR HENDRIKS, Department of Applied Physics, Eindhoven University of Technology, SUZANNE TE VELTHUIS, AXEL HOFFMANN, Argonne Natl Lab — The diffraction limit [1] is a fundamental barrier in optical imaging. It can be surpassed by the photonic nanojet phenomenon, generated by a lens-like dielectric micro-object [2]. Microspheres have been demonstrated as a powerful platform to challenge the diffraction limit by creating a virtual image with enhanced resolution and magnification [3,4]. Here we report on wide-field MOKE (Magneto-Optical Kerr effect) measurements harnessing this resolution enhancement. In-plane and perpendicular magnetized domains, probed with the longitudinal and polar Kerr effects, respectively, are imaged at increase spatial resolution. Our findings may serve as a way to combine the advantages of fast time resolution and versatile sample environment of optical measurements with smaller length scales.

[1] Lord Rayleigh, Philosophical Magazine Series 5, 8(49):261–274 (1879)

*Work at Argonne was supported by the US-DOE, Office of Science, MSED. Use of the Center for Nanoscale Materials was supported by the US-DOE, Office of Science, BES, under contract no. DE-AC02-06CH11357.
Magnetic Resonance Imaging* YOUNG JIN KIM (Presenter), IGOR M SAVUKOV, Los Alamos Natl Lab — Magnetic resonance imaging (MRI) in the ultra-low field (ULF) regime is a promising method for anatomical imaging with multiple advantages over conventional several-Tesla MRI. The leading high-sensitivity multichannel ULF MRI was realized only with multichannel superconducting quantum interference devices (SQUIDs); however, the need for cryogenic infrastructure is a serious drawback. We aim to develop an alternative, more practical ULF MRI based on a high-sensitivity multichannel atomic magnetometers (AMs) and multiple flux transformers (FTs). AMs are currently the most sensitive non-cryogenic magnetic-field sensors. Our approach represents the first ULF MRI implementation using the novel technique, which has many innovative features such as acceleration of MRI, a large array of sensors based on a single large atomic vapor cell, reducing the cost of sensors ~10 times, and flexible design based on FTs. In this talk, we will describe the basic principle and the design of our ULF MRI system.

*We acknowledge the support of the U.S. Department of Energy through the LANL Laboratory Directed Research Development program for this work
Ionically-controlled phase separation in cobaltite heterostructures

[Invited] GEOFFERY RIPPY, LACEY L TRINH, ALEXANDER MICHAEL KANE, ALEKSEY IONIN, MICAHEL LEE, University of California, Davis, RAJESH V CHOPDEKAR, Lawrence Berkeley National Laboratory, JOYCE CHRISTIANSEN-SALAMEH, University of California, Davis, DUSTIN GILBERT, University of Tennessee, ALEXANDER GRUTTER, NIST Center for Neutron Research, PEYTON MURRAY, University of California, Davis, MARTIN HOLT, ZHONGHOU CAI, Argonne National Laboratory, KAI LIU, Georgetown University, YAYOI TAKAMURA, ROOPALI KUKREJA (Presenter), University of California, Davis — Complex oxide heterostructures provide access to emergent functional and structural phases which are not present in the bulk constituent materials. Controlling ionic distribution and stoichiometry in complex oxide heterostructures has been utilized to significantly alter and tune the electronic, magnetic, and structural properties. Recently, deposition of a strong oxygen getter on top of an oxide thin film has emerged as a novel way to tailor oxygen stoichiometry and nanoscale functional properties. However, the role played by nanoscale morphology, i.e. phase separation and defects in these oxide thin films and heterostructures remains largely unknown. In this talk, I will focus on Gd/\text{La}_{0.67}\text{Sr}_{0.33}\text{CoO}_3 (LSCO) heterostructures due to the high oxygen ion conductivity, as well as the coupled magnetic and electronic properties of LSCO, which are strongly dependent on the oxygen stoichiometry. This combination of properties enable the ionic control of the functional properties of LSCO thin films through the presence of oxygen getter layers such as Gd. We utilize x-ray nanodiffraction to directly image the nanoscale morphology of LSCO thin films as they are progressively transformed from the equilibrium perovskite phase to the metastable brownmillerite (BM) phase with increasing Gd thickness. Our studies show the coexistence of perovskite and BM phases with a critical oxygen vacancy concentration threshold which leads to the formation of extended BM filaments. Strain maps reveal that the perovskite phase changes from compressive to tensile strain on opposite sides of a BM filament. Our studies provide an unprecedented nanoscale survey of the phase separation in the cobaltites and shed light on the formation of the metastable BM phase.

*University of California Davis, University of California Multicampus Research Programs and Initiatives (Grant No. MR-15-328528) and NSF (ECCS-1611424 and DMR-1905468).
"Magnetic Etch-a-Sketch" using the 1st-order phase transition in FeRh*

ISAIAH GRAY (Presenter), School of Applied and Engineering Physics, Cornell University, ANTONIO B MEI, Department of Materials Science and Engineering, Cornell University, YONGJIAN TANG, Department of Physics, Cornell University, JÜRGEN SCHUBERT, Peter Grünberg Institute (PGI-9) and Jara-Fundamentals of Future Information Technology, Forschungszentrum Jülich, DON WERDER, Cornell Center for Materials Research, Cornell University, JASON M BARTELL, Department of Materials Science and Engineering, Massachusetts Institute of Technology, DANIEL RALPH, Department of Physics, Cornell University, GREGORY FUCHS, School of Applied and Engineering Physics, Cornell University, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University — We demonstrate a novel approach for room-temperature rewritable magnetic patterning using the 1st-order phase transition from antiferromagnet (AF) to ferromagnet (FM) in FeRh. We employ epitaxial Fe$_{0.52}$Rh$_{0.48}$ films designed such that both phases are metastable at room temperature. Starting with the film in a uniform AF state, we write arbitrary patterns of FM phase using a focused pulsed laser with ~650 nm resolution. We image the FM patterns with anomalous Nernst microscopy and show that they are stable under magnetic field – at least up to 3 kOe – as well as elevated temperature up to ~315 K. The FM patterns can be written using a single picosecond laser pulse per pixel and can be fully erased by cooling the film below room temperature.


*This work was supported in part by the Cornell Center for Materials Research with funding from the National Science Foundation MRSEC program (DMR-1719875). This work made use of the Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM), supported by the NSF (No. DMR-1539918), and the Cornell Nanoscale Facility, a member of the National Nanotechnology Coordinated Infrastructure (NNCI) supported by the NSF (Grant No. ECCS-1542081).
**12:39PM G41.00006: Novel sample preparation and detection method for magnetic resonance force imaging of electron spins**

MICHAEL BOUCHER (Presenter), JOHN A MAROHN, Cornell University — Magnetic resonance force microscopy (MRFM) is a technique that opens up the possibility of extremely sensitive detection and imaging of electron spins, with sensitivity capable of detecting a single radical. In our experiment, we detect a change in magnetization of nitroxide radical probes as a shift in the frequency of a magnet-tipped cantilever. We discuss recent developments that have allowed us to overcome difficulties with this measurement. One difficulty is frequency noise from sample dielectric fluctuations interacting with charges on the cantilever tip. We have found that we can reduce this noise by applying a 10 nm metal coating over the sample. However, deposition of this metallic coating produces a “dead layer” in which nitroxide labels are no longer active. We show a new sample preparation technique which applies this coating without exposing sample radicals during metal deposition. Another difficulty is that the motion of the cantilever magnet causes a change in the resonance frequency of spins during the microwave pulses, which leads to image blurring and reduction in sensitivity. We show ways to “pause” cantilever motion during microwave application to prevent blurring and improve sensitivity.

*We acknowledge funding from the Army Research Office Grant W911NF1710247*

**12:51PM G41.00007: NV$^-$ center magnetometry using Bayesian statistics**

SERGEY DUSHENKO (Presenter), KAPILDEB AMBAL, University of Maryland, College Park/National Institute of Standards and Technology, ROBERT MCMICHAEL, National Institute of Standards and Technology — In magnetometry using NV$^-$ centers, we demonstrate order-of-magnitude speed up with Bayesian experimental design as compared to conventional frequency-swept measurements. The NV$^-$ center is a quantum defect with spin 1 and coherence time up to several milliseconds at room temperature. Zeeman splitting of NV$^-$ energy levels allows detection of the magnetic field via photoluminescence. It is an excellent platform for magnetometry with potential spatial resolution down to few nanometers and demonstrated sensitivity down to nT/Hz$^{1/2}$.

We compare conventional magnetic field measurement of fluorescence under pre-determined sweeps of microwave frequency with the measurement using a Bayesian statistics methodology. In the Bayesian experimental design, the frequency of each measurement is determined in real-time from utility predictions based on the accumulated experimental data. We report order of magnitude increase in the precision of magnetic field and hyperfine splitting determination for the same measurement time in the Bayesian scheme, compared with the conventional scheme.

*S.D., K.A. acknowledge support under the Cooperative Research Agreement between the University of Maryland and the National Institute of Standards and Technology, Award 70NANB14H209, through the University of Maryland.*
1:03PM G41.00008: Imaging nanoscale magnetization using scanning-probe magneto-thermal microscopy*  
CHI ZHANG (Presenter), JASON M BARTELL, JONATHAN KARSCH, ISAIAH GRAY, GREGORY FUCHS, Cornell University — High resolution, time-resolved magnetic microscopy is crucial for understanding novel magnetic phenomenon such as skyrmions, spinwaves, and domain walls. Currently, achieving 10-100 nanometer spatial resolution with 10-100 picosecond temporal resolution is beyond the reach of table-top techniques. To break free of the far-field diffraction limit, we have developed a near-field magnetic microscope based on magneto-thermo interactions: the time-resolved anomalous Nernst effect and the time-resolved longitudinal spin Seebeck effect. Our technique involves scanning a sharp gold tip within a near-field optical excitation. The resulting tip-sample interaction creates a nanoscale thermal gradient for magneto-thermal microscopy, and its extension to imaging an applied current density. We study the characteristics of near-field thermal excitation with a picosecond laser and demonstrate magnetic imaging of a multi-domain state. We present sub-100 nm spatial resolution from imaging current density around a nano-constriction. Our results suggest a new approach to nanoscale spatiotemporal magnetic microscopy in an accessible, table-top form to aid in the development of high-speed magnetic devices.

*We acknowledge support from AFOSR (FA9550-14-1-0243)

1:15PM G41.00009: Multi-axis cavity optomechanical torque characterization of magnetic microstructures and the contribution of the Einstein-de Haas effect  
JOSEPH LOSBY (Presenter), GHAZAL HAJISALEM, Univ of Calgary, KAYTE MORI, Physics, University of Alberta, GUSTAVO DE OLIVEIRA LUIZ, Univ of Calgary, VINCENT SAUER, MARK R FREEMAN, Physics, University of Alberta, PAUL BARCLAY, Univ of Calgary — Significant new functionality is reported for torsion mechanical tools aimed at full magnetic characterizations of both spin statics and dynamics in micro- and nanostructures. Specifically, multiple torque directions utilizing higher order mechanical modes are monitored, as is essential for study of anisotropic three-dimensional structures. The approach is demonstrated through application to shape and microstructural disorder-induced magnetic anisotropies in lithographically patterned permalloy, and will have utility for the determination of important magnetic thin-film and multilayer properties including interface anisotropy and exchange bias.

With the extension of torque magnetometry measurements into radio frequencies, the contribution of the Einstein-de Haas (EdH) effect can become comparable to the conventional magnetic cross-product signal. Through sensitive optomechanical detection of higher order mechanical modes, the torques owing to the EdH effect are elucidated, and offer a new method for exploring high frequency magnetic susceptibility in anisotropic structures.
Nano-engineered magnetic materials are of great interest for tuning magnetic interactions and because of their potential applications for next-generation spintronic devices. Nanoscale 3D magnetization textures such as inverse nickel metallaticates can be fabricated by infiltrating close-packed silica nanospheres with nickel. Such structures can support many distinct magnetic phases and topologies, leading to a new class of nanostructured magnetic metamaterials. Despite recent success in theoretical predicting and fabricating these materials, 3D characterization of their structure and properties remains very challenging due to the lack of suitable microscopy tools. We developed a new 3D nanoscale magnetic imaging capability that combines x-ray magnetic circular dichroism, ptychographic imaging, and vector tomography. Using this new magnetic vector ptycho-tomography method on a synchrotron beamline, we imaged a nickel magnetic metallatice sample to unveil the underlying structure and spin texture.

*We gratefully acknowledge support for this work by STROBE: A National Science Foundation Science & Technology Center, under Grant No. DMR 1548924.
1:39PM G41.00011: Scaling of domain cascades in stripe and skyrmion phases*  ARNAB SINGH, Saha Institute of Nuclear Physics, JAMES LEE (Presenter), Sonoma State University, KARINA E. AVILA, University of Illinois, Urbana-Champaign, YUAN CHEN, Lawrence Berkeley National Laboratory, SERGIO MONTOYA, ERIC FULLERTON, University of California, San Diego, PETER FISCHER, Lawrence Berkeley National Laboratory, KARIN ANDREA DAHMEN, University of Illinois, Urbana-Champaign, STEPHEN DOUGLAS KEVAN, Lawrence Berkeley National Laboratory, MILAN K. SANYAL, Saha Institute of Nuclear Physics, SUJOY ROY, Lawrence Berkeley National Laboratory — The origin of deterministic macroscopic properties often lies in microscopic stochastic motion. Magnetic fluctuations that manifest as domain avalanches and chaotic magnetization jumps exemplify such stochastic motion and have been studied in great detail. Here we report Fourier space studies of avalanches in a system exhibiting competing magnetic stripe and skyrmion phase using a soft X-ray speckle metrology technique. We demonstrate the existence of phase boundaries and underlying critical points in the stripe and skyrmion phases. We found that distinct scaling and universality classes are associated with these domain topologies. The magnitude and frequency of abrupt magnetic domain jumps observed in the stripe phase are dramatically reduced in the skyrmion phase. Our results provide an incisive way to probe and understand phase stability in systems exhibiting complex spin topologies.

*U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences: DE-AC02-05CH11231 (ALS, LBNL and MSMAG), and DE-SC0003678; Department of Atomic Energy, India, Raja Ramanna Fellowship.

1:51PM G41.00012: Ultra-Short-Period Undulators for the Next Generation X-ray Free Electron Lasers*  BERKIN GÜREL (Presenter), Faculty of Engineering and Natural Sciences, Sabanci University, OMER POLAT, Faculty of Engineering and Natural Sciences, Bahcesehir University, NILAY GUNDUZ AKDOGAN, Faculty of Engineering, Piri Reis University, OZAN AKDOGAN, Faculty of Engineering and Natural Sciences, Bahcesehir University — There is a growing interest on the compact XFELs to be used in applications such as medical science (surgery, fat removal), material science and military. In order to build a compact XFEL, constructing an undulator with sub-millimeter period ($\lambda_u$) is mandatory. Many problems arise due to miniaturization of undulators; such as keeping the magnetic field high while still having a considerable gap to minimize beam scraping. In this work, RADIA program has been employed for the modeling of sub millimeter period undulators ($20 \, \mu m < \lambda_u < 400 \, \mu m$) with three different magnet configuration; namely Up-Down ($\uparrow\downarrow\uparrow\downarrow\ldots$), Halbach (Wiggler) ($\uparrow\downarrow\uparrow\downarrow\leftarrow\uparrow\ldots$) and Hybrid ($\rightarrow\uparrow\leftarrow\downarrow\rightarrow\ldots$). Effects of sub-millimeter undulator period and gap on the magnetic field pattern of the undulator have been discussed.

*This work was supported by TUBITAK project: 118F319

Tuesday, March 3, 2020 11:15 AM - 2:15 PM
11:15AM G42.00001: Topological Magnetic-Spin Structures in Two-Dimensional Van Der Waals Cr$_2$Ge$_2$Te$_6^*$

MYUNG-GEUN HAN (Presenter), JOSEPH GARLOW, YU LIU, Brookhaven National Laboratory, HUIQIN ZHANG, Department of Electrical and System Engineering, University of Pennsylvania, DONALD DIMARZIO, MARK KNIGHT, NG Next, Northrop Grumman Corporation, CEDOMIR PETROVIC, Brookhaven National Laboratory, DEEP JARIWALA, Department of Electrical and System Engineering, University of Pennsylvania, YIMEI ZHU, Brookhaven National Laboratory — Long-range ferromagnetic order down to atomic layers provides an important degree of freedom in engineering two-dimensional (2D) materials and their heterostructure devices for spintronics, valleytronics and magnetic tunnel junction switches. Using direct imaging by cryo-Lorentz transmission electron microscopy we report that topologically nontrivial magnetic-spin states, skyrmionic bubbles, can be realized in exfoliated insulating 2D van der Waals Cr$_2$Ge$_2$Te$_6$. Due to the competition between dipolar interactions and uniaxial magnetic anisotropy, hexagonally-packed nanoscale bubble lattices emerge in the $ab$ plane by field cooling. Despite a range of topological spin textures arising due to pair formation and annihilation of Bloch lines, bubble lattices with single chirality are prevalent. Our observation of topologically-nontrivial homochiral skyrmionic bubbles in exfoliated vdW materials provides a new avenue for novel quantum states in atomically-thin insulators for magneto-electronic and quantum devices.

*This work was supported by the US Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division (Contract No. DE-SC0012704).
11:27AM G42.00002: Multiple ferromagnetic transitions and structural distortion in the van
der Waals ferromagnet VI₃ at ambient and finite pressures*  ELENA GATI (Presenter), YUJI
INAGAKI, Iowa State University, Ames Laboratory, TAI KONG, ROBERT J. CAVA, Princeton University, YUJI
FURUKAWA, SERGEY L. BUD’KO, PAUL C CANFIELD, Iowa State University, Ames Laboratory —
Magnetic van-der-Waals (vdW) materials are considered as promising candidate systems to
realize low-dimensional ferromagnetism in semiconductors. Here, we present a thermodynamic
(specific heat and magnetization) and microscopic NMR study on bulk single crystals of the
recently discovered ferromagnetic vdW material VI₃ at ambient and finite pressures [1]. Our
results show that VI₃ undergoes a structural transition, which is subsequently followed by two
ferromagnetic transitions at ambient pressure, giving rise to two distinct magnetically-ordered V
sites for low temperatures. Upon increasing pressure, the two magnetic transitions merge at p ~
0.6 GPa, and for even higher pressures (p ~ 1.25 GPa) merge with the structural transition. From
these observations, we infer that the magnetic structure in bulk single crystals of VI₃ is complex,
with magnetoelastic coupling being of significant importance.

*This work was carried out at Iowa State University and supported by Ames Laboratory, US DOE,
under Contract No. DE-AC02- 07CH11358. Work conducted at Princeton University was supported
by the NSF-sponsored PARADIGM program centered at Cornell University, Grant No. DMR-
1539918.

11:39AM G42.00003: First principles Calculation of Dzyaloshinskii–Moriya interaction in 2D
magnetic van der Waals heterostructures   KAI HUANG (Presenter), DING-FU SHAO, EVGENY Y
TSYMBAL, University of Nebraska - Lincoln — Magnetic skyrmions are nanoscale spin textures
promising for next-generation spintronic applications. Recent studies have demonstrated that
skyrmions can be generated at the interface between a ferromagnetic layer and a nonmagnetic
heavy-metal-based layer due to a large Dzyaloshinskii–Moriya interaction (DMI) induced by
broken inversion symmetry and strong spin-orbit coupling. This usually requires multilayer
heterostructures with sizable thickness, which limit the nanoscale application. Recent discoveries
of two-dimensional (2D) magnets and the related van der Waals heterostructures offer the
possibility for skyrmions to emerge at the atomic scale layer thickness. Here, we predict the
emergence of a large DMI in bilayer magnetic van der Waals heterostructures composed of a 2D
ferromagnetic metal Fe₃GeTe₂ monolayer and a nonmagnetic monolayer. Based on first-
principles density functional theory calculations, we find that the DMI, the exchange coupling,
and the magnetic anisotropy of the magnetic van der Waals heterostructures can be modulated
by the interfacial proximity effect, leading to the tunable skyrmion behaviors. Our work indicates
the 2D magnetic van der Waals heterostructures are promising platforms for the skyrmion-based
spintronics.
11:51AM G42.00004: Realization of very large Dzyaloshinskii-Moriya interaction and skyrmion states in two-dimensional Janus manganese dichalcogenides* JINGHUA LIANG
(Presenter), Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, WEIWEI WANG, HAIFENG DU, High Magnetic Field Laboratory, Chinese Academy of Sciences and University of Science and Technology of China, MAIRBEK CHSHIEV, Univ. Grenoble Alpes, CEA, CNRS, Spintec, ALBERT FERT, Unité Mixte de Physique, CNRS, Thales, University Paris-Sud, University Paris-Saclay, HONGXIN YANG, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences — The Dzyaloshinskii-Moriya interaction (DMI), which only exists in noncentrosymmetric systems, is responsible for the formation of exotic chiral magnetic states. However, it is absent in most theoretically predicted and experimentally confirmed two-dimensional (2D) magnetic thin films so far. In this report, we perform first-principles calculations to demonstrate that significant DMI can be obtained in a series of Janus monolayers of manganese dichalcogenides MnXY (X/Y = S, Se, Te, X ≠ Y) in which the difference between X and Y on the opposites sides of Mn breaks the inversion symmetry. In particular, the DMI amplitudes of MnSeTe and MnSTe are comparable to those of state-of-the-art ferromagnet/heavy metal (FM/HM) heterostructures. Moreover, by performing Monte Carlo simulations, we find that the MnSeTe and MnSTe monolayers can host stable skyrmion states with the application of a moderate external magnetic field. The present results pave the way for new device concepts utilizing chiral magnetic structures in specially designed 2D ferromagnetic materials.

*We acknowledge the from the NNSF of China (11874059), Zhejiang Province NNSF of China (LR19A040002), and Horizon 2020 Research and Innovation Programme under grant agreement no. 785219 (Graphene Flagship).

12:03PM G42.00005: Topological Spin Textures in Janus Monolayers of Chromium Trihalides Cr(I,X)₃* CHANGSONG XU (Presenter), Univ of Arkansas-Fayetteville, JUNSHENG FENG, School of Physics and Materials Engineering, Hefei Normal University, YOUSRA NAHAS, SERGEI PROHORENKO, Univ of Arkansas-Fayetteville, HONGJUN XIANG, Physics, Fudan University, LAURENT BELLAICHE, Univ of Arkansas-Fayetteville — Topological magnetic states are promising for ultra-dense memory and logic devices. Recent progresses in two-dimensional magnets encourage the idea to realize topological states, such as skrmions and merons, in freestanding monolayers. However, monolayers such as CrI₃ lack Dzyaloshinskii-Moriya interactions (DMI) and thus do not naturally exhibit skyrmions/merons but rather a ferromagnetic state. Here we propose the fabrication of Cr(I,X)₃ Janus monolayers, in which the Cr atoms are covalently bonded to the underlying I ions and top-layer Br or Cl atoms. By performing first-principles calculations and Monte-Carlo simulations, we identify strong enough DMI, which leads to not only helical cycloid phases, but also to topologically nontrivial states, such as the intrinsic domain wall skyrmions in Cr(I,Br)₃ and the magnetic-field-induced bimerons in Cr(I,Cl)₃. Microscopic origins of such spin textures are revealed as well.

*DOE ER-46612 and an Impact Grant from Arkansas Research Alliance.DARPA Grant No. HR0011727183-D18AP00010 (TEE Program). ARO grant W911NF-16-1-0227. NSFC (11825403), 2015CB921700, Eastern Scholar, Qing Nian Ba Jian Program, and Fok Ying Tung Education Foundation. 1908085MA10.
12:15PM G42.00006: Electrical excitation of superfluid- and string-like domain wall modes in layered van der Waal antiferromagnets*  MOHAMMAD MUSHFIQUR RAHMAN (Presenter), AVINASH RUSTAGI, Electrical and Computer Engineering, Purdue University, YAROSLAV TSERKOVNYAK, Physics & Astronomy, University of California, Los Angeles, PRAMEY UPADHYAYA, Electrical and Computer Engineering, Purdue University — Efficient excitation of magnons (collective spin excitation in magnetically ordered materials) has been a limiting factor in designing low-dissipation magnonic devices. The recent emergence of low-dimensional van der Waal magnets [such as CrI3] with demonstrated electrical control of magnetic order [Nature Mat. 17, 406 (2018)] opens up new opportunities in the field of magnonics. Motivated by these developments, we theoretically demonstrate the electrical excitation of superfluid- and string-like modes harbored by the antiferromagnetically coupled domain walls of bilayer CrI3. Furthermore, we show that dc magnetic fields provide a handle for selectively exciting the mode of choice.

*We acknowledge NSF grant ECCS 1810494

12:27PM G42.00007: Merons in Monolayer CrCl₃*  XIAOBO LU (Presenter), RUIXIANG FEI, LI YANG, Washington University, St. Louis — Noncollinear spin textures in low-dimensional magnetic systems such as skyrmions, magnetic bobbles and merons have been studied for decades with their extraordinary properties derived from their chirality and topological nature. Here, using first principles and Monte Carlo simulations, we propose that monolayer chromium chloride (CrCl₃) can be a promising candidate to observe paired magnetic vortex type and antivortex type topological defects, which are so-called merons. Through this paper, we demonstrate the existence of vortex and antivortex type meron pairings within the low temperature range (below 5K). Moreover, higher-order combinations of those meron pairs which are similar to the “quadrupole” excitations are also identified. Finally, including the in-plane and out-of-plane external magnetic field, we show the robustness of merons’ pairing and a rich phase space to tune the hybridizations between the ferromagnetism and meron excitations.

*The work at WUSTL are supported by the National Science Foundation (NSF) CAREER Grant No. DMR-1455346 and the Air Force Office of Scientific Research (AFOSR) grant No. FA9550-17-1-0304. The computational resources have been provided by the Stampede of TeraGrid at the Texas Advanced Computing Center (TACC) through XSEDE.
12:39PM G42.00008: Anomalous spin-Hall effect in 2D Cr-based materials* YURI DAHNOVSKY, ANDREI S. ZADOROZHNYYI (Presenter), Univ of Wyoming — We study the THE in various systems on 2D magnetic materials (CrI$_3$, CrCl$_3$, and CrBr$_3$). From the estimations a skyrmion size is about 30-40 nm. The computations of a spin Hall effect and magnetoresistance require the calculations of the nonequilibrium distribution function, which we will determine from the kinetic Boltzmann equation. The distribution function describes by a 4 × 4 matrix because of different spin projections and the spin-dependent momenta of conducting electrons. The matrix elements contain various parameters such as effective masses, exchange constants, etc., that will be found from the first principle calculations. The reason why such system exhibit topological Hall effect is because the scattering transition probability matrix has an antisymmetric part with respect to the scattering angle. The scattering asymmetry acts as an effective magnetic field, which sign can be either the same for both spin projections of an incident electron, hence leading to a topological charge Hall effect, or opposite for different electron spin projections, leading to the topological spin Hall effect.

*We acknowledge a grant (No. DE-SC0020074 from the US Department of Energy

12:51PM G42.00009: Skyrmions in TMD-based antiferromagnetic triangular lattices* ALDO RAELIARJAONA (Presenter), WUZHANG FANG, University of Nebraska - Lincoln, PO-HAO CHANG, Physics, University of Texas at El Paso, KIRILL BELASHCHENKO, ALEXEY KOVALEV, University of Nebraska - Lincoln — We study the adsorption of magnetic transition metal atoms (Cr, Mn, Fe, and Co) on top of a TMDs such as MoS2 or WSe2, where the transition metal atoms form a triangular lattice. We conducted Monte Carlo simulations and analytical studies to obtain and characterize the magnetic ground state and determine the phase diagram for systems with AFM triangular lattice. The Heisenberg exchange parameters, single-ion anisotropy constants, and Dzyaloshinskii-Moriya vectors were extracted from first-principles density functional calculations. We found that without external magnetic field spirals are the most stable textures. Furthermore, we demonstrate the possibility of stabilizing antiferromagnetic skyrmion lattices living on 3 sublattices in such system under the influence of an external magnetic field.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0014189.
Magnetically coupled nanomagnets have many potential applications including non-volatile memories, logic gates and sensors. In order to realize functional 2-D networks of coupled nanoscale magnetic elements such as those used for nanomagnet logic [1] and artificial spin ice [2], it is desirable to engineer effective lateral magnetic couplings in a controllable way. Up to now, this has been achieved by exploiting the long-range dipolar interaction. However, the dipolar interaction is non-local and scales inversely with the magnet volume, so limiting its use in applications involving nanometer sized structures and thin films. In this work, we demonstrate an alternative method to control the lateral coupling between adjacent magnetic nanostructures [3] based on the interfacial Dzyaloshinskii-Moriya interaction (DMI). In particular, we have patterned regions with in-plane (IP) and out-of-plane (OOP) magnetic anisotropy in a magnetic element using selective oxidation of Pt/Co/Al films, and the magnetization in the OOP and IP parts of the islands are chirally coupled via DMI arising from the Pt underlayer, giving either $\downarrow \rightarrow$ or $\uparrow \leftarrow$ configurations.

We have exploited this concept for various applications. For example, we have created stable synthetic lateral antiferromagnets, skyrmions with different numbers of IP rings and artificial spin ices based on a square lattice and kagome lattice. In addition, we have demonstrated field-free current-induced switching between multistate magnetic configurations in the chirally coupled thin-film nanomagnets via spin-orbit torques. Our work therefore provides a platform to design tailor-made arrays of correlated nanomagnets with a future perspective to achieve all-electric control of planar logic gates and memory devices.

**1:39PM G42.00011: Tuning Magnetic Order with Iron Intercalation in Transition Metal Dichalcogenides**  
CAOLAN JOHN (Presenter), Physics, Massachusetts Institute of Technology, SPENCER DOYLE, Physics, Harvard University, ERAN MANIV, JAMES ANALYTIS, Physics, University of California, Berkeley — The transition metal dichalcogenides are a class of two-dimensional materials currently under intense research due to their attractive electronic properties. Through the process of intercalation, magnetic atoms can be inserted between the layers of these materials to introduce long range magnetic order, enabling exploration of magnetism in these systems. I will present magnetization and thermodynamic measurements that indicate antiferromagnetic order in iron intercalated NbS$_2$. Crucially, we can use intercalation to control the strength of an emergent spin glass state below intercalation values of $x = 1/3$ in Fe$_x$NbS$_2$. The cooperation between this glassy phase and the antiferromagnetic order allow for the generation of substantial bias fields in the system.

*Caolan John was supported by the Haas Scholars Program and by the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant GBMF4374

**1:51PM G42.00012: Electrical switching in a magnetically intercalated transition metal dichalcogenide**  
ERAN MANIV (Presenter), NITYAN NAIR, CAOLAN JOHN, SPENCER DOYLE, JOSEPH ORENSTEIN, JAMES ANALYTIS, physics, University of California, Berkeley — Advances in controlling the correlated behavior of transition metal dichalcogenides have opened a new frontier of many-body physics in two dimensions. A field where these materials have yet to make a deep impact is antiferromagnetic spintronics – a relatively new research direction promising technologies with fast switching times, insensitivity to magnetic perturbations, and reduced crosstalk. Here, we present measurements on the intercalated TMD Fe$_{1/3}$NbS$_2$ which exhibits antiferromagnetic ordering below 42K. We find that remarkably low current densities of order $10^4$ A/cm$^2$ can reorient the magnetic order, which can be detected through changes in the sample resistance, demonstrating its use as an electronically-accessible antiferromagnetic switch. Fe$_{1/3}$NbS$_2$ is part of a larger family of magnetically intercalated TMDs, some of which may exhibit switching at room temperature, forming a platform from which to build tunable antiferromagnetic spintron devices.

*This work was supported as part of the Center for Novel Pathways to Quantum Coherence in Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.
2:03PM G42.00013: Evidence for a pressure-induced gapped spin-liquid ground state in a coupled ladder antiferromagnet \( \text{C}_9\text{H}_{18}\text{N}_2\text{CuBr}_4 \)†

TAO HONG (Presenter), Oak Ridge National Lab, TAO YING, Harbin Institute of Technology, QING HUANG, University of Tennessee, Knoxville, SACHITH DISSANAYAKE, Duke University, YIMING QIU, National Institute of Standards and Technology, MARK M TURNBULL, Clark University, ANDREY PODLESNYAK, YAN WU, HUIBO CAO, DAVID TENNANT, Oak Ridge National Lab, KAI SCHMIDT, Universität Erlangen-Nürnberg, STEFAN WESSEL, RWTH Aachen University — Here we present a comprehensive neutron scattering study on a spin-1/2 coupled ladder antiferromagnet \( \text{C}_9\text{H}_{18}\text{N}_2\text{CuBr}_4 \) (DLCB for short) under applied hydrostatic pressure. In DLCB, the inter-ladder coupling is sufficiently strong to drive the system to the long-range antiferromagnetic ordering phase below \( T_N=2 \) K [1]. Analysis of the spin Hamiltonian suggests that DLCB is close to the quantum critical point in two dimensions at ambient pressure and zero field [2]. Single-crystal neutron diffraction measurements under pressure suggest that the magnetic order breaks down above a critical pressure \( P_c \sim 1.0 \) GPa. By contrasting with quantum Monte Carlo calculations of the dynamic structure factor, the follow-up inelastic neutron scattering study above \( P_c \) reveals evidence of a gapped spin-liquid phase with the \( Z_2 \) topological order, characterized by excitation spectra of fully gapped visons and deconfined spinons.

References:

*This research used resources at the High Flux Isotope Reactor and Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory (ORNL).

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G43 DCOMP DAMOP DCMP: Precision Many-Body Physics IV: Novel Methods and Algorithms 702 - Evgeny Kozik, Kings Coll - Tag(s): Focus
11:15AM G43.00001: The variational and diagrammatic quantum Monte Carlo approach to the many-electron problem* [Invited] KUN CHEN (Presenter), KRISTJAN HAULE, Rutgers University, New Brunswick — Two of the most influential ideas developed by Richard Feynman are the Feynman diagram technique and his variational approach. Here we show that combining both, and introducing a diagrammatic quantum Monte Carlo method, results in a powerful and accurate solver to the generic solid state problem, in which a macroscopic number of electrons interact by the long-range Coulomb repulsion. We apply it to the quintessential problem of solid state, the uniform electron gas, which is at the heart of the density functional theory success in describing real materials, yet it has not been adequately solved for over 90 years. Our method allows us to calculate numerically exact momentum and frequency resolved spin and charge response functions. This method can be applied to a number of moderately interacting electron systems, including models of realistic metallic and semiconducting solids.

*This work is supported by the Simons Collaboration on the Many Electron Problem and NSF DMR-1709229.

11:51AM G43.00002: Modern diagrammatic many body techniques.* [Invited] RICCARDO ROSSI (Presenter), Simons Foundation, FEDOR SIMKOVIC, MICHEL FERRERO, Ecole Polytechnique — In this talk I will discuss recent progress on the development of unbiased diagrammatic techniques for strongly-correlated many-body systems. The formalism we have developed allows to elegantly and efficiently encode the fundamental structure of quantum-many theory using renormalized expansions as the building block. Within this framework it is easy to incorporate, for instance, well-established many-body approximations like Dynamical Mean Field Theory as the starting point of a perturbative expansion. In particular, I will present state-of-the-art results in two and three dimensional Fermi-Hubbard models away from half filling in the non-perturbative regime.

*Simons Foundation Many Electron Collaboration.

12:27PM G43.00003: Faster-than-the-Clock Quantum Monte Carlo* FEDOR SIMKOVIC (Presenter), MICHEL FERRERO, CPHT, Ecole Polytechnique, RICCARDO ROSSI, CCQ, Flatiron Institute — In this talk we present a way to naturally merge and extend Monte Carlo acceleration techniques with the sampling of set functions, which can be viewed as the partition function of a bosonic system. The algorithm is particularly suited for the Connected Determinant Diagrammatic Monte Carlo algorithm (CDet) as well as its extensions and generalizations. Our proposed algorithm is rejection-free and allows for variance and autocorrelation time reduction by making use of the exponential information contained in the full set structure. Finally, we present numerical results for the two-dimensional Hubbard model obtained with this technique.

*Simons Collaboration on the Many Electron Problem
12:39PM G43.00004: A light weight regularization for wave function parameter gradients in quantum Monte Carlo  SHIVESH PATHAK (Presenter), LUCAS WAGNER, University of Illinois at Urbana-Champaign — The parameter derivative of the expectation value of the energy is a key ingredient in variational quantum Monte Carlo (VMC) wave function optimization methods. A naive Monte Carlo estimate of this derivative suffers from an infinite variance which inhibits the efficiency of optimization methods which rely on a stable estimate of the derivative. In this work we derive a simple regularization of the naive estimator which is easy to implement and has a negligible bias. This regularization is trivial to implement in a standard VMC code without sampling complex distributions and it can be extrapolated to zero bias without extra computation.

12:51PM G43.00005: Measuring Rényi Entanglement Entropies in Lattice Worm Algorithm Quantum Monte Carlo*  EMANUEL CASIANO-DIAZ (Presenter), Univ of Vermont, CHRIS M HERDMAN, Physics, Middlebury College, ADRIAN DEL MAESTRO, Univ of Vermont — In this talk we report on an extension of lattice worm algorithm quantum Monte Carlo that allows for the exact simulation of interacting bosons at zero temperature. We will discuss the implementation of the SWAP technique within the lattice path integral framework that provides access to novel estimators, including the Rényi entanglement entropies without complete knowledge of the density matrix. This technology can be used to probe the scaling of entanglement between spatial subregions and may be useful in understanding the quantum information encoded in ultracold lattice gases that can be probed via a quantum gas microscope.

*This work was supported in part by the NSF under Grant No. DMR-1553991. Computations were performed on the Vermont Advanced Computer core supported in part by NSF Grant No. OAC-1827314.

1:03PM G43.00006: Diagrammatic Monte Carlo for Molecules  JIA LI (Presenter), MARKUS WALLERBERGER, EMANUEL GULL, Univ of Michigan - Ann Arbor — Electron correlations in chemical systems give rise to a wide range of interesting physical properties. Although traditional mean-field quantum chemical algorithms can reliably calculate ground state observables in many cases, finite temperature and spectral properties are only accessible with explicit inclusion of electron correlations. Diagrammatic Monte Carlo (DiagMC), which expands the physical observable in terms of connected Feynman diagrams and samples the resulting series stochastically, is a powerful technique for studying electron correlations and does not suffer from numerical sign problem which worsens with increasing system size. Recent developments in DiagMC algorithms have greatly improved their numerical efficiency. In this talk, I aim to introduce our DiagMC implementation for multi-orbital systems, and present our results when it is applied to realistic molecular systems.
1:15PM G43.00007: Hybridizing Pseudo-Hamiltonians and Non-local Pseudopotentials in Diffusion Monte Carlo*  
JARON KROGEL (Presenter), FERNANDO REBOREDO, Oak Ridge National Lab — Projector quantum Monte Carlo (QMC) methods are among the most accurate many body techniques to query the properties of the electronic ground state. Due to computational efficiency, non-local pseudopotentials (NLPPs) are used in QMC for all but light elements. This comes at the price of localization approximations (LAs) that can degrade total accuracy. An alternate pseudo-Hamiltonian (PH) approach that does not require LA was considered early in the QMC history of core pseudization [PRL 62 2088 (1989)], but was not adopted as producing adequate potentials was difficult. In this work, we explore the hybridization of NLPPs and PHs in an attempt to reduce the non-local components. For 3d transition metals we show that hybrid PHs can be as accurate as NLPPs, but with a much smaller non-local part. We find that a simple approach to partitioning scattering channels between the NLPP and PH components does not lead to a reduction of localization error, but instead aligns the behavior of the prevailing locality and T-moves approximations. Reasons for this behavior and possible avenues for direct minimization of localization error are discussed.

*This work is supported by the Materials Sciences & Engineering Division of the Office of Basic Energy Sciences, U.S. Department of Energy (DOE).

1:27PM G43.00008: Excitations with Diffusion Monte Carlo: a bottom-up approach.*  
FERNANDO REBOREDO (Presenter), Oak Ridge National Lab — The applications of diffusion Monte Carlo (DMC) have been largely focused on properties of the ground state. As a result, high quality methods to obtain and optimize the ground-state trial wavefunctions are available. However, since much of the phenomena in Solid State Physics is governed by low energy excitations, attempts to extend DMC for the calculations of excited states properties are also documented in the literature. Most of those attempts focus on the direct calculation of excitations. In this talk we will discuss an alternative approach: how to extract excited state properties as an observable of the many-body ground state evaluated within a standard DMC method. The theory will be tested in a model system and compared with exact solutions. The potential limitations of this indirect approach for large systems of interest for real material problems will be discussed.

*Research supported by the Materials Science and Engineering Division, Basic Energy Sciences, Department of Energy.

1:39PM G43.00009: Diagrammatic Monte Carlo for real materials*  
SAM AZADI (Presenter), Physics, King's College London, ARKADIY DAVYDOV, Physics, University of Zurich, EVGENY KOZIK, Physics, King's College London — We present a systematic method for reaching beyond the GW approximation by Diagrammatic Monte Carlo (DiagMC) for first-principle simulations of real materials. DiagMC is used to provide an efficient estimation of higher-order self-energy and polarisability diagrams to achieve a controlled solution for ab initio Hamiltonians.

*This work is supported by the Simons Foundation as a part of the Simons Collaboration on the Many Electron Problem.
1:51PM G43.00010: Evaluation of arbitrary Feynman graphs via algorithmic methods.*
JAMES P. F. LEBLANC (Presenter), Physics, Memorial U. of Newfoundland — Feynman diagrammatics is a powerful tool for the study of correlated electron systems. However, the formulation of diagrams in terms of Matsubara frequencies is not well suited to numerical computations due to an intrinsic inability to evaluate the unbounded Matsubara frequency integrals. In this talk we present an algorithm for fully symbolic evaluation of arbitrary Feynman diagrams that overcomes this issue, and many others. Further, from this perspective of analytics we identify a procedure for high order diagrams which allows for the optimal reduction of the sign problem. This is accomplished via invariant transformations that allow us to group diagrams whose integrands are analytically equal or analytically cancel.

*JPFL acknowledges the support of the Natural Sciences and Engineering Research Council of Canada (NSERC), RGPIN2017-04253.

2:03PM G43.00011: Diagrammatic Monte Carlo for attractively interacting fermions*
GABRIELE SPADA, Laboratoire Kastler Brossel, Ecole Normale Supérieure, RICCARDO ROSSI, Center for Computational Quantum Physics, Flatiron Institute, TAKAHIRO OHGOE, Department of Applied Physics, Waseda University, FEDOR SIMKOVIC, MICHEL FERRERO, Centre de Physique Théorique, Ecole Polytechnique, KRIS VAN HOUCKE, Laboratoire de Physique de l'ENS, Ecole Normale Supérieure, FÉLIX WERNER (Presenter), Laboratoire Kastler Brossel, Ecole Normale Supérieure — A major long-standing goal is the precise computation of properties of interacting many-fermion systems. By evaluating connected Feynman diagrams, the diagrammatic Monte Carlo approach works directly for infinite system size. Thanks to efficient Monte Carlo algorithms, one can reach high enough orders to observe convergence up to a small error bar, provided the diagrammatic series is sufficiently well behaved, if necessary after applying a divergent-series resummation procedure. A crucial ingredient is to use dressed propagators or vertices as building blocks of the diagrams, and to expand around an appropriate starting point. The functional integral formalism allows to justify the validity of such reorganized expansions and their resummability, even for a zero convergence radius. I will present results for two cases of experimental relevance: The normal phase of the unitary Fermi gas, and the superfluid phase of the attractive Hubbard model.

*Work supported by ERC Grant Critisup2

Tuesday, March 3, 2020 11:15 AM - 1:39 PM

Session G44 DCOMP: Van Der Waals Interactions in Molecules, Materials, and Complex Environments II 704 - Robert Distasio, Cornell University - Tag(s): Focus
**11:15AM G44.00001: The Role of Correlation Effects in Non-Valence Anions** [Invited]
KENNETH JORDAN (Presenter), SHIV UPADHYAY, ARAILYM KAIRALAPOVA, Univ of Pittsburgh — Non-valence anions are especially challenging for traditional electronic structure methods due to the need to use very large basis sets and to include high-order electron correlation effects. The most widely studied class of non-valence anions are dipole-bound anions for which the excess electron binds in the Hartree-Fock approximation provided a sufficiently flexible basis set is used. Even more challenging are non-valence correlation bound (NVCB) anions for which the excess electron does not bind in the absence of dispersion-like correlation effects between the excess electron and the electrons of the molecule or cluster. In my talk, ab initio and model Hamiltonian approaches for characterizing correlation effects in dipole-bound and NVCB anions will be analyzed. Although those anions have very extended charge distributions, we find that the dominant correlation contributions to the electron binding energies are shorter-range in nature than is generally believed.

*This research was funded by the National Science Foundation under grant CHE1762337.

**11:51AM G44.00002: Attracting Opposites: Promiscuous Ion-π Binding in the DNA Nucleobases**
BRIAN ERNST (Presenter), KA UN LAO, ANDREW G. SULLIVAN, ROBERT DISTASIO, Cornell University — Ion-π interactions between the face of a molecular π-system and a cation or anion are among the strongest non-covalent interactions known, with applications throughout biochemistry and structural biology, host-guest chemistry, as well as enzyme kinetics and organocatalysis. In this work, we perform a detailed theoretical case study of ion-π interactions in the DNA/RNA nucleobases by first demonstrating that these π-systems are promiscuous ion-π binders with the versatility to bind both cations (Li⁺/Na⁺) and anions (F⁻/Cl⁻). Using a novel SAPT-based energy decomposition analysis, we uncover the different physicochemical driving forces underlying the formation of cation- and anion-π complexes, as well as the crucial role played by charge penetration effects in anion-π systems. In doing so, a unified view of these rather distinct non-covalent binding motifs emerges with the finding that both cation- and anion-π complexes are strongly stabilized by an essentially ring-independent potential that can only be overcome by substantially unfavorable electrostatics. Interestingly, the analysis presented herein demonstrates that π-systems have an inherent propensity to bind both cations and anions, thereby implying that promiscuous ion-π binding should be quite common in nature.
12:03PM G44.00003: NENCI-2020: A Large Benchmark Non-Equilibrium Non-Covalent Interaction Database with Emphasis on the Repulsive Wall  ZACHARY SPARROW (Presenter), BRIAN ERNST, PAUL JOO, KA UN LAO, ROBERT DISTASIO, Cornell University — In this work, we present NENCI-2020: a benchmark database of non-equilibrium non-covalent interaction energies for a large and diverse set of intermolecular complexes. NENCI-2020 contains ~8,000 interaction energies computed with CCSD(T)/CBS, and includes 7 non-equilibrium intermolecular distances (spanning 0.7-1.1x the equilibrium separation) and 8 non-equilibrium angles (per distance) for ~150 complexes. Using SAPT2+, we demonstrate that NENCI-2020 contains a diverse array of intermolecular binding motifs, making this database well suited for testing and developing next-generation force fields, density functional theory (DFT) approximations, quantum chemical (QC) methods, and machine-learning based approaches. This is followed by a critical assessment of ~75 dispersion/van der Waals-corrected DFT and QC methods, in which we find that most approaches can describe interaction energies for equilibrium and farther-than-equilibrium configurations with chemical accuracy (i.e., to within 1 kcal/mol). More importantly, we find that nearly all methods suffer from a rapid and systematic increase in error as the intermolecular distances become small, thereby suggesting that more work will be needed to describe intermolecular potential energy surfaces with uniform accuracy.

12:15PM G44.00004: Ab initio evaluation of complexation energies for cyclodextrin–drug inclusion complexes  KENJI OQMHULA (Presenter), KENTA HONGO, RYO MAEZONO, TOM ICHIBHA, Japan Adv Inst of Sci and Tech — Within the framework of density functional theory (DFT), an appropriate incorporation of van der Waals (vdW) into the exchange correlation (XC) functional is important to accurately predict complexation energies of noncovalent systems. This point has not been widely verified in large host-drug systems. Here we benchmarked various DFT to evaluate complexation energies of host-guest complexes, three types of β-cyclodextrins and plumbagin (known as anti-cancer drug). We modeled these systems as follows: (1) DFT geometry optimization of individual guest and hosts, (2) their docking conformation search based on genetic algorithm with semi-empirical simulations, and (3) DFT geometry optimization of the docking system. Then single-point energy calculations were performed to evaluate complexation energies. Furthermore, we applied DMC (diffuse Monte Carlo) to validate the DFT results. We found M06-2X-D3 and CAM-B3LYP-D3 give almost the same energies for all the cases and they are both consistent with DMC within the error bar. From these results, we concluded that a proper incorporation of vdw and long-range exchange corrections into XC functionals is essential for describing the cyclodextrin-plumbagin systems.
Many-body dispersion effects and plasmonic correlations in the catalytic synchronization of a DNA-enzyme complex  MATTEO GORI (Presenter), Quantum Biology Laboratory, Howard University, Washington, DC, MARTIN STOEHR, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, University of Luxembourg, PHILIP KURIAN, Quantum Biology Laboratory, Howard University, Washington, DC — Long-range van der Waals dispersion forces could play a significant role in explaining the action of certain restriction enzymes inducing DNA double-strand breaks [J. Theor. Biol. 2016, 391, 102-112]. In particular, dipolar interactions among spatially separated nucleotides and enzymatic molecular subunits may be responsible for long-range synchronization of quantum electronic density fluctuations. Zero-point modes of such plasmon-like oscillations may promote double-strand breakage, in lieu of external chemical energy from ATP. Our analysis of Many-Body Dispersion (MBD) effects in the catalytic behavior of EcoRI, a sequence-specific DNA-targeting enzyme used widely in genomic science, offers clues for more refined investigations of the collective electron fluctuations (plasmon) in complex (bio)molecular systems [Chem. Soc. Rev. 2019, 48, 4118]. We present analysis of these MBD eigenmodes applied to EcoRI at different steps along the catalytic trajectory, including entropic measures of the degree of collectivity of each mode (i.e., its vectorial distribution in the atomic site basis) and other quantum information metrics, to understand the delocalization properties in Hilbert space and their implications for distant “plasmonic allostery” in 3+1-dimensional physical space.
Inversion Symmetry Breaking Probed by X-ray Absorption Spectroscopy in H-bonded Organic Ferroelectric Crystal

FUJIE TANG (Presenter), Department of Physics, Temple University, XUANYUAN JIANG, Department of Physics and Astronomy, University of Nebraska, HSIN-YU KO, Department of Chemistry, Princeton University, JIANHANG XU, Department of Physics, Temple University, MEHMET TOPSAKAL, Center for Functional Nanomaterials, Brookhaven National Laboratory, GUANHUA HAO, Department of Physics and Astronomy, University of Nebraska, ALPHA T. N’DIAYE, Advanced Light Source, Lawrence Berkeley National Laboratory, PETER A DOWBEN, Department of Physics and Astronomy, University of Nebraska, DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory, XIAOSHAN XU, Department of Physics and Astronomy, University of Nebraska, XIFAN WU, Department of Physics, Temple University — Molecular ferroelectrics (FE) based on ordering hydrogen bonds have potentially high electric polarization and ordering temperature compared with the conventional oxide FE materials. In particular, croconic acid (C5O5H2) with FE polarization of 30 μC/cm², plays a prototype of ferroelectric organic molecular solid, whose electric polarization is generated by proton transfer. We carry out X-ray absorption spectroscopy experiment at oxygen K-edge in croconic acid crystal. The experimental spectrum is well reproduced by the electron-hole excitation theory simulations from configuration generated by ab initio molecular dynamics simulation. When inversion symmetry is broken in ferroelectric state, the hydrogen bonding environment on the two bonded molecules become inequivalent. Such a difference is sensitively probed by the bound excitation in the pre-edge, which are strongly localized on the excited molecules. Our analysis shows that a satellite peak in the pre-edge will emerge at higher excitation energy which serves as a clear signature of ferroelectricity in the material.

This work was primarily supported by National Science Foundation through Awards No. DMR-1552287.

van der Waals Phonons in Molecular Crystals

SOMAYEH KHAZAEI (Presenter), ALEXANDRE TKATCHENKO, University of Luxembourg Limpertsberg — Low-frequency terahertz (THz) vibrations are ubiquitous in molecular materials throughout chemistry and biology [e.g. PRL 113, 055701; PRL 119, 097404]. Such delocalized vibrations play a key role in many phenomena, including entropic stabilization of molecular crystal polymorphs, protein folding, and signaling. However, our understanding of mechanisms behind THz vibrations in molecular materials is far from complete. Here we study a range of molecular crystals with DFT including many-body treatment of van der Waals (vdW) dispersion interactions (DFT+MBD). We find that THz vibrations are very sensitive to the correct treatment of electrostatic effects in DFT and explicit quantum-mechanical treatment of vdW interactions. We discuss a way to categorize vibrational modes in the THz range and show that these vibrations are crucial to achieve a better understanding of molecular materials.
First-principles studies of small molecule absorption kinetics in diamine-appended metal-organic frameworks

ALEX SMITH (Presenter), University of California, Berkeley, JEFFREY B NEATON, University of California, Berkeley; Molecular Foundry, Lawrence Berkeley National Laboratory; Kavli Energy Nanosciences Institute at Berkeley — Recently, a family of diamine-appended metal-organic frameworks (MOFs) has demonstrated selective and tunable adsorption via novel reversible non-Langmuir stepped isotherms, making them promising for carbon capture applications. Here, we use first principles van der Waals-corrected density functional theory calculations, as well as molecular dynamics and computations of NMR chemical shifts, to understand the structure, kinetics, and selectivity associated with the stepped isotherms in environments relevant to flue gas conditions. We compare binding energies with experiments, and predict intermediate and final structures to understand the measured isotherms. We focus on the role that SO2, a component of flue gas, plays in degrading MOF CO2 adsorption through studying SO2 binding energies and how SO2 disrupts the kinetics of CO2 adsorption. This work is supported by DOE, and computational resources are provided by NERSC.

Long-range Correlation Energy in the Interaction of Molecules with Surfaces

ALINA UMERBEKOVA (Presenter), MICHELE PAVANELLO, Rutgers University, Newark — By exploiting the fluctuation-dissipation theorem of DFT and a formally exact decomposition of the density-density linear response function evaluated at imaginary frequency, subsystem Density Functional Theory makes an excellent platform for developing non-local long-range correlation energy functionals [1,2]. We present a computational protocol to extract embedded C6 coefficients for molecules surrounded by complex environments from a real-time subsystem TDDFT simulation [3]. The C6 coefficients fully account for environmental screening effects through the many-body response [4]. We showcase a pilot calculation of the C6 coefficient of Benzene adsorbed on monolayer MoS2 and we show a surface enhancement of the van der Waals interaction between two benzene molecules nearby a MoS2 surface of 11 meV compared to the interaction estimated from C6 coefficients derived from isolated benzene molecules.

1:27PM G44.00010: Reproducibility of Molecular Adsorption Potential Energy Surfaces

LUKAS HÖRMANN (Presenter), ANDREAS JEINDL, OLIVER T. HOFMANN, Institute of Solid State Physics, Graz University of Technology — The adsorption of molecules on surfaces depends on a variety of mechanisms: Covalent bonds, charge transfer and van-der-Waals (vdW) interactions shape the potential energy surface (PES), making it key to understanding molecule-substrate interfaces. To describe these interfaces with density functional theory, one can choose from many different exchange correlation functionals and vdW correction schemes. To explore how robust the PES is in relation to the choice of method, we present a benchmark of common local, semi-local and non-local functionals in combination with various vdW corrections for perylenetetracarboxylic dianhydride (PTCDA) on Ag(111), one of the most frequently studied system.

Using only about 50 DFT calculations as input data, an in-house developed Gaussian process regression algorithm generates PESs with DFT accuracy. This allows us to analyze the PES's features, such as positions and energies of minima and saddle points, in detail. Comparing the results from different exchange correlation functionals allows us to identify trends and differences between the approaches. Finally, we compare key features, such as local minima, with experimental data to determine a “quality seal” for the different functionals and vdW corrections.

Tuesday, March 3, 2020 11:15 AM - 1:51 PM

Session G45 DCOMP DCP: Modeling the electrochemical interface and aqueous solutions II 706 - Luana Pedroza, Univ Federal do ABC - Tag(s): Focus
First-principles electrochemistry with grand-canonical DFT and continuum-solvation methods

RAVISHANKAR SUNDARARAMAN (Presenter), Materials Science and Engineering, Rensselaer Polytechnic Institute — First-principles calculations combining density-functional theory (DFT) and continuum solvation models have been highly successful in enabling the theoretical design of liquid-phase catalyst materials. The application of such methods to heterogeneous catalysis in electrochemical solid-liquid interfaces has however been far more challenging for two reasons. First, conventional continuum solvation methods designed for finite molecular systems are not readily applicable to solid-liquid interfaces with metal or oxide surfaces. Second, processes at these interfaces continuously exchange electrons with the electrode, which makes the charge states of the surface difficult to determine.

I will present recent developments in continuum solvation methods that enable simultaneously accurate treatment of solid surfaces and molecules in electrochemical interfaces. Additionally, by automatically equilibrating charge at a fixed electrochemical potential, new 'grand-canonical DFT' algorithms and software (JDFTx) facilitate realistic description of processes in these interfaces. Together, these methods enable first-principles prediction of electro- and photo-catalysis mechanisms for energy conversion, and of the surface structures and dynamics in battery materials. With clean prototypical electrochemical measurements as a benchmark, I will outline the present capabilities, pending challenges and necessary future developments in first-principles electrochemistry.

The nanoscopic structure of Pt-water electrified interface under applied potential

CLOTILDE CUCINOTTA (Presenter), Imperial College London — In this talk I will introduce some issues connected with the simulation of electrified interfaces at the nanoscale focusing in particular on modelling the effect of an applied potential to an electrochemical cell. I will present a new methodology to model charged electrodes and highlight some recent progress in the simulation of the double layer of the fundamental Pt-water interface and its response to changes of potential applied to the cell. We reveal that the metal/surface charging cannot be described using a traditional simple capacitor model and that the double layer nanoscopic structure, mass density and charge distribution, strongly depend on the applied potential.

*EP/P033555/1 Towards a Parameter-Free Theory for Electrochemical Phenomena at the Nanoscale (NanoEC)
In this presentation, we will discuss how a combination of ab-initio simulations and in-situ characterizations could be used to access to such information and how one could reduce uncertainty in interpreting the experimental data. The key is to use ab-initio simulations as link between multiple observables that are not linearly dependent each other, which may be used to avoid a misinterpretation due to accidental agreement on one observable. We will show the examples based on oxidation of III-V semiconductor surfaces induced by water and oxygen.

*Part of this work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. TAP, BCW and TO are supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Fuel Cell Technologies Office. XZ and SP acknowledge the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences under Award Number DE-FC02-04ER15533 (NDRL No: 5152).
12:15PM G45.00004: Activating 2D materials for hydrogen evolution reaction (HER) by electron doping*  NAIRWIT KARODAK (Presenter), OLIVIERO ANDREUSSI, Physics, University of North Texas — The two-dimensional materials have emerged as an effective electrocatalysts for Hydrogen evolution reaction in the recent few decades.[1] However, the database of such materials is limited so far mostly to family of transition metal dichalcogenides and MXenes. Moreover, majority of these need prior activation by defect engineering or elemental doping. In this presentation, we show an electron doping pathway to enhance the electro-catalytic efficiency of two-dimensional material surfaces towards HER. A high-throughput computational scheme has been employed, starting from a large computational database of the easily exfoliable compounds.[2] By exploiting continuum embedded density functional theory and Grand Potential Simulation techniques, we studied the H⁺ electrosorption reaction thermodynamics and the aqueous stability of the 2D materials at different applied potentials and pH.[3,4] Our results allow to identify some promising materials, which show potential catalytic activity and considerable stability at reducing potentials and acidic pH.

References

*University of North Texas

12:27PM G45.00005: Probing Pseudocapacitive response of MXene electrodes for energy storage from first principles*  FRANCISCO MARQUES DOS SANTOS VIEIRA (Presenter), Pennsylvania State University, YASUAKI OKADA, Murata Manufacturing, NATHAN D KEILBART, JAMES GOFF, Pennsylvania State University, KOSUKE SHIRATSUYU, Murata Manufacturing, ISMAILA DABO, Pennsylvania State University — Pseudocapacitive devices are able to store and release electrical energy by virtue of the rapid and reversible redox reactions which occur at the electrode surfaces. The family of transition metal carbides and nitrides, MXenes, show promise as pseudocapacitive electrodes. As the performance, power and energy densities, of the pseudocapacitive device is predicated on the quantity of lithium-ion adsorption onto the surface of the MXene, we are interested in the effects of MXene composition and solution properties on this phenomenon. We perform voltage-dependent cluster expansions to study reversible lithium-ion adsorption in realistic environments. The cluster expansions are fit with semi-local density functional calculations in implicit solvent. Preliminary results show that lithium-ion pseudocapacitance is sensitive to the dielectric constant of the solution and extent of surface electrification through electrochemical double layer capacitance. Our results also suggest that solvents with higher lithium reduction potentials that stabilize the lithium-ions in solution can extend the potential window of the pseudocapacitive electrode.

*MuRata Manufacturing
12:39PM G45.00006: Understanding water/silicon carbide interfaces using first principle simulations

FILIPPO SAVAZZI (Presenter), GIANCARLO CICERO, Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino, MARCO GOVONI, Materials Science Division, Argonne National Laboratory, GIULIA GALLI, Pritzker School of Molecular Engineering, University of Chicago — Interfaces between water and solid surfaces are key to many technological applications, including electrochemical devices, the fabrication of membranes for water purification and sensors for biomedical devices. Here we consider a bio-compatible material, SiC, of interest for biosensing and electrochemistry applications. We investigated the interaction of water with its hydrophobic and hydrophilic interfaces using first principles molecular dynamics and the Qbox code (http://qboxcode.org/). We report results on band offsets between the solid and the liquid and their dependence on the atomistic structure of the interface, which in turn is related to the hydrophobic or hydrophilic character of the solid termination. In addition, we will discuss the effect of an external applied electric field at the interface, to understand how the interface properties are modified under typical electrode working conditions.

*Part of this work was supported as part of the Advanced Materials for Energy-Water Systems (AMEWS) Center, an Energy Frontier Research Center funded by DOE/BES.

12:51PM G45.00007: Continuum models to handle electrolyte solutions effects in first-principles simulations of materials

OLIVIERO ANDREUSSI (Presenter), Department of Physics, University of North Texas — Continuum models of solvation have played a crucial role in quantum chemistry simulations and are now starting to be popular for the computational characterization of solvated, possibly electrified, interfaces. Recent advances in the field opened the possibility of modeling heterogeneous catalysis and electrochemistry in a first-principles-based framework, where the multiscale nature of the developed approaches provides a significant reduction of the computational burden while retaining a good accuracy. Nonetheless, extending continuum approaches to condensed-matter simulations present non-trivial issues, related to the complexity of the electrostatic problem in charged 2D interfaces and to the open structure of many crystalline substrates. Here we will present some of our recently proposed approaches to overcome these limitations, in particular focusing on a hierarchy of methods to describe the electrochemical diffuse layer. Moreover, handling environment effects through continuum embedding allows us to exploit a rigorous grand canonical approach to study the thermodynamic properties of electrochemical interfaces, thus overcoming some limitations of the computational-hydrogen electrode technique. Applications to noble metal (electro-)catalysis and beyond will be presented.
1:03PM G45.00008: Engineering Trimetallic Core-shell Nanoclusters for CO₂ Electro-reduction at Low Overpotentials  RAFIA AHMAD (Presenter), King Abdullah Univ of Sci & Tech (KAUST) — Storing energy in chemical bonds and finding an electrochemical catalyst to reduce CO₂ to hydrocarbon fuels such as CH₄ would provide an ideal solution for discontinuous renewable energy sources. Commercially used pure copper catalysts are known to possess the best Faradaic yield capacity (up to 50%) for CO₂ conversion to CH₄, however these require large overpotentials to perform this transformation. Using density functional theory (DFT), we tailor TMₓNi₁₃₋ₓ@Cu₄₂ (TM = 3d transition metals; x = 3, 6, and 9) nanoclusters to catalyze CO₂ electro-reduction to CH₄ with lower overpotentials than commercial catalysts. Among these, Sc₅(6)Ni₈(7)@Cu₄₂ possess unprecedented low overpotentials, ~0.17 V below standard potential value (SPV). The given core compositions ensure the optimal position of d-band center of Cu, which is required for better interaction with π orbital of CHO than with CO. This results in better stabilization of CHO, giving exergonic CO reduction. Estimated statistical coverage of CHO exceeds CO by 60% at ambient conditions on Sc₅Ni₈@Cu₄₂, ensuring CO₂ conversion to high end fuel CH₄ without CO poisoning. The energetics of the reaction pathway and the overpotential values are relatively unchanged with the inclusion of implicit aqueous solvent.

1:15PM G45.00009: Adsorption of small gas molecules on a single Pt atom supported by pristine graphene: diffusion Monte Carlo study  JEONGHWAN AHN (Presenter), IUE GYUN HONG, KonKuk Univ, HYEONDEOK SHIN, ANOUAR BENALI, Computational Science Division, Argonne National Laboratory, YONGKYUNG KWON, KonKuk Univ — We have used diffusion Monte Carlo (DMC) method to study adsorption of small gas molecules on a single Pt atom supported by pristine graphene. Firstly, we obtain Pt-graphene binding energy curves as a function of the vertical distance between Pt and graphene for three different adsorption sites (bridge, on-top, hollow), from which the equilibrium binding energies and distances are determined. Our DMC results are compared with DFT results based on several different density functionals, which reveals that PBE and rVV10 results show good agreement with our DMC results for both equilibrium energies and distances. For molecular adsorption on the Pt-graphene complex, we observe significant overestimation in DFT binding energies compared to the DMC ones. In the case of O₂ adsorption, the spin degrees of freedom are considered along with geometries. While DFT predicts the lowest-energy structure of a spin-triplet side-on configuration where the molecular axis of O₂ is parallel to the graphene sheet, DMC finds that the spin-singlet side-on configuration with the molecular axis being slightly tilted toward graphene is the lowest-energy state. The DMC calculations are currently in progress to examine diffusion path of O₂ and catalytic performance of Pt-graphene complexes.
1:27PM G45.00010: Morphological stability of electrodeposition through a viscoelastic coating*  PAUL RUDNICKI (Presenter), XIAN KONG, JIAN QIN, Stanford Univ — Lithium metal anodes, the key component of several emerging lightweight, energy-dense battery chemistries, continue to suffer from serious safety and cycle life concerns due to dendritic lithium growths. A promising approach toward dendrite suppression is to insert a viscoelastic polymeric interphase between the anode and the separator. Good coating layers have been empirically found to exhibit instantaneous elastic response and adaptability to volume change, but no mechanistic understanding was established. We develop a continuum model to study the effects of a polymer coating on the morphological dendritic instability by explicitly incorporating the viscoelastic response and the dielectric permittivity of the polymer. The effects of charging current density and overpotential during cycling are explored, and the coating properties and battery operation conditions for stable, uniform lithium growth and long cycle life are discussed.

*This material is based upon work supported by the N.S.F. Graduate Research Fellowship under Grant No. DGE-1656518, the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U.S. D.O.E. through the Battery500 Consortium, the 3M Non-Tenured Faculty Award, and the Hellman Scholar Award.

1:39PM G45.00011: Field-Aware Interfaces in Continuum Solvation  MATTHEW TRUSCOTT (Presenter), OLIVIERO ANDREUSSI, Univ of North Texas — The continuum embedding approach has seen a rapid influx of interest from the condensed matter community in recent years. We present here a number of additions to the modelling of continuum interfaces that aim to provide an implicit consideration of charged species and compounds with highly polarized regions in an effort to further expand on the capabilities of continuum models, especially in the treatment of electrochemical interfaces. These advances follow recent approaches of using the electric field as an effective proxy for the localized charge surrounding a specific region. This “field-aware” approach is applied to the recently proposed soft-sphere continuum solvation (SSCS) method, wherein the radius of each soft-sphere composing the interface is readjusted as a function of the field flux through its surface, as well as the self-consistent continuum solvation (SCCS) method, whose interface definition is modified by the normal component of the electric field. In both cases, a complex dependence of the interface function on both the electronic and ionic degrees of freedom of the solute is introduced. Analytic derivatives of the new interface are thus implemented during optimization procedures (SCF and geometry optimization).

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G46 GMAG DMP: Pyrochlores II: Spin Liquids  708 - Oleg Tchernyshyov, Johns Hopkins University - Tag(s): Focus
Dynamics of a pyrochlore quantum spin liquid NaCaNi$_2$F$_7$*

SHU ZHANG (Presenter), Physics, University of California, Los Angeles, HITEME CHANGLANI, Florida State University, KEMP PLUMB, Brown University, OLEG TCHERNYSHYOV, Johns Hopkins University, RODERICH MOESSNER, Max-Planck Institute for the Physics of Complex Systems — The Heisenberg antiferromagnet on a pyrochlore lattice is a well-known model realizing a classical spin-liquid state at low temperatures [1]. Much less is known about the quantum version of this model. The spin-1 pyrochlore material NaCaNi$_2$F$_7$ is well described by a weakly perturbed Heisenberg Hamiltonian [2]. It shows no magnetic order down to extremely low temperatures, making it a prime candidate for a three-dimensional quantum spin liquid. Inelastic neutron scattering has revealed a lack of magnetic Bragg peaks and a broad continuum of excitations incompatible with a conventional magnetically ordered state. We combine analytical theory and numerical approaches to elucidate the nature of this enigmatic spin-liquid state [3]. The three approaches---molecular dynamics simulations, stochastic dynamical theory and linear spin wave theory---reproduce remarkably well the energy and momentum dependence of the experimental inelastic neutron scattering intensity with the exception of the lowest energies. Our study offers the following picture of spin dynamics in this system. This frustrated magnet is slowly moving through a (very large) manifold of degenerate ground states lacking long-range order. This slow motion is driven by medium- and high-energy spin waves with Bose statistics. We discuss two surprising aspects and their implications for quantum spin liquids in general: the complete lack of sharp quasiparticle excitations in momentum space and the success of the linear spin wave theory. Similar conclusions have been reached independently about a $S=3/2$ "pyrochlore" antiferromagnet MgCr$_2$O$_4$ [4].


*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331.
11:51AM G46.00002: Magnetic field dependence of magnetic correlations in a pyrochlore Heisenberg antiferromagnet  ALBERTO DE LA TORRE (Presenter), Brown University, JASON W. KRIZAN, Princeton University, GUANGYONG XU, NIST, ROBERT J. CAVA, Princeton University, KEMP PLUMB, Brown University — Recent neutron experiments on the S=1 pyrochlore NaCaNi$_2$F$_7$ [1] revealed a dynamic structure factor exhibiting pinch points and a continuum of high energy magnetic excitations. These signatures point towards a magnetic ground-state which can be described by an almost ideal Heisenberg antiferromagnet on the pyrochlore lattice. Although a highly degenerate ground state its expected at low temperatures, disorder freezes the spin degrees of freedom so that a specific spin configuration is preferred [2]. How disorder induces a frozen spin state in this Coulomb phase [3] remains to be fully understood. We present here a set of neutron scattering measurements in NaCaNi$_2$F$_7$ as a function of external magnetic field. Above a threshold field, $H > 2$ T, a long-range ordered magnetic field polarized phase emerges. I will discuss the magnetic field and temperature evolution of magnetic correlations in NaCaNi$_2$F$_7$ through this polarized phase.


12:03PM G46.00003: Ultrasound Velocity Measurements in Bond-Disordered Pyrochlore Magnet NaCaCo$_2$F$_7$  TADADATAKA WATANABE (Presenter), HIROYA KATO, Nihon Univ - Tokyo, YOSHIKAKI HARA, Nat Inst Tech Ibaraki Col, JASON W. KRIZAN, ROBERT J. CAVA, Princeton Univ — Pyrochlore cobalt fluoride NaCaCo$_2$F$_7$ is a geometrically frustrated magnet, which exhibits spin freezing below $T_f \sim 2.4$ K while the Weiss temperature is $\theta_W \sim -140$ K. The spin-freezing behavior in this compound is considered to be due to the presence of bond randomness which is generated by the random occupation of Na$^+$ and Ca$^{2+}$ ions on the pyrochlore A sites. We perform ultrasound velocity measurements in a single crystal of NaCaCo$_2$F$_7$. Temperature ($T$) dependence of the bulk modulus $C_B = (C_{11} + 2C_{12})/3$ exhibits Curie-type $-1/T$ softening upon cooling below $\sim 20$ K down to $T_f$, which should be a precursor to the lattice distortion at $T_f$. And this softening is suppressed by the application of magnetic field, indicating that the spin freezing is driven by the spin-lattice coupling. For the bond-disordered frustrated NaCaCo$_2$F$_7$, the softening in the breathing elastic mode of $C_B$ above $T_f$ suggests that the spin freezing, or the release of frustration is a result of the enhancement of the bond randomness driven by the spin-lattice coupling.
12:15PM G46.00004: Low energy excitations in Tb$_2$Ti$_2$O$_7$ with [111] magnetic field*  XINSHU ZHANG (Presenter), SEYED KOOHPAYEH, PETER ARMITAGE, Johns Hopkins University — The pyrochlore magnet Tb$_2$Ti$_2$O$_7$ has shown exotic magnetic properties and has been considered to be a quantum spin liquid. Although Tb$_2$Ti$_2$O$_7$ has been studied for decades, low energy experiments with magnetic field along [111] are rare. We perform time-domain terahertz spectroscopy on high quality Tb$_2$Ti$_2$O$_7$ crystal to study the crystal field excitations as a function of magnetic field with very high resolution. The excitations behaves significantly different below and above a critical field, indicating a phase transition around 2.5 T. We also observed the discrepancy between two polarization channels. Our work provides insight into this very intriguing material.

*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331

12:27PM G46.00005: THz spectroscopy study of the rare-earth pyrochlore Tb$_2$Ti$_2$O$_7$* KIRILL AMELIN (Presenter), TOOMAS ROOM, URMAS NAGEL, National Institute of Chemical Physics and Biophysics, EVAN CONSTABLE, Institute of Solid State Physics, TU Wien, ZHE WANG, Institute of Physics II, University of Cologne, YANN ALEXANIAN, JULIEN ROBERT, RAFIK BALLOU, SOPHIE DEBRION, Institut Néel, CNRS — Tb$_2$Ti$_2$O$_7$ is unique rare-earth pyrochlore in that it does not exhibit theoretically predicted long-range magnetic order down to the lowest measured temperatures below 100 mK. Instead, a fluctuating spin-liquid state with short-range correlations persists, while strong spin-lattice coupling occurs. As a manifestation of this coupling, the two lowest crystal electric field (CEF) level doublets separated by approximately 1.5 meV = 0.42 THz have been shown to couple to a transverse acoustic phonon. Such a vibronic process is accompanied by hybrid magnetoelastic excitations, which have been previously detected by neutron scattering and THz spectroscopy.

We measured absorption of THz radiation in a single crystal at the temperatures 3 K and 60 K combined with magnetic fields up to $B = 15$ T applied along the local [111] axis. The $B$ dependence of the crystal field excitations gives us the opportunity to accurately describe the CEF spectrum including the vibronic process, and to see how it is transformed by a static magnetic field.

*We acknowledge the Estonian Ministry of Education and Research under Grant No. IUT23-03, and the European Regional Development Fund project TK134.
12:39PM G46.00006: Probing Multipolar Quantum Spin Liquids in non-Kramers Pyrochlore Materials with Magnetostriction.* ADARSH PATRI, University of Toronto, MASASHI HOSOI (Presenter), University of Tokyo, SUNGBIN LEE, Korea Advanced Institute of Science and Technology, YONG-BAEK KIM, University of Toronto — Quantum spin liquids (QSLs) and Multipolar ordered states (MPOs) both share the property of being notoriously difficult to detect with conventional probes. Recently, lattice-based techniques are proposed as novel probes to detect MPOs. Motivated by this success, we investigate the possibility of detecting QSL when it arises from interacting multipolar moments. In this talk, we theoretically propose that spin-lattice coupling can be used as a powerful tool to probe such multipolar QSL phases.

*This work was supported by NSERC of Canada, and Canadian Institute for Advanced Research. Y.B.K. is supported by the Killam Research Fellowship of the Canada Council for the Arts. M.H. is supported by JSPS Overseas Challenge Program for Young Researchers.

12:51PM G46.00007: Half-moon quantum spin liquid in a spin-1/2 J₁-J₂-J₃a Heisenberg antiferromagnet on the pyrochlore lattice PRATYAY GHOSH, Paul Scherrer Institut, TOBIAS MÜLLER, University of Wuerzburg, JOHANNES REUTHER, Physics Department, Freie Universitaet Berlin, RONNY THOMALE, University of Wuerzburg, MICHEL J P GINGRAS, University of Waterloo, YASIR IQBAL (Presenter), Indian Institute of Technology Madras — We investigate the quantum Heisenberg model on the pyrochlore lattice for spin-1/2 in the presence of antiferromagnetic nearest-neighbor J₁, second nearest-neighbor J₂, and third nearest-neighbor J₃a exchange interactions. By employing the pseudofermion functional renormalization group method, we find, that the quantum Coulomb spin liquid of the J₁ only model is robust along the line J=J₂=J₃a up till J/J₁~0.22, thus extending its classical region of stability. Similarly, for J/J₁>0.22, we find an absence of long-range magnetic order down to T=J₁/100, however, the bowtie features now give way to half-moons as seen in the static spin susceptibility profile, thus pointing to the realization of a ‘half-moon’ quantum spin liquid. At the point J/J₁=1/2, which features a sub-extensively degenerate classical ground-state manifold, we show that quantum fluctuations fail to break this degeneracy stabilizing a quantum spin liquid. In stark contrast to this finding, in the corresponding classical model, thermal fluctuations are known to select a collinear antiferromagnetically ordered state via the order-by-disorder mechanism. Hence, we present a rare scenario wherein thermal and quantum fluctuations act differently.
Experimental signatures of a three-dimensional quantum spin liquid in effective spin-1/2 Ce$_2$Zr$_2$O$_7$ pyrochlore* [Invited]  BIN GAO (Presenter), TONG CHEN, DAVID W TAM, CHIEN-LUNG HUANG, Rice Univ, KALYAN SASMAL, University of California, San Diego, DEVASHIBHAI ADROJA, ISIS Facility, STFC Rutherford-Appleton Laboratory, FENG YE, HUIBO CAO, GABRIELE SALA, MATTHEW STONE, Neutron Scattering Division, Oak Ridge National Laboratory, CHRISTOPHER BAINES, JOEL BARKER, Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, HAOKU HU, Rice Univ, JAE-HO CHUNG, Department of Physics, Korea University, XUANGHAN XU, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, MANIVANNAN NALLAIYAN, STEFANO SPAGNA, Quantum Design Inc., M BRIAN MAPLE, University of California, San Diego, ANDRIY NEVIDOMSKYY, EMILIA MOROSAN, Rice Univ, GANG CHEN, Department of Physics and Center of Theoretical and Computational Physics, The University of Hong Kong, PENGCHENG DAI, Rice Univ — A quantum spin liquid (QSL) is an exotic state of matter where unpaired electrons’ spins, although being entangled, do not show magnetic order even at the zero-temperature. Because such a state may be important to the microscopic origin of high-transition temperature superconductivity and useful for quantum computation, the experimental realization of QSL is a long-sought goal in condensed matter physics. Although neutron scattering experiments on the two-dimensional QSL candidates ZnCu$_3$(OD)$_6$Cl$_2$ and YbMgGaO$_4$ have found evidence for the hallmark of a QSL at very low temperature - a continuum of magnetic excitations, the presence of site disorder complicates the interpretation of the data. Recently, the three-dimensional (3D) Ce$^{3+}$ pyrochlore lattice Ce$_2$Sn$_2$O$_7$ has been suggested as a clean, effective spin-1/2 QSL candidate, but the evidence of a spin excitation continuum is missing due to the lack of single crystals. Here we use alternating current magnetic susceptibility, thermodynamic, muon spin relaxation ($\mu$SR), and neutron scattering experiments on single crystals of Ce$_2$Zr$_2$O$_7$, a compound isostructural to Ce$_2$Sn$_2$O$_7$, to demonstrate the absence of magnetic ordering/spin-glass down to 20 mK and the presence of a spin excitation continuum at 35 mK. With no evidence of oxygen deficiency and chemical disorder seen by diffuse scattering measurements and neutron diffraction, Ce$_2$Zr$_2$O$_7$ may be a 3D pyrochlore lattice QSL material with minimum magnetic and nonmagnetic chemical disorder.

*US DOE BES
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Interplay between magnetic exchange, multipolar interactions and virtual crystal field fluctuations in non-Kramers pyrochlore magnets

WEN JIN (Presenter), MICHEL J P GINGRAS, University of Waterloo, HALLAS ALANNAH, University of British Columbia, JONATHAN GAUDET, Johns Hopkins University, BRUCE D. GAULIN, McMaster University — It has been shown that multipolar degrees of freedom can play a vital role in causing exotic phases in pyrochlore magnets, such as octupoles in Kramers Nd$^{3+}$ or Ce$^{3+}$ ions and quadrupoles in non-Kramers Pr$^{3+}$ and Tb$^{3+}$ ions. Terbium-based pyrochlores are peculiar for hosting virtual crystal field excitation (VCFE) due to the small energy separation between the two low-lying crystal electric field doublets. Here we consider a two-doublets system with magnetic bilinear exchange and electric quadrupole-quadrupole interaction. Via a mean field approach, we show that the proposed model exhibits complex dipolar and quadrupolar phases. Different dipolar order parameters coexist due to VCFE, which also leads to a “parasitic” ferroquadrupolar order accompanying the dominant antiferroquadrupolar order. We find for a set of model parameters locating the system near the dipolar/quadrupolar phase boundary that, upon cooling, such system may undergo a two-step thermal transition into the ultimate low-temperature dipolar phase with an intermediated quadrupolar ordered state. We also propose a range of acceptable parameters for the Tb$_2$Ge$_2$O$_7$ pyrochlore that allows us to reproduce some of the main inelastic neutron scattering features.
1:51PM G46.00010: Crystal Field Excitations in Raman Spectra of Pr-based Pyrochlores*

YUANYUAN XU (Presenter), Department of Physics and Astronomy, Johns Hopkins University, TAKUMI OHTSUKI, The Institute for Solid State Physics, The University of Tokyo, HUIYUAN MAN, Department of Physics, Stanford University, NAN TANG, The Institute for Solid State Physics, The University of Tokyo, SANTU BAIDYA, Department of Physics and Astronomy, Rutgers University, HONGBIN ZHANG, Institut für Materialwissenschaft, Technische Universität Darmstadt, SATORU NAKATSUJI, The Institute for Solid State Physics, The University of Tokyo, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, NATALIA DRICHKO, Department of Physics and Astronomy, Johns Hopkins University — Interplay of strong electron correlations and spin-orbit coupling leads to exotic magnetic phases in rare earth pyrochlores. Here we present a study of Pr$_2$Ir$_2$O$_7$ and Pr$_2$Zr$_2$O$_7$, which show magnetic interactions but no ordering down to low temperatures [1-3]. We performed low temperature Raman scattering spectroscopy study of Pr$_2$Ir$_2$O$_7$ and Pr$_2$Zr$_2$O$_7$ single crystals to probe crystal field excitations and phonons. A comparison of crystal field excitations in these two materials reveals a splitting in the Pr$^{3+}$ crystal field doublet at 57 meV in Pr$_2$Zr$_2$O$_7$, possibly originating from the magneto-elastic coupling induced vibronic state. An anomalous broadening of this crystal field excitation is observed in Pr$_2$Ir$_2$O$_7$. A comparison of phonon spectrum to the density functional theory calculations demonstrates an anomalous broadening/splitting of the $E_g$ phonon mode corresponding to the Ir-O-Ir (Zr-O-Zr) bending. We discuss relevance of our findings to magnetic properties of these materials.


*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331

2:03PM G46.00011: Probing Emergent Excitations in Pr$_2$Hf$_2$O$_7$ with Thermal Conductivity

JENNIFER REID (Presenter), SHAUN FROUDE-POWERS, University of Waterloo, ALEXANDROS SAMARTZIS, BELLA A C I LAKE, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, ROBERT HILL, University of Waterloo — Pr$_2$Hf$_2$O$_7$ (PHO) is a quantum spin ice candidate with a non-Kramers doublet ground state that displays evidence of dynamic spin ice behaviour [1][2]. We report thermal conductivity measurements of single crystal samples of PHO as a function of temperature between 50 mK and 50 K and magnetic field up to 12 T. A combination of high magnetic field measurements and measurements of different sized samples are used to identify the lattice contribution. We interpret our results considering current theoretical predictions for exotic excitations in quantum spin liquids, such as emergent photons, magnetic monopoles and visons [3].


Tuesday, March 3, 2020 11:15 AM - 2:15 PM
Non-magnetic Origin of Spin Hall Magnetoresistance in Pt films and Epitaxial NiO/Pt bilayers  

ALEXANDRA CHURIKOVA (Presenter), DAVID BONO, BRIAN NELTNER, Massachusetts Institute of Technology MIT, LARRY SCIPIONI, ADAM SHEPARD, PVD Products, Inc., ANGELA WITTMANN, FELIX BUETTNER, Massachusetts Institute of Technology MIT, TY NEWHOUSE-ILLIGE, JAMES GREER, PVD Products, Inc., GEOFFREY BEACH, Massachusetts Institute of Technology MIT  

— Recently, electrical control of the magnetic order in antiferromagnetic insulators (AFIs) with a Pt overlayer as a spin current source has been a subject of great interest [1-4], as it allows for ultra-low power control of the magnetic order. However, the detection and nature of purely AFI magnetoresistive switching remains elusive [5-6]. Here, we show that the Pt signal has a strong bias due to the device-dependent current distribution and subsequent electromigration. We determine the effect of current density and magnetic layer thickness on the spin Hall magnetoresistance magnitude and signal shape of both Pt films and NiO(111)/Pt bilayers grown on sapphire substrate. The signal in both materials has a strong temperature dependence, and an exponential dependence on current, indicating the presence of thermally activated mechanisms. We suggest that more sophisticated techniques that directly probe the magnetic order are required to infer information about the AF magnetic state in such systems.

11:27AM G47.00002: Anisotropic Magnetoresistance and Nontrivial Spin Magnetoresistance in Pt/α-Fe₂O₃ Bilayers*  
SISHENG YU (Presenter), YANG CHENG, ADAM S AHMED, MENG LIN ZHU, JIN WOO HWANG, FENG YUAN YANG, Ohio State Univ - Columbus — Recently antiferromagnetic insulators (AFM) play an import role in spintronic research including the spin superfluid and long distance spin transport. However, magnetic proximity effect (MPE) has not been conclusively observed in antiferromagnet based systems. In this work, we observed anomalous Hall effect and anisotropic magnetoresistance in angular dependent magnetoresistance (ADMR) measurements in Pt on antiferromagnetic (AF) α-Fe₂O₃ (0001) epitaxial thin films at 10 K, which provide evidence for the MPE[1]. The Néel order of α-Fe₂O₃ and the induced magnetization in Pt show a unique ADMR compared with all other FM and AF systems. A macrospin response model is established and can explain the AF spin configuration and all main ADMR features in the Pt/α-Fe₂O₃ bilayers.


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11:39AM G47.00003: Magnetic anisotropy in a single crystal antiferromagnetic thin film*  
SAIMA SIDDIQUI (Presenter), University of Illinois at Urbana-Champaign, JOHN PEARSON, Argonne National Laboratory, AXEL HOFFMANN, University of Illinois at Urbana-Champaign — Antiferromagnetic (AF) materials promise to show magnetization dynamics, including switching, at ultra-high frequency and thus are of immense interest for next generation memory and logic applications. Besides, spin waves in AF insulators propagate very efficiently. However, electrically reading the states of the AF materials is not easy. Recently, spin Hall magnetoresistance (SMR) has been identified as one of the promising ways to access the surface states of the AF insulators. In this work, we deposit α-Fe₂O₃ (200 nm)/Pt (6 nm) on (11-20) Al₂O₃. We measure SMR of Pt Hall bar on Fe₂O₃. Below Morin transition temperature, we observe positive and negative magnetoresistance in the Pt/Fe₂O₃ bilayers depending on the direction of the electrical currents at the spin flop transition. This identifies that SMR can clearly determine the anisotropy of thin film AF insulators. We will show the detail study of the dependence of magnetoresistance on angular fields at different temperatures. Our study reveals important physical phenomena in AF Fe₂O₃ thin film.

*This work was supported by the Department of Energy, Office of Science, Materials Science and Engineering Division and by the NSF through U of Illinois at Urbana-Champaign Materials Research Science and Engineering Center DMR-1720633.
11:51AM G47.00004: Néel vector switching in enhanced-\(T_N\) magnetoelectric thin films* 
ATHER MAHMOOD (Presenter), WILL ECHTENKAMP, JUNLEI WANG, CHRISTIAN BINEK, University of Nebraska - Lincoln — Controlling magnetism by electrical means is a key challenge in the field of spintronics and essential for energy efficient devices in computing. Voltage-controlled switching of magnetization is manifested through boundary magnetization in \(\text{Cr}_2\text{O}_3\) and promises non-volatile spintronic memory and logic devices. In pure \(\text{Cr}_2\text{O}_3\), switching of the state variable takes place through magnetoelectric reversal of the Néel vector but the operation is limited to \(T< 307\) K. In contrast, in B-doped \(\text{Cr}_2\text{O}_3\), toggling of antiferromagnetic states is demonstrated in zero magnetic field between 300 and 400K. Various mechanisms including concentration dependent \(T_N\)-enhancement, voltage-controlled anisotropy, spin-canting, and a Néel spin orbit torque are simultaneously activated. Our results demonstrate that B-doping turns magnetoelectric \(\text{Cr}_2\text{O}_3\) into a high-\(T_N\) multi-functional material with electrically switchable Néel vector enabling CMOS compatible ultra-low power antiferromagnetic spintronics which operates in zero magnetic field.

*This work was supported in part by the MURI program, by nCORE, a subsidiary of the SRC, by AMML and NSF, and by MRSEC. The research was performed in part in the Nebraska Nanoscale Facility, and NCMN which are supported by the NSF and the Nebraska Research Initiative.

12:03PM G47.00005: Voltage Controlled Anisotropy in Boron-doped \(\text{Cr}_2\text{O}_3\) thin films*  
WILL ECHTENKAMP (Presenter), Ather Mahood, Christian Binek, University of Nebraska - Lincoln — Voltage controlled magnetization is a promising route for next-generation low-energy magnetic recording and logic devices. Utilizing magnetoelectric chromia (\(\text{Cr}_2\text{O}_3\)) based heterostructures, electric control of ferromagnetic exchange bias has been achieved up to the bulk Néel temperature of 307 K. Recently, it has been shown the Néel temperature of chromia can be increased to 400 K by boron doping. Moreover, boron doping could also introduce spin canting and enhance voltage controlled anisotropy which has been predicted in pure chromia, transforming B-doped chromia into a high-\(T_N\) multi-functional material. Here the spin flop transition of chromia is investigated and inferences about the crystal anisotropy are drawn. Utilizing low-temperature spin-flop magnetic measurements in B-doped chromia thin films, voltage controlled anisotropy is investigated for the first time in these films, with significant implications for future spintronic devices.

*This work was supported in part by the MURI program, by nCORE, a subsidiary of the SRC, by AMML and NSF, and by MRSEC. The research was performed in part in the Nebraska Nanoscale Facility, and NCMN which are supported by the NSF and the Nebraska Research Initiative.
12:15PM G47.00006: Antiferromagnetic Domain Dynamics in Nickelate Heterostructures
SANGJAE LEE (Presenter), JUAN JIANG, Yale University, GILBERTO F L FABBRIS, CLAUDIO MAZZOLI, Brookhaven National Laboratory, ANKIT DISA, Yale University, MARK DEAN, Brookhaven National Laboratory, FREDERICK J WALKER, CHARLES H AHN, Yale University — Understanding the energetics of the antiferromagnetic (AF) domains and the timescale of their fluctuations in a magnetic material are important for its application in spin-based electronics. NdNiO₃ (NNO) undergoes an AF transition at ~150K, and thus it serves as an oxide platform to study and engineer its AF ground state. We investigate how dimensional confinement leads to phase fluctuations in atomically layered (NdNiO₃)ₘ/(NdAlO₃)ₙ heterostructures through x-ray photon correlation spectroscopy (XPCS). The speckle patterns arising from coherent x-ray scattering provide the information on long- and short- ranged correlations for different heterostructures with varying thickness of nickelate layers, m, and aluminate layers, n. We find that the dynamics of the AF domain boundaries are dramatically enhanced as the dimensionality of the NNO layers are reduced, approaching the 2D limit. The dynamics of AF domain fluctuations in the heterostructure can be further tailored by tuning the interlayer coupling of nickelate layers. Our study demonstrates a path to characterize any long-range orders in quantum materials under dimensional effect and enables us to control AF domain configurations in oxide heterostructures.
12:27PM G47.00007: Spin transport in antiferromagnetic insulators: progress and challenges [Invited]  DAZHI HOU (Presenter), Hefei National Laboratory for Physical Sciences at the Microscale (HFNL), University of Science and Technology, China, ZHIYONG QIU, Dalian University of Technology, Dalian, China, JOSEPH BARKER, School of Physics and Astronomy, University of Leeds, KEI YAMAMOTO, Japan Atomic Energy Agency, OLENA GOMONAY, Institute of physics, Johannes Gutenberg Universität Mainz, Mainz, Germany, EIJI SAITOH, University of Tokyo — Spin transport is the key process for the operation of spin-based devices, which has been the focus of the spintronics research in the last two decades. Conductive materials such as semiconductors and metals, in which the spin transport relies on electron diffusion, were employed as the channels for spin transport in most studies. Due to the absence of conduction electron, insulators were excluded from the candidates for spin current channel before 2010. However, since the demonstration of the spin transmission through ferromagnetic insulator, it was realized that insulators with magnetic ordering can also serve as channels for spin transport[1]. In this talk I would like to introduce our recent progress of spin transport in antiferromagnetic insulators, e.g., the observations of temperature dependence of spin transmission, and spin current switching[2,3]. I would like to discuss the challenges for developing the functionality of antiferromagnetic insulator as well[4].


1:03PM G47.00008: Spin Transport in Multiferroic BiFeO$_3$ thin films*  HONGRUI ZHANG (Presenter), XIAOXI HUANG, YEN-LIN HUANG, RAMAMOORTHY RAMESH, Department of Materials Science and Engineering, University of California, Berkeley — Creation, detection, manipulation of spin current are the core issues in the spintronics field. In general, spin current can be manipulated by tuning charge current. BiFeO$_3$ is a multiferroic material, which has a strong magneto-electric coupling. We study spin-current transmission in La-doped BiFeO$_3$ (LBFO) thin films by using a trilayer device that sandwiches a LBFO thin film between a magnetic CoFe and a strong spin orbit coupling SrRuO$_3$ layer. Spin current transmission in LBFO thin films can be controlled by the electric field and La-doping concentration through changing antiferromagnetic spin orientation. The control of pure spin current by multiferroic materials may provide a new route towards next-generation electronics.

*This work is supported by an ARO-MURI
1:15PM G47.00009: Unleashing antiferromagnetic fluctuations for charge and spin responses of pseudo-spin-half square-lattice  LIN HAO (Presenter), JUNYI YANG, HAN ZHANG, University of Tennessee, Knoxville, DEREK MEYERS, Brookhaven National Laboratory, HIDEAMARU SUWA, ZHENTAO WANG, University of Tennessee, Knoxville, MARK DEAN, Brookhaven National Laboratory, CRISTIAN BATISTA, JIAN LIU, University of Tennessee, Knoxville — While manipulation of antiferromagnetic (AFM) order arises to the forefront of spintronics, it is a long-standing fundamental problem lying at the heart of correlated electron physics. Here we will present a series of exciting findings in pseudo-spin-half square-lattice systems, which are implemented as artificial layered iridates [(SrIrO$_3$)$_1$/SrTiO$_3$]$_m$ to engage with a staggered magnetic field effect (STMF) due to strong spin-orbit interaction. By tuning the SrTiO$_3$ spacer, the AFM structure of the Mott insulating state can be engineered [Phys. Rev. Lett. 119, 027204 (2017)]. With $m = 1$, the STMF leads to an intriguing positive anomalous magnetoresistance that probes the AFM susceptibility, because of the strong interplay between charge and longitudinal spin fluctuations [Nat. Commun. Accepted (2019)]. Upon driving the AFM structure to the two-dimensional limit at $m = 2$, while the ordering temperature is significantly reduced by strong critical fluctuations, the STMF allows an external field of only a thousandth of the superexchange interaction to greatly suppress the AFM fluctuations and enable a giant response of the AFM order [Nat. Phys. 14, 806 (2018)].

1:27PM G47.00010: Intrinsic Exchange Bias in Epitaxial CoFe2O4 thin film* DETIAN YANG (Presenter), XIAOSHAN XU, YU YUN, Physics & Astronomy, University of Nebraska-Lincoln — Exchange bias (EB), traditionally known as an interface phenomenon between ferro- or ferrimagnetic (FM) materials and antiferromagnetic (AFM) materials, has been successfully applied in magnetic storage and spintronic devices. Recently, surprising “intrinsic” EB (IEB) effects without a nominal AFM layer have drawn much attention. To ascertain the mechanism of IEB, we grew CoFe2O4 thin films epitaxially on sapphire (0001) substrates by pulsed laser deposition and studied its magnetometry by superconducting quantum interference device. In this single film, magnetization loops indicate the coexistence of a soft and a hard FM component, while the observed EB effect ---their clear shifts from the origin, suggest the existence of another AFM component. Analyses based on Preisach model demonstrate that only the hard FM component contributes to the EB. Thickness and temperature dependent EB and coercivity signatures are also extracted from these triple-component hysteresis loops. Our experiment suggests a potential application of adjustable EB and provide new platforms to study the elusive mechanism of intrinsic EB.

*This work was supported by the NSF DMR-1454618
1:39PM G47.00011: Fabrication of GeNi$_2$O$_4$, GeCu$_2$O$_4$, and MgCr$_2$O$_4$ Epitaxial Thin Films*
FANGDI WEN (Presenter), DENIS VASIUKOV, MIKHAIL KAREEV, XIAORAN LIU, LIANG WU, Rutgers University, New Brunswick, PADRAIC SHAFER, ELKE ARENHOLTZ, Lawrence Berkeley National Laboratory, Advanced Light Source, JAK CHAKHALIAN, Rutgers University, New Brunswick — In the AB$_2$O$_4$ spinel system with B site magnetic, a rich variety of magnetic and orbital frustration has been observed. Highlighted phenomena like spin-liquid phase and field-induced novel phase transitions were seen in these single-crystal systems extensively. Here we report on the first growth of the (001)-oriented GeNi$_2$O$_4$, (001)-oriented GeCu$_2$O$_4$ and (111)-oriented MgCr$_2$O$_4$. All fabricated films were characterized by X-ray diffraction and X-ray photoelectron spectroscopies confirming both crystalline epitaxy and chemical stoichiometry. Synchrotron-based X-ray absorption spectroscopies were also carried out to prove the correct electronic state. The availability of single-crystalline thin films can pave the road to understand the magnetic ordering of differently-oriented spinels in an ultra-thin limit.

*This work was supported by the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant No. GBMF4534, and by the Department of Energy under Grant No. DESC0012375. This research used resources of the Advanced Light Source, which is a Department of Energy Office of Science User Facility under Contract No. DEAC0205CH11231.

1:51PM G47.00012: Designing complex exchange interaction pathways in spinel films using entropy stabilization*
THOMAS ZAC WARD (Presenter), ALESSANDRO MAZZA, Oak Ridge National Laboratory, BRIANNA MUSICO, University of Tennessee, ELIZABETH SKOROPATA, YOGESH SHARMA, WENRUI ZHANG, Oak Ridge National Laboratory — Magnetic behaviors in AB$_2$O$_4$ spinels are dictated by the magnetic exchange interactions within and between the tetrahedral and octahedral sublattices. Functionality is then tied directly to the distribution and type of cations present within the unit cell. We will present our recent work developing entropic stabilization to synthesize single-crystal high entropy spinel oxide films of the AB$_2$O$_4$ type, where the cation sites are populated by 5 or more elements. We will describe how cation selection can be used to modify the type and strength of exchange interactions present in the crystal lattice. Lab-scale magnetic and structural characterization combined with beamline-based x-ray spectroscopy and neutron diffraction demonstrate the presence of highly tunable and varied magnetic responses; including: room temperature ferrimagnetic insulating states, surface-stabilized spin textures, tunable compensation points, and extraordinarily high strain-induced magnetic anisotropy.

*This work was supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
2:03PM G47.00013: Tunable electronic and magnetic properties in Eu$_{1-x}$La$_x$TiO$_3$ (0< x <1) 
HYUNGKI SHIN (Presenter), Department of Physics, University of British Columbia, BRUCE DAVIDSON, FENGMIAO LI, CHONG LIU, Quantum material institute, University of British Columbia, RONNY SUTARTO, Canadian Light Source, KE ZOU, Department of Physics, University of British Columbia — We explore the magnetic transitions and electronic structures of strained Eu$_{1-x}$La$_x$TiO$_3$ (0<x<1) grown by oxide molecular beam epitaxy (MBE). In bulk, undoped EuTiO$_3$ (Ti$^{4+}$) is insulating and antiferromagnetic with a Néel temperature of ~ 5.5 K, while LaTiO$_3$ (Ti$^{3+}$) is a Mott insulator with a Néel temperature of ~ 160K. Previous experiments of doping EuTiO$_3$ or LaTiO$_3$ thin films show novel emergent states, such as ferromagnetism, skyrmions, and metal-insulator transition. We show the studies of high-quality thin films of Eu$_{1-x}$La$_x$TiO$_3$ from x = 0 to x = 1. With a different ratio of Eu$^{2+}$/La$^{3+}$, we observe a series of transitions in the films. We will complete the phase diagram of this system.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G48 DCMP: Superconductivity in Low Dimensional Systems II

11:15AM G48.00001: Dimensionality of the Zeeman energy in conductors* RICHARD KLEMM (Presenter), AIYING ZHAO, Physics, Univ of Central Florida, QIANG GU, Physics, University of Science and Technology Beijing, TIMOTHY HAUGAN, Wright-Patterson Air Force Base, US Air Force Research Laboratory — The Dirac equation is extended for a relativistic electron or hole in an orthorhombically-anisotropic conduction band with effective masses $m_j$ for j=1,2,3 with geometric mean $m_g=(m_1m_2m_3)^{1/3}$. Its covariance is established with general proper and improper Lorentz transformations. The non-relativistic Hamiltonian is evaluated to order $1/(mc^2)^4$, where $mc^2$ is it's Einstein rest energy. For the magnetic induction $B$ in the crystallographic direction $\hat{e}_j$, the Zeeman $g$ factor is $2m(m_j/m_g^3)^{1/2}$. While propagating in a monolayer two-dimensional conduction band, $g$ is much less than 2 for $B$ parallel to the monolayer, as observed recently in superconducting monolayer NbSe$_2$, $B_{c2,||}$ of which appears to violate the `"Pauli limit" by a order of magnitude. In one-dimensional chain conductors of atomic thickness, $g$ is small for all $B$ directions while the particle is in its conduction band. The precise form for the quantum spin Hall energy is also found for a particle in a two-dimensional metal.

*Supported by the National Natural Science Foundation of China through Grant No. 11874083. A. Z. is supported by the China scholarship council. R. A. K. was supported by the AFOSR through their summer faculty fellowship program.
Controlling the charge dispersion of a nearly-open superconducting island

ARNO BARGERBOS (Presenter), WILLEMIJN UILHOORN, QuTech, Delft University of Technology, BERNARD VAN HECK, CHUNG-KAI YANG, Quantum Lab Delft, Microsoft, PETER KROGSTRUP, Quantum Materials Lab Copenhagen, Microsoft, LEO P KOUWENHOVEN, GIJS DE LANGE, ANGELA KOU, Quantum Lab Delft, Microsoft — Isolation from the environment determines the extent to which charge is confined on an island, which manifests experimentally through Coulomb oscillations such as charge dispersion. In superconducting circuits, the link to the environment has typically been formed from tunnel junctions. If instead a transparent ballistic junction forms the link between the superconducting island and the environment, Coulomb oscillations are predicted to suppress far more rapidly than for tunnel junctions due to imaginary-time Landau-Zener tunneling. Here we investigate the charge dispersion of a nanowire transmon hosting a quantum dot in the junction. We observe rapid suppression of the charge dispersion consistent with the scaling law resulting from diabatic transitions between Andreev bound states. We also observe greatly improved qubit coherence times at the point of highest charge dispersion suppression. Our observations further our fundamental understanding of charging effects in superconductors and suggests novel approaches for building charge-insensitive qubits.

This work has been supported by funding from the Dutch Research Council (NWO) and the Microsoft Quantum initiative.

Calorimetric Observation of Magnetic-Field-Induced High-Field FFLO Superconducting Phase in λ-(BETS)$_2$GaCl$_4$

NATHANAEL FORTUNE (Presenter), Physics, Smith College, ANDREAS RYDH, Physics, Stockholm University, JOYCE ELLEN PALMER-FORTUNE, Physics, Smith College, CHARLES C AGOSTA, Physics, Clark University, AKIKO KOBAYASHI, Chemistry, Nihon University — When an external magnetic field is applied parallel to the conducting layers in quasi-2D organic superconductors, a phase transition to a new, high-field, superconducting state with a spatially modulated superconducting order parameter can occur at the Clogston-Chandrasekhar paramagnetic limit $H_p$, as first predicted by Fulde, Ferrell, Larkin, and Ovchinnikov (FFLO). Candidate FFLO phases have been identified through NMR, RF penetration depth, magnetic torque, and transport measurements in a number of organic superconductors; in the case of the archetypal 2D organic superconductor κ-(BEDT-TTF)$_2$Cu(NCS)$_2$, corroborating evidence has been provided by the calorimetric observation of a first order phase transition at $H_p$ into a new high-field, higher-entropy superconducting phase. This evidence has been lacking, however, in other candidate FFLO systems. We report here low-temperature specific heat measurements in a second expected FFLO organic superconductor: λ-(BETS)$_2$GaCl$_4$. For field-angles within 0.5° of plane-parallel, we observe an enhancement of the upper critical field superconducting phase boundary $H_{c2}(T)$, a calorimetric signature of pancake vortex formation with decreasing field at $H_p$, and a field-induced phase transition between the upper and lower superconducting states.
11:51AM G48.00004: Anomalous Metallic Phase in Tunable Destructive Superconductors*
SAULIUS VAITIEKENAS (Presenter), PETER KROGSTRUP, CHARLES MARCUS, Center for Quantum Devices and Microsoft Quantum Lab--Copenhagen, Niels Bohr Institute, University of Copenhagen — The Little-Parks effect---a flux-dependent modulation of the transition temperature in multiply connected superconductors---results from the quantization of fluxoid through holes in superconductors. In hollow superconducting cylinders with diameter smaller than the superconducting coherence length, flux-induced supercurrents can give rise to the destructive Little-Parks effect, characterized by repeated reentrant quantum phase transitions between superconducting and metallic phases. Here, we use axial and transverse magnetic fields to control the crossover between the conventional and destructive Little-Parks regimes in nanowires with an epitaxial Al shell fully surrounding InAs core. The observed dependence on flux, transverse field, temperature, and current bias is in excellent agreement with theory. Near the crossover between the conventional and destructive regimes, an anomalous metal phase is found. The anomalous metallic phase is characterized by a field-controllable, temperature-independent resistivity between adjacent superconducting lobes.


*This research was supported by Microsoft, and the Danish National Research Foundation.

12:03PM G48.00005: Study of 2D superconductivity at oxide interfaces by microwave resonators  YILDIZ SAGLAM (Presenter), EDOUARD LESNE, DANIEL BOTHNER, FELIX SCHMIDT, Delft University of Technology, MARC GABAY, Paris-Saclay University, ANDREA CAVIGLIA, GARY STEELE, Delft University of Technology — The emergent two-dimensional electron system (2DES) formed at the interface between LaAlO3 (LAO) and SrTiO3 (STO) insulating oxides has been a subject of great interest in condensed matter physics during the last decade. Recently, (111)-oriented LAO/STO interfaces have been shown to exhibit an electronic correlation driven reconstruction of its band structure and a two-dimensional superconducting (SC) ground state, both tunable by electrostatic field-effect. Superconducting coplanar waveguide (SCPW) resonators are tools of exquisite sensitivity for probing low energy excitations in quantum materials, due to their intrinsic low ohmic losses and high-quality factors, highly relevant to quantum technology platforms. Here, in order to study the superconducting state at the LAO/STO(111) interface, we designed embedded SCPW resonators whose microwave resonance frequency can be tuned by electrostatic gating, manifesting a change of the 2DES’ superfluid density through a large change of its kinetic inductance. This allows us to map the SC phase diagram in a detection scheme that goes beyond traditional resistive measurements. Our work highlights the potential of such an approach to the fundamental study of superconductivity in complex materials.
12:15PM G48.00006: Ising superconductors: the interplay of magnetic field, triplet channels and disorder*  
DAVID MÖCKLI (Presenter), MAXIM KHODAS, The Racah Institute of Physics, The Hebrew University of Jerusalem — We study the superconducting instability in disordered non-centrosymmetric monolayers with intrinsic Ising spin-orbit coupling (SOC) subjected to an in-plane Zeeman magnetic field. The pairing interaction contains the channels allowed by crystal symmetry, such that in general, the pairing state is a mixture of singlet and triplet Cooper pairs. The joint action of SOC and Zeeman field selects a specific in-plane \( \mathbf{d} \)-vector triplet component to couple with the singlets, which gains robustness against disorder through the coupling. The out-of-plane \( \mathbf{d} \)-vector component, that in the clean case is immune to both the Zeeman field and SOC is obliterated by a small impurity scattering rate. We formulate the quasi-classical theory of Ising superconductors and solve the linearized Eilenberger equations to obtain the pair-breaking equations that determine the Zeeman field - temperature dependence of the continuous superconducting transition. Our discussion emphasizes how the Zeeman field, SOC and disorder affect the different superconducting order parameters, and we show how the spin-fields inevitably induce odd-frequency pairing correlations.

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Phys. Rev. B 99, 180505(R), 2019

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Israel Science Foundation, Grant No. 1287/15

GAURAV CHAUDHARY (Presenter), ZHIQIANG WANG, KATHRYN LEVIN, University of Chicago — In this talk we discuss the signatures of the pseudogap effects seen in transport studies of superconducting magic angle twisted bilayer graphene (MATBG). They should be viewed as rather natural; quite generally pseudogap phenomena are widely observed in very thin superconducting films of conventional materials such as Pb and TiN, high \( T_c \) cuprate superconductors and in interfacial superconductors. The pseudogap regime is characterized by two distinct temperature scales corresponding to the onset of phase coherence, i.e. \( T_{BKT} \) and the onset of pairing, i.e. \( T^* \). Here we develop the pairing fluctuation theory of the Berezinskii-Kosterlitz-Thouless (BKT) transition for the MATBG, demonstrating how pseudogap effects are enhanced in two dimensional superconductors. Moreover, they do not require anomalously strong attractive pairing mechanisms as proposed for the 3D cuprates. Using our theory along with the transport estimates for the pairing onset temperature \( T^* \), we quantify the expected strength of the pairing and fluctuations for the MATBG superconductors. Finally, we propose new tunneling based experiments from one two dimensional system to another, which can further probe the pseudogap phenomena.
12:39PM G48.00008: Quantum transport of atomically thin $1T_d$-MoTe$_2$  XIRUI WANG (Presenter), KENJI YASUDA, Massachusetts Institute of Technology MIT, DANIEL A RHODES, Columbia University, TAKEHITO SUZUKI, Massachusetts Institute of Technology MIT, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, JOSEPH G CHECKELSKY, Massachusetts Institute of Technology MIT, JAMES C HONE, Columbia University, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology MIT — There has been growing interest in the study of crystalline 2D superconductors, especially those with low carrier densities with gate tunability. Recently, it is reported that monolayer $1T_d$-MoTe$_2$ exhibits superconductivity with transition temperature of 8 K [1], much enhanced from the bulk whose $T_c = 0.1$ K [2], and higher than the isostructural monolayer $1T_d$-WTe$_2$ with its $T_c = 0.7$ K [3,4]. Whereas monolayer MoTe$_2$ is inversion-symmetric, inversion-symmetry is broken in bilayer MoTe$_2$ due to the stacking arrangement, which can change the superconducting properties. Here we will report the quantum transport properties of bilayer and monolayer MoTe$_2$, for a better understanding of its superconductivity, and pursuing topologically non-trivial state in this platform.


12:51PM G48.00009: Strong pairing in two dimensions: Pseudogaps, domes, and other implications*  KATHRYN LEVIN (Presenter), James Franck Institute, University of Chicago, XIAOYU WANG, National High Magnetic Field Laboratory, QIJIN CHEN, University of Science and Technology of China — The recent interest in superconductivity of strongly correlated 2D materials is driven by exciting discoveries of novel superconductors such as magic-angle twisted bilayer graphene (MATBG), FeSe monolayers and transition metal dichalcogenides. These are generally thought to be distinct from BCS-Eliashberg superconductors, and can be argued, from the Uemura plot, to be intermediate between BCS and Bose-Einstein condensation (BCS-BEC). In this talk we compute the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature $T_{BKT}$ and pairing onset $T^*$ as a function of pairing interaction strength $g$ and of density using this crossover theory. Rather than solving directly for the phase stiffness parameter we follow the literature on atomic Bose systems (which is based on a Quantum Monte Carlo analysis) and which constrains the total phase space density at the transition. Our results for $T_{BKT}$ compare favorably with Fermi gas experiments and yield the expected BCS and BEC asymptotes for a film with lattice dispersion. Given the measured $T_{BKT}$, we provide estimates for the pairing gap and for $T^*$ in concrete systems such as MATBG.

*Supported by NSF (grant # DMR-1420709) and NSF of China (grant #11774309)
In situ mutual inductance measurement of superconducting atomic films: Si(111)-√7 × √3-In and monolayer FeSe on SrTiO₃  
MING-CHAO DUAN (Presenter), YANFU WU, GANG YAO, CANHUA LIU, JINFENG JIA, Shanghai jiao Tong Univ — Many of the novel 2D superconducting films with highly crystalline structure and atomic thickness, fabricated in ultrahigh vacuum chambers, are highly vulnerable to air exposure, making it difficult to measure intrinsic superconducting properties such as zero resistance and perfect diamagnetism with ex situ experimental techniques. To realize vacuum-based measurements, we developed a multifunctional scanning tunneling microscope. The conventional STM probe in the microscope can be switched, under vacuum conditions, to a two-coil probe that can detect whether a material exclude magnetic flux. By using this in situ mutual inductance technique, for the first time, we succeeded in detecting the intrinsic diamagnetic response in both two-atomic-layer indium film on a Si(111) surface and monolayer FeSe films on SrTiO₃. The Si(111)-√7 × √3-In films is expected as a conventional superconductor according to previous STM study. Our diamagnetic measurements verify that the low-temperature variation of penetration depth in Si(111)-√7 × √3-In films follows the BCS theory in the dirty limit. On the other hand, the behavior of monolayer FeSe films on SrTiO₃ in the external magnetic field indicates a vortex melting picture.

Multi-carrier states in the Peierls electron-phonon model  
ALBERTO NOCERA (Presenter), University of British Columbia, JOHN SOUS, Departments of Physics and Chemistry, Columbia University, MONA BERCIU, University of British Columbia — Motivated by the discovery of light polarons and bipolarons in the Peierls electron-phonon model on a one dimensional lattice [1], we numerically study few-carrier states (up to six) using the density matrix renormalization group method. Our results show that a bipolaron liquid is a stable ground state in a wide range of phonon frequencies and electron-phonon interaction strengths. More interestingly, we provide numerical evidence that this homogeneous multi-carrier state for a sufficiently large electron-phonon coupling strength becomes unstable in favor of a multi-polaron complex suggestive of phase separation. We provide analytical arguments in support of our numerics based on an effective multi-body interaction between electrons mediated by phonons [2]. We finally show preliminary results for the case of two coupled chains and discuss the implications of the results for two dimensional systems.

1:27PM G48.00012: Bi$_2$Sr$_2$CaCu$_2$O$_8$ single crystal exfoliation, characterization, and manipulation*  PEDRO MERCADO LOZANO (Presenter), QIANG LI, Condensed Matter Physics and Material Science Division, Brookhaven National Laboratory, YOUNG JAE SHIN, Center for Functional Nanomaterials, Brookhaven National Laboratory, GENDA GU, Condensed Matter Physics and Material Science Division, Brookhaven National Laboratory — Bi$_2$Sr$_2$CaCu$_2$O$_8$ (BSCCO) is a high T$_c$ cuprate superconductor whose layered crystal structure allows the study of thickness dependence of its superconducting properties down to mono-layer. We developed a process to manipulate and analyze BSCCO single crystal and bi-crystal junctions at different film thickness. First, thickness characterization was performed through profile extraction with atomic force microscopy (AFM). A transfer stage was then used to isolate individual flakes of varying thickness in order to study their magnetic response on a SQUID magnetometer. Thin films of less than 100 nm were found to maintain their superconducting properties, which can be inferred from the observation of Meissner effect on the samples. Finally, by using the transfer stage, different layers of BSCCO were rotated around the c-axis and stacked on top of each other. These manipulations enable the study of superconducting properties of bi-crystal junction as a function of the twist angle and the layer thickness.

*This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

1:39PM G48.00013: An unexpected charge doping mechanism for quasi-one-dimensional ACr$_3$As$_3$ superconductors  KEITH TADDEI (Presenter), LIURUKARA D SANJEEWA, Oak Ridge National Lab, BING-HUA LEI, YUHAO FU, University of Missouri, QIANG ZHENG, Oak Ridge National Lab, DAVID SINGH, University of Missouri, ATHENA S. SEFAT, CLARINA RELOJ DELA CRUZ, Oak Ridge National Lab — In the race to find topological materials, superconductivity has found renewed interest as potential hosts of Majorana Fermions. However, realizing such states is non-trivial requiring for instance Cooper pairs with finite orbital-momentum or Dirac-like dispersions in the normal state. Recently, a new family of quasi-1D superconductors $A_{1.2}$Cr$_3$As$_3$ ($A$= Alkali metal) was discovered which is interesting in these regards for realizing spin-triplet superconductivity and having Dirac-like crossings near $E_F$. However, its study has been hampered due to extreme air sensitivity and an inability to charge dope. Here, we report results of diffraction studies and DFT work on KCr$_3$As$_3$ which solve both these problems. We show that the reported growth technique inherently intercalates H into the quasi-1D CrAs tubes and that the H acts as an electron donor. Furthermore, we reveal that the reported discrepancy in sample behavior (with some superconducting and others spin-glasses) is actually due to the amount of H. This work suggests a new stoichiometry KH$_{1-x}$Cr$_3$As$_3$, which is air stable and provides a charge doping mechanism. This allows for tuning between frustrated magnetism and superconductivity in a quasi-1D material as well as a potential route to reach the predicted Dirac points.
1:51PM G48.00014: Textured one-dimensional superconducting nanostructures*  
ROBERT LYNN, KRISTINE UNG, LEO V SEMENTILLI, NINA MARKOVIC (Presenter), Goucher College — We have fabricated one-dimensional superconducting nanostructures with precisely controlled texture. The fabrication method that combines nanoscale shadow mask deposition with in situ controlled etching allows nanoscale features to be drawn directly onto the substrate. By controlling the speed with which the shadow mask is translated over the substrate, we can vary the thickness of the nanostructure as it is being deposited. The thickness modulation allows us to control the shape of the superconducting wavefunction in these nanostructured wires, which can be detected in electrical transport measurements at low temperatures and in magnetic field.

*This work was supported in part by National Science Foundation under DMR-1663683 and the Croatian Science Foundation under HRZZ IP-2016-06-2289 C3TiNN.

2:03PM G48.00015: New Method for Identifying the FFLO State in λ-(BETS)$_2$GaCl$_4$ Using Sample Rotation*  
BRETT LARAMEE (Presenter), RAJU GHIMIRE, CALVIN BALES, Clark University, WILLIAM A CONIGLIO, National High Magnetic Field Laboratory, CHARLES C AGOSTA, Clark University, JOHN A SCHLUETER, National Science Foundation, AKIKO KOBAYASHI, Nihon University — The FFLO state is a state of inhomogeneous superconductivity that exists at high magnetic fields. In specific crystals, the point where Cooper pairs begin to break due to paramagnetic effects, $H_p$, happens before reaching the ultimate critical field, $H_{c2}$. We will present rf penetration depth measurements on the quasi-2D layered organic superconductor λ-(BETS)$_2$GaCl$_4$ (BETS) using a tunnel diode oscillator. The quasi-2D structure of BETS makes features such as $H_{c2}$, the FFLO phase transition, and vortex effects like the lock-in effect highly sensitive to the angle that the conduction planes make with the external field. By rotating the sample in a constant external magnetic field, we can locate points on the FFLO phase line that are not easily identifiable via field sweeps. In addition, we will visualize the FFLO phase transitions in BETS by showing a Field−Angle phase diagram at very low temperature (60 mK). With the addition of this new technique, we have begun constructing a full 3D Field−Angle−Temperature phase diagram of the FFLO state.

*We acknowledge funding from NSF DMR-1905950.
A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-11157490 and the state of Florida.
11:15AM G49.00001: Quantum Synchronization and Superconductivity  JONATHAN CURTIS (Presenter), VICTOR GALITSKI, University of Maryland, College Park — Synchronization is a phenomenon whereby weak interactions between oscillators enables a macroscopic phase coherence to develop. While this phenomenon is well known in the context of classical dynamical systems, its extension to quantum oscillators has been relatively un-explored. In this talk we will consider a model where the quantum oscillators are realized by a local superconducting order parameter. We will then study under what circumstances interactions lead to synchronization of the phase, enhancing the phase coherence and superconductivity of the sample.

11:27AM G49.00002: Theory of the nonlinear susceptibility of layered superconductors: application to strontium ruthenate*  FEI CHEN (Presenter), DAMJAN PELC, MARTIN GREVEN, RAFAEL FERNANDES, University of Minnesota — Probing superconducting fluctuations (SF) in unconventional superconductors is essential to elucidate their nature. Much work has been done to elucidate the contributions from SF to the conductivity and the linear susceptibility, disentangling them from normal state contributions can be challenging. An alternative that has been recently explored is to measure the nonlinear susceptibility via third-order magnetic response, which is believed to be dominated by SF above $T_c$. Here, we present a phenomenological theoretical model for the nonlinear susceptibility of layered superconductors. Our model, based on the Lawrence-Doniach functional, predicts power-law behaviors in distinct temperature and magnetic field regimes. Comparison with data from conventional BCS superconductors reveals an excellent agreement between theory and experiment. The same does not happen, however, for oxide superconductors, such as the strontium ruthenate $\text{Sr}_2\text{RuO}_4$ [D Pelc et al., Nat. Commun. 10, 2729 (2019)]. We show that inclusion of disorder can capture some of the experimental features. Finally, we discuss the limitations and possible extensions of our model.

*Supported by the U. S. Department of Energy through the University of Minnesota Center for Quantum Materials, under Award No. DE-SC-0016371.
11:39AM G49.00003: Current induced Non equilibrium states In NbTi superconducting Bridge

KHALIL HARRABI (Presenter), King Fahd Univ KFUPM, JEAN PAUL MANEVAL, Physics Department, ENS, Paris, France, LPA —

We report on the discrimination between dissipative states in NbTi superconducting filament on polished crystalline Al2O3 using current driven pulse technique. A current pulse larger than the depairing current ($I_c$) initiates a dissipation in a localized spot. The non-equilibrium state described by the two dissipative mechanism pinpointed as hot spot or phase slip center. A voltage underlines the collapse of the superconductivity show up after a certain delay time $t_d$. We found that the hostspot occurs at low temperature, the phase slip center close to the transition temperature, and proved that a hot spot is ignited by a phase slip center. The thermal relaxation time was ratiocinated from fitting the experimental data with the Time-Dependent Ginzburg-Landau (TDGL) theory due to M. Tinkham at low and high temperature.

*K.H gratefully acknowledges the support of the King Fahd University of Petroleum and Minerals, Saudi Arabia, under the SB181006 DSR project.

11:51AM G49.00004: Photo-Manipulation of Superconductivity in an Extended Hubbard Model

WEI-CHIH CHEN (Presenter), Department of Physics, University of Alabama at Birmingham, YAO WANG, Department of Physics, Harvard University, CHENG-CHIEN CHEN, Department of Physics, University of Alabama at Birmingham — Photo-induced phase transition is a promising approach to engineering material properties and has been demonstrated experimentally in several strongly correlated systems. Here, we numerically study intertwined orders involving charge, spin, and superconductivity in an extended Hubbard model by exact diagonalization on a 16-site square cluster. Our ground-state phases at various carrier doping match previous studies based on mean-field and functional renormalization group methods. On top of the equilibrium ground states, we then investigate the non-equilibrium dynamics of various orders during and after a realistic pump pulse. We found that these intertwined orders and superconducting pairing symmetries can be selectively manipulated through light polarization, frequency, and amplitude. This work shows that using ultrafast light to control superconductivity of desired pairing symmetry is possible.

*This work is supported by NSF Award No. OIA-1738698.
12:03PM G49.00005: Charged fluctuators as a limit to the microscopic and macroscopic coherence of superconductors  
NICOLAS BOURLET (Presenter), CEA-Saclay, HÉLÈNE LE SUEUR, CNRS, ARTIS SVILANS, ANIL MURANI, CEA-Saclay, LAURENT BERGE, LOUIS DUMOULIN, CSNSM, CNRS, PHILIPPE JOYEZ, CEA-Saclay — By analyzing experiments on thin-film resonators of NbSi and TiN, we shed light on a novel decoherence mechanism at work in disordered superconductors. This decoherence is caused by charged Two Level Systems (TLS) which couple to the conduction electrons in the BCS ground state, inducing fluctuations of the kinetic inductance. Standard theories of mesoscopic disordered conductors are used to describe this effect, linking electronic (microscopic) decoherence and electromagnetic (macroscopic) decoherence in superconductors. This model is compared to the so called Generalised Tunelling Model (GTM), used to describe the impact of fluctuating TLS on the dielectric properties of the resonators. Given the omnipresence of charged TLS in solid-state systems, these decoherence mechanisms affects all experiments involving disordered superconductors, and even more so for devices with smaller cross-sections through the new mechanism presented here. In particular, we show it easily explains the poor coherence observed in quantum phase slip experiments and may contribute to lowering the quality factors in disordered superconductor resonators.

12:15PM G49.00006: Analytical Noise Spectra for Chiral d-Wave Superconducting Heterostructures*  
COREY OSTROVE (Presenter), LINDA E REICHL, University of Texas at Austin — We present analytical expressions for the noise spectrum of a chiral d-wave/normal/chiral d-wave Josephson junction. The scattering matrix is derived from the Bogoliubov de-Gennes equations without use of the Andreev approximation. We use the derived scattering coefficients to calculate the current-current correlation function directly and from this the noise spectrum (and in particular the shot noise contribution) is generated. The effects of the chiral nature of the order parameter in the scattering and noise properties of the structures are investigated and are compared to those of those of the non-chiral d-wave order parameter. Recent experimental work has produced a number of candidate materials hypothesized to have chiral d-wave order parameters, which makes theoretical characterization of these structures of particular importance.

*This work is supported by Welch Foundation Grant No. F-1051
JOHN ZASADZINSKI (Presenter), Illinois Institute of Technology, BEVERLY LOWELL, Physics, Northwestern University, NOAH SAMUELSON, Illinois Institute of Technology. — The above-gap, SIN tunneling spectral dip (bosonic mode) feature in the bilayer cuprate Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) is highly reproducible and its doping dependence links it to the resonance spin excitation. SIS junctions on Bi2212 reveal a strongly enhanced dip strength and symmetric, decreasing conductance backgrounds, indicating the elastic tunneling origin of the bosonic mode and the connection to the pairing self-energy. The observation of similar bosonic mode features in the tunneling spectra of Fe-based superconductors and other cuprate superconductors is discussed. Scanning tunneling spectroscopy (STS) on FeSe reveals a similar background shape to Bi2212 indicating the symmetric bosonic mode features also are dominated by elastic tunneling. Disorder effects which show up as a depairing rate, $\Gamma$, in the fitting of the density of states (DOS) become increasingly important for lower Tc single-layer cuprates. It is demonstrated that SIS break junctions and intrinsic c-axis junctions allow the observation of a bosonic mode in strongly disordered Bi2201 with Tc values $\leq$ 5K. The scaling of $\Omega$ with Tc over nearly two decades, and over two different classes of superconductors suggests that the bosonic mode is a universal signature of unconventional superconductivity.

12:39PM G49.00008: Dynamics of phase coherence in superconducting cuprates upon mid-infrared photoexcitation*  
ANGELA MONTANARO (Presenter), FRANCESCA GIUSTI, DANIELE FAUSTI, Univ of Trieste - Trieste. — Superconducting fluctuations in optimally-doped cuprates are known to survive well above the critical temperature, making these systems a perfect playground to investigate the possibility of transiently controlling superconductivity through ultrashort light pulses. While it has been widely shown that high photon energy electromagnetic fields melt the superconducting phase [1], there are evidences that mid-infrared photoexcitation can trigger the onset of superconductivity in regions of the phase diagram in which the system is not superconducting at the equilibrium [2,3]. We performed measurements on optimally-doped Y-Bi2212 by a 3-pulse technique which allows to disentangle these two effects. The approach is based on selectively destroying the superconducting state using a visible pump, and then further exciting the sample by means of a mid-infrared source. By probing the system through a broadband supercontinuum, we reveal the details of the transient dynamics of the condensate phase coherence solely driven by mid-infrared pulses with photon energy close to the superconducting gap.


*ERC Starting Grant (677488)
12:51PM G49.00009: Josephson phenomena in Van der Waals heterostructures* LIAM FARRAR (Presenter), Physics, University of Bath, GEETHA BALAKRISHNAN, Physics, University of Warwick, SIMON J BENDING, Physics, University of Bath —

It is well established that a dissipationless supercurrent can flow across a junction at the interface between two superconductors due to a phenomenon known as the Josephson effect. This concept has recently been extended to 2D superconductors, where Josephson effects have been successfully measured at the interface between two misaligned NbSe2 flakes [1]. In this talk we discuss progress made in the formation of Josephson junctions between electrodes with different superconducting order parameters by two methods; homojunctions formed by stacking two exfoliated flakes of the same superconductor with a well-defined twist angle, and heterojunctions formed by stacking two different superconductors (eg. NbSe2, NbS2, BSSCO). These structures behave as underdamped Josephson junctions, exhibiting strong zero-bias supercurrents as well as clear signatures of the superconducting gaps. Finally, we will discuss the applications of this approach to the formation of more complex superconducting devices such as superconducting quantum interferometer devices (SQUIDS).


This work was supported by EPSRC, UK (EP/L015544/1).

1:03PM G49.00010: Vortex effects as an indication of a transition to the FFLO state* CALVIN BALES (Presenter), Physics, Brown University, RAJU GHIMIRE, Clark University, VESNA F MITROVIC, Physics, Brown University, JOHN A SCHLUETER, National Science Foundation, AKIKO KOBAYASHI, Nihon University, CHARLES C AGOSTA, Clark University — The FFLO state is an exotic superconducting state that allows materials to remain in a superconducting state at higher fields than the paramagnetic limit where a magnetic field would normally break the singlet state of the Cooper pairs. The angular dependence of the rf penetration depth of the sample relative to the field is sensitive to distinct data signatures such as vortex lock-in where the Josephson vortices are very lightly pinned and increase the penetration depth. This presentation will discuss the process by which we were able to analyze these vortex data signatures as an indication of vortex lock-in and the transition to the FFLO state. The analysis of angular and field sweeps as well as the transformation from angular sweeps to field sweeps and vice versa make evident the validity of the features we are seeing as well as the connections between the features and vortex motion. This presentation will focus on the results of measurements of λ-(BETS)2GaCl4 and κ-(ET)2Cu(NCS)4 superconductors.

*We acknowledge funding from NSF DMR-1905950. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-11157490 and the state of Florida.
1:15PM G49.00011: Imaging dissipative current in superconducting Niobium film using scanning SQUID susceptometry  ELI MUELLER (Presenter), JOHN ROBERT KIRTLEY, RUBY SHI, HUIYUAN MAN, KATHRYN ANN MOLER, Stanford Univ — The quasiparticle density of states is a strong diagnostic of the superconducting gap and may be observed as dissipation in two coil mutual inductance experiments. Mutual inductance experiments have typically been limited to millimeter spatial resolution and therefore measure nonzero impedance resulting from motion of vortices. Susceptibility measurements with greater spatial resolution may be able to detect the additional dissipation resulting from scattering of excited quasiparticles. Scanning Superconducting QUantum Interference Device (SQUID) susceptibility measurements offer micron scale spatial resolution with the in-phase component measuring superfluid density and the quadrature component measuring dissipation. In this talk, we report on micron scale scanning SQUID susceptometry measurements on a Niobium film in an effort to observe the frequency and temperature dependence of quasiparticle scattering. Successfully observing the temperature dependence of quasiparticle excitations in Niobium would be a proof of concept to measure dissipation in unconventional superconductors with micron scale spatial resolution.

1:27PM G49.00012: Dynamic Evolutions of Flux Distributions in a Superconductor by a Pulsed Current*  HODAKA KUROKAWA (Presenter), YUTO KINOSHITA, FUYUKI NABESHIMA, MASASHI TOKUNAGA, ATSUTAKA MAEDA, Univ of Tokyo — The dynamics of vortices in a superconductor has long been investigated because of its practical importance for the application of the superconducting magnets. The direct imaging of flux-density distributions must be powerful for the understandings of the dynamics of vortices. However, observations of the time-evolution of the flux-density distributions have been scarcely reported. From this viewpoint, it is still unclear how the static state of vortices collapses into the flow state. Hence, we observed the changes of flux–density distributions in a superconductor by a pulsed current with the magneto-optical microscopy. The flux-density distributions in a NbN film were measured up to 10000 frames per second. We investigated for different initial flux distributions in a comparative manner; the field-cooled state, the remanent state, the zero-field-cooled (ZFC) state. In the remanent state and the ZFC state, local reconfiguration of vortices occurred even below the critical current, which was qualitatively explained within the critical state model. However, some deviations between experiments and the theory were observed in the ZFC state, indicating that the current flows in the sample even far below the critical current.

*JSPS Grant-in-Aid for JSPS Fellows Grant Number JP19J11421
1:39PM G49.00013: Effect of electron irradiation on rf-susceptibility of ferromagnetic superconductor EuFe$_2$(As,P)$_2$* SUNIL GHIMIRE (Presenter), KYUIL CHO, MAKARIY A TANATAR, Ames Laboratory, TSUYOSHI TAMEGAI, Department of Applied Physics, University of Tokyo, RUSLAN PROZOROV, Ames Laboratory — High resolution AC magnetic susceptibility was measured in single crystals of ferromagnetic superconductor (T$_C$=24K, T$_{Curie}$=18K), EuFe$_2$(As,P)$_2$ using tunnel diode resonator (TDR) in zero and in finite external DC magnetic fields. The same sample was irradiated with 2.5 MeV electrons at a dose that caused substantial changes of all features. Based on these and literature results, the intricate interplay between superconductivity and ferromagnetism in this unique system will be discussed.

*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract # DE-AC0207CH11358.

1:51PM G49.00014: Rotational transition, domain formation, dislocations and defects in vortex systems with combined six- and 12-fold anisotropic interactions* MACIEJ W OLSZEWSKI, MORTEN ESKILDSEN (Presenter), Department of Physics, University of Notre Dame, CHARLES REICHHARDT, CYNTHIA REICHHARDT, Theoretical Division, Los Alamos National Laboratory — We introduce a new model for a pairwise repulsive interaction potential of vortices in a type-II superconductor, consisting of superimposed six- and 12-fold anisotropies. Using numerical simulations we study how the vortex lattice configuration varies as the magnitudes of the two anisotropic interaction terms change. A triangular lattice appears for all values, and rotates through 30° as the ratio of the six- and 12-fold anisotropy amplitudes is varied. The transition causes the VL to split into domains that have rotated clockwise or counter-clockwise, with grain boundaries that are "decorated" by dislocations consisting of five- and seven-fold coordinated vortices. We also find intra-domain dislocations and defects, and characterize them in terms of their energy cost.

*This work was supported in part by the Notre Dame Center for Research Computing. Work at the University of Notre Dame was supported by the US DOE, Office of Basic Energy Sciences, under Award No. DE-SC0005051. Part of this work was carried out under support by the US DOE through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of the US DOE (Contract No. 892333218NCA000001).

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G50 DCMP: Quantum Criticality Theory Mile High Ballroom 1C - Eun-Gook Moon, KAIST
11:15AM G50.00001: Quantum Criticality of Semi-Dirac Fermions  MIKOLAJ URYSZEK (Presenter), ELLIOT CHRISTOU, Univ Coll London, AKBAR JAEFARI, Western New England University, FRANK KRUGER, Univ Coll London, BRUNO UCHOA, University of Oklahoma — Two-dimensional semi-Dirac fermions are quasiparticles that disperse linearly in one direction and quadratically in the other. We investigate instabilities of semi-Dirac fermions toward charge and spin density wave and superconducting orders, driven by short-range interactions. We analyze the critical behavior of the Yukawa theories for the different order parameters using Wilson momentum shell renormalization group. We generalize to a large number of fermion flavors, N, to achieve analytic control in 2+1 dimensions and calculate critical exponents at one-loop order, systematically including universal 1/N corrections. The anomalous dimension of the fermion fields vanishes in the large N limit, consistent with a recovery of Fermi-liquid behaviour. However, many other unusual features persist. We show that this is a consequence of non-analytic terms in the mean-field free energy of semi-Dirac fermions.

11:27AM G50.00002: Quantum Criticality of Multiband Polar Metals*  PAVEL VOLKOV (Presenter), PIERS COLEMAN, PREMALA CHANDRA, Department of Physics and Astronomy, Center for Materials Theory, Rutgers University — Quantum criticality in metallic systems leads to a variety of exotic behaviors, that sensitively depend on the type of the transition. The case of a polar transition in a metal, structurally identical to a ferroelectric transition in an insulator, has received attention recently due to the discovery of a number of metallic compounds where a polar order exists.

We show that quantum criticality of multiband polar metals is of particular interest, as a strong coupling of the charge carriers to the critical mode can be realized near the band crossings in momentum space. We provide a comprehensive classification of the possible emerging quantum critical behaviors and find evidence for strong interaction effects and, in some cases, non-Fermi liquid physics. The critical properties are found to depend on the type of band crossing as well as dimensionality. Experiments, that can allow to probe the emergent behavior, and implications for existing materials are discussed.

*P. Volkov is supported by a Rutgers Center for Materials Theory Postdoctoral Fellowship.
11:39AM G50.00003: Deconfined quantum criticality in the 2D J-Q model*  BOWEN ZHAO  
(Presenter), Boston Univ, ANDERS W SANDVIK, Boston Univ/ IOP-CAS, Beijing — The deconfined quantum critical point (DQCP) was proposed as a new scenario for quantum phase transitions fifteen years ago [1] and is still an enigmatic concept, with no general consensus on its existence. To test the DQCP proposal, which is based on a quantum field theory that cannot be solved, numerical studies of various lattice models have been considered. While no direct signs of discontinuities have been observed in the finite-size scaling, there are scaling anomalies that have led to speculations of a weak first-order transition described by a non-unitary conformal field theory [2]. Another possibility is that the transition is continuous but violates standard scaling laws. The observed finite-size scaling violations can be described phenomenologically by a scaling form with two relevant fields that are tuned by the same parameter in the Hamiltonian [3]. We will discuss recent work aimed at high-precision tests of this type of scaling by doing large scale calculation of the J-Q model which can realize the quantum phase transition between the antiferromagnetic state and a valence-bond solid state.


*This work is supported by NSF Grant No. DMR-1710170 and the Simons Foundation.

11:51AM G50.00004: Quantum Critical Ballistic Transport in Two-Dimensional Fermi Liquids*  MANI CHANDRA (Presenter), GITANSH KATARIA, DESHDEEP SAHDEV, Quazar Technologies — We show that the ballistic regime in two-dimensional Fermi liquids is a quantum critical point (QCP) on the regime boundary separating Ohmic and hydrodynamic transport. The QCP corresponds to a free conformal field theory (CFT) with a dynamical scaling exponent $z = 1$. Its nontrivial aspects emerge in device geometries with shear, wherein the regime has an intrinsic universal dissipation, a nonlocal current-voltage relation, and exhibits the critical scaling of the underlying CFT. The Fermi surface has electron-hole pockets across all angular scales and the current flow has vortices at all spatial scales. The scale-invariant spatial structure is much richer than that of an interaction-dominated hydrodynamic regime, which only has a single vortex at the device scale. We animate the emergence of critical spatial (vimeo.com/365020115) and Fermi surface (vimeo.com/364982637) fluctuations as experimental parameters are tuned to the QCP. The vortices clearly demonstrate that Pauli exclusion alone can produce collective effects, with low-frequency AC transport mediated by vortex dynamics (vimeo.com/366725650).

*We thank gpueater.com for providing us with GPU (AMD Radeon) cloud instances.
12:03PM G50.00005: Collusion of Interactions and Disorder at the Superfluid-Insulator Transition: A Dirty 2d Quantum Critical Point*  HART GOLDMAN (Presenter), University of Illinois at Urbana-Champaign, ALEX THOMSON, California Institute of Technology, LAIMEI NIE, University of Chicago, ZHEN BI, Massachusetts Institute of Technology — We study the stability of the Wilson-Fisher fixed point of the quantum O(2N) vector model to quenched disorder in the large-N limit. While a random mass is strongly relevant at the Gaussian fixed point, its effect is screened by the strong interactions of the Wilson-Fisher fixed point. This enables a perturbative renormalization group study of the interplay of disorder and interactions about this fixed point. We show that, in contrast to the spiralling flows obtained in earlier double-ε expansions, the theory flows directly to a quantum critical point characterized by finite disorder and interactions. The critical exponents we obtain for this transition are in remarkable agreement with numerical studies of the superfluid-Mott glass transition. We additionally discuss the stability of this fixed point to scalar and vector potential disorder and use proposed boson-fermion dualities to make conjectures regarding the effects of weak disorder on dual Abelian Higgs and Chern-Simons-Dirac fermion theories when N=1.

*NSF GRFP under Grant No. DGE-1144245, the Kadanoff Fellowship at the University of Chicago, the Pappalardo Fellowship at MIT, the Walter Burke Institute for Theoretical Physics at Caltech, and the Caltech IQIM (Gordon and Betty Moore Foundation Grant GBMF1250).

12:15PM G50.00006: Deconfined quantum critical point in the extended Hubbard model: a sign-problem-free quantum Monte Carlo study  XUN CAI (Presenter), BOHAI LI, Tsinghua University, ZIXIANG LI, University of California, Berkeley, HONG YAO, Tsinghua University — Deconfined quantum critical point (DQCP) describes a type of quantum phase transitions at T=0 beyond Landau paradigm, where a continuous transition appears between ordered phases with incompatible broken symmetries. Convincing evidences of DQCP in correlated fermionic systems are scarce. Here we study the quantum phase diagram and phase transition on an extended Hubbard model of fermions on the square lattice. By performing determinant quantum Monte Carlo simulation, we establish the ground-state phase diagram of this model, and more intriguingly, show convincing evidence of a continuous phase transition between valence-bond-solid (VBS) and antiferromagnetic (AF) phases when the interaction strength is varied. We believe that our study provides a novel platform for the investigation of DQCP in the strongly correlated fermionic systems.
12:27PM G50.00007: Deconfined quantum criticality and emergent SO(5) symmetry in fermionic systems  
ZIXIANG LI, UC Berkeley, SHAOKAI JIAN, HONG YAO (Presenter), Tsinghua University — Deconfined quantum criticality with emergent SO(5) symmetry in correlated systems remains elusive. Here, by performing numerically-exact state-of-the-art quantum Monte Carlo (QMC) simulations, we show convincing evidences of deconfined quantum critical points (DQCP) between antiferromagnetic and valence-bond-solid phases in the extended Hubbard model of fermions on the honeycomb lattice with large system sizes. We further demonstrate evidences of the SO(5) symmetry at the DQCP. Moreover, it is the first time that the critical exponents obtained at the DQCP are consistent with the rigorous conformal bounds. Consequently, we establish a promising arena of DQCP with emergent SO(5) symmetry in interacting systems of fermions. Its possible experimental relevances in correlated systems such as graphene-family materials will be discussed briefly [1].

[1] Zi-Xiang Li, Shao-Kai Jian, and Hong Yao, arXiv:1904.10975

12:39PM G50.00008: Exploring a quantum critical point in the 3D Hubbard model using the dynamical cluster approximation  
SAMUEL KELLAR (Presenter), KA-MING TAM, Louisiana State University, Baton Rouge — This research simulates the single band three dimensional Hubbard Model using the dynamical cluster approximation. Away from half-filling the system appears to undergo a quantum phase transition driven by the chemical potential or doping level. The quasiparticle weight, extracted from the self-energy, is used to identify the emergence of a Fermi liquid phase. At lower fillings the quasiparticle weight maintains a finite value consistent with a Fermi liquid state. Nearer to half-filling the quasiparticle weight tends towards zero suggesting a non-Fermi liquid state. We also search for evidence of a marginal Fermi liquid state, a signature of the quantum criticality. In order to complete this simulation efficiently the continuous time quantum Monte Carlo method is run on a massively parallel simulation.

12:51PM G50.00009: Many-body chaos in the antiferromagnetic quantum critical metal  
PETER LUNTS (Presenter), Simons Foundation, AAVISHKAR PATEL, Physics, Berkeley — Recently, the scrambling rate as defined from the exponential growth of regularized out-of-time-ordered correlators has been used as a measure of integrability in quantum many-body systems. We compute the scrambling rate at the antiferromagnetic (AFM) quantum critical point, using the fixed point theory of Phys. Rev. X 7, 021010 (2017). At this strongly coupled fixed point, there is an emergent small control parameter $w$ that is a ratio of natural parameters of the theory. The strong coupling is unequally felt by the two degrees of freedom: the bosonic AFM collective mode is heavily dressed by interactions with the electrons, while the electron is only marginally renormalized. The scrambling rates of both degrees of freedom are linear in temperature (up to logarithms), but come with very different powers of $w$, indicating the different "degrees of integrability" of the two sectors of the theory. Although the interaction strength is of order unity, the larger Lyapunov exponent is still parametrically smaller than the universal upper bound. We also show that due to the non-local nature of the boson propagator, its effective "butterfly velocity" of the chaos front is infinite.
1:03PM G50.00010: Monopole hierarchy at a quantum critical point between a Dirac spin liquid and an antiferromagnet*  

ERIC DUPUIS (Presenter), WILLIAM WITCZAK-KREMPA, Universite de Montreal — Certain frustrated 2D quantum magnets may be described at low energy by a Dirac spin liquid (DSL) which is a version of quantum electrodynamics with 2N flavors of two-component gapless Dirac spinons. A DSL also hosts monopole excitations due to the compactness of the emergent U(1) gauge field. These drive the confinement of the spinons. We revisit the hierarchy among monopole operators with different quantum numbers at the quantum critical point (QCP) between a DSL and an antiferromagnet. By obtaining the scaling dimension of monopole operators while constraining their spin quantum number, we explicitly show their organization into multiplets of the QCP flavor symmetry group SU(2)xSU(N). We also discuss 1/N corrections to the scaling dimension of monopoles at a critical point between a DSL and a chiral spin liquid.

*É.D. is funded by an Alexander Graham Bell CGS from NSERC. W.W.-K. is funded by a Discovery Grant from NSERC, a Canada Research Chair, a grant from the Fondation Courtois, and a “Établissement de nouveaux chercheurs et de nouvelles chercheuses universitaires” grant from FRQNT.

1:15PM G50.00011: The Hall Effect and Dynamical Scaling about the Quantum Critical Point in Elemental Chromium  

STEPHEN ARMSTRONG (Presenter), DANIEL SILEVITCH, THOMAS F ROSENBAUM, California Institute of Technology — Elemental chromium is a spin-density-wave (SDW) antiferromagnet that can be tuned through a second order quantum phase transition by the application of 10 GPa of pressure. A nesting condition in the paramagnetic Fermi surface partially gaps the Fermi surface and forms the SDW. Since the Hall coefficient directly probes properties of the Fermi surface, it is an effective tool to investigate the evolution of the Fermi surface in the quantum critical regime, where there are indications of strong-coupling physics. In the low temperature limit, the Hall coefficient varies rapidly with pressure across the quantum critical point. By extending this measurement to higher temperatures, we are able to track the P-T dependence of this crossover and test analogies to the pseudogap phase in the superconducting cuprates. The temperature dependence of the width of this crossover constrains theories of dynamical scaling at the quantum critical point.
1:27PM G50.00012: Optical Conductivity of the Two Dimensional Anti-ferromagnetic Quantum Critical Metal* ASHUTOSH SINGH (Presenter), ANTON BORISSOV, SUNG-SIK LEE, McMaster University — In the two-dimensional anti-ferromagnetic quantum critical metal, coherent quasi-particle(s) ceases to exist at the hot spots due to strong coupling with soft spin fluctuations. Over an intermediate energy scale, physical responses of the non-Fermi liquid is controlled by the nesting angle between patches of Fermi surface connected by the anti-ferromagnetic wavevector. For instance, the anomalous dimension of electron(s) at the hot spots defined over an intermediate energy scale decreases with decreasing nesting angle due to an increased damping of spin fluctuations by particle-hole excitation. In this work, we compute the optical conductivity of the non-Fermi liquid state as a function of the nesting angle. Remarkably, the weight of the conductivity that scales anomalously with frequency due to the soft spin fluctuations is enhanced as the nesting angle decreases. This is attributed to the fact that the increased number of electrons that are subject to scattering with spin fluctuations overcompensates the decreased scattering rate of individual electrons.

*National Science and Engineering Research Council of Canada (NSERC) and by the Canadian Institute for Advanced Research (CIFAR) (Canada).

1:39PM G50.00013: Quantum criticalities with lattice vibrations* SANGEUN HAN (Presenter), Department of Physics, KAIST, JUNHYUN LEE, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park, EUN-GOOK MOON, Department of Physics, KAIST — Quantum criticality is one of the most important concepts in modern condensed matter physics, as novel physics may arise in the vicinity of the quantum critical point by quantum fluctuations. These fluctuations inevitably couple to lattice vibrations in real materials due to the lattice structures. It is well understood that a class of thermal continuous transitions on lattices is eventually destabilized by either macroscopic instability of lattice structures or induced first-order symmetry breaking transitions. However, for the quantum phase transition, little is known about its consequences. Here, we demonstrate that such interplay between quantum criticality and lattice vibration leads to a new class of quantum many-particle phenomena. Moreover, we suggest a new stability condition for these criticalities which generalizes the specific-heat criterion of thermal transitions to a quantum version. Our results suggest a new direction to find novel quantum criticalities in nature.

*This work was supported by the JQI-NSF-PFC (JL).
1:51PM G50.00014: Novel Criticality of Dirac Fermions from Lattice Symmetry Breaking
FRANK KRUGER (Presenter), ELLIOT CHRISTOU, Univ Coll London, FERNANDO DE JUAN, IKERBASQUE
— We consider the role of spontaneous lattice symmetry breaking in strongly interacting two
dimensional Dirac systems. The fermion induced quantum (multi-)criticality is described by Dirac
fermions coupled to a dynamical order parameter that is composed of mass and emergent
gauge fields. This is illustrated for the example of translational symmetry breaking due to charge-
density wave order on the honeycomb lattice. Using a renormalization-group analysis we find
that the putative emergent Lorentz invariance is violated. Finally, we identify that topological
phase transitions are well described by this effective field theory.

*F. K. acknowledges financial support from EPSRC under Grant EP/P013449/1.

2:03PM G50.00015: Kardar-Parisi-Zhang universality from soft gauge modes
VIR BULCHANDANI (Presenter), University of California, Berkeley — The emergence of superdiffusive spin
dynamics in integrable classical and quantum magnets is well established by now, but there is no
generally valid theoretical explanation for this phenomenon. A fundamental difficulty is that the
hydrodynamic fluctuations of conserved quasiparticle modes are purely diffusive. We propose a
"hydrodynamic Higgs mechanism" in isotropic integrable magnets, which generates soft gauge
modes that are decoupled from the quasiparticle sector. We show that the coarse-grained time
evolution of these modes lies in the Kardar-Parisi-Zhang universality class of dynamics.

Tuesday, March 3, 2020 11:15 AM - 1:39 PM

Session G51 DCMP DMP: Graphene: Electronic Structure and
Interactions III; Moire, Correlations, & Topology

Mile High Ballroom 1D - Dmitry Shcherbakov, Ohio State Univ - Columbus

11:15AM G51.00001: Electronic Collective Modes in Twisted Bilayer Graphene
NICHOLAS WERNER (Presenter), ANDREAS BILL, Department of Physics & Astronomy, California State University,
Long Beach, CA 90840 — Twisted Bilayer Graphene (TBLG) is a structure composed of two
graphene sheets stacked with a relative twist angle between them. Cao et al. [Nature 556, 43
(2018)] reported the discovery of a superconducting state in TBLG at a "magic angle" of about
1.05°. There is no consensus yet on the mechanism that causes this state.
We study electronic collective modes in bilayer graphene at various twist angles with a particular
emphasis on low-energy plasmons. The calculation is performed for two band structures: the
tight-binding model that displays a long-range periodic Moiré pattern at commensurate twist
angles, and the continuum model that allows for the calculation of collective modes at and near
the magic angle. We discuss the implications of the electronic collective modes spectrum for
superconductivity in twisted bilayer graphene.
11:27AM G51.00002: Charge Smoothening and Band Flattening due to Hartree corrections in Twisted Bilayer Graphene  LOUK RADEMAKER (Presenter), Univ of Geneva, PAULA MELLADO, Adolfo Ibáñez University, Chile, DMITRY ABANIN, Univ of Geneva — Doping twisted bilayer graphene away from charge neutrality leads to an enormous buildup of charge inhomogeneities within each Moiré unit cell. Here we show, using unbiased real-space self-consistent Hartree calculations on a relaxed lattice, that Coulomb interactions smoothen this charge imbalance by changing the occupation of earlier identified ‘ring’ orbitals in the AB/BA region and ‘center’ orbitals at the AA region. For hole doping, this implies an increase of the energy of the states at the \( \Gamma \) point, leading to a further flattening of the flat bands and a pinning of the Van Hove singularity at the Fermi level. The charge smoothening will affect the subtle competition between different possible correlated phases.

11:39AM G51.00003: Electrostatic Tuning of the Coulomb Interaction in Single Layer Graphene  NICHOLAS DALE (Presenter), RYO MORI, IQBAL UTAMA, CLAUDIA FATUZZO, University of California, Berkeley, JONATHAN DENLINGER, Advanced Light Source, CONRAD STANSBURY, SIHAN ZHAO, KYUNGHOO LEE, University of California, Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute of Materials Science, FENG WANG, ALESSANDRA LANZARA, University of California, Berkeley — The Landau-Fermi Liquid Theory maps an interacting liquid of electrons to a non-interacting gas of quasiparticles. This picture breaks down in Graphene, because the bare Coulomb interaction is preserved near the charge neutrality point. In this talk, I will discuss recent in-operando angle-resolved photoemission studies on single layer graphene where we directly visualize modifications of its electronic band structure upon tuning the Fermi Energy.

11:51AM G51.00004: Streamlining twisted bilayer graphene measurements*  JOE FINNEY (Presenter), AARON SHARPE, ARTHUR W BARNARD, CONNIE HSUEH, ELI J FOX, Stanford Univ, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, MARC KASTNER, MIT, DAVID GOLDHABER-GORDON, Stanford Univ — Twisted bilayer graphene (TBG) has emerged as a promising platform for studying strongly correlated physics. When the twist angle is near the magic angle of approximately one degree, transport measurements have revealed a host of interesting phenomena including correlated insulating states, superconductivity, and ferromagnetism. However, fabricating and effectively measuring TBG samples remains challenging. The twist angle varies widely from sample to sample, and even from contact to contact within the same sample. In this work, I present a few tools we have used in order to streamline the process of making and measuring TBG samples, along with some interesting results encountered along the way.

*This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.
Twisted bilayer graphene has recently gained significant attention due to the discovery of superconductivity and correlated insulating behavior near the magic angle of 1.1 degrees. Other twisted 2D van der Waals heterostructures are expected to host similar phenomena. Thus, methods for consistent and precise fabrication of twisted 2D materials are essential to enable their further study. We discuss the dry transfer technique that enables high accuracy rotational alignment that we have used to fabricate magic angle twisted bilayer graphene devices for scanning probe microscopy measurements. Using low temperature scanning tunneling microscopy and spectroscopy, we have verified the localization properties of the flat bands and directly probed the correlated insulating states at commensurate filings. These results can lead to a better understanding of the local electronic properties of magic angle twisted bilayer graphene.

The work at the University of Arizona was supported by the National Science Foundation under grants DMR-1708406 and EECS-1607911

Recently, signatures of quantum anomalous Hall states with spontaneous ferromagnetism were observed in twisted bilayer graphenes (TBGs) near 3/4 filling [Science 365, 605-608 (2019), arXiv: 1907.00261]. Importantly, it was demonstrated that an extremely small current can switch the direction of the magnetization. This opens the prospect of realizing low energy dissipation magnetic memories. However, the mechanism of the current-driven magnetization switching is poorly understood as the charge currents in graphene layers are generally believed to be non-magnetic. In this work, we demonstrate that, in TBGs, the twist-induced reduction of lattice symmetry allows a charge current to generate net orbital magnetization at a general filling factor through magnetoelectric effects. Substrate-induced strain and sublattice symmetry breaking further reduce the symmetry such that an out-of-plane orbital magnetization can be generated. Due to the large non-trivial Berry phase of the bands, the orbital magnetization of a Bloch state can be as large as tens of Bohr magnetons and therefore a small current would be sufficient to generate a large orbital magnetization. We further demonstrate how the charge current can switch the magnetization of TBGs as observed in experiments.

HKRGC
It has been recently established that optoelectronic and non-linear transport experiments can give direct access to the dipole moment of the Berry curvature in non-magnetic and non-centrosymmetric materials. Thus far, non-vanishing Berry curvature dipoles have been shown to exist in materials with substantial spin-orbit coupling where low-energy Dirac quasiparticles form tilted cones. Here, we prove that this topological effect does emerge in two-dimensional Dirac materials even in the complete absence of spin-orbit coupling. In these systems, it is the warping of the Fermi surface that triggers sizeable Berry dipoles. We show indeed that uniaxially strained monolayer and bilayer graphene, with substrate-induced and gate-induced band gaps respectively, are characterized by Berry curvature dipoles comparable in strength to those observed in monolayer and bilayer transition metal dichalcogenides.

References:


Interlayer electron-electron (el-el) and electron-phonon (el-ph) interactions emerge from the coupling of atomic layers in 2D heterostructures and are essential for describing their physical properties. The additional possibility of controlling the twisting angle between layers opens new possibilities for tunable devices. Raman spectroscopy is a fundamental tool to investigate el-ph interactions and the possibility of using multiple-excitation spectroscopy allows the distinction between intralayer and interlayer el-ph interactions. We will discuss a resonance Raman study of twisted bilayer graphene (TBG) samples with different twisting angles and measured using different laser lines. Results show that the extra Raman peaks that appear in the spectra come from different physical mechanisms: the intralayer process, where the el-ph scattering occurs in a single graphene layer and the other layer only imposes a periodic potential that scatters the excited electron, and the interlayer el-ph process, where the scattering occurs between states in the Dirac cones of adjacent graphene layers.
12:51PM G51.00009: Atomistic Calculation of Electron-Phonon Coupling in Twisted Graphene Layers

YOUNG WOO CHOI (Presenter), HYOUNG JOON CHOI, Department of Physics, Yonsei University, Seoul, 03722, Korea — We investigate electron-phonon coupling in twisted graphene layers based on atomistic calculations of electronic structure, phonon dispersion, and electron-phonon matrix elements. First, we calculate twisted double bilayer graphene (TDBG). Then, we analyze the characteristics of important phonon modes that have strong contributions to the total coupling strength. Also, we compare the electron-phonon coupling in TDBG and magic-angle twisted bilayer graphene in the context of the recent experimental observations of superconductivity in these systems. Our work provides microscopic understanding of the electron-phonon coupling in twisted graphene layers, which is a basis for explaining superconducting mechanism of these systems.

*This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2018-CRE-0097). Y.W.C. acknowledges support from NRF of Korea (Global Ph.D. Fellowship Program NRF-2017H1A2A1042152).

1:03PM G51.00010: Observation of Substrate Induced Multiple Dirac Cones in Graphene/ SiC Heterostructure

QIANGSHENG LU (Presenter), JACOB COOK, XIAOQIAN ZHANG, GUANG BIAN, Univ of Missouri - Columbia — The coupling between epitaxial graphene layers and various substrates give rise to many interesting phenomena such as the energy gap at the Dirac node and double Dirac cones. Electronic structure of graphene is modulated by the substrate effects. In this work, we measured the electronic structure of bilayer graphene/SiC heterostructure. Apart from the duplicated Dirac cones arising from the interaction with the interfacial reconstruction, 24 additional Dirac cones are clearly observed by angle-resolved photoemission spectroscopy (ARPES) within the 1st Brillouin zone of graphene. These 24 Dirac cones are directly generated from the coupling between graphene layers and the supporting SiC lattice, a result consistent with our tight-binding simulations. This work paves the way for understanding the direct electronic coupling between graphene and SiC substrates.

*This work is supported by the US National Science Foundation (NSF-DMR#1809160).

1:15PM G51.00011: Localized doping through lithium intercalation in twisted bilayer graphene

DANIEL LARSON (Presenter), GEORGIOS TRITSARIS, STEPHEN CARR, EFTIMIOS KAXIRAS, Harvard University — Lithium atoms intercalating between layers of graphene show an energetic preference for regions of AA stacking. Density functional theory calculations employing commensurate supercells with twist angles of 7.3° and 2.5° are used to study the energetics, atomic relaxation, and electronic structure of Li intercalation in twisted graphene bilayers, with results extrapolated to the magic angle.
1:27PM G51.00012: Scanning Tunneling Microscopy Studies of Electronic Correlations in Magic Angle Twisted Bilayer Graphene*  YOUNGJOON CHOI (Presenter), YIRAN ZHANG, HARPREET ARORA, ROBERT POLSKI, Caltech, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, STEVAN NADJ-PERGE, Caltech — Discovery of superconductivity and correlated insulating states in the magic angle (~1.1 deg) twisted bilayer graphene sparked the search for other broken symmetry states in this system. Previously we used scanning tunneling microscopy (STM), to investigate interaction effects at charge neutrality, spectroscopic gaps originating from insulating states at the half and quarter filling, and signatures of spatial ordering [1]. In this talk, we will present our latest STM results and discuss spatial spectroscopic maps revealing new insights into this system.


*This work was supported by NSF (DMR 1744011 and DMR 1753306). YC was supported by Kwanjeong Educational Foundation.

G51.00013: Hofstadter butterfly and quantum Hall effect in twisted double bilayer graphene*  JOHN A. CROSSE, Arts and Sciences, NYU Shanghai, MIKITO KOSHINO, Department of Physics, Osaka University, PILKYUNG MOON (Presenter), Arts and Sciences, NYU Shanghai — In this talk, I will discuss the energy spectrum and quantum Hall effect in twisted double bilayer graphene (TDBG, a pair of Bernal-stacked bilayer graphenes stacked with a rotational stacking fault). The electronic band structures of TDBG with AB-AB configuration and AB-BA configuration look similar in the absence of magnetic field, but their topological nature are different [1]. Therefore, the twins of AB-AB and AB-BA TDBG exhibit very different spectrum in magnetic field, by directly reflecting the difference in Chern numbers of the two pair structures [2]. For example, the first gap in the electron side of AB-AB TDBG remains opened in increasing magnetic fields, while that of AB-BA TDBG vanishes at some points due to the non-zero valley Chern number in AB-BA TDBG.


*J.A.C and P.M. were supported by NYU Shanghai (Start-Up Funds), NYU-ECNU Institute of Physics at NYU Shanghai, and New York University Global Seed Grants for Collaborative Research. J.A.C. acknowledges support from National Science Foundation of China Grant No. 11750110420. This research was carried out on the High Performance Computing resources at NYU Shanghai.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G52 DMP: Focus Topic: Surface, Interface, and Thin Film Science of Organic Molecular Solids I Mile High Ballroom 1E - Daniel Dougherty, North Carolina State University - Tag(s): Focus
11:15AM G52.00001: Using Deposition Rate to Control Liquid Crystal-like Order in Vapor Deposited Organic Glasses*  
CAMILLE BISHOP (Presenter), University of Wisconsin - Madison, JACOB THELEN, National Institute of Standards and Technology, YUHUI LI, University of Wisconsin - Madison, ELIOT H GANN, National Institute of Standards and Technology, MICHAEL TONEY, SLAC National Accelerator Laboratory, LIAN YU, University of Wisconsin - Madison, DEAN DELONGCHAMP, National Institute of Standards and Technology, MARK EDIGER, University of Wisconsin - Madison — Physical vapor deposition can prepare glassy materials with high degrees of structural anisotropy compared to liquid-cooled glasses. In this work, Posaconazole, a molecule with no known liquid crystal phases, is vapor-deposited to create smectic-like glasses with a high degree of orientational and positional order [Bishop et. al. PNAS 116, 21421 (2019)]. Deposition parameters are varied to prepare glasses with a range of liquid crystal-like order. We show that increasing the substrate temperature and decreasing the deposition rate have the same effect upon vapor-deposited glass structure, and describe the relationship using a “Deposition Rate-Substrate Temperature Superposition”. We expect that this superposition principle can be used to understand surface dynamics during vapor deposition, in order to optimize structural order in glasses for organic electronic applications.

*This research was primarily supported by NSF through the University of Wisconsin Materials Research Science and Engineering Center (DMR-1720415).

11:27AM G52.00002: 2D organic layers on surfaces: self-assembly and electronic structure*  
[Invited] SYLVIE RANGAN (Presenter), ROBERT ALLEN BARTYNSKI, Rutgers University, New Brunswick — Understanding the basic mechanisms leading to the formation of 2D organic layers on surfaces, either via Van der Waals, ionic or covalent interactions, is a necessary step toward the development of controlled and ordered organic layers, for technological applications such as homogeneous doping of graphene or 2D organic topological insulators. Using a combination of scanning tunnel microscopy, various electron spectroscopies techniques and ab-initio calculations, we have studied several aspects of the self-assembly and reactivity of particularly interesting model systems: Zinc tetraphenylporphyrins (ZnTPP) on single crystal surfaces.

First, we have explored the delicate balance of forces during the self-assembly process of ZnTPPs on metal single crystal surfaces. It is shown that molecule/molecule and molecule/surface interactions, as well as accumulated surface stress, all play an important role in determining self-assembly. In particular, it is shown that self-assembly can be kinetically trapped into metastable phases different from typical equilibrium outcomes. Furthermore, it is possible to generate under certain conditions on self-assembled ZnTPP arrays, surface mediated chemistry that leads, to site-selective dehydrogenation and intramolecular covalent bond creation. Intermolecular dehydrogenation is also possible, and if directed properly could lead to tunable highly ordered 2D covalent structure.

*The authors aknowledge funding from NSF CHE-1446389, DOE DE-AC02-05CH11231 and NSF CHE-1904648.
12:03PM G52.00003: Electric field manipulation of the molecular spin state of a Fe(II) spin crossover complex  GUANHUA HAO (Presenter), Department of Physics and Astronomy, University of Nebraska - Lincoln, AARON MOSEY, Physics Department, Indiana University Purdue University-Indianapolis, XUANYUAN JIANG, Department of Physics and Astronomy, University of Nebraska - Lincoln, ALPHA T. N'DIAYE, Advanced Light Source, Lawrence Berkeley National Laboratory, XIN ZHANG, JIAN ZHANG, Department of Chemistry, University of Nebraska–Lincoln, RUIHUA CHENG, Physics Department, Indiana University Purdue University-Indianapolis, XIAOSHAN XU, PETER A DOWBEN, Department of Physics and Astronomy, University of Nebraska - Lincoln — The spin crossover (SCO) phenomenon, in 3d transition metal compounds, has potential applicability in molecular spintronic devices for low-cost flexible memory. Isothermal changes of the electronic structure has now been achieved for the Fe(II) spin crossover complex \([\text{Fe(H}_2\text{B(pz)}_2\text{bipy)}_2]\), where pz = tris(pyrazol-1-yl)-borohydride and bipy = 2,2'-bipyridine, by external electric fields. This isothermal voltage-controlled switching is evident in thin film bilayer structures where the molecular spin crossover film is adjacent to a molecular ferroelectric thin film (the tested examples being polyvinylidene fluoride hexafluoropropylene or croconic acid (C$_5$H$_2$O$_5$)). These organic ferroelectric substrates appear to lock the spin crossover molecular complex largely in the low or high spin state depending on the direction of ferroelectric polarization, in both a planar two terminal diode structure and for a transistor structure. Moreover, the spin state change is observed to be accompanied by a conductance change, where higher conductance occurs at a high spin state while lower conductance is observed for a low spin state, and is seen to be nonvolatile, i.e. the spins state is retained in the absence of an applied electric field.

12:15PM G52.00004: Expanding the surface chemistry synthetic toolkit: facile carbon (sp$^2$)-nitrogen(sp$^2$) bond formation on Au[111] and Ag[111]  RAYMOND BLACKWELL (Presenter), ILYA PISKUN, University of California, Berkeley, JOAQUIM SOMOZA, Max Planck Institute for the Structure and Dynamics of Matter, FANGZHOU ZHAO, STEVEN LOUIE, University of California, Berkeley, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter, FELIX FISCHER, University of California, Berkeley — Surface assisted synthesis offers a unique pathway towards the creation of atomically precise nanostructures that cannot be achieved in solution. The Ulmann coupling—where surface stabilized radicals form covalent bonds prior to polymerization or cyclization—has emerged as a promising route for accessing novel architectures, in particular graphene nanoribbons where the electronic structure is intimately linked with the atomic structure. This reaction, however, has been limited to the formation of C-C bonds, restricting its overall scope. The ability to create novel linkages on the surface would allow for a deeper understanding of the interplay between atomic and electronic structure. Here we demonstrate facile C-N bond formation on different coinage metal surfaces at substantially lower temperatures than polymerization and subsequent C-C bond formation. Scanning tunneling microscopy and spectroscopy (STM/STS) performed conjointly with first-principles calculations confirm the desired product. The mechanism for C-N formation will be discussed along with strategies for the synthesis of extended 1-dimensional structures.
**12:27PM G52.00005: Scanning Tunneling Microscopy and Spectroscopy of Heterotriangulene-based 2D Polymers**

ZACHERY ENDERSON (Presenter), HARSHA VARDHAN MURALI, RAGHUNATH DASARI, TIMOTHY C PARKER, SETH R. MARDER, HONG LI, QINGQING DAI, SIMIL THOMAS, JEAN-LUC E BREDAS, PHILLIP N FIRST, Georgia Inst of Tech — Bottom-up synthesized covalent organic frameworks (COFs) provide a means to customize the properties of a 2D polymer from its monomer precursors. The 2D-crystalline DTPA (dimethylmethylene-bridged triphenylamine) COF is synthesized on Au(111) or Ag(111) through Ullman-type coupling. Theory predicts that the as-grown closed-shell electronic structure is semiconducting. Heating in vacuum selectively cleaves methyl groups from the monomer bridge sites, but leaves the framework intact, creating a COF resembling an ultra-flat covalent network of triangulene molecules. Enticing electronic properties are predicted, depending on the specific termination of the bridge sites. Calculations for a H-terminated case indicate that the “radical” COF will be a half-metal (fully spin-polarized density of states at the Fermi energy). Using an LT-STM, we present new information on the bridge configuration of the demethylated structure, on the electronic structure of the DTPA COF in its closed-shell (methylated) and “radical” (demethylated) forms, and on the interaction between the COF and substrate.


*Funded by the United States Army Research Office under grant number W911NF-15-1-0447 (MURI).*

**12:39PM G52.00006: Enhancement of Magnetoelectric Coupling in Ferroelectric Vinylidene Fluoride/Ferroelectric Cobalt by insertion of a dielectric layer of Magnesium Oxide.*

AASHISH SUBEDI (Presenter), KEITH D FOREMAN, SHIREEN ADENWALLA, University of Nebraska - Lincoln — Poly (vinylidene fluoride), or PVDF combines the advantages of organic based electronics with the useful bi-stable polarization characteristic of ferroelectricity. Magnetoelectric coupling between PVDF, and ferromagnetic cobalt thin films has been well established. Because VDF thin films may be deposited in vacuum, the interface between Co and VDF is clean and sharp, with little to no oxidation. We studied magnetoelectric coupling in these heterostructures, with VDF deposited directly on Co without breaking vacuum. This pristine interface resulted in very weak magnetoelectric coupling. The introduction of oxides of cobalt between these layers from exposure in air resulted in an increase in the surface coupling but presented challenges of surface purity and irreproducibility. Thus, we investigated the effect of controlled growth of a dielectric with high K, MgO. We focus on the growth and heat treatment of MgO on ferromagnetic cobalt. Consequently, we examine the interfacial interaction between the Cobalt, MgO and VDF layers and analyze how this affects the out of plane magnetic anisotropy of Cobalt.

*Research supported by NSF ECCS-1101256, MRSEC DMR-1420645 and UCARE-UNL.*
**12:51PM G52.00007: Electric Field Control of Molecular Charge State in a Single-Component 2D Organic Nanoarray**  
AGUSTIN SCHIFFRIN, DHANEESH KUMAR (Presenter), YUEFENG YIN, NIKHIL MEDHEKAR, CORNELIUS KRULL, Monash Univ — Quantum dots (QD) with an electric-field-addressable charge state are promising for digital information storage, single-electron transistors and quantum computing. Semiconductor QDs often offer limited control on size and composition, and low potential for scalability or miniaturization. Owing to their tunability and self-assembly capability, organic molecular building blocks can be used for the synthesis of two-dimensional (2D) QD arrays. Here, we report the self-assembly of 9, 10-dicyanoanthracene (DCA) molecules on Ag(111) into periodic 2D arrays, where the molecular charge state (neutral or negative) can be altered – individually and depending on the adsorption site – by the local electric field of a scanning tunneling microscope tip. Charging is enabled by an effective DCA/Ag(111) tunneling barrier and electric-field-driven electron population of the lowest unoccupied molecular orbital (LUMO). Subtle site-dependent variations of the DCA adsorption height result in a spatial modulation of the molecular polarizability, dielectric constant and LUMO energy level alignment, giving rise to a spatially dependent likelihood of charging. Our work offers potential for high-density 2D self-assembled arrays of QDs whose charge state can be addressed individually by an electric field.

**1:03PM G52.00008: Low Energy Electron Interactions with Aliphatic and Aromatic Self-assembled Monolayers on Au(111)**  
CARL VENTRICE (Presenter), SUNY Polytechnic Institute, JODI GRZESKOWIAK, University at Albany-SUNY — Electron scattering experiments have been performed on SAMs of the aliphatic molecule decanethiol and the aromatic molecule biphenylthiol grown on Au(111) via vapor phase deposition. The molecules take on either a lying down (LD) or standing up (SU) geometry, depending on coverage. From LEED, the crystal structure of both the LD phase and SU phase SAMs grown from both types of molecules is easily disrupted upon electron irradiation. Changes in peak intensities and positions of the TPD and XPS spectra indicate that the C-S bonds are cleaved for both molecules upon electron irradiation. In the SU phase of the aliphatic molecule, a large chemical shift in the C-1s and large reduction in the hydrocarbon fragments of the TPD spectra are observed. The LD phase of the aliphatic molecule and both phases of the aromatic molecule show only subtle changes to the spectra. The relative insensitivity of these SAMs to electron beam damage is attributed to charge delocalization effects. For the LD phase of the aliphatic molecule, excess charge is easily quenched since it is in direct contact with the metallic substrate. For the aromatic molecule, conjugated double bonds within the aromatic rings allow for excess charge delocalization, resulting in a lower probability for C-C bond breakage.
1:15PM G52.00009: Interface properties of FePc adsorbed on Ag (100) with and without NaCl monolayer

M. Jabrane 1,2, M.Y. El Hafidi1, M. El Hafidi1, A. Kara2

Laboratoire de la physique la matière condensée, Faculty of Sciences Ben M’Sik, Hassan II University*

MEYSOUN JABRANE (Presenter), Univ of Central Florida — For spintronic based technologies, current research focuses on developing novel nanoscale materials that combines molecular magnetism with organic spintronic devices. In this context, we studied magnetic properties of Iron-Phthalocyanine (FePc) adsorbed on various metallic surfaces. We found that FePc loses its magnetization when deposited on Cu(111) and Ag(111) with a charge transfer of 0.7e and 0.8e towards the molecule, respectively. Therefore, the interaction between FePc and the substrates affects the properties of the molecule. To circumvent the loss of FePc magnetic state, we suggest adding a monolayer of an insulator.

In this work, we tackle a full comparison of the geometric, magnetic and electronic properties of FePc/Ag(100) with and without an insulator. We have opted to use NaCl as insulator because its lattice constant is compatible to that of Ag. The calculations are performed using Density Functional Theory (DFT) and taking into account Vdw functionals to improve the description of the interactions.

*Partial support is provided from the U.S. Department of Energy Basic Energy Science under Award number DE-SC0007045. This research used computational resources of NERSC, as well as UCF-Stokes. Funding is provided from Amideast under Fulbright Joint Supervision award.

1:27PM G52.00010: Electric-field assisted nucleation processes of croconic acid films*

YIFAN YUAN, XUANYUAN JIANG, SHASHI PODDAR (Presenter), XIAOSHAN XU, University of Nebraska - Lincoln — Growth of organic thin films using physical vapor deposition typically follows a three-dimensional mode, resulting in a rough surface, which undermines their application potentials. To address this issue, we have studied the effect of electric field and temperature on the growth dynamics, especially the heterogeneous nucleation process, of croconic acid (CA) films, taking advantage of the large dipole of the molecules and the ferroelectric polarization of the molecular crystals. We found that the nucleation rate has a maximum at an intermediate temperature, and the electric field shifts the maximum nucleation rate towards the lower temperature. An analysis using classical nucleation theory suggests that the electric field decreases sublimation temperature, increases the wetting angle, and decreases the surface diffusion barrier. These results provide important insight into the growth of molecular crystal films under electric fields and pave a way to fabricate films with better surface characteristics for molecular ferroelectric films.

*The authors acknowledge the support from the National Science Foundation through the Materials Research Science and Engineering Center (Grant No. DMR-1420645).
Memory devices are responsible for a significant fraction of the energy consumed in electronic systems—typically 25% in a laptop and 50% in a server station. Reducing the energy consumption of memories is an important goal. For the evolving field of artificial intelligence the compatible devices must simulate a neuron. In the organic memristors based on Ru centred phenyl azo pyridine, spin coated on oxide surfaces, the device performance exceeds the ITRS roadmap specification significantly demonstrating the viability of this system for practical applications. More than that, the redox states of the molecules can be studied in operando using Raman and UV-Vis spectroscopies leading to a clear mechanistic understanding. By enhancing the interface fields the switching energies of the devices could approach atto Joules at sub-10 nm dimension. These molecular devices are extremely stable and reproducible—significant improvement from conventional organic electronics.

How could we “see” the processes that occur in complex atomic-scale heterogeneous interfaces? It was suggested that Surface-enhanced Raman spectroscopy presents a keen approach for studying such systems, implying utilization of the Chemical Enhancement (CE). The latter is expected to report all information about the interfacial electronic coupling, however, a substantial learning curve is ahead before that information can be fully understood. The case of Graphene Enhanced Raman Spectroscopy (GERS) appears to be particularly intriguing. A delocalized electron system of graphene coupled with localized electronic states of organic adsorbates makes a significant challenge for understanding their Raman spectroscopy. We present a systematic computational study of Tetracyanoquinodimethane (TCNQ) adsorbed on graphene. This talk will report about simulations of surface-enhanced Raman spectra along with the supporting electronic structure analysis, focusing on the interfacial charge transfer and electron-phonon coupling. The application of a wide range of external electric biases allows us to modulate the charge transfer across the interface and reveal its role in corresponding changes of Raman spectra.
Comparitive STM and LEED study of the self-assembly of theobromine on Au(111) and few layer graphene on SiC(0001)*  

ISMAIL BALTACI (Presenter), MALTE SCHULTE, CARSTEN WESTPHAL, Experimental Physics, TU Dortmund University — Graphene has unique electronic and structural properties and is of interest in a broad range of applications. The functionalization of graphene by molecular adsorbates enables applications like organic sensors and solar cells. As the weak interaction between substrate and adsorbate is important, graphene and Au(111) are suitable substrates due to their low reactivity. Compounds of the xanthine group have a great effect on the human central nervous system resulting in energy arousal and increased cognitive function\textsuperscript{1,2}. Hence they are of great significance for applications in pharmacology, toxicology, and biochemistry\textsuperscript{3,4}.

Here we present the first experimental results of the xanthine derivate theobromine weakly bonded to graphene and to Au(111) at room temperature. The molecule layers are characterized utilizing STM and LEED to compare the self-assembly on Au(111) and on graphene. The molecule structures show different domains and also the existence of glide planes.


*Thanks Nordrhein-Westfalen for financial support.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G53 APS: 2D Synthesis and Characterization  
Mile High Ballroom 1F - Fei Hui, Technion - Israel Institute of Technology - Tag(s): Focus

Towards room-temperature v magnetic semiconductors [Invited]  
YOUNG-HEE LEE (Presenter), IBS Center for Integrated Nanostructure Physics, Institute for Basic Science, Sungkyunkwan University — The ferromagnetic state in van der Waals two-dimensional (2D) materials has been reported recently in the monolayer limit. Intrinsic CrI\textsubscript{3} and CrGeTe\textsubscript{3} semiconductors reveal ferromagnetism but the T\textsubscript{c} is still low below 60K. In contrast, monolayer VSe\textsubscript{2} is ferromagnetic metal with T\textsubscript{c} above room temperature but incapable of controlling its carrier density. Moreover, the long-range ferromagnetic order in doped diluted chalcogenide semiconductors has not been demonstrated at room temperature. The key research target is to realize the long-range order ferromagnetism, T\textsubscript{c} over room temperature, and semiconductor with gate tunability. Here, we unambiguously observe a ferromagnetic hysteresis loop together with magnetic domains above room temperature in diluted V-doped WSe\textsubscript{2}, while maintaining the semiconducting characteristic of WSe\textsubscript{2} with a high on/off current ratio of five orders of magnitude. Some examples of other magnetic 2D materials are also presented.
Polymer-Free Transfer of 2D Materials onto III-V Semiconductor Surfaces for Scanning Probe Microscopy and Molecule-Encapsulation Experiments*  

LIHY BUCHBINDER (Presenter), Department of Physics, University of New Hampshire, SARA MUELLER, JAY A GUPTA, Department of Physics, The Ohio State University — A tabletop, dry touch-transfer method that employs van der Waals forces was used to transfer multi- to few-layer flakes of hexagonal boron nitride (hBN) and graphite onto cleaved, atomically flat GaAs (110) and InSb (110) surfaces. This method offers a cleaner alternative to current polymer-involved transfer methods, which leave polymer traces on the sample surface and require an extensive cleaning process for scanning probe microscopy (SPM) study.

An attractive application of this touch-transfer method is the encapsulation of target molecules between the semiconductor surface and graphene flakes for scanning tunneling microscopy (STM) studies. The conductivity of graphene allows us to probe the electronic states of otherwise challenging molecules and explore their possible applications. We present results of encapsulation of deionized water droplets between GaAs (110) and thinned graphite, characterized by atomic force (AFM), scanning electron (SEM), and optical microscopy techniques. Further studies will utilize nano-squeegeeing techniques using contact-mode AFM to control the placement of trapped water molecules.

*Funding for this research was provided by the Center for Emergent Materials: an NSF MRSEC under award number DMR-1420451.

Improved contacts to two-dimensional materials for extracting emergent properties  

CURT RICHTER (Presenter), Physical Measurement Laboratory, National Institute of Standards & Technology, SIYUAN ZHANG, Theiss Research and The National Institute of Standards and Technology, NICHOLAS B. GUROS, Department of Chemical and Biomolecular Engineering, University of Maryland and The National Institute of Standards and Technology, SON LE, Theiss Research and The National Institute of Standards and Technology, ARVIND BALIJEPALLI, CHRISTINA HACKER, Physical Measurement Laboratory, National Institute of Standards & Technology — It is critical to control the properties of electrical contacts to two-dimensional (2D) material systems such as twisted bilayer graphene or superconducting 2D systems in order to probe and properly extract their emergent quantum properties. We present here effective routes for contact engineering. It has been demonstrated that TMD monolayers can be effectively doped by using molecular reductants and oxidants introduced onto the surface from solution. [1] In this study, we investigated the effects of molecular doping and contact engineering on the 2D/metal interfaces and charge transport properties of MoS$_2$ devices. We show that MoS$_2$ p-type FETs can only be achieved through combining molecular doping and high-work function metals (e.g. Pd) [2]. We have demonstrated an exposed material forming gas cleaning anneal that effectively decreases deleterious organic contamination arising during fabrication as evidenced by uniform and improved field-effect transistor (FET) performance metrics [3] such as field-effect mobility and threshold voltage. [1] S. Zhang, et al., Adv. Mater. 30, 1802991 (2018); [2] S. Zhang et al., Appl. Phys. Lett. 115, 073106 (2019); [3] N. Guros, et al., ACS Appl. Mater. Interfaces. 11, 16683 (2019).
Graphene has attracted significant interest in recent years. Observation of unconventional superconductivity in twisted bilayer graphene, topological quantum phases, and observation of even denominator FQHE states are some of the exciting new findings [1]. The challenge lies in obtaining large enough single layers of graphene that can be used for device fabrication. Since graphene is sensitive to the surrounding environment, leaving the sample at ambient conditions would heighten the interactions with water and oxygen, increasing impurities and defects. Encapsulating graphene provides significant improvement to the quality of samples. Here we discuss the fabrication and characterization of graphene samples covered from h-BN prepared by mechanical exfoliation and dry transfer method. Optical microscope and AFM imaging were employed in determining the thickness of samples. We studied the transport properties of several µm scale graphene devices with a different number of layers and different geometries. Further, we examine the effect of current annealing on such devices.


*This work was supported by the Army Research Office (W911NF-15-1-0433), and the National Science Foundation (NSF ECCS 1710302).
12:27PM G53.00005: Metallicity of 2H-MoS$_2$ Induced by Au Hybridization*  BRANDON BLUE (Presenter), Physics and Nanoscience Technology Center, University of Central Florida, GLENN JERNIGAN, Naval Research Laboratory, DC, DUY LE, Physics and Renewable Energy and Chemical Transformations Cluster, University of Central Florida, JOSE FONSECA, Naval Research Laboratory, DC, STEPHANIE LOUGH, JESSE E THOMPSON, DARIAN SMALLEY, Physics and Nanoscience Technology Center, University of Central Florida, TALAT RAHMAN, Physics and Renewable Energy and Chemical Transformations Cluster, University of Central Florida, JEREMY ROBINSON, Naval Research Laboratory, DC, MASA ISHIGAMI, Physics and Nanoscience Technology Center, University of Central Florida — The interaction between bulk metal contacts and two-dimensional (2D) transition metal dichalcogenides (TMDs) has a critical influence on overall device performance in a variety of potential applications. This interaction has been studied extensively in the past, especially in the case of molybdemenum disulfide (MoS$_2$), with seemingly contradictory results. In this work, we directly exfoliate monolayer MoS$_2$ onto bulk Au and anneal the resulting heterostructure under ultra-high vacuum (10$^{-10}$ Torr, UHV) to 450 °C. After annealing, the MoS$_2$ monolayer is observed under scanning tunneling microscopy/spectroscopy (STM/STS) to remain in its 2H lattice configuration, yet with regions ranging from fully gapped to metallic. This observation is corroborated by ex situ Raman and photoemission spectroscopies, which show no signs of the otherwise expected 1T or 1T’ structural phase transitions. Theoretical calculations suggest the previous band-gap tuning observed in MoS$_2$-Au heterostructures is due to hybridization and chemical bonding at the S-Au interface, which can completely close the band-gap of 2H-MoS$_2$ at sufficiently short S-Au distances.

* D.L. and T.S.R. are supported in part by U.S. Department of Energy Grant DE-FG02-07ER46354.

12:39PM G53.00006: Reversible hydrostatic strain in graphene/gold nanoparticles hybrid material induced by laser irradiation*  ANDRÁS PÁLINKÁS (Presenter), Nanostructures Laboratory, Centre for Energy Research, Budapest, Hungary — Gold nanoparticles (NPs) were prepared on SiO$_2$ substrate by local annealing of gold thin films using focused laser beam. CVD-grown graphene was transferred onto the prepared NPs. Subsequent Raman-spectroscopy measurements were performed on the samples using different laser powers. We used higher laser intensity (6 mW) to locally anneal the hybrid material. Low laser powers (0.6 mW) were used to characterize the doping and the strain formed in the same areas both before and after local heating. While we found that higher intensity laser irradiation increased gradually the doping and the defect concentration in SiO$_2$-supported graphene, the same irradiation procedure did not induce such irreversible effects in the graphene supported by Au NPs. Moreover, the laser irradiation induced dynamic hydrostatic strain in the graphene on Au NPs, which turned out to be completely reversible. These results point out the role of the substrate in the resistance of graphene against laser irradiation, and can have implications in the development of graphene/plasmonic nanoparticle based high temperature sensors.

*The Authors acknowledge financial support from the NKFIH Office in Hungary, through the Grant K 119532 and KH 129587, and from the Korea-Hungary Joint Laboratory for Nanosciences.
12:51PM G53.00007: Environmental effects on optoelectronic properties of heterostructures of 2D materials  ATIKUR RAHMAN (Presenter), VRINDA NARAYANAN, GOKUL M. A., TAMAGHNACHOWDHURY, Department of Physics, IISER Pune, — We have developed a simple method to fabricate large-area MoS\(_2\) monolayer devices. We will discuss the fabrication of various heterostructures using monolayer MoS\(_2\) as one of the components. Due to the 2D nature of MoS\(_2\), the coulomb screening is less effective and the electronic and optoelectronic properties of these heterostructures depend strongly on the local environment. We will discuss how various characterization methods such as low-frequency noise, dielectric and transient photoresponse can be used to get a deeper understanding of the details of the charge transport mechanism in these systems.

1:03PM G53.00008: Electronic and Optoelectronic Properties of Indium Tin Selenide (In\(_{1-x}\)Sn\(_x\)Se)*  PRASANNA PATIL (Presenter), ROBINSON KARUNANITHY, Department of Physics, Southern Illinois University Carbondale, OLLI PITKANEN, Microelectronics Research Unit, Faculty of Information Technology and Electrical Engineering, University of Oulu, SIDONG LEI, Department of Physics and Astronomy, Georgia State University, POOPALASINGAM SIVAKUMAR, Department of Physics, Southern Illinois University Carbondale, KRISZTIAN KORDAS, Microelectronics Research Unit, Faculty of Information Technology and Electrical Engineering, University of Oulu, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University Carbondale — Selenide based binary- and ternary-layered compounds show exotic physical properties beneficial for developing them for future electronic & opto-electronics based applications.\(^1\) For example; few-layered Indium Selenide (InSe) has attracted attention due to presence of direct band gap and hence its impressive photo-responsive properties.\(^1\) It was also shown that ternary layered alloys such as Copper Indium Selenide (Culn\(_7\)Se\(_{11}\)) possess properties that can be harnessed for developing fast photodetectors.\(^2\) In this talk, we will report on the electronic and optoelectronic properties of few-layered Indium Tin Selenide (In\(_{1-x}\)Sn\(_x\)Se) presented. Specifically, a comparison of the key parameters associated with electronic and optoelectronic properties of In\(_{1-x}\)Sn\(_x\)Se with \(x = 0, 0.05, 0.1\) and 1 will be presented and discussed.

References:
2. S. Ghosh et al., 2D Mater. 5, 015001 (2018)

*ST and PDP acknowledges the support from Indo-U.S. Virtual Networked Joint Center Project on “Light Induced Energy Technologies: Utilizing Promising 2D Nanomaterials (LITE UP 2D)” through the grant number IUSSTF/JC-071/2017. PDP acknowledges the support provided by the Graduate School, Southern Illinois University Carbondale through the Doctoral Fellowship.
Dispersive Thermometry with a Graphene Josephson Junction

RAJ KATTI (Presenter), HARPREET SINGH ARORA, Caltech, OLLI SAIRA, Brookhaven National Laboratory, EWA REJ, MATTHEW MATHENY, MICHAEL ROUKES, STEVAN NADJ-PERGE, Caltech — Graphene, with its vanishing heat capacity and weak electron-phonon coupling at cryogenic temperatures, is a promising material for ultrasensitive calorimetry and single-photon detection. Here, we present dispersive thermometry measurements performed on a tunable graphene Josephson Junction (gJJ) integrated into a resonant microwave circuit. In contrast to DC detection methods that rely on the switching of the gJJ to its resistive state, this approach allows for continuous temperature readout. We will discuss device operation and show results in both the electron- and hole-doped regimes. Our results represent a step towards fast detection of low-energy photons and phonons.

*This work has been partially supported by a Gist-Caltech memorandum of understanding. S. N-P also acknowledges support from the IQIM (NSF Physics Frontiers Center).

Characterization of nonlinear screening in ionic liquid gated graphene multilayers via infrared spectroscopy

JIHO KIM, Physics, University of Seoul, MARCELO KURODA (Presenter), Physics, Auburn University, JIWON JEON, BYOUNGJU LEE, KWANGNAM YU, EUNJIP CHOI, Physics, University of Seoul — We quantify charge distributions in turbostratic few-layer graphene combining broadband infrared transmittance spectroscopy and analytical models. We show that the non-invasive experimental technique provides layer-resolved charge density profiles in regimes of interest for energy storage applications accessed using ionic-liquid gating. More importantly, we obtain unambiguous evidence of nonlinear screening of graphene which varies with thickness and charge density. Our results present good agreement with our theoretical model that accounts for the electrostatic coupling between layers and quantum capacitance of graphene. The proposed capacitor network model suggests that the effective channel capacitance increases with multilayer thickness but saturates after three layers, underscoring graphene’s qualities for ultrathin charge storage applications. Our work suggests that the combination of ionic liquid gating and infrared transmission spectroscopy may prove useful to the study of charge distributions in two-dimensional material systems.

*This work was supported by the National Research Foundation (NRF) grant funded by the Korean government (MSIT) (No. NRF-2017R1A2B4007782).
1:39PM G53.00011: Lithium intercalation of Black Phosphorous: Ex-situ and in-situ Raman Spectroscopy Study*  
   MANTHILA RAJAPAKSE (Presenter), MD RAJIB KHAN MUSA, USMAN ONUMINYA ABU, GAMINI U SUMANASEKERA, MING YU, JACEK BOGDAN JASINSKI, Univ of Louisville — Black phosphorous is emerging as a promising two-dimensional (2D) material which can be used as a host material for many intercalants. A systematic study on Li intercalation of black phosphorous was done using both in-situ and ex-situ electrochemical cells using black phosphorous as the cathode material. Galvanostatic discharge of dedicated in-situ electrochemical cell for Raman spectroscopy were used to study time evolution of vibrational modes under lithiation. Other than the peak broadening which is a result of structural expansion, it was observed that peaks corresponding to all three atomic vibrational modes $A_{1g}$, $B_{2g}$ and $A_{2g}$ were red-shifted as a result of lithiation. Peaks $B_{2g}$ and $A_{2g}$ shifted more towards lower wavenumbers whereas peak $A_{1g}$ shifted only 50% with respect to the other two, suggesting that Li ions prefer to be intercalated in-plane, along zig-zag and armchair directions than out-of-plane direction. Additional Transmission Electron Microscopy images were used to confirm the associated structural changes and Density Functional Theory (DFT) calculations were used to build a theoretical model for the phenomena.  

*This project is funded by US department of Energy  

1:51PM G53.00012: Study of Interface States and Dielectric Permittivity of Two-dimensional Tungsten Diselenide by Impedance Measurements*  
   FIDA ALI (Presenter), YANG ZHENG, SEKHAR BABU MITTA, WON JONG YOO, Nano-science and technology, Sungkyunkwan University — The dielectric permittivity of material holds great importance for understanding the intrinsic material properties and meanwhile, it's a critical design parameter for the design of novel device structure. In this article, we studied the capacitance-voltage (C-V) and conductance-voltage (G-V) characteristics of 2-D semiconducting WSe$_2$ based metal-insulator-semiconductor-metal capacitors under varying gate voltage ($V_G$), frequency and temperature. The obtained C-V and G-V results show a strong dependence on applied $V_G$, frequency (1 kHz to 1 MHz), and temperature (78K to 300K). From frequency-dependent C-V response, we extracted interface state density ($D_{it}$) by using the high-low frequency method, where $D_{it}$ values ranging from $3.8 \times 10^{10}$ to $3.6 \times 10^{12}$ cm$^{-2}$eV$^{-1}$ in the depletion region. Furthermore, we calculated the real ($\varepsilon'$), imaginary ($\varepsilon''$) parts of the dielectric constant and loss tangent (tan$\delta$) using C-V and G-V results. The results show that the values of $\varepsilon'$, $\varepsilon''$ and tan$\delta$ decrease with increasing frequency and increase with increasing temperature.  

*This work was supported by Global Research Laboratory Program (2016K1A1A2912707) and Global Frontier R&D Program (2013M3A6B1078873) both funded by Ministry of Science, ICT & Future Planning via National Research Foundation of Korea (NRF).
ANDREY SUSHKO (Presenter), KRISTIAAN DE GREVE, TROND I ANDERSEN, GIOVANNI SCURI, Physics, Harvard University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, PHILIP KIM, Physics, Harvard University, HONGKUN PARK, Chemistry and Chemical Biology, Physics, Harvard University, MIKHAIL LUKIN, Physics, Harvard University — The optical and electronic properties of van der Waals (vdW) heterostructures depend strongly on the atomic stacking order of the constituent layers. This is exemplified by Mott insulator states in ABC-stacked graphene, and topologically protected states along AB/BA boundaries in bilayer graphene. Moreover, periodic variation of local atomic registry, known as moiré patterns, has given rise to superconductivity in twisted bilayer graphene and exotic exciton states in TMD heterobilayers. However, the nm-scale moiré structure is typically indirectly deduced, because the conventional imaging technique, transmission electron microscopy (TEM), requires sample preparation that is incompatible with most optical and transport measurements. We present a method to directly image the local stacking order in complete vdW devices, including hBN-encapsulation, top- and bottom- graphite gates, and standard Si-substrates. Using this method, we demonstrate imaging of reconstructed moiré patterns in stacked TMDs, ABC/ABA stacking order in graphene multilayers, and AB/BA boundaries in bilayer graphene. Furthermore, we show that optical properties of the TMD are conserved after imaging, enabling correlation of local stacking order with optical and electronic properties.

*Hertz, PD Soros Fellowships

Tuesday, March 3, 2020 11:15 AM - 2:03 PM

Session G54 DCMP: Fractional Quantum Hall Effect and Composite Fermions Mile High Ballroom 2A - Yaroslaw Bazaliy, Univ of South Carolina
11:15AM G54.00001: Bloch Ferromagnetism of Composite Fermions  MD. SHAFAYAT HOSSAIN (Presenter), Princeton University, TONGZHOU ZHAO, SONGYANG PU, Department of Physics, Pennsylvania State University, M A MUEED, MENG MA, KEVIN VILLEGAS ROSALES, EDWIN CHUNG, LOREN PFEIFFER, KENNETH WEST, K. W. BALDWIN, Princeton University, JAINENDRA JAIN, Department of Physics, Pennsylvania State University, MANSOUR SHAYEGAN, Princeton University — The magnetic properties of the ground state of a low-density, 2D electron system (2DES) have been a topic of intense theoretical and experimental speculation and controversy, because the physics here is governed by strong correlations. Bloch predicted a fully spin-polarized ground state for a dilute fermionic system in 1929. However, such a state has eluded experimental realization for the last nine decades. Here we present an experimental realization of the elusive interaction-driven spin polarization in a dilute, 2D fermionic system, namely composite fermions (CFs). CFs are exotic quasiparticles, each composed of an electron and two flux quanta, formed in the half-filled Landau level of a 2DES. We determine the spin-polarization of these CFs via direct measurements of the CFs’ Fermi wavevector. We find that at high electron densities ($n_e$), the CFs are fully spin-polarized, consistent with previous experiments. As we lower $n_e$, the CFs lose their magnetization, also as expected. Remarkably, however, as $n_e$ is further reduced, the CFs make a sudden transition and become fully spin-polarized. This spontaneous magnetization of CFs closely resembles the Bloch ferromagnetism. We also performed theoretical calculations that provide a semi-quantitative understanding of the phenomenon.

11:27AM G54.00002: Hall viscosity of composite fermions*  SONGYANG PU (Presenter), Pennsylvania State University, MIKAEL FREMLING, Utrecht University, JAINENDRA JAIN, Pennsylvania State University — Hall viscosity, also known as the Lorentz shear modulus, has been proposed as a topological property of a quantum Hall fluid. Using a recent formulation of the composite fermion theory on the torus [1], we evaluate the Hall viscosities for a large number of fractional quantum Hall states at filling factors of the form $\nu=n/(2pn\pm1)$ [2], where $n$ and $p$ are integers. The calculated Hall viscosities $\eta^A$ agree with the expression $\eta^A = hS\rho/8\pi$, where $\rho$ is the density and $S$ is the ‘`shift“ in the spherical geometry [3]. We show that the Hall viscosity for $\nu=n/(2pn+1)$ may be derived analytically from the microscopic wave functions providing some assumption. This derivation is applicable to a class of states in the parton construction, which are products of integer quantum Hall states with magnetic fields pointing in the same direction [4].


*S.P. and J.K.J. was supported in part by the U. S. Department of Energy, Office of Basic Energy Sciences, under Grant No. DE-SC0005042. M.F. was supported by the D-ITP consortium.
11:39AM G54.00003: Fractional Chern insulators in magic-angle twisted bilayer graphene in the Hofstadter regime*  BARTHOLOMEW ANDREWS (Presenter), ALEXEY SOLUYANOV, Univ of Zurich — We apply a perpendicular magnetic field to the minimal effective two-orbital Fermi-Hubbard model describing the low-energy physics of twisted bilayer graphene at the first magic angle. Through the use of a Peierl's substitution, we determine the Landau level splitting and study the structure of the resulting Chern sub-bands for a range of magnetic flux per plaquette. We identify the minimal examples of low-energy topological flat sub-bands in this framework. We show that, with the inclusion of a density-density interaction, fractional Chern insulator states can be realized solely within these flat bands. Specifically, we characterize the $\nu = 1/3$ Laughlin state through the use of change pumping, spectral flow, entanglement scaling, and CFT edge state counting; and we analyze its dependence on band flatness. Ultimately, we comment on the requirements for the observation of fractional Chern insulators for this system in experiment.

*This project was funded by the Swiss National Science Foundation.

11:51AM G54.00004: Quantum Well Width Dependence of the Fractional Quantum Hall Energy Gaps  KEVIN VILLEGAS ROSALES (Presenter), PRANAV T MADATHIL, EDWIN CHUNG, K. W. BALDWIN, KENNETH WEST, LOREN PFEIFFER, MANSOUR SHAYEGAN, Princeton University — The fractional quantum Hall effect (FQHE) stems from the strong short-range Coulomb interaction in a two-dimensional (2D) electron system at high magnetic fields. However, the Coulomb interaction is softened in realistic samples which contain quasi-2D systems with a finite (non-zero) electron layer thickness. This softening leads to a weakening of the FQHE states, as manifested in a lowering of their energy gaps in both experiments [1] and calculations [2,3]. Here we present measurements of the energy gaps, from the temperature dependence of the magnetoresistance minima, of several fractional states in the lowest Landau level as a function of the width of the confining square quantum well. Our samples have a fixed density ($n \approx 1 \times 10^{11}$ cm$^{-2}$) while the width of the confining GaAs well varies between 20 and 80 nm. This is in contrast to measurements reported in [1] where the electrons were confined to parabolic Al$_x$Ga$_{1-x}$As quantum wells. The gaps in our measurements change in magnitude when plotted versus the GaAs well width. We contrast our results with numerical calculations that include the role of finite layer thickness [2,3].

12:03PM G54.00005: Achievement of Systematically Higher Transport Mobilities for a Large Range of Two-dimensional Electron Densities in GaAs Quantum Wells*  LOREN PFEIFFER (Presenter), EDWIN CHUNG, K. A. VILLEGAS-ROSALES, K. W. BALDWIN, KENNETH WEST, MANSOUR SHAYEGAN, Princeton University — For the range of two-dimensional (2D) electron densities between $1.5 \times 10^{10} \text{ cm}^{-2}$ and $1.4 \times 10^{11} \text{ cm}^{-2}$, we report measurements that confirm a ~60 to 70 % increase in the transport mobility of remotely-doped GaAs quantum wells compared to all previous GaAs material. A characteristic example of this development is the 2D transport mobility at an electron density of $1 \times 10^{11} \text{ cm}^{-2}$ in a 50 nm quantum well. Previously, in this type of sample the electron mobilities were limited to $\sim 1.8 \times 10^{7} \text{ cm}^{2}\text{V}^{-1}\text{s}^{-1}$; now we have grown several with transport mobilities reaching $\sim 3.0 \times 10^{7} \text{ cm}^{2}\text{V}^{-1}\text{s}^{-1}$. We attribute these results to our program of high-temperature in-situ bakes that have cleaned our AlGaAs barrier material of oxygen impurities, and to the use of large-area cryogenic cold-plates operating at 17 K in the vacuum sump of our molecular beam epitaxy chamber. When cooled to temperatures below 100 mK, the magnetotransport data of the $1 \times 10^{11} \text{ cm}^{-2}$ samples described above are remarkable, displaying clear quantum Hall features at the Landau level filling factors $\nu = 11/23, 12/25$, and even $13/27$.

*Work supported by the NSF (Grants DMR 1709076, ECCS 1906253, and MRSEC DMR 1420541), the DOE Basic Energy Sciences (Grant DE-FG02-00-ER45841), and the Gordon and Betty Moore Foundation (Grant GBMF4420).

12:15PM G54.00006: Renormalization Group Flow of Dirac Composite Fermions at Half Filling*  JONATHAN SAN MIGUEL (Presenter), Stanford Univ, HART GOLDMAN, Physics, University of Illinois, Urbana-Champaign, PRASHANT KUMAR, SRINIVAS RAGHU, Stanford Univ — We compare the effects of gauge field fluctuations between different composite fermion descriptions of the half-filled Landau level: the Halperin-Lee-Read (HLR) theory of non-relativistic composite fermions and the theory of Dirac composite fermions recently proposed by Son. While the Dirac theory is explicitly particle-hole symmetric, the HLR theory contains a fluctuating statistical gauge field which appears to break particle-hole symmetry. To better characterize this distinction, we present a renormalization group study of these theories in the presence of Coulomb interactions, using a controlled expansion both in the number of fermion species and the width of the Coulomb potential. In particular, we pay close attention to the effects in the HLR theory that break particle-hole symmetry. We find that both theories are described by marginal Fermi liquid fixed points and compare their universal features.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant Numbers DGE-1144245 and DGE-1656518, and by the DOE Office of Basic Energy Sciences, contract DE-AC02-76SF00515.
Heterostructure Design for High Two-dimensional Electron Density in GaAs/AlGaAs Quantum Wells at Large Hydrostatic Pressures

EDWIN CHUNG (Presenter), Princeton University, SHUAI YUAN, YANG LIU, Peking University, K. W. BALDWIN, KENNETH WEST, MANSOUR SHAYEGAN, LOREN PFEIFFER, Princeton University

The application of hydrostatic pressure to GaAs/AlGaAs heterostructures has been a topic of great interest due to the possibility of achieving a $g$-factor $\approx 0$ in high-quality, two-dimensional electron systems (2DESs). Despite the exciting prospect of studying electron-electron interactions in the absence of spin splitting, there are very few experimental reports on this subject. This is because in standard modulation-doped GaAs/AlGaAs heterostructures, the 2DES density decreases significantly as the magnitude of hydrostatic pressure applied to the system is increased. Here, we present a heterostructure design that circumvents such density degradation, so that high-density, high-quality 2DESs can be obtained at large hydrostatic pressures. We show that by implementing this scheme, the 2DES density only decreases by $\sim 4 \times 10^{10}$ cm$^{-2}$ even at a hydrostatic pressure of 8.2 kbar. This is a factor of $\sim 4$ improvement compared to conventional structures. We will also present low-temperature magnetotransport data that demonstrate the high quality of our samples at large hydrostatic pressures.

*Work supported by the NSF (Grants DMR 1709076, ECCS 1906253, and MRSEC DMR 1420541), the DOE Basic Energy Sciences (Grant DE-FG02-00-ER45841), and the Gordon and Betty Moore Foundation (Grant GBMF4420).

Diagnosis of universal geometric responses of fractional quantum Hall liquids

WEI ZHU (Presenter), Westlake University, DONNA SHENG, California State University Northridge, ZHAO LIU, Zhejiang University, LIANGDONG HU, Westlake University

Geometric response of topological quantum liquids is expected to reveal rich phenomenon. However, explicit demonstration or identification of the geometric response in a microscopic model is very challenging. Here, we demonstrate that Dehn-twist deformation is able to reveal both the universal modular properties and the microscopic features. We provide numerical evidences for various fractional quantum Hall (FQH) states, including fermionic and bosonic Laughlin states, Hierarchy states, Halperin states and Moore-Read states, by means of exact diagonalization calculations. We conclusively show, geometric transformation applied on torus geometry gives rise to a viscosity related Berry phase, which reflects the geometric metric of elementary FQH droplets. It also captures intrinsic modular information like topological spin and chiral central charge. These findings not only provide a unified description of Berry phase induced by geometric deformation, but also provide a systematical way to inspect the incompressibility of a gapped topological order in the projected Landau level.
12:51PM G54.00009: Particle-hole symmetry of the fractional quantum Hall effect in the lowest Landau level* EDUARDO PALACIOS (Presenter), MICHAEL R PETERSON, California State University, Long Beach — Electrons confined to two-dimensions experience the fractional quantum Hall effect (FQHE) at low electron densities, high magnetic fields, and low temperatures. FQHE states are topologically ordered phases characterized by the electron filling factor $\nu$ which is the electron number divided by the Landau level degeneracy. Alternatively, under particle-hole conjugation of a spin-polarized system confined to a single Landau level one can consider the system in terms of holes (the absence of an electron) with a hole filling factor of $\nu_h = 1 - \nu$. Naively, if the system maintains particle-hole symmetry, then the FQHE at filling factor $\nu$ will also occur at $1 - \nu$ with all the same properties. However, realistic effects such as Landau level mixing can break particle-hole symmetry at the level of the Hamiltonian through the inclusion of three-body terms. We study the nature of particle-hole symmetry on the FQHE in the lowest Landau level under realistic conditions numerically using exact diagonalization.

*This project is supported in part by National Science Foundation Grant --#1508290

1:03PM G54.00010: Identification of topological orders in fractional quantum Hall state at $\nu=1/4$* KWOK WAI MA (Presenter), Brown University — The nature of the fractional quantum Hall state at quarter filling in a wide quantum well is still under debate. Both one-component non-Abelian and two-component Abelian orders have been proposed to describe the system. Interestingly, these candidates received support from different experiments under disparate conditions. In this article, we focus on non-Abelian orders from Cooper pairing between composite fermions and the Abelian Halperin-(5,5,3) order. We discuss and predict systematically different experimental signatures to identify them in future experiment. In particular, we address the Mach-Zehnder interferometry experiment and show that it can identify the recently proposed 22111 parton order.

*This work was supported by the National Science Foundation under Grant No. DMR-1607451
1:15PM G54.00011: Anomalous nematic states in half-filled high Landau levels*  XIAOJUN FU (Presenter), QIANHUI SHI, MICHAEL ZUDOV, University of Minnesota, GEOFF C GARDNER, JOHN WATSON, MICHAEL MANFRA, Purdue University, K. W. BALDWIN, LOREN PFEIFFER, KENNETH WEST, Princeton University — It is well established that the ground states of a two-dimensional electron gas with half-filled high (N ≥ 2) Landau levels are compressible charge-ordered states, known as quantum Hall stripe (QHS) phases. The generic features of QHSs are a maximum (minimum) in a longitudinal resistance $R_{xx}$ ($R_{yy}$) and a non-quantized Hall resistance $R_H$. This talk will report on emergent minima (maxima) in $R_{xx}$ ($R_{yy}$) and plateau-like features in $R_H$ in half-filled $N ≥ 3$ Landau levels. Remarkably, these unexpected features emerge at temperatures considerably lower than the onset temperature of QHSs, suggestive of a new ground state.

*The work at Minnesota (Purdue) was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award \# ER 46640-SC0002567 (DE-SC0020138). L.N.P. and K.W.W. of Princeton University acknowledge the Gordon and Betty Moore Foundation Grant No. GBMF 4420, and the National Science Foundation MRSEC Grant No. DMR-1420541. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement Nos. DMR-1157490, DMR-1644779 and the State of Florida.

1:27PM G54.00012: Strain-induced resistance anisotropy near the FQHE v=5/2 in two-dimensional GaAs single quantum wells*  ALEXANDER STERN (Presenter), Max Planck Inst, BRIAN CASAS, Department of Physics and Astronomy, University of California Irvine, JOHANNES POLLANEN, Department of Physics and Astronomy, Michigan State University, JAMES EISENSTEIN, Department of Physics, California Institute of Technology, KENNETH WEST, LOREN PFEIFFER, Department of Electrical Engineering, Princeton University, JING XIA, Department of Physics and Astronomy, University of California Irvine — We report strain-dependent low temperature magnetotransport measurements of a two-dimensional electron gas (2DEG) confined in GaAs single quantum wells. The samples are mounted to a piezoelectric-based strain device with which we can, in situ, apply and vary tensile strain. With this apparatus, we have achieved strain as large as ~0.5% in GaAs quantum wells at cryogenic temperatures. We find that increasing strain causes the magneto-resistance of the 2DEG confined in the quantum well to become anisotropic near the filling factor $v = 5/2$. Additionally, we find that the effects of strain are highly dependent on the magnitude of the magnetic field applied. These anisotropic states are metastable and resume an isotropic state after a temperature dependent decay.

*The work at UC Irvine is supported by NSF Grant No. DMR- 1350122
Density Functional Theory of the Abelian Anyon Gas

YAYUN HU
(Presenter), Pennsylvania State University, GANPATHY MURTHY, Department of Physics and Astronomy, University of Kentucky, SUMATHI RAO, Harish-Chandra Research Institute, Homi Bhabha National Institute, JAINENDRA JAIN, Pennsylvania State University — A Kohn-Sham density functional theory of composite fermions takes into account the flux attached to composite fermions in a self-consistent fashion [1]. We extend this method to treat a system of many anyons. We construct a series of states that do not involve the center of mass excitations, and explore behavior in the vicinity of the fermionic statistics. We compare the energy obtained from our DFT calculation with exact energies known for small systems and find a qualitative and semi-quantitative agreement. Our method provides an understanding of the existing exact result and also a self-consistent way to calculate the ground state properties of the anyon gas in the thermodynamic limit.


This work is supported in part by DOE under Grant no. DE-SC0005042 and by the China Scholarship Council.

From CFT matrix product states to parent Hamiltonians

MATHEUS SCHOSSLER (Presenter), Washington University, St. Louis, SUMANTA BANDYOPADHYAY, Stockholm University/Nordita, ALEXANDER SEIDEL, Washington University, St. Louis — We study frustration free (FF) Hamiltonians of fractional quantum Hall (FQH) states from the point of view of the Matrix-product-state (MPS) representation of their ground/excited states. There is a wealth of solvable models relating to FQH physics, which, however, is mostly derived and analyzed from vantage point of first quantized "analytic clustering properties". In contrast, one obtains long-ranged FF lattice models when these Hamiltonians are studied in an orbital basis, which is the natural basis for the MPS representation of FQH state that has been of much interest lately. The connection between MPS-like states and frustration free parent Hamiltonians is central guiding principle in the construction of solvable lattice models, but thus far, only for short range Hamiltonians and MPS of finite bond dimension. The situation in the FQH context is fundamentally different. Here we expose the direct link between the infinite-bond-dimension MPS structure of Laughlin and Moore-Read-type CFT states and their parent Hamiltonians. Possible uses for states that lack a representation with nice analytic clustering properties are discussed.

SB acknowledges support from the European Research Council under the European Unions Seventh Framework ERS-2018-SYG 810451 HERO.
**G54.00015: Manifestations of the Uniform Berry Curvature in the Physics of Composite Fermions**

GUANGYUE JI (Presenter), JUNREN SHI, Peking University — It was proposed that the composite fermion is subject to a uniform Berry curvature in the momentum space [1]. Based on the picture, we theoretically consider a number of possible manifestations of the uniform Berry curvature. We show that the presence of the Berry curvature induces a shift in the commensurability condition of the geometrical resonance experiments. We argue that the shift had actually been observed in experiments. We further show that an electrostatic modulation, which is equivalent to a modulation of the Chern-Simons field of composite fermions, and the modulation of an externally applied magnetic field, yield different commensurability conditions. Moreover, we determine the low-frequency and long wavelength electromagnetic responses of a composite fermion system, and find results different from both the Halperin-Lee-Read theory and Son's Dirac theory.


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**Tuesday, March 3, 2020 11:15 AM - 2:15 PM**

**Session G55 DCMP: Transport and thermodynamic properties of topological systems: I** Mile High Ballroom 2B

**11:15AM G55.00001: Evidence of topological gap opening in the surface state of Bi$_2$Se$_3$ by proximity to a magnetic insulator**

SATYAKI SASMAL (Presenter), MATHIMALAR S, RAJASEKHAR P, ARCHIT BHARDWAJ, SAURABH CHAUDHARY, Tata Institute of Fundamental Research, Centre for Interdisciplinary Sciences, Hyderabad, BISWARUP SATPATI, Saha Institute of Nuclear Physics, KARTHIK RANAN, Tata Institute of Fundamental Research, Centre for Interdisciplinary Sciences, Hyderabad — Out-of-plane magnetism at the Bi$_2$Se$_3$/EuS interface is experimentally demonstrated and theoretically proposed [1,2,3], that is expected to break time-reversal-symmetry of topologically protected surface states (SSs). However, an exchange gap (EG) opening at the Dirac point due to proximity effect of the magnetic insulator (MI), EuS, is not observed before using transport studies, primarily due to dominant bulk conduction over the SSs. By using bottom gate voltage and external magnetic field studies, we report evidence of a metal-to-insulator transition at Bi$_2$Se$_3$/EuS interface, attributed to the opening of EG, with the signature of half-integer quantum Hall effect when Fermi level is tuned into the EG [4]. Our study also shows a gate-controlled enhanced interface magnetism at Bi$_2$Se$_3$/EuS interface which we attribute to the conduction carrier-mediated RKKY interactions [3]. Our efforts in this direction with suitable MI/TI/MI device will possibly allow us to demonstrate a switchable topological electronic device using magnetic proximity effect studies.


*We thank TIFR-Hyderabad, SERB, DAE and ECR grant.*
Evidence for a conducting surface state in FeSi

YUHANG DENG (Presenter), YUANKAN FANG, SHENG RAN, University of California, San Diego, WEIWEI XIE, Louisiana State University, SHEN WANG, SHIRLEY MENG, CHRISTIAN T WOLOWIEC, IVAN SCHULLER, University of California, San Diego, HONGBO LOU, SHUBIN LI, QIAOSHI ZENG, Center for High Pressure Science & Technology Advanced Research, JOHN SINGLETON, Los Alamos National Laboratory, ALEXANDER BREINDEL, M BRIAN MAPLE, University of California, San Diego — Electrical transport measurements on high quality single crystals of FeSi show a crossover from semiconducting to metallic behavior at 19 K ($T_c$). This metallic temperature dependent resistivity points to a conducting surface ground state of FeSi, supported by the impact of surface-to-volume ratio on the resistivity of the sample, and the absence of features in specific heat at low temperature [1]. We further explore this surface state using high field magnetoresistance, high pressure, and magnetic field modulated microwave spectroscopy (MFMMMS). Surprisingly, the surface sensitive MFMMMS measurement of FeSi shows an anomaly near $T_c$ with a signature typically associated with superconducting transitions. Based on the similarities in magnetoresistance between FeSi and the possible topological Kondo insulator SmB$_6$, FeSi could be a possible topological insulator.


Magnetotransport and weak anti-localization signatures in band-engineered 3D topological insulator pn-heterostructures

THOMAS MAYER (Presenter), HEDWIG WERNER, FLORIAN SCHMID, JOHANNES ZIEGLER, ELISABETH RICHTER, RALF FISCHER, University of Regensburg, REBECA DIAZ-PARDO, TU Munich, JUN FUJII, IVANA VOBOJNIK, Elettra-Sincrotrone Trieste, DIETER KARL WEISS, University of Regensburg, CHRISTIAN BACK, TU Munich, MATTHIAS KRONSEDER, DOMINIQUE BOUGEARD, University of Regensburg — To experimentally harness the novel physics arising from topological surface states (TSS) in 3D topological insulators (3D TIs) it is crucial to develop control over key band structure parameters. At the same time, controlling the contribution of bulk bands to transport has represented a major experimental challenge.

In this contribution, we combine band structure engineering in Bi-based heterostructures with alloy composition-tuning to provide experimental access to single TSS. In a vertical pn-heterostructure of 3D TIs, intrinsic band bending is introduced to create an internal depletion zone. It will not only induce compensation of unintentional charges, but also lead to an isolation of the top TSS from parasitic bulk background. We present pn-heterostructures with \((\text{Bi}_{1-x}\text{Sb}_x)_2(\text{Te}_{1-y}\text{Se}_y)_3\) as the p-type layer. Varying \((x,y)\) provides extensive control over the position of the Dirac point and the Fermi level. Moreover we observe a significant reduction of bulk carriers, compared to e.g. \(\text{Bi}_2\text{Se}_3\). We analyze our heterostructures in magnetotransport and angle-resolved photoemission spectroscopy (ARPES). Furthermore we discuss our conclusions in the light of the Hikami-Larkin-Nagaoka theory for weak anti-localization signatures observed in the longitudinal magneto-resistance.

Weak Antilocalization and Anisotropic Magnetoresistance in Topological Bi\(_2\)Te\(_x\)Se\(_{3-x}\) Thin Films

GREGORY STEPHEN (Presenter), Laboratory for Physical Sciences, OWEN VAIL, Army Research Lab, JIWEI LU, University of Virginia, PATRICK TAYLOR, Army Research Lab, ADAM FRIEDMAN, Laboratory for Physical Sciences — Topological materials, such as the quintessential topological insulators in the Bi\(_2\)X\(_3\) family \((X = O, S, Se, Te)\), are extremely promising for beyond Moore’s Law computing applications where alternative state variables and energy efficiency are prized. It is essential to understand how the topological nature of these materials changes with growth conditions and, more specifically, chalcogen content. In this study, we investigate the evolution of the magnetoresistance of \(\text{Bi}_2\text{Se}_{3-x}\text{Te}_x\) for varying chalcogen ratios as a function of both temperature and angle of applied field. Weak antilocalization (WAL), an indicator of topological surface states, is observed to weaken with Te substitution. We also demonstrate that the anisotropy of the WAL follows the Tkachov-Hankiewicz model of magnetoconductance in topological insulators rather than a more trivial \(\sin\theta\) dependence. This model, which is a generalization of the Hikami-Larkin-Nagaoka model, allows for measurement of both coherence length and skin depth of the conducting surface states. These results show the surface states in \(\text{Bi}_2\text{Se}_3\) to be most isolated from the bulk states, with quality degrading through Te substitution.
12:03PM G55.00005: Quantum Oscillations in Topological Insulator β-Ag2Te with High Mobility*  PENGLIANG LENG, XIAOYI XIE (Presenter), FAXIAN XIU, Physics, Fudan University — Stimulated by the fascinating properties discovered in topological insulators, topological quantum materials have become an exciting frontier in condensed matter physics and materials science. In this study, we claim a developed growth scheme to synthesize single crystalline (β-Ag$_2$Te) nanoplates with tunable Fermi levels by chemical vapor deposition (CVD). We systematically studied the transport measurement, showing that the atomic ratio of Ag and Te can significantly change the Fermi level of Ag$_2$Te nanoplates which achieves highest reported mobility ($\sim$50000 cm$^2$/V*s), and significant quantum oscillations appear. By analyzing the frequency and amplitude of the quantum oscillation, we can obtain various parameters in Ag$_2$Te, and push back the energy band structure.


*Our research was supported by National Natural Science Foundation of China (grant nos. 11474058, 11874116, 61674040)

12:15PM G55.00006: Anomalous quantum oscillations in topological insulators  AREG GHAZARYAN (Presenter), Institute of Science and Technology Austria, EMILIAN NICA, ONUR ERTEN, Department of Physics, Arizona State University, POUYAN GHAEMI, Department of Physics, City College of the City University of New York — Quantum oscillations are routinely used to determine the Fermi surface (FS) in metallic systems. In topological insulators, quantum oscillations can originate from the FS of the edge states. We analyze such quantum oscillations when the chemical potential lies close to the edge of either bulk conduction or valence bands. We compare and contrast these with standard cases for edge states with 2D electron-gas and Dirac dispersions, respectively. We discuss candidate systems where deviations from the standard cases are expected to occur. We comment on the possible implications for quantum oscillations observed in topological Kondo insulators.
**12:27PM G55.00007: Detection of hole pockets in type-II Weyl semimetal MoTe$_2$ from Shubnikov-de Haas quantum oscillations**

YAJIAN HU, Department of Physics, The Chinese University of Hong Kong, WING YU, Department of Physics, City University of Hong Kong, KWING LAI, Department of Physics, The Chinese University of Hong Kong, DAN SUN, FEDOR BALAKIREV, National High Magnetic Field Laboratory, Los Alamos National Laboratory, KING YAU YIP, WEI ZHANG, ESTEBAN I PAREDES AULESTIA, Department of Physics, The Chinese University of Hong Kong, RAJVEER JHA, RYUJI HIGASHINAKA, TATSUMA D. MATSUDA, Department of Physics, Tokyo Metropolitan University, YOICHI YANASE, Department of Physics, Kyoto University, YUJI AOKI, Department of Physics, Tokyo Metropolitan University, SWEE GOH (Presenter), Department of Physics, The Chinese University of Hong Kong — The bulk electronic structure of T$_d$-MoTe$_2$ features large hole Fermi pockets at the Brillouin zone center (Γ) and two electron Fermi surfaces along the Γ-X direction. However, the large hole pockets, whose existence has important implications for the Weyl physics of T$_d$-MoTe$_2$, had never been conclusively detected in quantum oscillations. In this presentation, we report an unambiguous detection of these elusive hole pockets via Shubnikov-de Haas (SdH) quantum oscillations. At ambient pressure, the quantum oscillation frequencies for these pockets are 988 T and 1513 T, when the magnetic field is applied along the c-axis. The quasiparticle effective masses $m^*$ associated with these frequencies are 1.50 $m_e$ and 2.77 $m_e$, respectively, indicating the importance of Coulomb interactions in this system. We further measure the SdH oscillations under pressure. At 13 kbar, we detected a peak at 1798~T with $m^* = 2.86$ m$_e$. Relative to the oscillation data at a lower pressure, the amplitude of this peak experienced an enhancement, which can be attributed to the reduced curvature of the hole pockets under pressure. Combining with DFT + $U$ calculations, our data shed light on why these important hole pockets had not been detected until now.

**12:39PM G55.00008: Magnetothermoelectricity of topological semiconductor ZrTe$_5$**

JUNBO ZHU (Presenter), CHANGMIN LEE, TAKEHITO SUZUKI, Massachusetts Institute of Technology MIT, SHIANG FANG, Harvard, NUH GEDIK, JOSEPH G CHECKELSKY, Massachusetts Institute of Technology MIT — We report a comprehensive study of electric, thermoelectric, thermodynamic measurements and angle resolved photoemission spectroscopy (ARPES) of the topological insulator candidate ZrTe$_5$. The single crystals grown by a chemical vapor transport method exhibit transport properties characterized by the electronic band structure with a small band gap that is observed by ARPES. The thermoelectricity has a significant response to magnetic field exceeding 300%, for which we discuss the mechanism along with the unique properties of bands deduced from the fermiology.
12:51PM G55.00009: Resonant and Magnetic Doping in Topological Insulator Bi$_2$Se$_3$*

BRANDI WOOTEN (Presenter), Ohio State Univ - Columbus, PATRICK TAYLOR, US Army Research Laboratory, JOSEPH P C HEREMANS, Ohio State Univ - Columbus — Topological insulators (TI) are bulk insulators with topologically protected, electrically conducting surface states. Unfortunately, “practical” topological protection is observed rarely. Interactions between bulk and surface electrons result in surface electrons having short lifetimes and experiencing strong dephasing that impedes possible applications, e.g., in quantum computing. We exploit resonant doping to reduce the bulk carrier concentration to meet the Mott criterion for the metal-insulator transition: the number of electrons due to unintentional doping, $n_D$, must be less than the critical carrier concentration, $n_c$. Se vacancies make Bi$_2$Se$_3$ heavily n-type, and the Mott criterion is not reached. By adding resonant dopant Sn to Bi$_2$Se$_3$, the density of states is widened at the top of the valence band, decreasing $n_c$ by an order of magnitude, allowing for the Mott criterion to be satisfied. Seebeck measurements show a sign change for Sn-doped Bi$_2$Se$_3$ as temperature is reduced, hinting that this approach works. Further, we plan to add magnetic dopant, Mn, and perform in-field transport measurements.


*Funding: CEM, NSF-DMR-1420451

1:03PM G55.00010: Identification of massive and topological surface states in the 3D topological insulator tensile strained HgTe

VALENTIN L. MÜLLER (Presenter), DAVID MAHLER, LUKAS LUNCZER, JONAS WIEDENMANN, WOUTER BEUGELING, HARTMUT BUHMANN, LAURENS W MOLENKAMP, University of Wurzburg — Topological surface states (TSS) with their linear dispersion and spin momentum locking constitute an interesting playground for basic research and future applications and have been identified in the topological insulator tensilely strained HgTe by magnetotransport measurements [1]. While the TSS are created due to the inversion of the bulk bands, additional surface states of different origin have been reported in gated devices of the topological insulator and the Dirac semi-metal phase of HgTe [2, 3]. These additional surface states are formed due to the shape of the electrochemical potential introduced by the electric field of the gate and are of general interest, since they can also be present in other topological materials. They are called massive Volkov-Pankratov states (VPS) after their first report in Ref. [4]. Here we present the unambiguous identification and manipulation of the different surface states, namely the TSS and the massive VPS, in the topological insulator HgTe by means of magnetotransport using top- and backgated devices as well as modulation doping.

1:15PM G55.00011: Transport evidence of Dirac dispersion in PbBi$_2$Te$_4$ 3D topological insulator* PRIYANATH MAL (Presenter), GANESH BERA, DEPARTMENT OF PURE AND APPLIED PHYSICS, GURU GHASIDAS VISHWAVIDYALAYA, KONI, Guru Ghasidas Vishwavidyalaya, BIPUL DAS, DEPARTMENT OF PHYSICS, National Changua University of Education, ARCHANA LAKHANI, UGC-DAE CSR Indore, G. R. TURPU, DEPARTMENT OF PURE AND APPLIED PHYSICS, GURU GHASIDAS VISHWAVIDYALAYA, KONI, Guru Ghasidas Vishwavidyalaya, C. V. TOMY, DEPARTMENT OF PHYSICS, IIT BOMBAY, PRADIP DAS, DEPARTMENT OF PURE AND APPLIED PHYSICS, GURU GHASIDAS VISHWAVIDYALAYA, KONI, Guru Ghasidas Vishwavidyalaya — The non-trivial nature of the surface states in PbBi$_{2-x}$Fe$_x$Te$_4$ is evident from the observations of the Shubnikov-de Haas (SdH) oscillations with π berry phase. Lower effective mass obtained from the Lifshitz-Kosevich fit and higher mobility values determined from the Dingle analysis confirmed the surface origin of the oscillations. An elongated band outside the surface Fermi surface is identified for pure sample and is absent for doped specimens. Combined SdH oscillations and Hall effect studies reveal the shifting of the Fermi level of PbBi$_2$Te$_4$ towards the Dirac point with successive Fe doping. Progressive decrease of the Fermi wave vector (k) and corresponding Fermi energy (E) with Fe doping can be fitted well with straight line, reveals the linear nature of the E-k diagram i.e. Dirac dispersion of topological surface states in PbBi$_2$Te$_4$. The observed weak anti-localization corroborates the spin-momentum locking as the consequence of π Berry phase acquires by the spin upon moving round the Dirac point and is consistent with SdH oscillations.

*PM thanks to CSIR for SRF award. PD, PM acknowledge the DST for supporting through project no. SR/FTP/PS-197/2012. PD, GRT acknowledging UGC-DAE CSR and IUAC for the project, no. CSR-IC-MSRSR-22/CRS-230/2017-18/1311 and IUAC/XIII.7/UFR-64315.

1:27PM G55.00012: Theory of drude-like nonlinear thermoelectric responses in quantum many-body systems XU YANG (Presenter), YING RAN, Boston College — A well-defined Drude peak in the linear electrical response is a fundamental feature of good metals, which has served as a basic probe of quantum materials irrespective of whether correlation is strong or not. We theoretically investigate Drude-like physics in general second-order nonlinear thermoelectric responses in time-reversal invariant noncentrosymmetric quantum many-body systems. The physical interpretations of the corresponding Drude weights are clarified, and the Drude relaxation time is discussed in the framework of the memory matrix technique. In particular, in linear responses the Drude weight is known to be related to the adiabatic derivative of the current with respect to twisted boundary conditions; while in the nonlinear case we find that the Drude weights are related to the adiabatic derivatives of dissipationless linear responses. In addition, we prove a general nonlinear reciprocal relation, and discuss nonlinear generalizations of the Lorentz ratio. Our results generalize the nonlinear Hall effect pointed out by Sodemann and Fu, and hold irrespective of whether quasiparticle descriptions are valid at low energies or not, indicating that nonlinear thermoelectric responses can serve as additional probes of strongly correlated systems such as non-Fermi liquids.
1:39PM G55.00013: Universal transport signatures of the topological phase transition in Majorana wires* AARON CHEW (Presenter), Caltech, WENYU HE, Hong Kong University of Science and Technology, JASON F. ALICEA, Caltech — Detecting the predicted magnetic-field-driven topological phase transition in proximitized nanowires is a key problem in the ongoing quest for unambiguous signatures of Majorana zero modes. We investigate the transport properties of a junction between a Luttinger liquid lead and a proximitized nanowire held at the topological phase transition. Upon fine-tuning a single parameter at the interface, the junction can realize a novel nontrivial fixed point at which electrons in the lead split into two propagating Majorana fermions, one that perfectly transmits into the critical nanowire and one that reflects. We introduce a bosonized framework for this fixed point and extract universal conductance signatures of the topological phase transition. We also comment on applications to tunneling into the edge of a two-dimensional topological superconductor.

*Army Research Office Grant Award W911NF-17-1-0323; NSF grant DMR-1723367; U.S.-Israel BSF Grant No. 2016258; the Israel Science Foundation; Caltech Institute for Quantum Information and Matter, an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation through Grant GBMF1250; Walter Burke Institute for Theoretical Physics at Caltech; Gordon and Betty Moore Foundation's EPIQS Initiative, Grant GBMF8682 to JA.

1:51PM G55.00014: Anomalous magnetotransport at a two-dimensional correlated electron system EDOUARD LESNE (Presenter), YILDIZ SAGLAM, THIERRY VAN THIEL, Delft University of Technology, PIERRE BRUNEE, Paris-Saclay University, ANA MONTEIRO, GARY STEELE, Delft University of Technology, MARC GABAY, Paris-Saclay University, ANDREA CAVIGLIA, Delft University of Technology — The emergent two-dimensional electron system (2DES) formed at the interface between LaAlO\textsubscript{3} (LAO) and SrTiO\textsubscript{3} (STO) insulating oxides has been a subject of great interest in condensed matter physics over the last decade. Recently, the (111)-oriented STO based 2DES has attracted further attention due to its sixfold orbital and lattice symmetry whereby two consecutive planes form a dense honeycomb lattice of Ti 3\textit{d} orbitals, a host candidate for prospective topologically non-trivial electronic phases. Furthermore, we have demonstrated that the (111)-LAO/STO interface exhibits an electronic correlation driven reconstruction of its band structure, and a two-dimensional superconducting groundstate, both tunable by electrostatic field-effect.

In this work, we report on the magnetotransport properties of the 2DES in both in-plane and out-of-plane magnetic field. In the planar Hall effect configuration we observe strongly gate-dependent large non-saturating magnetoresistive signal, with further plateau structures, when the sourced current is parallel to the applied external magnetic field. We tentatively relate the observed anomalous electronic transport to the complex band structure of the (111)-LAO/STO 2DES, exhibiting a number of avoided $d_{xz}$-$d_{yz}$-$d_{xy}$ band crossings, sources of Berry phase.
2:03PM G55.00015: Resistively detected nuclear magnetic resonance in topological insulators* ZEKUN ZHUANG (Presenter), VESNA F MITROVIC, JOHN BRADLEY MARSTON, Brown University — Topological insulators (TI) possess helical edge or surface states that are protected by both time-reversal symmetry and topology. We will present our proposal to use resistively detected nuclear magnetic resonance (RDNMR) to characterize Dirac fermions at the edge or surface of the TI. The effects of nuclear spins on the edge state conductance in both 2-D and 3-D TIs will be presented.

*We acknowledge Grant NSF OIA-192199.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G56 DCMP: Strange Metals Mile High Ballroom 2C - Yu He

11:15AM G56.00001: Coexisting Strange Metal and Fermi Liquid Collective Excitations in Sr$_2$RuO$_4$* ALI HUSAIN (Presenter), MATTEO MITRANO, MELINDA S RAK, SAMANTHA RUBECK, University of Illinois at Urbana-Champaign, HONGBIN YANG, Department of Chemistry and Chemical Biology, Rutgers University, FUMIHIKO NAKAMURA, Department of Education and Creation Engineering, Kurume Institute of Technology, CHANCHAL SOW, YOSHITERU MAENO, Department of Physics, Graduate School of Science, Kyoto University, PHILIP EDWARD BATSON, Department of Physics and Astronomy, Rutgers University, PETER MICHAEL AbbAMONTE, University of Illinois at Urbana-Champaign — The strange metal is an enigmatic phase found in numerous strongly correlated systems distinguished by violations of Fermi liquid and Boltzmann transport theories. Using momentum-resolved EELS (M-EELS), we previously showed that, while charge excitations of a Fermi liquid are known to propagate as plasmons with well-defined energy and momentum, the strange metal Bi$_{2.1}$Sr$_{1.9}$CaCu$_2$O$_{8+x}$ (Bi-2212) exhibits a featureless continuum of non-propagating charge fluctuations exhibiting simple scaling laws. Here, we present M-EELS results on Sr$_2$RuO$_4$ showing that it exhibits both a strange metal continuum and a well-defined low-energy collective mode below 100 meV propagating at near the Fermi velocity. Strikingly, the dispersion of this mode is strongly renormalized at low temperature where transport measurements indicate the onset of Fermi liquid behavior. These results suggest that Sr$_2$RuO$_4$ exhibits a crossover between Fermi liquid-like behavior at low energy and strange metal behavior at high energy, with the two sectors in coexistence. We also present new transmission M-EELS experiments validating the bulk origin of these observations.

*This work was supported by DOE grant DE-FG02-06ER46285. P.A. acknowledges support from Gordon and Betty Moore Foundation EPiQS grant GBMF-4542.
11:27AM G56.00002: Classical Glasses, Black Holes, and Strange Quantum Liquids* DAVIDE FACOETTI (Presenter), GIULIO BIROLI, JORGE KURCHAN, Ecole Normale Superieure, DAVID REICHMAN, Columbia University — From the dynamics of a broad class of classical mean-field glass models we construct a quantum model with finite zero-temperature entropy, a quantum transition at zero temperature, and a time-reparametrization (quasi-)invariance in the dynamical equations for correlations. The low eigenvalue spectrum of the resulting quantum model is directly related to the structure and exploration of metastable states in the landscape of the original classical glass model. This mapping reveals deep connections between classical glasses and the properties of SYK-like models.

*Work supported by the Simons Foundation, Grant Nos. #454943 (Jorge Kurchan), #454935 (Giulio Biroli), #454951 (David Reichman). DF was partially supported by EPSRC (CANES, EP/L015854/1) and ERC (grant n.723955 - GlassUniversality).

11:39AM G56.00003: A hydrodynamical description for transport in the strange metal phase of cuprates ANDREA AMORETTI (Presenter), Univ of Genova — High temperature superconductors are strongly coupled systems which present a complicated phase diagram with many intertwined phases appearing at the same time. This makes it difficult to understand the mechanism which generates their singular transport properties (see e.g. [1]). Hydrodynamics, which mostly relies on the symmetries of the system without referring to any specific microscopic mechanism, constitutes a promising framework to analyze these materials.

In this talk I will show that in the strange metal phase of the cuprates, a whole set of transport coefficients are described by a universal hydrodynamic framework once one accounts for the effects of quantum critical charge density waves. I will compare the theoretical prediction with the measured DC transport properties of Bi-2201 close to optimal doping, proving the validity of our approach. Our argument can be used as a consistency check to understand the universality class governing the behavior of cuprate high temperature superconductors.

References:
11:51AM G56.00004: Strange metallic magnetotransport in electron-doped cuprates*
NICHOLAS PONIATOWSKI (Presenter), TARAPADA SARKAR, PAMPA R MANDAL SARKAR, RICHARD GREENE, University of Maryland, College Park — The infamous linear-in-T resistivity seen in hole-doped cuprates has become the hallmark of strange metallicity, but a more expansive strange metal phenomenology exists in the electron-doped compounds. Linear-in-T resistivity and linear-in-H magnetoresistivity are observed at low temperatures, in stark contrast to conventional Fermi-liquid behavior, and at high temperatures an anomalous $T^2$ resistivity is observed. In this talk, we discuss other signatures of strange metallicity at higher temperatures (50-300 K) in these compounds as evidenced by magnetotransport experiments.

*This work is supported by the NSF under Grant No.DMR-1708334 and the Center for Nanophysics and Advanced Materials (CNAM).

12:03PM G56.00005: Ubiquitous power law behaviour in the self energy of Strange Metals*
STEEF SMIT (Presenter), Univ of Amsterdam — The high temperature superconducting state in cuprates is born out of the strange metal phase, showing resistivity linear in temperature, contravening Fermi liquid theory for metals. Theoretical understanding of this phase is limited, despite decades of research. Recently, the Anti-de Sitter/Conformal Field Theory (AdS/CFT) approach has been proposed to hold the answer, something we set out to test. ARPES experiments are able to determine the normal state electron lifetime (described by a self-energy) in a k-resolved manner. In a 2015 arXiv post (1), laser-ARPES data from BSCCO-2212 proposed that the E- and T-dependence of the self-energy are power-laws. This got the AdS/CFT community excited, as this behaviour comes out of their calculations. We have carried out analogous ARPES experiments on clean, single-layer BSCO-2201 systems over a wider range of T and E, obtaining some of the highest quality data ever recorded on these materials. This work presents the accurately extracted self-energies vs. energy and temperature, and often made assumptions such as k-independent self-energies are discussed. (1) Reber et al, arXiv (2015)

*This work is part of the programme Strange Metals with project number 167, which is (partly) financed by the Dutch Research Council (NWO)
12:15PM G56.00006: Microscopic origin of the `strange' metal* KYUNGMIN LEE (Presenter), Natl High Magnetic Field Lab, AAVISHKAR PATEL, University of California, Berkeley, NANDINI TRIVEDI, The Ohio State University, SUBIR SACHDEV, Harvard University — We study a disordered Anderson-Hubbard lattice model of strongly interacting fermions. We obtain the space and time dependent electron Green’s function by numerically summing the `melon’ diagrams. We show the emergence of two `fluids’: (i) a fraction of sites, with weaker hopping than the background, hybridize with a constellation of neighboring sites and nucleate islands, and behave similar to the Sachdev-Ye-Kitaev model; (ii) the remaining background electrons scatter off SYK islands, and display strange metal transport with a linear-in-temperature resistivity, and singular spectral widths down to zero temperature with no coherence scale.

*K. L. and N. T. have been supported by the Department of Energy Grant No. DE-FG02-07ER46423. A.A. P. and S. S. have been supported by the Department of Energy Grant No. DE-SC0019030.

12:27PM G56.00007: Incoherent Strange Metal Sharply Bounded by a Critical Doping in Bi2212* SU-DI CHEN (Presenter), Stanford Univ, MAKOTO HASHIMOTO, SLAC National Accelerator Laboratory, YU HE, Stanford Univ, DONGJOON SONG, National Institute of Advanced Industrial Science and Technology, Japan, KEJUN XU, JUNFENG HE, THOMAS DEVEREAUX, Stanford Univ, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, Japan, DONGHUI LU, SLAC National Accelerator Laboratory, JAN ZAANEN, Leiden University, the Netherlands, ZHIXUN SHEN, Stanford Univ — In normal metals, macroscopic properties are understood using the concept of quasiparticles. In the cuprate high-temperature superconductors, the metallic state above the highest Tc is found to be very different and called the “strange metal”. To study this state, we use angle-resolved photoemission spectroscopy to directly measure its spectral function. With increasing doping across a temperature-independent critical value pc ~ 0.19, we observe a dramatic change near the Brillouin zone boundary where the strange metal characterized by incoherent spectral function abruptly reconstructs into a more conventional metal with quasiparticle-like excitations. This sharp reconstruction signals the incoherent strange metal as a distinct state of matter. Furthermore, above the temperature scale of superconducting fluctuations, we find that the pseudogap — the anomalous suppression of low-energy spectral intensity with decreasing temperature — also sharply collapses at the very same pc. This suggests that the pseudogap is a low-temperature phenomenon associated with the incoherent strange metal.

*This study is supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract DE-AC02-76SF00515.
The optical conductivity of (K,Rb,Cs)Fe$_2$As$_2$: hidden temperature behaviors and electronic correlations strength  
RICARDO LOBO (Presenter), ESPCI Paris - PSL, CNRS, Sorbonne University — We measured the temperature dependence of the optical reflectivity in undoped XFe$_2$As$_2$ iron pnictides, where X = K, Rb, and Cs. A two-Drude analysis of the data quantitatively describes the Kramers-Kronig obtained optical conductivity of all compositions. From this analysis, we extracted the scattering rate and effective mass for each Drude contribution. Both our parameters and the overall optical conductivity are compared to first principles DMFT calculations. We discuss the temperature behavior of the scattering rate as a function of X and show that a hidden linear behavior emerges from the decomposition of the optical conductivity. The comparison of the full optical conductivity to DMFT calculations allows us to infer the evolution of the electronic correlations strength with ionic replacement. Collaborators: L. de' Medici, (ESPCI Paris, France), F. Hardy, A.A. Haghighirad (Karlsruhe Institute of Technology, Germany)

12:51PM G56.00009: $^{13}$C NMR measurement of $\theta$-(BEDT-TTF)$_2$I$_3$ in non-Fermi liquid region  
KAZUYA MIYAGAWA (Presenter), HIDEAKI MURASE, TAKURO SATO, Univ of Tokyo, MASAFUMI TAMURA, Tokyo University of Science, KAZUSHI KANODA, Univ of Tokyo — The BEDT-TTF salts with $\theta$-type molecular arrangement, $\theta$-(BEDT-TTF)$_2$X, which have a triangular lattice show a wide variety of electronic states (charge order insulator, charge glass state, metal) according to monovalent anion, X. Among them, the X=I$_3$ salt is considered to be in a typical metal because quantum oscillations are observed at low temperatures [1]. On the other hand, in the optical spectrum, normal Drude response was not observed above 100 K. So the salt is different from a simple Fermi liquid picture at high temperature [2]. Recently, we report increase of resistance noise near 50 K-180 K, where the resistance exceeds the Mott limit [2,3]. In this study, the $^{13}$C NMR spectra and the 1/$T_2$, which captures slow fluctuations in the order of kHz were measured. In the salt showing charged glass, the 1/$T_2$ has a peak, which is thought to be associated with the glass formation process [4]. On the other hand, in X=I$_3$ salt, the temperature dependence of 1/$T_2$ is very weak and the absolute value remained small. There was also no significant increase in linewidth. This means that the spectral density of fluctuation in the kHz range is small. [1] M. Tamura et al., JPSJ (1994). [2] K. Takenaka et al., PRL (2005). [3] T. Sato et al., Nat. Mat. (2019). [4] K. Miyagawa et al., JPSJ (2019).
Machine learning of non-Fermi liquid transport in quantum critical metals

GEORGE DRISCELL (Presenter), Cornell University, SAMUEL LEDERER, CARSTEN BAUER, SIMON TREBST, University of Cologne, EUN-AH KIM, Cornell University — Anomalous transport, such as T-linear resistivity (a hallmark of non-Fermi liquid behavior), is a ubiquitous feature of strongly correlated metallic systems, but famously difficult to understand theoretically. For relevant simple models, the transport computations of even numerically exact Monte Carlo simulations are subject to enormous systematic errors and come at great additional computational cost. Building on earlier work, we apply quantum loop topography (QLT) and supervised learning on quantum Monte Carlo data to examine the Fermi liquid to non-Fermi liquid crossover in models of both Ising nematic and spin density wave quantum criticality. Previous work on these models has demonstrated this crossover using measurements of correlation functions at nonzero imaginary time separation. Our results, using only equal time measurements, show good agreement with these previous results at dramatically lower computational cost. Hence, QLT-based machine learning can accelerate the exploration of parameter space in search for non-Fermi liquid behavior by obviating the need for expensive dynamical measurements.

Normal state properties of quantum-critical metals at finite temperatures

AVRAHAM KLEIN (Presenter), University of Minnesota, YONI SCHATTNER, Stanford University, EREZ BERG, Weizmann Institute of Science, ANDREY CHUBUKOV, University of Minnesota — Recent years have seen an intense effort to study models of fermionic quantum criticality and superconductivity via sign-problem-free quantum Monte Carlo. These studies found a number of puzzling features, which are in qualitative disagreement with quantum-critical-scaling theories and, in particular, cast doubt on the validity of Eliashberg-type approaches to quantum criticality. I will discuss how thermal fluctuations destroy the nice scaling properties of quantum-critical systems and show that after generalizing Eliashberg theory to account for thermal fluctuations many of the qualitative disagreements vanish. This work provides concrete guidelines for analyzing ongoing numerical work.

Supermetal

HIROKI ISOBE (Presenter), LIANG FU, Massachusetts Institute of Technology MIT — We study the effect of electron interaction in an electronic system with a high-order Van Hove singularity, where the density of states shows a power-law divergence. Owing to scale invariance, we perform a renormalization group (RG) analysis to find a nontrivial metallic behavior where various divergent susceptibilities coexist but no long-range order appears. We term such a metallic state as a supermetal. Our RG analysis reveals noninteracting and interacting fixed points, which draws an analogy to the $\varphi^4$ theory. We further present a finite anomalous dimension at the interacting fixed point by a controlled RG analysis, thus establishing an interacting supermetal as a non-Fermi liquid.
**1:39PM G56.00013: A symmetry-breaking analysis for non-Fermi liquids induced by order fluctuations in correlated electron systems**  
ZHENG-SU SHE (Presenter), RONG LI, Peking Univ —  
Correlated electron systems display multi-order fluctuations, which are thought of the origin for non-Fermi liquids. Here, we present a symmetry-breaking analysis for establishing this relationship. Specifically, we establish a sequence of symmetry-breakings under increasing temperature with varying orders such as density wave, nematicity and loop current in cuprates. In particular, we propose that the underlying order for strange metal (SM) is vortex fluctuation, as a fluctuating loop current excited by thermal fluctuations and field. Furthermore, a theory for scattering rate by multi-order fluctuations is constructed based on a symmetry analysis of multi-dimensional Hamiltonian with elements determined by length order function (i.e. orders' periodicity). It then yields a formula for resistivity, i.e., \( \rho = \rho_a + (\rho_b^2 + \alpha^2 T^2 + \beta^2 B^2)^{1/2} \), capturing the scaling transition from \( T^2 \) in pseudogap phase to \( T \) in SM phase, as well as anomalous magnetoresistance near quantum critical point. We report the validation evidence of dozens of cuprate samples. The most remarkable outcome is the revelation of the role of a length order function in linking macroscopic resistivity to microscopic fluctuating orders, which is essential for understanding anomalous transport in correlated electron systems.

**1:51PM G56.00014: The role of electron-electron collisions for charge and heat transport at intermediate temperatures**  
WOO-RAM LEE, Univ of Alabama - Tuscaloosa, ALEXANDER FINKELSTEIN, Texas A&M University, KAREN MICHAELI, The Weizmann Institute of Science, GEORG SCHWIETE (Presenter), Univ of Alabama - Tuscaloosa —  
We study electric, thermal and thermoelectric transport in correlated electron systems in the intermediate temperature regime, in which elastic and inelastic scattering are both important. To this end, we study the Boltzmann equation in the presence of an electric field and a temperature gradient for two cases: First, when electron-electron collisions are treated within the relaxation-time approximation while the full momentum dependence of electron-impurity scattering is included and, second, when the electron-impurity scattering is momentum-independent, but the electron-electron collisions give rise to a momentum-dependent inelastic scattering rate of the Fermi-liquid type. We find that the inelastic relaxation rate enters the electric conductivity and the Seebeck coefficient only when the momentum dependence of the electron-impurity collisions is included. Specifically, we show that inelastic processes only mildly affect the electric conductivity, but can generate a non-monotonic dependence of the Seebeck coefficient on temperature and even a change of sign. Thermal conductivity always depends on the inelastic scattering rate even for a constant elastic relaxation rate.

*This work is supported by DOE, ISF, NSF, and the College of Arts and Sciences at the University of Alabama.*
2:03PM G56.00015: Charge Transport in the Non-ergodic Extended phase of Quasi-periodic systems
SOUMI GHOSH (Presenter), JYOTSNA GIDUGU, SUBROTO MUKERJEE, Indian Institute of Science — We study the transport properties and the spectral statistics of a one-dimensional closed quantum system of spinless fermions in a quasi-periodic potential which produces a single particle mobility edge. For such systems, it has been shown that many body eigenstates can be of three different kinds: extended and ETH (energy thermalization hypothesis) obeying (thermal), localized and ETH violating (many body localized) and extended and ETH violating (non-ergodic extended). Here we investigate the non-ergodic extended phase from the point of view of level spacing statistics and charge transport. We calculate the DC conductivity and the low frequency conductivity $\sigma(\omega)$ and show that both are consistent with sub-diffusive transport. This is contrasted with diffusive transport in the thermal phase and blocked transport in the MBL phase.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G57 DMP: Electronic and Optical Properties of 2D Materials II
Mile High Ballroom 3A - Xiaoxiao Zhang, University of Florida - Tag(s): Focus

11:15AM G57.00001: First-principles simulation of inelastic electron beam-matter interactions and their effect on knock-on damage cross sections* ANTHONY YOSHIMURA (Presenter), Rensselaer Polytechnic Institute, DAVID LINGERFELT, PANCHAPAKESAN GANESH, JACEK JAKOWSKI, Oak Ridge National Laboratory, MICHAEL LAMPARSKI, JOEL GIEDT, Rensselaer Polytechnic Institute, BOBBY SUMPTER, Oak Ridge National Laboratory, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Electron irradiation by transmission electron microscopy is an effective method for engineering the properties and morphology of 2-dimensional (2D) materials with a high degree of spatial control. It follows that many computational models have been developed to predict the rates of atomic displacements in 2D materials under such irradiation. However, while current models give reasonable predictions for conductors, they often vastly underestimate the displacement rates in insulators. In this work, we combine density functional theory with quantum electrodynamics to demonstrate how the consideration of electron-electron scattering can lead to the prediction of significantly higher displacement rates in gapped materials, reducing the disparity between theory and experiment. This new model would be a boon for materials engineers, allowing for the controlled manipulation of any 2D material for targeted functionality.

*This work was funded by the National Science Foundation (Award 1608171)
11:27AM G57.00002: A comparison study between the Lennard-Jones and DRIP potentials for friction of graphene layers*  
WOO KYUN KIM (Presenter), HUYAN LI, Univ of Cincinnati —  
Graphene is a one-atom thick 2-D material and has huge potential as a solid lubricant for small length scale devices such as nano/micro-electro-mechanical systems. Atomistic simulations such as molecular dynamics is a popular tool to study the frictional behaviors of graphene layers and it is of critical importance to accurately describe the interlayer interactions in order to give a reliable prediction on the friction of graphene. Here, two interatomic potentials, Lennard-Jones (LJ) potential and dihedral-angle-corrected registry-dependent interlayer (DRIP) potential, are examined to model interlayer interactions in friction simulations of multilayer graphene structures. While both potentials have similar attractive interactions, DRIP models the repulsive interaction by considering transverse distance and dihedral angle. In this study, we investigate the friction properties between two pristine graphene layers. The simulation results reveal that friction forces of the DRIP models are about one order of magnitude larger than those of the LJ models. It turns out that the modification of the repulsive term in DRIP introduces additional energy corrugations which increase the friction force.

*This work was in part supported by NSF CMMI 1662666.

11:39AM G57.00003: Structural studies of Ni-doped MoS$_2$ monolayers and polytypes using density functional theory (DFT)*  
RIJAN KARKEE (Presenter), ENRIQUE GUERRERO, DAVID STRUBBE, University of California, Merced — The structure of MoS$_2$ with strong covalent bonds in plane and weak van der Waals interactions out of plane gives rise to interesting properties for applications such as solid lubricants, optoelectronics, sensors, and electrochemical devices. Transition metal doping is found to improve the performance in tribology [MR Vazirisereshk et al., Lubricants 7, 57 (2019)] and hydrodesulfurization. We study the structure and properties of Ni-doped MoS$_2$ in the 1H and 1T monolayer and 2H and 3R bulk polytypes, using density functional theory (DFT). We calculated the formation energy of Ni at different sites (Mo and S substitution, intercalation/adsorption) to identify the most energetically favorable ones, and analyzed the energy for layer separation and the energetics of interlayer sliding. We studied the effect of Ni doping on local bonding and lattice structure at different dopant concentrations to assess possible phase changes. This work gives insight into the previously unclear structure, properties, and solid lubrication performance of Ni-doped MoS$_2$.

*Merced nAnomaterials Center for Energy and Sensing, MERCED cluster at UC Merced and NERSC supercomputer at LBNL
11:51AM G57.00004: Electrochemical Properties of Pt-Graphene Hybrid System: DFT Modeling Approach  JI IL CHOI (Presenter), SEUNG SOON JANG, Georgia Inst of Tech — Epitaxially grown Pt thin film on a graphene template is found to have a few monolayer thickness with structural stability comparable to Pt(111) surface and promising electrochemical activity. The newly synthesized thin film shows the crystalline Pt structure of quadrilateral polygon in monolayer stacking, and simple cubic-like (SC-L) stacking in bi-layer film. In this study, we present a computational research on the unique architecture of the graphene templated epitaxial platinum layers in support of the remarkable recent progress. Recently proposed strongly constrained and appropriately normed (SCAN) density function study (DFT) is employed to investigate the materials characteristics. Electrochemical activities of the system are evaluated in terms of the free energy variation in oxygen reduction reaction (ORR). In architectures, Pt exhibits registry with the C-C bridge sites along the armchair and zigzag directions forming strong covalent bonds. Here, the details of the atomistic/electronic structures and binding energies are discussed. Interestingly, the ORR can occur on both Pt and graphene surfaces. This would provide a good strategy for 1) the protection of metallic catalyst and 2) tune the electronic structure of catalyst.

12:03PM G57.00005: Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons  ZHONGCAN XIAO (Presenter), North Carolina State University, CHUANXU MA, Oak Ridge National Laboratory, WENCHANG LU, North Carolina State University, JINGSONG HUANG, LIANGBO LIANG, KUNLUN HONG, AN-PING LI, BOBBY SUMPTER, Oak Ridge National Laboratory, JERRY BERNHOLC, North Carolina State University — Atomically precise synthesis of graphene nanoribbons (GNRs) may enable GNR-based nanoelectronics. We investigated GNR synthesis from DBBA molecular precursors on an Au(111) surface [1]. The growth process consists of dehalogenation/polymerization followed by cyclodehydrogenation. We investigated the latter using the nudged elastic band method within DFT. Our studies found that the metal substrate: (i) enhances the reaction energetics because adsorption of the product (GNR) on Au (111) is stronger than the adsorption of the reactant (polyanthrylene), and (ii) acts as a catalyst to lower the energy barriers for cyclodehydrogenation. In comparison, an underlying adsorbed GNR screens the metal substrate and hinders on-top GNR growth by lowering the adsorption energy and increasing the energy barriers. We also investigated electronic levels of various intermediate structures and found that molecular orbitals play an important role in directing the reaction, e.g., the injected electrons (or holes) lower the energy barrier through arenium ion effect. These findings provide new insight into GNR growth and offer guidance for the design of new graphitic structures.

**12:15PM G57.00006: Electronic Structure of twisted kagome lattice**

**ERIC SUAREZ MORELL**
(Presenter), Federico Santa Maria Technical University, FELIPE CASTRO DE LIMA, ROBERTO HIROKI MIWA, Universidade Federal de Uberlandia —

We have studied how a generic bilayer kagome lattice behave upon layer rotation. We employed a Tight Binding model with one orbital per site and found (i) for low rotational angles, and at low energies, the same flat bands structure like in twisted bilayer graphene; though, for a larger value of the magic angle.

Moreover, (ii) at high energies, due to the superstructure symmetry regions, we found the characteristics three band dispersion of the kagome lattice. In the latter, its band width decreases for lower angles confining them within a few meV. Therefore, we found in twisted kagome lattice the coexistence of two sets of flat bands in different energies and lying in different spatial regions of the bilayer system. The calculations are done for a generic kagome lattice, nonetheless we used a ratio between inter and intra layer nearest hopping similar to the value obtained in the studies of a kagome bilayer structure of Fe$_3$Se$_2$ [1] to fit experimental results.


*FONDECYT Regular 1170921*

**12:27PM G57.00007: 2D Memory Physics and Applications**

**[Invited] DEJI AKINWANDE**
(Presenter), University of Texas at Austin — This work presents the latest research progress on the atomic-level details of non-volatile resistance switching (NVRS) in 2D memory devices, otherwise known as atomristors. In particular, we will focus on memory characteristics and atomistic imaging and transport studies, together with the first principle calculations to elucidate the underlying physics. These studies provide one to one correlation between the structural and electronic properties of defects and their role in the resistance switching mechanism.

Applications from information storage to RF communication to neuromorphic computing will be highlighted.

*This work is supported in part by a PECASE, and an NSF grant.*
1:03PM G57.00008: Excitonic effects in optical-field-driven quasi 2D materials from time-dependent GW approach* [Invited] YANG-HAO CHAN (Presenter), Lawrence Berkeley National Laboratory, DIANA QIU, FELIPE H. DA JORNADA, STEVEN LOUIE, Physics, Unviersyt of California, Berkeley — Atomically thin quasi two-dimensional (2D) insulating materials exhibit novel exciton physics due to ineffective screening, quantum confinement, and topological effects. Such exciton physics has recently been studied in details experimentally and theoretically. Going beyond near-equilibrium set-up, one expects that excitonic effects also dominate the responses of out-of-equilibrium systems and can lead to interesting phenomena in optically-driven 2D materials. Using a newly developed real-time, non-equilibrium Green function method within the adiabatic GW approximation, we show that, for non-centrosymmetric 2D semiconductors, excitonic effects give rise to a strong DC current, the so-called shift current, upon even sub-bandgap frequency CW light illumination through a second-order nonlinear optical process. The frequency-dependent shift current coefficients can be enhanced by orders of magnitude by the strong e-h interactions, producing a bulk photovoltaic effect (i.e., without having to have a p-n junction) of promise for applications with appropriate materials. Furthermore, we show that, in optical-field-driven angle-resolved photoemission spectroscopy (ARPES) experiments, the energy and wavefunction of excitons may be measured directly under achievable laboratory conditions. With optical pump frequencies close to the resonance frequency for exciton excitations, distinct excitonic features manifest themselves dramatically as modulated replicas of the involved valence band states. We also find that, at higher pump intensity, the quasiparticle band energies are renormalized due to the driving optical fields.

*This work was supported by the Center for Computational Study of Excited State Phenomena in Energy Materials (C2SEPEM), which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231.
1:39PM G57.00009: Valley Polarization in Superacid-Treated Monolayer MoS$_2$* RUIJIE LI, YIFEI LI, HUIFENG TIAN, PEIQI LIAO, LEI LIU (Presenter), Department of Materials Science and Engineering, College of Engineering, Peking University, Beijing 100871, P. R. China — Point defects play a critical role in numerous phenomena such as transport, optical, and optoelectrical properties. With a lower dimensionality, due to reduced dielectric screening the interplay between charge carriers, excitons, and point defects becomes stronger in the two-dimensional materials, such as monolayer transition metal dichalcogenides (TMDCs). TMDCs have shown the fascinating spin-valley-coupled physics, which is strongly related to the lifetime of photoexcited exciton and the polarization decay time. Recently the superacid treatments have been demonstrated to increase the life time of excitons in monolayer MoS$_2$. The valley properties of treated MoS$_2$ monolayers are largely unexplored. With the variable temperature steady state PL and polarization-resolved PL spectroscopy, we show the robust absorption of superacid molecules and unexpectedly enhanced defect-bound emission under high vacuum under low temperature. The unaffected valley polarization of monolayer MoS$_2$ emphasizes the exciton trapping effect by the shallow defect levels. Our finding paves the way for the understanding of point defeat engineering for monolayer TMDCs.

*Supported by National Natural Science Foundation of China (11974001, U1932153) and Beijing Natural Science Foundation (2192022, Z190011).

1:51PM G57.00010: Anomalous CDW response in high mobility magnetic 2D material GdTe$_3$ KENNETH BURCH (Presenter), YIPING WANG, Boston college, SHIMING LEI, LESLIE SCHOOP, Princeton University — Most known magnetic van der Waals (vdW) materials are insulating or semiconducting. It is crucial to find materials with magnetic order and high-mobility for high-speed spintronic device making. Anti-ferromagnet GdTe$_3$ satisfies both down to 2D limits. It also exhibits an incommensurate charge density wave (CDW) but the role of it in GdTe$_3$ properties is still unclear. Here, we report the recent temperature and polarization dependent Raman study of GdTe$_3$, we will talk about the coupling between CDW mode and the existing phonons.
Resonant and Bound States of Charged Defects in Two-Dimensional Semiconductors*

JOHANNES LISCHNER (Presenter), MARTIK AGHAJANIAN, Imperial College London, BRUNO SCHULER, KATHERINE COCHRANE, JUN-HO LEE, CHRISTOPH KASTL, JEFFREY B. NEATON, ALEXANDER WEBER-BARGIONI, Lawrence Berkeley National Laboratory, ARASH A. MOSTOFI, Imperial College London — A detailed understanding of charged defects in two-dimensional semiconductors is needed for the development of ultrathin electronic devices. Here, we study negatively charged acceptor impurities in monolayer WS$_2$ using a combination of scanning tunnelling spectroscopy and large-scale atomistic electronic structure calculations. We observe several localized defect states of hydrogenic wave function character in the vicinity of the valence band edge. Some of these defect states are bound, while others are resonant. The resonant states result from the multi-valley valence band structure of WS$_2$, whereby localized states originating from the secondary valence band maximum at $\Gamma$ hybridize with continuum states from the primary valence band maximum at $K/K'$. Resonant states have important consequences for electron transport as they can trap mobile carriers for several tens of picoseconds.

*We acknowledge support by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, the Swiss National Science Foundation under project number P2SKP2 171770 and by the Air Force Office of Scientific Research Hybrid Materials MURI under award number FA9550-18-1-0480.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G58 DCP DCOMP DPOLY DCMP: DFT and Beyond V Mile High Ballroom

3B - Carsten Ullrich, Univ of Missouri - Columbia - Tag(s): Focus
Weizmann Institute of Science — Optical and excited-state phenomena are key ingredients in functional materials characterization, dominating emerging applications in broad areas of photophysics. Excited-state properties, including linear and non-linear light absorption, as well as radiative and non-radiative exciton decay processes, are strongly related to the material structure and composition. Recent experimental advances allow a controlled fabrication of structurally complex materials, along with close tracking of excited-state processes in them. However, a theoretical realization of the underlying interactions and subsequent design rules in such materials is highly challenging, as it demands a predictive description of the involved excitations, strongly depending on the structural perturbation. In this talk, I will describe a computational assessment of the relation between excitonic phenomena and material structure and design, using many-body perturbation theory within the GW and Bethe-Salpeter equation (GW-BSE) approach. I will discuss the effect of atomic defects and heterostructures on the excitonic properties in layered transition metal dichalcogenides (TMDs), where the structural complexity leads to mixed transitions between states of different nature and localization, determining unique and tunable selection rules and absorption. I will further present a GW-BSE-based approach to study exciton transport with relation to material structure and symmetry, demonstrated on selected systems of varying dimensionalities.

Many-body perturbation theory (MBPT) has emerged as a state-of-the-art approach for quantitatively accurate prediction of (opto)electronic properties of materials. However, the computational cost of MBPT motivates the search for simpler methods, particularly those based on density functional theory (DFT), to enable the study of larger and more complex systems. In particular, tuned and screened range-separated hybrid (SRSH) hybrid methods have been shown to provide MBPT accuracy at the cost of hybrid DFT for many materials. We test the accuracy of time-dependent (TD)SRSH for describing the optoelectronic properties of defective semiconductors by the study of point defects in bulk GaN. We first show that the predicted quasiparticle gap and low-energy excitation spectra of (TD)SRSH and MBPT agree well in pristine GaN and GaN containing a single nitrogen vacancy, establishing the accuracy of the method. Aided by the reduced computational cost of (TD)SRSH, we then report on a series of technologically relevant point defects in GaN. This study indicates that TDSRSH is a computationally feasible approach for quantitatively accurate first-principles modeling of defective semiconductors.

*We acknowledge funding from U.S. Department of Energy, Office of Science, Award #DE-SC0018080
12:03PM G58.00003: UNDERSTANDING EXCITONS IN STACKED PERYLENE DIIMIDE DERIVATIVES*  
ALIYA MUKAZHANOVA (Presenter), Materials Science and Engineering, Boston University, KASIDET JING TRERAYAPIWAT, Department of Chemistry, Boston University, SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University — π-stacked organic chromophores are promising class of materials for optoelectronics with their electronic properties strongly dependent on the chemical structure of the molecule and inter-molecular interactions. Here, we investigate the optical properties of recently synthesized stacked perylene diimide derivatives via time-dependent density functional theory with a Franck-Condon Herzberg-Teller approximation of vibronic effects, validating our approach by comparison to measurement. By stacking the molecules along a DNA-like backbone and varying the number of stacked molecules from one to three, we determine the role of inter- and intra- molecular interactions on the nature of optical excitations. We determine that for stacked molecules, ground-state vibrational excitations play an important role in the optical absorption spectrum, which we account for via molecular dynamics. Additionally, we apply a nonadiabtic dynamics method to study the role of the backbone on evolution of excited-states. We demonstrate that inter-molecular interactions and backbone strongly influence optical properties, providing new design strategies for efficient optoelectronic materials.

*The authors acknowledges financial support from the National Science Foundation (DMR-1610031, DMR-1847774).

12:15PM G58.00004: First-principles investigations of structure and vibrations of c(4x2) PF₃ on Cu(001)  
NIMA KARIMITARI (Presenter), STEVEN LEWIS, University of Georgia — We use first-principles density functional theory (DFT) to study the structure and vibrational dynamics of PF₃ on the Cu(001) surface in the c(4x2) geometry. This system presents a unique opportunity to consider the complex interplay at work when a molecule with 3-fold symmetry binds to a surface with 4-fold symmetry. Our calculations find an upright structure for the PF₃ molecules, in contrast to experimental claims. The phonon analysis reveals an interesting coupling between adsorbate modes, surface mods and bulk modes. We will present detailed calculational evidence, including phonon density of states and projected density of states to support the rich structural and vibrational behavior that this system affords.
12:27PM G58.00005: First-principles simulations of photocatalytic systems for hydrogen production*  SAMUEL LEMAY (Presenter), GABRIEL ANTONIUS, Hydrogen Research Institute, Université du Québec à Trois-Rivières — Hydrogen offers a green alternative to fossil fuels, as it can be used in combination with fuel cells to propel an electric vehicle. In order to assist the design of photocatalytic systems for hydrogen production, we perform first-principles calculations of the electronic structure of several catalysts and attempt to predict their efficiency for hydrogen evolution reactions. One class of catalysts are coordination complexes composed of a metallic atom surrounded by organic ligands. In the present work, we focus on Co(bpy)2 and Co(bpym)2 where (bpy) is a bipyridine ligand and (bpym) is a bipyridine mimic. We rely on density functional theory (DFT) to compute the structural parameters of the molecules, their formation energy, and electronic energy levels. We aim to calculate the energy levels of the neutral, charged, and hydrogenated states of the molecules and compare it to cyclic voltammetry measurements.

*We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC), [funding reference numbers RGPIN-2019-07149 and DGECR-2019-00008], as well as support from Université du Québec à Trois-Rivières. The computational resources were provided by Calcul Québec and Compute Canada.

12:39PM G58.00006: The Dirac equation and its implications for density functional theory-based calculations of materials containing heavy elements  DANIEL A REHN (Presenter), JOHN M WILLS, ANN E MATTSSON, Los Alamos National Laboratory — Electronic structure calculations based on density functional theory (DFT) typically give quantitatively accurate predictions for ground-state properties of materials containing light elements. For materials containing heavy elements, relativistic effects play an increasingly important role and in principle, a formulation of DFT based on the Dirac equation is needed to properly incorporate relativistic effects. Working towards that goal, we have developed a code, called dirac-fp, that solves the Dirac-Kohn-Sham equations under the assumption of a vanishing orbital current. The dirac-fp code is based on the full potential linear muffin tin orbital (FP-LMTO) code RSPt, but solves the Dirac-Kohn-Sham equations throughout the entire computational cell. To assess the results of the Dirac-Kohn-Sham (Dirac) approach, we compare the ground state properties to the scalar relativistic (SR) and scalar relativistic+spin-orbit coupling (SR+SO) approaches for three different non-magnetic FCC materials: thorium, aluminum, and gold, in which relativistic effects should be strong, negligible, and intermediate, respectively. We find that only the Dirac approach is able to provide consistent results in the electronic structure and ground state properties across all three materials.
12:51PM G58.00007: Effect of functional -NH2 groups on sensitization of 3,6-diaminocarbazole towards Picric Acid VISHAL KUMAR (Presenter), SOUMITRA SATAPATHI, Indian Inst of Technology Roorkee — Due to the significance of explosive detection for homeland security and environmental protection, the research of new materials and methodologies for sensing electron-deficient explosive nitroaromatics is urgently imperative. In this paper we demonstrate an opto-chemical sensor for explosive detection by using a carbazole derivative, namely 3,6-diaminocarbazole (DAC) (Φf=49%), was synthesized through controlled nitration of the carbazole (Φf=42%) with fuming nitric acid. As a proof of concept, electron-deficient explosive molecule 2,4,6-trinitrophenol (TNP) is used as a model analyte to our sensor with LOD 3.7µM. In solution, PL signal from highly electron-rich DAC gets quenched upon addition of aliquots of TNP caused by photo-induced electron and resonance energy transfer i.e. quantified by Stern-Volmer constant (KS\text{V}= 4.1\times10^4 \text{ M}^{-1}) which is higher than KS\text{V}=3.3\times10^4 \text{ M}^{-1}, valuated for carbazole. The quenching mechanism was further established by time-resolved PL and steady state absorption spectroscopy which was found to be a mixture of static and dynamic in nature as lifetime of DAC (2.18 ns) is reduced to 1.24 ns for TNP. As a conclusion, results indicate that major response of this sensitivity enhancement to TNP originates from Föster Resonance Energy Transfer between DAC and TNP.

1:03PM G58.00008: Charge Transport Properties of Biomolecules* ABHISHEK AGGARWAL (Presenter), Indian Institute of Science - Dept of Physics, SAIENTAN BAG, Institute of Nanotechnology, Karlsruhe Institute of Technology, RAVINDRA VENKATRAMANI, Department of Chemical Sciences, Tata Institute of Fundamental Research, MANISH JAIN, PRABAL K MAITI, Indian Institute of Science - Dept of Physics — Double-stranded DNA (dsDNA) and dsRNA hold great promises in molecular electronics. We characterize the charge transport properties of dsRNA for different sequences and compare them with similar sequences of dsDNA in two extreme charge transport regimes – incoherent charge hopping regime and coherent electron transport regime. We find that the relative conductance of A-form dsRNA and B-form dsDNA depends on the mechanism of charge transport. This is attributed to various structural differences in dsDNA and dsRNA. We also study the effect of stretching and propose a method to detect conformational changes using electrical measurements. Despite the twist-stretch coupling of dsRNA and dsDNA being different under external force, dsRNA shows similar structural polymorphism to dsDNA under different pulling protocols. Our atomistic MD simulations show that overstretching dsRNA along the 3’ ends (OS3) leads to the emergence of S-RNA whereas overstretching along the 5’ ends (OS5) leads to melting of dsRNA. Using the dsRNA morphology from MD simulations, we use a multiscale method involving ab initio DFT calculations and Kinetic Monte Carlo (KMC) simulations to estimate the conductance of dsRNA and find that the conformational changes drastically affect its conductance.

*MHRD, IISc
1:15PM G58.00009: Cyanide Bridged Platinum-Iron Complexes as Cisplatin Prodrug Systems: Design and Computational Study  ARIELA KASPI-KANETI (Presenter), SRIJANA BHANDARI, BARRY DUNIETZ, Kent State Univ - Kent —

We present design principles of cyanide bridged Platinum-Iron complexes as novel Platinum(IV) anti-cancer prodrugs that bear the potential of high selectivity towards cancerous cells. The proposed molecular system can release up to six cisplatin anticancer agents per prodrug unit. This functionality of the prodrug is addressed through density functional theory (DFT) calculations that are presented as a demonstration of the proposed principle.

1:27PM G58.00010: Detection of DNA nucleotides with Nanopores and Nanogaps from 2D Materials beyond Graphene: First Principle Studies  BENJAMIN TAYO (Presenter), Univ of Central Oklahoma — Sequencing the DNA at the resolution of individual DNA bases is an important problem whose solution could lead to cost-effective methods for sequencing the DNA, leading to revolutions in the field of genomics and personalized medicine. We present the results of computational studies on nano-bioelectronic devices combining the superb properties of 2D materials beyond graphene with DNA nucleotides. We anticipate our studies to shed useful insights that can help to address two major challenges in current sequencing technologies: 1) strong coupling between 2D materials and nucleotides is expected to produce large signal-to-noise ratio compared to devices using graphene due to adsorption of nucleotides on graphene surface, or devices based on probing ionic currents, which often produce very low signal-to-noise ratio, 2) strong coupling between 2D materials and nucleotides is anticipated to produce large tunneling currents capable of accomplishing both spatial and temporal resolution at the single-base level. The performance of our proposed device for single-base sequencing will be evaluated by employing density functional theory and the nonequilibrium Green’s function method to investigate the transverse conductance properties of nucleotides inside the nanogap or nanopore.
1:39PM G58.00011: Electronic and optical properties of halide perovskite quantum dots: a DFT and TDDFT study. ATHANASIOS KOLIOGIORGOS (Presenter), Control Engineering, Czech Technical University in Prague, CHRISTOS GAROUFALIS, IOSIF GALANAKIS, SOTIRIOS BASKOUTAS, Materials Science, University of Patras —
Perovskite quantum dots (QDs) constitute a novel and rapidly developing field of nanotechnology with promising potential for optoelectronic applications. However, few perovskite materials for QDs and other nanostructures have been theoretically explored. In this study, we present a wide spectrum of different hybrid halide perovskite cuboid-like QDs with the general formula of ABX₃ (A = Cs, CH₃NH₃; B = Pb, Sn, Ge, Ca, Sr and X = Cl, Br, I) with varying sizes below and near the Bohr exciton radius. Density functional theory (DFT) and time-dependent DFT calculations were employed to determine their structural, electronic, and optical properties. Our calculations include both stoichiometric and non-stoichiometric QDs, and our results reveal several materials with high optical absorption and application-suitable electronic and optical gaps. Our results also reveal whether the stoichiometric or non-stoichiometric model is closer to experiment. Finally, we explore a computational approach for the study of resonance energy transfer between 2 nanostructures of different sizes. Our study highlights the potential as well as the challenges and issues regarding nanostructured halide perovskite materials, laying the background for future theoretical and experimental work.

1:51PM G58.00012: Efficient and Accurate Fully Relativistic Density Functional Treatment for Molecules and Periodic Solids* RUNDONG ZHAO (Presenter), VICTOR YU, Duke University, KIMBERLY ZHANG, University of California, Irvine, YUNLONG XIAO, Peking University, YONG ZHANG, WENJIAN LIU, Shandong University, VOLKER BLUM, Duke University — A fully relativistic density functional method (called quasi-four-component algorithm, Q4C) in combination with numeric atom-centered orbital (NAO) basis functions is presented. Q4C initially projects the atomic solution to (electron-only) positive-energy states and deals with only two components but restores the negative-energy component in a second step; it therefore retains the full precision of traditional four-component relativistic methods. While Q4C inherently reduces the dimension of the Hamiltonian matrix and correspondingly the computational demand in matrix diagonalization, the adoption of localized NAO basis functions further reduces the computational demand in real space operations, enabling us to explore large and complex systems containing heavy elements fully relativistically. Here, we report benchmarks for the properties of a series of common periodic materials and molecules. Additionally, the band structure of a much larger system, i.e. the 2D hybrid organic-inorganic perovskite (2D-HOIP) (4-FPEA)₂PbI₄ (containing 94 atoms per unit cell) is reported, showing the code’s applicability to large systems.

References:

*We thank Matthias Scheffler and FHI, Berlin, for supporting this work.
2:03PM G58.00013: An Electronic Structure Approach to Understand Charge Transfer & Transport in Organic Semiconducting Materials  SRIJANA BHANDARI (Presenter), Kent State Univ - Kent — Effective design of optoelectronic devices requires understanding of the role of the molecular environment. However, widely used forms of DFT and TDDFT fail to accurately describe the frontier orbital gap and charge transfer states of such molecular systems in the condensed phase. Recently we implemented a novel approach combining screened RSH (SRSH) with polarized continuum model (PCM), where long range electrostatic interactions are consistently screened by a 1/e factor (e is the solid-state dielectric constant). Using this new approach, we achieved a highly efficient quantum chemical procedure to obtain condensed phase IP and EA based on single molecule calculations and the correct charge transfer energies of a complex system.

Using this approach, we address molecular conductance where DFT has an established tendency to overestimate the conductance. Here, we develop the approach to address non-equilibrium conditions by using RSH functionals within NEGF formulation to study conductance. We then develop the approach to study NDR based on (phenylene ethynylene) derivatives.

We compare the RSH-NEGF results with alternative DFT-NEGF approaches to highlight the importance of using an approach based on physically significant frontier orbitals.

Tuesday, March 3, 2020 11:15 AM - 1:39 PM

Session G59 DMP: Ferromagnetic Kagome Metals Mile High Ballroom 3C

11:15AM G59.00001: Spin dynamics of the isotropic kagome ferromagnet Fe₃Sn₂  JEFFREY LYNN (Presenter), REBECCA DALLY, NIST Center for Neutron Research, National Institute of Standards and Technology, NIRMAL GHIMIRE, NISHCHAL THAPA MAGAR, Department of Physics and Astronomy, George Mason University, DANIEL PHELAN, JOHN MITCHELL, Materials Science Division, Argonne National Laboratory — The giant anomalous Hall effect in the itinerant kagome magnet Fe₃Sn₂ was recently attributed to massive Dirac fermions resulting in a Berry curvature in the ferromagnetic phase [1], with a topologically non-trivial field-dependent spin texture phase discovered[2], demonstrating an intimate relationship between the electronic and magnetic properties in this strongly correlated electron material. Here we present a new perspective on Fe₃Sn₂ by studying the magnetic excitations near \( q = 0 \) using inelastic neutron scattering. The results on polycrystalline samples show this material to be an isotropic ferromagnet near its \( T_C \) of 660 K, where we find a negligible spin gap, and large spin-wave stiffness. The moments initially point along the \( c \)-axis and slowly rotate over the course of several hundred degrees towards the \( ab \)-plane. This indicates the “soft” nature of the ferromagnet, which is at odds with the argument that anisotropy is responsible for some the materials’ properties elsewhere in phase space.

Additionally, magnetic susceptibility and magnetization measurements agree with our neutron diffraction results showing this sample does not undergo a re-entrant spin-glass phase as reported by some.

11:27AM G59.00002: Scanning Tunneling Microscopy Study of Fe$_3$Sn$_2$*  
JORGE OLIVARES RODRIGUEZ (Presenter), ANUVA AISHWARYA, LIN JIAO, VIDYA MADHAVAN, University of Illinois at Urbana-Champaign — The peculiar geometry of the Kagome lattice, composed of corner-sharing triangles, has been known to be a fertile ground for exotic quantum phases since theory predicts the possible coexistence of topological and frustrated magnetic states stemming from this structure. The recently rediscovered metallic ferromagnet Fe$_3$Sn$_2$, consisting of two kagome bilayers (Fe$_3$Sn) layers separated by a honeycomb Sn layer, is seemingly a good candidate to explore the interplay between frustrated magnetism and topological band structure due to recent reports which include the observation of massive dirac fermions and the anomalous Hall effect. In addition, it has also been reported that its electronic structure can be tuned by changing its magnetic moments or temperature, making it a viable candidate for spintronic applications. Here we present a scanning tunneling microscopy/spectroscopy study of Fe$_3$Sn$_2$ at low temperatures and under a magnetic field.

*We acknowledge the support from the U.S. Department of Energy under the grant number DE-SC0014335

11:39AM G59.00003: Defects in magnetic Weyl semimetal Co$_3$Sn$_2$S$_2$*  
QIANG ZOU (Presenter), MINGMING FU, MINA YOON, CNMS, Oak Ridge National Lab, RUI XUE, DAVID MANDRUS, University of Tennessee, Knoxville, ZHENG GAI, CNMS, Oak Ridge National Lab — In Co$_3$Sn$_2$S$_2$, a magnetic Weyl semimetal with kagome-lattice, the existence of bulk Weyl nodes, which are formed under broken inversion or time-reversal symmetry, creates nontrivial topological properties, for example, robust Giant anomalous hall effect. The surface–bulk correspondence ensures the bulk bands related topological “Fermi arc” surface bands dispersion. In this presentation, we use low temperature high magnetic field scanning tunneling microscope, spin polarized STM, and quasiparticle interference (QPI) to study the influence of local defects including magnetic and nonmagnetic vacancies and adatoms to the Weyl nodes movement. Co and Sn vacancies in the Kagome-lattice are identified, their behavior under magnetic field are studied. S adatoms in 1D forms are compared with individual adatoms. The interplay among topology, defects and magnetism are discussed for the understanding of the involved quantum phenomena.

*This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.
Temperature dependent conductivity in magnetic Weyl semimetal Co$_3$Sn$_2$S$_2$ with terahertz spectroscopy

ELIZABETH FULLER (Presenter), EVAN JASPER, YUFEI LI, ROLANO VALDES AGUILAR, Ohio State Univ - Columbus, RUI XUE, DAVID MANDRUS, University of Tennessee, Knoxville — The recently discovered Weyl semimetal, Co$_3$Sn$_2$S$_2$, is attractive for its intrinsic ferromagnetic behavior below $T_c \sim 175$ K with almost full spin polarization, i.e. half-metallicity. Previous studies$^{1,2}$ report evidence of a highly tunable, large anomalous Hall effect (AHE) with change in temperature. We utilize spectroscopic methods in the terahertz range to measure the optical conductivity in a single crystal Co$_3$Sn$_2$S$_2$ within the 8 K to 290 K temperature range. We observe a clear downward shift in the reflectance of the crystal with increasing temperatures near the ferromagnetic transition and a similar trend for low temperatures. We will discuss these measurements in the context of the Anomalous Hall conductivity that varies with shifts in Weyl node position.


*This work is supported by the Center for Emergent Materials, an NSF MRSEC, under grant DMR-1420451.

Fermi-arc diversity on surface terminations of the magnetic Weyl semimetal Co$_3$Sn$_2$S$_2$

NURIT AVRAHAM (Presenter), NOAM MORALI, PRANAB KUMAR NAG, RAJIB BATABYAL, Weizmann Institute of Science, LIU ENKE, Beijing National Laboratory, QIUNAN XU, YAN SUN, Max Planck Dresden, BINGHAI YAN, Weizmann Institute of Science, CLAUDIA FELSER, Max Planck Dresden, HAIM BEIDENKOPF, Weizmann Institute of Science — Bulk–surface correspondence in Weyl semimetals ensures the formation of topological “Fermi arc” surface bands whose existence is guaranteed by bulk Weyl nodes. By investigating three distinct surface terminations of the ferromagnetic semimetal Co$_3$Sn$_2$S$_2$, we verify spectroscopically its classification as a time-reversal symmetry-broken Weyl semimetal. We show that the distinct surface potentials imposed by three different terminations modify the Fermi-arc contour and Weyl node connectivity. On the tin (Sn) surface, we identify intra–Brillouin zone Weyl node connectivity of Fermi arcs, whereas on cobalt (Co) termination, the connectivity is across adjacent Brillouin zones. On the sulfur (S) surface, Fermi arcs overlap with nontopological bulk and surface states. We thus resolve both topologically protected and nonprotected electronic properties of a Weyl semimetal.
12:15PM G59.00006: Large anomalous Hall and planar Hall effect in magnetic Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$  
SHUO-YING YANG (Presenter), Max Planck Institute of Microstructure Physics, JONATHAN NOKY, JACOB D GAYLES, Max Planck Institute for Chemical Physics of Solids, FASIL KIDANE DEJENE, Max Planck Institute of Microstructure Physics, YAN SUN, Max Planck Institute for Chemical Physics of Solids, ENKE LIU, Institute of Physics, Chinese Academy of Science, MAZHAR ALI, Max Planck Institute of Microstructure Physics, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, STUART PARKIN, Max Planck Institute of Microstructure Physics — Weyl fermions are chiral massless fermions manifested in crystalline solids by spin split conduction and valence bands crossing at discrete points. Time-reversal-symmetry-broken Weyl semimetals (WSMs) have attracted particular attention because of their interesting interplay between intrinsic magnetism and topologically nontrivial electrons. In this work, we perform detailed transport studies on a magnetic Weyl semimetal, $\text{Co}_3\text{Sn}_2\text{S}_2$. Nanoplates as thin as 180 nm were grown via chemical vapor transfer methods. Through magneto-transport measurements, we report a large intrinsic anomalous Hall conductivity generated by a large Berry curvature from the Weyl nodes. The anomalous Hall conductivity is robust against both increased temperature and charge conductivity, reaching $\sim 1420 \text{ ohm}^{-1} \text{ cm}^{-1}$. In addition, we discuss the observation of a large planar Hall effect (PHE) in $\text{Co}_3\text{Sn}_2\text{S}_2$. We carefully examined all possible origins of the PHE including ferromagnetism, orbital magnetoresistance and the chiral anomaly. Our analysis reveals that even though negative magnetoresistance (NMR) was not seen, the observed PHE is chiral anomaly dominated. Our results show how multiple PHE contributions can be disentangled in a magnetic WSM system and suggest that PHE is a sensitive probe of Weyl transport.

12:27PM G59.00007: Exchange biased Anomalous Hall Effect driven by frustration in a magnetic Kagome lattice*  
ELLA LACHMAN (Presenter), RYAN MURPHY, NIKOLA MAKSIMOVIC, ROBERT KEALHOFER, SHANNON C HALEY, University of California, Berkeley, ROSS MCDONALD, Los Alamos National Laboratory, JEFFREY R LONG, JAMES ANALYTIS, University of California, Berkeley — $\text{Co}_3\text{Sn}_2\text{S}_2$ is a ferromagnetic Weyl semimetal that has been the subject of intense scientific interest due to its large anomalous Hall effect (AHE). We show that the coupling of this material's topological properties to its magnetic texture leads to a strongly exchange biased AHE, and argue that this is likely caused by coexistence of ferromagnetism and spin glass phases. The spin glass is being driven not by disorder, but by the geometric frustration intrinsic to the Kagome network of magnetic ions. Both phases are thought to originate from the Co spin system, in an interesting display of Exchange Bias emanating from a single magnetic phase. Magnetism plays an important role in the robustness of the QAHE in magnetically doped topological insulators, and may play a crucial role in unlocking the possibility of a QAHE in low-dimensional structures of $\text{Co}_3\text{Sn}_2\text{S}_2$.  
arXiv:1907.06651

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12:39PM G59.00008: High field quantum oscillation studies of Dirac electrons in iron-based kagome lattice metals*  LINDA YE (Presenter), MIN GU KANG, Massachusetts Institute of Technology, MUN K. CHAN, ROSS MCDONALD, National High Magnetic Field Laboratory, LANL, DAVID E GRAF, National High Magnetic Field Laboratory-Florida State University, ABRAHAM L LEVITAN, MINYONG HAN, Massachusetts Institute of Technology, DAVID CHARLES BELL, Harvard University, MADHAV PRASAD GHIMIRE, IFW Dresden, SHIANG FANG, Harvard University, JHIH-SHIH YOU, JORGE I. FACIO, IFW Dresden, EFTHIMIOS KAXIRAS, Harvard University, JEROEN VAN DEN BRINK, IFW Dresden, RICCARDO COMIN, JOSEPH G CHECKELSKY, Massachusetts Institute of Technology — The kagome lattice has long been theoretically known to harbor Dirac dispersions together with a dispersionless (flat) band. The relevance of the kagome lattice model in the context of electronic structures has recently been established in a class of binary hexagonal iron stannides, where Dirac dispersions derived from Fe 3d electrons are observed at Brillouin zone corners in photoemission studies [1,2]. Here we report high magnetic field quantum oscillation studies of Dirac electrons in these iron-based kagome metals including ferromagnetic Fe3Sn2 [3] and antiferromagnetic FeSn [2]. In Fe3Sn2 we observe a doublet of quasi-2D bulk Dirac electrons while a single bulk Dirac pocket is identified in FeSn. We further discuss the impact of crystallographic stacking and magnetic order on the Dirac electronic states in Fe3Sn2 and FeSn. References: [1] L. Ye, M. Kang et al., Nature 555 638-642 (2018). [2] M. Kang, L. Ye et al., arXiv/1906.02167, Nat. Mater. (in press). [3] L. Ye et al., Nat. Comm. 10, 4870 (2019).

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12:51PM G59.00009: Topological Chern bands for electrons and magnons realized in one Kagome ferromagnet: CoCu3(OH)6Cl2*  ZHUORAN HE (Presenter), GANG XU, Huazhong University of Science and Technology, BIAO LIAN, Princeton University — We study the topological electron bands and spinon bands in the ferromagnetic phase of CoCu3(OH)6Cl2. The Cu ions with fractional valence and magnetic moments form a 3D trigonal crystal stacked from 2D Kagome layers. A t-J model with spin-orbit coupling is constructed from the hybridized Wannier orbitals and studied using the Schwinger bosons to calculate the spinon bands. The Chern numbers of the electron and spinon bands reveal their nontrivial topological properties and implications on the spintronic transport properties are discussed. Our work provides an example for the study of interactions between two topological systems and sheds light on the understanding of correlated electrons in magnetic topological materials.

*The authors thank the support from the MOST and NSFC, the Thousand Young Talents Program, and cooperation with Princeton University.
1:03PM G59.00010: Electronic structure of a metallic ferromagnetic pyrite

IÑIGO ROBREDO
(Presenter), Donostia International Physics Center, NIELS SCHRÖTER, PSI, SEBASTIAN KLEMENZ, ROBERT KIRBY, Princeton, ANDREAS P SCHNYDER, MPI Stuttgart, AITOR BERGARA, EHU/UPV, VLADIMIR STROKOV, JONAS A. KRIEGER, TIANLUN YU, PSI, FERNANDO DE JUAN, MAIA G VERNIORY, Donostia International Physics Center, LESLIE SCHOOOP, Princeton — In this work we present combined experimental and theoretical results to elucidate electronic and magnetic properties of metallic cobalt pyrite CoS$_2$. On one side we reveal that the Density Functional Theory predicted band structure is in good agreement with angular resolved photoemission spectroscopy (ARPES) measurements, performed for the first time. Further studying its band structure we discovered that this material exhibits topological behaviour. Close to the Fermi level, we found a potential 'New Fermion', a 4-dimensional magnetic band crossing protected by cubic, non-symmorphic magnetic symmetries, along with several neighbouring Weyl fermions. We finally analyze the surface states and identify surface Fermi arcs.

1:15PM G59.00011: Systematic analysis of topological and magnetic properties of materials related to MnBi$_2$Te$_4$ by substitution

SUGATA CHOWDHURY (Presenter), KEVIN GARRITY, FRANCESCA TAVAZZA, MML, NIST — The search for materials with axion insulator phases has motivated extensive research about interactions between topological surface states and symmetry-breaking magnetic ordering, with possible applications in spintronics and quantum information. Recently, experimental and theoretical works have focused on MnBi$_2$Te$_4$, which is predicted to display this phase. In this work, we have looked at alternative elements in the same septuple layer structure by considered a series of 3d transitions metal from V to Ni as the magnetic element, as well as Sb for Bi and Se for Te. We study the topological properties and magnetic properties of new candidate materials. Our calculations reveal several potential topological materials, with properties depending on the filling of d electrons and the magnetic ordering. We also discuss the optical properties and electron phonon interactions of those materials. These types of stoichiometric magnetic materials are an excellent candidate for future topological devices.

1:27PM G59.00012: Phase transition from Mn-Bi$_2$Te$_3$ to MnBi$_2$Te$_4$

KEJING ZHU (Presenter), MENGHAN LIAO, YAN GONG, KE HE, QIKUN XUE, Tsinghua University — The realization of MnBi$_2$Te$_4$ film opens the vision to search rich topological effects in intrinsic magnetic topological insulator. In the cleaved single crystal samples, the high resolution angle-resolved photoemission spectroscopy (ARPES) shows the clear topological electronic structures, and the transverse resistance reaches quantization in a high external magnetic field. Those results indicate that 124 family materials can be an ideal platform for further exploring various topological phenomena. But in Mn-Bi-Te system, 124 structure is not the solely stable phase. Mn atoms can replace the position of Bi atoms to form a Mn doped Bi$_2$Te$_3$ phase. MnBi$_4$Te$_7$ and Mn$_2$Bi$_2$Te$_5$ are also predicted to be existed in this system. In order to give a clear phase diagram and give an instruction of growing Mn-Bi-Te material, we investigate the evolution of electronic energy band structures with increasing Mn doping level. We also study the temperature influence on the Mn-Bi-Te material.
G59.00013: Abnormal Negative Magnetoresistance and Exceptional Hall Component in Magnetic Weyl Semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$ Nanodevices*  

QI ZENG (Presenter), GANGXU GU, JIANLEI SHEN, ENKE LIU, WENHONG WANG, YONGQING LI, Chinese Academy of Sciences — Recently, the first magnetic Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$ has been discovered[1-3]. For topological related spintronics applications in low dimensions, the growth and physical researches of $\text{Co}_3\text{Sn}_2\text{S}_2$ thin films are highly desired. In this work, we synthesized single-crystalline $\text{Co}_3\text{Sn}_2\text{S}_2$ nanoflakes with thickness from 100 to 30 nm by chemical vapor method. The nanodevices were prepared by using microfabrication. The nanoflakes show stable Curie temperature around 181 K, high anomalous Hall conductivity of 800 S cm$^{-1}$, large coercive force up to 5.5 T, and high quality with RRR up to 20. At low temperatures, the decreased resistance is observed when the external magnetic field is lower than the coercive field and antiparallel to the internal magnetization, showing an abnormal negative magnetoresistance. Meanwhile, an exceptional Hall component, after subtracting the normal and anomalous Hall, is also found before the magnetic domain is switched. A value of this component is observed up to three times larger than the anomalous Hall contribution. Exotic behaviors were observed in magnetic Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$ nanodevices.


*NSFC: 11974394 and 51722106
G59.00014: Pressure Driven Topological and Quantum Phase Transition on Magnetic Weyl Kagome Lattice

QI ZENG, Chinese Academy of Sciences, Institute of Physics, QIUSHI YAO, Southern University of Science and Technology, JIANLEI SHEN, Chinese Academy of Sciences, Institute of Physics, HONGYI SUN, Southern University of Science and Technology, WENHONG WANG, Chinese Academy of Sciences, Institute of Physics, YONGGANG WANG, Center for High Pressure Science and Technology Advanced Research (HPSTAR), QIHANG LIU, Southern University of Science and Technology, ENKE LIU (Presenter), Chinese Academy of Sciences, Institute of Physics — Recently, the Shandite compound $\text{Co}_3\text{Sn}_2\text{S}_2$ has been proved as a magnetic Weyl semimetal[1-3]. $\text{Co}_3\text{Sn}_2\text{S}_2$ possesses the out-of-plane magnetic Kagome lattice formed by Co atoms, which dominates the behaviors of Weyl fermions in this system. In this work, we performed experiments and theoretical calculations under high pressures to study the evolution of the topological state in $\text{Co}_3\text{Sn}_2\text{S}_2$. Experimental results show that the Curie temperature, anomalous Hall conductivity, and coercitive force of Hall curves decrease with increasing pressure. The ordinary Hall coefficient changes sign at a critical pressure, producing a maximum of the carrier concentration and a switch of the carrier types. Around 40 GPa the magnetic order finally disappears and the system goes into the protection of time reversal symmetry, becoming a topological insulator phase above 40 GPa. The calculations further found that additional Weyl nodes emerge with increasing pressure, showing low- and high-pressure Weyl fermion states. The topological and quantum phase transition is observed under pressure in the magnetic Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$.


*NSFC: 11974394 and 51722106
G59.00015: On the anisotropies of magnetization and electronic transport of magnetic Weyl semimetal Co$_3$Sn$_2$S$_2$*  

JIANLEI SHEN (Presenter), QI ZENG, ENKE LIU, Chinese Academy of Sciences — Co$_3$Sn$_2$S$_2$, a quasi-two-dimensional system with kagome lattice, has been found as the first magnetic Weyl semimetal recently[1-3]. In this work, the anisotropies of magnetization and transport properties of Co$_3$Sn$_2$S$_2$ were investigated. High field measurement results indicate this semimetal shows a giant magnetocrystalline anisotropy with an out-of-plane saturation field of 0.9 kOe and an in-plane saturation field of 230 kOe at 2 K, showing a magnetocrystalline anisotropy coefficient $K_u$ up to $8.3 \times 10^5$ J m$^{-3}$, which indicates that it is extremely difficult to align the small moment of 0.29 μB/Co on the kagome lattice from $c$ axis to ab plane. The out-of-plane angular dependences of Hall conductivity further reveal strong anisotropies in Berry curvature and ferromagnetism, and the vector directions of both are parallel with each other. For in-plane situation, the longitudinal and transverse measurements for both $I \parallel a$ and $I \perp a$ cases show that the transport on the kagome lattice is isotropic. These results provide essential understanding on the magnetization and transport behaviors for the magnetic Weyl semimetal Co$_3$Sn$_2$S$_2$.


*NSFC: 11974394 and 51722106

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G60 DMP: Topological Materials: Semimetals and Higher Order States  Mile High Ballroom 4A - Darius Torchinsky, Temple Univ

11:15AM G60.00001: Ultrathin epitaxial Na3Bi films for topological electronics [Invited]  
MICHAEL FUHRER (Presenter), Monash University — Selected by Focus Topic Organizer (Seongshik Oh and Peter Armitage)
11:51AM G60.00002: Polymerized triptycene as a candidate material of higher-order topological insulator*  TOMONARI MIZOGUCHI (Presenter), MINA MARUYAMA, SUSUMU OKADA, YASUHIRO HATSUGAI, Univ of Tsukuba — Higher-order topological insulators (HOTIs) have attracted growing attention as a novel class of topological state of matter, where boundary states, protected by topological natures of Bloch wave functions in a bulk, appear at boundaries with co-dimension larger than one. So far, various theoretical models for HOTIs have been proposed, and it is highly desirable to search suitable materials to realize the HOTIs. In this presentation, we propose that a class of carbon-based materials called polymerized triptycene is a promising platform for a two-dimensional second-order topological insulator. The materials are composed of triptycene molecules and phenyl rings connecting the triptycene molecules. In this class of materials, the C₆ rings form a kagome-type network, which becomes a platform to realize the HOTI when introducing the “breathing” structure. We show by the analysis of the tight-binding model that the corner states appear under the appropriate choice of the sample edges. We also demonstrate that the corner states are topologically protected by the bulk topological invariant, or the Z₃ Berry phase, that characterizes HOTIs.

*This work is supported by the JSPS KAKENHI, Grant number JP17H06138 (T. M. and Y. H.), MEXT, Japan.

12:03PM G60.00003: Apatite as a higher-order topological insulator with 2/3-filled hinge states*  MOTOAKI HIRAYAMA, RIKEN, RYO TAKAHASHI, SATORU MATSUISHI, HIDEO HOSONO, SHUICHI MURAKAMI (Presenter), Tokyo Inst of Tech - Tokyo — In our previous work we have shown that electrides are suitable for achieving various topological semimetal phases [1]. In our presentation, we show that the apatite A₆B₄(SiO₄)₆, one of the one-dimensional electrides, realizes a higher-order topological insulator with 2/3-filled one-dimensional metallic hinge states. This is considered to be in the class of Cₙ-protected higher-order topological insulators proposed by Benalcazar et al. [2], but the hinge charge is different from that naively expected from their theory. This difference comes from the difference in the fundamental units constituting the crystal; the apatite crystal consists of triangular units, unlike hexagonal units assumed in Ref. [2]. We show how this difference affects topological properties of the system via crystal terminations.


*This work was supported by JSPS KAKENHI Grant Number 18H03678, and by the MEXT Elements Strategy Initiative to Form Core Research Center (TIES).
12:15PM G60.00004: Evidence of Higher Order Topology in WTe$_2$ from Josephson Coupling through Anisotropic Hinge States  YONG-BIN CHOI (Presenter), Department of Physics, POSTECH, Pohang, Republic Korea, YINGMING XIE, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, CHUI-ZHEN CHEN, Institute for Advanced Study and School of Physical Science and Technology, Soochow University, Suzhou 215006, China, JINHO PARK, Department of Physics, POSTECH, Pohang, Republic Korea, SU-BEOM SONG, Department of Materials Science and Engineering, Pohang University of Science and Technology, Pohang, Republic of Korea, JIHO YOON, Max Plank Institute for Microstructure Physics, Halle (Saale), Germany, BUMJOON KIM, Department of Physics, POSTECH, Pohang, Republic Korea, TAKASHI TANIGUCHI, KENJI WATANABE, Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Ibaraki, Japan, HU-JONG LEE, Department of Physics, POSTECH, Pohang, Republic Korea, JONGHWAN KIM, Department of Materials Science and Engineering, Pohang University of Science and Technology, Pohang, Republic of Korea, KIN CHUNG FONG, Raytheon BBN Technologies, Quantum Information Processing Group, Cambridge, MA 02138, USA, MAZHAR ALI, Max Plank Institute for Microstructure Physics, Halle (Saale), Germany, KAM TUEN LAW, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, GIL-HO LEE, Department of Physics, POSTECH, Pohang, Republic Korea — The noncentrosymmetric Td-WTe$_2$, previously known as a Type-II Weyl semimetal, is expected to have higher order topological phases with topologically protected, helical one-dimensional (1D) hinge states when their scarcely separated Weyl points get annihilated. However, the detection of these hinge states is difficult in the presence of the semimetallic behaviour of the bulk. Here, we spatially resolved the hinge states by analysing the magnetic field interference of supercurrent in Nb-WTe$_2$-Nb proximity Josephson junctions. The Josephson current along the $a$-axis of the WTe$_2$ crystal, but not along the $b$-axis, showed sharp enhancements at the edges of the junction; the amount of enhanced Josephson current was comparable to the upper limits of a single 1D conduction channel. Furthermore, the Josephson effect under microwave radiation, shows voltage doubling of Shapiro steps when Josephson current flows along the $a$-axis of WTe$_2$ crystal, which implies $4\pi$ periodicity of current phase relationship. Our experimental observations provide evidence of the higher order topological phase in WTe$_2$ and its corresponding anisotropic topological hinge states, in good agreement with theoretical calculations.

12:27PM G60.00005: Higher order topological insulators in anti-perovskites  YUAN FANG (Presenter), JENNIFER CANO, Stony Brook University — We prove that a family of anti-perovskite materials realize a higher order topological insulator (HOTI) phase, characterized by a previously introduced Z4 index. A tight binding model and a k.p model are used to capture the physics of the bulk, surface and hinge states of these anti-perovskites. A phase diagram of the Z4 index and weak topological invariant is obtained for the tight binding model. The mirror Chern number is also discussed. In order to reveal the gapless hinge states in the presence of mirror Chern surface states, several ways of opening the surface gap are proposed and confirmed by calculation, including cleaving the lattice to reveal a low-symmetry surface, building a heterostructure, and applying strain. Upon opening the surface gap, we are able to study the hinge states by computing the momentum space band structure and real space distribution of mid-gap states.
Transport evidence of triply degenerate nodal semimetal YRh$_6$Ge$_4$*

YANGLIN ZHU (Presenter), Department of Physics, Pennsylvania State University, XIN GUI, Department of Chemistry, Louisiana State University, YU WANG, Department of Physics, Pennsylvania State University, DAVID E GRAF, National High Magnetic Field Laboratory, WEIWEI XIE, Department of Chemistry, Louisiana State University, ZHIQIANG MAO, Department of Physics, Pennsylvania State University — Triply-degenerate nodal semimetal (TDNS) represents a new topological quantum state [1,2]. In this talk, we report our magnetotransport studies on YRh$_6$Ge$_4$, which was recently predicted to be a TDNS[3]. We find it exhibits remarkable signatures of a chiral anomaly, manifested by large negative longitudinal magnetoresistance, quadratic field dependence of magnetoconductance and planar Hall effect [4]. Furthermore, we have also observed Shubnikov-de Haas (SdH) quantum oscillations, the analyses of which reveals two point-like Fermi surfaces consistent with the calculated band structure; these pockets host nearly massless three-component fermions. These results suggest YRh$_6$Ge$_4$ may serve as a model system to probe the exotic properties of three-component fermions and understand their underlying physics.


*This work is supported by NSF under grants DMR 1917579 and 1832031.
12:51PM G60.00007: Cornering the zero mode: realization of an artificial electronic higher-order topological insulator*  MARLOU SLOT (Presenter), National Institute of Standards and Technology, SANDER KEMPKES, JETTE VAN DEN BROEKE, PIERRE CAPIOD, Utrecht University, VLADIMIR A BENALCAZAR, Pennsylvania State University, DARIO BERCIOUX, Donostia International Physics Center, DANIEL VANMAEELBERGH, CRISTIANE MORAIS SMITH, INGMAR SWART, Utrecht University — Quantum simulators are essential tools for understanding complex quantum materials. Platforms based on ultracold atoms in optical lattices and photonic devices have led the field so far, but the basis for electronic quantum simulators is now being developed. Here, we experimentally realize an electronic higher-order topological insulator (HOTI). More specifically, we create a breathing kagome lattice by manipulating carbon monoxide molecules on a Cu(111) surface using a scanning tunneling microscope [1]. We engineer alternating weak and strong bonds to show that a topological state emerges at the corner of the non-trivial configuration, but is absent in the trivial one. Different from conventional topological insulators, the topological state has two dimensions less than the bulk, denoting a HOTI. The corner mode is protected by a generalized chiral symmetry, leading to a particular robustness against perturbations. Our versatile approach to designing artificial lattices holds promise for investigating novel quantum phases of matter.


*This work was supported by the Dutch and Spanish Ministry of Science, ERC, and Eberly Research Fellowship.

1:03PM G60.00008: Systematic investigation of physical properties of YbB$_{6\pm x}$ using the combinatorial approach*  SEUNGHUN LEE (Presenter), XIAOHANG ZHANG, NAILA AL HASAN, HUILONG HOU, University of Maryland, College Park, SUCHISMITA SARKER, APURVA MEHTA, SLAC National Accelerator Laboratory, RICHARD GREENE, ICHIRO TAKEUCHI, University of Maryland, College Park — Rare-earth boride systems have gained tremendous interest for exploring exotic and novel physical phenomena such as mixed valence states, heavy fermion, strong correlation and superconductivity. Since samarium hexaboride (SmB$_6$) has turned out to be a topological insulator, ytterbium boride (YbB$_x$) systems have been intensively studied as another possible topological insulator. However, the existence of the topologically protected surface states of YbB$_6$ is yet to be confirmed, and the origin of the quantum oscillations in Kondo insulator YbB$_{12}$ remains unresolved. We are systematically investigating the physical properties of YbB$_{6\pm x}$ depending on stoichiometry using the thin-film combinatorial approach. The composition spread YbB$_{6\pm x}$ thin films were fabricated by the co-sputtering of YbB$_6$ and B targets. The composition mapping of the spread films is performed using wavelength dispersive X-ray spectroscopy (WDS), and synchrotron x-ray diffraction measurements are employed for structural mapping analysis. We will discuss the electrical behavior of YbB$_{6\pm x}$ with the change in the valence state of Yb ion depending on the stoichiometry.

*This work was supported by AFOSR No. FA9550-14-10332.
1:15PM G60.00009: The fate of topological properties in U-based materials*  FREDERICO BENEDETTO SANTOS (Presenter), JOE D THOMPSON, ERIC BAUER, SEAN THOMAS, FILIP RONNING, PRISCILA ROSA, Los Alamos National Laboratory — Recent reports on CeSbTe show that Weyl and Dirac topological states can be tuned by low magnetic fields, which provide a promising route for investigating the interplay between magnetism and topology [1]. Here we aim at increasing the degree of correlations in this system by replacing Ce with U atoms. Though USbTe has been investigated previously [2,3], little is known about its putative topological properties. In this talk, I will discuss the growth of USbTe single crystals and their physical properties characterization via thermodynamic and electrical transport measurements at ambient pressure and under applied pressure.


*Work at Los Alamos was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering.

1:27PM G60.00010: New kagome prototype materials: discovery of KV$_3$Sb$_5$, RbV$_3$Sb$_5$, CsV$_3$Sb$_5$*  BRENDEN ORTIZ (Presenter), University of California, Santa Barbara, LIDIA GOMES, University of Illinois at Urbana-Champaign, JENNIFER R MOREY, MICHAL J. WINIARSKI, Johns Hopkins University, MITCHELL BORDELON, University of California, Santa Barbara, JOHN S MANGUM, Colorado School of Mines, IAIN OSWALD, Colorado State University, JOSE RODRIGUEZ-RIVERA, NIST Center for Neutron Research, JAMES NEILSON, Colorado State University, STEPHEN WILSON, University of California, Santa Barbara, ELIF ERTEKIN, University of Illinois at Urbana-Champaign, TYREL MCQUEEN, Johns Hopkins University, ERIC TOBERER, Colorado School of Mines — With its unique and elegant structure, the kagome lattice is a key platform for the study of condensed matter physics. From quantum spin liquid candidates, topologically nontrivial phases, and Weyl semi-metal candidates, these materials are poised at the frontier of material science. The kagome metals, in particular, offer unique opportunities due to the delocalization of electrons and renormalization of the electronic and magnetic ground state. Recently we discovered a new class of kagome metals: KV$_3$Sb$_5$, RbV$_3$Sb$_5$, and CsV$_3$Sb$_5$, all of which crystallize in the P6/mmm space group and exhibit a structurally perfect kagome lattice of vanadium. Our work has indicated that these materials are prime candidates for correlated electron phenomenon (anomalous Hall, heavy fermion transport, etc.). Furthermore, the Fermi level is in close proximity to Dirac features, and we can demonstrate Fermi level tuning through deintercalation of the alkali metal. Our work indicates that KV$_3$Sb$_5$ and its cogeners are fruitful candidates for the exploration of exotic transport phenomena.

*California NanoSystems Institute, Elings Fellowship program
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PbPd$_3$ has been reported to host an interesting band structure that includes a dispersionless branch along the Γ-X line that could result in a large DOS near the $E_F$ and Dirac-like surface states.[1] Previous results on the Fermi surface topography of PbPd$_3$ suggest that the $E_F$ is roughly 50 meV above the flat bands.[2] This results in the flat bands only having a weak effect on the bulk properties, while the impact of the Dirac cone at the Γ-point is limited due to it being several hundred meV above the $E_F$. In order to access the flat bands, we doped Au on the Pb site to lower the $E_F$. As a result, a significantly enhanced thermopower has been achieved. Furthermore, we performed magnetoresistance and torque magnetometry measurements in magnetic fields up to 45 T to reveal the change in the Fermi surface as a result of doping. We will discuss detailed results of the Fermi surface topology measurements on these doped series and prospects for tuning the $E_F$ in the opposite direction to meet the Dirac cone.


*NHMFL is supported by National Science Foundation through NSF/DMR-1644779 and the State of Florida. KW acknowledges support of the Jack E. Crow Fellowship. JN and TS acknowledge support from NSF/DMR-1606952.
1:51PM G60.00012: The Bulk boundary Correspondence in 3d non-Hermitian Semimetals
ZHICHENG ZHANG (Presenter), ZHESEN YANG, JIANGPING HU, Chinese Academy of Sciences, Institute of Physics — Recently, both numerical and analytical methods are proposed to calculate the generalized Brillouin zone (GBZ) and explore the bulk-boundary correspondence in non-Hermitian systems. In this article, we apply these methods to the study of the bulk-boundary correspondence of non-Hermitian semimetal model. Concretely, we take two non-Hermitian semimetal models into account and assume open boundary condition in x, y, and z directions. In each case, we calculate the spectrums and GBZ with typical parameters and plot topological phase diagram with unit-circle Brillouin zone. We find that GBZ recovers the manifest consistency between OBC and PBC spectrums, and the topological phase diagram in x, y, and z direction open boundary condition is consistent with the projection of 3-dimensional (3d) topological phase diagram into corresponding direction. Besides, we compare the topological phase diagrams calculated with unit-circle Brillouin zone and GBZ, which clearly shows that GBZ recovers the bulk-boundary correspondence in non-Hermitian systems. The GBZ phase diagrams in x-direction and y-direction open boundary cases, there exist exceptional lines phases; and in z-direction open boundary case, we get the parameter space for topological nontrivial phase with winding number \( w = 1 \).

2:03PM G60.00013: Phonon Hall effect in nonmagnetic insulators
TAKUMA SAITO (Presenter), KOU MISAKI, HIROAKI ISHIZUKA, NAOTO NAGAOSA, Univ of Tokyo — Thermal Hall effect (THE), a phenomena in which the presence of magnetic field causes thermal current perpendicular to the temperature gradient, is a useful probe to detect current of charge-neutral particles in materials: excitation of spin or lattice motion. Recently, mechanisms of THE have been theoretically investigated to reveal how the charge-neutral particles are affected by magnetic moments or magnetic field. THE of phonons has been observed only in magnetic insulators [1], and previous studies have attributed the origin of THE to spin-phonon interaction, such as the Raman interaction [2] and magnon-phonon interaction [3]. In sharp contrast, our study shows that THE of phonon is possible even without magnetic moment. This is due to imperfect screening of magnetic field in crystals: negative charge of electrons and positive one of nuclei do not completely cancel each other when the correction beyond the adiabatic approximation is taken into account. For quantitative estimation, we calculated the THE in lattice models of band insulators.

Transport properties and flux pinning analysis of high-performance FeAs122 superconducting wires [Invited] YANWEI MA (Presenter), Institute of Electrical Engineering, Chinese Academy of Sciences — Iron-based superconductors (IBS), especially 122 type, are very promising candidates for high-field applications because of its ultra-high $H_{c2} > 70$ T at 20 K, low anisotropy ($g < 2$ for 122), and ease of fabrication. In recent years, tremendous progress has been made on the critical current density ($J_c$) of the 122-type IBS wires based on a powder-in-tube technique. Encouraging breakthroughs were made, including a high transport $J_c$ exceeding the practical level of $10^5$ A cm$^{-2}$ (at 4.2 K, 10 T), the first 100 meter-class wire and the first performance test of a 30 mm IBS inserted coil under a 24 T background field. More recently, the highest transport $J_c$ value has achieved 0.15 MA/cm$^2$ ($I_c = 437$ A) at 4.2 K and 10 T in densified and textured 122 tapes made by hot pressing. The transport $J_c$ measured at 4.2 K under high magnetic field of 27 T is still on the level of 55 kA/cm$^2$. Herein we compared the $T_c$ and $J_c$ distributions of the K-doped FeAs122 tapes by a calorimetric method. We found that hot-pressing provides a better environment for a complete chemical reaction and a more homogenous dopant distribution, which are beneficial to the global current of a superconductor. We further study the vortex dynamics of the hot-pressed high-$J_c$ tapes. We found that the magnetization relaxation rate below 10 K shows a temperature insensitive plateau with a value comparable to that of low temperature superconductors. Moreover, the relaxation rate below 20 K tends to saturate with the increasing field which is beneficial for high field application. We also highlight some remarkable advances relevant to practical applications, including mechanical strain properties, copper sheaths, multifilamentary fabrication, and superconducting joints.
Superconducting phase diagram of Ni-doped magnetically ordered superconductor RbEu(Fe\(_{1-x}\)Ni\(_x\))\(_4\)As\(_4\) for x ≤ 0.04 in pulsed fields up to 65 T* MATTHEW SMYLIE (Presenter), Hofstra University, KRISTIN WILLA, Karlsruhe Institute of Technology, YILMAZ SIMSEK, Sabanci University, JINKE BAO, Argonne National Laboratory, HENDRIK HEBBEKER, Hofstra University, WAI-KWONG KWOK, DUCK YOUNG CHUNG, Argonne National Laboratory, MERCOURI KANATZIDIS, Northwestern University, JOHN SINGLETON, FEDOR BALAKIREV, Los Alamos National Laboratory, ULRICH WELP, Argonne National Laboratory — The superconducting phase diagram of single-crystal RbEu(Fe\(_{1-x}\)Ni\(_x\))\(_4\)As\(_4\) for x = 0.02, 0.03, 0.04 has been measured in pulsed magnetic fields up to 65 T using a proximity diode oscillator technique. Doping lowers T\(_c\) and slightly lowers the superconducting anisotropy, but does not affect the Eu magnetic order. Upon doping, the curvature of phase boundaries for both H || ab and H || c remains remarkably consistent, indicating that the suppression of T\(_c\) is doping driven, not disorder driven. As in the parent compound, Pauli limiting dominates H\(_{c2}\)\(_{ab}\), whereas orbital limiting dominates H\(_{c2}\)\(_c\). The resultant high Maki parameter \(\alpha\) for H || ab is consistent with a possible FFLO state at low temperatures, but none is seen in the accessible field range.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. Part of this work is supported by the US DoE BES FWP Science in 100 T, and carried out at the National High Magnetic Field Laboratory, which is funded by NSF Cooperative Agreement DMR-1157490, the State of Florida and U.S. DoE.
ReEuFe₄As₄ is a Fe-base superconductor with a high transition temperature of $T_c \sim 37$ K that enters into a magnetic state at 15 K in which Eu-4f moments are helically ordered. In this state, in-plane ferromagnetically ordered Eu-planes undergo 90 deg rotation between layers resulting in a commensurate helix with a period of 4 c-axis lattice constant. This structure is easily polarized in fields of the order of several kOe resulting in a field-induced ferromagnet with a moment of 7 $\mu_B$/ (unit cell) coexisting with superconductivity. Nevertheless, most measurements to date have yielded no or only very weak coupling between superconductivity and magnetism. Using specific heat measurements in fields up to 14 T, we show that the $H_{c2}$-line exhibits clear downwards curvature in a temperature range close to $T_c$ where Ginzburg-Landau theory applies, amounting to a shift by $\delta T_c \sim 0.4$ K in 14 T $\parallel$ c. This effect can be captured quantitatively in a model in which the exchange fields from the field-induced polarization of the Eu-moments renormalize $T_c(H)$.

* The work at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division. The PPMS used for specific heat measurements was funded by NSF MRI grant 1828387.
12:15PM G61.00004: Angular dependent studies of vortex pinning and dynamics in RbEuFe₄As₄ single crystals with columnar defects*  IVAN NEKRASHEVICH (Presenter), Los Alamos Natl Lab, MATTHEW SMYLIE, Dept. of Physics and Astronomy, Hofstra University, ULRICH WELP, WAI-KWONG KWOK, ALEXEI KOSHELEV, JIN-KE BAO, DUCK YOUNG CHUNG, MERCOURI KANATZIDIS, Materials Science Division, Argonne National Laboratory, LEONARDO CIVALE, Los Alamos Natl Lab — We performed studies of vortex pinning and dynamics in RbEuFe₄As₄ single crystals with different densities and orientations of aligned columnar defects (CDs) introduced by heavy ion irradiation, as a function of temperature (T) and magnetic field strength (H) and orientation (Θ). Pristine crystals have a superconducting transition temperature \( T_c \sim 37K \) and a magnetic ordering transition of the Eu at \( T_m \sim 15K \), neither of which is changed by the irradiations. We developed a model to account for the modifications to the vortex critical state produced by the magnetic moments. Irradiated crystals exhibit large critical current densities \( J_c \) and a lock-in phase (where vortices remain fully trapped into the CDs even if \( H \) is tilted away from them), which is the fingerprint of correlated pinning. For large CDs densities (e.g. matching field \( B_\Phi \sim 10T \)) the lock-in phase spans an unusually large angular range and extends to fields above 2T. This allows us to investigate the angular variations of \( J_c \) and the creep rates associated with the expansion of half-loops and double-kinks inside the lock-in region, due to the changes in the pinning energy arising from the \(-B\cdot H/4\pi\) term in the free energy.

*Work funded by US DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

12:27PM G61.00005: Fermi Surface Folding and Surface Reconstruction in an Iron-Based Superconductor CaKFe₄As₄*  YONGQING CAI (Presenter), HUAN YANG, TAO XIE, CONG LI, YU XU, DINGSONG WU, GUODONG LIU, HUIQIAN LUO, H.-J. GAO, LIN ZHAO, XINGJIANG ZHOU, Chinese Academy of Sciences, Institute of Physics — High resolution angle resolved photoemission spectroscopy and scanning tunneling microscopy were carried on the CaKFe₄As₄ to study its electronic structure. CaKFe₄As₄ consists of parent compound CaFe₂As₂ and heavily hole doped KFe₂As₂ but with a high \( T_C \) of 35K. We found three hole-like pockets at the Brillouin zone center and two electron-like pockets around the Brillouin zone corner. We also discovered a large hole pocket around the Brillouin zone corner which has the same size as the outmost hole pocket at the Brillouin center. Using scanning tunneling microscopy, we determine that there exists × reconstruction in CaKFe₄As₄, which will lead to the folding of the hole pocket from Brillouin zone center to Brillouin zone corner. The implication of these observations related to other iron-based superconductors will be discussed.

*This work is supported by the National Key Research and Development Program of China (Grant No. 2016YFA0300300, 2017YFA0302900), the Strategic Priority Research Program (B) of the Chinese Academy of Sciences (Grant No.XDB25000000), the National Natural Science Foundation of China (Grant No. 11888101,11534007), and the Youth Innovation Promotion Association of CAS (Grant No. 2017013).
**12:39PM G61.00006: Scattering studies of the nature of long-range magnetic order coexisting with superconductivity in single-crystal RbEuFe$_4$As$_4^*$**  
ZAHIRUL ISLAM (Presenter), Argonne Natl Lab, OMAR CHMAISSEM, Northern Illinois University, ULRICH WELP, JONG WOO KIM, Argonne Natl Lab, HUIBO CAO, Oak Ridge Natl Lab, ALEXEI KOSELEV, Argonne Natl Lab, KRISTIN WILLA, Karlsruhe Institute of Technology, MATTHEW SMYLIE, Hofstra University, ZHU DIAO, Halmstad University, ANDREAS RYDH, Stockholm University, JINKE BAO, DUCK YOUNG CHUNG, Argonne Natl Lab, MERCOURI KANATZIDIS, Northwestern University, WAI-KWONG KWOK, STEPHAN ROSENKRANZ, Argonne Natl Lab — We present magnetic long-range order studied by x-ray scattering and magnetic neutron diffraction (MND) on a single crystal RbEuFe$_4$As$_4$ (RbEu1144) superconductor. In tetragonal RbEu1144 superconductivity (SC) appears at ~37 K followed by an antiferromagnetic (AFM) transition at $T_N$ ~15 K. Our diffraction studies revealed a long-range, fully coherent, and 3D ordered magnetic phase characterized by a single wavevector, $q=(0,0,1/4)$, which indicates a 4-unit-cell magnetic periodicity along the 4-fold $c$ axis. High-resolution x-ray scattering did not find any detectable structural distortions (e.g. orthorhombic) at low temperatures. Element-selective x-ray resonant scattering (XRS) and MND measurements indicated a helical magnetic order of full Eu$^{2+}$ moments locked into the $ab$ plane, without the presence of any ferromagnetism (FM). The use of charge-magnetic interference phenomena in XRS for measuring hysteresis and determining trapped magnetic field value is presented.

*Advanced Photon Source and High Flux Isotope Reactor are DOE Office of Science User Facilities operated by Argonne National Laboratory (ANL) and Oak Ridge National Laboratory, respectively. The work at Materials Science Division, ANL, was supported by the DOE, Office of Science, Materials Sciences and Engineering Division.*

**12:51PM G61.00007: Mechanism of helical interlayer magnetic structure in RbEuFe$_4$As$_4^*$**  
ALEXEI KOSELEV (Presenter), Argonne Natl Lab — Motivated by the discovery of helical magnetic structure in RbEuFe$_4$As$_4$ [1], we study interlayer ordering of magnetic moments in a material composed of spatially-separated superconducting and ferromagnetic layers [2]. We consider the interplay between the normal and superconducting indirect exchange interaction mediated by tunneling between the conducting layers. The normal interlayer interaction can be related with the 2D density of states of an isolated layer. For shallow bands, such interaction is ferromagnetic and short-range. On the other hand, the superconducting contribution always gives antiferromagnetic interaction and extends over several layers if the interlayer hopping energy exceeds the superconducting gap. The frustration between the normal and superconducting parts may lead to a spiral magnetic configuration. The 90$^\circ$ angle between the neighboring-layers moments observed in RbEuFe$_4$As$_4$ is caused by four-fold in-plane anisotropy. This model explains a physical origin of the magnetic spiral in RbEuFe$_4$As$_4$.


*This work was supported by the US DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.*
1:03PM G61.00008: Competition between spin-vortex crystal and superconductivity in Ni-doped CaKFe$_4$As$_4$*  ANDREAS KREYSSIG (Presenter), JOHN WILDE, Ames Laboratory, Iowa State University, Dept. of Physics and Astronomy, Ames, ANNA E. BÖHMER, Ames Laboratory, Iowa State University, Ames; Karlsruhe Institute of Technology, Karlsruhe, WEI TIAN, Oak Ridge National Laboratory, Oak Ridge, WILLIAM MEIER, Ames Laboratory, Iowa State University, Ames; Oak Ridge National Laboratory, Oak Ridge, BING LI, BENJAMIN G. UELAND, MINGYU XU, SERGEY L. BUD'KO, PAUL C. CANFIELD, ROBERT MCQUEENEY, ALAN I. GOLDMAN, Ames Laboratory, Iowa State University, Dept. of Physics and Astronomy, Ames — CaKFe$_4$As$_4$ is a member of the iron arsenide superconductors in which partial substitution of Ni for Fe shifts the ground state from superconducting to antiferromagnetically (AFM) ordered. Employing neutron diffraction we determined that the AFM order is a non-collinear, commensurate structure with a hedgehog spin-vortex crystal (SVC) arrangement in the Fe planes and a simple AFM stacking perpendicular to them. The long-range SVC order coexists with superconductivity, however, similar to the doped 122 compounds with collinear stripe AFM, the ordered magnetic moment is gradually suppressed as the superconducting order parameter develops. Almost complete suppression of the AFM order is observed in a sample close to the critical Ni concentration, resulting in a back-bending of the AFM-transition-temperature phase line as a function of concentration. This supports the notion that both collinear and non-collinear magnetism as well as superconductivity compete for the same Fermi-surface nested electrons in the iron arsenide superconductors.

*This work was supported by the U. S. DOE, BES, DMSE, under Contract DE-AC02-07CH11358. This research used resources at HFIR, a U. S. DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

1:15PM G61.00009: Magnetic susceptibility of realistic superconducting samples* RUSLAN PROZOROV (Presenter), MAKARIY A TANATAR, NAUFER M NUSRAN, KYUIL CHO, KAMAL JOSHI, SUNIL GHIMIRE, Ames Laboratory — Finite element numerical exploration of the Meissner-London equations was performed for realistic three-dimensional (3D) superconducting samples of non-ellipsoidal shape and, also, having internal textures. The goal was to establish the connection between the effective finite-size magnetic susceptibility, geometric parameters of the model and the intrinsic parameters such as London penetration depth. Theoretical results are compared with the experiments where the total magnetic susceptibility was measured using tunnel-diode resonator and local first critical field was measured using NV-centers in diamond optical magnetometry. The observed differences are attributed to the specific morphological features of iron-based superconductors and high-$T_c$ cuprates.

*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract # DE-AC02-07CH11358.
Cooperative response of the magnetic and superconducting subsystems in magnetic superconductor RbEuFe4As4* VITALII VLASKO-VLASOV (Presenter), ULRICH WELP, ALEXEI KOSHELEV, Argonne Natl Lab, MATTHEW SMYLIE, Hofstra University, JINKE BAO, DUCK YOUNG CHUNG, Argonne Natl Lab, MERCOURI KANATZIDIS, Northwestern University, WAI-KWONG KWOK, Argonne Natl Lab — We present magneto-optics and magnetization based studies of the magnetic flux evolution in single crystals of the magnetic superconductor RbEuFe4As4 during field cooling and warming, and magnetic field cycling at temperatures above and below the magnetic transition point, Tm. The vortex patterns emerging at T below and ~Tm on different crystal facets in the fields of different orientations, reveal a peculiar magnetization process, where the magnetic subsystem serves as an internal magnetic flux pump while the superconducting subsystem controls the entry of magnetic flux quanta into the bulk. The interplay of magnetic susceptibility amplifying the magnetic induction and vortex pinning attenuating the magnetic flux entry, results in a field and temperature dependent critical state that mimics a paramagnetic Meissner effect. The observed anisotropic vortex dynamics is associated with a peculiar fine scale Eu-spin helical structure modified by the vortex field and resulting in a nontrivial spatial current distribution, which yields a self-consistent inhomogeneous enhancement of the sample magnetization.

*The work was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division.

Temperature dependent resistivity in hole-doped Ba1−xKxFe2As2 subject to electron irradiation* MAKARIY TANATAR (Presenter), YONG LIU, T. A. LOGRASSO, RUSLAN PROZOROV, Ames Lab, MARCIN KONCZYKOWSKI, OLIVIE CAVANI, LSI, Ecole Polytechnique — Temperature dependence of in-plane and inter-plane electrical resistivity was studied in single crystals of hole doped iron based superconductor Ba1−xKxFe2As2 (0 ≤ x ≤ 1). Low temperature (20 K) irradiation with relativistic 2.5 MeV electrons was used to control residual resistivity of the samples. Matthiessen rule is found to be universally violated for all compositions and for both current flow directions. This is in stark contrast with electron doped Ba(Fe1−xCox)2As2 [1] and iso-electron substituted BaFe2(As1−xPx)2 [2]. Possible reasons for Matthiessen rule violation are discussed.


*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract # DE-AC02-07CH11358.
1:51PM G61.00012: Strain effect on the superconductivity of FeSe$_{0.5}$Te$_{0.5}$ thin films induced by mica substrate
YE GAO (Presenter), CHENGuang MEI, MIAO MENG, XI ZHANG, YONGGuANG ZHAO, Tsinghua University — Iron-based superconductors have attracted much attention because of their promising prospects in both applied and fundamental research. Iron chalcogenide superconductors, which have the simplest structure, play an important role in this field. It has been shown that pressure or strain has remarkable influence on their superconducting transition temperatures ($T_C$) [1, 2]. To further explore the strain effect, we grow epitaxial FeSe$_{0.5}$Te$_{0.5}$ (FST) thin films on muscovite mica substrates by pulsed laser deposition, because different strains can be induced by bending mica owing to the flexibility of mica after mechanical exfoliation [3]. It is shown that $T_C$ value of FST increases under compressive strain while decreases under tensile strain. It is also indicated that the relative orientations of electrical current and strain are important in the change of transport property. The results are discussed by considering different contributions. This work is helpful to understand superconducting mechanism of iron chalcogenide superconductors, and shows a great potential for novel applications with flexible superconductors.


2:03PM G61.00013: Spontaneous Nernst Effect in an Iron-based Topological Superconductor Fe$_{1+y}$Te$_{1-x}$Se$_x$  
LU CHEN (Presenter), ZIJI XIANG, COLIN B TINSMAN, Univ of Michigan - Ann Arbor, GENDA GU, Brookhaven National Laboratories, LU LI, Univ of Michigan - Ann Arbor — We report on a study of Nernst effect in an iron-based superconductor Fe$_{1+y}$Te$_{1-x}$Se$_x$. We observe a zero-field Nernst effect that appears around the superconducting transition temperature $T_C$. This spontaneous Nernst signal does not follow the temperature and field dependence of the thermal power and occur only in the temperature range near $T_C$ where the superconducting fluctuation is strong and vortex liquid is robust. This intrinsic spontaneous Nernst signal indicates the violation of time reversal symmetry (TRS) in the superconducting state. The TRS in Fe$_{1+y}$Te$_{1-x}$Se$_x$ may be broken by pinning flux introduced by the interstitial iron impurity. To further understand the role of excess Fe atoms, we study a series of Fe$_{1+y}$Te$_{1-x}$Se$_x$ single crystals that have different $T_c$ and different levels of excess Fe concentrations and demonstrate how they affect the spontaneous Nernst effect signal.

Tuesday, March 3, 2020 11:15 AM - 2:03 PM

Session G62 DMP: Nanostructures and Metamaterials V  Mile High Ballroom 4C - Xiaobo Yin, Lawrence Berkeley National Laboratory
11:15AM G62.00001: Soft porous polymer materials, a new range of acoustic metasurfaces*

KATERINA KAMPIOTI (Presenter), JACQUES LENG, CNRS Bordeaux — In 2011 a new range of 2D materials, widely known as metasurfaces, has emerged. These planar metamaterials of subwavelength thicknesses, capable of wave front shaping, consist of a single or several layers of artificial structure1.

In general, metasurfaces are engineered by assembling arrays of deep sub wavelength building blocks. Here, we present a bottom-up approach which is based on soft-porous material: the dependence of the refractive index of soft porous polymer materials with their porosity enable us to fabricate acoustic gradient-index (GRIN) metasurfaces1. Yet, their fabrication requires photo-polymerization of the thin film, which is made difficult by the presence of porogenic agents that scatter light. We will present a rational approach to understand the coupling between photo-chemistry and light scattering (in scattering media), and we will illustrate how the use of grayscale lithography facilitates the generation of this high precision microstructures.


*This work was funded and performed within the project BRENNUS ANR-15-CE08-0024.

11:27AM G62.00002: Self-Assembly of Poly(ethylene glycol)-Functionalized Gold Nanorods at the Vapor/Liquid Interface*

HYEONG JIN KIM (Presenter), WENJIE WANG, Ames laboratory, Iowa State University, WEI BU, ChemCARS, The University of Chicago, SURYA MALLAPRAGADA, DAVID VAKNIN, Ames laboratory, Iowa State University — Using surface sensitive synchrotron X-ray diffraction, we report on the self-assembly of gold nanorods (AuNRs) into 2D films at the vapor/liquid interface. The films are facilitated by grafting the AuNRs with poly(ethylene glycol) (PEG). Grazing incidence small angle X-ray scattering (GISAXS) and specular X-ray reflectivity (XRR), show that PEG-AuNRs in aqueous suspensions migrate to the vapor/liquid interface in the presence of salt, forming a uniform monolayer with planar-to-surface orientation. Furthermore, the 2D assembled PEG functionalized AuNRs exhibit short range order into rectangular symmetry with side-by-side and tail-to-tail nearest-neighbor packing. The effect of PEG chain length and salt concentration on the 2D assembly are also reported.

11:39AM G62.00003: Temperature-induced self-assembly and crystallization of gold nanorods*  DAVID VAKNIN (Presenter), HYEONG JIN KIM, WENJIE WANG, ALEX TRAVERSET, SURYA MALLAPRAGADA, Ames Laboratory, Iowa State University — We report on temperature-induced and improved assembly and crystallization of gold nanorods (AuNRs) that are grafted with poly(ethylene glycol) (PEG) in electrolytic suspensions. Small angle X-ray scattering (SAXS) reveals that elevating the temperature of dispersed PEG-AuNRs suspensions in the presence of electrolytes or poly-electrolytes spontaneously induces the assembly of the AuNRs into hexagonal superlattices. Surprisingly, we find that the lattice constant of the crystalline AuNRs significantly decreases and crystal quality improves by increasing the temperature of the suspensions. Implications of the results for engineering new nanomaterials are discussed.


11:51AM G62.00004: Laser-written nanograting deep inside silicon*  AQIQ ISHRAQ (Presenter), RANA ASGARI SABET, ONUR TOKEL, UNAM - National Nanotechnology Research Center, Bilkent University — Functional optical elements fabricated on the surface of silicon (Si) constitute fundamental building blocks of Si-photonics. For fabrication of these elements, generally conventional lithography and etching techniques are used. We recently demonstrated a laser-writing method that enables direct creation of buried or “in-chip” optical elements inside the wafer [1]. This direct laser-writing method had enabled 3D optical elements at 1-µm resolution [1]. Here, we expand the technique for demonstrating the first in-chip nanogratings crated in Si, realized without damaging the wafer surface. In order to achieve this, we exploit the ‘non-diffracting’ nature of Bessel beams, and infrared laser pulses of ~5 ns, 1.55 µm where Si is transparent. The crystal structure is modified in the form of periodic rod-like structures with structure-widths 250 nm to 1-micrometer, resulting in grating efficiencies up to 45%. These in-chip optical elements constitute the first examples of a larger class of emerging in-chip nano-photonic components, that can potentially lead to novel infrared elements at the nanoscale.


* Bilim Akademisi (BAGEP Award)
12:03PM G62.00005: Large Area Superhydrophilic Silicon Surface Texturing using Nanosecond Laser Pulses  
NANCY VERMA (Presenter), Light and Matter Physics Department, Raman Research Institute, Bengaluru, India, K. K. ANOOP, Department of Physics, Cochin University of Science and Technology, Cochin, India, PRIYA DOMINIC, REJI PHILIP, Light and Matter Physics Department, Raman Research Institute, Bengaluru, India — We report experimental investigations of large area laser micro/nano texturing of silicon (100) targets by Nd: YAG laser pulses (λ=532 nm, τ =7 ns) addressing the wetting behavior of processed silicon surface. In particular, ns laser surface processing is used to develop hierarchical surface structures by the line scanning method to create parallel micro-channels with proper overlap between the lines at different laser pulse fluence ranging from 2 J/cm$^2$ to 4 J/cm$^2$. We observe that the bottom of craters formed due to single and multipulse laser irradiations are rather flat, but some concentric nano-ripple features are present along the rim of the craters, resulting in the formation of multiscale surface morphology. The topography of the samples is investigated using AFM and SEM, whereas the wetting property is measured through sessile drop contact angle measurements. The combination of microscale channels written by parallel line scan, with self-organized surface patterns and random nanoparticles decoration, formed on the surface allow developing highly hydrophilic silicon surfaces with contact angle values reaching around 5°, presenting potential interest for superwetting applications.

12:15PM G62.00006: Growth Kinetics of Metal Nanowires and Nanoplates*  
KRISTEN FICHTHORN (Presenter), ZIHAO CHEN, JUNSEOK KIM, Pennsylvania State University — Metal nanocrystals have gained tremendous attention due to their superior performance in various applications, ranging from selective catalysis to electronic devices to plasmonic applications. For these and many other applications, the properties of the nanocrystals are highly sensitive to their shape. However, it remains a challenge to achieve high shape selectivity in solution-phase syntheses. I will discuss our efforts to understand the growth of Cu and Ag nanocubes, nanowires and nanoplates, which is facilitated by the inclusion of halide ions (chloride, bromide, and iodide) in the synthesis protocol. We use ab initio thermodynamics based on quantum density-functional theory (DFT) to demonstrate how these halides create thermodynamic driving forces for cubes, plates and wires, by selectively altering surface energies. Using a combination of DFT and the theory of absorbing Markov chains, we demonstrate how halides affect surface diffusion and interfacet transport to drive the growth of particular nanoshapes in the presence of halide. Our results agree with experiment and indicate a promising way to exact control over nanocrystal synthesis.

*This work is funded by the Department of Energy, Office of Basic Energy Sciences, Materials Science Division, Grant DEFG02-07ER46414.
Molecular dynamics simulation of silicon nanowires with oxide layers under uniaxial tension

WENTING XU (Presenter), WOO KYUN KIM, Univ of Cincinnati — The size-dependent brittle-to-ductile transition (BDT) of silicon is an important scientific topic, but its underlying mechanism is still unclear. Silicon nanostructures such as nanowires have been widely used in electronics and optoelectronics applications and have also been used to study the BDT phenomenon of silicon in both experiments and simulations. While silicon is spontaneously oxidized when exposed to air, most of the previous simulation studies have neglected the effect of oxide layers on BDT. In this work, we employ the molecular dynamics (MD) simulation method to study the influence of oxide layers on the BDT of silicon nanowires under uniaxial tension loading. The oxide layers are created by inserting oxygen atoms into the Si-Si bonds from the nanowire surface and several key factors such as nanowire diameter, thickness of oxide layers, temperature, and strain rate are considered. The MD simulation results reveal the effect of oxide layers on the plastic deformation of silicon nanowires and elucidate its atomic-scale mechanisms.

Porous Silica Cluster Collision Molecular Dynamics

ERIC SWITZER (Presenter), ANIKET BHATTACHARYA, Univ of Central Florida — Silica nanoparticles are theorized to exist in the interstellar medium, where collision velocities range over several orders of magnitude. We report molecular dynamics simulation studies of the coalescence of small (approx. 2 nm) porous silica clusters with each other for a range of velocities and initial cluster porosities. Our use of the ReaxFF bond-order potential allows us to account for bond dynamics during the collision. We vary cluster porosity through the random removal of silica base units during the cluster formation stage and monitor post-collision structural dynamics. We compare both the pair correlation function and structure factors of prepared porous clusters as verification of our preparation method. We use simulation data to study the evolution of post-collision cluster morphology characterized in terms of final porosities and fractal dimensions as a function of the initial range of porosities and velocities. We compare our results with similar studies using different potentials during collision processes.
12:51PM G62.00009: Granular aluminum meandered superinductors for quantum circuits

PLAMEN KAMENOV (Presenter), WEN-SEN LU, KONSTANTIN KALASHNIKOV, THOMAS J DINAPOLI, Rutgers University, New Brunswick, MATTHEW T BELL, University of Massachusetts, Boston, MICHAEL GERSHENSON, Rutgers University, New Brunswick — We report on the optimization, fabrication, and characterization of superinductors made of meandered nanowires of strongly disordered (granular) Aluminum [1]. Superinductors are essential for numerous superconducting quantum circuits operating at millikelvin temperatures. We succeeded in increasing the self-resonance frequency of superinductors by the optimization of its in-plane dimensions. These compact superinductors are beneficial for a wide range of applications, from superconducting circuits for quantum computing to microwave elements of cryogenic parametric amplifiers and kinetic-inductance photon detectors. We have also demonstrated that the superinductors based on granular Aluminum films can be integrated in “hybrid” superconducting circuits containing conventional Al-Al2O3-Al Josephson junctions.


*The work at Rutgers University was supported by the NSF award DMR1708954 and the ARO award W911NF-17-C-0024. The work at the University of Massachusetts Boston was supported in part by a 2019 Google Faculty Research Award and NSF Awards No. ECCS-1608448, DUE-1723511, and DMR-1838979.

1:03PM G62.00010: Characterization of Spin-Thermal Environment Interaction Leading to Nuclear Quadrupolar Spin Relaxation

SANGHAMITRA NEOGI (Presenter), MANOJ SETTIPALLI, University of Colorado, Boulder — The control of spin dynamics at the nanoscale is crucial for quantum technologies based on spin qubits. Quadrupolar nuclei with spin > ½ facilitates creation of N-qubit systems, the representation of many qubits with one nuclear species. Additionally, nuclei with strong quadrupole moments can be used to perform QIP with NQR. However, the strong quadrupole couplings lead to faster spin relaxation and stronger dissipation due to spin-environment interaction. It is crucial to analyze the effect of local environment fluctuations on spin-environment relaxation (SER) to correctly predict the evolution of the qubits implemented by the quadrupolar spins. The prediction of quadrupolar relaxation time (T1) in alkali halides improved considerably due to the inclusion of realistic phonon density of states, over approximate phonon dispersions. However, the predicted T1 is still off by an order of magnitude compared to measured data. Here, we extend the formulation by incorporating the full dispersion relations of thermal phonons to describe T1. Our study provides a framework to characterize the thermal noise affecting the nuclei spin qubits. We anticipate that this work will lead to tailoring the relaxation time by controlling phononic environment of the spin qubits.
1:15PM G62.00011: Spin transport in ferromagnet-InSb nanowire quantum devices

ZEDONG YANG (Presenter), BRETT HEISCHMIDT, School of Physics and Astronomy, University of Minnesota, SASA GAZIBEGOVIC, GHADA BADAWY, DIANA CAR, Eindhoven University of Technology, PAUL CROWELL, School of Physics and Astronomy, University of Minnesota, ERIK BAKKERS, Eindhoven University of Technology, VLAD PRIBIAG, School of Physics and Astronomy, University of Minnesota — Semiconductor nanowires (NWs) such as InSb are a leading platform for realizing future Majorana zero modes based on quantum computing\(^1\). However, the appliance of external magnetic fields can suppress the superconductivity and place geometric restrictions on the device. These challenges can be circumvented by integrating magnetic elements with the NWs. In our experiments, by fabrication ferromagnetic contacts, we investigate spin transport across InSb NWs in a quasi-1D ballistic regime\(^2\). Hysteretic magnetoconductance can be observed proving spin-polarized transport across the NWs. Moreover, we show that electrostatic gating tunes the observed hysteretic signal and also reveals a transport regime where the device acts as a spin filter.


*Supported primarily by the Department of Energy under Award No. DE-SC-0019274. Nanowire growth was supported by the European Research Council (ERC HELENA 617256), and the Dutch Organization for Scientific Research (NWO).

1:27PM G62.00012: Optical Properties of Monolayer Bismuthene under Electric Field based on First-principles Calculations

WEI CHIEH LIU (Presenter), LIANGLIANG XU, MING-CHIEH LIN, Department of Electrical and Biomedical Engineering, Hanyang University, TSAN-CHUEN LEUNG, Department of Physics, National Chung Cheng University, HUA-YI HSU, Department of Mechanical Engineering, National Taipei University of Technology — Monolayer bismuthene has extraordinary optoelectronic, catalytic, and biocompatible properties, and potential as a 2D topological insulator. When monolayer bismuthene deposited on the surface of the object to form sufficiently thin, there is a stable form of a low buckling hexagonal structure. If the thickness of the crucible becomes thinner than the Fermi wavelength, there may be a transition from a semimetal to a semiconductor due to the quantum confinement effect. So this could be a promising low-dimensional thermoelectric material. The monolayer bismuthene is a p-type semiconductor, but the hole concentration arising from the intrinsic defects is very low and hard to control. It is found that the optical properties can be changed dramatically by applying external electric field. In this work, the energy band structure, density of states, and optical constants of bismuthene have been calculated using the first-principles calculations based on density functional theory (DFT). With applying an electric field, the optical properties of bismuthene are determined and compared to those calculated from the tight-binding model. The controlled optical properties of monolayer bismuthene may have some applications in optoelectronics, either combined with other 2D or topological materials.
1:39PM G62.00013: Shadowing of epitaxial superconductors on selectively grown in-plane semiconductor wires for advanced quantum devices  
JOON SUE LEE (Presenter), University of Tennessee Knoxville, MIHIR PENDHARKAR, CONNOR DEMPSEY, SUKGEUN CHOI, ARANYA GOSWAMI, University of California Santa Barbara, HAO WU, PO ZHANG, University of Pittsburgh, ROY OP HET VELD, ERIK BAKKERS, Eindhoven University of Technology, SERGEY M FROLOV, University of Pittsburgh, CHRIS J PALMSTROM, University of California Santa Barbara — In superconductor-semiconductor systems, a clean interface between superconductor and semiconductor is crucial for quantum transport studies. Advances in epitaxial Al growth on low-dimensional semiconductors have resulted in enhanced features of superconducting proximity effect. In addition, development of clean junctions by in-situ shadowing has led to further improvement of superconducting features in 1D nanowire-based systems. Here we demonstrate a shadowing scheme of epitaxial superconductors on in-plane quantum wires by selective-area growth. Shadow wall structures are pre-fabricated next to wire-shape trenches. After epitaxial growth of semiconductor wires on the trenches, Al deposition is carried out at an angle between 40 and 60 degrees from the normal direction of the substrate. The shadowing of Al results in clean Al-semiconductor junctions based on the shape of the shadow wall structures. This shadow scheme can be applied to any selective-area growth wires by various techniques such as molecular beam epitaxy, chemical beam epitaxy, and metalorganic vaporphase epitaxy. We further discuss transport studies in devices prepared by this scheme as well as deposition of another superconductor with a higher superconducting transition temperature.

1:51PM G62.00014: Synthetic Weyl Points and Chiral Anomaly in Majorana Devices  
PANAGIOTIS KOTETES (Presenter), Institute of Theoretical Physics, Chinese Academy of Sciences, MARIA TERESA MERCALDO, University of Salerno, MARIO CUOCO, CNR-SPIN — We demonstrate how to design various nonstandard types of Andreev-bound-state (ABS) dispersions, via a composite construction relying on Majorana bound states (MBSs). Here, the MBSs appear at the interface of a Josephson junction consisting of two topological superconductors (TSCs). Each TSC harbors multiple MBSs per edge by virtue of a chiral or unitary symmetry. We find that, while the ABS dispersions are $2\pi$ periodic, they still contain multiple crossings which are protected by the conservation of fermion parity. A single junction with four interface MBSs and all MBS couplings fully controllable, or networks of such coupled junctions with partial coupling tunability, open the door for topological band structures with Weyl points or nodes in synthetic dimensions, which in turn allow for fermion-parity (FP) pumping with a cycle set by the ABS-dispersion details. In fact, in the case of nodes, the FP pumping is a manifestation of chiral anomaly in 2D synthetic spacetime. The possible experimental demonstration of ABS engineering in these devices further promises to unveil new paths for the detection of MBSs and higher-dimensional chiral anomaly. 

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G63 DMP DCMP FIAP: Defects in Gallium Oxide and Nitride  
High Ballroom 4D - Anderson Janotti, University of Delaware - Tag(s): Focus
Gallium oxide is an emerging ultra-wide bandgap semiconductor that holds enormous promise for devices needed to operate in extreme conditions, including high electric fields, high temperatures and radiation environments. Attributes such as its ~ 4.8 eV bandgap, ease of n-type doping, ability to synthesize AlGaO alloys to enable heterostructure devices, availability of melt-grown large area Ga2O3 substrates, and device figures of merit that theoretically exceed more mature wide bandgap technologies based on SiC and GaN, all contribute to rapid acceleration of research in this area. To date, Ga2O3 materials and devices are being grown using a wide range of epitaxial methods, and identifying point defects that are associated with growth conditions, and discriminating between impurity and native physical sources are key to guiding the advancement of material quality so that Ga2O3 can reach its ultimate properties desired for applications in RF power electronics and UV optoelectronics. This presentation focuses on the ongoing investigation of defect states in the Ga2O3 bandgap using a range of defect spectroscopy methods that enable comprehensive characterization of deep level defects across the entire ~ 4.8 eV bandgap. Deep level optical spectroscopy, deep level transient (thermal) spectroscopy and admittance spectroscopy are applied to Ga2O3 materials and devices grown by MBE, MOCVD, LPCVD and EFG methods to enable a quantitative comparison of how defect introduction varies with growth method. High energy particle radiation is used to distinguish native from impurity-based defect states provides further differentiation regarding physical sources. Identification of which defects contribute to important properties for device transport, such as carrier compenstation and electron mobility, is discussed.

*This work is sponsored by the Defense Threat Reduction Agency (DTRA HDTRA1-17-10034) and the Air Force Office of Scientific Research (FA9550-18-1-0059 and FA9550-18-1-0479).
11:51AM G63.00002: Ab initio studies on segregation of n-type dopants and vacancies near beta-Ga2O3(010) surface  JINGYANG WANG (Presenter), Materials Science and Engineering, Stanford University, PAULETTE CLANCY, Chemical and Biomolecular Engineering, Johns Hopkins University — Beta-Ga2O3 is a wide-bandgap semiconductor with important electronic and optoelectronic applications. It has been observed that upon extended period of thermal annealing, certain types of n-type dopants such as Sn show strong tendency of segregation towards Ga2O3 surfaces, even forming a secondary SnO2 phase. Using density functional theory, we conducted a comprehensive study on the thermodynamic preference of common n-type dopants (Si_Ga, Ge_Ga, Sn_Ga) and intrinsic defects (V_Ga, V_O) both near the (010)-surface and in the bulk of Ga2O3. The key findings are: (1) in bulk Ga2O3, Si prefers to occupy tetrahedral over octahedral Ga site (by -0.60 eV), Sn shows the opposite preference (by -0.90 eV), and Ge have almost equal preference on either Ga site; (2) Si and Ge shows weaker likelihood of segregation towards Ga2O3(010) surface (-0.14 eV for Si, -0.11 eV for Ge) than Sn (-0.25 eV), while both V_Ga and V_O assume strong tendency of segregation (< -0.4 eV); (3) all dopant species (Si, Ge, Sn) show significantly decreased (increased) segregation energy with the presence of surface V_Ga (V_O); (4) co-doping with Si or Ge in the second-nearest-neighbor configuration can raise the segregation energy of Sn. The implications for experimental processing conditions will be discussed.

12:03PM G63.00003: Electronic properties of the Ga2O3-Fe2O3 system  SHOAIB KHALID (Presenter), Department of Physics and Astronomy, University of Delaware, FERNANDO SABINO, ANDERSON JANOTTI, Department of Material Science and Engineering, University of Delaware — Fe2O3 has attracted a lot of interest due to its interesting electronic, chemical and magnetic properties, with applications in photoelectrochemical cells, gas sensor, and Li ion batteries. It is readily available as one of the most abundant material found on earth. On the other hand Ga2O3 is a wide-band-gap semiconductor promising for high power electronic devices and UV blind photodetectors. Here we present results for the electronic structure of Fe2O3 and Ga2O3 in both monoclinic and corundum phases using different exchange correlation functionals. We show how the valence and conduction band edges change with respect to the vacuum level depending upon the choice of functional used for Fe2O3 and Ga2O3. We discuss their band alignments, and the electronic structure and stability of the Ga2O3-Fe2O3 alloys. Finally, we discuss the possibility of forming a p-n heterojunction with p-Ga2O3 and n-Ga2O3 and its characteristics.
Unusual Formation of Point Defects and Their Complexes in Ultra-wide Band Gap Beta-Ga2O3

JARED JOHNSON, Ohio State Univ - Columbus, ZHEN CHEN, Cornell University, JOEL VARLEY, Lawrence Livermore National Laboratory, CHRISTINE JACKSON, ESMAT FARZANA, AARON AREHART, HSIEN-LIEN HUANG, STEVEN RINGEL, Ohio State Univ - Columbus, CHRIS VAN DE WALLE, University of California, Santa Barbara, DAVID MULLER, Cornell University, JINWOO HWANG (Presenter), Ohio State Univ - Columbus — Beta-Ga2O3 has unique advantages including high breakdown voltage and availability as bulk substrates, which make it a viable candidate for next-generation power device applications. We present the first direct microscopic observation of the unusual formation of interstitial-divacancy complexes within beta-Ga2O3 lattice using atomic resolution scanning transmission electron microscopy. We observed that cation atoms are present in multiple interstitial sites, and each interstitial atom is paired with two adjacent vacancies. The observed structure is consistent with density functional theory calculation, which predicts them to be compensating acceptors. The number of the complexes increase as a function of Sn doping, which matches with the increase of the trap state at Ec - 2.1 eV measured using deep level optical spectroscopy, strongly suggesting that the defects correspond to that trap level. We also show that two neighboring complexes can further relax the structure in between, creating more cation vacancies. Our finding provides new crucial information on the exact structural origin of the properties of beta-Ga2O3 that has been unobtainable using other methods.

*We acknowledge support by the Department of Defense, Air Force Office of Scientific Research GAME MURI Program.

Donor and acceptor properties in Ga2O3 polymorphs

JOHN LYONS (Presenter), DARSHANA WICKRAMARATNE, Center for Computational Materials Science, United States Naval Research Laboratory, JOEL VARLEY, Lawrence Livermore National Laboratory — An ultra-wide band gap and substrate availability make Ga2O3 an attractive power electronic material. But questions still remain as to how best control its electrical conductivity through impurity doping. In this work, we evaluate the properties of acceptor and donor dopants in Ga2O3 polymorphs using first-principles calculations based on hybrid density functional theory. Hole localization and low-lying valence bands are exhibited by all Ga2O3 phases, causing deep acceptor behavior for all impurities considered. These polymorphs also share other properties, such as similar positions of the deep oxygen vacancy defect levels. In contrast, cation-site donors (such as C, Si, Ge, and Sn) are found to be shallow. These donors do exhibit defect transition levels above the Ga2O3 conduction band minimum, which may become relevant if Ga2O3 is alloyed with aluminum and the band gap increases.

*This work was supported by the NRL/ONR Base Research Program. DW was supported by a NRC associateship at the US NRL.
12:39PM G63.00006: Optical Properties of Acceptor Impurities in Ga$_2$O$_3$  INTERÓN CHATRATIN
(Presenter), FERNANDO SABINO, Department of Materials Science & Engineering, University of Delaware, PAKPOOM REUNCHAN, Department of Physics, Kasetsart University, ANDERSON JANOTTI, Department of Materials Science & Engineering, University of Delaware — Ga$_2$O$_3$ has attracted great attention as a promising material for high power electronic applications due to a very large band gap, high breakdown voltage and ability to be doped n-type. The Ga$_2$O$_3$ Baliga’s figure of merit is only lower than that of diamond. Most importantly, large single crystals of Ga$_2$O$_3$ are available, facilitating epitaxial growth. Although p-type Ga$_2$O$_3$ have not been demonstrated as acceptor impurities tend to introduce deep acceptor levels, they can be used to make semi-insulating layers, and that can be useful in device designing. The deep levels of acceptor impurities in ultra-wide-band gap oxides are often difficult to probe experimentally. To facilitate the experimental characterization of the acceptor impurities, we employed hybrid density-functional calculations to investigate the optical transitions of acceptor impurities in monoclinic Ga$_2$O$_3$. We constructed configuration coordinate diagrams to determine the absorption and emission energies that can be compared with the optical absorption and photoluminescence measurements. The results show that all impurities exhibit deep acceptor transitions. The calculated emission energies are compared with the available experiment data.

12:51PM G63.00007: Transition levels for impurities in β-Ga$_2$O$_3$*  SUMAN BHANDARI
(Presenter), MARY ZVANUT, Univ of Alabama - Birmingham — Bulk Ga$_2$O$_3$ is of interest for both electronic and optical applications. However, the large number of different impurities often complicates understanding of the basic material properties. Confusion can be minimized by directly monitoring individual impurities using photo-induced electron paramagnetic resonance (EPR). Specifically, the present work tests the validity of several proposed defect levels in Fe-doped and Mg-doped β-Ga$_2$O$_3$ crystals by identifying each impurity, Fe$^{3+}$, Mg$^0$, and Ir$^{4+}$ with an EPR spectrum. The EPR intensity for the impurity is monitored during illumination from 1500 to 300 nm at 30 K or 130 K, and changes are associated with ionization. A photo-threshold between 2.0 and 2.3 eV where Ir$^{4+}$ increases and Fe$^{3+}$ decreases is assigned to the Ir$^{3+/4+}$ defect level, and one between 1.2 and 1.5 eV where Fe$^{3+}$ increases is assigned the Fe$^{2+/3+}$ level after consideration of the lattice relaxation. Ongoing study of the Mg-doped samples indicates that Mg$^0$ decreases between 1.6 and 1.9 eV, consistent with reported levels for Mg$^{-}/0$; however the photon energy dependence for the generation of the neutral Mg$^0$ is not yet clear. The presentation will describe procedure and analysis details, particularly for the curious case of neutral Mg.

*This work is supported by NSF-1904325
1:03PM G63.00008: Bismuth-alloyed Ga₂O₃ as a novel p-type transparent conducting oxide
XUEFEN CAI (Presenter), FERNANDO P. SABINO, ANDERSON JANOTTI, University of Delaware, SUHUAI WEI, Beijing Computational Science Res Ctr — Ga₂O₃ is a wide-band-gap semiconductor that has attracted great attention for applications in power electronics and UV-blind detectors. It is easy to make it n-type by adding Si, Ge, or Sn, yet difficult (or impossible) to make it p-type unless its electronic structure is fundamentally changed. Here we show that adding a few percent of Bi to Ga₂O₃ leads to an intermediate valence band that is sufficiently high in energy to enable p-type doping. Using first-principles calculations we study the electronic structure of Bi-alloyed Ga₂O₃ and the doping efficiency of possible acceptor impurities in this system. Specifically, we discuss the results for Mg, Zn, and Cu acceptors in (BiₓGa₁₋ₓ)₂O₃, including their most favorable incorporation sites, formation energies, and transition energy levels. We show that dilute (BiₓGa₁₋ₓ)₂O₃ alloys could be good candidates for novel p-type transparent conducting oxide that will create new opportunities in Ga₂O₃-based device design.

1:15PM G63.00009: Direct Imaging on Strain Relaxation of MBE-grown Single Phase alpha-(Al,Ga)₂O₃ on m-sapphire Substrate in Atomic Resolution Using Scanning Transmission Electron Microscopy
CELESTA CHANG (Presenter), Department of Physics, Cornell University, RIENA JINNO, DEBDEEP JENA, HUILI GRACE XING, Electrical and Computer Engineering, Cornell University, DAVID ANTHONY MULLER, Applied and Engineering Physics, Cornell University — MBE-grown corundum structured alpha-Ga₂O₃ on c-plane sapphire substrates often contains considerable amount of beta-Ga₂O₃ due to c-plane facets. Recently, a successful MBE-growth of pure alpha-(Al, Ga)₂O₃ on m-plane sapphire was reported. Here, we show the relaxation mechanism of such films by performing strain analysis with scanning transmission electron microscopy (STEM). The films are partially relaxed through dislocation cores at the interface, some of which tend to climb up into the film. High angle annular dark field (HAADF)-STEM images in plan-view shows the formation of very thin gamma-Ga₂O₃ at the interface occupying less than 1% area density. Owing to its defect spinel-type structure that requires two cation vacancies, gamma-Ga₂O₃ is believed to form naturally at the interface to accommodate the strain arising from lattice mismatch.

*This material is based on the work supported by the Cornell Center for Materials Research (CCMR) Shared Facilities, which are supported through the NSF MRSEC program (No.DMR-1719875). This work is supported by the Cornell/AFOSR ACCESS center of excellence (No. FA9550-18-1-0529).
1:27PM G63.00010: Ultrafast Optical Measurement of Defect Dynamics in \( \beta \)-Ga\(_2\)O\(_3\) using Supercontinuum Pump-Probe Spectroscopy.* ARJAN SINGH (Presenter), OKAN KOKSAL, NICHOLAS TANEN, DEBDEEP JENA, HUILI XING, FARHAN RANA, Cornell University — Ga\(_2\)O\(_3\) polymorphs have shown great promise for high power devices. \( \beta \)-Ga\(_2\)O\(_3\) has a large number of intrinsic and extrinsic defects with poorly understood properties. Non-equilibrium optical spectroscopy has proven to be a valuable tool in studying midgap defects in materials. In this work, we use optical pump-probe spectroscopy that employs a supercontinuum pulse to probe the defects and their ultrafast dynamics in a wide energy interval within the material bandgap. Our results show transient absorption of the probe pulse by midgap defects that is highly polarization selective. Our results show that hole capture times of defects scale with their separation in energy from the valence band with defects furthest away from the valence band exhibiting the slowest hole capture rates. Temperature dependence of hole capture rates indicate a thermally activated capture process involving lattice relaxation (multi-phonon process) that can be fitted with a Mott-Seitz expression. We present models to explain the nature of these defects and the ultrafast dynamics associated with the capture of photoexcited carriers by these defects.

*The research was funded by AFOSR ACCESS grant FA9550-18-1-0529.

1:39PM G63.00011: X-ray diffraction studies of GaN p-i-n structures for high power electronics* ALEXANDRA ZIMMERMAN (Presenter), JIAHENG HE, GUANJIE CHENG, DAVIDE DEL GAUDIO, JORDAN OCCENA, Materials Science and Engineering, University of Michigan, FABIAN NAAB, Michigan Ion Beam Laboratory, University of Michigan, MOHSEN NAMI, BINGJUN LI, JUNG HAN, Department of Electrical Engineering, Yale University, RACHEL GOLDMAN, Materials Science and Engineering, University of Michigan — Although silicon-based electronics are used to power light-emitting diodes and electric vehicles, their utility in high power applications is limited by a low breakdown voltage. The most promising alternative power devices consist of vertical GaN devices, which often require regrown active regions. In this work, we examine the p-i interface of a series of GaN p-i-n structures prepared with and without ex-situ ambient exposure and/or chemical etching. For the “in-situ” GaN structure, elastic recoil detection analysis (ERDA) revealed the highest interfacial \([H]\) and Rutherford backscattering shows the highest density of displaced Ga atoms, likely due to efficient incorporation of Mg\(_{Ga}\). Here, we report on x-ray diffraction studies of the crystallinity of the GaN p-i-n structures. The full width at half max (FWHM) of phi and omega scans were used to quantify the mosaicity and threading dislocation (TD) densities at the p-i interfaces. Interestingly, the lowest screw-type dislocation density and highest edge-type dislocation density are observed for the “in-situ” GaN structure. The relationship between interfacial \([H]\), displaced Ga, and screw- and edge-type dislocations will be discussed.

*We gratefully acknowledge the support of ARPA-E through AWD0000191.
Influence of interfacial defects on the electronic states at GaN p-i-n diode interfaces

GUANJIE CHENG (Presenter), JIAHENG HE, ALEXANDRA ZIMMERMAN, DAVIDE DEL GAUDIO, Department of Materials Science and Engineering, University of Michigan, FABIAN NAAB, Michigan Ion Beam Laboratory, University of Michigan, MOHSEN NAMI, BINGJUN LI, JUNG HAN, Department of Electrical Engineering, Yale University, RACHEL GOLDMAN, Department of Materials Science and Engineering, University of Michigan — Although silicon-based electronics are used for light-emitting diodes and electric vehicles, their utility in high power applications is limited by a low breakdown voltage. A promising alternative is vertical GaN devices, but these require regrown active regions. Here, we report on the influence of regrowth processing steps on interfacial defects and their electronic signatures. A comparison of GaN p-i-n structures prepared with and without ex-situ ambient exposure and/or chemical etching reveals the highest interfacial near-band edge (NBE) and donor-acceptor pair (DAP) cathodoluminescence (CL) emission from the in-situ structures. Interestingly, elastic recoil detection analysis (ERDA) and Rutherford backscattering spectroscopy reveal the lowest interfacial [H] but the highest fraction of displaced Ga atoms, suggesting efficient incorporation of Mg$_{Ga}$. On the other hand, for the ex-situ structures, minimal interfacial [H] is observed, and the highest surface NBE and DAP CL emission is apparent. Finally, for the etched/regrown structures, ERDA reveals the highest interfacial [H], and significant yellow CL emission is observed. We will discuss relationships between interfacial [H], the fraction of displaced Ga atoms, CL emission features, and diode performance.

Study of carbon-related point defects in C-doped GaN using photo-induced electron paramagnetic resonance spectroscopy

SUBASH PAUDEL (Presenter), MARY ZVANUT, Univ of Alabama - Birmingham, MICHAL BOCKOWSKI, Institute for High Pressure Physics, Police Academy of Sciences — Incorporation of carbon impurities in GaN creates semi-insulating substrates. However, the role of carbon has not been fully understood. We used photo-induced electron paramagnetic resonance (EPR) to study point defects in mm thick free-standing 10$^{17}$-$10^{19}$ cm$^{-3}$ C-doped GaN. An isotropic signal at $g \approx 1.987$ was observed at 3.5 K with an intensity which increases with carbon concentration, indicating the signal represents a C-related defect. In $[C] < 6 \times 10^{17}$ cm$^{-3}$ samples, additional signals, a neutral donor with $g_{par}=1.951$ and $g_{per}=1.950$, and an anisotropic signal with $g_{par} \approx 2.121$, were observed. The intensity of the C-related and the donor signal start to increase at 2.75 eV and decrease at 0.95 eV. The same quenching threshold for C-related and donor signals suggests that 0.95 eV represents the energy required to excite an electron to C-related defects. The ionization threshold, 0.95 eV, is consistent with the predicted value for (-/0) transition level of C$_{N}$. The decrease in donors during quenching is one order of magnitude less than the decrease in C-related defects, which suggests the change in C-related defects is not solely controlled by the donor but also by other defects such as $g_{par} \approx 2.121$ defect.

The work at UAB was supported by the National Science Foundation, NSF/DMR 1606765.
Session G64 DMP: Strong Correlation, Competing Phases, and Spin-Orbit Interactions in Complex Oxide Heterostructures

11:15AM G64.00001: Electronic reconstruction at the interface of SrIrO$_3$ and SrRuO$_3$

JOCIENNE NELSON (Presenter), NATHANIEL SCHREIBER, Cornell University, ALEXANDRU BOGDAN GEORGESCU, Center for Computational Quantum Physics, Flatiron Institute, BERIT GOODGE, CYRUS ZELEDON, LENA FITTING KOURKOUTIS, Cornell University, ANDREW MILLIS, ANTOINE GEORGES, Center for Computational Quantum Physics, Flatiron Institute — The interface between SrIrO$_3$ and SrRuO$_3$ has been the focus of much attention due to reports of emergent phenomena including the topological Hall effect and magnetic skyrmions. However, due to the presence of electron correlations, strong spin orbit interactions, and ferromagnetism, the electronic structure of the interface is challenging to predict and understand. Here we employ a combination of oxide molecular-beam epitaxy, in situ angle-resolved photoemission spectroscopy, scanning transmission electron microscopy, and density functional theory to investigate heterostructures of SrIrO$_3$/SrRuO$_3$. We perform a systematic investigation of the electronic structure of (SrIrO$_3$)$_n$(SrRuO$_3$)$_{20}$, spanning n = 1 to 10 to investigate the electronic reconstruction as a function of distance from the interface.

11:27AM G64.00002: Breaking Symmetries to Create a Robust Room-Temperature Ferrimagnetic Ferroelectric in LuFeO$_3$/CoFe$_2$O$_4$ Superlattices [Invited]

DARRELL SCHLOM (Presenter), Materials Science and Engineering, Cornell University — Materials that exhibit simultaneous order in their electric and magnetic ground states hold tremendous promise for use in next-generation, low-power memory and logic devices in which electric fields control magnetism. Such materials are, however, rare as a consequence of the competing requirements for ferroelectricity and magnetism, and until recently BiFeO$_3$ was the only material with this functionality at room temperature. Interface materials are a way to overcome these competing requirements, as was recently demonstrated for (LuFeO$_3$)$_m$/LuFe$_2$O$_4$ superlattices [J.A. Mundy et al. Nature 537 (2016) 523–527]. The rumpling imposed by the geometric ferroelectric hexagonal LuFeO$_3$ imposes a local distortion on the neighboring LuFe$_2$O$_4$—a distortion that removes the mirror symmetry that the LuFe$_2$O$_4$ layers would otherwise have. This breaking of symmetry enables the LuFe$_2$O$_4$ to become simultaneously ferrimagnetic and ferroelectric. This rumpling is distinct from strain engineering because no macroscopic strain is involved. In this presentation we extend this atomically engineered design methodology to LuFeO$_3$/CoFe$_2$O$_4$ superlattices producing a robust ground state that is simultaneously ferroelectric and ferrimagnetic at temperatures well above room temperature.

* The work reported was performed in collaboration with the groups of Elke Arenholz (Advanced Light Source, LBNL), Julie A. Borchers (NIST), Craig J. Fennie (Cornell), Lena F. Kourkoutis (Cornell), Steven A. McGill (National High Magnetic Field Laboratory), David A. Muller (Cornell), Julia A. Mundy (Harvard), Janice L. Musfeldt (University of Tennessee), Ramamoorthy Ramesh (UC Berkeley), William D. Ratcliff (NIST), Peter Schiffer (Yale), and Andreas Scholl (Advanced Light Source, LBNL).
12:03PM G64.00003: Metal-insulator transition and charge transfer in complex oxide heterostructures from DFT+DMFT  
SOPHIE BECK (Presenter), CLAUDE EDERER, Materials Theory, ETH Zurich — We study the interplay between several control mechanisms on the emerging functionalities of complex oxide thin films and heterostructures composed of different early transition metal oxides, including correlated metals, Mott insulators and band insulators, using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). We discuss several examples where factors, such as e.g. lattice mismatch-induced epitaxial strain, dimensional confinement, and multilayer engineering lead to modifications of structural as well as electronic properties, that give rise to a variety of phases not present in the corresponding bulk compounds.

In particular, we address multilayers composed of materials that share the same B-site atom, such as, for example, LaVO3/SrVO3 and LaTiO3/CaTiO3, where the electronegativity difference leads to charge transfer from the higher valent to the lower valent transition metal cation, rendering the interface to be more metallic than the bulk constituents on a length scale of few unit cells in good agreement with experimental results. We draw a conceptual comparison to other types of heterostructures and give an overview on interface effects in early transition metal oxides.

12:15PM G64.00004: Long-range magnetic reconstruction of J_\text{eff} = 1/2 pseudospins in Sr_2IrO_4 via 5d-4d interfacial interactions with Sr_2RuO_4  
MARYAM SOURI (Presenter), University of Kentucky, CHRISTOPHER DIETL, Argonne National Laboratory, EKATERINA PAERSCHKE, University of Alabama at Birmingham, GABRIEL A CALDERON ORTIZ, The Ohio State University, SUJAN SHRESTHA, University of Kentucky, JINWOO HWANG, The Ohio State University, GANG CAO, University of Colorado at Boulder, JONG WOO KIM, JUNG HO KIM, Argonne National Laboratory, AMBROSE SEO, University of Kentucky — Sr_2IrO_4 has attracted attention for its relativistic Mott insulating states originating from strong spin-orbit coupling (SOC) and electron-correlation. The strong SOC in iridates entangles the magnetic moments and orbital degrees of freedom, making the system sensitive to external stimuli.

We report the magnetic properties of Sr_2IrO_4 driven by 5d-4d interfacial interactions with Sr_2RuO_4. We have synthesized Sr_2IrO_4 thin films on Sr_2RuO_4 single crystal substrates by pulsed laser deposition. This heterostructure has never been studied before. We have observed the magnetic properties of this heterostructure are distinct from Sr_2IrO_4 thin-films under similar strain (-0.5 %) and Sr_2IrO_4 bulk crystals. Resonant inelastic x-ray scattering has revealed an anisotropic softening of magnetic excitations in the Sr_2IrO_4/Sr_2RuO_4, where the modified magnon dispersion indicates enhanced longer-range interactions between the J_\text{eff} = 1/2 pseudospins of Sr_2IrO_4. Note that this long-range magnetic reconstruction occurs throughout the entire Sr_2IrO_4. Our results imply the strong interfacial interactions between 5d iridates and 4d ruthenates. The approach of synthesizing epitaxial thin films on unconventional single crystal substrates opens a new direction of studying strongly correlated systems.
12:27PM G64.00005: Effect of Misfit Dislocation in SrIrO$_3$ heterostructures* ZHEN WANG (Presenter), DAVID A HOWE, PRAHALD SIWAKOTI, MOHAMMAD SAGHAYEZHIAN, Louisiana State University, Baton Rouge, YIMEI ZHU, Brookhaven National Laboratory, E WARD PLUMMER, JIANDI ZHANG, Louisiana State University, Baton Rouge — Iridates benefit from a large spin-orbit coupling where the Ir-O bond geometry strongly impacts both electronic and magnetic properties leading to topologically non-trivial spin textures. The coupled spin and charge combined with interface engineering provides a unique opportunity to harvest the expected magnetoelectric coupling in BaTiO$_3$ (BTO)/ SrIrO$_3$ (SIO) superlattices where induced non-centrosymmetricity is present. A clear picture of the microstructures at interface is required for understanding the intrinsic structure-property relationship. By using scanning/transmission electron microscopy, we studied the structural feature of the BTO/SIO superlattices on SrTiO$_3$ (001) substrate. Misfit dislocations are found in the superlattices to compensate the large lattice parameter and octahedra rotation mismatch between BTO and SIO. Due to the gradual relaxation of mismatch strain, the density of the misfit dislocation changes as a function of the superlattice thickness, and it almost disappears under a certain thickness. Moreover, the effect of the misfit dislocation on the magnetic property will also be discussed.

*Supported by the US Department of Energy (DOE) under Grant No. DOE DE-SC0002136.

12:39PM G64.00006: Nanophotonic Engineering of Reconfigurable Vanadium Dioxide Phases* DUSTIN SCHRECONGOST, YINXIAO Xiang, West Virginia University, HAI-TIAN ZHANG (Presenter), ROMAN ENGEL-HERBERT, Penn State Univ, CHENG CEN, West Virginia University — The metal-insulator transition in VO$_2$ has extended applications in active optoelectronics and metasurfaces. Recently we have shown that by using scanning probe lithography techniques, various insulating and metallic VO$_2$ phases can be manipulated on-demand in nanoscale. Here we study the plasmonic properties of a room-temperature monoclinic metal phase of VO$_2$ and explore planar structure designs for desired optical functionalities. As a proof of concept, reconfigurable optical polarizers and plasmonic spatial modulators have been demonstrated. These results showcase the potential of building programmable nanophotonic devices on a monolithic correlated material platform.

*Experimental work at West Virginia University was supported by the Department of Energy Grant No. DE-SC-0010399 and National Science Foundation Grant No. NSF-1454950. The work at Pennsylvania State University was supported by the National Science Foundation through Grant No. DMR-1352502 and the Penn State MRSEC program DMR-1420620.
12:51PM G64.00007: Characteristic Lengths of Interlayer Charge-Transfer in Correlated Oxide Heterostructures*  
GANESH JI OMAR (Presenter), ARIANDO ARIANDO, Natl Univ of Singapore — Electronic devices in the form of high mobility conducting channel with charge carriers can be regulated through the internal charge transfer or chemical doping. Here, we demonstrate the effect of a crystalline LaFeO$_3$ buffer layer on amorphous and crystalline LaAlO$_3$/SrTiO$_3$ heterostructures with a different characteristic length of interlayer charge transfer. The LaFeO$_3$ buffer layer acts as an energetically favored electron acceptor in both LaAlO$_3$/SrTiO$_3$ systems, resulting in modulation of interfacial carrier density and hence metal-to-insulator transition. Such different critical LaFeO$_3$ thicknesses are explained in terms of distinct characteristic lengths of the redox-reaction-mediated and polar-catastrophe-dominated charge transfer, controlled by the interfacial atomic contact and Thomas-Fermi screening effect, respectively. Our results not only shed light on the complex interlayer charge transfer across oxide heterostructures but also establish a new route to precisely tailor the charge-transfer process at a functional interface by atomically engineered buffer layers.

*This research is supported by the Agency for Science, Technology and Research (A*STAR), National University of Singapore (NUS) and the Singapore National Research Foundation (NRF).

1:03PM G64.00008: Synthesis and characterization of freestanding Sr$_2$IrO$_4$ epitaxial thin films  
SUJAN SHRESTHA (Presenter), MARYAM SOURI, MATTHEW COILE, Department of Physics and Astronomy, University of Kentucky, JIWOONG KIM, Department of Physics, Pusan National University, JOHN G CONNELL, Department of Physics and Astronomy, University of Kentucky, JONG WOO KIM, Advanced Photon Source, Argonne National Laboratory, AMBROSE SEO, Department of Physics and Astronomy, University of Kentucky — Mott insulating states in Sr$_2$IrO$_4$ have attracted substantial interest due to the coexistence of strong spin-orbit interactions and electron correlation. To understand the effect of strain on Sr$_2$IrO$_4$, we have synthesized freestanding Sr$_2$IrO$_4$ epitaxial thin films. We have deposited Sr$_2$IrO$_4$ thin films on water-soluble Sr$_3$Al$_2$O$_6$ buffer layers$^1$ using pulsed laser deposition. XRD and RSM show that the Sr$_3$Al$_2$O$_6$ buffer layer is strained compressively and Sr$_2$IrO$_4$ thin films follow the in-plane lattice constants of the buffer layer. However, the width of rocking curve of freestanding Sr$_2$IrO$_4$ thin films is about three times greater than as-grown Sr$_2$IrO$_4$ thin films. Also, the in-plane lattice constants of freestanding Sr$_2$IrO$_4$ thin films are slightly larger than Sr$_2$IrO$_4$ single crystals, presumably due to the introduction of defects during delamination. The optical spectra of freestanding Sr$_2$IrO$_4$ thin films show the blue shift of $J_{\text{eff}} = \frac{1}{2}$ interband optical transitions compared to Sr$_2$IrO$_4$ thin films grown on SrTiO$_3$. The blueshift is consistent with the result of tensile strained Sr$_2$IrO$_4$ thin films.
Freestanding Sr$_2$IrO$_4$ thin films offer an opportunity to study their properties under large strain by combining with piezoelectric or mechanical devices.

1:15PM G64.00009: Epitaxial Growth of Perovskite Vanadates*  JASON HOFFMAN (Presenter), JENNIFER E. HOFFMAN, Harvard University — Perovskite vanadates have recently attracted significant attention for their wide-range of functional properties. Below around 140 K, LaVO$_3$ undergoes a structural transition, and becomes an orbitally ordered antiferromagnetic insulator. SrVO$_3$, on the other hand, is a strongly correlated paramagnetic metal. In this work, we use oxygen-plasma assisted molecular beam epitaxy (MBE) to deposit epitaxial LaVO$_3$ and SrVO$_3$ thin films on insulating SrTiO$_3$ substrates. We use *ex-situ* x-ray diffraction and magnetotransport measurements to compare the properties of (001) and (111)-oriented samples. We also discuss the behavior of LaVO$_3$ / SrVO$_3$ heterostructures, where above-room-temperature ferromagnetism has been reported and ferroelectricity has been predicted.

*This work supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319 and the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant No. GBMF4536.

1:27PM G64.00010: Metal-Insulator Transition in Strongly Correlated Quantum Confined SrVO$_3$ Superlattices*  ALYN JAMES (Presenter), Univ of Bristol, MARKUS AICHHORN, Institute of Theoretical and Computational Physics, Graz University of Technology, JUDE LAVEROCK, Univ of Bristol — Superlattices (such as SrVO$_3$/SrTiO$_3$) have many interesting physical phenomena influenced by orbital degeneracy, quantum confinement, interfaces and electron-electron correlations to name a few. The use of varying the number of SrVO$_3$ layers in superlattices gives a way to tune the strongly localized electron-electron correlations and the metal-insulator transition (MIT). These local correlations are beyond the predictive capabilities of standard density functional theory (DFT) calculations. Therefore, dynamical mean field theory (DMFT) needs to be used in conjunction with DFT (the DFT+DMFT method) to model these local correlations.

This talk will discuss our ongoing work on using the DFT+DMFT method to understand the fundamental electron correlation physics in previous experimental data of SrVO$_3$/SrTiO$_3$ superlattices. We investigate the effects on the correlated electron behavior of varying the thickness of SrVO$_3$ layers and propose a potential mechanism behind the MIT in these systems.

*A. D. N. J. gratefully acknowledges the financial support of the UK EPSRC (EP/L015544/1).
1:39PM G64.00011: Variable-temperature infrared microscopy of conducting oxide interfaces
STEFANO GARIGLIO (Presenter), WEIWEI LUO, MARGHERITA BOSELLI, JEAN-MARIE POUMIROL, IVAN ARDIZZONE, JEREMIE TEYSSIER, DIRK VAN DER MAREL, JEAN-MARC TRISCONE, ALEXEY B KUZMENKO, Univ of Geneva — Probing the local transport properties of two-dimensional electron systems confined at buried interfaces requires a non-invasive technique with a high spatial resolution. Using a scattering-type scanning near field optical microscopy, we study the conducting LaAlO$_3$/SrTiO$_3$ interface from room temperature down to 6 K [1]. We observe that the near-field optical signal is highly sensitive to the transport properties of the electron system. According to our model, such sensitivity originates from the interaction of the AFM tip with coupled plasmon–phonon modes.


1:51PM G64.00012: Direct imaging of the internal Bloch-components of polar-skyrmions and anti-hedgehogs in oxide heterostructures* YU-TSUN SHAO (Presenter), Applied and Engineering Physics, Cornell University, SUJIT DAS, Materials Science and Engineering, University of California, Berkeley, RUIJUAN XU, Applied Physics, Stanford University, SWATHI CHANDRIKA, Applied and Engineering Physics, Cornell University, HAROLD HWANG, Applied Physics, Stanford University, RAMAMOORTHY RAMESH, Materials Science and Engineering, University of California, Berkeley, DAVID ANTHONY MULLER, Applied and Engineering Physics, Cornell University — Emergent topological textures in ferroelectric heterostructures such as polar vortices and skyrmions has been the playground for exploring new phases and phenomena, exhibiting exotic functionalities including emergent chirality and local negative capacitance. These topologies can be realized in superlattices of (PbTiO$_3$)$_n$/(SrTiO$_3$)$_n$, either on a rigid substrate or fully lifted-off as 2D-like membranes. The electric analog of magnetic skyrmions, nm-scale polar-skyrmion bubbles, was recently observed yet their local dipole configurations and response to external stimuli are less explored. Results of electron diffraction-imaging show that the in-plane polarization curling direction is preserved (counter-clockwise, CCW) whether the skyrmion bubbles are elongated, merged, or broken apart under the perturbation of a focused electron probe. Furthermore, an ordered skyrmion square lattice appeared when heated to 373 K, in which a CCW curling dipole moment was surrounded by arrays of anti-hedgehogs and clockwise curling dipole moments.

*Research supported by AFOSR Hybrid Materials MURI (FA9550-18-1-0480), facilities support from the NSF (DMR-1429155, DMR-1719875).
2:03PM G64.00013: Self-doping in Sr2VO4/Sr2IrO4 superlattice*  YUHAO GU (Presenter), JIANGPING HU, Institute of Physics, Chinese Academy of Sciences, HANGHUI CHEN, Department of Physics, New York University Shanghai — Searching for high transition temperature superconductivity in non-cuprate materials has always been one of the focus topics in condensed matter physics. Theoretically, Sr2IrO4 has been proposed as a promising candidate to induce high Tc superconductivity because of the similarity of its electronic structure to that of cuprates [1]. Experimentally, surface-electron doped Sr2IrO4 exhibits spectroscopic signatures that are consistent with a superconducting gap but a zero-resistance state is yet to be found [2,3]. Here we artificially design a Sr2VO4/Sr2IrO4 superlattice, composed of VO2 layer and IrO2 layer alternating along the c-axis. Our ab initio calculations show that only V-dxy band and Ir-J=1/2 band cross the fermi level, forming a coupled two-dimensional Hubbard model with self-doping. The superlattice can be used as an effective way to electron dope iridates without introducing chemical disorder.


*H.C. acknowledges the funding of National Natural Science Foundation of China (Grant No. 11774236) and NYU University Research Challenge Fund.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G65 DMP: Defects and Dopants in Low Dimensional Materials
Mile High Ballroom 4F - Jinkyoung Yoo - Tag(s): Focus

11:15AM G65.00001: Covalent Quantum Defects of Carbon Nanotubes: A New Material for Quantum Information Science*  HAN HTOON (Presenter), Center for Integrated Nanotechnologies, Materials Physics and Applications Division, LOS ALAMOS NATL LAB — sp³ defects of single wall carbon nanotubes (SWCNTs), often referred to “organic color centers”,¹ are rapidly emerging as a new material system for chemistry, physics, materials science, engineering and quantum technologies. These defects are created via covalent bonding of organic functional groups to the sp² lattice of SWCNTs and display quantum mechanical properties in a way similar to color centers of solid state systems. In this talk, I will provide a brief over view on our recent accomplishments in understanding and controlling quantum optical properties of this new material system. Specifically, I will cover (1) unique molecularly tunable electronic structures of these covalent quantum defects², (2) demonstration of room temperature single photon emission at 1.55 µm telecommunication wavelength with 0.99 single photon purity,³ ⁴ and (3) single defect magneto PL experiment revealing hidden spin sensitive electronic fine structure states.

¹ Nat. Photon 11, 535 2017; ² Nat. Chem. 10, 1089 2018; ³ Nat. Photon. 11, 577 2017; ⁴ Nat. Mater. 17, 663 2018;

*This work was supported by DOE BES QIS infrastructure grant LANLBES22.
11:51AM G65.00002: Carrier recombination mechanisms at quantum point defects in wide band gap two-dimensional materials*  
TYLER SMART (Presenter), Physics, University of California, Santa Cruz, FENG WU, JUNQING XU, YUAN PING, Chemistry and Biochemistry, University of California, Santa Cruz — The identification and design of defects in two-dimensional (2D) materials as promising defect based qubits and single photon emitters requires a deep understanding of the underlying carrier recombination mechanisms. Yet, the dominant mechanism of carrier recombination at defects in 2D materials has not been well understood. In order to address these concerns, we developed first-principles methods to calculate the radiative and nonradiative recombination rates at defects in 2D materials, using h-BN as a prototypical example. We reveal the carrier recombination mechanism at defects in 2D materials being mostly dominated by defect-defect state recombination. In particular, we disentangle the nonradiative recombination mechanism into key physical quantities: the zero-phonon line and Huang-Rhys factor. At the end, we identified that strain can effectively tune the electron-phonon coupling at defect centers and drastically change the nonradiative recombination rates. This work serves as a general platform for understanding carrier recombination at defects in 2D materials, while providing pathways for engineering of quantum efficiency.


*This work is supported by NSF DMR-1760260 and DMR-1747426.

12:03PM G65.00003: Curvature-driven atomic localization and dipole alignment of quantum emitters in h-BN  
DONGGYU YIM (Presenter), MIHYANG YU, GICHANG NOH, JIEUN LEE, HOSUNG SEO, The Energy System, Ajou Univ — Hexagonal boron nitride (h-BN) has recently emerged as a promising materials platform for developing various solid-state quantum technologies. In particular, a number of color centers in h-BN have been found to be stable and bright single-photon-emitters (SPEs) operating at room temperature, which are crucial elements for quantum optical applications. In this talk, we combine first-principles theory and experiment to investigate the intimate relation between curvature in h-BN and atomic localization of SPEs. We use density functional theory to calculate the energetically stable configuration of various defect models of the SPEs in a buckled h-BN plane with different curvatures. We show that the vacancy-derived point defects in h-BN prefer to form in the highest-curvature area of the buckle and we find that the high curvature induces a dimer reconstruction for the atoms surrounding vacancy. Our result provides not only a microscopic understanding on the recent experimental observations of the SPEs being located in h-BN buckles but also strongly suggests that the atomic origin of the SPEs may be vacancy-derived. We also discuss several key features of the SPEs formed on h-BN buckle such as dipole orientation, which would be helpful to design future experiments of the SPEs in h-BN.
12:15PM G65.00004: Excitons and Radiative Lifetimes at Point Defects in Hexagonal Boron Nitride from First Principles* SHIYUAN GAO (Presenter), HSIAO-YI CHEN, MARCO BERNARDI, Caltech — Point defects in hexagonal boron nitride (hBN) have been recently investigated as promising single-photon emitters. Previous theoretical work has proposed candidate atomic structures for these localized emitters using density-functional theory (DFT) calculations, which focused on the defect formation energy, symmetry, and single-particle electronic transitions. Here, we use DFT plus the GW-Bethe-Salpeter equation method to compute the ground and excited states of a set of candidate hBN defect structures. Our calculations can predict the band gap, excitons and radiative lifetimes of the various defects, while including anisotropic dielectric screening and spin-orbit interaction effects. We show that the radiative lifetime can differ by orders of magnitude among different candidate structures, and it can be used as an effective physical quantity to rule out candidate defects. We analyze our results for the most promising structure, which exhibits energy and radiative lifetime in very good agreement with experiment. Through a statistical analysis, we comment on the likelihood that our calculations can successfully identify the structure behind the single-photon emitters observed experimentally.

*This work was supported by the Department of Energy under Grant No. DE-SC0019166.

12:27PM G65.00005: Ab initio theory of negatively charged boron vacancy qubit in hBN* VIKTOR IVÁDY (Presenter), GERGELY BARCZA, GERGŐ THIERING, Wigner Research Center for Physics, SONG LI, City University of Hong Kong, HANEN HAMDI, ÖRS LEGEZA, Wigner Research Center for Physics, JYH PIN CHOU, City University of Hong Kong, ADAM GALI, Wigner Research Center for Physics — Highly correlated orbitals coupled with phonons in two-dimension are identified for paramagnetic and optically active boron vacancy in hexagonal boron nitride by first principles methods which are responsible for recently observed optically detected magnetic resonance signal. We report on ab initio analysis of the correlated electronic structure of this center by density matrix renormalization group and Kohn-Sham density functional theory methods. By establishing the nature of the bright and dark states as well as the position of the energy levels, we provide a complete description of the magneto-optical properties and corresponding radiative and non-radiative routes which are responsible for the optical spin polarization and spin dependent luminescence of the defect. Our findings pave the way toward advancing the identification and characterization of room temperature quantum bits in two-dimensional solids.

Reference

Boron Dangling Bonds as Single Photon Emitters in Hexagonal Boron Nitride

MARK TURIANSKY (Presenter), University of California, Santa Barbara, AUDRIUS ALKAUSKAS, Center for Physical Sciences and Technology (FTMC), LEE BASSETT, University of Pennsylvania, CHRIS VAN DE WALLE, University of California, Santa Barbara — Defects in semiconductors are an attractive candidate to realize quantum information applications such as quantum computing and cryptography, as well as nanoscale sensing. Hexagonal boron nitride (h-BN) is a desirable host for these quantum defects due to its two-dimensional crystal structure, excellent stability, and wide band gap. Single-photon emission has been observed in h-BN from point defects in the lattice, but microscopic identification of the underlying defect has proved elusive. In this work, we employ hybrid density functional theory to demonstrate that the properties of boron dangling bonds are consistent with the experimental reports. Specifically, doubly occupied boron dangling bonds give rise to optical emission at 2.06 eV with a Huang-Rhys factor of 2.3. The emission is linearly polarized, with indirect excitation into the conduction band explaining the lack of dipole alignment seen in experiment. The boron dangling bond possesses a metastable triplet state, which can be used to realize spin-sensing applications.

This work is supported by NSF.

Influence of the environment on the coherence properties of spin-defects in low-dimensional solids and nanostructures: a computational study

MYKYTA ONIZHUK (Presenter), University of Chicago, MENG YE, Department of Physics, Tsinghua University, GIULIA GALLI, University of Chicago — Several recent studies have shown that in three-dimensional materials (e.g. diamond and SiC), at low temperature and in the presence of a large magnetic field, the central spin decoherence is mainly due to the fluctuating magnetic field induced by nuclear spin flip-flop transitions. Hence the interaction between electronic defects with the nuclear spin bath of the crystal is the dominant one in determining spin-defect decoherence times. However, in the case of two-dimensional (2D) and nanostructured semiconductors, the interaction with the environment, for example a supporting substrate, is expected to significantly affect spin-coherence times. We present a computational study aimed at understanding environmental effects on coherent lifetimes of spin-defects. We evaluated coherence functions using the Cluster Correlation Expansion method, and we computed the Hahn-echo $T_2$ time – an important metric for qubit performance – for spin defects in 2D transition metal di-chalcogenides [1] interacting with various substrates, and for nanodiamonds with different surface terminations.


This work was supported by the Center for Novel Pathways to Quantum Coherence in Materials, an Energy Frontier Research Center funded by DOE/BES.
1:03PM G65.00008: Carbon dimers as the source of 4.1 eV luminescence in hexagonal boron nitride*

MAZENA MACKOIT-SINKEVICIENE, Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania, MAREK MACIASZEK, Faculty of Physics, Warsaw University of Technology, Poland, CHRIS VAN DE WALLE (Presenter), University of California, Santa Barbara, AUDRIUS ALKAUSKAS, Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania — Hexagonal boron nitride (h-BN) is an exciting material for electronics and optoelectronics, as well as for quantum information applications. h-BN samples typically display bright luminescence with a zero-phonon line (ZPL) at 4.1 eV, and single-photon emission associated with this line has been observed. The source of the luminescence has been intensely debated, though there seems to be broad agreement that carbon is involved. We propose that the carbon dimer, C\textsubscript{B}–C\textsubscript{N}, gives rise to this ubiquitous narrow luminescence band. Such carbon dimers have actually been observed in transmission electron microscopy. Our first-principles calculations, based on hybrid density functional theory, show that the neutral state of the dimer is stable over a wide range of electron chemical potentials. The calculated ZPL energy, Huang-Rhys factor, and radiative lifetime are all close to the experimental values. The optical transition occurs between two localized π-type defect states, with the lower-lying state localized on C\textsubscript{N}, while the higher-lying state is localized on C\textsubscript{B}. We find the transition to be dipole allowed with polarization in the h-BN plane.

*Work supported by the Research Council of Lithuania, the EU’s Horizon 2020 Programme, and NSF.

1:15PM G65.00009: Gate-defined quantum dots in monolayer and bilayer WSe\textsubscript{2}: Part I, Fabrication*

JEB STACY (Presenter), SHIVA DAVARI DOLATABADI, ALEJANDRO MERCADO TEJERINA, JEREMY TULL, RABINDRA BASNET, KRISHNA PANDEY, MD NABI, Physics, Univ of Arkansas-Fayetteville, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, JIN HU, HUGH CHURCHILL, Physics, Univ of Arkansas-Fayetteville — Gate-defined quantum dots in monolayer and bilayer WSe\textsubscript{2} are a platform for novel quantum transport and quantum optoelectronic investigations of WSe\textsubscript{2}, as well as for potential applications in coherent valleytronics. In this presentation, we discuss design considerations and implementations for the fabrication of ~100 nm diameter gate-defined, p-type quantum dots in monolayer and bilayer WSe\textsubscript{2}. The devices were controlled using a combination of bottom confining gates and a top accumulation gate, with hBN used for gate insulation and encapsulation of the WSe\textsubscript{2}. Top hBN and WSe\textsubscript{2} were transferred onto Pt for reliable p-type bottom contact.

*We acknowledge support from AFOSR award FA-9550-16-1-0203
1:27PM G65.00010: Gate-defined quantum dots in monolayer and bilayer WSe$_2$: Part II, Measurement*  
SHIVA DAVARI DOLATABADI (Presenter), JEB STACY, ALEJANDRO MERCADO TEJERINA, JEREMY TULL, RABINDRA BASNET, KRISHNA PANDEY, MD NABI, Physics, Univ of Arkansas-Fayetteville, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, JIN HU, HUGH CHURCHILL, Physics, Univ of Arkansas-Fayetteville — Gate-defined quantum dots in monolayer and bilayer WSe$_2$ are a platform for novel quantum transport and quantum optoelectronic investigations of WSe$_2$, as well as for potential applications in coherent valleytronics. In this presentation, we discuss low-temperature electronic transport measurements of p-type gate-defined quantum dots in monolayer and bilayer WSe$_2$. These devices are operated with gates above and below the WSe$_2$ layer so that carriers are accumulated in the WSe$_2$, then selectively depleted to define the dot. We report observations of Coulomb blockade as well as excited state spectroscopy of confined holes in WSe$_2$ dots. 

*We acknowledge support from AFOSR award FA-9550-16-1-0203.

1:39PM G65.00011: A carbon dimer defect as a spin qubit candidate in hexagonal boron nitride: an ab-initio study  
JOOYONG BHANG (Presenter), DONGGYU YIM, Department of Energy Systems Research, Ajou University, Suwon, Gyeonggi 16499, Korea, HE MA, GIULIA GALLI, Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637, USA, HOSUNG SEO, Department of Energy Systems Research, Ajou University, Suwon, Gyeonggi 16499, Korea — Hexagonal boron nitride has been recently found to host a variety of quantum defects that are potentially useful for advancing solid-state quantum technologies. However, optically addressable spin quantum bits (qubits), such as the diamond NV center, have not yet been reported in h-BN. In this talk, we propose a carbon dimer(C$_2$) defect as a promising candidate of optically active spin qubit in h-BN. We use first-principles density functional theory to investigate its structural and electronic properties. We show that the C$_2$ defect features a non-zero spin ground state (S=1), arising from defect-induced deep levels in the band gap of the host material, and localized unpaired electrons. We calculate the defect formation energy of the C$_2$ defect and other C-related defects in h-BN and we show that the C$_2$ defect is energetically stable. To assist potential future experiments, we report the zero-phonon line, the zero-field splitting tensor, and the hyperfine tensor of the C$_2$ defect at various DFT levels of theory, including the HSE hybrid functional. Our study aimed at searching coherent spin qubits in h-BN can be potentially applied to a wide variety of other two-dimensional van der Waals materials systems.
1:51PM G65.00012: Ab initio design and control of quantum emitters in low-dimensional materials

CHITRALEEMA CHAKRABORTY (Presenter), CHRISTOPHER CICCARINO, PRINEHA NARANG, Harvard University — The formation of atomic defects is unavoidable in 2D materials with currently available growth techniques\(^1\). Nevertheless, a myriad of functionalities in modern optoelectronic and nanophotonic devices leverage quantum defects including the recent demonstration of single photon emitters in 2D materials\(^2\). In parallel, advances in scanning probe techniques provide opportunities to directly create, manipulate and characterize defects down to the atomic scale in 2D materials\(^3\). We predict optically active quantum defects in 2D transition metal dichalcogenides from first-principles. We will discuss the excited state defect configuration(s) and the corresponding electron-phonon interactions\(^4\) to quantify the optical efficiency of emitters via the Huang-Rhys factor. Our work presents a pathway for maximizing the optical efficiency of designer quantum emitters in low-dimensional systems and provides a deterministic choice for defect creation at the atomic scale\(^3\).


*This work was supported by DOE ‘Photonics at Thermodynamic Limits’ Energy Frontier Research Center under grant DE-SC0019140.

2:03PM G65.00013: Mie Resonant Dielectric Metastructure based Quantum Optical Circuits Integrated with Single Photon Source: A new paradigm for Quantum Information Processing

SWARNABHA CHATTARAJ (Presenter), JIEFEI ZHANG, Univ of Southern California, SIYUAN LU, IBM Thomas J. Watson Research Center, ANUPAM MADHUKAR, Univ of Southern California — Realization of scalable optical quantum information processing systems requires optical circuits built around on-chip single photon sources (SPS) in spatially regular arrays\(^1\) to provide the needed light manipulating functions of enhancement of SPS emission rate, control on emission directionality, guiding, splitting and recombining to enable on-chip controlled photon interference and entanglement. To this end we have introduced use of light manipulating units (LMU) based on metastructures of subwavelength dielectric building blocks in which a collective Mie mode provides all the above noted functions while eliminating mode mismatch between the components of the network, including the SPS\(^2\). In this talk we present FEM based simulation and design of such SPS-LMUs that result in two types of entanglement over large on-chip distances: (1) path-entanglement via interference of photons from distinct SPSs, and (2) emergence of coherence and entanglement via direct photon-mediated long-range coupling resulting in super-radiance with ~2-fold decay rate enhancement of the coupled SPSs\(^3\).


*Funded by ARO W911NF-15-1-0025
11:15AM G66.00001: Spin-triplet superconducting state in the nearly ferromagnetic compound UTe2 [Invited]  SHENG RAN (Presenter), University of Maryland, College Park — Our recent discovery of the novel spin-triplet superconductivity in UTe2 [1] has inspired a lot of interests in the community. Superconducting state of UTe2 closely resembles that of ferromagnetic superconductors, but the normal state is paramagnetic with no indication of magnetic ordering. Unusual properties of $H_c^2$, NMR Knight shift, and specific heat strongly indicate that the superconductivity in UTe2 is carried by spin-triplet pairs. Even more striking, superconductivity reenters in the magnetic field of 45 tesla and persists up to 65 tesla, reflect a new kind of exotic superconductivity rooted in magnetic fluctuations and quantum dimensionality [2]. Application of pressure reveals a two-fold enhancement of this unusual superconductivity, which is closely related to the suppression of Kondo coherence [3]. In this talk, I will review our recent results on UTe2.


11:51AM G66.00002: Field- and pressure-induced phenomena in novel spin-triplet superconductor UTe2* [Invited]  DAI AOKI (Presenter), Tohoku Univ — We present our recent results on the novel spin-triplet superconductor UTe2, which is at the verge of the ferromagnetic order. The huge upper critical field exceeding the Pauli limit indicates the spin-triplet state. For the field along b-axis, the field reentrant superconductivity is observed up to $H_m \sim 35$T, where the first order metamagnetic transition occurs. The field reentrant superconductivity in UTe2 is similar to that observed in ferromagnetic superconductors, namely URhGe and UCoGe. Applying the pressure in UTe2, the superconducting transition temperature splits and the mulitple superconducting phase is detected in the AC calorimetry measurements. We overview the results on UTe2 comparing with ferromagnetic superconductors, and show our perspective. This work was done in collaboration with G. Knebel, A. Pourret, J.P. Brison, D. Braithwaite, Q. Niu, M. Valiska, J. Flouquet, A. Nakamura, F. Honda, Y. Homma, D.XLi, Y. Shimizu, Y. J. Sato, A. Miyake, S. Imajo, S. Kohama, M. Tokunaga, H. Harima, W. Knafo, I. Sheikin, C. Paulsen, Y. Tokunaga, S. Kambe, H. Sakai, S. Fujimori, K. Ishida, G. Nakamine, S. Kitagawa.

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TRISTIN METZ (Presenter), SEOKJIN BAE, Center for Quantum Materials, University of Maryland, SHENG RAN, I-LIN LIU, NIST Center for Neutron Research, YUN SUK EO, WESLEY T FUHRMAN, Center for Quantum Materials, University of Maryland, DANIEL AGTERBERG, Physics, University of Wisconsin, Milwaukee, STEVEN ANLAGE, Center for Quantum Materials, University of Maryland, NICHOLAS BUTCH, NIST Center for Neutron Research, JOHNPIERRE PAGLIONE, Center for Quantum Materials, University of Maryland — Low-temperature electrical and thermal transport, magnetic penetration depth, and heat capacity measurements were performed on single crystals of the actinide superconductor UTe$_2$ ($T_c$=1.6K) to determine the structure of the superconducting energy gap. Heat transport measurements performed with currents directed along both crystallographic a- and b-axes reveal a vanishingly small residual fermionic component of the thermal conductivity. The magnetic field dependence of the residual term follows a quasi-linear increase consistent with the presence of nodal quasiparticles, rising rapidly toward the a-axis upper critical field where the Wiedemann-Franz (WF) law is recovered. Together with a quadratic temperature dependence of the magnetic penetration depth up to $T/T_c$= 0.3, these measurements provide evidence for an unconventional spin-triplet superconducting order parameter with point nodes positioned along the crystallographic a-axis. Millikelvin specific heat measurements reveal an upturn below 300 mK that is well described by a divergent quantum-critical contribution to the density of states (DOS). Modeling this contribution with a $T^{-1/3}$ power law allows restoration of the full entropy balance in the superconducting state and reveals a perfect $T^3$ power law for the electronic DOS below $T_c$ which is consistent with the point nodal gap structure determined by thermal conductivity and penetration depth measurements.
1:03PM G66.00004: Electronic band structure of triplet superconductor UTe₂ from angle resolved photoemission spectroscopy* [Invited] L. ANDREW WRAY (Presenter), New York Univ NYU, LIN MIAO, Southeast University, SHOUZHENG LIU, YISHUAI XU, ERICA KOTTA, New York Univ NYU, SHENG RAN, NIST Center for Neutron Research, JOHNPIERRE PAGLIONE, Univ of Maryland-Colege Park, JONATHAN DENLINGER, Lawrence Berkeley National Laboratory, NICHOLAS BUTCH, NIST Center for Neutron Research — The compound UTe₂ has recently been shown to realize spin triplet superconductivity from a non-magnetic normal state. This has sparked intense research activity, including theoretical analyses that suggest the superconducting order parameter to be topologically nontrivial. However, the underlying electronic band structure is a critical factor for these analyses, and remains poorly understood. I will present high resolution angle resolved photoemission (ARPES) measurements covering multiple planes in the 3D Brillouin zone of UTe₂, revealing distinct Fermi pockets from two light electron bands and one heavy band. Electronic symmetries and many-body ordering instabilities will be discussed in comparison with numerical simulations.

*This research used resources of the Advanced Light Source, which is a DOE Office of Science User Facility under contract no. DE-AC02-05CH11231. Work at NYU was supported by the MRSEC Program of the National Science Foundation under Award Number DMR-1420073. Synthesis and analysis instrumentation at NYU is supported by NSF under MRI-1531664, and by the Gordon and Betty Moore Foundation’s EPIQS Initiative through Grant GBMF4838. This work was supported by the Gordon and Betty Moore Foundation’s EPIQS Initiative through Grant GBMF4419 (synthesis), and the Maryland Center for Nanophysics and Advanced Materials.

1:39PM G66.00005: Coexistence of ferromagnetic fluctuations and superconductivity in the actinide superconductor UTe₂* [Invited] JEFF SONIER (Presenter), Simon Fraser Univ — We report low-temperature muon spin relaxation/rotation (μSR) measurements on single crystals of the actinide superconductor UTe₂. Below 5 K, we observe a continuous slowing down of magnetic fluctuations that persists into the superconducting state, but find no evidence of long-range or local magnetic order down to millikelvin temperatures. The temperature dependence of the dynamic relaxation rate is consistent with spin fluctuations for a three-dimensional weak itinerant ferromagnetic metal, and suggests UTe₂ is close to a ferromagnetic quantum critical point. Our μSR results also indicate that the superconductivity coexists with the magnetic fluctuations and similar to other actinide-based superconductors, UTe₂ has a very low superfluid density.

*Acknowledged support from NSERC of Canada, DOE, Office of Basic Energy Sciences, the Gordon and Betty Moore Foundation’s EPIQS Initiative & NIST.

Tuesday, March 3, 2020 11:15 AM - 2:15 PM

Session G67 DCMP: Quantum Valley Hall Edge Channels: Highways for Electrons, Photons, and Surface Plasmons Four Seasons 2-3 - Long Ju, Massachusetts
11:15AM G67.00001: Topological valleytronics using kink states in bilayer graphene: a valley valve and beam splitter [Invited] JING LI (Presenter), Los Alamos National Laboratory — Two-dimensional honeycomb lattices possess a valley degree of freedom, the control of which offers opportunities to realize topologically protected edge modes to transport electrons without dissipation, and potentially contribute to new paradigms of electronics, namely valleytronics. In this talk, I will describe how we realize valley-momentum locked topological 1D channels, i.e. quantum valley Hall kink states, at internal line boundaries of two artificial domains of Bernal stacked bilayer graphene with opposite band gaps via asymmetrical gating [1]. These kink states possess mean free path of a few µm at B=0, and their helicity (±1) can be conveniently controlled by changing the gating polarity. In an all electrically defined “cross” device with 4 channels, I will demonstrate reconfigurable ballisitic waveguides of the kink states, and valleytronic operations such as valley valve and electron beam splitter that exploit topological protection [2]. Kink states can ballistically transmit through two channels with aligned helicity (on state), while get blocked between channels with opposite helicity (off state). The on/off ratio reaches 800% at B=0, and it doesn't require valley-polarized current to operate, instead relying on the control of topology. In a B-field, Fermi energy becomes a knob to continuously tune the current splitting ratio of kink states in two propagation directions, resembling the function of a quantum point contact for quantum Hall edge states. The versatile control and potential scalability of the kink states open the door to many exciting possibilities in low dimensional topological applications.


11:51AM G67.00002: Polaritons in Moire Superlattices of Graphene and Boron Nitride [Invited] DMITRI BASOV (Presenter), Physics, Columbia University — Electronic properties of graphene can be drastically altered when it is laid upon another graphene layer, resulting in a moiré superlattice. The relative twist angle between the two layers is a key tuning parameter of the interlayer coupling in thus-obtained twisted bilayer graphene (TBG). We studied the propagation of plasmon polaritons in TBG by infrared nano-imaging. The atomic reconstruction occurring at small twist angles transforms the TBG into a network of conducting channels that act as efficient reflectors of plasmon polaritons. The analysis of plasmonic images allows one to infer the conductivity of the domain walls in moire superlattices. TBG at small twist angles effectively acts a natural plasmon photonic crystal for propagating nano-light. We observed similar nano-optical effects in other twisted van der Waals crystals including hexagonal boron nitride. In hBN, domain walls modify the response of phonon polaritons.
12:27PM G67.00003: Topological photonics: slow light and solitons* [Invited] MIKAEL RECHTSMAN (Presenter), SEBABRATA MUKHERJEE, JONATHAN GUGLIELMON, Pennsylvania State University — In this talk we will describe the realization of chiral edge states for photons in a photonic Floquet topological insulator, employing optical waveguide arrays. We will describe how such topological states can be used to simultaneously overcome two shortcomings of slow-light systems, namely disorder-induced scattering (and Anderson localization) as well as low bandwidth. We will show how optical nonlinearity can be used to realize Gross-Pitaevskii-type interactions, and a resulting soliton that spectrally resides in a topological band gap.

*M. C. R. acknowledges the National Science Foundation under Grant No. ECCS-1509546, the Charles E. Kaufman Foundation (a supporting organization of the Pittsburgh Foundation) and the Office of Naval Research under YIP program, Grant No. N00014-18-1-2595.

1:03PM G67.00004: The electron thickness of graphene [Invited] KLAUS ENSSLIN (Presenter), ETH Zurich — The van-der-Waals stacking technique enables the fabrication of heterostructures, where two conducting layers are atomically close. In this case, the finite layer thickness matters for the interlayer electrostatic coupling. Here we investigate the electrostatic coupling of two graphene layers, twisted by 22 degrees such that the layers are decoupled by the huge momentum mismatch between the K and K' points of the two layers. We observe a splitting of the zero-density lines of the two layers with increasing interlayer energy difference. This splitting is given by the ratio of single-layer quantum capacitance over interlayer capacitance C and is therefore suited to extract C. We explain the large observed value of C by considering the finite dielectric thickness d of each graphene layer and determine d=2.6 Angstrom. In a second experiment we map out the entire density range with a Fabry-Pérot resonator. We can precisely measure the Fermi-wavelength in each layer, showing that the layers are decoupled. We find that the Fermi wavelength exceeds 600nm at the lowest densities and can differ by an order of magnitude between the upper and lower layer. These findings are reproduced using tight-binding calculations.

This work was done in collaboration with Peter Rickhaus, Ming-Hao Liu, Marcin Kurpas, Annika Kurzmann, Yongjin Lee, Hiske Overweg, Marius Eich, Riccardo Pisoni, Takashi Tamaguchi, Kenji Wantanabe, Klaus Richter, and Thomas Ihn

1:39PM G67.00005: Atomic and electronic reconstruction at van der Waals interface in twisted 2-D materials [Invited] HYOBIN YOO (Presenter), Sogang University — Controlling the interlayer twist angle in two-dimensional (2-D) van der Waals (vdW) heterostructures offers an experimental route to create moire superlattices. One can realize exotic electronic states by adjusting the width of the electronic bands with a tunable moire length scale. However, in the small twist angle regime, vdW interlayer interaction can cause significant structural reconfiguration at the interface, creating the arrays of domain structures. In this talk, we will discuss the atomic reconstruction at twisted vdW interfaces and its effect on electronic structure and electrical transport behavior. Moreover, one can tune the domain topology at the reconstructed interface using 2-D vdW crystals that has lower symmetry. We will discuss the connection between crystal symmetry and tunable domain topology.
Session G68 DQI: Superconducting Qubit Quantum Simulation and Algorithms

11:15AM G68.00001: Quantum Supremacy: Benchmarking the Sycamore Processor [Invited]
KEVIN SATZINGER (Presenter), Google Inc - Santa Barbara — The promise of quantum computers is that certain computational tasks might be executed exponentially faster on a quantum processor than on a classical processor. A fundamental challenge is to build a high-fidelity processor capable of running quantum algorithms in an exponentially large computational space. Here we report the use of a processor with 53 programmable superconducting qubits. In our Sycamore processor, each qubit interacts with four neighbors in a rectangular lattice using tunable couplers. A key systems engineering advance of this device is achieving high-fidelity single- and two-qubit operations, not just in isolation but also while performing a realistic computation with simultaneous gate operations across the entire processor. We benchmark the Sycamore processor using cross-entropy benchmarking, a scalable method to evaluate system performance. Our largest system benchmarks feature circuits that are intractable for classical hardware, culminating in the demonstration of quantum supremacy. Furthermore, the fidelities from full-system benchmarks agree with what we predict from individual gate and measurement fidelities, verifying the digital error model and presenting a path forward to quantum error correction.

Nature 574, 505-510 (2019)

11:51AM G68.00002: Quantum supremacy using the Sycamore processor
CHARLES NEILL (Presenter), Google Inc - Santa Barbara — The promise of quantum computers is that certain computational tasks might be executed exponentially faster on a quantum processor than on a classical processor. A fundamental challenge is to build a high-fidelity processor capable of running quantum algorithms in an exponentially large computational space. Recently, our team has demonstrated a dramatic speedup relative to all known classical algorithms providing an experimental realization of quantum supremacy on a computational task. In this talk, I will focus on the hardware details of the Sycamore processor and how this device enabled supremacy-quality two-qubit gates.
Electromagnetic fields possess zero point fluctuations (ZPF) which lead to observable effects such as the Lamb shift and the Casimir effect. In the traditional quantum optics domain, these corrections remain perturbative due to the smallness of the fine structure constant. To provide a direct observation of non-perturbative effects driven by ZPF in an open quantum system we wire a highly non-linear Josephson junction to a high impedance transmission line, allowing large phase fluctuations across the junction. Consequently, the resonance of the former acquires a relative frequency shift that is orders of magnitude larger than for natural atoms. Detailed modelling confirms that this renormalization is non-linear and quantum. Remarkably, the junction transfers its non-linearity to about 30 environmental modes, a striking back-action effect that transcends the standard Caldeira-Leggett paradigm. This work opens many exciting prospects for longstanding quests such as the tailoring of many-body Hamiltonians in the strongly non-linear regime, the observation of Bloch oscillations, or the development of high-impedance qubits.

*The speaker thanks the ANR-16-CE24-0005, ANR-14-CE26-0018, ANR-15-IDEX-02 and the CFM foundation
Quantum simulation in circuit QED: Observation of quantum many-body effects due to zero point fluctuations - II: Experiment*  

SEBASTIEN LEGER (Presenter), JAVIER PUERTAS, KARTHIK SRIKANTH BHARADWAJ, REMY DASSONVILLE, JOVIAN DELAFOREST, FARSHAD FOROUGHI, VLADIMIR MILCHAKOV, LUCA PLANAT, OLIVIER BUISSON, CÉCILE NAUD, WIEBKE GUICHARD, SERGE FLORENS, Institut Neel, IZAK SNYMAN, Wits University, NICOLAS ROCH, Institut Neel — Electromagnetic fields possess zero point fluctuations (ZPF) which lead to observable effects such as the Lamb shift and the Casimir effect. In the traditional quantum optics domain, these corrections remain perturbative due to the smallness of the fine structure constant. To provide a direct observation of non-perturbative effects driven by ZPF in an open quantum system we wire a highly non-linear Josephson junction to a high impedance transmission line, allowing large phase fluctuations across the junction. Consequently, the resonance of the former acquires a relative frequency shift that is orders of magnitude larger than for natural atoms. Detailed modelling confirms that this renormalization is non-linear and quantum. Remarkably, the junction transfers its non-linearity to about 30 environmental modes, a striking back-action effect that transcends the standard Caldeira-Leggett paradigm. This work opens many exciting prospects for longstanding quests such as the tailoring of many-body Hamiltonians in the strongly non-linear regime, the observation of Bloch oscillations, or the development of high-impedance qubits.

*The speaker thanks the ANR-16-CE24-0005, ANR-14-CE26-0018, ANR-15-IDEX-02 and the CFM foundation.

Analog quantum simulation of a Kondo impurity with superconducting circuits  

NICHOLAS GRABON (Presenter), ROMAN KUZMIN, NITISH JITENDRAKUMAR MEHTA, University of Maryland, College Park, MOSHE GOLDSTEIN, Tel Aviv University, VLADIMIR MANUCHARYAN, University of Maryland, College Park —

A particular quantum simulator can be used to access the many body properties of the Kondo problem [1]. We created the first experimental realization of this quantum simulator. The simulator is comprised of a high impedance Josephson junction waveguide connected to a fluxonium qubit at its end. The fluxonium hosts a fluxon mode that can be far detuned from any of the other transitions. It can thus be considered as a two level system that then acts as the spin in the simulated Kondo model. This spin couples to a continuum of modes in the waveguide, which acts as the bath, thus completing the model. We study the spectra of inelastic and elastic scattering of the waveguide photons which are expected to reveal the many body correlation functions of the Kondo model.

12:39PM G68.00006: Simulating a Dirac particle with coupled transmon circuits* ELISHA SVETITSKY (Presenter), NADAV Y KATZ, Hebrew University of Jerusalem — The core concept of quantum simulation is the mapping of an inaccessible quantum system onto a controllable one by identifying analogous dynamics. We map the Dirac equation of relativistic quantum mechanics in 3+1 dimensions onto a multi-level superconducting Josephson circuit. Resonant drives determine the particle mass and momentum and the quantum state represents the internal spinor dynamics, which are cast in the language of multi-level quantum optics. The degeneracy of the Dirac spectrum corresponds to a degeneracy of bright/dark states within the system and particle spin and helicity are employed to interpret the multi-level dynamics. We simulate the Schwinger mechanism of electron-positron pair production by introducing an analogous electric field as a doubly degenerate Landau-Zener problem. All proposed measurements can be performed well within typical decoherence times. This work opens a new avenue for experimental study of the Dirac equation and provides a tool for control of complex dynamics in multi-level systems.

*This work is supported by the European Research Council Project No. 335933.

12:51PM G68.00007: Quantum Simulation of Hyperbolic Space with Circuit Quantum Electrodynamics: From Graphs to Geometry* IGOR BOETTCHER (Presenter), PRZEMYSLAW BIENIAS, RON BELYANSKY, ALICIA KOLLAR, Joint Quantum Institute, University of Maryland, College Park, MD 20742, USA, ALEXEY V GORSHKOV, Joint Center for Quantum Information and Computer Science, NIST/University of Maryland, College Park, MD 20742, USA — We give a quantum field theoretic perspective on recent breakthrough experiments in circuit quantum electrodynamics, where hyperbolic lattices are realized with superconducting resonators and photons are tricked into believing that space is hyperbolic. We show how these finite lattice geometries can be mapped onto quantum field theories in continuous negatively curved space. We use this as a computational tool to quantitatively reproduce ground state energy, spectral gap, and correlation functions of the noninteracting lattice system by means of analytic formulas on the Poincare disk, and show how conformal symmetry emerges for large lattices. I will discuss how interaction effects can be induced by coupling qubits to the hyperbolic lattice. This sets the stage for studying interactions and disorder on hyperbolic graphs, and to resolve fundamental open problems at the interface of interacting many-body systems, quantum field theory in curved space, and quantum gravity using tabletop experiments.

*This work was supported by DoE BES Materials and Chemical Sciences Research for Quantum Information Science program, NSF Ideas Lab on Quantum Computing, DoE ASCR Quantum Testbed Pathfinder program, ARO MURI, ARL CDQI, NSF PFC at JQI, NSERC, and FRQNT.
Demonstration of programmable quantum simulations of lattice models using a superconducting parametric cavity

JAMAL BUSNAINA (Presenter), JIMMY SHI-HUN HUNG, M.V. MOGHADDAM, CHUNG WAI SANDBO CHANG, A.M. VADIRAJ, Institute for Quantum Computing and Department of Electrical Engineering, University of Waterloo, HADISEH ALAEIAN, Physikalisches Institut, Universität Stuttgart, ENRIQUE RICO, Department of Physical Chemistry, University of the Basque Country, C.M. WILSON, Institute for Quantum Computing and Department of Electrical Engineering, University of Waterloo — There has been a growing interest in realizing quantum simulators for important physical systems where perturbative methods are ineffective. The scalability and flexibility of circuit quantum electrodynamics (cQED) make it a promising platform for implementing various types of simulators, including lattice models of strongly-coupled field theories. With this in mind, we use a multimode superconducting parametric cavity to create programmable lattices of bosonic modes by parametrically pumping at mode-difference frequencies. The choice of pump frequencies allows changing the graph of the lattice in situ. Further, the resulting hopping terms induced between the modes can be made complex by controlling the relative phases of the parametric drives. This enables us to study a wide variety of interesting lattice models. For instance, controlling the total loop phase in closed plaquettes allows us to simulate the motion of particles in a static gauge field, including producing nonreciprocal transport. The system can also realize models with topological features such as the bosonic Creutz ladder. In this talk, we present experimental results on a variety of different small lattice models.

Quantum simulation of a spin chain with superconducting circuits

QUENTIN FICHEUX (Presenter), AARON SOMOROFF, NITISH JITENDRAKUMAR MEHTA, ROMAN KUZMIN, University of Maryland, College Park, IVAR MARTIN, Argonne National Laboratory, MAXIM G VAVILOV, University of Wisconsin-Madison, VLADIMIR MANUCHARYAN, University of Maryland, College Park — An Ising chain is one of the simplest many-body systems to exhibit a quantum phase transition. In the presence of a transverse field and disorder, this model produces a rich variety of non integrable ground states giving rise to exotic phase transitions including many body localization and Anderson localization.

Initial experimental efforts to simulate this model have focused on cold atoms [1] and trapped ion systems [2,3] with limited coupling strength imposed by the laws of nature. Our experiment uses an artificial spin chain made of highly anharmonic fluxonium qubits [4] arranged on a lattice and coupled to one another by mutual inductance. While the transverse magnetic field and on-site energy can be tuned in situ, disorder and coupling strength can be adjusted at will by microfabrication enabling us to reach unprecedented parameter regimes.

A deeper understanding of the competition and resulting transitions between phases of matter could provide insights into the properties of complex materials and more generally into the many-body physics of quantum systems.

1:27PM G68.00010: Growth and preservation of entanglement in a many-body localized system  
BEN CHIARO (Presenter), University of California, Santa Barbara, BROOKS FOXEN, MATTHEW MCEWEN, JOHN M MARTINIS, AI Quantum, Google — 
We use programmable superconducting qubit quantum processors to provide a detailed survey of the many-body localized (MBL) phase for both 1D and 2D lattice geometries. We demonstrate disorder induced ergodicity breaking by studying the transport properties of excitations as the system evolves under a Bose-Hubbard Hamiltonian. Further, we use interferometric techniques to establish effective non-local interactions in our localized system. Beyond demonstrating these defining features of MBL we directly observe the slow growth of von Neumann entanglement entropy. From density matrix measurements we also compute the entanglement of formation and use this information to provide a spatial and temporal map of entanglement. Finally, starting with a maximally entangled Bell state embedded in an MBL environment, we measure the capability of an MBL system to preserve this quantum correlation and characterize its degradation in response to a remote excitation.

1:39PM G68.00011: Approximating finite-temperature dynamic correlation functions on quantum computers  
JEFFREY COHN (Presenter), IBM Research-Almaden, KHADIJEH NAJAFI, Virginia Tech, BARBARA JONES, IBM Research-Almaden, JAMES FREERICKS, Georgetown University — Dynamic correlation functions such as single particle Green's functions, linear response functions, or dynamical susceptibilities serve as a foundational tool kit for studying strongly correlated quantum systems. Ideally, a quantum computer will be able to extract these functions for systems sizes that are intractable on classical computers. When it comes to studying these functions at finite temperature the main bottleneck comes from the resource overhead and circuit complexities required in preparing each Gibbs sample. We present a framework aimed at alleviating this bottleneck by optimizing a series of approximations. Specifically, we sample from a series of time averaged embedded clusters initially in their respective local Gibbs states. After extracting each approximate dynamic correlation function we employ Richardson extrapolation where the error expanded in the series is determined by the total number of sub-clusters used in each approximation. We obtain higher order estimates for each distinct path of approximations. We can optimize even further by weighting each distinct path by how closely each path fits the proper fluctuation theorem. We demonstrate this toolbox numerically using exact diagonalization of the Hubbard model on small clusters.
1:51PM G68.00012: Band engineering for quantum simulation with superconducting circuits
CHRISTIE CHIU (Presenter), ANDREW HOUCK, Princeton University — Quantum simulation has been implemented on a variety of experimental platforms such as neutral atoms, ions, quantum dots, and superconducting circuits, each offering unique features. Superconducting circuits can and have been used to realize artificial photonic materials in a wide range of lattice geometries and graph connectivities, due to the flexibility of on-chip fabrication. In addition, photon-photon interactions are highly tunable using nonlinearities such as superconducting qubits, leveraging the vast toolkit developed for quantum computation. Here I report on recent progress towards engineering flat bands for studies of strongly correlated many-body physics.

*This research was supported by the Princeton Materials Science Postdoctoral Fellowship and the ARO MURI program.

G68.00013: Propagation and Localization of Collective Excitations on a 24-Qubit Superconducting Processor
YANGSEN YE (Presenter), University of Science and Technology of China — Superconducting circuits have emerged as a powerful platform of quantum simulation, especially for emulating the dynamics of quantum many-body systems. Here we construct a Bose-Hubbard ladder with a ladder array of 20 qubits. We then use pairs of controllable qubits to study the dynamics of the ladder model. We investigate theoretically and demonstrate experimentally the dynamics of single- and double-excitation states with distinct behaviors. We observe linear propagation of photons in the single-excitation case. The double-excitation state, initially placed at the edge, localizes; while placed in the bulk, it splits into two single-excitation modes. Our work paves the way to simulation of exotic logic particles by subtly encoding physical qubits and exploration of rich physics by superconducting circuits.

Tuesday, March 3, 2020 12:30 PM - 2:00 PM

Session H01 APS: Students Lunch with the Experts Lobby D - Tag(s): Careers, Industry, Undergrad Friendly
12:30PM H01.00001: Students Lunch with the Experts — Students may sign up to enjoy a complimentary box lunch while participating in an informal and stimulating discussion with a physics expert.

Tuesday, March 3, 2020 2:00 PM - 2:00 PM

Session H71 : Poster Session II (2:00pm - 5:00pm) Exhibit Hall C/D - Tag(s): Poster, Undergrad Friendly
H71.00001: CONDENSED MATTER PHYSICS —
H71.00002: WITHDRAWN ABSTRACT —
H71.00003: Hydrodynamic Transport in Near Magic Angle Twisted Bilayer Graphene*

MOHAMMAD ZARENIA (Presenter), Univ of Missouri - Columbia, INDRA YUDHISTIRA, Yale-NUS College, SHAFFIQUE ADAM, National University of Singapore & Yale-NUS College, GIOVANNI VIGNALE, Univ of Missouri - Columbia — Using the semiclassical quantum Boltzmann theory and employing the Dirac model with twist angle-dependent Fermi velocity we obtain results for the electrical resistivity, the electronic thermal resistivity, the Seebeck coefficient, and the Wiedemann-Franz ratio in near magic angle twisted bilayer graphene, as functions of doping density (around the charge-neutrality-point) and modified Fermi velocity. The Fermi velocity-dependence of the relevant scattering mechanisms, i.e. electron-hole Coulomb, long-ranged impurities, and acoustic gauge phonons is considered in detail. We find a range of twist angles and temperatures, where the combined effect of momentum-non-conserving collisions (long-ranged impurities and phonons) is minimal, opening a window for the observation of strong hydrodynamic transport. Several experimental signatures are identified, such as a sharp dependence of the electric resistivity on doping density and a large enhancement of the Wiedemann-Franz ratio and the Seebeck coefficient.

*This work was supported by the U.S. Department of Energy (Office of Science) under grant No. DE-FG02-05ER46203. The work in Singapore is supported by the National University of Singapore Young Investigator Award (R-607-000-094-133).

H71.00004: Detecting superconductivity out-of-equilibrium*

BENEDIKT FAUSEWEH (Presenter), Los Alamos National Laboratory, SEBASTIAN PAECKEL, ALEXANDER OSTERKORN, Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany, THOMAS KOEHLER, Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden, DIRK MANSKE, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany, SALVATORE MANMANA, Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — Pump-probe experiments on cuprates and similar systems suggest the existence of a transient superconducting state far above the critical temperature. This poses the question how to reliably identify the emergence of superconductivity, out-of-equilibrium. In our contribution we investigate this point by studying the non-equilibrium dynamics in an extended Hubbard model and by computing various observables, which are used in theory and experiment to identify superconductivity. We specifically show, that the time-dependent optical conductivity is not sufficient to distinguish between a dynamical induced superconductor or an enhanced metallic state. In turn, we suggest to utilize time-resolved ARPES experiments in the two-particle channel to probe for superconducting signatures.

*B.F. and D.M. thank the Max Planck-UBC-UTokyo Center for Quantum Materials for financial support. T.K.’s contribution was partially funded through an ERC Starting Grant under grant agreement No. 758935. We acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) through SFB/CRC1073 (projects B03 and B07) and Research Unit FOR 1807 (project P7). This work was supported in part by the Los Alamos National Laboratory LDRD Program.

H71.00005: WITHDRAWN ABSTRACT
H71.00007: Stimulated electron-electron interaction in cavities* HONGMIN GAO (Presenter), FRANK SCHLAWIN, DIETER JAKSCH, University of Oxford — Electron interactions mediated by the exchange of virtual bosonic excitations form a central cornerstone in quantum many-body theory where they are responsible for many-body phases such as superconductivity [1,2]. More recently, interactions mediated by excitations with photonic character, such as exciton-polaritons [3,4] and transverse cavity photons [5] have also been tipped to lead to superconductivity. We propose a novel scheme to engineer stimulated electron interactions in any 2D electron system coupled to a cavity under driving. The interaction can be tuned to be attractive (or repulsive) and lead to Cooper instability at temperature up to ~1K. Our scheme opens up a new avenue for on-demand quantum material engineering.


*This work is supported by the European Union’s Seventh Framework Programme (FP7/2007-2013)/ERC Grant Agreement No. 319286 Q-MAC.

H71.00008: First-principles study on the electronic structures of ternary TMDC alloys in monolayer and multilayer forms* JUN NARA (Presenter), WENTONG GENG, TAKAHISA OHNO, National Institute for Materials Science — Transition metal dichalcogenides (TMDCs) have attracted great attention for their potential application in many fields including light-emitting diodes and photo detectors. The possibility in controlling the stacking sequence of different kind of TMDC layers by means of van der Waals epitaxy enables us to design novel materials through electronic structure engineering. Recently, two-dimensional lateral heterostructures have been successfully synthesized by Sahoo et al. [1], providing us a new freedom in heterostructure design other than sequential stacking. We have investigated the electronic structures of a monolayer and multilayers of ternary alloys made of Mo\(_{(1-x)}\)W\(_x\)S\(_2\) by using PHASE/0 [2], a first-principles electronic structure calculation code. We obtain a direct energy band gap whose width is smaller than both MoS2 and WS2. Details of the results will be given in the presentation.

We used the NIMS Numerical Materials Simulator for the calculations.


*This work was supported by Innovative Science and Technology Initiative for Security, ATLA, Japan.
H71.00009: Electronic states and Coulomb excitations of $\alpha$-$T_3$ zigzag nanoribbons  
PAULA FEKETE (Presenter), US Military Academy at West Point, ANDRII IUROV, Medgar Evers College of the City University of New York, GODFREY GUMBS, Hunter College of the City University of New York, DANHONG HUANG, Air Force Research Laboratory, Kirtland Airforce Base, Albuquerque, NM — We have examined all possible non-equivalent types of edge terminations for pseudospin-1 $\alpha$-$T_3$-based nanoribbons. Our results show that all of their fundamental electronic properties depend significantly on both the hopping parameter $\alpha$ and the particular geometry of their edge. For all non-equivalent edge terminations, we have calculated the electronic wave functions, Coulomb potential, and plasmon dispersion relations. We also report on the dependence of the plasmon dispersion on the electron doping concentration for zigzag edged nanoribbons.

H71.00010: Ultrafast nonlinear electron dynamics in gapped graphene*  
AHMAL ZAFAR (Presenter), SEYYEDEH AZAR OLIAEI MOTLAGH, ARANYO MITRA, FATEMEH NEMATOLLAHI, VADYM APALKOV, MARK I STOCKMAN, Georgia State University — We theoretically study the ultrafast electron dynamics in gapped graphene. Graphene consists of two equivalent sublattices and has both inversion and time-reversal symmetries. Breaking the inversion symmetry in graphene opens the bandgap and makes sublattices inequivalent. Gapped graphene is used as a model for a broad class of two-dimensional materials, including transition metal dichalcogenides. The ultrafast electron dynamics in gapped graphene is induced by a linearly polarized ultrafast optical pulse applied perpendicular to graphene monolayer. Our results show that the residual, i.e., after the pulse, conduction band (CB) population, which characterizes the irreversibility of the electron dynamics, is large and shows interference fringes in the reciprocal space. The finite bandgap in graphene makes the electron dynamics partially reversible, which manifests itself in smearing of the interference fringes in the CB population distribution.

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National Science Foundation (NSF)sub-award No T883032,Federal Award No. EFMA-1741691
Department of Energy (DOE)DE-FG02-01ER15213
Department of Energy (DOE)DE-SC0007043
Air Force Office of Scientific Research (AFOSR)sub-award No. 24086151,Federal Award No. FA9550-15-1-0037
H71.00011: Ultrafast field-driven currents in gapped graphene*  ARANYO MITRA (Presenter), SEYYEDEH AZAR OLIAEI MOTLAGH, AHMAL ZAFAR, FATEMEH NEMATOLLAHI, VADYM APALKOV, MARK I STOCKMAN, Georgia State University — We study theoretically interaction of a linearly polarized ultrashort and ultrafast optical pulse with gapped graphene monolayer. A finite conduction band population and corresponding electric currents are generated during the pulse. In gapped graphene, inversion symmetry is broken, and while one axis, is still the axis of symmetry (y-axis), the other axis (x-axis) is no longer so, which results in generation of non-trivial currents. When the incident pulse is polarized along x-axis, both the longitudinal and transverse currents are generated. Our results show that both currents strongly depend on the bandgap. The generated electric currents transfer electrical charge and make the gapped graphene electrically polarized. The transferred charge in longitudinal direction has monotonic dependence on the field amplitude and weak dependence on the bandgap, while in transverse direction, the transferred charge shows non-monotonic dependence on the field amplitude.

*Office of Naval Research (DOD)N000-14-17-1-2588
National Science Foundation (NSF)sub-award No T883032,Federal Award No. EFMA-1741691
Department of Energy (DOE)DE-FG02-01ER15213
Department of Energy (DOE)DE-SC0007043
Air Force Office of Scientific Research (AFOSR)sub-award No. 24086151,Federal Award No. FA9550-15-1-0037

H71.00012: Optical absorption spectrum for $\alpha\mc{T}_3$ materials interacting with light.  DIPENDRA DAHAL (Presenter), The Graduate Center, City University of New York, GODFREY GUMBS, Physics and Astronomy, Hunter College, City University of New York, ANDRII IUROV, Physics and Astronomy, Medgar Evers College, City University of New York, DANHONG HUANG, Air Force Research Laboratory — We have investigated the optical absorption properties of $\alpha\mc{T}_3$ materials, interacting with linearly and circularly polarized irradiation. The peaks in the optical absorption spectra and the plasmon modes show strong dependence on the hopping parameter $\alpha$ and a relatively moderate dependence on the strength of light-matter interaction, as well as on the polarization of the incoming off-resonance dressing field.
Temperature dependence of van Hove singularity excitons in atom thick semiconductors*  
GARRETT BENSON (Presenter), VIVIANE ZURDO COSTA, NEAL BORDER, SHIRIN JAMALI, San Francisco State Univ, KENTARO YUMIGETA, MARK BLEI, SEFAATTIN TONGAY, Materials Science and Engineering, Arizona State University, ANDREW ICHIMURA, AKM SHAH NEWAZ, San Francisco State Univ — Atomically thin semiconducting transition metal dichalcogenides (TMDs) are emerging as a new platform for exploring two-dimensional exciton physics. These excitons play a crucial role in determining the light-matter interactions of a semiconducting material, such as absorption, photoluminescence, and electroluminescence. In addition to direct-band gap transition excitons (known as $A$- and $B$- excitons), there also exists a pair of van Hove singularity (vHS) assisted excitonic transitions, known as the $C$- and $D$- excitons. Currently it is not known how these vHS excitons modify at different temperature. To bridge the knowledge gap, we probed the temperature dependence of both direct-band gap and vHS excitons via photocurrent spectroscopy. We observed that all the excitonic peaks shift to lower energy as the temperature decreases. Moreover, we observed that the rate of shift for vHS excitons differs significantly from the rate of shift for the direct-band gap excitons. This study advances our understanding of the intrinsic properties of excitons in 2D TMDs.

*This research is supported by a Department of Defense Award (ID: 72495RTREP) and a National Science Foundation Grant ECCS1708907.

Steering valley-polarized emission of monolayer MoS$_2$ sandwiched in plasmonic antennas  
TE WEN (Presenter), HU AIQIN, School of Physics, Peking University, YANG CHEN, CHENG-WEI QIU, Department of Electrical and Computer Engineering, National University of Singapore, QIHUANG GONG, GUOWEI LV, School of Physics, Peking University — Monolayer transition metal dichalcogenides (TMDCs) have intrinsic spin-valley degrees of freedom, making it appealing to exploit valleytronic and optoelectronic applications at the nanoscale. Here, we demonstrate that a chiral plasmonic antenna consisting of two stacked gold nanorods (GNRs) can modulate strongly valley-polarized photoluminescence (PL) of monolayer MoS$_2$ in a broad spectral range at room temperature. The valley-polarized PL of the MoS$_2$ with the antenna can reach up to ~48% accompanied with more than three orders of magnitude enhancement of PL intensity. Also, the $K$ and $K'$ valleys under opposite circularly polarized light excitation exhibit different emission intensities and directivities in the far-field, which can be attributed to the valley-dependent exciton modulation by the chiral antenna in both excitation and emission processes. The distinct features of the ultra-compact hybrid suggest potential applications for valleytronic and photonic devices, chiral quantum optics, and high-sensitive detection.
H71.00015: Electron transport through pair of Graphene-Superconductor junctions*
SHAHRRUKH SALIM, RAHUL SURESH MARATHE, SANKALPA GHOSH (Presenter), Indian Inst of Tech-New Delhi — Electron transport across Graphene-Superconductor (GS) junctions have recently attracted a lot of attention [1] after it was pointed out that the Andreev processes in such junction holds distinct features as compared to Andreev processes in Normal metal-Superconductor junction because of the ultra relativistic dispersion of the charge carriers in Graphene. In this work we analyze transport properties through a pair of such junctions that can be either GSG or SGS form due to Andreev and normal processes. In one part of the work we compare such transport with certain optical phenomena such as Goos-Hanchen shift [2] and discuss its experimentally verifiable features. We also investigate the formation of the Andreev Bound States (ABS) in heterojunctions like SGS, and explore its connection with the transport properties; Josephson current.

References:

*Shahrukh Salim is funded by MHRD, Govt. of India

H71.00016: Strain Imaging of Laterally-Stitched Monolayers by Nonlinear Optical Microscopy*
CHUN AN CHEN (Presenter), YING-YU LAI, KUAN-CHANG CHIU, CHEN PO-HAN, YI-HSIEN LEE, YU-TING LIN, YI-CHENG CHIANG, I-TUNG CHEN, National Taiwan Normal Univ — Strain configuration is significant to crystal structure and performance of monolayer two-dimensional lattice. Heterojunction of various monolayer transition metal dichalcogenides (TMD) is emergent route to induce unique symmetry and strain configurations. Here, we realize the synthesis of diverse in-plane artificial lattice by lateral stitching of different monolayer TMD using sequential CVD growth. Highly oriented strain patterns are observed and studied by second harmonic generation imaging of the TMD multijunctions. Strain pattern with lateral and vertical heterostructures are studied using angle resolved second harmonic generation, which is practical to correlate unique properties by direct probing symmetry and strain configuration of monolayer TMDs.

*The authors acknowledge support from AOARD grant (co-funded with ONRG) FA2386-16-1-4009, Ministry of Science and Technology (MoST-106-2119-M-007-023-MY3; MoST-105-2112-M-007-032-MY3, 107-2923-M-007 -002 -MY3), and Academia Sinica Research Program on Nanoscience and Nanotechnology, Taiwan.
H71.00017: Synthesis and enhanced magnetoresistance of WTe$_2$ single crystals*  \textbf{YU-TING LIN} (Presenter), CHUN-AN CHEN, CHEN PO-HAN, I-TUNG CHEN, YI-CHENG CHIANG, YI-HSIEN LEE, Materials Science and Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan — Tungsten ditelluride (WTe$_2$) is one of the low symmetry two-dimensional materials and exhibits extremely large magnetoresistance (XMR) below 10K. Understanding of novel properties in the materials is highlighted to induce unique properties at elevated temperature. Study of the temperature dependent MR is essential for real applications and deep insights. Most reported studies on fundamental issues are mainly achieved in exfoliated WTe$_2$ (for reduced disorders) which is encapsulated with h-BN layers (for ideal interfaces). Here, we demonstrate synthesis and enhanced performances of the synthesized WTe$_2$ single crystals. Tunable thickness and high crystallinity of the WTe$_2$ are achieved using promoter-assisted CVD. A large MR of the CVD-grown WTe$_2$ is experimentally realized.

*We acknowledge support from AOARD grant (co-funded with ONRG) FA2386-16-1-4009, Ministry of Science and Technology (MOST 108-2112-M-007-006-MY3, MOST 107-2923-M-007-002-MY3, MOST 106-2119-M-007-023-MY3, and MOST 105-2112-M-007-032-MY3), and Academia Sinica Research Program on Nanoscience and Nanotechnology (AS-iMATE-107-11), Taiwan.

H71.00018: Carbonaceous magnetic nanocomposites*  \textbf{DEREJE SEIFU} (Presenter), Morgan State Univ, SHASHI P KARNA, WMRD, US ARL, HAIPING HONG, EE, SDSMT — Ferromagnetic nanoparticles when in proximity to low-dimension carbonaceous structures, such as 1D carbon nanotubes and 2D graphene, induce ferromagnetism in the latter through spin-orbit coupling and exchange interaction. Taking advantage of these interaction, we have created carbonaceous magnetic nanocomposites using carbon nanotubes and multilayer graphene that exhibit enhanced magnetic properties compared to the pristine nanoparticles [1-3]. The Magnetic nanoparticles studied included Fe, Fe$_2$O$_3$, Fe$_3$O$_4$, Co$_3$O$_4$, and CoFe$_2$O$_4$ on both carbon nanotubes and multilayered graphene. Structural and magnetic studies showed that magnetic enhancement occurred by proximity effect.


*The corresponding author D.S acknowledges the support of ARL-W911NF-19-2-0222.
H71.00019: Nonlinear Electrical and Linear Optical Properties of Layered Graphene Oxide
DEJAN MAKSIMOVSKI, Colgate University, N. G. HALLFORS, Biomedical Engineering, KUST, ABDEL ISAKOVIC (Presenter), Colgate University — We measured a significant, two orders of magnitude decrease in the resistance of layered (5 - 100 nm) reduced graphene oxide. The resistance drops as the number of layers increases, lending a notion to the influence of out-of-plane transport being modulated by modifications to the changes in electronic structure, as additional layers are added. These changes are observed for line and area resistance, as well, indicating that geometry doesn't play major role. In parallel with this result, we report spectroscopic study (Raman, FTIR) on the same samples, where the ratio of spectral D (1350 cm\(^{-1}\)) and G (1580 cm\(^{-1}\)) features shows unusual dependence on the thickness (the number of layers of graphene oxide), in that it mimics the dependence of the resistance on thickness. Detailed spectroscopic study of various bonds (some sp\(^2\) related, some not) shows a number of features that are potentially relevant for explanation of observed resistance behavior. The role of carbon vacancies is also studied, showing that the bonding of molecules external to graphene oxide becomes modified in the presence of vacancies. AFM and electron microscopy studies complement these findings and show how layered graphene oxide large area, nanoscale thickness scale structures evolve with controlled defects.

H71.00020: Towards an electrically driven single photon source made from a carbon nanotube
DUBLIN NICHOLS (Presenter), DUY NGUYEN, ETHAN MINOT, Oregon State Univ — On-demand single photon sources have potential applications in quantum cryptography, quantum computing, and metrology. In particular, there is a need for devices that can be integrated into an on-chip network and can produce indistinguishable photons on-demand. Such devices would enable practical designs for all-optical quantum computers. We aim to create electrically driven single photon sources using individual semiconducting carbon nanotubes with sp\(^3\) defects. Novel aspects of our device design include integration with van der Waals heterostructures, and the use of electrostatic gating to form p-n junctions. I will show why this is a promising platform, and discuss our progress towards fabricating a working prototype.
H71.00021: Transport in armchair graphene nanoribbons and in ordinary waveguides
MUHAMMAD ZUBAIRM (Presenter), Department of physics, Concordia University, MOUSA BAHRAMI, Department of Computer Science and Mathematics, Nippising University, PANAGIOTIS VASILOPOULOS, Department of physics, Concordia University — We study dc and ac transport along armchair graphene nanoribbons using the k.p spectrum and eigenfunctions and general linear-response expressions for the conductivities. Then, we contrast the results with those for transport along ordinary waveguides. In all cases, we assess the influence of elastic scattering by impurities, describe it quantitatively with a Drude-type contribution to the current previously not reported, and evaluate the corresponding relaxation time for long- and short-range impurity potentials. We show that this contribution dominates the response at very low frequencies. In both cases, the conductivities increase with the electron density and show cusps when new subbands start being occupied. As functions of the frequency, the conductivities in armchair graphene nanoribbons exhibit a much richer peak structure than in ordinary waveguides: in the former, intraband and interband transitions are allowed, whereas in the latter, only the intraband ones occur. This difference can be traced to that between the corresponding spectra and eigenfunctions.

*M.Z. and P.V. acknowledge the support of the Concordia University under Grant No. VB0038 and Concordia University Graduate Fellowship.

H71.00022: Electronic Structure Study of Halogen and Gold Halide Doped Carbon Nanotubes
MD LATIFUR RAHMAN, MD HASIBUL AMIN, AHMED ZUBAIRM (Presenter), Electrical and Electronic Engineering, Bangladesh University of Engineering and Technology — Achieving high electrical conductivity of carbon nanotubes (CNTs) through doping will facilitate its application in power transmission cable and nanoelectronic interconnects. Here, we report extremely efficient p-doping of CNT using halogen and gold halide molecules. Using ab initio theoretical calculations based on density functional theory, we investigated the effect of dopants, such as I\textsubscript{2} and AuCl\textsubscript{3}, on the electronic band structure of semiconducting and metallic CNTs. We found that both I\textsubscript{2} and AuCl\textsubscript{3} introduces states between the first Van Hove singularities of conduction and valance bands. I\textsubscript{2} was reported being an efficient dopant for CNTs. From our calculations, we confirm that large Fermi level shift occurs for both I\textsubscript{2} and AuCl\textsubscript{3} doping. Though the Fermi shift is much larger for AuCl\textsubscript{3} doping. Moreover, transmission function calculations reveal that a few fold increase in available quantum channels exists for AuCl\textsubscript{3} doping compared to I\textsubscript{2} doping. Therefore, gold halide such as AuCl\textsubscript{3} can be a perfect candidate as a dopant molecule of CNTs to produce conductors with ultra-high conductivities.
H71.00023: Investigating single-walled carbon nanotube films for LEDs and lasers*  
MARK STEGER (Presenter), BRYON LARSON, KIRA THURMAN, ANDREW FERGUSON, JEFFREY L BLACKBURN, National Renewable Energy Laboratory — Carbon nanotubes (CNT) offer interesting optoelectronic properties including engineered conductivity and tunable infrared emission. CNTs have been extensively studied as carrier transport layers for OLEDs or as single-nanotube LEDs. Here, we investigate LED and laser architectures using CNT films as a bulk active emitter layer tunable in the near IR. We investigate the intrinsic stability of the emitter layer and optimize device structure.

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H71.00024: Phase segregation and superconductivity in Cu doped Ni$_{2-x}$Cu$_x$NbSn Heusler alloys  
BRANDON REESE (Presenter), MAHMUD KHAN, Miami University — Heusler alloys exhibit numerous exotic properties including superconductivity that can be systematically controlled via manipulation of their stoichiometry and elemental doping. It has been reported that partial substitution of Ni by Cu in Ni$_{2-x}$Cu$_x$ZrGa results in a systematic reduction of T$_{C}$. Considering this observation it is interesting to explore the effect of Cu doping on the superconducting properties of other Heusler alloys. Therefore, we have performed an experimental study on the superconducting properties of partially Cu doped Ni$_{2-x}$Cu$_x$NbSn materials. Ni$_2$NbSn has 29 valence electrons per formula unit and 7.25 valence electrons per atom. The material exhibits a superconducting phase transition at T$_{C}$ = 3.4 K. A series of Ni$_{2-x}$Cu$_x$NbSn materials were synthesized by arc-melting and annealing techniques. All materials were characterized by x-ray diffraction, dc magnetization, and transport measurements. Interestingly, a Cu concentration of 2.5% resulted in phase segregation of the system. Two superconducting transitions were observed in all compounds at temperatures near T$_{C1}$ = 17.8 K, and T$_{C2}$ = 3.4 K. Magnetization data has confirmed type-II superconductivity for each sample at both T$_{C1}$ and T$_{C2}$. 

1 Dharma Raj Basaula, Jeffrey Brock, Mahmud Khan, AIP Advances 8, 055704 (2018).
H71.00025: Gapless spin liquid state and quantum phase diagram in the spin-1/2 $J_{1}$-$J_{2}$ square Heisenberg model  WEN-YUAN LIU (Presenter), physics, Chinese Univ of Hong Kong, SHOUSHU GONG, physics, Beihang University, ZHENGCHENG GU, physics, Chinese Univ of Hong Kong — The spin-1/2 $J_{1}$-$J_{2}$ square Heisenberg model is one of the most interesting and also challenging quantum spin models, due to the strongly frustrated interactions. It is of the primary candidate models to study quantum spin liquid (QSL). Despite intensively studied in the past 30 years, the nature of the intermediate nonmagnetic phase is still under great debates. Especially, whether the intermediate phase is a QSL is currently a matter of great concern to the community. A recent DMRG calculation suggests that the intermediate region is a valence bond state. However, the DMRG method is essentially a one-dimensional method. Recently, we developed an efficient and accurate finite projected entangled pair states (PEPS) method, which can deal with a very large system in high precision. With this state-of-the-art tensor network based method, we find it is a spin liquid phase for a large region of the nonmagnetic phase, and spin correlations of the spin liquid decay in a power law form, indicating it is gapless. Methodologically, we give the first solid PEPS calculation beyond DMRG. By comparing with DMRG in details, we provide a direct numerical evidence to explicitly demonstrate the conceptual advantage of PEPS over DMRG for large 2D systems.

H71.00026: Thermodynamic properties of a spin-1/2 Heisenberg model on the triangular lattice  KAZUHIRO SEKI (Presenter), SEIJI YUNOKI, RIKEN — By using the numerically exact diagonalization technique and a block-extended version of the finite-temperature Lanczos method, we study thermodynamic properties, such as entropy, specific heat, and uniform susceptibility, of a spin-1/2 Heisenberg model on the triangular lattice with the nearest-neighbor exchange interaction $J$ and the four-spin exchange interaction $J_c$. Our calculations on small clusters containing up to 36 spins have found that, differently from the pure triangular-lattice ($J_c=0$) case, the temperature dependence of the specific heat exhibits a pronounced double-peak structure for finite and moderate $J_c/J$.

H71.00027: Monte Carlo Study of Three-dimensional Flat-Band Ferromagnetism in a Diamond Lattice*  JUNJIA ZHANG, ERIC J BOBROW (Presenter), YI LI, Johns Hopkins University — We study the p-orbital bands in the orbital-active diamond lattice. This system features doubly-degenerate flat bands at each momentum in the Brillouin zone as well as dispersive bands exhibiting nodal-line semimetal behavior. Due to the suppression of kinetic energy, strong correlation effects lead to ferromagnetism in the flat bands, which can be mapped to a modified percolation problem. We investigate the transition between the paramagnetic and ferromagnetic phases in the flat bands via Monte Carlo simulation.

*This work is supported by NSF CAREER DMR-1848349 and in part by the Alfred P. Sloan Research Fellowships.
H71.00028: A highly sensitive TES spectrometer for resonant elastic/inelastic X-ray scattering study of quantum materials  SANG JUN LEE (Presenter), SLAC - Natl Accelerator Lab, SANGJUN LEE, University of Illinois Urbana Champaign, YOUNG-IL JOE, NIST, HAI HUANG, SLAC - Natl Accelerator Lab, WILLIAM B DORIESE, NIST, JASON KNIGHT, DONGHUI LU, SLAC - Natl Accelerator Lab, JOEL N ULLOM, PAUL SZYPRYT, DANIEL SWETZ, NIST, PETER MICHAEL ABBAMONTE, University of Illinois Urbana Champaign, JUN-SIK LEE, SLAC - Natl Accelerator Lab — Resonant inelastic X-ray scattering (RIXS) as well as resonant elastic X-ray scattering (REXS) have been appreciated as compelling techniques in research of quantum materials. It is because the techniques deliver element-, site-, and valence-specific information through a resonance-enhanced photon-in/photon-out process. Conventionally, grating-based spectrometers have been used to measure the scattered photons in RIXS/REXS in the soft X-ray regime. However, we often experience a lack of sensitivity when a weak signal needs to be detected. Here, we introduce a novel method to overcome such difficulty using transition-edge sensors (TESs). A spectrometer built upon an array of TESs has detection efficiency that is orders of magnitude larger than a conventional grating spectrometer and has shown a spectral coverage broader than 1 keV and a moderate energy resolution of 1.5 eV (FWHM) at 500 eV. A TES spectrometer was recently integrated with the soft X-ray scattering setup at beamline 13-3 of the Stanford Synchrotron Radiation Lightsource (SSRL) and was successfully commissioned. In this poster, we will present new results taken with this new RIXS/REXS + TES approach. We believe that this approach can bring impacts to a wide range of quantum materials studies.

H71.00029: WITHDRAWN ABSTRACT  —

H71.00030: Evidence for effects of nitrogen exposure on the Bi$_2$Se$_3$ density of states  MICHAEL GOTTSCHALK (Presenter), Michigan State University, MAL-SOON LEE, Pacific Northwest National Laboratory, ERIC GOODWIN, Michigan State University, THOMAS CHASAPIS, MERCOURI KANATZIDIS, Northwestern University, S D MAHANTI, STUART TESSMER, Michigan State University — Bi$_2$Se$_3$ is a topological insulator widely used for scientific studies due in part to the ease with which it can be cleaved, exposing a clean surface for study. Typically the materials exhibit n-type doping attributed to selenium vacancies which results in a shift of the Dirac point to between 100 and 300 meV below the Fermi level. Using room temperature scanning tunneling microscopy (STM), we observed evidence for a shift in the expected density of states spectra when crystals first cleaved in a helium gas environment became exposed to ultra high purity N$_2$ gas. The shift brings the Dirac point 50 meV closer to the Fermi level. We will also present density functional theory calculations supporting the picture that nitrogen can bind to the selenium vacancies and shift the density of states. Finally, we will present data showing the time scale over which the exposure occurs.
**H71.00031: Measurement of fractional charge at disclination defects in higher-order topological crystalline insulators**

CHRISTOPHER PETERSON (Presenter), TIANHE LI, TAYLOR L HUGHES, GAURAV BAHL, University of Illinois at Urbana-Champaign — Topological crystalline insulators (TCIs) are known to host quantized fractional charge at boundaries and defects, which is topologically protected by bulk crystalline symmetries. Recently, this bulk-boundary correspondence was extended by the discovery of higher-order TCIs, which may host quantized fractional charge at a boundary of their boundary. Here, we use arrays of microwave resonators to experimentally study higher-order TCIs on lattices with disclination defects. Introducing a disclination defect to a finite lattice is equivalent to inserting or removing one or more sectors, changing the total number of corners and consequently introducing an overall fractional charge. Since the total charge in a lattice must remain an integer, the disclination core is expected to also host fractional charge to compensate. We experimentally measure C4-symmetric higher-order TCIs on square lattices having disclinations with positive and negative Frank angles, which respectively have 5 and 3 corners. We find that, in both cases, the disclination core does indeed host fractional charge, such that the total charge of the lattice is an integer. Furthermore, we show that there are gapless bound states associated with the defect.

*We acknowledge support from the US National Science Foundation.

**H71.00032: Topological surface states in strained Cd3As2 thin films**

PABLO VILLAR ARRIBI (Presenter), Argonne Natl Lab, TIMO SCHUMANN, SUSANNE STEMMER, University of California, Santa Barbara, ANTON BURKOV, University of Waterloo, OLLE HEINONEN, Argonne Natl Lab — Cd3As2 is a Dirac semi-metal with two Dirac nodes near the Γ point in the first Brillouin zone aligned along the crystallographic c-axis. The structure of Cd3As2 is rather complicated with a large unit cell and it is typically grown along the (112) direction, which does result in a projection of the Fermi arc states on the (112) surface. The Dirac points are protected by inversion and C4 symmetry about the tetragonal c-axis. In recent experiments, the inversion symmetry can be broken in thin films, and the C4 symmetry can be broken by a bi-axial strain perpendicular to the c-axis [1]. This brings up the question of what happens to the Fermi arc states in the ultra-thin film limit and in the presence of broken symmetries. We are using a simple description of the low energy physics to examine the behavior of the Fermi arc states. As an example, when inversion symmetry is broken, so is the symmetry of the Fermi arc states near the Dirac points, and the two-fold degeneracy of the Dirac cones is lifted.


*This work was supported U.S. Department of Energy Office of Science, Office of Basic Energy Sciences.
**H71.00033: Chiral Anomaly and Temperature Effects in Tilted Doped Weyl Semi-metals: Dichroism And Dynamic Hall Angle**

ASHUTOSH SINGH (Presenter), JULES P CARBOTTE, McMaster University

We calculate the absorptive part of the dynamic conductivity for both right and left handed circular polarized light in the Kubo formalism. Due to finite contribution from the imaginary part of Hall conductivity, we observe dichroism in certain frequency regime. Including the effect of chiral pumping creates difference in chemical potential in the positive and negative chirality nodes, which leads to additional regions of frequencies where dichroism remains finite. We have also considered the case of a non-centrosymmetric Weyl semi-metal in which the two nodes are displaced in energy by an amount ±Q₀. This also modifies the dichroism in a similar fashion. Further, with increase in temperature (T), the boundaries of the regions of finite dichroism become smeared out in energy and extend beyond their original range for T = 0 and at the same time the dichroism is reduced. When T is increased to be of the order of the chemical potential associated with the doping, the dichroism vanishes. We have also extended the work to include the frequency variation of dynamic Hall angle for both zero and finite temperature cases.

*National Science and Engineering Research Council of Canada (NSERC) and by the Canadian Institute for Advanced Research (CIFAR) (Canada).

**H71.00034: Ultrafast optical current in Weyl semimetals**

FATEMEH NEMATOLLAHI, VADYM APALKOV (Presenter), MARK I STOCKMAN, Georgia State University

We study theoretically the nonlinear response of Weyl semimetals to an ultrashort optical pulse. Such strong electric field induces a finite conduction band population near the Weyl points in the reciprocal space. Also, the optical pulse causes current in the system both during and after the pulse.

*1-Office of Naval Research (DOD); N000-14-17-1-2588
2-Emory University, subcontracted by the National Science Foundation (NSF); T883032 is the subaward number; the Federal Award no. is EFMA-1741691
3-Department of Energy (DOE); DE-FG02-01ER15213
4-Department of Energy (DOE); DE-SC0007043
5-University of Central Florida, subcontracted by the Air Force Office of Scientific Research (AFOSR); 24086151 is the subaward number; the Federal Award no. is FA9550-15-1-0037*
**H71.00035: Sign Change in the Anomalous Hall Effect and Strong Transport Effects in a 2D Massive Dirac Metal Due to Spin-Charge Correlated Disorder***  
AYDIN KESER (Presenter), School of Physics, University of New South Wales, ROBERTO RAIMONDI, Department of Physics, Universita Roma Tre, DIMITRIE CULCER, School of Physics, University of New South Wales — The anomalous Hall effect (AHE) is highly sensitive to disorder in the metallic phase. Here we show that statistical correlations between the charge-spin disorder sectors strongly affect the conductivity and the sign or magnitude of AHE. As the correlation between the charge and gauge-mass components increases, so does the AHE, achieving its universal value, and even exceeding it, although the system is an impure metal. The AHE can change sign when the anticorrelations reverse the sign of the effective Dirac mass, a possible mechanism behind the sign change seen in recent experiments.

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**H71.00036: Strain-engineering of Topological Type-II Dirac Semimetal NiTe$_2$***  
ANTONIO MANESCO (Presenter), Kavli Institute of Nanoscience, Delft University of Technology, PEDRO P. FERREIRA, LUCAS EDUARDO CORRÊA, ANTONIO JEFFERSON DA SILVA MACHADO, GABRIELLE WEBER, LUIZ T. F. ELENO, University of Sao Paulo — The electronic, elastic and topological properties of the equilibrium and strained type-II Dirac semimetal NiTe$_2$ were studied within the scope of density functional theory. This bulk transition metal dichalcogenide harbor a tilted symmetry-protected Dirac cone from p-orbital bands in the vicinity of the Fermi level. The projected electronic structure and group analysis suggest that single orbital-manifold band inversion can be assigned as the mechanism behind the present topologically non-trivial states. Also, several applied strain modes are shown to be an effective route to tuning this bulk electronic trends. For instance, a small uniaxial strain along z-direction is enough to approach Dirac fermions into the Fermi energy and suppress another usual non-relativistic bands from the Fermi surface. Through our investigations, we propose a static-control of the electronic states by the intercalation of light-metal monovalent species into the van der Waals gap. We also present a low-energy effective model and discuss effects of external fields and low-dimensionality.

*We gratefully acknowledge the financial support by São Paulo Research Foundation, grants 2016/10167-8, 2019/07082-9, 2018/10835-6 and 2019/05005-7.
**H71.00037: Nonlinear Anomalous Hall Effect in Type I Weyl Metals**

AYDIN KESER (Presenter), DIMITRIE CULCER, University of New South Wales, ARC FLEET — Within the framework of linear response, Anomalous Hall Effect (AHE) in time reversal (TR) invariant systems is prohibited, yet in inversion symmetry (P) breaking system, AHE second order in the applied fields is expected.

The Fermi sea contribution to both linear and nonlinear AHE in Weyl semimetal is due to Berry dipoles and multipoles, however, in a doped metallic phase free carrier contribution at each node is large when the cone is tilted. We calculate the second order optical AHE conductivity in tilted Weyl nodes and characterize disorder contributions in the DC limit of first and second order AHE. We discuss the implications of our findings in the context of P-breaking TR-invariant system of Weyl nodes at nonzero chemical potential.

*This research was supported by the Australian Research Council Centre of Excellence in Future Low-Energy Electronics Technologies (project CE170100039) and funded by the Australian Government.*

**H71.00038: Hybrid Dispersion Dirac semimetal and Hybrid Weyl phases in Luttinger Semimetals: A dynamical approach**

SAYED ALI AKBAR GHORASHI (Presenter), William & Mary — We show that hybrid Dirac and Weyl semimetals can be realized in a three-dimensional Luttinger semimetal with quadratic band touching (QBT). We illustrate this using periodic kicking scheme. In particular, we focus on a momentum-dependent drivings (nonuniform driving) and demonstrate the realization of various hybrid Dirac and Weyl semimetals. We identify a unique hybrid dispersion Dirac semimetal with two nodes, where one of the nodes is linear while the other is dispersed quadratically. Next, we show that by tilting QBT via periodic driving and in the presence of an external magnetic field, one can realize various single/double hybrid Weyl semimetals depending on the strength of external field. Finally, we note that in principle, phases that are found in this work could also be realized by employing the appropriate electronic interactions.


*NSF DMR-1455233 CAR, ARO W911NF-18-1-0290, ONR.*

**H71.00039: WITHDRAWN ABSTRACT**

**H71.00040: 3D quantum Hall effect: Theories and recent progress**

FANG QIN, Southern University of Science and Technology, CHUNMING WANG, Shanghai Normal University, HAIZHOU LU (Presenter), Southern University of Science and Technology, XINCHENG XIE, Peking University — The quantum Hall effect is one of the most important discoveries in condensed matter physics. Usually, the quantum Hall effect happens in 2D. A 3D quantum Hall effect has been a long-sought phase of matter. Recently, the quantized Hall resistance has been observed 3D crystals of Cd3As2 and ZrTe5 and can be attributed to the Weyl orbit and charge density wave mechanisms, respectively. In this talk, we will introduce the theories and recent progress of 3D quantum Hall effect.
**H71.00041: Point contact Andreev reflection spectroscopy on possible chiral superconductor UTe$_2$**

SEUNGHUN LEE (Presenter), XIAOHANG ZHANG, SHENG RAN, RICHARD GREENE, University of Maryland, College Park, NICHOLAS BUTCH, National Institute of Standards and Technology, JOHNPIERRE PAGLIONE, ICHIRO TAKEUCHI, University of Maryland, College Park — Recent findings on a heavy-fermion superconductor, UTe$_2$ such as 1) an exceptionally large and anisotropic upper critical field, 2) a large residual Sommerfeld coefficient, 3) the reentrant superconducting phase in a high magnetic field, and 4) pressure-enhanced superconductivity, have attracted great attention as indication of spin-triplet superconductivity. Scanning tunneling microscopy/spectroscopy measurements and microwave surface impedance measurement on UTe$_2$ have suggested presence of the chiral edge state and normal fluid at the surface as evidence for the chiral spin-triplet pairing symmetry of the superconducting order parameter in UTe$_2$. To further investigate the superconducting order parameter, we are performing point contact Andreev reflection (PCAR) measurements on single-crystal UTe$_2$. PtIr and Nb tips are used to form N(I)/S and S(I)/S point-contact junctions, respectively. Evolution of conductance spectra as a function of temperature, magnetic field, and tip pressure will be discussed.

*This work was supported by AFOSR No. FA9550-14-10332.

**H71.00042: A New Frontier in Superconductivity: a Study of Hybridized Gold Clusters**

AJIT HIRA (Presenter), JOSE PACHECO, MATILDA FERNANDEZ, BRIDGET ORTIZ, Northern New Mexico College, TOMMY CATHEY, Lockheed Information Systems — In this research we utilize a combination of the tools of ab initio quantum mechanics and the tools of molecular dynamics, the Hubbard Model to study clusters of the compounds Au$_m$X$_n$ (X = atom of a different species; 1 <= m <= 10; and 1 <= n <= 10). We also looked for enhanced absorption characteristics that have sometimes been found at sub-gap frequencies when coupling is decreased. Topological superconductors are of great interest because of the active ongoing experimental efforts to study exotic physics such as Majorana zero modes. These systems have excitations with non-Abelian exchange statistics, which can be a path to quantum information processing. Our calculations reveal two of the signatures of superconductivity at temperatures close room temperature, but not all the signatures. Further calculations are planned in attempts to place our findings on a more firm footing. Such calculations are important in light of the recent reports of room-temperature superconductivity from experimentalists in India. We also discuss the possibility of superconductivity mechanisms other than the formation of cooper pairs.

*The New Mexico AMP program, funded by the NSF, supported some of our work.*
Topological semimetals exhibiting Dirac and Weyl fermions, which support low-energy quasi-particles in condensed matter physics, have been attracting intense research interest because of the exotic properties they possess like high magnetoresistance and high carrier mobilities. The transition metal diarsenides such as MoAs$_2$ and WAs$_2$ have been reported to feature very large magnetoresistance suggesting the possibility of topological quantum state in these materials. Here, we present the systematic electronic structure measurements of TAs$_2$ (T = Mo, W) by using angle-resolved photoemission spectroscopy (ARPES) complemented by first-principles calculations. We observe a single Dirac surface state in MoAs$_2$, which switches to trivial state for different cleaving surface. Interestingly, no Dirac surface state is observed in WAs$_2$, despite its high magnetoresistance, highlighting the role of spin-orbit coupling in the electronic structure. Our study thus provides a new perspective on how cleavage plane and spin-orbit coupling drive changes in the electronic structures in low-symmetry systems.

*This project is supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0415 and the National Science Foundation (NSF) CAREER award DMR-1847962.
**H71.00044: Long-Lived Quantum Well State Excitation and Surface Photovoltage Interplay in Topological Insulator**

SAMUEL CIOCYS (Presenter), ALESSANDRA LANZARA, RYO MORI, University of California, Berkeley — Topological insulators with Fermi levels doped into the bulk-gap exhibit strong surface band-bending and long-lived surface photovoltage (SPV) effects. Furthermore, in-situ surface doping of the topological insulators Bi2Se3 and Bi2Te3 can lead to strong Rashba-split quantum well states. In this study, we have combined bulk-doping and surface-doping to obtain both a strong surface photovoltage and spin-momentum locked quantum well states. Remarkably, Time- and angle-resolved photoemission spectroscopy reveals an additional pump-induced quantum well state that persists for 100s of picoseconds and coincides with the surface photovoltage, as well as time-dependent modifications to the quantum well states. Our work demonstrates that topological insulators are an exemplary foundation for tunable spin-textures with complex dynamics.

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**H71.00045: Kagome bands disguised in a coloring-triangle lattice**

SHUNHONG ZHANG (Presenter), University of Science and Technology of China, MENG KANG, Wuhan University, HUAQING HUANG, University of Utah, WEI JIANG, University of Minnesota, XIAOJUAN NI, University of Utah, LEI KANG, Beijing Computational Science Research Center, SHUNPING ZHANG, HONGXING XU, Wuhan University, ZHENG LIU, Tsinghua University, FENG LIU, University of Utah — The kagome bands hosting exotic quantum phases generally and understandably pertain only to a kagome lattice. This has severely hampered the research of kagome physics due to the lack of real kagome-lattice materials. Interestingly, we discover that a coloring-triangle (CT) lattice, named after color-triangle tiling, also hosts kagome bands. We demonstrate first theoretically the equivalency between the kagome and CT lattices, and then computationally in photonic (waveguide lattice) and electronic (Au overlayer on electride Ca2N surface) systems by first-principles calculations. The theory can be generalized to even distorted kagome and CT lattices to exhibit ideal kagome bands. Our findings open an avenue to explore the alluding kagome physics.

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**H71.00046: Observation of Dirac state in DySb**  
KLAUSS DIMITRI (Presenter), MD MOFAZZEL HOSEN, GYANENDRA DHAKAL, Univ of Central Florida, BAOKAI WANG, Physics, Northeastern University, FIROZA KABIR, CHRISTOPHER SIMS, SABIN REGMI, Univ of Central Florida, ERIC BAUER, FILIP RONNING, Condensed Matter and Magnet Science Group, Los Alamos National Laboratory, ARUN BANSIL, Physics, Northeastern University, MADHAB NEUPANE, Univ of Central Florida — Extreme magnetoresistance (XMR), magnetic and structural phase transition, and possible non-trivial topological phases in the rare-earth monopnictide family have recently invigorated intense research interest. Recent reports have experimentally revealed the presence of a Dirac-like semimetallic phases in some lighter rare earth monopnictide materials. Here we present a systematic ARPES study as well as first-principles calculations of DySb, a potential candidate for hosting a Dirac semi-metal phase. Our studies reveal two hole-like Fermi surface pockets present at the zone center (Gamma) point as well as two elliptical electron-pockets present in the zone corner (X) point of the Brillouin zone (BZ). Interestingly, Rashba-split states are observed at the (X) point of the BZ in a certain momentum direction, which is further supported by our first-principles calculations. A Dirac state is also observed at the (X) point of the BZ in the vicinity of the magnetic transition temperature. Our study opens a new direction to look for Dirac semi-metal states in other members of the rare earth monopnictide family.

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**H71.00047: Infrared absorptions in gate-tuned twisted bilayer graphene**  
KWANGNAM YU, Univ of Seoul, NGUYEN VAN LUAN, TAESOO KIM, Center for Integrated Nanostructure Physics, Institute for Basic Science (IBS), Sungkyunkwan University, JIWON JEON, JIHO KIM, Univ of Seoul, PILKYUNG MOON, New York University Shanghai and NYU-ECNU Institute of Physics at NYU Shanghai, YOUNG-HEE LEE, Center for Integrated Nanostructure Physics, Institute for Basic Science (IBS), Sungkyunkwan University, EUNJIP CHOI (Presenter), Univ of Seoul — We show that the infrared transmission spectrum of electrically gated twisted bilayer graphene (TBG) manifests dramatic changes such as the splitting of the interlinear-band absorption step, the shift of the inter-van Hove singularity transition peak, and the emergence of a very strong intravalence (intraconduction) band transition. These anomalous optical behaviors demonstrate that non-rigid band reconstruction occurs by the ion-gel gating due to layer-dependent Coulomb screening that is confirmed by our band structure calculations. We discuss the implications of such effect on the superconductivity of TBG, and also on possible applications as electro-optical device.
We theoretically investigate periodically driven two dimensional semimetal in high frequency regime and demonstrate the possibility of realizing both Floquet Topological Insulator featuring Floquet edge states and Floquet higher order topological insulating phase, accommodating topological corner modes. Topological phase transition takes place with the external drive where Chern number changes from +1 to -1 with the change of drive amplitude in case with broken time-reversal symmetry (T) due to circularly polarized light. When discreet four-fold rotation symmetry (C_4) is broken by adding a mass perturbation alongwith broken T, the quadrupolar moment Q_{xy} is found to have a quantized value 0.5 and topological corner modes arise in the system which is characterization of second order topological insulator. The nature of the Floquet corner modes with the increase of external drive is examined.
**H71.00049: Higher-order Topological Phases in Dynamical Optical Lattices**

HAIPING HU (Presenter), George Mason Univ, BIAO HUANG, Physics and Astronomy, University of Pittsburgh, ERHAI ZHAO, George Mason Univ, W.VINCENT LIU, Physics and Astronomy, University of Pittsburgh — We propose a versatile framework to dynamically generate Floquet higher-order topological insulators by multi-step driving of topologically trivial Hamiltonians. Two analytically solvable examples are used to illustrate this procedure to yield Floquet quadrupole and octupole insulators with zero and/or \( \pi \)-corner modes protected by mirror symmetries. Furthermore, we introduce dynamical topological invariants from the full unitary return map and show its phase bands contain Weyl singularities whose topological charges form dynamical multipole moments in the Brillouin zone. Combining them with the topological index of Floquet Hamiltonian gives a pair of \( \mathbb{Z}_2 \) invariant \( \nu_0 \) and \( \nu_\pi \) which fully characterize the higher-order topology and predict the appearance of zero- and \( \pi \)-corner modes. Our work establishes a systematic route to construct and characterize Floquet higher-order topological phases.

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H71.00050: Stable Higgs Modes in Fulde-Ferrell-Larkin-Ovchinnikov States*  
ZHAO HUANG (Presenter), Los Alamos National Laboratory, CHIN-SEN TING, Texas Center for Superconductivity, University of Houston, JIAN-XIN ZHU, SHIZENG LIN, Los Alamos National Laboratory — Higgs boson is an elementary particle in the Standard Model that was discovered experimentally in 2012. The Higgs boson is massive thus requiring a huge particle collider to enable its discovery. An elementary excitation, analogous to Higgs boson, can also appear in superconductors as a consequence of the U(1) symmetry breaking. Akin to its cousin in particle physics, the Higgs boson in superconductors is very massive, which renders it short lived by decaying into quasiparticle continuum. This raises a question of how to stabilize the Higgs mode in superconductors. Here we study the Higgs mode in thin-film superconductors with spatially inhomogeneous superconducting order parameter, known as the Fulde-Ferrell-Larkin-Ovchinnikov state. By deriving an effective action for the small amplitude fluctuation in the ground state manifold, we obtain the dispersion for the Higgs mode. We find that the Higgs mode becomes massless and more stable at finite momentums.

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H71.00051: Superconductivity Suppression in Disordered Films: Interplay of Proximity to the Two- and Three-Dimensional Localization  
DANIIL ANTONENKO (Presenter), MIKHAIL SKVORTSOV, Skolkovo Institute of Science and Technology — We revisit the problem of superconductivity suppression in homogeneously disordered thin films. Andersons theorem stating that the critical temperature is insensitive to the degree of disorder is violated in the vicinity of the Anderson localization transition. For strongly disordered films, the interplay between disorder and interaction effectively suppresses the BCS coupling constant, thereby reducing the critical temperature. For strictly 2D films, superconductivity suppression is coming from large scales (similar to the 2D localization), and summation of the leading logarithms can be performed with the help of Finkelsteins renormalization group. For thicker and sufficiently dirty films, there exists an additional effect originating from small scales (similar to the 3D localization). We calculate the corresponding contribution to the shift of the critical temperature and discuss its importance in the context of experimental situation.

H71.00052: WITHDRAWN ABSTRACT —
**H71.00053: Shape-driven conductivity in graphene**  
**BENJAMIN KATZ** (Presenter), **VINCENT CRESPI**, Pennsylvania State University — A graphene surface is presented which has a non-vanishing density of states at the Fermi level. This is driven by defects in the sheet structure: these defects are solely odd-membered rings, forced upon the system by topological constraints due to its shape, which is a series of cones and saddles. These defects sufficiently distort the electronic structure of pure graphene such that the density of states at the Fermi level is significant. The system, physically, is globally flat--there is no net gaussian curvature--and the density of states is calculated via first principles. The system further possesses multiple stable surface configurations accessible via mechanical inversion of the cones, each with different densities of states.

*Research conducted under support from the 2DCC-MIP at Penn State, funded by NSF grant DMR-1539916.*

**H71.00054: Electric-field screening in multilayer graphene**  
**NIKITA TEPLIAKOV** (Presenter), **QUANSHENG WU, OLEG V. YAZYEV**, Ecole Polytechnique Federale de Lausanne — Electronic properties of multilayer graphene are now routinely controlled using out-of-plane applied electric fields thus enabling novel electronic and optoelectronic devices. In this work, we perform first-principles calculations with explicitly applied external electric field of varying strength on a large number of multilayer graphene models including twisted configurations. We show that multilayer graphene with $N > 3$ layers features a highly nonlinear electric-field screening and nonsymmetric distribution of the electrostatic potential. We further develop a highly accurate parameterization of the tight-binding model for describing multilayer graphene that includes both the electric-field screening and crystal-field splitting effects. Our work is important for the design of devices based on multilayer graphene as it provides quantitative description of the electric-field screening in this system.

**H71.00055: First Principles dielectric spectroscopy of graphene in a tera-Hz frequency region**  
**TOMOYUKI HAMADA** (Presenter), **JUN NARA, TAKAHISA OHNO**, International Center for Materials Nanoarchitechtonics, National Institute for Materials Science — The complex dielectric function $\varepsilon_1 + i\varepsilon_2$ of graphene were calculated from its electronic structure by using a first principles broadband dielectric spectrometer *UVSOR* (Universal Virtual Spectrometer for Optoelectronic Research) [1-3]. The $\varepsilon_2$ was calculated by considering the direct inter-band transitions of electrons of graphene between its conduction and valence bands including those between the two-hold degenerated bands at its Dirac point. Calculations showed that the $\varepsilon_2$ of graphene is proportional to $1/\omega$ ($\omega$ is incident photon frequency) in a low frequency region where the electron transitions in the Dirac cone occurs and that it positively diverges as $\omega \to 0eV$. The optical spectra of graphene in a frequency region from 1 to 30 tera (T) Hz were calculated. Calculated optical absorption coefficients showed that graphene is a weak absorber of THz electro-magnetic waves. Details of calculations and calculation results will be given in the presentation.

*This work was supported by Innovative Science and Technology Initiative for Security, ATLA, Japan.*
**H71.00056: Stokes and anti-Stokes Raman scattering in mono- and bilayer graphene**  
CONG XIN (Presenter), PING-HENG TAN, State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences — Stokes and anti-Stokes Raman spectroscopy associated with the intervalley double resonance (DR) process in carbon materials is a unique technique to reveal the relationship between their characteristic electronic band structures and phonon dispersion. Here, we report the Stokes and anti-Stokes Raman scattering of the 2D mode in pristine graphene. The excitation energy ($E_{ex}$)-dependent frequency discrepancy between anti-Stokes and Stokes components of the 2D mode ($\Delta \omega(2D)$) is observed, which is in good agreement with the theoretical results. $E_{ex}$-dependent $\Delta \omega(2D)$ is attributed to the nonlinear dispersion of the in-plane transverse optical (iTO) phonon branch near the K point, confirmed by the nonlinear $E_{ex}$-dependent frequency of the 2D mode ($\omega(2D)$) in the range of 1.58–3.81 eV. The wavevector-dependent phonon group velocity of the iTO phonon branch is directly derived from $\Delta \omega(2D)$. We also report Stokes and anti-Stokes Raman scattering of the D mode in defected graphene and the 2D mode in bilayer graphene associated with intervalley DR Raman processes.

**H71.00057: Progress in quantum transport study of magic-angle twisted bilayer/bilayer graphene**  
HYEON-WOO JEONG (Presenter), JINHO PARK, SU-BEOM SONG, JONGHWAN KIM, Pohang Univ of Sci & Tech, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, GIL-HO LEE, Pohang Univ of Sci & Tech — Magic-angle twisted bilayer/bilayer graphene (TBBG) has shown various kinds of correlated electronic phases including superconductivity, ferromagnetism, Mott insulator [1, 2]. First, we discuss our dry transfer technique for making atomically clean TBBG with so-called tear-and-stack process. In our experiment, we measured the electron-electron interaction induced Mott insulating state at half fillings. We also observed the signature of superconducting phase near Mott insulating phase, and investigated by measuring temperature dependence and magnetic field dependence of current-voltage characteristics. As twist angle uniformity is crucial to form a macroscopic superconducting phase [3], we discuss our efforts and progress in realizing more homogeneous twist angle in TBBG devices.

REFERENCES:
H71.00058: Hydrodynamic Transport Theory of a non-Galilean invariant Electron Liquid*
ANTON ANDREEV, University of Washington, Seattle, SONGCI LI (Presenter), ALEX LEVCHENKO, University of Wisconsin - Madison — We develop a hydrodynamic transport theory of a non-Galilean invariant electron liquid in the presence of smooth inhomogeneities with emphasis on graphene. We computed the transport coefficients near charge neutrality point and showed a break down of the Wiedemann Franz law, resembling the observations in Crossno et al. Science 351, 1058, (2016). We studied magnetotransport phenomena and showed that the magnetoresistance is positive and quadratic in weak fields. Lastly, we examined magnetothermal transport phenomena and derived the Nernst and Ettingshausen coefficients.

*The work was suppported by DOE-BES Award No. DE-FG02-07ER46452 (A. A), NSF Grants No. DMR-1653661 and No. DMR-1743986 (S. L and A. L).

H71.00059: Growth Evaluation of Wafer-based Au-catalyzed GaAs Nanowires on GaAs(111)B Substrates with Different Patterning Conditions using µ-Raman Characterization
SE-JEONG PARK (Presenter), Korea ITS Application R&D Center, Korea I.T.S. Co., Ltd., JEUNG HUN PARK, Andlinger Center for Energy and the Environment, Princeton University — We report the relation between the catalyst patterning conditions and the intensity of the 1st order Raman active modes in Au-catalyzed GaAs nanowires. Au-patterned GaAs(111)B substrates were prepared by e-beam Litho with varying patterning conditions and GaAs NWs were grown via VLS process using a solid-source MBE. To understand the effects of the preparation conditions and resulting morphologies on the optical characteristics of 1st order TO and LO phonon modes of GaAs, the NWs were characterized by µ-Raman and SEM as a function of the e-beam dose rate, inter-dot spacing, and pattern size. The Ensembles of single crystalline NWs covered with different Au-thickness showed a downshift and asymmetric broadening of the TO and LO phonon peaks relative to GaAs bulk modes. The TO and LO intensity were clearly increased as well as the relatively higher peak shift and broadening of Raman spectra from the 100 nm pattern in response to the dose rate change. We have shown that not only the identifications of the changes in GaAs LO and Arsenic anti-site peaks are good indicators to characterize the quality of as-grown GaAs NWs but Raman spectroscopy is a powerful tool for characterizing chemical, structural, and morphological information of as-grown NWs within the supporting substrate.
H71.00060: Enabling Novel Approach to a controlled Fabrication of Freestanding Nanomaterials using Two Direct-Writing Technologies  KEITH MCCORMACK (Presenter), NICK SCHAPER, Saint Louis University, NICK LAVRIK, IVAN KRAVCHENKO, Oak Ridge National Laboratory, MARIA F. PANTANO, University of Trento, IRMA KULJANISHVILI, Saint Louis University — Owing to their unique properties, nanoscale materials, such as nanotubes, nanowires, and 2D layered nanomaterials are emerging as key building blocks of the next generation technologies. Practical implementation of such nanomaterials necessitates their successful incorporation with well-established processes for fabrication of electrical and mechanical devices, often integrated with silicon microstructures. Typically, nanomaterials are synthesized on host substrates and transferred onto the target substrates or devices. In this work, we combine mask-free “direct-write patterning” (DWP) approach for synthesis of nanomaterials at desired locations, and the direct laser writing (DLW) technique, which is based on 2-photon polymerization, to allow for the fabrication of micro-bridge structures with sub-micrometer resolution and nanolithographic patterning of catalysts for in-situ growth of nanoscale 1D or 2D materials. We will discuss our recent results on controlled preparation of 1D and 2D nanostructures with desired morphology using DWP and DLW, as well as the characterization data from Raman, AFM, and SEM measurements. Acknowledgement. A portion of this research was conducted at the ONRL Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

H71.00061: Thermal Hall Effect Measurements on U\textit{Pt}$_3$*  LUKE PRITCHARD-CAIRNS (Presenter), ANDREW HUXLEY, Physics, University of Edinburgh — The heavy fermion material U\textit{Pt}$_3$ is arguably the best understood unconventional superconductor to date, and has been shown to possess multiple superconducting phases [1,2]. Despite this, the symmetry of the superconducting order parameter is still somewhat up for debate, with experimental evidence for both the $E_{2u}$ [3] and $E_{1u}$ [4] representations.

Recent theoretical work has shown that the superconducting state of U\textit{Pt}$_3$ should exhibit a measurable thermal Hall effect [5], the magnitude of which is proportional to the orbital momentum of the superconducting order parameter. This implies that the thermal Hall coefficient should change when moving between the A and B phases. Furthermore, a sufficiently accurate measurement of the thermal Hall effect may be able to distinguish between the $E_{2u}$ and $E_{1u}$ representations.


*I acknowledge studentship funding from EPSRC under the grant number EP/P013686/1.
H71.00062: Muon spin rotation and relaxation in Pr$_{1-x}$Nd$_x$Os$_4$Sb$_{12}$: superconductivity and magnetism in Pr-rich alloys* PEI-CHUN HO (Presenter), Physics, California State University, Fresno, DOUGLAS E MACLAUGHLIN, Physics, University of California, Riverside, M BRIAN MAPLE, Physics, University of California, San Diego, LEI SHU, Physics, Fudan University, ADRIAN HILLIER, ISIS Neutron and Muon Sources, Science & Technology Facilities Council, OSCAR BERNAL, Physics, California State University, Los Angeles, TATSUYA YANAGISAWA, Physics, Hokkaido University, P. K BISWAS, ISIS Neutron and Muon Sources, Science & Technology Facilities Council, JIAN ZHANG, CHENG TAN, Physics, Fudan University, SHOJI D HISHIDA, Physics, California State University, Fresno, TAYLOR MCCULLOUGH-HUNTER, Physics, Hokkaido University — The Pr-rich end of the alloy series Pr$_{1-x}$Nd$_x$Os$_4$Sb$_{12}$ has been studied using muon spin rotation and relaxation. The end compound PrOs$_4$Sb$_{12}$ is an unconventional heavy-fermion superconductor, which exhibits a spontaneous magnetic field in the superconducting phase associated with broken time-reversal symmetry. No spontaneous field is observed in the Nd-doped alloys for x ≥ 0.05. The superfluid density is insensitive to Nd concentration, and no Nd$^{3+}$ static magnetism is found down to the lowest temperatures of measurement. Together with the slow suppression of the superconducting transition temperature with Nd doping, these results suggest anomalously weak coupling between Nd spins and conduction-band states. [1]


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H71.00063: Elastic properties of hidden order in URu$_2$Si$_2$ are reproduced by staggered nematic order* JARON KENT-DOBIAS (Presenter), MICHAEL MATTY, BRAD J RAMSHAW, Cornell University — We develop a phenomenological mean field theory of the hidden order phase in URu$_2$Si$_2$ as a "staggered nematic" order. Several experimental features are reproduced when the order parameter is a nematic of the B$_{1g}$ representation, staggered along the c-axis: the topology of the temperature-pressure phase diagram, the response of the elastic modulus (C$_{11}$ – C$_{12}$) / 2 above the hidden-order transition at zero pressure, and orthorhombic symmetry breaking in the high-pressure antiferromagnetic phase. In this scenario, hidden order is characterized by broken rotational symmetry that is modulated along the c-axis, the primary order of the high-pressure phase is an unmodulated nematic state, and the triple point joining those two phases with the high-temperature paramagnetic phase is a Lifshitz point.

*This research was funded in part by NSF grants DMR-1719490 and DMR-1719875.
H71.00064: Electron temperature modulation at the 2D electron system in the GaAs/AlGaAs under microwave photoexcitation*  THARANGA NANAYAKKARA (Presenter), U. KUSHAN WIJEWARDENA, ANNIKA KRIISA, SAJITH WITHANAGE, RAMESH MANI, Georgia State University, CHRISTIAN REICHL, WERNER WEGSCHEIDER, Laboratorium für Festkörperphysik, ETH Zürich — The magnetotransport measurements have been performed on the 2D electron system at GaAs/AlGaAs heterojunctions to understand the influence of the microwave photoexcitation on the spin splitting of the Shubnikov-de Haas oscillations at low temperatures (<1 K). The purpose of the study is to examine the temperature modulation of the electrons under microwave photoexcitation by examining observable spin splitting- and variation thereof under photoexcitation- at high filling factors. In this study, a multicomponent Lifshitz-Kosevevich\(^1\) type function has been applied to describe the magnetotransport data, and relevant results will be presented here.


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H71.00065: Translation symmetry broken groundstates near quantum hall edge at \(\nu = 2\)*

AMARTYA SAHA (Presenter), GANPATHY MURTHY, Univ of Kentucky — Edge reconstruction for the 2D electron gas in a magnetic field at \(\nu = 2\) has been studied by Dempsey, Gelfand, and Halperin[1], who found that when the confining potential is softened the two spin polarized channels spatially separate. Using the time dependent Hartree Fock (TDHF) method we found that the collective excitations of this type of groundstate becomes unstable if we decrease the edge potential’s slope beyond certain limit. This analysis is similar to what Franco and Brey[2] did for the \(\nu = 1\) edge. We found two groundstates, charge density wave (CDW) and spin textured edge (STE). These phases not only have lower energy but also screens the background potential better than than the earlier proposed groundstate[1]. Finally, we study the collective excitations of these phases using TDHF method.


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H71.00066: Two- and three-electron bubbles in Al$_x$Ga$_{1-x}$As/Al$_{0.24}$Ga$_{0.76}$As quantum wells*
XIAOJUN FU (Presenter), QIANHUI SHI, MICHAEL ZUDOV, University of Minnesota, GEOFF C GARDNER, JOHN WATSON, MICHAEL MANFRA, Purdue University — We report on transport signatures of eight distinct bubble phases in the $N = 3$ Landau level of an Al$_x$Ga$_{1-x}$As/Al$_{0.24}$Ga$_{0.76}$As quantum well with $x = 0.0015$. These phases occur near partial filling factors $\nu \approx 0.2$ (0.8) and $\nu \approx 0.3$ (0.7) and have $M = 2$ and $M = 3$ electrons (holes) per bubble, respectively. We speculate that a small amount of alloy disorder in our sample helps to distinguish these broken symmetry state in low-temperature transport measurements.

*The work at Minnesota (Purdue) was supported by the US Department of Energy, Office of Science, Basic Energy Sciences, under Award No. ER 46640-SC0002567 (DE-SC0006671). A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreements No. DMR-115749 and No. DMR-1644779 and the State of Florida.

H71.00067: Ballistic electrons splashing down in a Fermi sea of a 1-dimensional quantum Hall liquid*
RAMIRO RODRIGUEZ (Presenter), FRANCOIS PARMENTIER, SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette cedex, France, DARIO FERRARO, Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16146, Genova, Italy & SPIN-CNR, Via Dodecaneso 33, 16146, Genova, Italy, PREDEN ROLLEAU, SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette cedex, France, ULF GENNSER, ANTONELLA CAVANNA, Centre de Nanosciences et de Nanotechnologies (C2N), CNRS, Université Paris-Sud, Université Paris-Saclay, 91120 Palaiseau, France, MAURA SASSETTI, Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16146, Genova, Italy & SPIN-CNR, Via Dodecaneso 33, 16146, Genova, Italy, FABIEN PORTIER, SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette cedex, France, DOMINIQUE MAILLY, Centre de Nanosciences et de Nanotechnologies (C2N), CNRS, Université Paris-Sud, Université Paris-Saclay, 91120 Palaiseau, France, PATRICE ROCHE, SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette cedex, France — The one-dimensional, chiral and dissipationless edge channels of the quantum Hall effect are good candidates to form the electrical analogue of optical fibers, which allows to coherently manipulate the propagation of single electronic wave packets. However Coulomb interactions between neighboring edge channels can lead to energy relaxation. We explore this phenomenon by measuring the energy distribution function of quasiparticles emitted at well-defined energy in an edge channel at filling factor $\nu = 2$. Our setup relies on a pair of electrostatically defined quantum dots, used as energy-resolved emitter and detector, tunnel coupled to an edge channel. We show that, on sub-micron lengths, quasiparticles undergo a strong relaxation with a survival probability dropping exponentially with their energy. Remarkably, this relaxation preserves the position and width of the quasiparticle peak in the energy distribution function. Furthermore, at intermediate lengths, we observe a marked revival of the peak at high injection energy. Our findings are qualitatively compatible with the conventionally considered theories, however new ingredients such as dissipation seem crucial in order to provide a more quantitative comparison.

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Single crystal growth of Bi2212 with different Bi/Sr ratio for terahertz waves emitters

MAYU NAKAYAMA (Presenter), TAKANARI KASHIWAGI, TAKAYUKI IMAI, SYUNGO NAKAGAWA, GENKI KUWANO, YUKINO ONO, TOMOYUKI SHIZU, YOUTA KANEKO, SHINJI KUSUNOSE, JEONGHYUK KIM, MANABU TSUJIMOTO, University of Tsukuba, TAKASHI YAMAMOTO, QuTech Delft University of Technology, HIDETOSHI MINAMI, University of Tsukuba, TAKASHI MOCHIKU, National Institute for Materials Science, HIRONORI NAKAO, Institute of Materials Structure Science, High Energy Accelerator Research Organization, KEK, HIROSHI EISAKI, SHIGEYUKI ISHIDA, The National Institute of Advanced Industrial Science and Technology, YUKIO HASEGAWA, The university of Tokyo, RICHARD KLEMM, University of Central Florida, KAZUO KADOWAKI, University of Tsukuba — The Bi-based copper oxide high-temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) has a nonstoichiometry composition expressed as Bi$_{2+x}$Sr$_{2-x}$CaCu$_2$O$_{8+\delta}$. We consider that the disorder of the insulating layer due to this nonstoichiometric composition (Bi/Sr) affects the CuO$_2$ layer and consequently changes in the superconducting transition temperature and the in-plane residual resistance. The intrinsic Josephson junctions (IJJs) constructed in Bi2212 have been thought to be affected by a crystallographic disorder. For the application of Bi2212 single crystals to terahertz wave emitters (Bi2212-THz emitters) based on IJJs, we evaluated the disorder mainly from the viewpoint of crystal structure. Specifically, we prepared single crystals of Bi2212 with different Bi/Sr ratio and subsequently the oxygen was controlled by post annealing. And the physical properties of the crystals have been examined by using X-ray techniques. We also study the device characteristics of Bi2212-THz emitters made by different ratio of (Bi/Sr) and the obtained results are compared at this moment. We will discuss these characteristics in details in the meeting.
H71.00069: Quantum Signatures in Superconducting-to-Normal Switching Experiments on a Multigap Superconducting Junction* ROBERTO RAMOS (Presenter), University of the Sciences, STEVEN CARABELLO, Penn State Harrisburg, JOSEPH LAMBERT, National Radio Astronomy Observatory, WENQING DAI, Apple, DANIEL CUNNANE, NASA Jet Propulsion Laboratory, QI LI, Pennsylvania State University, KE CHEN, XIAOXING XI, Temple University — We review the results of our tunneling spectroscopy experiments\(^1\) which demonstrated microwave resonant activation in a multi-gap superconductor. We had measured histograms of superconducting-to-normal switching events in hybrid Josephson heterojunctions (MgB\(_2\)/I/Pb and MgB\(_2\)/I/Sn) at sub-Kelvin temperatures. When microwaves were coupled to the junctions, we observed peaks superposed on the histograms - features consistent with microwave resonant activation. This demonstrates microwave resonant activation in a novel superconducting multigap system where one superconducting electrode is multi-gap and the other superconducting electrode is single-gap. In this system, we have observed signatures of quantum behavior such as the Lorentzian shape of the escape rate enhancement, a saturation in the width of the switching current distribution at low temperatures, and evidence of multi-photon transitions.


*R.C. Ramos acknowledges support from the National Science Foundation DMR 1555775 and the Charles Kaufman Foundation.*
H71.00070: Nonlinear behaviour of confined superfluid helium.∗ EMIL VARGA (Presenter), VAISAKH VADAKKUMBATT, ALEXANDER SHOOK, JOHN DAVIS, Univ of Alberta — Superfluid Helmholtz resonators provide a versatile tool for the study of both superfluid $^4$He and $^3$He under microscopic confinement. They have proven to be effective at measuring the superfluid fraction [1] and enabled detection of emergent phases under confinement in superfluid $^3$He [2]. We extend previous experiments into the strongly driven regime where the resonance is nonlinear. The nature of the nonlinear behaviour depends on the isotope of helium, and on the phase in superfluid $^3$He.

For superfluid $^4$He, the nonlinearity is due to turbulence, which at relatively high temperatures closely approximates two-dimensional turbulence of discrete point vortices even though the confinement is significantly larger than the coherence length.

For the case of superfluid $^3$He, the coherence length is comparable to the confinement and a new phase appears [2]. Here, the qualitative nature of the nonlinearity (i.e., nonlinear dissipation vs. Duffing resonance) changes with the superfluid phase, enabling phase identification.


∗The University of Alberta; Natural Sciences and Engineering Research Council, Canada (Grants RGPIN-04523-16, DAS-492947-16, CREATE-495446-17); and Canada Foundation for Innovation.

H71.00071: Dynamics of $^3$He in a quasi-1D environment using $^4$He-plated MCM-41: NMR Studies∗ CHAO HUAN, JOHNNY ADAMS (Presenter), MARC LEWKOWITZ, NAOTO MASUHARA, Department of Physics and NHMFL, University of Florida, DONALD CANDELA, Department of Physics and NHMFL, University of Massachusetts Amherst, NEIL SULLIVAN, Department of Physics and NHMFL, University of Florida — We utilize pulsed NMR techniques to study the dynamics of $^3$He atoms in quasi-1D. The quasi-1D structure was formed within the nanochannels of mesoporous MCM-41 plated with a monolayer of $^4$He. Measurements were carried out between 0.030K < T < 3.0K, with a $^3$He line density of 0.1Å⁻¹. Direct measurement of the nuclear spin magnetization as a function of temperature show the effect of degeneracy more pronounced in a quasi-1D system compared to 3D systems. Studies of the nuclear spin-lattice interaction show a characteristic peak at 2$T_F$, while the nuclear spin-spin interaction show unusual temperature dependencies below 0.5K.

∗This research was carried out at the National High Magnetic Field Laboratory's High B/T Facility which is supported by NSF Grant DMR 1644779 and by the State of Florida.
H71.00072: Enhancement of critical current density in a superconducting NbSe₂ step junction  
XIN HE (Presenter), YAN WEN, CHENHUI ZHANG, ZHIPING LAI, King Abdullah Univ of Sci & Tech (KAUST), EUGENE M CHUDNOVSKY, Physics Department, Lehman College and Graduate School, XIXIANG ZHANG, King Abdullah Univ of Sci & Tech (KAUST) — We investigate the transport properties of a NbSe₂ nanodevice consisting of a thin region, a thick region and a step junction. We find the critical current density has similar values for both the thin and thick regions away from the junction, while the critical current density of the thin region of the junction increases to approximately 1.8 times as compared with the values obtained for the other regions. We attribute such an enhancement of critical current density to the strong vortex pinning at the surface step.

H71.00073: Optimizing the Lumped Element Resonator via changing the total capacitance and the coplanar waveguide distance for effective magnon-photon coupling*  
YUZAN XIONG (Presenter), Electronic and Computer Engineering, Oakland University, YI LI, TOMAS POLAKOVIC, RALU DIVAN, JOHN PEARSON, Argonne National Laboratory, HONGWEI QU, Electronic and Computer Engineering, Oakland University, ZHILI XIAO, WAI-KWONG KWOK, Argonne National Laboratory, WEI ZHANG, Electronic and Computer Engineering, Oakland University, VALENTYN NOVOSAD, Argonne National Laboratory — Controllable superconducting quantum circuits with strong coupling strength is a key ingredient in the study of magnon-photon coupling in hybrid magnonic systems. The circuit's impedance is a crucial factor for optimizing the magnon-photon coupling as it strongly affects the current-flow pattern. Here, we explore the low-impedance lumped element resonator which is capacitively side-coupled to the signal line of a coplanar waveguide, by altering key parameters that were characterized with a triple-axis vector magnet at 1.5 K. The resonance frequencies are found to be inversely proportional to the circuit's total capacitance. The coupling strength is mostly affected by the distance between them. We identified a critical coupling strength, which suggests an optimal quality-factor along with a minimum insertion loss. Our studies reveal an alternative route to increase the susceptibility of magnon-photon coupling.

*The thin-film fabrication and low-temperature measurement were supported by the DOE, Materials Science and Engineering Division. The experimental design and analytical modeling were supported by AFOSR under grant no. FA9550-19-1-0254. The use of the CNM, an Office of Science user facility, was supported by the U.S. DOE, BES, under Contract No. DE-AC02-06CH11357.
**H71.00074: Transfer of Electron Exergy and Thermal Energy in Magnetic Field**

ANDREI SERGEEV (Presenter), US Army Rsch Lab - Adelphi, MICHAEL REIZER, 5614 Naiche Rd., Columbus, OH 43213, USA — Electrons placed in magnetic field create magnetization currents with kinetic and magnetic energy, which is an important part of the electron exergy. Even in the presence of an external thermal field the magnetization currents are dissipationless and, therefore, they do not produce entropy. However, temperature dependence of magnetization involve the magnetization currents into thermal phenomena in rather sophisticated way, which includes transformations of bulk currents into surface currents and interaction between magnetization currents. We review and revise the transfer of electron exergy and thermal energy in magnetic field, including Poynting vector, Onsager relations, Nernst and Ettingshausen effects in superconductors. Recent experiments with single magnetic vortices directly confirm our theoretical conclusions.

*The work is supported by the Army Research Laboratory. Research of AS was accomplished under Cooperative Agreement No. W911NF-18-2-0222.*

**H71.00075: Dependence of physical properties on Bi/Sr ration and oxygen content of Bi$_{2+x}$Sr$_{2-x}$CaCu$_2$O$_{8+\delta}$**

SYUNGO NAKAGAWA (Presenter), TOMOYUKI SHIZU, Univ of Tsukuba, HIRONORI NAKAO, Institute of Materials Structure Science, High Energy Accelerator Research Organization, TAKANARI KASHIWAGI, MAYU NAKAYAMA, JEONGHYUK KIM, TAKAYUKI IMAI, MANABU TSUJIMOTO, Univ of Tsukuba, YUKIO HASEGAWA, The university of Tokyo, SHIGEYUKI ISHIDA, HIROSHI EISAKI, The National Institute of Advanced Industrial Science and Technology, TAKASHI MOCHIKU, National Institute for Materials Science, KAZUO KADOWAKI, Univ of Tsukuba — In order to extract the fundamental physical properties of high transition temperature (high-$T_c$) superconductors, one needs to take account of the details of real materials which possibly affect their properties. In the case of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212), non-stoichiometry due to the intersubstitution between Bi and Sr atoms exists, yielding its composition Bi$_{2+x}$Sr$_{2-x}$CaCu$_2$O$_{8+\delta}$. Accordingly, the number of hole carries ($n_h$) as well the magnitude of chemical inhomogeneity depends on $x$ and $\delta$ (oxygen content). In order to evaluate the precise $x$- and $\delta$- dependence of the physical properties, high-quality single crystals of Bi2212 with $x=0.10, 0.15,$ and 0.20 were grown by the Travelling-Solvent Floating Zone (TSFZ) method. The $\delta$ values were systematically changed by annealing the as-grown crystals under various conditions. To evaluate $n_h$, we performed XAFS measurements, in which the pre-peak intensity of the oxygen K-edge absorption spectra is known to a measure of $n_h$. We have successfully established the relationship between $n_h$ and $T_c$ of the Bi2212 system with different amount of chemical inhomogeneity ($x$'s). The details of these characteristics will be presented in the meeting.
H71.00076: In-plane ordering of O vacancies in a high-\(T_c\) cuprate superconductor with compressed Cu-O octahedrons: an automated cluster expansion study  
YUNHAO LI  
(Presenter), SHIQIAO DU, ZHENGYU WENG, ZHENG LIU, Tsinghua University — A recently discovered 73K cuprate superconductor \(\text{Ba}_2\text{CuO}_{4.5}\) implies that intact CuO\(_2\) planes are not absolutely necessary in achieving high-T\(c\) superconductivity. Featuring an exceptional Jahn-Teller distortion, wherein the CuO\(_6\) octahedrons are compressed along the \(c\) axis, O vacancies in this material prefer to reside in the CuO\(_2\) plane, which significantly modify the 2D square lattice. By combining first-principles total energy calculation with the automated structure inversion method, the effective cluster interactions of O vacancies are mapped out. Around \(\delta=0.8\), where the superconductivity was observed experimentally, we predict that the O vacancies form a long-range order, which slice the CuO\(_2\) plane into 1D chains and two-leg ladders. The latter was not known to exist in other cuprates. A Monte Carlo simulation is performed based on the effective cluster interaction model, showing that such an ordering pattern is stable up to \(~900\) K. Our results put forth a concrete structural basis to discuss the underlying superconducting mechanism.

H71.00077: Superconductivity in PbBe Multilayer Thin Film*  
THOMAS NOTT (Presenter), JAMES G STOREY, JEFFERY TALLON, JOHN KENNEDY, Victoria Univ of Wellington — It was recently proposed by X. H. Zheng et al [1], that hetero-structures of Pb and Be would exhibit high-temperature superconductivity at 36K due to Beryllium's high Debye temperature and low mass. To investigate this we have alternately grown thin films of Pb and Be in a layered structure by the use of a vacuum evaporator. Layers were approximately 10nm each for a total film thickness of <100nm. Magnetisation measurements show a transition at \(~10\)K, slightly above the bulk T\(c\) of Pb, which persists to fields significantly higher than the critical field of Pb. This shows promise for Pb-Be layered systems and may be further improved with thinner, higher quality layers.


*Funded by the Macdiarmid Institute of New Zealand
H71.00078: Pressure effects on superconductivity and anomalous transition in triangular lattice CuIr$_2$Te$_4$* 

HUNG-DUEN YANG (Presenter), HUNG-CHENG WU, YI-CHIEH CHUNG, TING-WEL GUO, ZONG-HENG YANG, D. CHANDRASEKHAR KAKARLA, Natl Sun Yat Sen Univ, LIANGZI DENG, MELISSA GOOCH, CHING (PAUL) W CHU, Texas Center for Superconductivity, University of Houston — Geometrical spin-frustrated systems play an important role in condensed matter physics. Recently, a proposed charge-density-wave (CDW) along with superconductivity (SC) in CuIr$_2$Te$_4$ was reported [1] through the resistivity and magnetization measurements. It motivated us to further study the competitions between CDW and SC under external hydrostatic pressure. The CuIr$_2$Te$_4$ was synthesized by the solid-state reaction method and characterized using X-ray diffraction (XRD) and magnetization measurements. XRD pattern confirmed the major phase of CuIr$_2$Te$_4$ and the anomalous transition ($T_s \sim 200$ K) along with SC transition below $T_c \sim 3$ K in zero-field-cooling cycle was observed. The preliminary results are in agreement with the previous report [1]. Under the external pressure, both transitions ($T_s$ and $T_c$) exhibit a systematic change, suggesting that a significant competition between anomalous transition and SC occurs in CuIr$_2$Te$_4$. The nature of anomalous transition in CuIr$_2$Te$_4$ will be discussed.

Reference:


H71.00079: Structure and magnetism of Fe$_{68.8}$Pd$_{31.2}$*

ANUPAM SINGH (Presenter), SANJAY SINGH, School of Materials Science and Technology, Indian Institute of Technology (BHU), Indian Institute of Technology (BHU), RAJEV RAWAT, UGC-DAE Consortium for Scientific Research, Indore, DHANANJAI PANDEY, School of Materials Science and Technology, Indian Institute of Technology (BHU), Indian Institute of Technology (BHU) — Fe-Pd based magnetic shape memory alloys show magnetic as well as structural (martensitic) transition [1]. In the martensite phase these alloys exhibit large magnetic field induced strain about $\sim 3\%$ due to which these alloys can be used as magnetic actuators [2]. We present here the results of sample preparation, compositional analysis, X-ray diffraction (XRD) measurements and magnetic measurements. The sample is prepared by arc-meting technique and composition (Fe$_{67.4}$Pd$_{32.6}$) was verified through Energy Dispersive Analysis of X-rays. The Rietveld refinement shows that room temperature structure is cubic with space group Fm-3m and exhibit tetragonal phase at low temperature. The martensite transition observed around temperature T$\sim 235$ K, where a sharp drop in the magnetization is observed and also confirmed by low temperature XRD. A very low thermal hysteresis of the martensite phase transition makes this system important for various applications.

References

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**H71.00080: Tuning the electronic and magnetic properties of Heusler alloys: A theoretical and experimental investigation**

DANIEL WINES (Presenter), FATIH ERSAN, Univ of Maryland-Baltimore County, RABIN MAHAT, SHAMBHU K KC, SUDHIR REGMI, UPAMA KARKI, University of Alabama, PRAHALAD PADHAN, Indian Institute Of Technology, ARUNAVA GUPTA, PATRICK LECLAIR, University of Alabama, CAN ATACA, Univ of Maryland-Baltimore County — Half metallic Heusler alloys have attracted recent attention because they are suitable materials for information storage and spintronics applications. This work presents a detailed experimental and theoretical study on a series of Fe$_{3-x}$V$_x$Ge, Fe$_{3-x}$Cr$_x$Ge, Co$_2$Fe$_{1-x}$V$_x$Ge, and Co$_2$$_{2-x}$V$_x$FeGe (0 ≤ x ≤ 1) Heusler alloys. To study these alloys, we used the cluster expansion formalism, which uses density functional theory (DFT) calculated energies as a training set, and ultimately gives us the energetics of an alloyed system as a function of concentration. We employed DFT calculations at the GGA and GGA+U level to calculate the energetic stability and the structural, electronic, mechanical and magnetic properties of each alloyed system at specific alloying ratios. Experimental measurements for these materials such as stability, lattice parameter and magnetic moment are in agreement with our calculations. Our results also confirm the half metallicity of certain alloyed materials. The findings of this study not only confirm previous experimental measurements, but can aid future experimentalists and manufacturers in the synthesis of other Heusler alloys with specific desired properties.

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**H71.00081: Structure-Property Relationships in Nanocarbon-Al Composites Made by an Electrocharging Assisted Process**

MADELINE MORALES (Presenter), XIAOXIAO GE, CHRISTOPHER KLINGSHIRN, Materials Science & Engineering, University of Maryland, College Park, DANIEL COLE, US Army Research Laboratory, Aberdeen Proving Ground, LOURDES SALAMANCA-RIBA, Materials Science & Engineering, University of Maryland, College Park — Carbon nanostructures are a growing area of research due to their excellent mechanical, electrical and thermal properties. Electrocharging assisted processing of a novel class of materials, termed “covetics,” presents a practical option for macroscale production of nanocarbon-metal composites. This process incorporates carbon on the order of a couple weight percent in metals where carbon solubility is in the low ppm range. Increased tensile strength and electrical conductivity have been measured in Al covetics; however, there is minimal understanding of the structure-process-property relationship and there is high variability in measured properties among trials. We have found that the activated carbon precursor is converted to sp$^2$ graphitic carbon with increased crystallite size. XRD and XPS show no measurable formation of carbide phases. The local electromechanical behavior measured by nanoindentation and AFM gives insight into a fundamental understanding of the improved properties in covetics, and is used to improve the fabrication process for maximal increase in electrical conductivity and tensile strength.

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**H71.00082: Ab initio investigation of solid-solid interfaces**  
MICHAEL WOODCOX (Presenter), MANUEL SMEU, Binghamton University — Because a material can be engineered to satisfy a particular need through alloying, there are other properties of that material that may not be fully understood, or may be ignored entirely. While these materials may standalone as an excellent solution to a particular problem, when they interact with other materials it may drastically alter their effectiveness. In this work, we have used density functional theory (DFT) and *Ab Initio* Molecular Dynamics (AIMD) to investigate solder-substrate interfaces. This method is being developed to provide fundamental understanding of the atomic-scale interactions occurring at the solder joints and the impact that they have on the strength and stability of the interface. Using first principles to explore these larger systems we hope to provide a level of insight into the nature of soldering, the formation of intermetallic compounds, and an enhanced resolution of forces at the interface that would help to optimize industrial needs while also exploring the limits of system sizes that can be investigated using these methods.

**H71.00083: Magnetic and Microstructure Properties of Co-doped rapidly solidified Ni\textsubscript{50}Mn\textsubscript{25-x}Co\textsubscript{x}Ga\textsubscript{25} Heusler alloys**  
IMADDIN AL-OMARI (Presenter), Dept. of Physics, Sultan Qaboos University, Muscat PC 123, Oman — Cobalt-doped melt-spun ribbons of Ni\textsubscript{50}Mn\textsubscript{25-x}Co\textsubscript{x}Ga\textsubscript{25} were prepared to study the influence of cobalt on the magnetic properties of the NiMnGa based Heusler alloy. Bulk specimens were also prepared for a comparative study. The bulk specimens and the melt spun ribbons were annealed at 900 deg. C for 5 hours followed by quenching. Microstructural studies revealed an extensively twinned structure which is beneficial for magnetic field induced strain. The magnetization measurements showed a reduction in the moment with an increase in the cobalt content from 78.4 emu/g to 52.7 emu/g for Co (x=6) and Co (x=10), respectively. A reduction was also observed in the T\textsubscript{C} when cobalt content was increased from Co (x=6) (T\textsubscript{C} =386K) to Co (x=10) (T\textsubscript{C} =263K).

*We thank Sultan Qaboos University for the support provided during this study.*
H71.00084: Local structure analysis of long-period stacking ordered (LPSO) structure phase-containing Mg alloys by X-ray absorption spectroscopy*  MAIKO NISHIBORI (Presenter), KOHEI FUJINO, KAKERU NINOMIYA, Kyushu Univ — Long-period stacking (LPSO) type Mg alloy [1] has the structure modulation and concentration modulation of the atomic arrangement in long period, and is different from the hcp structure which is a pure Mg crystal structure. In LPSO-Mg alloy, kinks are formed due to the introduction of a significant difference in grain orientation in the crystal accompanying plastic deformation, which leads to material strengthening. However, the mechanism of kink formation and its strengthening has not yet been clarified. In this study, the changes in the local structure of solid solution atoms during the formation of LPSO-phase and the kink deformation were investigated by x-ray absorption spectroscopy. As a result, the central atom of L12 cluster of LPSO-phase contained in Mg alloy was identified, and the possibility of re-diffusion of solid solution atoms by kink deformation was suggested.

*Materials were provided by Prof. K. Hagiwara of Osaka University, Prof. M. Yamasaki and Prof. Y. Kawamura of Kumamoto University. XAS measurements were performed at SPring-8 BL27SU (2019B1433, 2019B1765) and SAGA-LS BL11 (1905029F). This work was supported by MEXT/JSPS KAKENHI, Grant Numbers JP19H05130.

H71.00085: Characterization of Fatigue with the Field Theory of Deformation and Fracture
CONOR MCGIBBONEY (Presenter), SANICHIRO YOSHIDA, NAOYA FUJISHIMA, SHUN TAKAHASHI, Chemistry and Physics, Southeastern Louisiana University, TOMOHIRO SASAKI, Mechanical Engineering, Niigata University — We conducted physical experiments with metal specimens undergoing fatigue loading. Using the optical interferometric technique Electronic Speckle-Pattern Interferometry (ESPI) we analyzed the temporal behavior of the displacement pattern formed while the specimen was experiencing cyclic loads. In traditional Fatigue Analysis of aircraft wings, cracks are formed due to oscillatory loads, these cracks propagate through a structure, and a failure occurs when stresses on these cracks are above a material's ultimate strength. ESPI data from our physical experiments indicates that shear instability is related to dislocation dynamics and it can be observed by unstable temporal behavior of the displacement field, leading us to a more formal physical description of fatigue. From the viewpoint of wave dynamics described by the Field theory of Deformation and Fracture we can describe the transition from deformation to fracture in solids. Deriving field equations that govern the displacement field of solids under deformation, we conducted numerical simulations based on our physical experiments. Our hypothesis is that the Field Theory of Deformation and Fracture characterizes fatigue on a fundamental theoretical level.
H71.00086: Non-noble metal Ni-Mo alloys with special electronic structure as a cocatalyst for alternative Pt in photocatalysis*  XIN HAN (Presenter), LIN AN, CHENGYI HOU, QINGHONG ZHANG, HONGZHI WANG, College of Materials Science and Engineering, Donghua University — Noble metals are often used as cocatalysts in photocatalysis due to their special electrical properties. However, the high cost of noble metals severely limits the development and application of photocatalytic technology. Therefore, the development of non-noble metal cocatalysts is of great significance in the field of photocatalysis. In this work, noble-metal-free Ni-Mo alloys with different Ni/Mo ratios were developed and used as cocatalyst to replace the noble metal Pt using g-C$_3$N$_4$ as a substrate. Experimental results show that the optimal Ni$_4$Mo$_6$/g-C$_3$N$_4$ photocatalyst has a photocatalytic H$_2$ production rate of up to 1785 μmol/g/h, which is about 37 times higher than that of pure g-C$_3$N$_4$, and comparable to that of the Pt/g-C$_3$N$_4$. The improved photocatalytic performance can be attributed to the presence of Ni-Mo alloys with special electronic structure, which effectively promotes the separation of photogenerated e$^-$/h$^+$ pairs.

*This work was financially supported by the China Scholarship Council and the Fundamental Research Funds for the Central Universities and Graduate Student Innovation Fund of Donghua University.

H71.00087: Non-saturating, Sub-Liner Magnetoresistance in bulk Ge$_2$Sb$_2$Te$_5$*  MING YIN (Presenter), BRANDON LACEY, Benedict College, LEI WANG, Yale University, TIMIR DATTA, Univ of South Carolina — Phase Change materials (PCM) rapidly and reversibly switch or transform between amorphous and crystalline states. This microscopic repositioning of the system in the lattice level may give rise to large macroscopic differences in physical properties; these changes in technologically important electrical, thermal and optical parameters were discovered in 1960's. Ambient temperature operable PCM's are utilized in electronic flash memory drives and in optical data storage devices. Previously we have reported on a well-known PCM alloy Ge$_2$Sb$_2$Te$_5$; where, based on Noritheim-Gorter like scaling between Seebeck coefficient (S) and electrical conductivity (σ) we have argued the existence of two distinct types of scattering. Here we report the high magnetic field magnetoresistance in poly-crystalline specimens Ge$_2$Sb$_2$Te$_5$, especially in the low temperature regime. We observe a relatively strong increase in the ohmic resistance in response to the applied magnetic field, about 150% increase between 0 - 18 T. The transport data can be precisely described by empirical functions, however, the behavior does not follow the well-known Kholer's rule. Overall, the field dependence is sub-linear but does not quite saturates up to 18 T even in the sub-kelvin range.

*DOE DE-NA0002630
H71.00088: Charge transport properties of ZnO, MgO, and CdO alloys* NICK BOECKER (Presenter), MACK ADRIAN DELA CRUZ, GARY PENNINGTON, Towson Univ — Monte Carlo based simulations of charge transport are used to investigate how important electrical properties of doped monoxide metals can be manipulated through alloying. Results include the effects of phonon, impurity, and alloy scattering on the carrier mobility in alloys of ZnO, MgO, and CdO. The electronic structure of the alloys is determined using the virtual crystal approximation and the non-local empirical pseudopotential method, which agrees well with electronic experimental data of these materials. Results have potential applications in optoelectronic devices.

*We acknowledge support from NSF Grant DMR 1709781 and from the Jess and Mildred Fisher College of Sciences and Mathematics at Towson University.

H71.00089: Temperature dependence of the anomalous Nernst effect in a Ni-Mn-Ga system* AVIRUP DE (Presenter), IISER Pune, SANJAY SINGH, School of Materials Science and Technology, IIT BHU, SUNIL NAIR, IISER Pune — Ni-Mn-Ga alloys, well-known for showing large magnetic shape memory effect, undergoes various phase transitions upon cooling, sensitive to their compositional variations. In this work, we report a detail investigation of the off-stoichiometric Ni$_{1.95}$Mn$_{1.05}$Ga through various magnetic, electronic, and thermal characterizations. Of particular, anomalous Nernst effect (ANE) studies are presented for the first time in these class of material, revealing that the ANE is very sensitive across the pre-martensitic transition in comparison to other transport measurements. With the ANE being sensitive to changes at the Fermi surface, we infer the link of structural modulations with the modulation of the Fermi surface via its nesting features. Moreover, the large ANE-signal at room temperature and the significant drop across the martensitic transition could also be promising for many spintronics applications.

*AD is thankful to UGC, Government of India, for providing financial support through a Senior Research Fellowship. S.N. acknowledges funding support by the Department of Science and Technology (DST, Government of India) under the DST Nanomission Thematic Unit Program (SR/NM/TP-13/2016).
H71.00090: Effect of heat treatment on current induced mixed dynamic metal-insulator phase in needle-like VO$_2$ single crystals.  BERTINA FISHER (Presenter), LARISA PATLAGAN, GEORGE M. REISNER, Technion - Israel Institute of Technology — Sliding domains in the current induced mixed Metal-Insulator phase of VO$_2$ single crystals are very sensitive on the crystal quality. Following measurements aimed to test this sensitivity were performed on an initially virgin needle-like crystal:
1. d.c. I-V measurements under steady state conditions (adequate load resistance in the NDR regime) carried out at ambient temperature on a VO$_2$ single crystal under the microscope while sliding domains were recorded on videos.
2. R(T) measurements during three heating-cooling cycles between room temperature and 355 K.
3. Repeated d.c. I-V measurements under same conditions as in 1 with video recording of sliding domains.

The results show:

a. Slow cycling through the transition have a healing effect on the sample: R(T) becomes reproducible and the activation energy in the insulating state is highest.
b. The damping term in $u(J)$ ($u$-sliding velocity and $J$-current density) after heat treatment, is practically zero in contrast to its finite value before.
c. The energetics of sliding domains emission, determined by $P(f)$ ($P=IV$- the power, $f$-the frequency) shows that the energy per domain emission decreases with increasing $f$ before heat treatment, but remains high and constant thereafter. This motivates studying samples with controlled imperfections.

H71.00091: Effect of heat treatment on the current induced dynamic mixed metal-insulator phase in needle-like VO$_2$ single crystals.  BERTINA FISHER (Presenter), LARISA PATLAGAN, GEORGE M. REISNER, Technion - Israel Institute of Technology — Sliding domains in the current induced mixed metal insulator phase of VO$_2$ single crystals are very sensitive on the crystal quality. Following measurements aimed to test this sensitivity were performed on an initially virgin needle-like crystal:
1. d.c. I-V measurements under steady state conditions (adequate load resistance in the NDR regime) carried out at ambient temperature on a VO$_2$ single crystal under the microscope while sliding domains were recorded on videos.
2. R(T) measured during three heating-cooling cycles between room temperature and 355 K.
3. Repeated d.c. I-V measurements under same conditions as in 1 with video recording of sliding domains.

The results show:

a. Slow cyclings through the transition have a healing effect on the sample: R(T) becomes reproducible and the activation energy in the insulating state is highest.
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c. The energetics of sliding domains emission, determined by $P(f)$ ($P=IV$- the power, $f$-the frequency) show that the energy per domain emission decreases with increasing $f$ before heat treatment, but remains high and constant thereafter. This motivates studying samples with controlled imperfections.
H71.00092: Mottness Collapse in 1T-TaS$_{2-x}$Se$_x$ Transition-Metal Dichalcogenide: An Interplay between Localized and Itinerant Orbitals*  
SHUANG QIAO (Presenter), Beijing Computational Science Research Center, XINTONG LI, Tsinghua University, XIANHUI CHEN, Nanjing University, JIAN WU, YAYU WANG, ZHENG LIU, Tsinghua University — The layered transition-metal dichalcogenide 1T-TaS$_2$ has been recently found to undergo a Mottinsulator-to-superconductor transition. By combining scanning tunneling microscopy measurements and first-principles calculations, we investigate the atomic scale electronic structure of the 1T-TaS$_2$ Mott insulator and its evolution to the metallic state upon isovalent substitution of S with Se. We identify two distinct types of orbital textures—one localized and the other extended—and demonstrate that the interplay between them is the key factor that determines the electronic structure. In particular, we show that the continuous evolution of the charge gap visualized by scanning tunneling microscopy is due to the immersion of the localized-orbital-induced Hubbard bands into the extended-orbital-spanned Fermi sea, featuring a unique evolution from a Mott gap to a charge-transfer gap.

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H71.00093: Evolution of the metallic state of LaNiO$_3$ with thickness as observed with β-detected NMR  
VICTORIA KARNER (Presenter), ARIS CHATZICHRISTOS, DAVID L CORTIE, DEREK FUJIMOTO, ROBERT F KIEFL, University of British Columbia, PHILIP C. P. LEVY, TRIUMF, RYAN M. L. MCFADDEN, University of British Columbia, GERALD MORRIS, MATT PEARSON, MONIKA K STACHURA, TRIUMF, GEORG CHRISTIANI, FRIEDERIKE WROBEL, BERNHARD KEIMER, EVA BENCKISER, ALEXANDER BORIS, Max Planck Institute for Solid State Research, W ANDREW MACFARLANE, University of British Columbia — A unique set of electronic and structural conditions allow for high-$T_c$ superconductivity in the cuprates.

It has been postulated that LaNiO$_3$/LaMO$_3$ (M = Al, Ti, Ga) superlattices (SLs) could share enough of these properties to support a related superconducting state[1]. LaNiO$_3$ is the only one of the rare-earth nickelates (RNiO$_3$) that remains a paramagnetic metal at all temperatures.

Here, we present β-detected NMR measurements on LaNiO$_3$/LaAlO$_3$ SLs. Specifically, we will address the evolution of the metallic phase of LaNiO$_3$ with decreasing sample thickness.

References:
Polariton Optical Transistor based on a MoSe$_2$-WS$_2$ Heterogenous Bilayer embedded in an Optical Microcavity at Room Temperature*  

PATRICK SERAFIN (Presenter), GERMAN KOLMAKOV, New York City College of Technology — Exciton polaritons in an optical microcavity were shown to be a platform for the design of working elements for optical transfer and processing circuits such as optical transistors and switches. In this report, we considered a three-way superposition of cavity photons, direct excitons and indirect excitons in a bilayer semiconducting system; that is, exciton dipolaritons. Using the forced diffusion equation, we studied the room-temperature dynamics of dipolaritons in a transition-metal dichalcogenide (TMD) heterogeneous bilayer embedded in an optical microcavity. Specifically, we considered a MoSe$_2$-WS$_2$ heterostructure, which encompasses Y and Ψ-shaped channels guiding the dipolariton propagation. We demonstrated that optical signals propagating in the channels can be effectively redistributed between the branches of the channels by applying the driving voltage \( \sim 2\)V/mm to one of the TMD layers. Our findings open the route to the design of an efficient room temperature polariton based optical transistor.

*This work was supported in part by the Department of Defense under the grant No. W911NF1810433.

WITHDRAWN ABSTRACT —

Polariton Formation and Propagation in an Optical Microcavity with Embedded Transition Metal Dichalcogenide with Disorder*  

SHAINA E RAKLYAR (Presenter), YAMUNA PAUDEL, New York City College of Technology, YURI LVOV, Rensselaer Polytechnic Institute, DAVID WAYNE SNOKE, University of Pittsburgh, GERMAN KOLMAKOV, New York City College of Technology — Transition-metal dichalcogenides (TMD) provide a platform for optoelectronic applications at room temperatures due to strong light-matter interactions and exciton stability. By considering the coupled dynamics of cavity photons and TMD excitons, we numerically studied exciton-polariton formation and propagation in an optical microcavity with an embedded TMD layer. Specifically, we studied the case where the TMD excitons are affected by a short-scale (10-100 nm) random potential due to the interactions with the environment inside the cavity. To characterize the stability of the polaritonic states in the system, we numerically calculated the energy of eigen modes in a cavity as a function of the wave number, \( E(k) \). In our poster, we present our findings and, in particular, we discuss the crossover from the polaritonic modes formed at weak disorder to strongly broadened photonic and excitonic modes at strong disorder. We also discuss the polariton formation and propagation in a cavity where the TMD layer is non-uniform and consists of a set of separate, topologically disconnected microflakes.

*This work was supported in part by the Department of Defense under the grant No. W911NF1810433.
H71.00097: Peculiar electron-phonon coupling in hBN/WS$_2$ heterostructures* MIAO-LING LIN (Presenter), State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China, YU ZHOU, HAI LI, Key Laboratory of Flexible Electronics and Institute of Advanced Materials, Jiangsu National Synergetic Innovation Center for Advanced Materials, Nanjing Tech University, 30, WANG YAO, Department of Physics and Centre of Theoretical and Computational Physics, University of Hong Kong, Hong Kong, China, PING-HENG TAN, State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China — The electron-phonon coupling (EPC) in materials is the key to the fundamental research, underlying many novel quantum behaviors. van der Waals heterostructures (vdWHs) provide new platform to reveal the intrinsic interactions between electrons and phonons. Here we report the cross-dimensional EPC between the three-dimensional (3D) layer-breathing (LB) phonons in a thick hBN/WS$_2$ vdWH up to hundreds of layers and two-dimensional (2D) electrons of its few-layer WS$_2$ constituent. New LB modes are resonantly enhanced in hBN/WS$_2$ vdWHs when the excitation energy approached the C exciton energy of WS$_2$ constituent. This cross-dimensional EPC strength is consistent with the phonon wavefunction projection between the layer-extended bulk-like LB modes in hBN/WS$_2$ vdWHs and the LB modes strongly coupled with the C exciton in the corresponding standalone WS$_2$ flakes, which can be further confirmed by the interlayer bond polarizability model in vdWHs. This work suggests additional possibilities to manipulate EPC in vdWHs for new quantum phenomena.

Reference:

*National Key Research and Development Program of China (Grant Nos 2016YFA0301204); National Natural Science Foundation of China (Grant Nos 11874350, 11434010 and 11474277).
**H71.00098: Nano-lasing from Zn-doped GaAs nanowires on Iron (Fe) substrate**

GYANAN AMAN (Presenter), Department of Electrical Engineering and Computer Science, University of Cincinnati, Cincinnati, OH 45221, U.S.A, CHIAWEI TU, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, U.S.A, MYKHAYLO LYSEVYCH, HOE TAN, CHENNUPATI JAGADISH, Department of Electronic Materials Engineering, Research School of Physics and Engineering, Australian National University, Canberra ACT, 0200, Australia, HEIDRUN SCHMITZER, Department of Physics, Xavier University, Cincinnati, OH 45207, MARTIN FRAENZL, Department of Physics, University of Leipzig, 04103 Leipzig, Germany, MARC CAHAY, Department of Electrical Engineering and Computer Science, University of Cincinnati, Cincinnati, OH 45221, U.S.A, HANS PETER WAGNER, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, U.S.A — We investigated optically pumped lasing from highly zinc-doped GaAs nanowires (NWs) on an iron (Fe) substrate at 5 K cryostat temperature. The conically shaped GaAs NWs possess an 8 nm thick Al$_2$O$_3$ layer around it to reduce Schottky band-banding. The NWs were optically excited with 150 fs laser pulses generated from Ti-Sapphire centered at a wavelength of 720 nm. The lasing output versus excitation power (L-L) of the lasing NWs shows the characteristic S shaped curve. Lasing NWs on Fe have a length of more than 4 µm with tip and base diameters of ~300 and~500 nm, respectively. Shorter NWs did not provide sufficient modal gain to exceed the plasmonic losses in the Fe film. The emission spectrum reveals two or three longitudinal modes, which resonate within the gain spectrum. The threshold power for NW lasers on Fe substrate were higher than for NWs on Au or glass due to significantly higher losses in the Fe film. FDTD simulations reveal that the hybrid plasmonic mode of lasing NWs on Fe has a predominantly photonic character. In a further step, we will investigate if an applied magnetic field influences the lasing behavior in GaAs NWs on Fe substrate.

*The support of the Australian Research Council and URC is kindly acknowledged.

**H71.00099: Epsilon-near-zero plasmonic nanowaveguides to achieve efficient resonance energy transfer and quantum entanglement**

CHRITOS ARGYROPOULOS (Presenter), YING LI, University of Nebraska - Lincoln — The efficient entanglement and strong resonance energy transfer between optical dipole emitters randomly distributed in a photonic system over extended time periods and long distances remain a key challenge. The main reasons are the extremely weak dipole-dipole interactions, decoherence, and dephasing between the emitters caused by radiative and nonradiative losses. We tackle this problem by proposing a practical plasmonic waveguide system to engineer both the temporal (entanglement) and spatial (resonance energy transfer and superradiance) coherent emission dynamics by an ensemble of emitters. The proposed nanoscale plasmonic waveguide system, that exhibits an effective epsilon-near-zero (ENZ) response, can simultaneously achieve the efficient inter-emitter entanglement and large enhancement of resonance energy transfer in elongated distances, long time scales, and, even more importantly, independent of the emitters' nanoscale positions [Y. Li, A. Nemilentsau, and C. Argyropoulos, “Resonance Energy Transfer and Quantum Entanglement Mediated by Epsilon-Near-Zero and Other Plasmonic Waveguide Systems,” Nanoscale 11, 14635, 2019]. Our presented results are expected to be useful for the future quantum communication and information plasmonic-based nanodevices.

*NSF DMR-1709612
H71.00100: Tuning photonics structure by integrating with 2D materials* KAI HAO (Presenter), ROBERT SHREINER, AMY BUTCHER, ALEXANDER A HIGH, University of Chicago — Monolayer transition metal dichalcogenides (TMDCs) exhibit exceptional coupling to light and large electrical tunability, which make them perfect candidates for optoelectronics applications. We demonstrate the integration of TMDCs and photonic structures. Due to the strong coupling between the TMDCs and tightly confined light fields, the optical properties of the photonic structures are significantly modified. By electrically tuning the TMDCs, we can control the coupling between them and realize on demand tuning of the photonic structures. This study sheds light on future applications of TMDCs in on-chip photonics.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1746045

H71.00101: Critical tuning of Luttinger liquid interactions through control of ion impurities* ANDREAS MICHELESEN (Presenter), Physics and Materials Research Science Unit, University of Luxembourg, MANUEL VALIENTE, Institute for Advanced Study, Tsinghua University, NIKOLAJ TZINNER, Aarhus Institute for Advanced Studies, Aarhus University, ANTONIO NEGRETTI, Zentrum für Optische Quantentechnologien, Fachbereich Physik, Universität Hamburg — Introducing ionic impurities into a Luttinger liquid (LL) of neutral atoms modifies the effective atom-atom interaction. By tuning characteristic parameters of the system, namely the short range phases of the atom-ion polarization potential and the relative density of atoms and ions, we show that the effective interaction of the LL can be tuned across a wide spectrum of values. Remarkably, the introduction of ions allows an interaction which is initially attractive to become effectively repulsive. We demonstrate this by finding the ground state of an atom-ion system using DMRG and extracting the LL parameter and the speed of sound. The LL theory models the low-energy physics of a gas of cold atoms in a one-dimensional trap, and thus these results are experimentally relevant for the recent advances in bringing different atomic species together in hybrid quantum systems.

*Aarhus University Research Foundation, the Carlsberg Foundation through a Carlsberg Distinguished Associate Professorship grant, the Cluster of Excellence ‘The Hamburg Centre for Ultrafast Imaging’ (DFG) - EXC 1074 - project ID 194651731, the Cluster of Excellence ‘Advanced Imaging of Matter’ (DFG) - EXC 2056 - project ID 390715994, and the National Research Fund, Luxembourg, under grant ATTRACT 7556175
**H71.00102: First-principles calculation of the electronic nematicity in FeSe**

XUANYU LONG (Presenter), Institute for Advanced Study, Tsinghua University, SHUNHONG ZHANG, International Center for Quantum Design of Functional Materials (ICQD), Hefei National Laboratory for Physical Sciences at the Microscale, and Synergetic Innovation Center of, FA WANG, International Center for Quantum Materials, School of Physics, Peking University, ZHENG LIU, Institute for Advanced Study, Tsinghua University — We report a density functional theory calculation that produces the nonmagnetic electronic nematic state in FeSe, without explicit breaking of the tetragonal lattice symmetry. We incorporate orbital-resolved interactions by +U and hybrid functional, and precondition the initial wavefunction to find local energy minima with spontaneous symmetry breaking. The lowest-energy nematic state we find features an anti-ferro hexadecapolar charge order, instead of a simple ferro-orbital order, which is important to produce the correct Fermi surface topology in FeSe. We propose that the weak inversion symmetry breaking induced by this multipolar order can be detected by high-precision measurement of the band dispersion as well as second-harmonic generation.

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**H71.00103: WITHDRAWN ABSTRACT**

**H71.00104: Bogoliubov-de Gennes analysis of superconducting gap in nanowires and nanotubes**

GERMAN LOPEZ (Presenter), CHUMIN WANG, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico — Most quantum theories of superconductivity have been formulated in the reciprocal space by taking the advantage of translational symmetry. Such symmetry is absent in many nanostructured superconductors, whose study requires a real space approach such as the Bogoliubov-de Gennes formalism [1]. In this work, the inhomogenous superconducting gap [2,3] in nanostructures is studied by means of a simple attractive Hubbard model. The results show a unique critical temperature for each nanostructure despite the variation of its local superconducting gap and the spectral average of such gap over the chemical potential location grows when its coordination number diminishes. The latter suggests that the superconductivity in nanostructures could be enhanced by the quantum confinement of electrons, which reduces its kinetic energy and accentuates the potential one.

This work was partially funded by UNAM-PAPIIT-IN110020 and CONACyT-252943. Computations were performed at Miztli of DGTIC-UNAM. G.E.L. thanks the support from UNAM-PAEP 2020.

H71.00105: Effects of percolation on the superconductor-insulator transition in thin films*
KRISTINE UNG, ROBERT LYNN, SAMUEL SHAPIRO, NINA MARKOVIC (Presenter), Goucher College —
Thin films of superconductors are known to undergo a quantum phase transition into the
insulating state as a function of disorder and magnetic field, but the nature of the transition has
been debated for decades. In order to investigate the effects of percolation and rare
superconducting regions on the superconductor-insulator transition in thin films, we have
fabricated a series of nanostructured films with controlled vicinity to the percolation threshold.
We will show how the measurements of resistance as a function of temperature and magnetic
field correlate to the physical texture of the films.

*This work was supported in part by National Science Foundation under DMR-1663683 and the
Croatian Science Foundation under HRZZ IP-2016-06-2289 C3TiNN.

H71.00106: Domains, Domain Walls, and Phase Slips in the Nearly-Commensurate Charge
Density Wave Phase of 1T-TaS₂*
BONING YU (Presenter), MANOJ K SINGH, BISHNU SHARMA, MICHAEL BOYER, Clark University —
The nearly-commensurate charge density wave (CDW) state of 1T-TaS₂ consists of hexagonally ordered domains. Within these domains, the CDW state is
commensurate with the lattice. However, there are domain walls which include phase slips in the
CDW state between neighboring domains. Here we combine our scanning tunneling microscopy (STM) data of the nearly-commensurate CDW state with computer simulations to study, at the
atomic-scale, domains, domain ordering, and phase slips at domain walls in 1T-TaS₂. In particular,
we examine how these features manifest themselves in Fourier transforms of STM topographic
images.

*We acknowledge support from NSF Grant number DMR-1904918.
**H71.00107: The low frequency surface slasmons in multicoaxial NIM cables: Zero magnetic field**

MANVIR KUSHWAHA (Presenter), Rice Univ, BAHRAM DJAFE.I-ROUHANI, Physics, USTL — 
Employing an elegant response function theory\(^1\)\(^-\)\(^3\), which does not require matching of the messy boundary conditions, 
we investigate the surface plasmon excitations in the multicoaxial cylindrical cables made up of negative-index metamaterials. The multicoaxial cables with dispersive metamaterial components exhibit a 
rather richer (and complex) plasmon spectrum with each interface supporting two modes: one 
TM and the 
other TE for \(m\neq 0\) (the integer order of the Bessel function). The cables with nondispersive 
metamaterial components 
bear a different tale: they do not support simultaneously both TM and TE modes over the whole 
range 
of propagation vector. The computed local and total density of states enable us to substantiate 
spatial positions 
of the modes in the spectrum. Such quasi-one-dimensional systems as studied here should prove 
to be the milestones 
of the emerging optoelectronics and telecommunications systems. 1. M.S. Kushwaha, B. Djafari- 
Rouhani, 

**H71.00108: Harnessing the magneto-optics in quantum wires for observing the quantum pinch effect**

MANVIR KUSHWAHA (Presenter), Rice Univ — Here, we report on a two-component, 
cylindrical, quasi-one-dimensional quantum plasma subjected to a \textit{radial} confining harmonic 
potential and an applied magnetic field in the symmetric gauge. It is demonstrated that such a 
system as can be realized in semiconducting quantum wires offers an excellent medium for 
oberving 
the quantum pinch effect at low temperatures. An exact analytical solution of the problem allows 
us to make significant observations: surprisingly, in contrast to the classical pinch effect, the 
particle density as well as the current density display a \textit{determinable} maximum before 
attaining a minimum at the surface of the quantum wire. The effect will persist as long as the 
equilibrium pair density is sustained. Therefore, the technological promise that emerges is the 
route to the precise electronic devices that will control the particle beams at the nanoscale\(^1\). 1. 
M.S. 
**H71.00109: Nanoporous Metal Foams as Efficient Particulate Filters**

JAMES MALLOY (Presenter), KAI LIU, Georgetown University — Nanostructured metal foams offer exciting potential for applications in diverse fields such as catalysts, electronics, heat exchange, structural materials, and filtration due to their extremely high surface area to volume ratios. We have achieved a variety of metallic foams using electrochemical methods, with strong mechanical stability and tunable porosity and density (0.1%-30% of bulk density) [1]. Uniaxial compression tests reveal significantly varying structural strengths depending on the relative density. Additional physical characteristics and applications have been explored. We have also investigated using such foams as efficient filtration membranes for micron and sub-micron sized particles. Over 99% of airborne micron sized particles are found to be filtered after passing through just 1 mm of metallic foam. The foams are also found to be effective for filtering out deep submicron particles. The pressure drops across the foams are found to vary depending on the bulk density of the foam; with the lower density foams being comparable to commercial HEPA filters.


*This work has been supported by the Georgetown Environmental Initiative Impact Program.

**H71.00110: Sub-5 nm patterning via self-assembly and template-assisted assembly of colloidal nanocrystals**

AUSTIN KELLER (Presenter), CHERIE KAGAN, CHRISTOPHER B MURRAY, DIAN, University of Pennsylvania — We explore using colloidal lithography and conventional fabrication tools for patterning substrates at and below the 5 nm scale. Our processing pathway combines bottom-up methods using inorganic nanocrystal (NC) synthesis and self-assembly techniques with top-down nanofabrication techniques. A pattern is established by the size, shape, and arrangement of discrete NC building-blocks, and the density is determined by the interparticle spacing of each element. The collective arrangement of each element sets the ensemble pattern, where each NC serves as a discrete hard etch mask. We explore self-assembly at a liquid-air interface and topographic template-assisted capillary assembly methods to establish the NC patterns. This pattern is transferred to the underlying substrate using inductively couple plasma reactive ion etching, and a selective chemical wet etch is used to remove any remaining mask material after pattern transfer. The NC systems explored are Fe₃O₄ spheres, TiO₂ rods, and GdF₃ rhombic plates with CF₄ and Cl₂ plasma etch chemistries. The goal of our pathway is to implement innovative processing methods into already well-established fabrication methods and technology, while maintaining process simplification and enabling wider access to patterning at the deep nanoscale.
H71.00111: Skyrmions on a sphere shell  DELARAM NEMATOLLAHI (Presenter), KIERAN MULLEN, Univ of Oklahoma — Skyrmions, as small electronic spin-structures, provide a window into strongly interacting many electron systems. The existence of these spin-textures has been studied in quantum Hall (QH) ferromagnets, in which the kinetic energy of the electrons is quenched by the strong external magnetic field. The large angular momentum (l) single particle states on the surface of a sphere are similarly degenerate in energy as a function of their z component (m) for fixed (l). This makes electrons on a sphere an interesting system for studying spin textures. Using Hartree-Fock theory, we initially force a skyrmionic texture on the system by applying a small “scaffolding” field that couples to the spins to produce a texture and investigate the stability of the spin-structure as the field goes to zero. We study the dependence of the skyrmion stability on the number of electrons, the choice of interactive potential, and material parameters.

H71.00112: Metallic density of states in the spin liquid RuCl$_3$.*  ANDREAS RYDH, university of stockholm, ALI BANGURA, Natl High Magnetic Field Lab, KIMBERLY MODIC, max planck dresden, GREGORY SCOTT BOEBINGER, Natl High Magnetic Field Lab, BRAD J RAMSHAW, Cornell, ROSS MCDONALD, Los Alamos Natl Lab, ARKADY SHEKHTER (Presenter), Natl High Magnetic Field Lab — We use resonant line-width spectroscopy and SiN nanocalorimeters to measure specific heat of a small (~1μg mass) RuCl$_3$ sample. The low-temperature limit of C/T is metallic-like, with an extrapolated Sommerfeld coefficient corresponding to a density of states of about 100 mJ/molK$^2$, consistent with Majorana fermions of about 10meV bandwidth. We discuss the field- and angular evolution of this metallic density of states. Finally we examine thermodynamics of the AFM boundary, as well as AFM spin waves in RuCl$_3$.

*NSF through DMR-1157490

H71.00113: Heat Capacity Studies of Nano-Confined Argon*  ERIN MARLOWE (Presenter), Indiana Univ - Bloomington — The effect of confinement on the thermodynamic properties and phase transitions of liquids and solids in confinement has been of long-standing interest and recent interest has focused on the effects of dimensionality. Hydrogen has been of interest due to the importance of quantum effects, in particular zero-point motion, and has been studied extensively in a variety of porous media. Argon is a good model for hydrogen as it will exhibit similar behaviors, in general, to hydrogen. Furthermore, it is important to understand the behavior of noble gasses in confinement as it may be useful for understanding gasses like hydrogen. Templated porous materials, such as MCM-41, provide an attractive model system for studying the effects of confinement due to their highly uniform one-dimensional pores with variable pore size. Unfortunately, the minimum pore diameter is typically limited to a few nanometers which limits our ability to approach the one-dimensional limit. We will present measurements of the heat capacity of argon confined in MCM-41.

*This work was supported by the NSF through grants DMR-1809027.
H71.00114: Effects of Metamaterial Engineering on Properties of Ultrathin Layers of NbTiN

JONATHON CARTELLI (Presenter), WILL KORZI, Department of Physics Astronomy and Geosciences, Towson University, ANNE-MARIE VALENTE-FELICIANO, Jefferson Lab, JOSEPH PRESTIGIACOMO, MICHAEL OSOFSKY, United States Naval Research Laboratory, IGOR SMOLYANINOV, Saltenna LLC, VERA N SMOLYANINOVA, Department of Physics Astronomy and Geosciences, Towson University — Application of the metamaterial dielectric function engineering is capable of enhancing superconducting properties in type I superconductors such as aluminum and tin, leading to the tripling of the critical temperature $T_c$ in Al-Al$_2$O$_3$ epsilon near zero (ENZ) core-shell metamaterial superconductors. Similar effects have been observed in hyperbolic (superconductor/dielectric) metamaterials [1]. Here, we report on the effects of metamaterial dielectric function engineering on superconducting properties of ultrathin layers of NbTiN. NbTiN/AlN multilayers with varied number of layers and layer thicknesses were fabricated. Dielectric constants of these metamaterials were measured via polarization reflectometry will be reported. Correlation of the results of the transport measurements and the hyperbolic properties of the multilayers will be discussed.


*This work was supported by the DARPA grant W911NF1710348.

H71.00115: Introducing a new noncentrosymmetric superconductor: Zr$_3$Ir

SAJILESH K P (Presenter), PHYSICS, IISERB, D SINGH, P. K BISWAS, muon, ISIS pulse neutron and muon source, R P SINGH, PHYSICS, IISERB — An intrinsic momentum dependent antisymmetric spin-orbit coupling (ASOC) in noncentrosymmetric (NCS) systems arising due to lack of inversion center in the crystal structure gives way to numerous unusual superconducting properties [1]. The Fermi surface in these systems becomes nondegenerate in the presence of spin-orbit coupling, giving a plausibility to form an admixed superconducting order parameter. This breaks the conventional notion of even parity spin-singlet and odd parity spin-triplet order parameter, leading to the high upper critical field, anisotropic superconducting gap, and time-reversal symmetry breaking [1]. We report a new NCS compound Zr$_3$Ir, crystallizes in a tetragonal $\alpha$-V3S structure. The magnetization, specific heat, and muon spin rotation confirm s-wave superconductivity, having a transition temperature $T_c = 2.3$ K. Muon spin relaxation confirms the preservation of time reversal symmetry in the superconducting ground state [2].

References

*We acknowledge Science and Engineering Research Board, Government of India for the financial support and we also thank ISIS, STFC, UK for the beam time to conduct the $\mu$SR experiments.
Probing the superconducting ground state of noncentrosymmetric superconductors using muon spectroscopy: A case of Re-based compounds

DEEPAK SINGH (Presenter), Rutherford Appleton Lab, R P SINGH, Department of Physics, Indian Institute of Science Education and Research Bhopal, India, ADRIAN HILLIER, P. K BISWAS, Rutherford Appleton Lab, SOURAV MARIK, Laboratory Crismat, UMR6508 CNRS, Normandie University, France, SAJILESH K P, Rutherford Appleton Lab — Noncentrosymmetric superconductors (NCSs) with broken inversion symmetry has a direct influence on the superconducting properties of the system. In particular, NCSs with α-manganese structure has attracted much attention recently, after the discovery of time reversal symmetry breaking (TRSB) in all the members of the Re$_6$X (X = Ti, Hf, Zr) family [1,2]. Its persistence and the independent nature of the particular transition metal, points to a key role played by Re. To test such a hypothesis, and to ascertain the possible relevance of the noncentrosymmetric structure to TRSB in Re-based NCSs, we proceeded with a twofold study. On one hand, we studied the Re$_6$X family of compounds using muon spectroscopy, whereas, on the other hand we also studied the NbOs$_2$ compound, which doesn't contain Re as the primary element and adopts similar α-Mn structure with superconducting transition temperature $T_c = 2.7$ K [3]. The results of muon spin relaxation/rotation measurements strongly suggests that the local electronic structure of Re is crucial for understanding the TRSB superconducting state in Re$_6$X.


Physical properties of (Mn$_{1-x}$Fe$_x$)Si at x=0.15 along the critical trajectory

ALLA E PETROVA, Institute for High Pressure Physics, SERGEY YU GAVRILKIN, Lebedev Physical Institute, DIRK MENZEL, Technische Universität Braunschweig, SERGEI STISHOV (Presenter), Institute for High Pressure Physics — We report results of studying the magnetization, specific heat and thermal expansion of a single crystal with nominal composition (Mn$_{1-x}$Fe$_x$)Si with x=0.15. We found no thermodynamic evidences in favor of a second order phase transition in this material. The trajectory corresponding to the present composition of (MnFe)Si is a critical one, i.e. approaching quantum critical point at lowering temperature, but some properties may feel the cloud of helical fluctuations bordering the phase transition line.

*AEP and SMS greatly appreciate financial support of the Russian Foundation for Basic Research (grant No. 18-02-00183) and the Russian Science Foundation (grant 17-12-01050).
Investigation of quantum criticality in $\alpha$-RuCl$_3$ by means of dilatometry

ANJA WOLTER, SEBASTIAN GASS, LAURA T. CORREDOR, VILMOS KOCSIS (Presenter), Leibniz Institute for Solid State and Materials Research Dresden, LUKAS JANSSEN, MATTHIAS VOJTA, Institute of Theoretical Physics, Technical University of Dresden, PAULA J KELLEY, STEPHEN E NAGLER, Neutron Scattering Division, Oak Ridge National Laboratory, DAVID MANDRUS, Material Science and Technology Division, Oak Ridge National Laboratory, BERND BUECHNER, Leibniz Institute for Solid State and Materials Research Dresden — The quantum spin liquid candidate $\alpha$-RuCl$_3$ shows field-induced quantum criticality around $\mu_0 H_c \sim 7$-8 T, where the antiferromagnetic zigzag phase is suppressed [1,2]. Such behavior can be studied via the characteristic divergence in the temperature and field dependence of the Grüneisen parameter [3]. Here, we present high-resolution thermal expansion $\alpha$, magnetostriction $\lambda$, and specific-heat ($C_p$) measurements, performed on single crystals of $\alpha$-RuCl$_3$. The length changes were measured parallel to the $c$ axis stacking direction for magnetic field perpendicular to the $c$ axis up to 15 T. The extracted Grüneisen parameter $G = \alpha / C_p$ shows typical hallmarks for quantum critical behavior, with $G$ diverging in a characteristic manner at $\mu_0 H_c = 7.8(1)$ T. Furthermore, our thermodynamic investigations show clear evidence for the existence of three different low-temperature phases in the examined field range in line with recent magnetocaloric and neutron diffraction measurements [4]. We present calculations for thermal expansion and Grüneisen parameter in a minimal lattice model.


Percolation and Quantum Criticality: a New Universality Class

SEAN FAYFAR (Presenter), ALEX BRETAÑA, WOUTER MONTFROOIJ, Physics, University of Missouri Columbia, THOMAS HEITMANN, The Missouri Research Reactor, University of Missouri Columbia — We present the results of computer simulations on a class of percolation systems that form a new universality class. We show the results for the critical exponents for this new class, based on simulations of two- and three-dimensional lattices consisting of half a billion sites, and discuss the ensuing modified scaling laws. This new percolation system, dubbed Protected Percolation, differs from standard site percolation in that once a cluster breaks off the percolating cluster, its sites become protected and cannot be removed; thus, only sites from the lattice spanning cluster can be removed. This restriction closely mimics the situation in chemically doped quantum critical systems where isolated magnetic clusters are protected from (further) Kondo screening. Initial results indicate that Protected Percolation violates the Harris Criterion, which leads to a natural explanation as to why universal critical exponents for quantum phase transitions have been elusive.
H71.00120: Validity of Harris criterion for two-dimensional quantum spin systems with quenched disorder* JHAO-HONG PENG (Presenter), LENG-WEI HUANG, DENG-RUEI TAN, FU-JIUN JIANG, National Taiwan Normal Univ — Inspired by the recent results regarding whether the Harris criterion is valid for quantum spin systems, we have simulated a two-dimensional spin-1/2 Heisenberg model on the square lattice with a specific kind of quenched disorder using the quantum Monte Carlo (QMC) calculations. The considered quenched disorder has a tunable parameter $0 \leq p \leq 1$ which can be considered as a measure of randomness. Interestingly, when the magnitude of $p$ increases from 0 to 0.9, at the associated quantum phase transitions the value of the correlation length exponent $\nu$ grows from a number compatible with the O(3) result 0.7112(5) to a number slightly greater than 1. In other words, by varying $p$, $\nu$ can reach an outcome between 0.7112(5) and 1 (or greater). Moreover, among the studied values of $p$, all the associated $\nu$ violate the Harris criterion except the one corresponding to $p=0.9$. Considering the form of the employed disorder here, the above described scenario should remain true for other randomness if it is based on the similar idea as the one used in this study. This is indeed confirmed by our preliminary results stemming from investigating another disorder distribution.

*This work is partially supported by the "Ministry of Science and Technology" of Taiwan (Grant No. MOST 108-2112-M-003 -012 -MY2).

H71.00121: Percolation Physics in doped and stochioetric Quantum Critical System ALEX BRETAÑA (Presenter), SEAN FAYFAR, WOUTER MONTFROOIJ, Physics, University of Missouri - Columbia, THOMAS HEITMANN, The Missouri Research Reactor, University of Missouri - Columbia — We argue that spontaneous fragmentation of the magnetic lattice in strongly correlated electron systems close to the quantum critical point accounts for most of the observed non-Fermi liquid behavior. Upon cooling, magnetic fragmentation of the Kondo lattice is caused by a distribution of Kondo temperatures, which in turn originate from small variations in interionic separations (0.05-0.1 Å). This temperature-dependent fragmentation transforms the magnetic lattice to a percolation system resulting in the creation of isolated clusters which dominate the low-temperature response of quantum critical systems. We argue the validity of this new scenario for the physics near a QCP using literature data on systems where interionic distances have been modified by means of chemical doping (e.g., UCu$_4$Au) as well as stoichiometric systems where zero-point phonons are responsible for such variations (e.g., CeRu$_2$Si$_2$). The percolation physics describing QCP-systems represents a new universality class (see Fayfar et al.). This new class appears to violate the Harris criterion, thereby providing a natural explanation for the lack of universality of the critical exponents observed in QCP-systems.
Many-Body Localization in Central Spin.* MARCOS TRIVELATO (Presenter), CARLOS EGUES, Sao Carlos Institute of Physics at the University of Sao Paulo, JOHN SCHLIEermann, Institute for Theoretical Physics, University of Regensburg, JOAO VITOR IGNACIO COSTA, Sao Carlos Institute of Physics at the University of Sao Paulo — We investigate many-body localization in a periodic one dimensional Heisenberg chain, with a central spin interacting equally with each spin in the chain. The chain is subject to a uniaxial quenched disorder field. Apart from a detailed analysis of the phase diagram, we study the time evolution of nonlocal out-of-time-ordered correlators to diagnose the information scrambling in the dynamics of the system.

*This work was supported by the Brazilian agencies CNPq, CAPES and FAPESP grant 2016/08468-0.

Multi-Layer Restricted Boltzmann Machine Representation of 1D Quantum Many-Body Wave Functions HUAN HE, YUNQIN ZHENG (Presenter), ANDREI BERNEVIG, Princeton University, GERMAN SIERRA, Universidad Autónoma de Madrid, Instituto de Física Teórica, UAM-CSIC — We consider representing two classes of 1D quantum wave functions of spin systems, including the AKLT and CFT correlator wave functions, in terms of multi-layer restricted Boltzmann machines. In our prescription, the AKLT wave function can be exactly represented by a 2-layer restricted Boltzmann machine with five hidden spins per visible spin. The construction can be generalized to prove that any MPS wave function on \( N \) unit cells with finite bond dimension can be approximated by a 2-layer restricted Boltzmann machine with \( O(N) \) hidden spins within an error which scales linearly with \( N \). The Haldane-Shastry wave function or a chiral boson CFT correlator wave function, as any Jastrow type of wave functions, can be exactly written as a 1-layer Boltzmann machine with \( O(N^2) \) hidden spins and \( N \) visible spins. Applying the cumulant expansion, we further find that the chiral boson CFT correlator wave function (with small vertex operator conformal dimension \( \alpha \), i.e., \( \alpha < 0.1 \)) can be approximated, within 99.9\% accuracy up to 22 visible spins, by a 1-layer RBM with \( O(N) \) hidden spins. The cumulant expansion also suggests that the hidden spins of the restricted Boltzmann machine can be interpreted as the conformal tower of the chiral boson CFT on the cylinder.
H71.00124: Puzzling "bad metal" resistivity and optical conductivity of normal-state cuprates: an emergent Bose liquid perspective  
LONG ZOU, Shanghai JiaoTong University, ZIJIAN LANG, Tsung-Dao Lee Institute & Shanghai JiaoTong University, SHENGTAO JIANG, Shanghai JiaoTong University, WEI KU (Presenter), Tsung-Dao Lee Institute & Shanghai JiaoTong University — We investigate anomalous normal-state in-plane resistivity and optical conductivity of cuprates by using multi-orbital bose-liquid model. Specifically, we assume that the charge carriers in cuprate are tightly bound pre-formed pairs. We show the low-energy optical spectrum involving both intra- and inter-band excitation. While inter-band excitation explain the continuous spectrum and its contribution around the van-Hove singularities of the pre-formed pairs can reproduce the experimental observed onset near 1000cm⁻¹, the intra-band excitation will mainly contributes to low frequency conductivity and gives rise to linear resistivity without saturation. Instead of considering about the mean free path, we demonstrate this universal bad metal behavior originate from the continuously decreasing height of low-frequency peak since its weight transfers to high energy region with temperature. Our study reveals the bosonic nature of the low-energy carriers and provides a strong support for the picture of tightly bound preformed pairs in describing the high-temperature superconductivity and other low-energy physics of the cuprates.

H71.00125: "Time-reversal symmetry breaking in topological superconductor Sr₀.₁Bi₂Se₃"  
P. NEHA, K. S. JAT (Presenter), School of Physical Sciences, Jawaharlal Nehru University (JNU), Delhi India, TANMOY DAS, Department of Physics, Indian Institute of Science Bangalore India, S. PATNAIK, School of Physical Sciences, Jawaharlal Nehru University (JNU), Delhi India — We report on the detection of the TRS breaking in the topological superconductor Sr₀.₁Bi₂Se₃, probed by zero-field μSR measurements. The TRS breaking provides strong evidence for the existence of a spin-triplet pairing state. The existence of TRS breaking is also verified by longitudinal-field μSR measurements, which negates the possibility of magnetic impurities as the source of TRS breaking. The temperature-dependent superfluid density deduced from transverse-field μSR measurements yields nodeless superconductivity with low superconducting carrier density and penetration depth λ = 1622(134) nm. From the microscopic theory of unconventional pairing, we find that such a fully gapped spin-triplet pairing channel is promoted by the complex interplay between the structural hexagonal warping and higher order Dresselhaus spinorbit-coupling terms. Based on Ginzburg-Landau analysis, we delineate the mixing of singlet- to triplet-pairing symmetry as the chemical potential is tuned far above from the Dirac cone. Our observation of such spontaneous TRS breaking chiral superconductivity on a helical surface state, protected by the TRS invariant bulk topology, can open avenues for interesting research and applications.
**H71.00126: Tight-binding Models for Two-dimensional Allotropes of Bismuth based on Wannier Functions**

QILE LI (Presenter), Materials Science and Engineering, Monash University, JACKSON SMITH, Physics, RMIT University, YUEFENG YIN, CHUTIAN WANG, Materials Science and Engineering, Monash University, MYKHAILO V. KLYMENKO, JARED H. COLE, Physics, RMIT University, NIKHIL MEDHEKAR, Materials Science and Engineering, Monash University — Recently two-dimensional allotropes of bismuth have attracted significant attention in the study of topological materials due to the strong correlation between their crystalline symmetry and electronic band topology.

This connection has been studied previously by directly transferring the empirical tight-binding models of semi-metallic bulk bismuth to its two-dimensional counterparts. However, this approach fails to describe the electronic structure of two-dimensional bismuth correctly. Therefore, new physical models are required when considering the two-dimensional forms of bismuth. In this study, we have constructed tight-binding models based on the Wannier representations derived from the Bloch states in first principles calculations. We have successfully reproduced the band features for three types of two-dimensional bismuth allotropes (Bi(111), Bi(110) and bismuthene) with minimal tight-binding parameters. We have verified the accuracy of the model by calculating band representations and topological invariants. We expect these simple but accurate tight-binding models can help to examine the electronic transport in these systems more effectively in the future.

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**H71.00127: Probing black hole-like quasinormal modes in quantum Hall point contact geometries**

SURAJ HEGDE, Max Planck Institute for the Physics of Complex Systems, VARSHA SUBRAMANYAN (Presenter), BARRY BRADLYN, SMITHA VISHVESHWARA, Physics, University of Illinois at Urbana-Champaign — Recently it was shown by the authors that quantum Hall systems under the influence of an external saddle potential can realize the inverted harmonic oscillator (IHO), which is of importance in its own right and in the context of black hole physics [*]. A key feature of this potential is the occurrence of the resonant states/quasinormal modes (QNM) that decay in time via a finite outward flux. In this talk, we explore the directions for feasible experimental realisation and detection of these states. We analyze the bounded scattering potential of the Pöschl-Teller model whose scattering matrix has a resonant pole structure comparable to the IHO. We study quantities such as the non-escape probability that could be amenable to measurement and extraction of the decay rates of QNMs. We propose time-resolved measurements in quantum Hall point contact architectures for experimentally probing these wave packet scattering phenomena.

H71.00128: Probing the stability of Shastry Sutherland lattice in $\text{Er}_2\text{Pd}_2\text{Sn}$ and $\text{Er}_2\text{Pd}_2\text{In}$

GICELA SAUCEDO SALAS (Presenter), University of Texas, El Paso, SAHU BAIDYANATH, ANDRE MICHAEL STRYDOM, University of Johannesburg, STUART CALDER, Oak Ridge National Laboratory, HARIKRISHNAN S NAIR, University of Texas, El Paso — The group of 2:2:1 compound crystalizing in the $\text{Mo}_2\text{FeB}_2$ structure type, more commonly known as $R_2T_2X$ intermetallic ($R =$ rare earth, $T =$ transition metal, $X =$main group), have been reinvestigated recently owing to the spin liquid state in the underlying Shastry-Sutherland lattice (SSL) formed by the $R$ [1, 2]. Our motivation in investigating this compound is to explore the interplay of frustration and quantum criticality. For this study we have selected less-investigated $\text{Er}_2\text{Pd}_2\text{In}$ and $\text{Er}_2\text{Pd}_2\text{Sn}$. X-ray powder diffraction studies and subsequent Rietveld refinements confirmed that the compounds were phase-pure and crystallized in the tetragonal $\text{Mo}_2\text{FeB}_2$ structure. Both the compounds obeyed Curie-Weiss law in the paramagnetic regime, as judged from magnetic susceptibility data, which indicated anti-ferromagnetism. Specific heat data on both the compounds revealed a double peak indicating complex magnetic structure and phase transitions. We will present a detailed analysis of the magnetization and specific heat on both $\text{Er}_2\text{Pd}_2$(Sn/In). This motivated our current neutron diffraction experiment to determine the magnetic structure of these SSL compounds to probe for novel magnetic phases.

H71.00129: Thermoelectric transport in electronic systems at low and intermediate temperatures*

ZAHIDUL ISLAM JITU (Presenter), WOO-RAM LEE, Univ of Alabama - Tuscaloosa, ALEXANDER FINKELSTEIN, Texas A&M University, KAREN MICHAELI, The Weizmann Institute of Science, GEORG SCHWIETE, Univ of Alabama - Tuscaloosa — Measurements of thermoelectric transport in correlated electron systems probe different aspects of the many-body dynamics compared to electric and thermal transport. Here, we study theoretically how electron-electron interactions influence the Seebeck coefficient (thermopower) in disordered conductors when the phonon-drag is negligible. In particular, we discuss the regime of intermediate temperatures, where inelastic electron-electron collisions and elastic scattering on impurities occur at similar rates, and the low-temperature regime, where impurities provide the dominant scattering mechanism.

*This work is supported by DOE, ISF, NSF, and the College of Arts and Sciences at the University of Alabama.
H71.00130: Valence Transition in CeOs$_4$Sb$_{12}$ and Its T-H Phase Diagram*  PEI-CHUN HO
(Presenter), Physics, California State University, Fresno, JOHN SINGLETON, MARCELO JAIME, NHMFL, LANL, KATHRIN GOETZE, MATTHEW PEARCE, PAUL GODDARD, Physics, University of Warwick, KALYAN SASMAL, M BRIAN MAPLE, Physics, University of California, San Diego, TATSUYA YANAGISAWA, Physics, Hokkaido University — The filled skutterudite compound CeOs$_4$Sb$_{12}$ displays Kondo insulating behavior accompanied by a ~1 K Spin-Density-Wave order state. Recently it has also been suggested as a potential topological insulator. In penetration depth and magnetic susceptibility measurements, we found a Fermi-surface reconstruction in CeOs$_4$Sb$_{12}$ and an unusual phase boundary in the temperature $T$ vs magnetic field $H$ diagram associated with the valence transition from the Ce$^{4+}$ to Ce$^{3+}$ state, denoted as an L and an H phase, respectively. Based on the experimental features from magnetostriction, magnetoresistance, and high $T$ skin depth, a newly modified $T$-$H$ phase boundary of the L to H phases becoming much broader than what originally thought.\cite{1,2} The cyclotron mass of the conduction electron has a significant enhancement below ~35 T.

\cite{1} arXiv:1907.09181 \cite{2} PRB 94, 205140 (2016).

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H71.00131: Kondo effect in a spin-orbit coupled quantum wire under the influence of an external magnetic field  EDSON VERNEK (Presenter), Physics and Astronomy, Ohio University, GEORGE B MARTINS, Physics, Federal University of Uberlândia, ROK ZITKO, Jozef Stefan Institute — We performed a detailed study of the Kondo effect occurring in a quantum dot coupled to a nanowire with Rashba and Dresselhaus spin-orbit couplings (SOC) subjected to an external magnetic field. We report the results for local static and dynamic physical properties of the dot in the Kondo regime obtained through the Numerical Renormalization Group method. Despite the SOC-induced magnetic anisotropy of the bands, the local quantum dot properties remain isotropic in the spin space at zero external field. However, when an external magnetic field is applied to the system, clear fingerprints of the SOC-induced anisotropy are revealed through the quantum dot physical properties that become dependant on the direction of the field. We demonstrate that the quantitative evaluation of this SOC-induced anisotropy, measured by tunneling spectroscopy techniques, can be used to determine the ratio of Rashba and Dresselhaus SOC strengths in the wire.
H71.00132: Effect of pseudospin-1 fermions on the RKKY interaction in α-T₃ lattice

GODFREY GUMBS (Presenter), Hunter college, ANDRII IUROV, Medgar Evers college, DANHONG HUANG, Air Force Research Lab — The interaction energy for the indirect-exchange or Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between magnetic spins localized on lattice sites of the α-T₃ model is calculated using linear response theory. In this model, the AB-honeycomb lattice structure is supplemented with C atoms at the centers of the hexagonal lattice. This introduces a parameter alpha for the ratio of the hopping integral from hub-to-rim and that around the rim of the hexagonal lattice. A valley and alpha-dependent retarded Green's function matrix in momentum-energy space is generated using the (A,B,C) lattice basis forming the low-energy Hamiltonian. The corresponding coordinate space Green's functions not only depend on which sublattice (A,B or C) the interacting spins are located but the cut-off wave vector used in the Fourier transform integral restricted to lie within the first Brillouin zone (B.Z.).

H71.00133: Plasmon dispersion in semimetallic pseudospin-1 α-T₃-based nanoribbons

ANDRII IUROV (Presenter), Medgar Evers College, PAULA FEKETE, West Point, US Military Academy, LIUBOV ZHEMCHUZHNA, DIPENDRA DAHAL, GODFREY GUMBS, Hunter college, DANHONG HUANG, Air Force Research Lab — We have calculated the electronic states, Coulomb potential energy, dynamical polarizability and the plasmon dispersion relations for both intrinsic and extrinsic semimetallic armchair graphene nanoribbons in α-T₃ materials. Our obtained results depend on both the parameter α, which is the ratio of the interaction strength and hopping coefficients between the hub and rim-atoms of the hexagonal lattice, and the number of atoms across the nanoribbon. The corresponding results for the dice lattice and graphene are also discussed as limiting cases of our work.

H71.00134: Suspended Nanowire Devices as Templates for Size-selected Nanocluster Networks*

PATRICK EDWARDS (Presenter), MARKO S. CHAVEZ, MOHAMED Y. EL-NAGGAR, VITALY V KRESIN, Physics, Univ of Southern California —

The study of metallic clusters at the nano-scale has revealed many finite-size effects not present in bulk materials, including electron shell structure, enhanced surface plasmon resonance, cluster-cluster charge tunneling, and Josephson current in potential superconducting arrays. Many of these features have been analyzed spectroscopically in the gas phase and via probe microscopy on surfaces, but an ongoing challenge is arranging size-selected nanoclusters into device geometries which would enable the exploration and optimization of transport phenomena based on their unique properties. We propose the use of suspended nanowire devices as scaffolds for organizing nanocluster assemblies. We will describe progress toward the fabrication and characterization of nanocluster chains supported by carbon nanotubes and by isolated bacterial flagella, both of which offer unique environments to study morphological and electronic properties of clusters on surfaces. Future work with such devices, employing varying nanocluster materials and tuned deposition conditions, will make it possible simultaneously to optimize the properties both of individual size-selected particles and of their nanoscale assemblies and networks.

*This work was supported by the NSF.
H71.00135: Resonant Scattering of Light from Dielectric Nanopillars AMINATOU DABOKEMP (Presenter), HUIZHONG XU, Department of Physics and Astronomy, San Francisco State Univ — The use of plasmonic nanoparticles dispersed in a visibly transparent polymer matrix has recently emerged as a promising alternative approach to realize transparent display [1]. The localized surface plasmon resonance of these particles allows them to selectively scatter light at certain wavelengths. However, their performance is limited due to the inherent absorption in these plasmonic particles. In this study, we use finite element method to study scattering of light from titanium dioxide nanopillars. Due to the large refractive index contrast between the nanopillar and its surrounding medium, strong resonant scattering can be achieved across the entire visible spectrum by varying its dimensions. As a result of zero absorption and sharp resonances, the figure of merit of these structures for transparent display applications is found to exceed values previously reported for plasmonic nanoparticles. Furthermore, the angular distribution of light scattered from these structures can be tuned by varying their dimensions. These nanopillar structures may be used to create novel metasurfaces with applications in metalenses, see-through head-up displays, and smart glasses.


H71.00136: Patterned Fabrication of Dielectric Nanopillar Arrays for Single Molecule Spectroscopy Applications* PATRICK DELEAR (Presenter), CHELSEA HOWARD, JOSEPH CHANDLER, BRIAN LE, OSKAR GARCIA, HUIZHONG XU, Department of Physics and Astronomy, San Francisco State Univ — The ability to guide and confine light on a scale much smaller than the wavelength of light opens up a variety of applications in fields including information processing, nanoscale imaging and lithography, and single molecule spectroscopy. For example, our previous studies have demonstrated the efficient guiding of visible light through 50-nm-diameter zinc oxide nanowire waveguides. However, the lengths of these zinc oxide nanowires are not well controlled due to the chemical synthesis method used, prohibiting their application in devices for single molecule spectroscopy. In this study, we use nanofabrication techniques to demonstrate the fabrication of titanium oxide nanopillars with controlled diameter and length. The use of these titanium oxide nanopillar waveguides for single molecule studies with fluorescence correlation spectroscopy at micromolar concentrations is probed and its application in studying the dynamics of protein molecules on cell membranes will be explored.

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H71.00137: The magneto-optics in quantum wires comprised of vertically stacked quantum dots: A calling for the magnetoplasmon qubits  MANVIR KUSHWAHA (Presenter), Rice Univ — A deeper sense of advantages over the planar quantum dots and the foreseen applications in the single-electron devices and quantum computation have given vertically stacked quantum dots (VSQD) a width of interest. Here, we embark on the collective excitations in a quantum wire made-up of vertically stacked, self-assembled InAs/GaAs quantum dots in the presence of an applied magnetic field in the symmetric gauge. The gauge invariance is preserved. The Fermi energy is observed to oscillate as a function of the Bloch vector. Remarkably, the intersubband single-particle continuum splits into two with a collective excitation propagating within the gap. This is attributed to the (orbital) quantum number owing to the applied magnetic field. Strikingly, the alteration in the well- and barrier-widths can enable us to customize the excitation spectrum in the desired energy range. These findings demonstrate, for the very first time, the viability and importance of studying the VSQD subjected to an applied magnetic field\(^1\). The technological promise that emerges is the route to devices exploiting magnetoplasmon qubits as the potential option in designing quantum gates for the quantum communication networks.


H71.00138: One-phonon resonant Raman scattering in a nanowire in presence of an external electric field  MARICELA FERNÁNDEZ LOZADA (Presenter), Univ de Sonora, RICARDO BETANCOURT RIERA, RENÉ BETANCOURT RIERA, Fisica, Instituto Tecnológico de Hermosillo, RAÚL RIERA AROCHE, Univ de Sonora — In this work, the emission spectra for a one-phonon resonant Raman scattering process in a semiconductor nanowire of GaAs with a cylindrical symmetry in the presence of an external transversal and homogeneous electric field, as a mechanism for controlling the electron states and the selection rules due to confinement, are presented. The theoretical model considers single parabolic conduction and valence bands which are split into a sub-bands system due to confinement and electric field. We have considered Frölich type Hamiltonian for the electron-phonon interaction and only Stokes process, where the Comas-Trallero model for a free-standing wire has been used. Moreover, the electron intermediate states correspond to uncorrelated electron-hole pairs. As a result, the emission spectra corresponding to different laser energies and the selection rules for the process are discussed. The electric field produces the appearance of transitions linked to phonon oscillation modes where despite using dipole approximation in the electron-photon interaction.
H71.00139: Carrier dynamics in ultrathin gold nanowires: Role of Auger processes

GYAN PRAKASH (Presenter), Department of Physics, Indian Institute of Science, Bangalore, SUBHAJIT KUNDU, AHIN ROY, N RAVISHANKAR, ABHISHEK K SINGH, Materials Research Center, Indian Institute of Science, Bangalore, A K SOOD, Department of Physics, Indian Institute of Science, Bangalore — Carrier dynamics in metallic nanostructures is strongly influenced by their confining dimensions. Gold nanoparticles of size $\sim 2$ nm lie at the boundary separating metallic and non-metallic behavior. Here, we examine the carrier dynamics in high aspect ratio ultrathin gold nanowires (Au-UNWs) of average diameter $\sim 2$ nm using pump (3.1 eV) and coherent white-light continuum as a probe in the spectral range of 1.15 eV to 2.75 eV. We find that the transient carrier dynamics in Au-UNWs under extreme excitation regime is slower than predicted by the often used two-temperature model. Systematically probing the dynamics by varying the pump intensity from weak to strong excitation regime reveals that the mechanism of carrier relaxation through electron-phonon observed so far in larger size Au nanostructures is not sufficient in the Au-UNWs. We show that the reduced screening of e-e interaction due to spilling of conduction band and localization of core (d band) electrons at the surface promotes Auger heating.

*Department of Science and Technology (DST) and Council of Scientific and Industrial Research (CSIR), India

H71.00140: Extending classical computational electrodynamics to quantum domain

CHRISTOPHER SILFIES (Presenter), JIANTAO KONG, Rutgers University, Camden — The Finite-Difference Time-Domain (FDTD) method [1] is widely used to simulate electromagnetic response of metallic structures, where abrupt boundary between materials is always assumed. However, when the scale is down to nanometer or even smaller, the non-abrupt electron density profile at metal surface causes problems, which are the so called nonlocal effects [2] (wavenumber-dependence) in plasmonics and nanophotonics research. We developed an approach [3] accounting for the non-abrupt surface profile, effectively extending the conventional FDTD method to nonlocal domain. This extension is still within the fast classical calculation scheme, but with the quantum mechanical surface plasmonic effects covered to first order. We utilized this approach to simulate on a few typical nanostructures, and the results on resonance shift and field enhancement agree very well with experiments and other ab initio calculations (e.g. DFT) in literature.


*This work has been supported by the new faculty start-up fund of Rutgers, the State University of New Jersey, Camden.
H71.00141: Cuboid Arrays as Surface Enhanced Raman Spectroscopy*  
ROSSHELL LAMUG (Presenter), AFTAB AHMED, California State University, Long Beach — Surface-enhanced Raman spectroscopy (SERS) allows for the enhancement of intrinsically weak Raman signal and thus enables the detection of analytes at single-molecule level and chemical specificity. Despite remarkable advancements in specificity and sensitivity however, SERS still suffers from a loss of signal that depends critically on techniques for nanofabrication. In this project, we use cuboid arrays as an ideal platform for a SERS substrate. This study investigates plasmonic materials and structural parameters of the array to achieve resonant enhancement of the local electric field. Our previous studies, using Finite Difference Time Domain method, revealed promising Raman enhancement factors, approaching $10^8$ using self-assembled arrays of gold nanocubes. These enhancement factors can be further improved with outside parameters such as hybridization of material and using a waveguide arrangement structure. The outcome of this work is the development of a low-cost user-friendly SERS substrate with high sensitivity, and stability. This work will broadly impact the field by assisting in the optimization of powerful multidisciplinary chemical sensing devices.

*This material is based upon work supported in part by the NIH Grant: CSULB MARC U*STAR; NIH Award No.: NIGMS T34 GM008074

H71.00142: Plasmon-induced efficient hot carrier generation in graphene on gold ultrathin film with periodic array of holes: Ultrafast pump-probe spectroscopy*  
GYAN PRAKASH (Presenter), RAJESH KUMAR SRIVASTAVA, SATYENDRA NATH GUPTA, A K SOOD, Department of Physics, Indian Institute of Science, Bangalore — Surface plasmon polaritons (SPPs) due to their inherent property of nanoscale confinement and localization, smaller than the interacting light wavelength, show strong light-matter interaction. Here, using ultrafast transient absorption spectroscopy we show that a high density of hot-electrons can be generated in graphene, through a strong interaction in a hybrid plasmonic structure of graphene with 3D gold hole array. Notably, pump-induced reflectivity shows significant signatures in the spectral window corresponding to extraordinary optical transmission resonances of gold hole array originating from the carrier dynamics in graphene. A comparative study of the graphene on gold film with and without hole array confirms the highly efficient direct plasmon-induced hot carrier generation in graphene.

*Department of Science and Technology (DST) and Council of Scientific and Industrial Research (CSIR), India
H71.00143: Effect of temperature and defects on the mechanical and electronic properties of stacked van der Waals materials: The example of boron carbo-nitride  
SIBY THOMAS (Presenter), MOHSEN ASLE ZAEEM, Mechanical Engineering, Colorado School of Mines, Golden, CO-80401, USA — We demonstrate how the temperature and defects affect the electronic and mechanical properties in van der Waals bound low-dimensional systems, with the example of monolayer boron carbo-nitride (BCN). Molecular dynamics simulation reveals that as a hetero-structure of h-BN and graphene, the C-C bond in the BCN is responsible for an improved full width at half maximum (FWHM) compared to graphene, which ensures the structural integrity of the BCN monolayer. Besides, consistent with graphene and h-BN, the in-plane lattice parameter of BCN shows thermal contraction over a wide range of temperatures and exhibits a system size dependence. Further, the density functional theory calculations show that electronic bandgap varies substantially (between 0.73 and 1.2 eV) with the presence of Stone-Wales defects whereas it possess metallic character with the presence of vacancy defects. In addition, a tensile test analysis reveals that the elastic modulus and Poisson's ratio of monolayer BCN are anisotropic and decrease (increase) with the application of uniaxial tensile (compressive) strain which is beneficial for many technological applications.

H71.00144: Manipulating charge transfer from core to shell in CdSe/CdS/Au heterojunction quantum dots*  
EXIAN LIU (Presenter), KANISHKA P KOBBEKADUWA, PAN P ADHIKARI, Physics and Astronomy, Clemson University, OU CHEN, Department of Chemistry, Brown University, JIANBO GAO, Physics and Astronomy, Clemson University — Core/shell Quantum dots (QDs) or nanorods decorated with metal nanoparticles such as gold (Au) and platinum (Pt) have considerable applications in photocatalysis and optoelectronics. The shell medium plays a key role in tuning charge transfer and recombination process from core to metal domain. However, the study of influence of shell, which addresses the interplay between intrinsic excitons and shell-related surface states in trap-related core/shell/metal QD is currently lacking. In addition, the band offset between the core and shell that relies on temperature parameter also impacts the charge carrier transfer and recombination, but how do charge transfer and recombination vary with temperature still remains unclear.

Aim to comprehensively understand the interplay between charge transfer and recombination mechanisms in CdSe/CdS/Au heterojunction nanocrystals, we study these systems with temperature-dependent steady-state photoluminescence (PL) and time-resolved PL. We manipulate the charge transfer to shell surface by varying the tunneling barrier height resulted from temperature variation, and the barrier width resulted from shell thickness variation. These mechanisms are manifested by an intrinsic exciton emission and trap emission in the near-infrared range.

*Clemson University
**H71.00145: Molecular migration in poly(vinyl alcohol) mixtures**

KATARZYNA MAJERCZAK

(Presenter), ZHENYU JASON ZHANG, Univ of Birmingham — Fluorescence techniques, both Fluorescence Recovery After Photobleaching and Fluorescence Correlation Spectroscopy were used to investigate the migration characteristics of small molecules in thin films composed of poly(vinyl alcohol) (PVA), glycerol and surfactants of various headgroup chemistry. We found that the diffusion kinetics of a molecular probe, Rhodamine B, is determined by both molecular arrangement within the film and the magnitude of charged intermolecular interactions. Addition of glycerol initially increases PVA chain flexibility, but inhibits probe movement once its concentration exceeds 44 wt% due to onset of noncompatibility between the two components. The presence of surfactants in the system was found to reduce the diffusivity of RhB in PVA matrix, which is consistent with that in bulk solutions. The reduced diffusion is likely due to steric inhibition for nonionic surfactants. However, the fine balance between inter-molecular interactions and steric inhibition governs the diffusivity of RhB when cationic or anionic surfactants are present in the matrix.

*This research was funded by School of Chemical Engineering, University of Birmingham, and EPSRC (grant number EP/P007864/1).

**H71.00146: Ab initio calculations on the depassivation reaction of H⁺ at a-SiO₂/Si(100) interfaces**

PEI LI (Presenter), Beijing Computational Science Res Ctr — Hydrogen is widely used to passivate the dangling bonds generated in the thermo xidation process, which significantly improves the electronic quality of the Si/SiO₂ interface. It may, however, make the devices vulnerable in certain environments. For example, ionization radiation may convert the excess hydrogen induced in the fabrication process to protons, and then the later may migrate to the interface and depassivate the dangling bonds saturated by hydrogen. In this study, the depassivation of \( P_{b1} \) and \( P_{b0} \) defects generated in amorphous SiO₂/Si(100) interfaces is investigated quantitatively. For \( P_{b1} \) defects, the proton detaches from the oxygen atom and then activates the defect. The forward reaction barrier is ~0.4 eV. After the reaction, the energy of the system decreases by 0.85 eV. The depassivation of \( P_{b0} \) defects is more unpredictable, because the proton may be trapped by other atoms or bonds during the long reaction path due to the location of the defect. In our simulation, the proton can be captured by Si-O-Si or Si-Si bond, and form threefold-coordinated O atom defect or Si-H⁺-Si bridge bond, respectively. The energy of the intermediate products is lower than the desired ones.
Perfect absorption in lossy anisotropic materials* SANJAY DEBNATH (Presenter), EVGENII NARIMANOV, Purdue Univ — Current state of art for perfect absorption is based on manipulating the incoming wave (which needs to be coherent) or the medium (needs to match impedance at optical frequency) or both. We show (Opt. Express. 27, 9561-9569 (2019)) perfect absorption of incoherent plane wave by planar semi-infinite slab based on the Brewster phenomenon. Lossless isotropic media support Brewster wave but cannot absorb energy. On the other hand, introducing loss in the medium causes Brewster wave to evolve directly into the leaky Zenneck surface wave. We demonstrate that anisotropic media with extra degrees of freedom in material parameters can bring the Zenneck wave back to Brewster wave even in the presence of loss. Our approach identifies potential classes of lossy anisotropic media who support this behavior and shows that the operating frequency of the proposed system is independent of physical dimensions. Our results show that many existing natural materials exhibit this effect at different frequencies from far-infrared to deep ultraviolet regimes.

*We acknowledge NSF(1629276-DMR), and Gordon and Betty Moore Foundation.

Femtosecond laser-induced structural dynamics of Nickel (111) single crystal. An ultrafast time-resolved x-ray diffraction study. RUNZE LI (Presenter), PETER M. RENTZEPIS, Texas A&M University — Femtosecond, 8.04 KeV x-ray pulses, generated from a table-top system, are used to probe the lattice dynamics of 100 nm and 150 nm Ni (111) single crystals grown on sapphire substrates and irradiated with 800 nm, 100 fs laser pulses. At pump fluencies below the damage and melting threshold, we observed lattice contraction due to the formation of a blast force, and coherent acoustic phonons with a period of 35 ps and 46 ps for the 100 nm and 150 nm Ni (111) films, respectively. The spatiotemporal distribution of electron, spin, and lattice temperatures within the 150 nm thick nickel single crystal was also simulated using the three-temperature model. In addition to the ultrafast heating within the skin depth, this study also revealed the tens of picoseconds time required for heating the hundred nanometer bulk of the Ni (111) single crystal.
Magneto-Dielectric investigation in partially disordered Tb$_2$CoMnO$_6$ thin film

RAJESH MANDAL (Presenter), Physics, Indian Institute of Science Education and Research, Pune, MOHIT CHANDRA, MALVIKA TRIPATHI, R.J. CHAUDHARY, Indore Centre, UGC-DAE Consortium for Scientific Research, VASILY MOSHNYAGA, I. Physikalisches Institut, Georg-August-Universität Göttingen — Relaxor ferroelectrics are recognized as a family of disordered or partially ordered materials that are classified as a special class of dipolar glass with the formation of weakly interacting polarized nano domains (PNR) below a certain temperature. They are distinguished from normal ferroelectric materials in terms of broad transition in the temperature dependent dielectric constant and the dispersion of the transition temperature with applied frequency. Here we report the observation of magneto-dielectrically coupled ferroelectric relaxation at quite high temperature (200K) in Tb$_2$CoMnO$_6$/STO(100) double perovskite thin film. Partially B site disordered film has been grown by means of a metal-organic aerosol deposition (MAD) technique. This material is reported as ferromagnetic insulator with $T_C$ around 90K. Here we observe an enhanced transition temperature of 110K due to in plane strain. The deviation from the Curie-Weiss law far above $T_C$ indicates the development of short range spin correlation which is getting coupled with the electric dipoles present in the system.

*Erasmus Plus grant (EU) and DST, India

A comparative study of characteristics of ZnO TFT for various substrate and fabrication parameters

SHAHIDUL ASIF (Presenter), Missouri State Univ — Several ZnO TFTs (thin-film field-effect transistors) are developed for assessing the characteristics as an FET under different fabrication parameters and substrate materials. These ZnO TFTs are grown using pulsed laser deposition in different substrate temperatures (300-700°C), in different oxygen pressures, and with or without annealing between 400-700°C. The substrates are n-type Silicon with SiO$_2$ insulating layer, and in some samples, they were accompanied by an additional HfO$_2$ film layer as a high dielectric material. All the TFTs have bottom-gate structure while the drain, source, and gates are equipped with gold electrodes fabricated by the sputtering method. The films are analyzed by XRD, Raman spectroscopy and photoluminescence as a verification of the presence of ZnO. Using an experimental set-up, the transfer and I-V characteristics are measured whereas the gate voltage is swept over a range of ~10-50 V. To assess the effectiveness of ZnO material for using in a TFT, the field-effect mobility, the drain current density, etc. are measured. Finally, the TFTs are tested for application in high frequency sweeping (1kHz-1MHz) as the hysteresis nature and power gain cut-off frequencies are compared.
H71.00151: Interface Orbital/Charge Reconstruction and Its Effect on Spin Orientation for (110)-La\textsubscript{2/3}Sr\textsubscript{1/3}MnO\textsubscript{3} Layer Sandwiched by LaCoO\textsubscript{3} Films*  FURONG HAN (Presenter), JIRONG SUN, Chinese Academy of Sciences, Institute of Physics — Here we made the first attempt to reveal the effect of orbital/charge reconstruction associated with interface engineering on spin degree of freedom. We took tensely strained (110)-LaCoO\textsubscript{3}/La\textsubscript{2/3}Sr\textsubscript{1/3}MnO\textsubscript{3}/LaCoO\textsubscript{3} trilayers as specimens, focusing on orbital reconstruction and accompanied effects. The most remarkable finding is the reordering of the energy levels of Mn-3d orbitals: the low-lying orbital becomes d\textsubscript{x2-y2} for sandwiched La\textsubscript{2/3}Sr\textsubscript{1/3}MnO\textsubscript{3} rather than d\textsubscript{3z2-r2} as expected for a bare La\textsubscript{2/3}Sr\textsubscript{1/3}MnO\textsubscript{3} film. Interlayer charge transfer via d\textsubscript{x2-y2} orbitals is further detected, which is the driving force for orbital reconstruction. Due to spin-orbit coupling, the charge/orbital reconstruction produces a chain effect on spin degree of freedom of the La\textsubscript{2/3}Sr\textsubscript{1/3}MnO\textsubscript{3} layer, resulting in a dramatic spin reorientation by 90° in film plane. The present work vividly demonstrates how to tune macroscopic properties of correlated oxides via the mutual coupling between different degrees of freedom.

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H71.00152: Observation of high electron mobility with significant spin-orbit coupling in rock-salt YbO epitaxial thin film*  TAKU YAMAMOTO, KENICHI KAMINAGA (Presenter), DAICHI SAITO, DAICHI OKA, TOMOTERU FUKUMURA, Tohoku University — We report the optical and electrical properties of ytterbium monoxide (YbO) epitaxial thin films with unusual valence state of Yb\textsuperscript{2+} (4f\textsuperscript{14}5d\textsuperscript{0}) [1]. Consistent with the chemical trends of ytterbium monochalcogenides, YbO thin films exhibited the narrow bandgap of 0.25 eV and the large crystal field splitting of 5d orbitals. Electrical resistivity was tunable by electron doping to 5d conduction band via the introduction of oxygen vacancies. Also, electron mobility at 300 K increased up to 13 cm\textsuperscript{2}V\textsuperscript{-1}s\textsuperscript{-1} with increasing electron carrier density. The weak antilocalization at low temperature observed in the heavily electron-doped YbO suggests significant spin-orbit coupling owing to the heavy Yb nucleus. [1] T. Yamamoto et al., Appl. Phys. Lett. 114, 162104 (2019). Selected as Featured.

*This work was supported by MEXT/JSPS (18H03872, 26105002) and the Mitsubishi Foundation.
**H71.00153: InN/AlN/Si (111) semiconductor-insulator-semiconductor (SIS) heterostructure for ultrafast optical fibre communication (1550 nm)**  
ARUN CHOWDHURY (Presenter), ROHIT PANT, Materials Research Centre, Indian Institute of Science, BASANTA ROUL, Central Research Laboratory, Bharat Electronics, DEEPEndRA KUMAR SINGH, KARUNA KAR NANDA, SALURU BABA KRUPANIDHI, Materials Research Centre, Indian Institute of Science — In this work, we report on InN/AlN/Si (111) SIS-based self-powered, and ultrafast photodetector, which works at an extremely important wavelength of 1550 nm (fibre communication). InN was grown on AlN/Si template by plasma-assisted molecular beam epitaxy. The heterostructure with a top-bottom (vertical) type of electrode configuration shows a responsivity of 3.36 µA/W with transit times in milliseconds range at zero bias. The variation of photocurrent with respect to power density is nonlinear with an exponent of 1.36, which might be attributed to the presence of traps at the interfaces. To further elucidate the nature of interface of the SIS heterostructure, a low-temperature vertical electrical transport behaviour was studied over a range of 100 – 400 K. It reveals that the barrier height (BH) is inhomogeneous in nature at the hetero-interface. It has been explained by assuming the presence of double Gaussian distribution of BH at the SIS interface based on thermionic emission theory. The double Gaussian distribution of the BH indicated the presence of traps at the interface which was already speculated from the photocurrent and power density relation of the photodetection studies.

**H71.00154: Graphene Doping in LiMnO$_4$ cathode of Lithium Ion Battery**  
NNAMDI ENE (Presenter), ERICA S WILEY, MEHMET ALPER SAHINER, Physics, Seton Hall University — Lithium ion batteries, due to their high-power density and high energy are being utilized more and more in present day electronic devices. One way we might improve the absorbance of these batteries is by reducing the band gap energy of the materials used as either the anode or the cathode. Graphene, having a crystalline, 2-dimensional and monoatomic structure has a high electrical conductivity. Graphene is also called a zero-band gap semiconductor. Previous research supports the reduction in the band gap energy by the introduction of graphene as a dopant in thin films. (Elmas et al. 28) This research will thus seek to study the effects of graphene doping in the LiMnO$_4$ cathode region, to electronic energy configuration and the electrical performance of lithium ion thin films prepared by pulsed laser deposition.

H71.00155: Self-powered, broadband and ultrafast MoS$_2$/AlN/Si based photodetector*

DEEPEndra Singh (Presenter), Rohit Pant, Basanta RouL, Arun Chowdhury, Karuna Kar Nanda, Saluru Baba Krupanidhi, Indian Institute of Science — Heterostructures of ultrathin 2D layered materials and wide band gap semiconductors offer possibilities of high-performance electronic devices. The absence of a band gap in graphene, which limits its application as a switch, MoS$_2$ has attracted considerable attention in recent years due to its excellent optoelectronic properties, as well as the presence of a narrow band gap. Here, we have reported a self-powered, broadband and ultrafast photodetector based on MoS$_2$/AlN/Si heterostructure. MoS$_2$ thin film has been deposited on AlN template on n-Si(111) by pulsed laser deposition. The vertical transport of the heterostructure exhibits excellent photodetection properties at zero bias condition. The device shows a broadband photoresponse in the range of 300-1100 nm, with a maximum responsivity of 5.47 A/W at 900 nm. Transient analysis of the device at 900 nm shows an ultrafast detection, with rise/fall times of 12.5/14.9 μs. Band alignment studies of MoS$_2$ and AlN has been done by XPS and a band diagram of the heterostructure depicting the self-powered transport has been proposed.

*Council of Scientific & Industrial Research Deependra Kumar Singh acknowledges Council of Scientific & Industrial Research, New Delhi for providing senior research fellowship.

H71.00156: Understanding the negative compressibility in a 2D electron gas: Application to LaAlO$_3$/SrTiO$_3$*

Aditi D Mahabir (Presenter), Univ of North Florida, Alexander Balatsky, Nordic Institute for Theoretical Physics, Jason Haraldsen, Univ of North Florida — We investigate the effects of a two-band coupling on the negative compressibility for the two-dimensional electron gas. Using a homogeneous 2D electron model and a two-band description of the electron interactions, we examine the dependence of critical carrier density, dielectric constant, and effective mass on the negative compressibility of the 2D electron gas and compare results to the at the complex oxide interface of LaAlO$_3$/SrTiO$_3$. From our calculations, we show that the presence of interband coupling will produce a dramatic decrease in the polarizability and the critical carrier density of the 2DEG. Furthermore, we find that the ratio of the effective masses of the bands has a distinct and dramatic effect on the negative compressibility.

*This project is supported, in part, by the Institute for Materials Science at Los Alamos National Laboratory.
H71.00157: Epitaxial growth and interface band alignment studies of all oxide α-Cr$_2$O$_3$/β-Ga$_2$O$_3$ p-n heterojunction* SAHADEB GHOSH (Presenter), MADHUSMITA BARAL, Synchrotrons Utilization Section, Raja Ramanna Centre for Advanced Technology, Indore and HBNI, Mumbai, RAJIV KAMPARATH, Raja Ramanna Centre for Advanced Technology, R. J CHOWDHURY, SQUID-VSM and PLD Lab, UGC-DAE Consortium For Scientific Research, Indore, D. M PHASE, SEM and Beamline Lab, UGC-DAE Consortium For Scientific Research, Indore, S. D SINGH, TAPAS GANGULI, Synchrotrons Utilization Section, Raja Ramanna Centre for Advanced Technology, Indore and HBNI, Mumbai — Epitaxial growth of α-Cr$_2$O$_3$(p-type) on c-Al2O3 and β-Ga$_2$O$_3$ (n-type) on α-Cr$_2$O$_3$(p-type) has been carried out to make an all oxide epitaxial n-type β-Ga$_2$O$_3$/p-type α-Cr$_2$O$_3$ heterojunction using RF sputtering. A valence band offset of 3.38 ± 0.2 eV at the heterojunction is determined using Kraut's method. From the bandgap measurements of α-Cr$_2$O$_3$ and β-Ga$_2$O$_3$, the conduction band offset of 1.68 ± 0.2 eV at the heterojunction is obtained. Thus, the band alignment at this heterojunction is found to be staggered (Type-II), which leads to the confinement of electrons and holes in the β-Ga$_2$O$_3$ layer and α-Cr$_2$O$_3$ layer, respectively. Our results provide a pathway to design all oxide optoelectronic devices based on a p-n heterojunction consisting of n-type β-Ga$_2$O$_3$ and p-type α-Cr$_2$O$_3$.

*The authors are thankful to HBNI, RRCAT for financial support during the course of the work.

H71.00158: Quantum Correction to the Work Functions of Clean Tungsten Surfaces under Electric Fields LIANGLIANG XU (Presenter), YUE WANG, MING-CHIEH LIN, Department of Electrical and Biomedical Engineering, Hanyang University, TSAN-CHUEN LEUNG, Department of Physics, National Chung Cheng University, HUA-YI HSU, Department of Mechanical Engineering, National Taipei University of Technology — Tungsten has a relatively high work function, electron emission is largely limited. In this work, first-principles calculations are used to study the work functions of tungsten (100), (110), and (111) surfaces under different electric fields. We have carefully and systematically tested the convergence of density-functional-theory (DFT) calculations in the local-density approximation (LDA) and generalized-gradient approximation (GGA) with a plane-wave basis set with the projector-augmented wave (PAW) method as implemented in the Vienna ab initio simulation package (VASP). Detailed study of field emission by using VASP is performed and it is found when we increase the electric field strength, the work functions of tungsten surfaces are reduced accordingly. A new scaling law of work function reduction due to the charge transfer near the metal/vacuum interface caused by external electric field is obtained. The quantum effect is different from the classical Schottky effect of lowering work function due to an external electric field. With the quantum correction, the predictions of Richardson-Dushman and Fowler-Nordheim equations under strong electric fields for thermionic and field emissions, respectively can be improved.
**H71.00159: Picosecond laser ultrasonic measurements of elastic properties of transition metal dichalcogenides**

ETHAN MURRAY, MADELAINE PELLETIER, JACOB STULIGROSS, ELLIS THOMPSON, BRIAN DALY (Presenter), Vassar College, SENG HUAT LEE, Pennsylvania State University — We report ultrafast optical pump-probe measurements of sound velocity and attenuation for GHz frequency longitudinal acoustic strain pulses in MoSe$_2$ and WSe$_2$. High-quality bulk single crystals of 2H-MoSe$_2$ and WSe$_2$ were synthesized by chemical vapor transport with iodine as the transport agent. Thin layers with thicknesses ranging from a few nm up to a few hundred nm were then mechanically exfoliated onto sapphire or SiO$_2$/Si wafers. A degenerate optical pump-probe experiment was performed with a Ti: sapphire ultrafast laser with peak wavelength varied from 760 nm to 830 nm. At these wavelengths, the optical absorption in these crystals is strong enough that a high frequency acoustic strain pulse with frequency components approaching 100 GHz is generated. This picosecond ultrasonic pulse travels back and forth in the exfoliated layer and causes a reflectivity change that is measured by time-delayed probe pulses via the strong strain dependence of the optical properties. Longitudinal sound velocities as well as an upper bound on attenuation of 100 GHz phonons are determined by comparing reflectivity data to 1D simulations.

*We acknowledge the support of Vassar College’s NSF award DMR-1709521, and a sub-award through the 2DCC-MIP at Penn State - Prime Award: DMR-1539916.

**H71.00160: Ab-initio study of surface plasmons on palladium surfaces**

UNAI MUNIAIN (Presenter), DIPC, RUBEN ESTEBAN, DIPC and Ikerbasque, VYACHESLAV SILKIN, DIPC, Ikerbasque and UPV/EHU — Collective electronic excitations at metal surfaces lead to strongly localized electromagnetic fields that play a key role in numerous phenomena in physics, material science, biology or medicine [1]. In particular, surface plasmons are modes that appear in vacuum/metal boundaries, with a constant dispersion relation in the long-wavelength limit predicted by simple models [2]. However, in real metallic systems such predictions often fail. In particular, in many materials, when the non-local behavior of the electronic response is considered, additional collective modes characterized by significantly lower frequencies may appear [3]. In this work, we perform first-principles time-dependent density-functional calculations of the excitation spectra of the palladium surfaces, in order to establish the characteristics of its surface plasmons. We analyze the properties of the surface collective excitations using the surface response function, which is closely related to the permittivity of the material. Our results thus contribute to gaining a better understanding of the optical response of palladium structures.


*GV Project PI2017-30*
**H71.00161: Comparing Magnetron Sputtered ScN Films Grown on Sapphire ((10-10) and (1-102)) Substrates**

TOBIN MURATORE (Presenter), SAID ELHAMRI, Physics, University of Dayton, AMBER REED, JOHN CETNAR, Air Force Research Laboratory, DAVID C LOOK, Wright State University, KURT EYINK, HADLEY SMITH, ZACHARY BIEGLER, Air Force Research Laboratory — ScN films with high quality crystal structure and desirable carrier concentration have previously been grown on sapphire (0001) substrates. This study seeks to determine whether similarly high quality films can be grown on (101-0) and (1-102) orientated sapphire. The depositions for this study were carried out via reactive, unbalanced, DC magnetron sputtering. Previous growth of ScN on sapphire (0001) showed film quality is sensitive to sputtering conditions. This study seeks to determine what, if any, sputtering conditions can produce films of comparable quality to those grown on sapphire (0001) substrates on the lower symmetry surfaces. The impact of these growth conditions on the crystal quality and electrical properties were evaluated using x-ray diffraction and Hall-effect measurements. X-ray diffraction results indicate that growth on sapphire (1-102) is sensitive to temperature, with optimal growth occurring in a 40°C window. For (10-10) sapphire, similar crystal quality occurs over temperatures from 500-900°C. XRD also shows no conditions tested for either substrate displayed the single crystal growth present on (0001) sapphire.

*This research was supported the Air Force Office of Scientific Research through project FA9550-RYCOR490

**H71.00162: WITHDRAWN ABSTRACT** —

**H71.00163: Compression-rate dependent domain growth patterns in diacetylenic chiral lipids Langmuir films: choline vs. ethanolamine head-groups**

PRITAM MANDAL (Presenter), Durgapur Women's College — In this talk, we discuss domain growth in Langmuir monolayers of two diacetylenic lipids, one with choline and other with ethanolamine head group. We found that (i) Unlike a diacetylenic lipid, Diyne PE (23:2), the diacetylenic Diyne PC (23:2), does not form chiral hierarchal self-assembled patterns. (ii) Structured solid domains in Diyne PC (23:2) Langmuir layer forms within a lower temperature range than with Diyne PE (23:2). Comparing their domain morphology we argue that choline and ethanolamine head groups interact differently with water, influencing the packing-mode. (iii) For both lipids, the growth patterns depend on the compression speed. At lower compression-rate the condensed domains grow as fractal dendrites with straight backbone whereas at rapid compression rate, domains grow as curved claws developing branches as they grow. Since slow or rapid compression rate pushes the monolayer to different non-equilibrium state (different super-saturation), we reason that solid phase grow out of different metastable states, generating distinct morphology.

*I acknowledge the King Abdullah University of Science and Technology (KAUST), Thuwal-6900, KSA, where I first started this study as a postdoc.*
**H71.00164: Ultrasonic modification of hydrophobin bubbles and droplets for multiphase systems***  
ZHAOXIAN ZHANG (Presenter), PAUL RUSSO, SAAD BHAMLA, SAMYAK JAIN, UDITA RINGANIA, Georgia Inst of Tech — Cerato Ulmin(CU), a fungal protein classified as Hydrophobin, is an amphipathic surfactant which self-assembles at interfaces. CU can encapsulate air or oil in aqueous solutions to form non-spherical bubbles or droplets, similar to those formed by interfacial composite materials with solid-like surfaces. A sufficient dispersion of CU in water can create concentrated oil droplet/air bubble structures resembling complex multi-phase systems. These structures, which are observed to be stable for days, could have a variety of applications in emulsion engineering, reaction catalysis, and constructing multi-scale metastructures, among many others. Ultrasonic agitation was used to modify these structures, and it was discovered that the frequency of the ultrasound corresponded to the length scale of air-filled structures, by mechanism of Minnaert Resonance. With this method it was possible to select the size distribution of the air-filled structures. Oil-filled structures behaved differently, yet with sufficient ultrasound amplitude, it was possible to produce CU-oil nano-emulsions, likely by the mechanism of cavitation. The size and longevity of these nano-emulsions were studied by dynamic light scattering.

*Funding from Solvay through the MSE Research Scholars Program.

**H71.00165: Scanning Probe Microscopy of Two Dimensional Covalent Organic Frameworks***  
HARSHAVARDHAN MURALI (Presenter), ZACHERY ENDERSON, CAMERON FERIANTE, RAGHUNATH DASARI, HONG LI, SIMIL THOMAS, TIMOTHY C PARKER, JEAN-LUC E BREDAS, SETH R. MARDER, PHILLIP N FIRST, Georgia Inst of Tech — Covalent organic frameworks (COFs) are a new class of materials that can be designed to exhibit interesting physical, chemical and electronic properties. In this work, we study the growth and properties of single layer covalent organic frameworks that we synthesize on noble metal surfaces, typically via an Ullmann-like process accomplished through thermal deposition and annealing. An outstanding challenge in 2D-COF on-surface synthesis is to achieve long range, defect free crystalline order over hundreds of nanometers. Using scanning tunneling microscopy (STM), we probe COF growth and island formation under different preparation conditions, from monomer self-assembly to covalent bond formation. We also study the electronic properties of COF islands obtained in this process, including effects of finite size and substrate interaction, using scanning tunneling spectroscopy and comparisons to theoretical first-principles calculations.

*This work is funded by the United States Army Research Office under grant number W911NF-15-1-0447 (MURI).*
**H71.00166: Nanotribology of Phosphonium Phosphate Ionic Liquid: a Combined Atomic Force Microscopy and Surface Spectroscopy Study**  
FILIPPO MANGOLINI, ZIXUAN LI (Presenter), OSCAR MORALES-COLLAZO, University of Texas at Austin, JERZY T. SADOWSKI, Brookhaven National Laboratory, HUGO CELIO, ANDREI DOLOCAN, JOAN BRENNECKE, University of Texas at Austin — Ionic liquids (ILs) have recently gained considerable attention owing to their unique and tunable properties (e.g., wide electrochemical window, high thermal stability), which make them potentially useful for a range of applications, including batteries, fuel cells, catalysis, and lubrication. When IL are used as lubricants, the interface between the IL and the solid surface plays a pivotal role to determine the friction/wear response. Despite the weight of the studies published in the literature, remarkably little is still known about the structure of solid/IL interfaces and its relationship with the lubrication mechanism/performance of ILs. Here, we used atomic force microscopy (AFM) to visualize and quantify the processes occurring at sliding interfaces in situ, in single-asperity nanocontacts. The AFM experiments, in which a diamond tip was slid on steel in phosphonium phosphate ILs, indicated a significant friction reduction only after the removal of the native surface oxide from steel. Based on laterally-resolved ex situ analyses of the surface chemistry of steel by X-ray photoemission and low energy electron microscopy, and time-of-flight secondary ion mass spectrometry, a simple phenomenological model will be proposed to account for the observed lubrication behavior.

**H71.00167: WITHDRAWN ABSTRACT**

**H71.00168: Planar polymers under cylindrical confinement**  
DULCE VALENCIA (Presenter), Northwestern University — We show that the cylindrical confinement of a planar ribbon gives rise to the formation of stationary helical shapes, previously observed in molecular dynamics simulation studies of some planar polymers inside nanotubes. In the limit of small twisting deformations, we notice that a confined ribbon describes identical equilibrium configurations of an elastic rod on the plane. Also, every locally planar strip adsorbed on a cylinder is forced to follow a helical envelope, as its length increases. We also determine the forces and torques that sustain each ribbon equilibrium configuration through the equilibrium geometry and the confinement surface parameters.

*Northwestern University*
H71.00169: SAMPLE: Surface structure search enabled by coarse graining and statistical learning  LUKAS HÖRMANN (Presenter), ANDREAS JEINDL, ALEXANDER T. EGGER, MICHAEL SCERBELA, OLIVER T. HOFMANN, Institute of Solid State Physics, Graz University of Technology — Studying the electronic structure of organic monolayers on inorganic substrates requires knowledge about their atomistic structure. Such monolayers often display rich polymorphism arising from diverse molecular arrangements in different unit cells. The large number of possible arrangements poses a considerable challenge for determining the different polymorphs from first principles.

To meet this challenge, we developed SAMPLE[1-3], which employs coarse-grained modeling and machine learning to efficiently map the minima of the potential energy surface of commensurate organic adlayers. Requiring only a few hundred DFT calculations of possible polymorphs as input, we use Bayesian linear regression to determine the parameters of a physically motivated energy model. These parameters yield meaningful physical insight and allow predicting adsorption energies for millions of possible polymorphs with high accuracy.

We demonstrate SAMPLEs capabilities on the systems of naphthalene[1] and TCNE[2,3] on coinage metals where we predict the energetically most favorable polymorphs and compare them to experimental data.


H71.00170: Effects of Ligand Composition on Protein Corona Formation around, and the Surface Structure of, Au Nanoparticles  SAM HOFF (Presenter), University of Colorado, Boulder, DESIRÉ DI SILVIO, SERGIO MOYA, Soft Matter Nanotechnology Lab, CIC biomaGUNE, RONALD ZIOLO, Centro de Investigación en Química Aplicada, HENDRIK HEINZ, University of Colorado, Boulder — Coatings on nanoparticles in biological environments greatly impact the dynamics and stability of the nanoparticles. Destinations, and potential function of nanoparticles can be changed by attaching ligands to the nanoparticle surface. In this study, molecular dynamics is used to study how different ligands, and specifically different chemical end groups, alter the surface structure and dynamics of the ligands in solution. PEG2000, Alkyl-PEG600-Glucosamide, and Alkyl-PEG600-Butanamide and their specific interactions with Bovine Serum Albumin and Concanavalin A are studied in detail. The effects of altering the end group on Alkyl-PEG600-Butanamide to Propanamide and Ethanamide are explored, and is found to have a significant impact on the surface structure at the ligand-water interface, potentially altering nanoparticle interactions in solution, as well as protein corona formation. The CHARMM36-Interface force field is used throughout all simulations which yields interfacial properties directly comparable to experimental measurements. The study is expected to lead to new insight into how protein-ligand interactions work, as well as advancing understanding of how ligand conformations can affect their environmental interactions.
H71.00171: Selective studies of adsorption of Ag\textsubscript{8}M and Ag\textsubscript{14}M clusters (M = Au, Co and Pt) on alumina substrate*  ISABELLA LEVENSOHN KASTOR (Presenter), NUSAIBA ZAMAN, ABDELKADER KARA, Univ of Central Florida — Small silver clusters were used as catalyst for Li-air batteries, which controlled the rate of discharge at the cathode. The gap near the fermi energy was shown to control the oxygen reduction, an important reaction for LiO\textsubscript{2} formation. One can vary the size of the cluster to vary the gap, however, this “knob” provides limited variance. Hence, we study the effect of alloying in combination with size variation of Ag\textsubscript{8}M and Ag\textsubscript{14}M clusters (M = Au, Co and Pt). Using Density Functional Theory (DFT), we determine the most stable geometry of these bimetallic clusters and calculate the binding energies of these clusters on the alumina substrate. We explore how the gap at the Fermi level of the system varies as a function of elemental composition and size of the cluster. Bader charge analysis is also performed to probe how the charges are transferred between the cluster and the substrate. These preliminary studies will open the door for more systematic studies of alloy clusters of different size and stoichiometry for Li-O\textsubscript{2} battery cathode design as well as for general catalysis.

* Partial support is provided from the U.S. Department of Energy Basic Energy Science under Award number DE-SC0007045. This research used computational resources of NERSC, as well as UCF-Stokes.

H71.00172: Structural and magnetic transition in NiO(111) surface  WANDONG XING (Presenter), YANG ZHANG, Tsinghua University, FANYAN MENG, University of Science and Technology Beijing, JING ZHU, RONG YU, Tsinghua University — We report an experimental and theoretical analysis of the NiO(111) surfaces combining aberration corrected TEM and first-principles calculations. An unreconstructed O-terminated (1×1) surface and a reconstructed O-terminated surface (with the topmost Ni in tetrahedral sites, a wurtzite-like surface stacking) have been revealed. Here, the two surfaces are shown to be stabilized by charge compensation, arising from changing the valence state of the topmost Ni\textsuperscript{2+} into Ni\textsuperscript{3+} ions and providing the additional positive charges to the surface. In addition, it is found that the main difference between the two surface structures is the movement of the topmost Ni atoms from octahedral position to tetrahedral position, coupling to a spin transition from the low-spin state (Ni\textsuperscript{3+}-LS) to the high-spin state (Ni\textsuperscript{3+}-HS).
H71.00173: Using Machine Learning to Understand Mechanical Loss in LIGO Mirror Coatings
SAGADA PENANO (Presenter), KIRAN PRASAI, E.L. Ginztion Laboratory, Stanford University, JUN JIANG, ALEC MISHKIN, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, RICCARDO BASSIRI, MARTIN M. FEJER, E.L. Ginztion Laboratory, Stanford University
— The sensitivity of future generations of gravitational wave detectors such as LIGO will be limited by thermal noise from the mirror coatings on the test masses. A major source of thermal noise is the mechanical loss of the coatings. The mechanical loss at temperatures higher than 10 K is believed to be the result of thermally activated transition between two level systems (TLSs) in the amorphous coating. By using a multilayer perceptron neural network to understand the atomic structures of many computer-generated two-level systems (TLS) of amorphous tantala (a-Ta$_2$O$_5$), a prospective coating material, we aim to identify the structural motifs that contribute to mechanical loss. From an analysis of many independent TLSs, we can identify which atoms are most likely to relax by comparing changes in atomic energies and positions. Values that describe the structural features of these atoms can then be computed using angular and radial distribution functions. Using these predictions, a common pattern of relationship between structure and relaxation behavior can be extracted. The results will likely aid in understanding what gives rise to the measured values of mechanical loss and will help determine the best materials and deposition parameters for lower mechanical loss mirror coatings.

H71.00174: Invalidity of the BCS theory of superconductivity
JORGE HIRSCH (Presenter), University of California, San Diego — A theory that purports to describe the natural world can be proven invalid by either (a) an experimental result or (b) a theoretical proof that it is internally inconsistent. However BCS is special: it cannot be disproved by (a) because any superconductor yielding an experimental result that doesn't conform to BCS is simply declared to be 'unconventional'. Hence we are left with (b). In a process where the temperature of a type I superconductor in a magnetic field changes, the London penetration depth and hence the magnetic flux changes, generating a Faraday electric field. BCS theory predicts that the electric field gives rise to a normal current and as a consequence Joule heat is dissipated, in an amount that depends on the speed of the process, and it also predicts that the final state is independent of the speed of the process. I show that these two predictions cannot be simultaneously reconciled with the laws of thermodynamics. Therefore, BCS theory is internally inconsistent. I propose a resolution of this conundrum through physics that is not part of BCS theory.

H71.00175: WITHDRAWN ABSTRACT —
H71.00176: Numerical solution of the full-bandwidth Eliashberg equations including vertex corrections beyond Migdal's approximation  ALEX APERIS (Presenter), FABIAN SCHRODI, PETER OPPENEER, Uppsala University — We solve the full bandwidth and non-adiabatic Eliashberg equations for electron-phonon mediated superconductivity by fully including the first vertex correction in the electronic self-energy. The non-adiabatic equations are solved numerically without further approximations for a generic one band model system. We compare the results with outcomes of adiabatic Eliashberg calculations. Non-adiabatic contributions can increase, decrease or have negligible effect to the superconducting gap depending on the dimensionality of our system, the degree of non-adiabaticity and the coupling strength. We further examine effects on the transition temperature and the electron-phonon coupling constant. Our treatment opens up the possibility of systematically studying vertex correction effects in strongly coupled and/or adiabatic superconductors, such as the ones with high transition temperature.

H71.00177: Melting transition of the nematic state in an under-doped d-wave superconductor*  HONG-YI CHEN (Presenter), YU-YO CHEN, National Taiwan Normal Univ — We study the melting transition of smectic state in an under-doped d-wave superconductivity. We demonstrate that the transition is discontinuous to the nematic state by increasing the impurities. We calculate the entropy as a function of impurities which shows a sharp transition between the smectic and nematic states. We also show that the density-of-states at the Fermi energy emerges as the sub-gap induced by the SDW order is smeared out gradually. The transition between the smectic and nematic states is associated the reconstruction of the electronic Fermi surface. We calculate the superfluid density that exhibit a plateau and indicates that the nematic state development in d-wave superconductor is distinct from high-temperature pseudogap.

*MOST 107-2112-M-003-002

H71.00178: Finding the static critical exponent in YBa2Cu3O7 using critical current density  IOAN DASCALU (Presenter), MATTHEW C. SULLIVAN, Ithaca Coll — We grew thin films of hole-doped cuprate YBa2Cu3O7 (YBCO) using optimized pulsed laser deposition and patterned them into a meander wire with conventional photolithography techniques. We examined the normal-superconducting phase transition of the thin films via a critical scaling analysis of voltage vs current isotherms, where each measurement is the average of many reverse-polarity measurements. We expect the superconducting phase transition to obey critical (3D-XY) theory near the critical temperature and obey mean-field theory further from the critical temperature. We show that critical current density can access both the critical regime and the mean-field regime in a single sample. We present our results on the static critical exponent in both regimes for YBCO.
**H71.00179: Transport characteristics of type II Weyl semimetal MoTe\(_2\) thin films grown by chemical vapor deposition**

NIRAJ BHATTARAI (Presenter), ANDERW W FORBES, Physics, The Catholic University of America, RAJENDRA DULAL, Advanced Physics Laboratory, Institute for Quantum Studies, Chapman University, IAN L PEGG, JOHN PHILIP, Physics, The Catholic University of America — Theoretical calculations and experimental observations show MoTe\(_2\) is a type II Weyl semimetal, along with many members of transition metal chalcogenides family. We have grown highly crystalline large-area (upto 8mm X 4mm) MoTe\(_2\) thin films on Si/SiO\(_2\) substrates by chemical vapor deposition. Very uniform, continuous, and smooth 1T'-MoTe\(_2\) films were obtained as confirmed by scanning electron microscopy, atomic force microscopy, x-ray and Raman spectroscopy analyses. Measurements of the temperature dependence of longitudinal resistivity and current-voltage characteristic at different temperature are discussed. Unsaturated, positive quadratic magnetoresistance of the as-grown thin films has been observed at various temperatures below room temperature. Hall resistivity measurements confirm the majority charge carriers are holes. Using the single band model, carrier concentration was calculated to be \(2.38 \times 10^{21}\) holes cm\(^{-3}\) at 10 K, which is semimetallic, and increasing with temperature. These results will guide us in the way of pragmatic applications of thin films MoTe\(_2\) in future electronic devices.

**H71.00180: WITHDRAWN ABSTRACT**

**H71.00181: "Thickness dependent characteristics of Single Crystalline Bi:YIG Thin Film grown with different orientation"**

GANESH GURJAR (Presenter), School Of Physical Sciences, Jawaharlal Nehru University New Delhi India, VINAY SHARMA, Special Centre for Nanosciences, Jawaharlal Nehru University New Delhi India, SATYABRATA PATNAIK, School Of Physical Sciences, Jawaharlal Nehru University New Delhi India, BIJOY KUANR, Special Centre for Nanosciences, Jawaharlal Nehru University New Delhi India — The Magneto-Optical (MO) properties are increases when bismuth (Bi) is substituted in the YIG (Bi\(_{0.1}\)Y\(_{2.9}\)Fe\(_5\)O\(_{12}\), BYIG). BYIG films of two different thickness were grown with different orientation ([111] and [100]) by pulsed laser deposition (PLD) technique over single crystalline Gadolinium gallium garnet (GGG) substrates. The BYIG grown with [100] orientation was observed structurally better with lesser strain (around 40% lesser). As the thickness of film decreases, the size of lattice parameter is also slightly decreases and it is more (by 0.073%) for the film grown over GGG having [111] plane. Larger ferromagnetic resonance (FMR) line width is observed in [111] directed film (100 Oe) as compared to [100] directed film (60 Oe) and also it decreases with the film thickness (100 Oe to 47 Oe in [111] and 60 Oe to 39 Oe in [100] directed film). The value of net effective magnetization and Gilbert damping constant is observed to be increases with decrease in thickness of the film. The low Gilbert damping constant (1.53\(\times\)10\(^{-4}\), [100]) is observed as compared with (2.68\(\times\)10\(^{-4}\), [111]). Thus BYIG thin film grown on GGG along [100] direction shows better structural and magnetization characteristics and hence can be used for microwave devices such as microwave filter etc.
**H71.00182: Study of V/TiO$_2$ interface by X-ray Photoelectron Spectroscopy**

MIRANDA S MARTINEZ (Presenter), ANIL CHOURASIA, Texas A&M University, Commerce — The V/TiO$_2$ interface has been studied by the technique of x-ray photoelectron spectroscopy (XPS). Thin films of titanium were deposited on a quartz substrate and oxidized in situ to form TiO$_2$ overlayer. Thin films of vanadium were then deposited onto this TiO$_2$ substrate. The samples were annealed at 100, 200, 300, 400, and 500°C for fifteen minutes and were analyzed in situ by XPS. The titanium 2p, the vanadium 2p and the oxygen 1s core level analyzed for this purpose. The aluminum x-rays (energy = 1486.6 eV) were used as the source of excitation. The spectral data have been recorded at 45 degree take-off angle. The spectral data have been analyzed to estimate the chemical reactivity at the V/TiO$_2$ interface. The spectral features (shift in the core levels and the shape of the core level peaks) have been utilized. The chemical reactivity as a function of the thickness of the vanadium overlayer and the annealing temperature has been established and will be presented.

*Supported by Organized Research, TAMU-Commerce

**H71.00183: Au$_n$ cluster deposited on a TiO$_2$ (110) slab**

PABLO DE LA MORA (Presenter), Facultad de Ciencias, Universidad Nacional Autonoma de Mexico, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de Mexico, ESTHER AGACINO, FES Cuautitlan, Universidad Nacional Autonoma de Mexico — The unreactiveness of gold breaks down in the nanoscale, where it has a very strong catalytic activity. To study this, Au atoms are added in the 110 surface of the rutile, TiO$_2$. In this study gold atoms are added one by one to the surface and different configurations are energetically optimized. The objective is to study how the atoms interact with the rutile surface and when the 2D to the 3D transition happens. The Au$_4$ cluster deviates from the flat rhombus, thus beginning to have a 3D character, it is in the Au$_5$ where the 3D character is clearly obtained, forming triangular bipyramid. The study was done using the WIEN2k package.

*PAPIIT IN 115618
**H71.00184: Synthesis, Crystallography, Microstructure, Crystal defects and Optical Properties of (Fe-Ni) co-doped ZnO Thin Films prepared by sol–gel technique**

AHMAD ALSAAD (Presenter), QAIS AL-BATAINEH, A. AHMAD, A. BANI-SALAMEH, Jordan University of Science and Technology, Physics Department, ZAID ALBATAINEH, Department of Electronic Engineering, Yarmouk University, AHMAD TELFAH, Leibniz Institut für Analytische Wissenschaften — Zinc oxide (ZnO) and Iron-Nickel Fe-Ni co-doped ZnO thin films have been doped coated in glass sustrate using Sol Gel technique.

In addition, the microstructural properties and crystal imperfections of these samples were studied. X-ray diffraction (XRD) has been utilized to carry out these studies. XRD analysis revealed that these samples have a polycrystalline hexagonal wurtzite structure and nanometric dimensions. XRD-line profile analysis was used to study the microstructure and crystal defects of these nanoparticles. Crystallite size and microstrain were estimated using the Williamson–Hall method. It was observed that the crystallites sizes have increased as Fe-Ni concentrations were increased. However, strain in the thin films has decreased upon increasing Fe-Ni concentrations. Interestingly, the microstrain has decreased upon increasing Fe-Ni concentrations. The optical properties of the thin films were investigated using UV-Vis spectrometer measurements. The transmittance of the undoped ZnO was decreased upon increasing the concentration of Fe-Ni.

*Authors would like to thank Jordan University of Science and Technology for technical and financial support. We would like to thank Leibniz Institute in Germany for technical support.*

**H71.00185: Adsorption And Diffusion Properties of Aromatic Molecules on Silica/Ru(0001)**

MUHAMMAD SAJID (Presenter), WILLIAM KADEN, ABDELKADER KARA, Univ of Central Florida — Now a days, organic materials are replacing the conventional Si based ones in electronic devices due to being cheap, light weight and flexible. These devices are manufactured with metal contacts at both ends, providing support and/or electric conduction. Electronic properties at both ends are changed due to charge transfer at the interface affecting performance. In order to control charge transfer, we are investigating effects of inserting an inert layer separating the two. Using DFT with added vdW corrections and surface science spectroscopic techniques (XPS, LEED etc), we are studying adsorption of aromatic molecules on Ru(0001) with and without silica layer in between. Silica layer is shown to greatly inhibit adsorption strength and charge transfer at the interface. Using CI-NEB (Climbing Image Nudge Elastic Band) and TPD (Temperature Programmed Desorption) measurements, diffusion characteristics of molecules through pores of silica sheet and under the layer are thoroughly discussed. Comparison of simulation and experiment can provide better understanding of important processes at the interface.

*Partial support is from U.S. Department of Energy under Award number DE-SC0007045. Computational resources of NERSC and UCF-Stokes are used.*
H71.00186: Linking sprayability to thin-film performance in CNT-redox-polymer dispersions
KARTHIKA SURESH (Presenter), Chemical Engineering and Materials Science, University of Minnesota, Twin Cities, STEPHEN COTTY, XIAO SU, Department of Chemical & Biomolecular Engineering, University of Illinois, Urbana, MICHELLE A CALABRESE, Chemical Engineering and Materials Science, University of Minnesota, Twin Cities — Carbon nanotube (CNT)-loaded redox-polymer coatings are an attractive class of composite materials for charge storage devices, high-surface area ion-binding platforms, and selective redox mediated separation systems. While CNTs provides a nanoporous conductive network, the electroactivity of the redox-polymers grants these systems high pseudocapacitive charge-storage and ion recognition properties. Metallopolymers in particular are attractive due to their fast electron-transfer, synthetic tunability, and reversibility. However, processing CNT-metallopolymers to form uniform thin film coatings on large length scales is a substantial challenge. The sprayability, coatability, and printability of these dispersions are dictated by the extensional flow properties. Here, we link the extensional flow properties to the quality of the solution-processed thin film using capillary breakup extensional rheometry (CaBER) to capture filament formation and breakup. The CNT: polymer ratio, polymer molecular weight, polymer chemistry and solvent quality all impact the extensional rheology and corresponding thin film quality. Our results show a strong link between macroscopic flow properties, dispersion processability and final thin-film performance on the electrodes.

H71.00187: Oxidation of Tin as investigated by X-ray Photoelectron Spectroscopy*
ALLEN HILLEGAS, ANIL CHOURASIA (Presenter), Texas A&M University, Commerce — The oxidation of tin has been investigated by the technique of x-ray photoelectron spectroscopy. Thin films of tin were deposited on a silicon substrate by the e-beam technique. The films were oxidized in situ by exposing them to an atmosphere of oxygen at temperatures of 100, 200, 300, 400, and 500°C for various times. Aluminum x-rays (energy = 1486.6 eV) were used to record the spectra. The tin 3d and oxygen 1s core levels have been investigated. The spectral data (binding energy shift and the shape of the core level peaks) have been utilized to interpret the data. The growth of the oxide as a function of the substrate temperature and the oxygen pressure has been evaluated. The oxidation kinetics have been modelled to follow the growth of the oxide.

*Supported by Organized Research, TAMU-Commerce
**H71.00188: Fabrization of giant piezoelectric material Sm-doped Pb(Mg_{1/3}Nb_{2/3})O_3-PbTiO_3 single crystal film**

YIFEI FANG (Presenter), MIN XU, YIN HANG, Key Laboratory of High Power Laser Materials, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences — Sm-doped Pb(Mg_{1/3}Nb_{2/3})O_3-PbTiO_3 (Sm-PMN-PT) single crystal was recently reported as a new piezoelectric material with the highest piezoelectric charge coefficients which will have great applications on transducers and sensors in electromechanics [1]. In previous research, the piezoelectric mechanism in the material is believed that the local structural heterogeneity of relaxor ferroelectric crystals caused by Rare-earth element. However, the research on the thin film of this material is still lack. For further investigate the piezoelectric properties of Sm-PMN-PT thin film, we explored the methods to grow Sm-PMN-PT film on different substrates, such as YAlO_3, MgAl_2O_4, MgO. Furthermore, we analyzed and compared the differences in the transport properties and crystal structure between Sm-PMN-PT layers deposited onto different substrates. According to the calculation in Ref. [1], La^{3+} and Nd^{3+} was considered substituting the Sm ions in our future work. This research will promote the development of advanced piezoelectric devices.


**H71.00189: Fabrication of (Ga_{2}O_3)_{x}(Fe/Cr)_{y}(ZnSeTe /ZnSTe)_{1-x-y} film on quartz substrate**

YIFEI FANG (Presenter), SHULONG ZHANG, MIN XU, YIN HANG, Key Laboratory of High Power Laser Materials, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences — Mid-IR (MIR) band at ~3μm has attracted much attention for their wide applications in medical, biological, sensing technologies, etc. Ga_{2}O_3 is a wide band gap semiconductor material with fine electrical and luminescent properties, which has been widely used in photoelectric devices. Recently, an intriguing material (In_{2}O_3/Ga_{2}O_3)_{0.1}(Co)_{0.5}(ZnS/Se)_{0.4} has been reported[1] that which owns better optical and transport properties than its parent phase of Ga_{2}O_3 and In_{2}O_3. According to Ref [1], the reason of doping Co was the rich absorption and emission levels, good infrared optical properties, and room temperature ferromagnetic (RT-FM) property. However, compared with Co, transition metal Fe and Cr have wider FWHM of absorption, emission and luminescence spectrum, and even Fe has stronger RT-FM property than Co. Moreover, the different chalcogenide elements substitution might induce abundant properties which has been already verified by many researches in correlated system[2]. Hereby, we synthesized (Ga_{2}O_3)_{x}(Fe/Cr)_{y}(ZnSeTe /ZnSTe)_{1-x-y} film onto quartz substrate and investigated the structure, optical and transport properties.

**H71.00190: A route to atomically flat TiO2 terminated surfaces in SrTiO3 avoiding HF acid.**

DAKOTA BROWN (Presenter), JAMES PAYNE, MAITRI WARUSAWITHANA, Univ of North Florida — SrTiO3, known as a quantum paraelectric, is a very interesting quantum system. At the same time it is a widely used substrate to grow epitaxial oxide thin films. For the growth of high quality films and superlattices, it is imperative to have an atomically flat starting surface with a known surface termination. While the main technique for obtaining quasi-ideal SrTiO3 surfaces for growth of epitaxial thin films has been via an etching step that involves HF acid [Appl. Phys. Lett. 73, 2920 (1998)] followed by an anneal in flowing oxygen to around 1000 C, here we discuss an alternate process for obtaining atomically flat surfaces. Our process involves etching in a dilute HCl acid solution, which is known as a polishing etch for SrTiO3, and eliminates the use of HF acid and the need for the high temperature (1000 C) anneal. We will compare atomic force microscopy and RHEED images of SrTiO3 substrates prepared with our process involving dilute HCl acid with those prepared using the method involving HF acid. Our controlled experiments suggest that this process provides extremely smooth surfaces with very sharp step edges that are mostly oriented parallel to the crystallographic axes.

*Department of Physics, University of North Florida

**H71.00191: Intrinsic magnetic topological insulator phases in the Sb doped MnBi$_2$Te$_4$ bulks and thin flakes**

BO CHEN (Presenter), FUCONG FEI, FENGQI SONG, Nanjing Univ — Magnetic topological insulators (MTIs) offer a combination of topologically nontrivial characteristics and magnetic order and show promise in terms of potentially interesting physical phenomena such as the quantum anomalous Hall (QAH) effect and topological axion insulating states. However, the understanding of their properties and potential applications have been limited due to a lack of suitable candidates for MTIs. Here, we grow two-dimensional single crystals of Mn(Sb$_x$Bi$_{(1-x)}$)$_2$Te$_4$ bulk and exfoliate them into thin flakes in order to search for intrinsic MTIs. We perform angle-resolved photoemission spectroscopy, low-temperature transport measurements, and first-principles calculations to investigate the band structure, transport properties, and magnetism of this family of materials, as well as the evolution of their topological properties. We find that there exists an optimized MTI zone in the Mn(Sb$_x$Bi$_{(1-x)}$)$_2$Te$_4$ phase diagram, which could possibly host a high-temperature QAH phase, offering a promising avenue for new device applications.
**H71.00192: Gate-controlled anomalous Hall effect reversal in the magnetic topological insulator MnBi$_2$Te$_4$ device**

SHUAI ZHANG (Presenter), Nanjing Univ — Magnetic topological insulator, a platform for realizing quantum anomalous Hall effect, axion state and other novel quantum transport phenomena, has attracted a lot of interest. Recently, it is proposed that MnBi$_2$Te$_4$ is an intrinsic magnetic topological insulator, which may overcome the disadvantages in the magnetic doped topological insulator, such as disorder. Here we report on the gate-reserved anomalous Hall effect (AHE) in the MnBi$_2$Te$_4$ thin film. By tuning the Fermi level using the top/bottom gate, the AHE loop gradually decreases to zero and the sign is reversed. The positive AHE exhibits distinct coercive fields compared with the negative AHE. It reaches a maximum inside the gap of the Dirac cone, and its amplitude exhibits a linear scaling with the longitudinal conductance. The positive AHE is attributed to the competition of the intrinsic Berry curvature and the extrinsic skew scattering.

**H71.00193: Preparation of Few quintuple layers Bismuth selenide (Bi$_2$Se$_3$) by spin coated-coreduction approach (SCCA) and Optical nonlinearity was discussed**

WEI-HENG SUNG (Presenter), HSUAN-SEN WANG, Department of photonics, National Sun Yat-sen University, YUE ZHOU, Department of Physics, Jiangsu University of Science and Technology, HONG LIU, State Key Laboratory of Crystal Materials, Shandong University, CHAO-KUEI LEE, Department of photonics, National Sun Yat-sen University — Topological insulators (TIs) have been realized their functionality of saturation absorption (SA) for pulsing lasers. Recently, using spin coated-coreduction approach (SCCA) growth Bi$_2$Te$_3$ thin film, continuous wave mode locking (CWML) solid state laser with repetition rate as high as GHz has been demonstrated. Compared to Bi$_2$Te$_3$, Bi$_2$Se$_3$ has been theoretically and experimentally investigated with p-type nature, leading to greater potential to be a SA. However, the difficulty of preparing high optical thin film results in the less report about their application for pulsed lasers. In this study, large area topological insulator thin film Bi$_2$Se$_3$ (Bismuth Selenide) of few quintuple layers were prepared by spin coated-coreduction approach (SCCA). AFM image, TEM image, XPS, XRD, Raman pattern all show that the growth Bi$_2$Se$_3$ thin film is with high crystalline quality. In addition, the application of Bi$_2$Se$_3$ for pulsing solid state laser was studied and discussed as well.

*MOST106-2112-M-110-006-MY3*
H71.00194: Role of polarization force for coherent phonon generation within the Bi$_2$Te$_3$ thin film  MENG-CHING LEE (Presenter), TSUN-I CHEN, JIN-WEI LI, CHAO-KUEI LEE, Department of Photonics, National Sun Yat-sen University — To date, the generation mechanism of coherent phonon within the topological insulators is an important but still unconfirmed topic. In this work, using double pulse technique, the dynamic properties and possible mechanisms of the coherent phonon($A_{1g}^1$, $A_{1g}^2$, $E_{g}^2$) in Bi$_2$Te$_3$ were investigated. Among these three phonon modes, decreasing intensity and frequency as increasing temperature was observed, which can be attributed to the reducing temperature gradient, leading to thermal force generation mechanism. However, by analyzing the temporal evolution of the phonon frequency, the frequency of $E_{g}^2$ was gradually shifted to higher frequency rather than red shift trend observed in the $A_{1g}^1$ and $A_{1g}^2$. This indicates that an additional way for generating $E_{g}^2$ mode with nature of an-harmonicity might be inevitable. Here, the polarization force mechanism for $E_{g}^2$ mode was proposed and discussed in detail.

H71.00195: Strain induced tuning and annihilation of Dirac point in the topological insulator Bi$_2$Se$_3$ (001) surface.  SOUMENDRA DAS (Presenter), PRAHALLAD PADHAN, Indian Inst of Tech-Madras — Engineering the band gap and tuning the Dirac point (DP) of (001) surface of the 8 quintuple layers (QLs) thick Bi$_2$Se$_3$ were investigated by varying the strain through first principle density functional theory calculations, with and without the presence of spin-orbit coupling (SOC). The strain on the Bi$_2$Se$_3$ (001) surface primarily varies the band width, which changes the orbital population in the conduction and valence band. The tuning of the $p_z$ - orbital population of Bi on the (001) surface of the Bi$_2$Se$_3$ froms the Dirac cone at the $\Gamma$ point, which can be achieved under uniaxial, biaxial or volume conservation strain. Around 6% out-of-plane tensile strain annihilates the DP of the (001) surface of the Bi$_2$Se$_3$ which causes the loss of topological surface states. The anniliation of the DP occurs even at lower values of volume conservation strain. However, the DP feature is preserved for the entire range of biaxial strain. The DP moves towards the Fermi level for the increasing tensile strain under uniaxial and volume conservation configuration, but the similar displacement of DP occurs due to increasing compressive biaxial strain. The tuning of DP may provide a new pathway to control many physical properties of Bi$_2$Se$_3$ and shed light for its technological applications.

H71.00196: WITHDRAWN ABSTRACT  DONNA GREENE (Presenter), American Physical Society —
H71.00197: Core Reconstruction of Dislocations in layered-chalcogenide semiconductors (Bi2X3 - X = Te, Se, and S)*  
NESTOR FAJARDO (Presenter), RICARDO NUNES, Physics Department, UFMG - Brazil — The interest in the layered chalcogenide family Bi2X3 (X = Te, Se, and S) is due to their thermoelectric properties and the topology of their electronic structure. Understanding scattering of electronic carriers and phonons in such materials is crucial for devising strategies to improve their thermoelectric properties. A crucial step is the identification of the reconstruction patterns in the core of dislocations in these covalently-bonded systems. In this work, we investigate the single- and double-period core reconstruction of the 60-degree and the screw dislocations - both with Burguers vector parallel to the basal plane - in these materials. Issues of dissociation of the 60-degree and the screw dislocations into 30-degree and 90-degree partial dislocations will also be discussed.

*We express our gratitude to the brazilian agency: Consejo Nacional de Desenvolvimento Científico e Tecnológico (CNPq) for financial support and also to the Physics Department of the Universidad Federal de Minas Gerais.

H71.00198: WITHDRAWN ABSTRACT* —

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H71.00199: Refinement of High-Throughput Calculations for Rare Earth Topological Insulators  
GAVIN NOP (Presenter), JONATHAN SMITH, Iowa State University — Topological Insulators (TI) have become increasingly important in the condensed matter science of electronic band theory. We focus on inorganic topological insulators using advancements in “Topological Quantum Chemistry” (TQC) [Bradlyn et al., Nature 547, 298 (2017)], combined with “A Complete Catalog of High-Quality Topological Materials” [Vergniory et al., Nature 566, 480 (2019)], to narrow our search to predicted topological insulators. In the latter paper, a high-throughput calculation of electronic band structure was used to predict TI’s. The inorganic topological materials were down-selected to rare earth materials which require on-site electron correlation and spin orbit coupling to verify their band topology. To keep computations feasible, we restrict our materials search to binary and ternary compounds with appropriate crystal structures. Rare earth materials require high-quality density functional theory calculations in order to compute their electronic band structure. We produce such high-quality calculations for a down-selected representative set of rare earth crystals in order to refine and correct the TQC high-throughput predictions. G.N. is grateful for an assistantship in the US DOE Office of Science, Science Undergraduate Laboratory Internship program.
H71.00200: Aubry-Andre-Harper Model with on-site hopping and p-wave pairing*
MOHAMMAD YAHYAVI, BALAZS HETENYI, BILAL TANATAR (Presenter), Department of Physics, Bilkent University — We study an extended Aubry-André-Harper model with simultaneous modulation of hopping on-site potential and p-wave superconducting pairing. For the case of commensurate modulation of $\beta=1/2$ it is shown that the model hosts four different types of topological states: Adiabatic cycles can be defined which pump particles two types of Majorana fermions or Cooper pairs. In the incommensurate case we calculate the phase diagram of the model in several regions. We characterize the phases by calculating the mean inverse participation ratio and perform multifractal analysis. In addition we characterize whether the phases found are topologically trivial or not. We find an interesting critical extended phase when incommensurate hopping modulation is present. The rise between the inverse participation ratio in regions separating localized and extended states is gradual rather than sharp. When in addition the on-site potential modulation is incommensurate we find several sharp rises and falls in the inverse participation ratio. In these two cases all different phases exhibit topological edge states.

*This work is funded by TUBITAK and TUBA.

H71.00201: Dipolar Magnetoexcitons in $\alpha$-$T_3$ double layers in a high magnetic field
YONATAN ABRANYOS (Presenter), GODFREY GUMBS, Physics and Astronomy, Hunter College of CUNY, OLEG BERMAN, Physics, New York City College of Technology — We consider two parallel $\alpha$-$T_3$ layers separated by an insulating slab (e.g. SiO$_2$ or a hexagonal boron nitride (h-BN) insulating barrier) in a high magnetic field. The equilibrium system of local pairs of electrons and holes, spatially separated in these parallel $\alpha$-$T_3$ layers, correspondingly, can be created by varying the chemical potential using a bias voltage between two $\alpha$-$T_3$ layers or between two gates located near the corresponding $\alpha$-$T_3$ sheets (case 1) (for simplicity, we also call these equilibrium local e-h pairs as dipolar magnetoexcitons). In case 1 a dipolar magnetoexciton is formed by an electron on the Landau level 1 and hole on the Landau level $-1$. Dipolar magnetoexcitons with spatially separated electrons and holes can be created also by laser pumping (case 2) and by applying a perpendicular electric field. In case 2, a dipolar magnetoexciton is formed by an electron in the Landau level 1 and hole in the Landau level 0. We assume the system is in a quasi-equilibrium state. We study the collective properties and superfluidity of dipolar excitons in $\alpha$-$T_3$ double layers in a high magnetic field for both case 1 and case 2.
H71.00202: Smooth Evolution in Hall Coefficient in the Overdoped Cuprate Tl2201
CARSTEN PUTZKE (Presenter), University of Bristol, SIHAM BENHABIB, WOJCIECH TABIS, LNCMI Toulouse, JAKE AYRES, LIAM MALONE, University of Bristol, NIGEL HUSSEY, HFML Nijmegen - Radboud University, JOHN R. COOPER, University of Cambridge, ANTONY CARRINGTON, University of Bristol — Our understanding of the microscopic origin of superconductivity in the cuprates is dependent on our knowledge of the normal state. Recently a sharp transition in the carrier density was proposed, close to optimal doping in YBa$_2$Cu$_3$O$_{6+\delta}$ and Nd-doped La$_{2-x}$Sr$_x$CuO$_{4.1,2}$. This transition was argued to be tied to the Pseudogap endpoint $p^*$. Here we report a study of the high field Hall coefficient of the single-layer cuprate Tl$_2$Ba$_2$CuO$_{6+\delta}$ (Tl2201) which shows that $n_H(0)$ evolves smoothly in the overdoped, so-called strange metal, phase of cuprates. No evidence for a Pseudogap has to date been reported in this material. This raises the question for a universality of the proposed link between the Pseudogap endpoint and the transition in carrier density, from $p$ to $1+p$, inferred from the Hall coefficient. Rather the evolution of $n_H$ seems to correlate with the emergence of the anomalous linear-in-$T$ term in the in-plane resistivity. The presented data will shed new light on the evolution that the cuprates take from a Fermi liquid behavior to a strongly correlated, highly complex behavior in the underdoped side of the phase diagram.

H71.00203: Exploring the Josephson Scanning Tunneling Microscopy: Towards a Phase-Coherent Junction
MICHAEL DREYER, JOSEPH MURRAY (Presenter), WAN-TING LIAO, Laboratory for Physical Sciences, SUDEEP DUTTA, CHRISTOPHER J LOBB, FREDERICK C WELLSTOOD, University of Maryland College Park, ROBERT E BUTERA, Laboratory for Physical Sciences — Josephson scanning tunneling microscopy (JSTM) is performed by using a superconducting tip on a superconducting sample. The resulting Josephson junction (JJ) is usually too small in terms of critical current and capacitance to support phase coherence between the two superconductors. We are pursuing a concept to overcome that limitation by stabilizing the phase in the scanning junction with a larger JJ in a SQUID loop. We employ a home-built dual-tip STM with connected tips to implement the concept. We characterize the individual junctions by measuring standard $I(V)$ and $dI/dV$ curves, as well as $V(I)$ characteristics which are more common to the study of JJs. In the SQUID configuration, a flux bias of the SQUID should lead to a modulation of the critical current, thus proving the concept.
H71.00205: Mapping out the electronic and magnetic transitions in mixed-valent La$_{1-x}$Sr$_x$MnO$_3$ thin films*  JAMES PAYNE (Presenter), DAKOTA BROWN, THOMAS PEKAREK, MAITRI WARUSAWITHANA, Univ of North Florida — The rich phase diagram in mixed-valent manganites has been intensely studied in bulk crystals as a function of chemical doping. Here we study the effect of doping in La$_{1-x}$Sr$_x$MnO$_3$ thin films by varying the Sr/La ratio between samples. These thin films are grown using ozone assisted molecular beam epitaxy with carefully controlled stoichiometry for a range of doping from x = 0.0 to x = 0.5. Our electronic measurements reveal a crossover from a Mott insulator to a metallic ground state as x is increased. In the metallic ground state we observe a metal-to-insulator transition coincident with a ferromagnetic-to-paramagnetic ordering transition consistent with the double exchange interaction with higher, doping dependent transition temperatures compared to those reported for bulk La$_{1-x}$Sr$_x$MnO$_3$ crystals. We will also discuss the magnetic ordering transitions observed in the low doping regime (x<0.17) where an insulating ground state is observed and compare these transitions with those reported for bulk La$_{1-x}$Sr$_x$MnO$_3$ crystals.

*NSF Grant No. DMR-16-26332

H71.00206: Temperature-dependent Raman studies of a natural van der Waals heterostructure*  VIVIANE ZURDO COSTA (Presenter), Physics and Astronomy, San Francisco State University, SAM VAZIRI, Electrical Engineering, Stanford University, SHIRIN JAMALI, ADDISON MILLER, Physics and Astronomy, San Francisco State University, ANDREW IchIMURA, Chemistry and Biochemistry, San Francisco State University, ERIC POP, Electrical Engineering, Stanford University, AKM SHAH NEWAZ, Physics and Astronomy, San Francisco State University — Van der Waals heterostructures (vdWH) comprised of two-dimensional (2D) materials offer a platform to obtain designed materials with unique electronic properties. Research on 2D vdWH has so far been focused on fabricating such heterostructures by stacking individual 2D crystals, which leads to stacks with the presence of fabrication defects. Franckeite (Fr) is a naturally occurring vdWH comprised of two different alternately stacking semiconducting layers, that enables the study of a complex layered system where the crystal orientation between layers has been preserved. Unlike other layered sulfide-based materials, Fr is a grained-textured rock composed of few-millimeter flakes in random orientation. For this reason, exfoliation of thin flakes with a uniform and large surface area for optical characterization and transfer techniques is especially challenging. By precise manipulation of the starting flake in combination with different substrates we were able to increase the quality of exfoliation and obtain few-layer (< 5) Franckeite flakes with uniform surface areas of approximately 5 μm. Here we present results on the developed exfoliation technique and temperature-dependent Raman spectroscopy of Franckeite.

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H71.00207: Magnetism-induced Raman modes in two-dimensional CrI\textsubscript{3} atomic layers*
GAIHUA YE (Presenter), ZHIPENG YE, RUI HE, Texas Tech Univ, HYUN HO KIM, BOWEN YANG, ADAM TSEN, University of Waterloo, Canada, WENCAN JIN, SIWEN LI, LIUYAN ZHAO, University of Michigan — We studied CrI\textsubscript{3} atomic layers down to the monolayer limit using temperature and magnetic field dependent micro-Raman spectroscopy. Two sets of Raman modes at frequencies of ~76 and ~125 cm\textsuperscript{-1} are observed in CrI\textsubscript{3} atomic layers only in the antisymmetric channel below the magnetic phase transition temperature, suggesting that these two modes are related to the broken time reversal symmetry in the samples. By tracking the thickness dependence of both modes, we reveal that they are of the surface nature. Magnetic field dependent measurements of bilayer CrI\textsubscript{3} at 10 K further show that these modes disappear above the critical field of ~0.8 T. Possible origin of these two Raman modes is proposed.

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H71.00208: Strain tuned structural phase transition and optical switching in 1T-ZrS\textsubscript{2} and 1T-ZrSe\textsubscript{2}  
EDOARDO MARTINO (Presenter), Ecole Polytechnique Federale de Lausanne, FLORIAN LE MARDELÉ, University of Fribourg, KONSTANTIN SEMENIUK, Ecole Polytechnique Federale de Lausanne, DAVID SANTOS-COTTIN, University of Fribourg, FRANCESCO CAPITANI, Soleil Synchrotron, HELMUTH BERGER, LASZLO FORRO, Ecole Polytechnique Federale de Lausanne, ANA AKRAP, University of Fribourg — Strain is a versatile and powerful tool to manipulate electronic properties of 2D-materials. In addition to continuous tuning of the electronic band-structure, applied strain can drive a structural phase transition, generating new states with drastically different optical and electronic properties. While this has not been observed in the most actively investigated semiconducting transition metal dichalcogenides, 2H-MoS\textsubscript{2} and 2H-WSe\textsubscript{2}, we found strain-induced structural phase transitions to take place in 1T-ZrS\textsubscript{2} and 1T-ZrSe\textsubscript{2}, which possess optical and electronic properties similar to those of Mo- and W- compounds, but have different crystalline structure and orbital character. Our high-pressure Raman scattering, X-ray diffraction and optical absorption experiments revealed a reversible metallization of 1T-ZrSe\textsubscript{2} at 8 GPa and an irreversible transformation of 1T-ZrS\textsubscript{2} to a new semiconducting phase at 3 GPa, with smaller band gap by 1 eV (from 1.7 eV to 0.7 eV), a change that is optically evident. The study is complemented by structural investigation under pressure and \textit{ab initio} band structure calculations.

H71.00209: WITHDRAWN ABSTRACT —
H71.00210: Electrostatically control interfacial states for stackable electronics*  CHEN PO-HAN (Presenter), YU-TING LIN, CHUN-AN CHEN, YI-CHENG CHIANG, I-TUNG CHEN, YI-HSIEN LEE, National Tsing-Hua University — Semiconducting monolayer of transition metal dichalcogenides (TMD) is ideal fundamental unit for stackable electronics because of its excellent optoelectronic properties. However, further applications are hindered with various issues from trap states of the monolayers. Here we develop a method to effectively engineer trap states of the monolayer MoS2 for excellent optoelectronic performances, including ultrahigh photoresponsivity (R) of $10^2$–$10^4$ A/W, high sensitivity (D*) of $10^{11}$–$10^{12}$ Jones and large absorbance. A scalable image sensor array of CVD-grown MoS2 monolayer is demonstrated.

*AOARD grant (co-funded with ONRG) FA2386-16-1-4009

H71.00211: Large-Scale Synthesis of MoS$_2$ One-dimensional Nanostructures and Precision Manipulation*  YUN HUANG, ZEXI LIANG, KANG YU, University of Texas at Austin, PAULO FERREIRA, The department of Advanced Electron Microscopy, International Iberian Nanotechnology Laboratory, DONGLEI (EMMA) FAN (Presenter), University of Texas at Austin — In the family of two dimensional (2D) materials, molybdenum disulfide (MoS$_2$) has received immerse attention. Herein, we report a scalable approach to synthesize MoS$_2$ nanoribbons with controlled dimensions. Characterizations confirm the chemistry, morphology, and crystalline structures of materials obtained at different reaction stages, including MoO$_3$, MoS$_2$/MoO$_2$ hybrid, and MoS$_2$ nanoribbons. With the electric tweezers based on combined AC and DC electric fields, the MoS$_2$ nanoribbons can be readily manipulated with desired orientations along arbitrary trajectories, e.g. along a cat drawing. Moreover, it is found that the electromechanical behaviors of the particles obtained at different growth stages strongly correlate with their electric properties, the demonstration of which could be utilized to monitor and understand the synthetic process of targeted nanomaterials. This work may lead to a new paradigm in the large-scale fabrication of 2D materials with designed dimensions and inspire their innovative applications in nanorobotics, micro/nanoelectromechanical system devices (MEMS/NEMS), as well as molecule delivery and release.

*The research is supported by the National Science Foundation and Welch Foundation.
H71.00212: First Principles Electronic and Lattice Dynamics Calculations of TiSe$_2$ and TiTe$_2$

WARDA RAHIM (Presenter), University College London, PHILIP KING, University of St. Andrews, DAVID SCANLON, University College London — TiSe$_2$ bulk and monolayer both undergo a charge density wave (CDW) instability,$^{1,2}$ whereas only monolayer TiTe$_2$ undergoes a CDW transition.$^3$ We performed electronic structure and lattice dynamics calculations (Phonopy code)$^4$ for both of these Ti(IV) dichalcogenides using hybrid (HSE06)$^5$ density functional theory. We also mapped the potential energy surfaces$^6$ spanned by the imaginary mode eigenvectors to estimate the barrier associated with the transition and to track the route to the CDW phase. Our results successfully show that though TiTe$_2$ bulk has no lattice instability, its monolayer has an instability similar to, but much weaker than that seen in TiSe$_2$, highlighting the origin of a weak coupling CDW distortion brought about by a lattice instability. These results could have impact in understanding of CDW instabilities in other systems, particularly the methodology of following imaginary modes to track the transitions between phases.

$^2$Chen et al., Nat. Commun., 2015, 6, 8943
$^3$Chen et al., Nat. Commun., 2017, 8, 516

H71.00213: Controlling the stereospecific bonding motif of Au-thiolate links and assessment of their catalytic properties* MOHAMMED SABRI G. MOHAMMED (Presenter), LUCIANO COLAZZO, Donostia International Physics Center, AURELIO GALLARDO, The Czech Academy of Sciences, ZAKARIA M ABD EL-FATTAH, Al-Azhar University, JOSÉ A. POMPOSO, Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, PAVEL JELÍNEK, The Czech Academy of Sciences, DIMAS GARCÍA DE OTEYZA, Donostia International Physics Center — Organosulfur compounds at the interface of noble metals have long been proved to be extremely versatile systems. In this work we explore the formation of gold-thiolate-based organometallic structures from 1,4-bis(4-mercaptophenyl)benzene (BMB) deposited onto Au(111) surface. By controlling the on-surface reaction conditions we can selectively choose the resulting structures to be either arrays of cyclic Au$_3$BMB$_3$ units or linearly stacked nanowires, although the former turn out to be the thermodynamically favored products[1]. Most interestingly, co-deposition of alkyne-functionalized pyrene derivatives on this system reveals the catalytic activity of the R-S-Au-S-R vertices on alkyne coupling reactions.

Reference:

*The project leading to this contribution has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No 635919), from the Spanish Ministry of Economy, Industry and Competitiveness (MINECO, Grant No. MAT2016-78293-C6).
H71.00214: Optimal $U$ values for 3$d$ transition metal oxides within a SCAN+$U$ framework

SAI GAUTAM GOPALAKRISHNAN (Presenter), Mechanical and Aerospace Engineering, Princeton University, OLIVIA LONG, Physics, Princeton University, EMILY CARTER, Office of Chancellor, University of California Los Angeles — Redox-active transition metal oxides that can tolerate oxygen off-stoichiometry are crucial ingredients for generating renewable fuels via oxide-based solar thermochemical reactors. However, any predictive modeling, such as using density functional theory (DFT) calculations, needs to accurately describe the energetics of redox reactions involving transition metals, if new candidates are to be found. Recently, we found that the strongly constrained and appropriately normed (SCAN) exchange-correlation functional requires a Hubbard $U$ correction (determined, e.g., from experimental oxidation enthalpies) to accurately describe the ground state structure, magnetic moments, and electronic properties of Ce-, Mn-, and Fe-based systems. In the present work, we extend our approach to identify optimal $U$ values for other 3$d$ oxides within the SCAN+$U$ framework. Although the absolute magnitude of $U$ values required for all 3$d$ metals is lower than what is needed using a generalized gradient approximation+$U$ or a local density approximation+$U$ approach, we find that the addition of $U$ makes non-negligible improvements in ground state property predictions, particularly for Ti, V, Co, and Ni oxides, highlighting the importance of using a SCAN+$U$ framework.

H71.00215: Polarization dependence photoluminescence in flexible two-dimensional MoS$_2$ for lattice deformation characterization

YANGBOWEN LIU (Presenter), XIAN ZHANG, Mechanical Engineering, Stevens Inst of Tech — Since Nobel Physics Prize in 2010 about graphene, intense research endeavors have been paid worldwide to comprehend the intrinsic characteristics of two-dimensional (2D) materials and explore their cutting-edge applications in bioengineering, energy storage and conversion, and nanoelectronics. 2D heterostructures consisting of various 2D materials are receiving extensive interests nowadays. However, there is a lattice deformation when different 2D materials are stacked together. Characterization of each 2D layer’s lattice deformation facilitates with the optimized 2D device design. In this project, we study the rotation angle dependent photoluminescence (PL) of one atomic layer of 2D MoS$_2$ under a serious of external mechanical deformations. The PL shows a dependence with the sample rotation angle at stretched status. The intensities of two PL peaks (627 nm and 679 nm) have strong angle dependence and a serious of mechanical deformations (up to 10%) are performed. This research result can be used to accurately identify the value of lattice deformation in 2D heterostructures.

Reference:
**H71.00216: Optical measurements on phosphorus polymorphs.** CARLOS JOSAFAT CORDERO SILIS (Presenter), ELIZABETH CHAVIRA, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, THOMAS STEGMANN, Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, ADRIANA TEJEDA CRUZ, KARLA ERISETH REYES MORALES, MIGUEL ÁNGEL CANSECO MARTÍNEZ, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México — The anisotropic electronic structure of phosphorene makes it promising, for research and technological applications. Its polymorphs are White Phosphorus, which transforms into Red or Violet at 280 °C and 550 °C, and Black Phosphorus obtained from White applying pressure (12000 Bar) or trough catalysis. This research focuses on alternative synthesis methods for these, given their prohibitive cost, using common available materials.

Method 1: Matches’ heads were crushed with a blade to detach the material; it is then combusted in a Petri dish, mixed in 5 mL methanol for 30 h, at 26-32 °C, 45-47% humidity, and ground to a fine powder in an agate mortar. 146 mg were heated to 200 °C/65 h.

Method 2: Using tweezers and a cotton swab the strips are covered with acetone for a few seconds and scraped. The material is mixed in 20 mL acetone for 2 h, at 24 °C, 45 % humidity, air dried and ground to a fine powder. 118 mg were heated to 200 °C/65 h.

X-ray powder diffraction (XRD) analysis of the samples shows, for Method 1: SrP, Sr3P4O13, P2O5 and Sr2BrP. For Method 2: PBr5, and SrP. Simultaneous calorimetric and thermogravimetric analysis show the binary and ternary compounds observed by XRD. UV-Vis analysis shows the influence of the polymorphs and other impurities. Color changes are present.

**H71.00217: In-situ measurement of strain evolution in 2D materials on flexible substrates using Raman spectroscopy.** MARC MEZZACAPPA (Presenter), Mechanical Engineering, Saint Louis University, HENRY WRIGHT, DHEYAA ALAMERI, Physics, Saint Louis University, MARY CONLEY, Physics, Chemistry, Saint Louis University, CHI HOU LEI, Mechanical Engineering, Saint Louis University, IRMA KULJANISHVILI, Physics, Saint Louis University — Since its recent discovery, extensive research investigating the physical properties of Graphene and other similar two-dimensional (2D) materials has been performed. Graphene’s excellent mechanical properties, flexibility, and optical transparency make it a promising candidate for a variety of layered architectures and hybrid devices. A custom low profile testing device was designed and manufactured in-house for in-situ physical measurements of single and multilayer 2D materials on flexible substrates using Raman spectroscopy. The design of the device allows for accurate and consistent strain application of both uniaxial bending and uniaxial tension in 2D materials. Here we use the device to investigate bending induced strain evolution in 2D materials through observation of characteristic Raman spectra band shifts. 2D materials used here were prepared via chemical vapor deposition (CVD) and were transferred to the flexible substrates. Our results provide information on strain development, substrate interaction, and adhesion properties of the 2D material tested.

*Current affiliation for Dheyaa Alameri is University of Misan, Iraq.*
H71.00218: Study of Low Energy Electron Transparency of Graphene and Doped-Graphene via Electron Energy Analyzer*  MERID BELAYNEH (Presenter), Qatar Environment & Energy Research Institute — Merid Legesse,1 Vineet Mohanty,2 Mohamed Farhat, Brian Fu,2 Sabre Kais,3 Timothy S Fisher,4 and Fahhad Alharbi1
1Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha, Qatar.  
2Department of Mechanical Engineering, Purdue University, West Lafayette, Indiana, USA.  
3Department of Chemistry and Physics, Purdue University, West Lafayette, Indiana, USA.  
4Department of Mechanical and Aerospace Engineering & California Nano Systems Institute, University of California Los Angeles, Los Angeles, CA, USA

The electron transparency of graphene is investigated using Hemispherical Energy Analyzer. We further compare the results to numerically obtained values and find excellent agreement between the two. The measurements and calculations demonstrated that graphene is an excellent electron transparent material even at low electron kinetic energies where the transmission exceeds 90% with 12-eV energy. The experimental data and the model is used to extract the parameters of the experimental setup. There are some discrepancies about electron transparency of graphene in literature. By, detailed analysis, we showed that these are due to the sensitivity of the transmission on the experimental setup.

*Thanks, Qatar National Research Foundation for the support Grant No. NPRP X-107-1-027.

H71.00219: Structural, electronic, and optical properties of defect-containing MX2 monolayers from first principles*  JARON KROPP (Presenter), CAN ATACA, Univ of Maryland-Baltimore County — In this work, we investigate the role of defects on the modification of the structural, electronic, and optical properties of transition metal dichalcogenide (MX2: M=Mo,W; X=S,Se) nanosheets. Using the cluster expansion formalism and density functional theory (DFT), we calculate the energetics and magnetic ordering of MX2 monolayers with various concentrations of chalcogen vacancies. The energetically favorable structures with desired vacancy concentration are then investigated further to determine the effects on the electronic, magnetic, and optical properties including the exciton binding energies. The structures we obtained from cluster expansion are then used as training sets for our machine learning algorithm to predict large scale MX2 monolayers with desired vacancy concentration. We employ classical molecular dynamic simulations to study in the effect of vacancy defect concentration on the structural deformation of freestanding MX2 nanosheets and nanoribbons. We report that after certain vacancy concentration values, MX2 monolayers deform from planar structures to buckled structures. This work not only provides insight into realistic (i.e. CVD grown) MX2 monolayers, but also provides guidance for defect engineering for device applications of MX2 structures.

*NSF DMR-1726213
**H71.00220: Superconductivity in layered misfit chalcogenide BiSe-NbSe\(2\)**  
KAYA KOBAYASHI (Presenter), MASAHARU SHIRATA, JUN AKIMITSU, Okayama Univ — Layered misfit chalcogenides, (BiSe)\(_{1+\delta}\)(NbSe\(_2\)) is an anisotropic superconductor (T\(c=2.3\) K)\([1]\). The superconductivity is mostly carried out in NbSe\(_2\) layers, *i.e.* a superconducting NbSe\(_2\) layer is sandwiched by insulating BiSe layers. The situation for NbSe\(_2\) resembles the monolayer on a substrate, albeit the slight charge transfer is discussed from BiSe layers. We report the new structure of the series of the material, (BiSe)\(_{1+\delta}\)(NbSe\(_2\))\(_n\), and the enhancement of T\(c\) as the number of NbSe\(_2\) layers (n) increases.


*This work is supported by Grants-in-Aid for Scientific Research (Grant No. 18K03540, 19H01852).

**H71.00221: Piezoelectric domain walls in van der Waals ferroelectric CuInP\(_2\)Se\(_6\)**  
ANDRIUS DZIAUGYS, Vilnius University, JOHN A BREHM, Vanderbilt University, ALEX A PURETZKY, Oak Ridge National Lab, TIANLI FENG, Vanderbilt University, SABINE M. NEUMAYER, Oak Ridge National Lab, EUGENE ELISEEV, National Academy of Sciences of Ukraine, JURAS BANYS, Vilnius University, YULIAN VYSOCHANSKII, Institute of Solid State Physics and Chemistry, Uzhgorod, Ukraine, MICHAEL MCGUIRE, SERGEI V. KALININ, Oak Ridge National Lab, SOKRATES T PANTELIDES, Vanderbilt University, NINA BALKE, Oak Ridge National Lab, ANNA MOROZOVSKA, National Academy of Sciences of Ukraine, MICHAEL MCGUIRE, SERGEI V. KALININ, Oak Ridge National Lab, SOKRATES T PANTELIDES, Vanderbilt University, NINA BALKE, Oak Ridge National Lab, ANNA MOROZOVSKA, National Academy of Sciences of Ukraine, PETRO MAKSYMOVYCH (Presenter), Oak Ridge National Lab — Van der Waals layered chalcogenophosphates, such as CuInP\(_2\)S\(_6\) and AgInP\(_2\)S\(_6\), exhibit intriguing polar properties such as room temperature ferrielectric ordering, negative electrostriction, large elastic nonlinearity, proximity to ionic conductivity and multi-well ferroelectric potential, presumably due to a unique influence of the van der Waals gap. Here we will discuss anomalous properties of domain walls in ferrielectric selenophosphate CuInP\(_2\)Se\(_6\) detected using piezoresponse force microscopy. Whereas in ferroelectrics, including a structurally similar case of ferrielectric CuInP\(_2\)S\(_6\), electromechanical response and polarization vanish at the domain wall, the reverse is true in the case of CuInP\(_2\)Se\(_6\), so that piezoresponse vanishes everywhere but the domain wall. And yet, these domain walls can be manipulated by electric field. We propose the existence of an antiferroelectric phase in the near-surface layer of CuInP\(_2\)Se\(_6\), with locally enhanced polarization at antiferroelectric domain walls. Nature Comms. in review (2019).

*Experiments carried out at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, with addition support from CIEE / Baltic-American Freedom Foundation, DOE MSE at ORNL and University of Vanderbilt.
**H71.00222: Synthesis of Semiconducting Graphene Nanoribbons via Chemical Vapor Deposition**

ROBERT JACOBBERGER (Presenter), AUSTIN J WAY, VIVEK SARASWAT, MICHAEL ARNOLD, University of Wisconsin - Madison — Graphene nanoribbons (GNRs) are predicted to exhibit excellent charge and thermal transport, novel magnetic and spin-polarized edge states, and technologically useful bandgaps, provided that their edge structure and width are controlled with nearly atomic precision. However, producing GNRs with such a high degree of structural fidelity has been a major challenge. We have discovered a scalable technique to synthesize GNRs via the highly anisotropic crystal growth of graphene on Ge(001) during chemical vapor deposition. By tailoring the growth conditions, GNRs with nearly atomically-smooth armchair edges, tunable sub-10 nm widths, and lengths of hundreds of nanometers are synthesized. The GNRs are semiconducting with sizeable bandgaps and display high-performance charge transport at room temperature. By initiating growth from nanoscale seeds, arrays of GNRs with controlled placement and alignment are produced. GNRs are also grown on Si substrates by utilizing epitaxial Ge interlayers. This bottom-up method may provide a route for realizing state-of-the-art technologies based on semiconducting graphene.


**H71.00223: A Novel Opto-mechanical method for Large-scale Production of Boron Nitride Nanosheets in Water**

GAYATHRI H N (Presenter), JYOTI SHAKYA, PHANINDRA SAI, ARINDAM GHOSH, Indian Institute of Science — Hexagonal boron nitride (h-BN) is considered as most promising material for next generation microelectronic and other technologies. It can be easily integrated with other 2D materials such as graphene and molybdenum disulfide (MoS$_2$). The boron nitride nanosheet (BNNs) has lattice constant like that of graphene and a large electrical band gap. Also, it has an atomically smooth surface and large optical phonon modes. These qualities make it applicable as a substrate material for a high-performance graphene electronics and as an ideal nano filler in polymers for many application in polymer industry. To realize such applications at industrial level, the obvious task is to synthesize nanosheets in large scale. Here in we report synthesis of high quality BNNs in large quantities by a novel opto-mechanical method using water as a solvent, without adding any chemical or surfactants. The exfoliated BNNs have been extensively analysed for nanosheet area and thickness by SEM, AFM and Raman spectroscopy.

**References**

H71.00224: Mechanical and electrical properties of Ti$_3$C$_2$T$_x$ MXene single flakes

ALEXEY LIPATOV (Presenter), University of Nebraska - Lincoln, MOHAMED ALHABEB, A.J. Drexel Nanomaterials Institute, Drexel University, HAIDONG LU, University of Nebraska - Lincoln, BABAK ANASORI, A.J. Drexel Nanomaterials Institute, Drexel University, ALEXEI GRUVERMAN, University of Nebraska - Lincoln, YURY GOGOTSI, A.J. Drexel Nanomaterials Institute, Drexel University, ALEXANDER SINITSKII, University of Nebraska - Lincoln — Two-dimensional transition metal carbides and nitrides, known as MXenes, are a large class of materials that are finding numerous applications ranging from energy storage and electromagnetic interference shielding to water purification and antibacterial coatings. While bulk applications of MXenes are rapidly developing, their intrinsic physical property characterization through single-flake measurements remains a largely unexplored area of research. Here, we report the elastic properties of monolayers and bilayers of the most important MXene material to date, Ti$_3$C$_2$T$_x$ (T stands for surface termination) measured using nanoindentation with the tip of an atomic force microscope. The effective Young's modulus of a single layer of Ti$_3$C$_2$T$_x$ was found to be 0.33 ± 0.03 TPa, which is the highest among the reported values for solution-processed 2D materials, including graphene oxide. Individual Ti$_3$C$_2$T$_x$ flakes also exhibit a high conductivity of 4600±1100 S/cm and field-effect electron mobility of 2.6±0.7 cm$^2$/Vs. We found that the resistivity of individual flakes is only one order of magnitude lower than the resistivity of multilayer Ti$_3$C$_2$T$_x$ films, which indicates a surprisingly good electron transport through the surface terminations of different flakes, unlike in many other 2D materials.

H71.00225: Two relaxation rates in the in-plane THz conductivity of a clean Sr$_2$RuO$_4$ thin film

YOUCHENG WANG (Presenter), Institute of Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University, HARI NAIR, NATHANIEL SCHREIBER, Department of Materials Science and Engineering, Kavli Institute at Cornell for Nanoscale Science, Cornell University, JACOB RUF, LUDI MIAO, Laboratory of Atomic and Solid State Physics, Department of Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell University, DARRELL SCHLOM, Department of Materials Science and Engineering, Kavli Institute at Cornell for Nanoscale Science, Cornell University, PETER ARMITAGE, Institute of Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University — Understanding the metallic normal state of Sr$_2$RuO$_4$ could help solve puzzles about its unconventional superconducting state. The normal state of Sr$_2$RuO$_4$ is considered a clean Fermi liquid in the low temperature and low frequency limit. Herein we present time domain THz measurements of the optical conductivity of a highly clean, RRR (residual resistivity ratio) ≈ 53 epitaxial thin film, in which we find deviation from Fermi liquid scaling of a simple metal below 3 meV. The complex conductivity can be modeled with two Drude terms, the decay rate of both of which follows $T^2$ dependence. We discuss the physical implications of two conducting channels. We compare the results with our experiments on other metallic ruthenates including SrRuO$_3$ and CaRuO$_3$ with similar RRR.

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331.
H71.00226: Synthesis of 2D materials by direct heating of bulk sources*  DAVOUD HEJAZI (Presenter), RENDA TAN, SWASTIK KAR, Northeastern University — Synthesis of high-quality 2D materials usually requires reactors/furnaces of various levels of complexities. A simple method of growing 2D materials or their combined structures (heterostructure, alloys etc.) that is easy to set up and run can accelerate 2D research. We find that single and multilayered 2D materials of various types can be easily fabricated by direct thermal evaporation. This is in stark contrast with conventional vapor-phase techniques that require chemical reactions of precursors and flow of an inert carrier gas so, substantially reducing the cost and complexities. Sources of target nanomaterials are taken in commercial bulk form, reduced to powder, placed on a clean container in close proximity of target substrate in an inert atmosphere, then heated to and held at a range of material-specific high temperatures and durations. The nanomaterials evaporate and deposit directly on the substrate in the form of well-formed crystals. The synthesis methodology is much simpler than the other methods (CVD, MBE, etc.). We present detailed analysis (AFM, optical images, Raman, photoluminescence) of various types of 2D materials/structures possible via direct, mixed, and sequential evaporation of bulk powders.

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NEU Provost’s Tier 1 Interdisciplinary seed grant

H71.00227: WITHDRAWN ABSTRACT —

H71.00228: Structural and Physical Properties of “Field-Edited” Iridates*  GANG CAO (Presenter), HENGDI ZHAO, BING HU, NICK PELLATZ, YU ZHANG, DMITRY REZNIK, University of Colorado, Boulder — A great deal of theoretical work addressing exotic states for iridates has thus far met very limited experimental confirmation. The conspicuous discrepancies are due chiefly to the extreme susceptibility to structural distortions inherent in these materials. To fundamentally address this challenge, we have structurally “edited” these materials (borrowing the phrase “genome editing”) via application of magnetic field during single-crystal growth. Our results have demonstrated that the “field-edited” single crystals not only are much less distorted but also exhibit some long-sought phenomena absent in the same materials grown without a magnetic field. We present and discuss these results along with comparisons drawn from other relevant systems.

*This work is supported by NSF via grant DMR 1903888
**H71.00229: Electronic transport in graphene/RuCl$_3$ heterostructures**

(Presenter), EVERARDO MOLINA, Physics and Astronomy, California State University, Long Beach, VIKRAM NAGARAJAN, GILBERT LOPEZ, Physics, University of California, Berkeley, NICHOLAS BREZNAY, Physics, Harvey Mudd College, ROBERT KEALHOFER, Physics, University of California, Berkeley, ISAAC ARRIAGA, DEREK BERGNER, Physics and Astronomy, California State University, Long Beach, JAMES ANALYTIS, Physics, University of California, Berkeley, CLAUDIA OJEDA-ARISTIZABAL, Physics and Astronomy, California State University, Long Beach — Ruthenium Chloride (RuCl$_3$), a spin-orbit assisted Mott insulator, presents exciting physics thanks to spin-orbit entangled moments with interactions that are highly anisotropic, making it a close realization to the Heisenberg-Kitaev model. RuCl$_3$’s highly insulating character limits the accessible experimental techniques to those requiring bulk crystals, such as resonant magnetic scattering, magnetic susceptibility or heat capacity measurements. Here, we design and measure devices that implement few layers of RuCl$_3$ into an electronic device to form a Gr/RuCl$_3$ Van der Waals heterostructure (similar to heterostructures reported recently [1]) with the aim of studying in a quantum coherent regime, signatures of proximity effects between graphene and RuCl$_3$’s magnetic ordered state at low temperatures.


*This project is funded by The Department of Energy, award number: DE-SC0018154

**H71.00230: Qualitative Description of Magnetoelectric Coupling in Multiferroic BTO/CFO Janus Fibers**

SABA ARASH (Presenter), BRYAN CHAVEZ, Department of Physics and Astronomy, University of South Carolina, MATTHEW BAUER, JENNIFER ANDREW, Department of Materials Science & Engineering, University of Florida, THOMAS M CRAWFORD, YANWEN WU, Department of Physics and Astronomy, University of South Carolina — The magnetoelectric coupling dynamics in multi-phase multiferroic materials was investigated in a perovskite-spinel fiber system with Janus structure consisting of ferroelectric barium titanate (BTO) and ferrimagnetic cobalt ferrite (CFO). We observed strong evidence of such coupling from the distinct changes in the second harmonic generation signals under different applied magnetic field orientations. Here, we provide a clear qualitative description of how the electrical polarization of the BTO half is affected by the changes incurred in the magnetization of the CFO half in different groups of fibers. We observed that although the results vary for different fiber ensembles due to the memory of the initial system, the subsequent changes in the fiber system correlate qualitatively and can be understood in a systematic way with our simple dipole model.
H71.00231: Strain-based magneto-electric coupling effect induced orbital reconstruction and near room temperature ferromagnetic insulator state in PbZr$_{0.52}$Ti$_{0.48}$O$_3$/$\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ heterostructure  CHAO LIU (Presenter), Materials Science and Engineering, National University of Singapore — Multiferroic heterostructures attracts much attention due to fascinating potential applications in electric field control of magnetism and abundant physics significance. However, more and more fascinating phenomenon appearing near ferromagnetic/ferroelectric interface requires deeper investigation on this interface and the related coupling mechanism. Here, a near room temperature ferromagnetic insulator state in PbZr$_{0.52}$Ti$_{0.48}$O$_3$/$\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ heterostructures was reported by varying PbZr$_{0.52}$Ti$_{0.48}$O$_3$ thickness. Abnormal enlarged c/a ratio in La$_{0.67}$Sr$_{0.33}$MnO$_3$ by strain-based coupling effects, which lead to d$_{3z^2-r^2}$ orbital preferable occupancy and narrower e$_g$ bandwidth, was regarded as the dominant reason while valence change induced by charge-based coupling effects could be limited responsible considering short screening length. This work paves a deeper understanding of strain-based coupling effects across ferromagnetic/ferroelectric interface and enrich physics content in La$_{1-x}\text{Sr}_x\text{MnO}_3$ based electron strong correlated system.

H71.00232: Tunneling Transport in Gapped Graphene through a Bias-Tunable Potential Barrier* DANHONG HUANG (Presenter), Space Vehicles Directorate, Air Force Research Lab - Kirtland, FARHANA ANWAR, Center for High Technology Materials, University of New Mexico, ANDRII IUROV, Department of Physics and Computer Science, Medgar Evers College of City University of New York, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College of the City University of New York, ASHWANI SHARMA, Space Vehicles Directorate, Air Force Research Lab - Kirtland — We have investigated electron tunneling and transport properties for graphene through a non-square barrier with a finite slop in the potential profile. We have developed a new methodology based on the finite-difference solution of the scattering equations for a Dirac electron, and have also built a perturbation theory for the electron transmission for the case with a small slope. Both gapped and gapless graphene materials have been considered in our calculations. All these predicted properties are expected to have the highest importance for novel electronic and optical devices.

*DH would like to acknowledge the financial supports from the Air Force Office of Scientific Research (AFOSR) and the Laboratory University Collaboration Initiative (LUCI) program.
H71.00233: Gauging electronic transport in Sodium Iridate and Vanadium Triiodide thin crystals through graphene heterostructures*  EVERARDO MOLINA (Presenter), SARA QUBBAJ, Physics and Astronomy, California State University, Long Beach, VIKRAM NAGARAJAN, Physics, University of California, Berkeley, TAI KONG, Chemistry, Pinceton University, GILBERT LOPEZ, Physics, University of California, Berkeley, NICHOLAS BREZNAY, Physics, Harvey Mudd College, ROBERT KEALHOFER, Physics, University of California, Berkeley, DEREK BERGNER, ISAAC ARRIAGA, Physics and Astronomy, California State University, Long Beach, ROBERT J. CAVA, Chemistry, Pinceton University, JAMES ANALYTIS, Physics, University of California, Berkeley, CLAUDIA OJEDA-ARISTIZABAL, Physics and Astronomy, California State University, Long Beach - Sodium Iridate (Na$_2$IrO$_3$) presents exciting ground states thanks to the combination of electronic correlations, spin-orbit coupling, crystal field effects and a honeycomb arrangement of the iridium ions. Vandium triiodide (V$_3$I) on the other hand, constitutes a promising candidate for 2-D magnetism. Due to the highly insulating behavior of these materials, little progress has been made in terms of transport measurements. Here we explore an indirect transport measurement of thin exfoliated Na$_2$IrO$_3$ and V$_3$I crystals through a graphene heterostructure.

*This project was funded by the Department of Energy award number DE-SC0018154

H71.00234: Asymmetry strain induced superdomain structures in (101)-oriented Pb(Zr$_{0.2}$Ti$_{0.8}$)O$_3$ and PbTiO$_3$  SHENG-ZHU HO (Presenter), MENG-XUN XIE, YU-CHEN LIU, YU-HUAI LI, JAN-CHI YANG, YI-CHUN CHEN, Natl Cheng Kung Univ - Ferroelectric materials in room temperature have attracted great scientific and technological interests due to its huge potential for applications in nonvolatile memory devices. Lead zirconate titanate (Pb(Zr$_x$Ti$_{1-x}$)O$_3$, PZT) compounds, with remarkable ferroelectricity, is one of the most commonly studied system. Abundant previous researches have shown that ferroelectric domain structures of the PZT system would depend on the orientation of epitaxial substrate due to the strain effect. In this study, we investigated the domain structures of (101)-orientated tetragonal Pb(Zr$_{0.2}$Ti$_{0.8}$)O$_3$ (PZT) and PbTiO$_3$ (PTO) epitaxial films grown on cubic SrTiO$_3$ (110) substrates by vector piezoresponse force microscopy (vector-PFM). Interestingly, we observe superdomains with particular spontaneous polarizations on both PZT and PTO films which are under asymmetry strains from the substrate. However, comparing with those of (101)-orientated PTO, (101)-orientated PZT has more fine structures within one superdomain period, which are with polarization rotations along phi-direction observed by vector-PFM. As the result, we could further confirm the strain effect break the in-plane symmetry of the PZT and PTO films and and lead to the superdomain structures.
**H71.00235: Study of structural, electromagnetic and magnetoelectric properties of multiferroic composites**

BABLU CHANDRA DAS (Presenter), MD. FEROZ ALAM KHAN, M. A. MATIN, A.K.M. AKTHER HOSSAIN, Department of Physics, Bangladesh University of Engineering and Technology, Dhaka-1000, Bangladesh — Abstract

The composition $(1-x)\text{Ba}_{0.985}\text{Ca}_{0.015}\text{Zr}_{0.10}\text{Ti}_{0.90}\text{O}_3 + (x)\text{Ni}_{0.48}\text{Cu}_{0.12}\text{Zn}_{0.40}\text{Gd}_{0.04}\text{Fe}_{1.96}\text{O}_4$ (where $x = 0.0, 0.2, 0.4, 0.6$ and $1.0$) was prepared using the conventional solid state reaction method. The X-Ray diffraction analysis confirmed the coexistence of the two phases of the present research. Microstructural and surface morphology were studied by Field Emission Scanning Electron Microscopy (FESEM). Magnetic properties e.g. permeability, magnetic loss and quality factor have been calculated as a function of frequency. The dielectric properties such as dielectric constant and dielectric loss were measured as a function of frequency and temperature at room temperature. $M - H$ hysteresis loops and $P - E$ hysteresis loops confirm the ferromagnetic and ferroelectric nature of the composite samples. Variation of the ME coefficient ($\alpha_{ME}$) with the dc magnetic field was also measured for the multiferroic composite samples.

*This research was funded by CASR, Bangladesh University of Engineering and Technology (BUET).*

**H71.00236: Thermally Induced Metastable Inter-Ferroelectric Phase Switching in Mechanically Biased Single Crystal Relaxor Ferroelectrics**

PETER FINKEL (Presenter), United States Naval Research Laboratory, STEPHAN M YOUNG, UMKC, SAMUEL E LOFLAND, Rowan University, MARGO STARUCH, United States Naval Research Laboratory — In this work we examine a thermally induced metastable phase transition in mechanically biased piezoelectric $[\text{Pb(In}_{1/2}\text{Nb}_{1/2})\text{O}_3]_{0.24}[\text{Pb(Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3]_{0.46}[\text{PbTiO}_3]_{0.32}$ domain-engineered single crystals. Our results show a purely thermally-driven first order ferroelectric rhombohedral-to-orthorhombic phase transition accompanied by a large, sharp discontinuity in strain while the piezocrystal is held under mechanical compressive bias stress and variable electric field bias. We demonstrate this transition can be cycled repeatedly with a small thermal hysteresis ($< 3^\circ$C) under zero applied electric field with dynamic reversible strain jump of $\sim 0.25 \%$. Moreover, we show that the thermally driven phase switching behavior can be tuned by varying the bias stress and/or electric field, illustrating the path for establishing effective control parameters and conditions for potential future applications such as actuators, thermoelectric transducers and sensors.
Colossal Dielectric Constant Achieved via Acceptor-Donor doped ZnO Ceramic

DONG HUANG (Presenter), CHI-CHUNG LING, The University of Hong Kong — Materials having colossal dielectric constant (CDC) and low loss, with good frequency stability is crucial for device miniaturization and high-energy density storage application. Hu et al. recently reported a temperature and frequency independent CDC with a low dielectric loss in acceptor-donor co-doped TiO$_2$. The CDC is postulated to be originated from electron-pinned defect dipoles which is the acceptor-donor defect complex, though the detail mechanism and experimental evidence are lacking.

Li-Al co-doped ZnO, Zn$_{0.99}$(Li$_{0.1}$, Al$_{0.2}$)$_{0.033}$, ceramic exhibits CDC with good frequency stability, which have a dielectric constant $\sim$10$^4$ at 1 kHz. Impedance spectroscopy shows that the CDC phenomenon is not associated with the internal barrier capacitance (IBLC) effect. M"(f) spectrum obtained from electric modulus analysis reveals two relaxation processes P1 and P2. Frequency dependent ac conductivity data can be well fitted by the Correlated Barrier Hopping (CBH) model, showing that the CDC would be originated from the thermally activated electron hopping between two neighboring acceptor-donor defect sites over their Coulombic barrier. A simple model involving these acceptor-donor defect complex dipoles and the Cole-Davidson distribution of relaxation time can explain the CDC phenomenon.

WITHDRAWN ABSTRACT

The Effect of Semiconductor Nanostructures on the Performance of Nanometer-Thick Parallel Plate Capacitors*

MASOUD KAVEH (Presenter), NIKOLAS ROESKE, Physics and Astronomy, James Madison University, FAZEL BANIASADI, CHENGGANG TAO, Department of Physics, Virginia Tech, HOE TAN, MYKHAYLO LYSEVYCH, CHENNUPATI JAGADISH, Department of Electronic Materials Engineering, Research School of Physics and Engineering, Australian National University — We fabricate nanometer thick, parallel plate capacitors which have semiconductor nanostructures as their dielectric spacers and investigate their capacitance as a function of geometry and the type and thickness of spacer and metal plates. Selected semiconductors are SrTiO$_3$ nano-powder and GaAs and Si nanowires (NW) which have relatively high dielectric constants. 30 nm and 60 nm thick Au plates are fabricated on both solid glass and flexible poly(methyl methacrylate) substrate using an electron beam deposition system. The vertically aligned 50 nm diameter GaAs NWs were grown using the Au catalyzed vapor-liquid-solid method. The Si NWs are randomly oriented with an average diameter of 70 nm. The SrTiO$_3$ nano-particles are cubical with a width of around 30 nm. The reference sample, Au plates with air as dielectric, reveal capacitance in the pico-Farad order. However, capacitor structures with semiconductor dielectrics show an enhancement of the total capacitance, mainly explained by the semiconductor spacer weakening the effective internal electric field. Photoluminescence measurements on the semiconductors adjacent to Au plates also show an energy transfer from semiconductor excitons to plasmon oscillations in the Au plates.

*The support of the 4VA at JMU is kindly acknowledged.
H71.00240: Pretransitional Diffuse Neutron Scattering in Ferroelectric KTa$_{1-x}$Nb$_x$O$_3$*
GRACE YONG (Presenter), Loyola University Maryland, ROSS ERWIN, NIST/NCNR, OLEKSIY SVITELSKIY, Physics, Gordon College, JEAN TOULOUSE, Physics, Lehigh University, LYNN A BOATNER, Materials Science, ORNL, STEPHEN M SHAPIRO, Neutron Scattering, BNL — Pretransitional diffuse neutron scattering in ferroelectric KTa$_{1-x}$Nb$_x$O$_3$ occurs at (110), (111), and (130) with no diffuse scattering at (100), and (200). These observations will be discussed using the elastic structure factor and `uniform phase shift' description.

*NSF grant # 1709282
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H71.00241: The strong nonlinearity optical calculation of 3D Dirac semimetals.** TIANNING ZHANG (Presenter), YEE SIN ANG, Singapore University of Technology and Design — The optical nonlinearity of novel Dirac materials, such as graphene, have been extensively studied theoretically and experimentally in recent years. Due to the exceptionally strong light-matter interactions, Dirac material is promising in revolutionizing the functionality of photonic and optoelectronic device technology. In this work, we study the nonlinear optical response generated by the massless Dirac quasiparticles residing around the topologically-protected Dirac nodal points in three-dimensional (3D) Dirac topological semimetals in the terahertz frequency regime. Analytical expressions of third-order interband nonlinear optical conductivities are obtained based on semiclassical Boltzmann equation and quantum mechanical Floquet theory. Using Cd$_3$As$_2$ as an example, we demonstrate that the optical nonlinearity of 3D Dirac semimetal at terahertz frequency is comparable to that of the two-dimensional Dirac fermions in graphene. Importantly, the additional degree of freedom of 3D Dirac semimetal shall offer additional optical device design flexibility not found in atomically-thin graphene.

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XMUM Research Fund, Grant No. XMUMRF/2019-C3/IECE/0003
H71.00242: "Origin of Exceptional Magneto-resistance in Weyl Semimetal TaSb$_2$"* PAWAN KUMAR (Presenter), School Of Physical Sciences, Jawaharlal Nehru University New Delhi India, SUDESH SUDESH, Department of Physics, Banasthali University, Niwai Tonk Rajasthan India, GANESH GURJAR, SATYABRATA PATNAIK, School Of Physical Sciences, Jawaharlal Nehru University New Delhi India — We study magneto-transport properties in single crystals of TaSb$_2$, which is a topological semimetal. In the presence of magnetic field, the electrical resistivity shows onset of insulating behaviour followed by a plateau at low temperature. Such resistivity saturation is generally assigned to topological surface states but we find that aspects of extremely large magneto resistance and resistivity plateau are well accounted by classical Kohler's scaling. In addition, magneto-resistance in TaSb$_2$ shows non-saturating field dependence. Evidence for anomalous Chiral transport is provided with observation of negative longitudinal magneto-resistance. Shubnikov-de Haas oscillation data reveal two dominating frequencies, 201 T and 455 T. At low temperature, the field dependence of Hall resistivity shows non-linear behaviour that indicates the presence of two types of charge carriers in consonance with reported electronic band structure. Analysis of Hall resistivity implies extremely high electron mobility.

*P. Kumar, Sudesh and G. Gurjar acknowledges UGC-India for fellowship support. Authors are thankful to AIRF(JNU INDIA) for the access to PPMS and TEM facilities. S. Patnaik thanks SERB DST INDIA for the project EMR/2016/003998/PHY.

H71.00243: Ultrahigh conductivity in Weyl semimetal NbAs nanobelts* CHENG ZHANG, XIANGYU CAO (Presenter), FAXIAN XIU, Department of Physics, Fudan University — In two-dimensional (2D) systems, high mobility is typically achieved in low-carrier-density semiconductors and semimetals. Here, we discover that the nanobelts of Weyl semimetal NbAs maintain a high mobility even in the presence of a high sheet carrier density. We develop a growth scheme to synthesize single crystalline NbAs nanobelts with tunable Fermi levels. Owing to a large surface-to-bulk ratio, we argue that a 2D surface state gives rise to the high sheet carrier density, even though the bulk Fermi level is located near the Weyl nodes. A surface sheet conductance up to 5–100 S per is realized, exceeding that of conventional 2D electron gases, quasi-2D metal films, and topological insulator surface states. Corroborated by theory, we attribute the origin of the ultrahigh conductance to the disorder-tolerant Fermi arcs. The evidenced low-dissipation property of Fermi arcs has implications for both fundamental study and potential electronic applications.

*National Natural Science Foundation of China (grant nos. 11474058, 61674040 and 11874116)
**H71.00244: Suppression of magnetism and Seebeck effect in Na$_{0.875}$CoO$_2$ induced by Sb$_{Co}$ dopants**  MOHAMMED H. N. ASSADI, University of New South Wales, MARCO FRONZI (Presenter), IRCRE, Xi’an Jiaotong University, PAOLO MELE, Shibaura Institute of Technology — We examined the electronic properties of Sb-doped Na$_{0.785}$CoO$_2$ using density functional calculations based on GGA+U formalism. We demonstrated that Sb dopants were the most stable when replacing Co ions within the complex Na$_{0.875}$CoO$_2$ lattice structure. We also showed that the Sb$_{Co}$ dopants adopted the +5 oxidation introducing two electrons into the host Na$_{0.875}$CoO$_2$ compound. The newly introduced electrons recombined with holes that were borne on Co$^{4+}$ sites that had been created by sodium vacancies. The elimination of Co$^{4+}$ species, in turn, rendered Na$_{0.875}$(Co$_{0.9375}$Sb$_{0.0625}$)O$_2$ non-magnetic and diminished compound’s thermoelectric effect. Furthermore, The Sb$_{Co}$ dopants tended to aggregate with the Na vacancies keeping a minimum distance. Conclusions drawn here can be generalized to other highly oxidized dopants in Na$_x$CoO$_2$ that replace a Co.

**H71.00245: Temperature influence in the broadening parameter of photoreflectance spectras on GaAs doped with Ge and Sn as aged samples**  SAMUEL ZAMBRANO (Presenter), University of Magdalena, University of Guajira, GERARDO FONTHAL, Doctoral Program in Physical Sciences, University of Quindio, JOSE SIERRA, University of Magdalena, JOHN PRIAS, Doctoral Program in Physical Sciences, University of Quindio — Aged samples of GaAs doped with Ge and Sn growth by liquid phase epitaxy, show temperature influence in the broadening parameter of the photoreflectance spectras domined mainly by the photon-defects interactions. The samples were characterized via Raman spectroscopy, X-ray diffraction technique and scanning electron microscopy. The photoreflectance spectras were taken by varying temperatures from 20 to 300 K. Optical measurements suggest that increase temperature and increases broadening parameter, exhibiting changes in the photon-defects interactions, possibly attributed to increase in aging defects.

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**H71.00246: Investigation of the obscure spin state of Ti-doped CdSe**

JOHN DIMUNA (Presenter), TUCKER BOYETT, Univ of North Florida, ANANT K RAMDAS, IREK MIOTKOWSKI, Purdue University, THOMAS PEKAREK, JASON HARALDSEN, Univ of North Florida — Using computational and experimental techniques, we examine the nature of the 2+ oxidation state of Ti-doped CdSe. Through stoichiometry and magnetization measurements, the weakly-doped material of Cd$_{1-x}$Ti$_x$Se ($x = 0.0043$) shows the presence of a robust spin-1 magnetic state of Ti, which is indicative of a 2+ oxidation state. Given the nature of the Ti$^{2+}$ state, we investigate the electronic and magnetic states with density functional theory for a supercell of CdSe with an ultra-low concentration of Ti. We find that reproducing the magnetic moment of spin-1 requires an onsite potential of 4-6 eV must be included. Furthermore, the electronic structure and density of states show the presence of a Ti-$d$ impurity band above the Fermi level and a weakly metallic state for a $U = 0$ eV. However, the evolution of the electronic properties as a function of the Hubbard U shows that the Ti-$d$ drop below the Fermi around 4 eV with the onset of a semiconducting state. The impurity then mixes with the lower valence bands and produces the 2+ state for the Ti atom.

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**H71.00247: Understanding the spin-glass state through the magnetic properties of Mn-doped ZnTe**

ALEXANDRIA R ALCANTARA (Presenter), DINA MATEV, Univ of North Florida, ANANT K RAMDAS, IREK MIOTKOWSKI, Purdue University, THOMAS PEKAREK, JASON HARALDSEN, Univ of North Florida — To understand the spin-glass state of diluted magnetic semiconductors, we have examined the magnetic properties of Zn$_{1-x}$Mn$_x$Te using density functional theory and magnetization measurements. Utilizing the generalized gradient approximation, we investigate the dependence of the Hubbard onsite potential on the magnetization and electronic structure. We find that the ground state magnetic preference is antiferromagnetic and that the onsite potential is needed to harden the magnetic moment of $S = 5/2$. Furthermore, the system is clearly semi-conducting, which suggests that the spin-glass nature of the compound is produced through the magnetic exchange interactions through the $p$- and $d$-orbital hybridization.

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H71.00248: (Si)GeSn Semiconductors for integrated optoelectronics and quantum electronics

SIMONE ASSALI (Presenter), AASHISH KUMAR, MAHMOUD ATALLA, SALIM ABDI, SAMIK MUKHERJEE, ANIS ATTIAOUI, OUSSAMA MOUTANABBIR, Ecole Polytechnique de Montreal — Si-compatible photonic and opto-electronic devices operating at mid-infrared wavelengths can now be fabricated using Sn-containing group IV semiconductor (Si)GeSn alloys, directly grown on a Si substrate. The possibility to independently engineer strain and composition in this new class of semiconductors allows for a high degree of tunability of band structure and lattice parameter of the material, thus enabling a variety of multi-layer heterostructures and low-dimensional systems.

In this presentation, the recent progress in the epitaxial growth of metastable (Si)GeSn semiconductors in a CVD reactor will be discussed. The effect of the growth parameters on the structural and opto-electronic properties will be highlighted, ranging from the macroscopic scale down to the atomic-level, hence providing a deeper understanding of the fundamental properties of this material system. The relevance of (Si)GeSn semiconductors for Si-compatible mid-infrared opto-electronics will be discussed by correlating the material properties (crystalline quality, compositional profile, point defects, dopants incorporation and active carrier concentration) with the opto-electronic properties of p-i-n MIR photodetectors.


H71.00249: Long-lived modulation of plasmonic absorption by remote thermal injection*

JOHN TOMKO (Presenter), Univ of Virginia, EVAN RUNNERSTROM, North Carolina State University, YI-SIANG WANG, University of Southern California, JOSHUA NOLEN, Vanderbilt University, DAVID OLSON, Univ of Virginia, KYLE KELLEY, ANGELA CLERI, JOSH NORDLANDER, Pennsylvania State University, JOSHUA D CALDWELL, Vanderbilt University, OLEG PREZHDHO, University of Southern California, JON-PAUL MARIA, Pennsylvania State University, PATRICK HOPKINS, Univ of Virginia — Light interactions capable of inducing charge and energy transfer across interfaces are the fundamental basis for a multitude of technologies, including photocatalysis, energy harvesting, and photodetection. One of the more common mechanisms associated with these processes relies on injection of the charge carrier itself. In this work, we elucidate upon a novel means of of electronic energy injection that can be accessed by relying on non-equilibrium dynamics achievable at metal-semiconductor interfaces that has yet to be realized. This remote thermal injection (RTI) process is demonstrated through an ultrafast pump-probe technique that relies on monitoring the optical properties of a mid-infrared epsilon-near-zero cavity following optical excitation of a remote contact, providing a highly sensitive probe into the spatial variations of electron density and energy relaxation mechanisms in the heterostructure. These results are further supported via ab initio density functional theory (DFT) simulations.

*We acknowledge funding from the Army Research Office, Multidisciplinary University Research Initiative (Grant No. W911NF-16-1-0406)
H71.00250: *Investigation of Exciton-Phonon Coupling in Cesium Lead Bromide Perovskite Nanosheets with photoluminescence*  
Xiangzhou Lao (Presenter), Shijie Xu, The University of Hong Kong — Variable-temperature photoluminescence (PL) spectra of cesium lead bromide (CsPbBr$_3$) nanosheets were measured in a low temperature range of 5 to 40 K. In this interested low temperature range the measured PL spectra exhibit a main zero-phonon peak and its longitudinal-optical (LO) phonon sideband, and are quantitatively simulated using the multimode Brownian oscillator (MBO) model. Good agreement between theory and experiment enables us to determine several key parameters characterizing the exciton–phonon coupling, including the dimensionless Huang-Rhys factor $S$ accounting for the exciton-LO phonon coupling strength and the damping constant $\gamma$ for the phonon bath (quasi-continuous acoustic phonons) dissipation. It is found that Huang-Rhys factor $S$ peculiarly tends to diminish upon increasing the temperature, suggesting weakened exciton-LO phonon coupling in the interested low-temperature range. However, as often observed in solids, the damping constant $\gamma$ in the nanosheets increases almost linearly with the rise of temperature. This study may shed some light on the complex exciton-phonon scattering mechanisms in solids.

*This study was supported by the SRT on New Materials of HKU.

H71.00251: *Carrier Multiplication in Quasi-1D Nanosystems: A Time-Dependent Density Functional Theory Study*  
Junhyeok Bang (Presenter), Chungbuk Natl Univ — Carrier multiplication (CM) is a fundamental process in the electronic excited state, which generates multi-excitons from a single-photon absorption. CM has been intensively investigated for photovoltaic applications, because it can improve optoelectronic devices efficiency. However, CM is rarely witnessed in conventional semiconductors, calling for an unconventional material enhancing the CM. Here, using real-time time-dependent density functional theory, we show that CM occurs in quasi-one-dimensional (1D) nanosystems derived from 2-dimensional van der Waals materials. The origin of CM in quasi-1D, i.e., releasing the constraints of the CM process, are different from that in 0D nanosystems, i.e., phonon bottleneck. The results provide the way to control the excited carrier dynamics and CM in nanosystems.

*This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) (NRF-2018R1D1A1B07044564), the National Research Council of Science & Technology (No. CAP-18-05-KAERI).

H71.00252: WITHDRAWN ABSTRACT
H71.00253: Two-Exciton states in Cyanine Dimers on DNA Scaffolds  PAUL CUNNINGHAM (Presenter), SEBASTIAN A. DIAS, YOUNG C. KIM, DIVITA MATHUR, United States Naval Research Laboratory, DONALD L KELLIS, BERNARD YURKE, RYAN D PENSACK, WILLIAM B KNOWLTON, Boise State University, IGOR L. MEDINTZ, JOSEPH S. MELINGER, United States Naval Research Laboratory — The control of intermolecular coupling is a pathway towards achieving highly efficient energy transport in artificial light-harvesting networks. Similar requirements are also needed for the design of molecular wires and logic structures within the field of molecular excitonics. Here we report on the creation of cyanine dye homodimers on DNA scaffolds. The DNA provides a backbone to precisely control dye placement through covalent attachment and thereby the coupling strength, allowing the absorption and emission properties of the resulting dimers to be tailored. Through this strategy, we are able to realize delocalized one- and two-exciton states, the later of which is a first for a DNA-scaffolded system. Such multi-exciton states hold promise for entangled photon emission and molecular logic gates. Both the one- and two-exciton states are well described by molecular exciton theory when electron-vibrational coupling is accounted for. We also address the impact of molecular motion on the dynamics of these states, and identify a path towards greater control of these properties.

H71.00254: Exact Steady-state Solution of Electron Transport Through a Quantum System Coupled with Dissipative Electrodes*  TSE-MIN CHIANG (Presenter), LIANG-YAN HSU, Academia Sinica — In the framework of the Lindblad quantum master equation, we develop a theory which allows us to describe electron transport through a molecular junction coupled with dissipative electrodes. We generalize the theory of coherent quantum transport and include the electronic dissipation in electrodes. Moreover, we derive an exact solution of steady-state current and analyze the asymptotic behavior in the different limits of electronic dissipation. Furthermore, we obtain a Landauer-type formula and show that this formula can be reduced to the original Landauer formula in the condition of zero dissipation rate.

*This research was supported by Academia Sinica and the Ministry of Science and Technology of Taiwan (MOST 106-2113-M-001-036-MY3).
ANASTASIA SPIRIDONOVA (Presenter), The Graduate Center, City University of New York — Monolayer transition-metal dichalcogenides (TMDC) such as MoS$_2$, MoSe$_2$, WS$_2$ and Se$_2$ host a series of exciton Rydberg states denoted by the principal quantum number $n = 1, 2, 3$, etc. We study the 1$s$–2$s$ exciton Rydberg states in TMDC monolayers encapsulated by hexagonal boron nitride (hBN) under the action of a magnetic field. The exciton Rydberg states exhibit similar Zeeman shifts but distinct diamagnetic shifts from each other. Excitons in the magnetic field are described in the framework of the potential model. We have used the Keldysh potential to calculate the energies of exciton Rydberg states in hBN-encapsulated monolayers of MoS$_2$, MoSe$_2$, WS$_2$, and WSe$_2$ under varying magnetic field. Our calculations use as inputs the effective masses of electron and hole obtained in the framework of the density functional theory. The binding energies of exciton are calculated using the first-order perturbation theory, which gives good approximation only in the low magnetic field. These binding energies are comparable to experimental measurements. Our results are consistent with the other theoretical predictions.

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TUOMAS ROSSI (Presenter), PAUL ERHART, Department of Physics, Chalmers University of Technology, MIKAEL KUISMA, Department of Chemistry, University of Jyväskylä — Metal nanoparticles absorb light much more than their physical size would suggest due to the excitation of a localized surface plasmon resonance. After its excitation, the plasmon resonance decays into high-energy electrons and holes, which, combined with the large absorption cross section, make metal nanoparticles attractive hot-carrier generators for photocatalysis. In this presentation, we describe the femtosecond dynamics of localized surface plasmons in noble metal nanoparticles by using time-dependent density-functional theory (TDDFT). We track the plasmon formation and decay into hot carriers in terms of contributing electron-hole transitions [1,2]. By analyzing the resulting hot-carrier distributions down to atomic-scale detail, we shed light on the hot-carrier generation in catalytically-relevant edge and corner sites of nanoparticles [2].


*EU Horizon 2020 research and innovation programme, Marie Sklodowska-Curie grant No 838996
H71.00257: ABCs of strong exciton–plasmon coupling in 2D TMDCs*  AARON ROSE (Presenter), JEREMY R. DUNKLIN, LUCY METZROTH, HANYU ZHANG, ELISA M MILLER, JAO VAN DE LAGEMAAT, National Renewable Energy Laboratory — We present experimental details of strong exciton–plasmon coupling in 2D MoS$_2$ at the A-, B-, and C-excitons at room temperature. In one experiment, we show plasmon-mediated coherent hybridization of the A- and B-excitons. Rabi splitting of $\sim 70$ meV in $k$-space at each exciton is also shown. The observation of coherent coupling between different exciton energy levels in a valley-polarized material suggests the possibility of valleytronic quantum information transport and/or spin entanglement.

In another experiment we show giant Rabi splitting of 244 meV at the C-exciton, in $k$-space. This corresponds to 9.5% of the transition energy and approaches the ultrastrong coupling regime. We discuss the role the TMDC band structure plays in this large coupling and unique features of the C-exciton.

The band modification that materials experience under strong coupling can be useful for modifying chemical reaction pathways and rates. We discuss experimental design considerations and show results of strong coupling in aqueous electrolyte.

The experimental work is backed up by electromagnetic transfer matrix and coupled oscillator models.

*Funding was provided by DOE Basic Energy Sciences Solar Photochemistry Program.

H71.00258: Tunability of thermal conductivity in lead chalcogenide nanowire heterostructures by strain or alloying*  MACK ADRIAN DELA CRUZ (Presenter), NICK BOECKER, GARY PENNINGTON, Towson Univ —
In the past few years, work on lead chalcogenide alloys of PbSe, and PbTe has shown interesting tunability of electronic properties. PbTe-based materials have shown enhanced phonon scattering driven by a near ferroelectric phase transition mediated by strain or alloying. The thermal properties of such materials are of interest for thermoelectric applications. We consider a low-dimensionality heterostructure, the nanowire, which generally has a lower thermal conductivity compared to bulk. We consider a computationally efficient shell model to find the phonon dispersion of bulk, and approximate the nanowire phonon dispersion. Phonon transport is modeled with an energy deviational Monte Carlo formulation of the Boltzmann transport equation. We further consider layered alloys, with three different transition types between layers: abrupt, linear, and exponential. The considered phonon scattering mechanisms are phonon-phonon, boundary, defect, interface, alloy, and strain. We will report on the further tunability of thermal conductivity by manipulating nanowire heterostructures of these lead chalcogenide alloys.

*The authors acknowledge support from the NSF grant DMR 1709781 and support from the Jess and Mildred Fisher College of Science and Mathematics at Towson University.
**H71.00259: Imaging Nematic Transitions in Iron-Pnictide Superconductors with a Quantum Gas**  
FAN YANG, STEPHEN TAYLOR (Presenter), STEPHEN D EDKINS, JOHANNA PALMSTROM, IAN FISHER, BENJAMIN L LEV, Stanford Univ — The SQCRAMscope is a recently realized Scanning Quantum CRyogenic Atom Microscope that utilizes an atomic Bose-Einstein condensate to measure magnetic fields emanating from solid-state samples. Here, we combine the SQCRAMscope with an in situ microscope that measures optical birefringence near the surface of a sample to study iron-pnictide superconductors, where the relationship between electronic and structural symmetry-breaking resulting in a nematic phase is under debate. We conduct simultaneous and spatially resolved measurements of both bulk and surface manifestations of nematicity via transport and structural deformation channels, respectively. By performing the first local measurement of emergent resistivity anisotropy in iron pnictides, we observe a spatially inhomogeneous increase in the temperature at which optical birefringence appears near the surface over that at which anisotropic local transport appears within the bulk. This is consistent with the existence of a higher-temperature surface nematic transition, albeit one that emerges inhomogeneously. More broadly, these measurements demonstrate the SQCRAMscope's ability to reveal important insights into the physics of complex quantum materials.

*Supported in part by ONR and DOE.

**H71.00260: Monte-Carlo simulations of a random-field Ising-O(3) model**  
NATHANIEL PAGE (Presenter), THOMAS VOJTA, Missouri Univ of Sci & Tech — Many of the iron-based superconducting compounds undergo a structural phase transition and stabilize a stripe-like spin-order at low temperatures. We investigate the relation between the structural and magnetic phase transitions in these materials and study the effects of random strain commonly found in the samples. To do so, the magnetic properties of these materials are modeled via quasi-two dimensional Ising-O(3) model which describes both spin and nematic (stripe) degrees of freedom. Random strain is included via a random field term coupling to the nematic variables. We perform large-scale Monte Carlo simulations of this model to determine the phase diagram and characterize the phase transitions.

**H71.00261: Abstract Withdrawn**
H71.00262: Specific Heat Study in Iron Based Superconductors: A Theoretical Three-Orbital Model Analysis. MADHAVI AHALAWAT (Presenter), AJAY SINGH, Department of Physics, Indian Institute of Roorkee, India — The present work deals with the study of specific heat in superconducting state of iron based superconductors. In these materials, five 3d orbitals due to iron, Hund's coupling and electron correlations coexist and dominate electronic properties of these systems. Therefore, we have attempted the theoretical analysis based on three orbitals per site tight-binding model Hamiltonian containing hopping between orbitals, Hund's coupling and intra and inter orbital Coulomb interaction. We have employed Green's function technique within BCS mean field approximation to calculate the expressions of superconducting energy gap parameter and quasiparticle energies and used these results to calculate specific heat jump as a function of temperature and various parameters of the model Hamiltonian. Then we compared the results with the recent specific heat data and other relevant data of iron based superconductors.

References:

H71.00263: Contribution of substrate phonon to the superconductivity of 1 unit-layer FeSe on SrTiO$_3$ HOYEON JEON (Presenter), MINJUN LEE, Seoul National University, Seoul, Korea, JIN MO BOK, HAN-YONG CHOI, Sungkyunkwan University, Suwon, Korea, YUNKYU BANG, Pohang University of Science and Technology, Pohang, Korea, JUNGPIIL SEO, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu, Korea, JUNGSEOK CHAE, Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, Korea, YOUNG KUK, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu, Korea — A single unit-layer (1 UL) FeSe grown on SrTiO$_3$ is one of Fe-based superconductors and has a high superconducting transition temperature compared to bulk FeSe of which Tc is near 8K. To investigate interface effect, especially phonons of substrate, we used scanning tunneling microscope (STM) and measured local electron density of states (DOS) of 1 UL FeSe on SrTiO$_3$. Our results show that the spectral features depend on the phonon dispersions of FeSe as well as that of SrTiO$_3$. Phonon density of states and electron-phonon coupling constant were calculated according to Eliashberg theory.
H71.00264: S* Superconductivity in Electron-Doped Iron Selenide by Exchange of Hidden Spin Fluctuations* JOSE RODRIGUEZ (Presenter), Physics and Astronomy, California State University Los Angeles — The observation of spin resonances around the corner of the unfolded Brillouin zone in intercalated iron-selenide high-$T_c$ superconductors is consistent with the presence of low-energy hidden spin fluctuations in these materials. We develop an Eliashberg theory based on the exchange of hidden spin fluctuations by electrons in the principal $3d_{xz}$ and $3d_{yz}$ orbitals of the iron atom. At half filling, and in the absence of interactions, an electron-type Fermi surface exists at the center of the unfolded Brillouin zone and a hole-type Fermi surface exists at the corner of the unfolded Brillouin zone. As the interaction strength grows strong, Eliashberg theory predicts a Lifshitz transition to electron/hole Fermi surface pockets at the corner of the folded Brillouin zone. They are extremely faint because of wavefunction renormalization. The Eliashberg theory also predicts a rigid shift of the renormalized band structure upon electron doping, resulting in small but faint hole Fermi surface pockets, and in larger electron Fermi surface pockets. Last, the Eliashberg theory predicts an instability to S-wave Cooper pairing that alternates in sign between the electron-type and the hole-type Fermi surface pockets.

*This work was funded in part by the Air Force Office of Scientific Research.

H71.00265: Giant enhancement of critical current density at high field in superconducting (Li,Fe)OHFeSe films by Mn doping* DONG LI (Presenter), JIE YUAN, PEIPEI SHEN, Institute of Physics, Chinese Academy of Sciences, CHUANGYING XI, High Magnetic Field Laboratory, Chinese Academy of Science, JINPENG TIAN, SHUNLI NI, JINGSONG ZHANG, ZHONGXU WEI, WEI HU, ZIAN LI, LI YU, Institute of Physics, Chinese Academy of Sciences, JUN MIAO, School of Materials Science and Engineering, University of Science and Technology Beijing, FANG ZHOU, Institute of Physics, Chinese Academy of Sciences, LI PI, High Magnetic Field Laboratory, Chinese Academy of Science, KUI JIN, XIAOLI DONG, ZHONGXIAN ZHAO, Institute of Physics, Chinese Academy of Sciences — Critical current density ($J_c$) is one of the major limiting factors for high-field applications of iron-based superconductors. Here, we report that Mn ions are successfully incorporated into nontoxic superconducting (Li,Fe)OHFeSe films. Remarkably, the $J_c$ is significantly enhanced from 0.03 to 0.32 MA cm$^{-2}$ under 33 T, and the vortex pinning force density monotonically increases up to 106 GN m$^{-3}$, which is the highest record so far among all iron-based superconductors. Our results demonstrate that Mn incorporation is an effective method to optimize the performance of (Li,Fe)OHFeSe films, offering a promising candidate for high-field applications.

*This work was supported by the National Key Research and Development Program of China (Grant Nos. 2017YFA0303003, 2016YFA0300301, 2017YFA0302902, 2018YFB0704102); the National Natural Science Foundation of China (Nos. 11888101, 11834016, 11674374, 11574027); the Strategic Priority Research Program of Chinese Academy of Sciences (XDB25000000), the Strategic Priority Research Program and Key Research Program of Frontier Sciences of the Chinese Academy of Sciences (Grant Nos. QYZDYSSW-SLH001, QYZDY-SSW-SLH008)
Results of Point-Contact Spectroscopy Measurements of the Energy Gap of Phosphorus-doped Iron Pnictides BaFe$_2$(As$_{1-x}$P$_x$)$_2$* BRET CONTI (Presenter), KEERAN O RAMANATHAN, ERIK CAULEY, University of the Sciences, CHENGLIN ZHANG, YU SONG, GUOTAI TAN, PENGCHENG DAI, Rice University, ROBERTO RAMOS, University of the Sciences — The study of multi-band superconductivity has gained momentum over the past few years, especially with the advent of iron-based superconductors where multiple energy gaps have been observed. The observed energy gaps which are anisotropic largely depend on the way that the crystal has been grown and how contact is made to access tunneling directions. Soft point contacts to the crystals studied were carefully made using silver paint. We report the results of four-wire tunneling spectroscopy measurements of the energy gap of phosphorus-doped iron pnictides BaFe$_2$(As$_{1-x}$P$_x$)$_2$ where $x = 0.204$, 0.304, 0.25, 0.39, 0.43 and 0.69. The differential conductance $dI/dV$ of these samples exhibit broad peaks and shoulders with $\Delta_1 = 2$-5 meV, and $\Delta_2 = 7$-10 meV. Some of these results were reproducible over similar samples, correspond well with existing data from literature while other features appear new. We report temperature-dependent features that we are in the process of analyzing. These measurements were performed fully by undergraduates.

* R.C.R. acknowledges support from National Science Foundation Grant DMR-1555775 and the Charles Kaufman Foundation.
**H71.00267: Quantum phase transition between the quantum anomalous Hall liquid and insulator states**

CHANG LIU (Presenter), YUNBO OU, YANG FENG, GAOYUAN JIANG, WEIXIONG WU, SHAORUI LI, ZIJIA CHENG, KE HE, XUCUN MA, QIKUN XUE, YAYU WANG, Tsinghua University — The quantum anomalous Hall (QAH) effect has been discovered in magnetically doped topological insulator (TI) thin films in zero magnetic field. A fundamental question concerning the QAH effect is whether it is merely a zero-magnetic-field quantum Hall (QH) effect, or if it can host unique quantum phases and phase transitions that are unavailable elsewhere. Here we perform transport studies on more than 80 QAH samples with different level of disorders. We discover two novel quantum phases, namely the QAH liquid and anomalous Hall (AH) insulator, and the quantum phase transition between them driven by magnetic field. Surprisingly, a universal quantum resistance h/e² is observed at the coercive field of QAH liquid samples in the low disorder limit. We propose that the transmission between chiral edge states, tunable by disorder and magnetic field, is the key for unraveling the peculiar quantum transport phenomena in magnetic TIs.

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**H71.00268: High throughput screening of magnetic thermoelectric materials based on anomalous Nernst effect by first-principles study**

HIKARU SAWAHATA (Presenter), NAOYA YAMAGUCHI, SUSUMU MINAMI, FUMIYUKI ISHII, Kanazawa Univ — The thermoelectric conversion based on the anomalous Nernst effect (ANE) has attracted attention because the ANE realizes the high-density integration more easily compared to that based on the Seebeck effect. This effect is induced by the anomalous Hall conductivity (AHC), and if the AHC changes drastically as a function of the Fermi level, we expect the large ANE [1]. In this study, we implemented the method of computing AHC in metallic systems efficiently [2] to OpenMX code, and we performed high-throughput screening, searching for two-dimensional ferromagnetic materials which have the large Nernst coefficient by the first-principles calculation.

**H71.00269: The evolution of magnetism in intrinsic magnetic insulator material**

*MnBi$_2$Te$_4$(Bi$_2$Te$_3$)$_n*  
FUCONG FEI (Presenter), Nanjing University — Magnetic topological insulators (MTIs) are promising platforms for the observation of quantum anomalous Hall effect (QAHE), which is a long-expected dissipationless quantum transport phenomenon without applying external magnetic field. The recent progress on intrinsic MTI materials shed new light on the observation of higher temperature of QAHE. Here we grow the high-quality single crystals of three promising intrinsic MTI candidates MnBi$_2$Te$_4$(Bi$_2$Te$_3$)$_n$ ($n = 0, 1, 2$). By magnetic measurement, we discover that the all three compounds show anti-ferromagnetic (AFM) behavior, while the magnetic transition temperature decreases when increasing the value $n$. Meanwhile, by transport measurement, anomalous Hall effect can be observed in all three samples and the behaviors are correspondingly consistent with the magnetic measurements. The AFM coupling becomes weaker since the critical magnetic field for anti-ferromagnetism to ferromagnetism transition becomes lower when increasing $n$, and net ferromagnetic moment retains in $n = 1$ and 2 under low temperature. We believe that the tunable magnetic and transport properties by controlling the component ratio in MnBi$_2$Te$_4$(Bi$_2$Te$_3$)$_n$ provide an ideal platform to investigate the high-temperature QAH phase and the related physics.

**H71.00270: Topological Electronic Structure and Its Temperature Evolution in Antiferromagnetic Topological Insulator MnBi$_2$Te$_4**

YUJIE CHEN (Presenter), Tsinghua University, LIXUAN XU, ShanghaiTech University, JIAHENG LI, Tsinghua University, YIWEI LI, University of Oxford, HONGYUAN WANG, ShanghaiTech University, CHAOFAN ZHANG, National University of Defense Technology, HAO LI, YANG WU, Tsinghua University, AIJI LIANG, CHENG CHEN, ShanghaiTech University, SUNGWON JUNG, CEPHISE CACHO, Diamond Light Source, YUANHAO MAO, National University of Defense Technology, SHUAI LIU, MEIXIAO WANG, YANFENG GUO, ShanghaiTech University, YONG XU, Tsinghua University, ZHONGKAI LIU, ShanghaiTech University, LEXIAN YANG, YULIN CHEN, Tsinghua University — The intrinsic magnetic topological insulator MnBi$_2$Te$_4$ exhibits rich topological effects such as quantum anomalous Hall effect and axion electrodynamics. Here, by combining the use of synchrotron and laser light sources, we carry out comprehensive and high-resolution angle-resolved photoemission spectroscopy studies on MnBi$_2$Te$_4$ and clearly identify its topological electronic structure. In contrast to theoretical predictions and previous studies, we observe topological surface states with diminished gap forming a characteristic Dirac cone. We argue that the topological surface states are mediated by multidomains of different magnetization orientations. In addition, the temperature evolution of the energy bands clearly reveals their interplay with the magnetic phase transition by showing interesting differences between the bulk and surface states, respectively. The investigation of the detailed electronic structure of MnBi$_2$Te$_4$ and its temperature evolution provides important insight into not only the exotic properties of MnBi$_2$Te$_4$, but also the generic understanding of the interplay between magnetism and topological electronic structure in magnetic topological quantum materials.
**H71.00271: Multifold Weyl nodes in a nonsymmorphic garnet compound**

HYO-SUN JIN (Presenter), KWAN-WOO LEE, Division of Display and Semiconductor Physics, Korea University — In condensed matters, now, many systems show linear band crossings of 4-fold Dirac nodes or 2-fold Weyl nodes, which have been sought for a long time in high energy physics. Recently, multifold nodes, which have no high energy counterpart, have been also proposed, e.g., 3-, 6-, and even 8-fold Weyl nodes. However, except triple-node points, no experimental realization has been successful yet. In this presentation, we will introduce an interesting real system with various exotic Weyl nodes, lying not far away from the Fermi energy.

Using first principles calculations, we will address a nonsymmorphic ferrimagnetic garnet insulator with the \textit{Ia-3d} space group (No.230). In the absence of spin-orbit coupling (SOC), this system shows various magnetic multifold Weyl nodes, in particular, of 4- and 6-folds. These nodes with nonzero Chern numbers are due to a combination of several crystalline symmetries including inversion and glide reflection symmetries. Furthermore, we will discuss on the topological nature of the unconventional Weyl nodes by an effective Hamiltonian analysis.

*This research was supported by NRF-2019R1A2C1009588

**H71.00272: Decoupling of electronic thermal conductivity and electrical conductivity in the magnetic nodal semimetal CeAlGe**

FEI HAN (Presenter), QUYNH NGUYEN, THANH NGUYEN, RICARDO PABLO PEDRO, ANUJ APTE, NINA ANDREJEVIC, MINGDA LI, Massachusetts Institute of Technology MIT — Wiedemann-Franz (WF) law is a robust empirical law stating that the ratio between the electronic thermal conductivity and electrical conductivity is related by a universal Lorenz number. For conventional materials, this law is strictly obeyed even when the electronic thermal conductivity and electrical conductivity are suppressed by magnetic fields. In the magnetic nodal semimetal CeAlGe, we observed a decoupling of electronic thermal conductivity and electrical conductivity.

CeAlGe possesses a ferrimagnetic ordering in the ab plane below 4.5 K. The magnetic field applied along the c axis diminishes the ferrimagnetic ordering and induces a ferromagnetic ordering along the c axis. At a certain temperature, the positive magnetoresistance (MR) originating from the enhanced electron cyclotron motion and the negative MR originating from the spin reorientation compensates completely, which makes the MR is zero at this temperature. However, at this temperature, the thermal conductivity does not keep a constant as expected by the WF law. In contrast, we found the magnetic field suppressed the thermal conductivity to the largest extent at this temperature. This indicates a new mechanism dominating the relationship between the electronic thermal conductivity and electrical conductivity.
**H71.00273: Magneto-transport properties of antiferromagnetic Weyl semimetal CuMnSb**

VIPIN NAGPAL (Presenter), SATYABRATA PATNAIK, School of Physical Sciences, Jawaharlal Nehru University-New Delhi — The electrical resistivity and magneto-transport properties of reported magnetic Weyl semimetal CuMnSb is studied. CuMnSb with an antiferromagnetic transition at 60K is synthesized using solid state reaction technique and crystallizes in cubic lattice structure with space group F-43m (216). No abrupt change in resistivity is observed below the transition under the application of 5T field. A highest non-saturating MR of 4% is observed at 5K and 6T. It is analyzed that MR in CuMnSb arises from the contribution of linear field $B$ dependence as well as the parabolic $B^2$ term.

*V. Nagpal acknowledge UGC NET-JRF, UGC New Delhi for financial support. S. Patnaik thanks funding support of SERB, DST-FIST and DST-PURSE programs of Government of India.

**H71.00274: Molecular beam epitaxy growth of (MnSb$_2$Te$_4$)(Sb$_2$Te$_3$)$_n$ SL/QL sequences**

IDO LEVY (Presenter), HAIMING DENG, STEVEN ALSHEIMER, LIA KRUSIN-ELBAUM, MARIA C TAMARGO, The City College of New York — Recent predicted intrinsic magnetic topological materials in the MB$_2$T$_4$-family (where M = V, Mn, Ni or Eu, B = Bi or Sb, T = Te, Se, or S) show a great promise for realizing intrinsic axion insulators and quantum anomalous Hall (QAH) insulators. These materials modify the B$_2$T$_3$ crystal structure forming septuple layers (SL) in the form of T-B-T-M-T-B-T. Not all of the listed magnetic TI candidates have been yet explored, and thus far out-of-plane surface magnetization was only found in MnBi$_2$Te$_4$ and MnSb$_2$Te$_4$. Both materials are antiferromagnetic (AFM) in the bulk and not suitable for QAH unless they have odd number of SLs. Recent studies in MnBi$_2$Te$_4$ have shown that separating SLs with Bi$_2$Te$_3$ quintuple layers (QL) turns an AFM into a ferromagnet (FM). Here we show that through layer-by-layer growth using molecular beam epitaxy (MBE) we can control the SL/QL sequence. We describe the conditions for which MnSb$_2$Te$_4$/Sb$_2$Te$_3$ sequence is ferromagnetic with $T_c$ higher than that in the Bi-based SL/QL sequence, as witnessed by large anomalous Hall signal with coercive field $\sim$0.1 T at 2 K. The structural (TEM and HR-XRD) characterization and the optimization of the SL/QL sequence will be presented.

*This work was supported by NSF Grant Nos. DMR-1420634 and HRD-1547830.
H71.00275: First-principles theory of Cr-vacancy in BaZrO$_3$ as a solid-state qubit candidate

JAEWOOK LEE (Presenter), HOSUNG SEO, Ajou Univ — Recently, remarkable advances have been made in the development of solid-state quantum bits (qubits), which are the basic hardware units of quantum information processing. One of the leading solid-state qubit platforms is the nitrogen-vacancy (NV) center in diamond. Furthermore, a significant interest has been emerging in the literature to develop such defect-based qubits in diverse wide-gap semiconductors for broadening the scope of the solid-state quantum information. In this study, we explore a Cr-O vacancy complex in BaZrO$_3$ as a potential solid-state qubit candidate. We use first-principles density functional theory to examine the stability and the electronic and spin properties of the Cr-O vacancy pair in BaZrO$_3$. To investigate the stability of the defect in various charge states, we calculate the defect formation energy of Cr-vacancy in BaZrO$_3$. In addition, we use HSE06 hybrid functionals to accurately calculate the defect level diagram and the zero-phonon line of the Cr-O vacancy. In the poster, we also discuss the recent progress and challenges in computational design of new defect qubits in complex wide-gap materials.

H71.00276: Magnetic-field and tunable-barrier effects on charge transport in DNA heterostructures

YONG JOE (Presenter), ALAA ALSAID, IBTISAM ABU ALKHAYR, Ball State University — The tunable barrier and magnetic field effects are studied in the electron transport of the double-stranded DNA molecular electronic structure. Our theoretical approach involves the application of the two-dimensional tight-binding Schrödinger equation to calculate transmission and electric current through the nearest-neighbors of twenty base-pairs’ DNA. A combination of G-C and A-T base-pairs of DNA, which can be considered as a barrier and a well, forms a superlattice in semiconductor heterostructures and exhibits a miniband whose width depends on the strength of the barriers and energy level of the wells. We also incorporate a variation of magnetic field flux density into the hopping integrals as a phase factor and observe Aharonov-Bohm (AB) oscillations in the transmission. It is shown that for non-zero magnetic flux, the transmission zero leaves the real-energy axis and moves up into the complex-energy plane. We also point out that both the hydrogen bonds between the base pair and the coupling between leads and DNA with flux variations play a role to determine the periodicity of AB oscillations in the transmission.
**H71.00277: Non-Hermitian Thermal Emitters using Metal-Semiconductor Hybrid Resonators**

CHLOE F DOIRON, GURURAJ NAÎK (Presenter), Rice Univ — Thermal emitters always have absorption losses and hence are open systems. Open systems are non-Hermitian and are best described by non-Hermitian physics. Here, we develop a non-Hermitian description of resonant thermal emitters and thereby take advantage of absorption loss in the system. Further, the non-Hermitian description provides new design tools such as symmetry, phase, and topology to control the properties of the thermal emission. We demonstrate such a thermal emitter using coupled plasmonic and photonic resonators. A lossless silicon photonic resonator is coupled to a lossy tungsten plasmonic resonator via a spacer. As the spacer thickness is increased, the thermal emission from the device held at 1000 K exhibits a transition from PT-symmetric to symmetry-broken phase through an exceptional point. The thermal emission from the device breaks the trade-off between emission brightness and spectral selectivity and simultaneously achieves both. Further, we show that the internal phase of resonators is a powerful tool to control the thermal emission from this device. Overall, this work is an unorthodox approach towards designing not only thermal but also other nanophotonic light sources.

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**H71.00278: The effect of van der Waals force on two-dimensional SiC/GeC heterostructures**

SAFIA ABDULLAH R ALHARBI, MING YU (Presenter), Univ of Louisville — The effect of van der Waals interaction on two-dimensional (2D) SiC/GeC heterostructures has been studied based on the density functional theory. The van der Waals interaction is considered by employing the semi-empirical correction scheme of Grimme [1], which is used in optimizing the equilibrium interlayer distance and binding energy between 2D monolayers. We found that for the layered SiC/GeC heterostructure with the C-Ge (Si-C) species order, the cohesive energy as a function of interlayer distance is about 0.03 eV per unit cell lower than that with the C-C (Si-Ge) species order, for both AA and AB stacking. Further findings show that the interlayer electrostatic forces mainly stabilize the equilibrium distance for the C-Ge (Si-C) species ordering, and vdW interactions only make the system attain a lower cohesive energy. On the other hand, vdW forces stabilize the interlayer distance for the C-C (Si-Ge) species order. These preliminary results suggest that interlayer electrostatic forces may play a role in ionic-like multilayer heterostructures.


*We acknowledge the finding support by Arts and Sciences Research and Creative Activities Grant at University of Louisville.
H71.00279: Experimental studies of nonlinear optics of self-assembled hyperbolic metamaterials  
WILL KORZI (Presenter), JONATHON CARTELLI, BRYAN AUGSTEIN, KENT HESS, Department of Physics, Astronomy, and Geosciences, Towson University, NAVEEN KADASALA, STEPHEN BLAMA, MARY SAJINI DEVADAS, Department of Chemistry, Towson University, VERA N SMOLYANINOVA, Department of Physics, Astronomy, and Geosciences, Towson University, IGOR I SMOLYANINOV, Saltenna LLC and University of Maryland — Sub-wavelength confinement of light in nonlinear hyperbolic metamaterials due to formation of spatial solitons has attracted much recent theoretical attention because of its seemingly counter-intuitive behavior. In order to achieve self-focusing in a hyperbolic wire medium, a nonlinear self-defocusing Kerr medium must be used as a dielectric host. It was demonstrated that this behavior finds natural explanation in terms of analogue gravity in effective “optical spacetime”, which can be used to describe nonlinear optics of a hyperbolic wire medium. In this work we will report first experimental observation of this effect using iron-cobalt ferrofluid-based self-assembled hyperbolic metamaterials subjected to external magnetic field.

H71.00280: Enhancing the Light Emission of Colloidal Quantum Dots with Dual-band Absorbers Based on Metasurfaces  
DONGFANG LI (Presenter), CHUN-CHIEH CHANG, AJAY SINGH, JENNIFER A HOLLINGSWORTH, HOU-TONG CHEN, Los Alamos National Laboratory — Quantum dots (QDs) are essential light emitters with great tunability of spectrum and find important technological applications in various areas, including light-emitting devices, photovoltaics, and bioimaging. The recent advance of metamaterials has enabled the direct control of the light emission properties with patterned ultrathin metallic films, ranging from enhanced light emission and modified fluorescence spectrum to well-defined polarization and unidirectional radiation. However, the outcoupling efficiency of two-dimensional (2D) QD-based optoelectronic devices is still limited. Here we propose and demonstrate the enhancement of the light emission of QD-based 2D optoelectronic devices at around telecom wavelengths by employing dual-band perfect absorbers based on plasmonic metasurfaces. The two resonant peaks of the absorber simultaneously match the absorption and radiation wavelengths of non-blinking “giant” QDs at the telecom regime, thus enhancing the excitation pump meanwhile maintaining the efficient outcoupling of the light emission. These findings will not only benefit technological applications of QD-based optoelectronic devices but also offer better understanding of the fundamental physical mechanisms of light-matter interactions.
**H71.00281: High-Yield Production of Nanoplatelet Bi$_2$Te$_3$ via Supercritical Ball Milling in Carbon Dioxide**

MOHAMED ATWA (Presenter), Okinawa Institute of Science and Technology, TESSUI NAKAGAWA, Department of Chemistry, University of the Ryukyus, MAKOTO SCHREIBER, YOSHINORI OKADA, Okinawa Institute of Science and Technology — Nanoplatelet Bi$_2$Te$_3$ is highly desired as a starting powder for the consolidation of bulk nanostructured thermoelectric legs, as low-dimensional Bi$_2$Te$_3$ has long been expected to result in a higher Seebeck coefficient and lower thermal conductivity, leading to an unprecedented enhancement in the thermoelectric figure of merit (zT) in this material. The production of few-layer Bi$_2$Te$_3$ nanoplatelets has thus far mainly been limited to low-yield hydrothermal synthesis techniques. Studies have suggested that Bi$_2$Te$_3$ degrades in the presence of water, making such hydrothermal techniques inherently non-ideal for the production of high thermoelectric performance Bi$_2$Te$_3$ nanoplatelets. In this study, we show that gram-yield quantities of few-layer Bi$_2$Te$_3$ nanoplatelets are preferentially exfoliated along the basal plane using a novel, “all-dry” supercritical carbon dioxide (scCO$_2$) ball milling technique. We will discuss advantages of our method in terms of the size, morphology, and crystallinity of the resulting nanoplatelets are compared against conventional ball milling techniques.

**H71.00282: Tuning structural and electronic properties of α-Te tubular nanostructures by uniaxial strain**

YANRONG GUO, JINJIN WANG, SONGYOU WANG, Optical Science and Engineering, Fudan University, Shanghai 200433, China, YU JIA, School of Physics and Engineering, Zhengzhou University, Zhengzhou 450001, China, WAN-SHENG SU (Presenter), National Taiwan Science Education Center, Taipei 11165, Taiwan — Tellurene, a new member of two-dimensional family materials, shows outstanding photoelectric characteristics. Here, a first-principles calculation is employed to explore the effect of uniaxial strains on the electronic properties for α-Te tubular nanostructures with various tube sizes. Under compressive and tensile strains of 10%, the atomic structures of α-Te tubular nanostructures have not been destroyed, demonstrating they have good flexibility. Interestingly, we found armchair (5,5) α-Te tubular nanostructures experience an intriguing semiconductor–metal transition at a certain strain, while other α-Te tubular nanostructures are semiconductor with modulable band gap. The electronic properties of α-Te tubular nanostructures under strain modulation can help to understand the properties of new nanomaterials comprehensively, paving the way for future optoelectronic applications.

*W.-S. Su would like to thank the Ministry of Science and Technology for financially supporting this research under Contract No. MOST-108-2112-M-979-001. Support from the National Centers for Theoretical Sciences and High-performance Computing of Taiwan in providing significant computing resources to facilitate this research is also gratefully acknowledged.*
H71.00283: Thermal drift induced artifacts in AFM atomic lattice images*  DONGHYEON MOON (Presenter), BO RAM JEON, SUENNE KIM, Hanyang Univ — Two-dimensional materials are emerging as next-generation ultra-thin semiconductor device materials. The electronic band structure of these materials is strongly perturbed by mechanical strain. Therefore, many studies on the strain engineering of two-dimensional materials have been conducted recently. The aim of these studies is to control the electronic and optical properties of two-dimensional materials. To determine the effect of strain, it is necessary to investigate the atomic lattice structure accurately. Various scanning force microscopy (SFM) techniques have been used to observe these two-dimensional crystal lattices. In this study, we show that artifacts due to thermal drift in AFM measurements can impede accurate structural interpretation related to strain. In other words, distorted images can lead to incorrect scientific conclusions on the critical strain issues in these atomically thin two-dimensional materials.

*D.M., B.R.J., and S.K. were financially supported by the National Research Foundation (NRF) of Korea grant funded by the Korea Government (2017R1D1B04036381).

H71.00284: Phonon dispersion curves for three new MoS$_2$ type monolayers.*  FERNANDO MAGANA (Presenter), GERARDO-JORGE VAZQUEZ FONSECA, ERICK GARCES GARCIA, Univ Nacl Autonoma de Mexico — Using ab initio calculations based on density functional theory, we obtained new structures for MoS$_2$ type monolayers: NbS$_2$, MoP$_2$ and NbP$_2$, not previously reported in the literature. These proposed structures were relaxed to their minimum energy configuration. Then, we calculated the phonon dispersion curves for each one of them. We exhibit the differences with respect of MoS$_2$. The Quantum-Espresso package [1] was used with norm conserving pseudo potentials.


*We thank Dirección General de Asuntos del Personal Académico de la Universidad Nacional Autónoma de México, partial financial support by Grant IN-111807 and we also thank Miztli Super-Computing center the technical assistance.
We present a theoretical study of second harmonic generation (SHG) in structured metamaterials; particularly, an array of cross-shaped vacuum inclusions within a silver host. We calculate the nonlinear susceptibility tensor, for a large number of geometrical configurations for the inclusions. We demonstrate that both, the SHG intensity and the resonance peaks are highly sensitive to even subtle changes in the geometry that break the centrosymmetry of the array of inclusions. We presented the results for calculation of non linear susceptibility of second order for a metamaterial composed by silver host and cross-shaped inclusions of vaccum. The dielectric functions of both materials are known. The intensity in nonlinear susceptibility tensor depends on the variation in the symmetry of the metamaterial. We present the three non-zero components of that tensor, calculated by Haydock Recursive Method.

*This work was supported by DGAPA-UNAM under Grants No. IN113016 and No. IN111119 (WLM) and by CONACyT under scholarship 589138 (U.R.M.).

Recent studies have hinted at the importance of dynamic interactions between electronic states and the lattice in organic-inorganic 2D perovskites (2DPs). It is thus critical to understand the interplay between structure and properties during light excitation and in operating devices. Here, we investigate these effects by exploring the 2DPs phase space in terms of both layer thickness and interlayer organic spacer rigidity. We reveal the relation between structural and photophysical properties in 2DPs by correlating structural and optoelectronic spectroscopy at the sub-micron scale and under magnetic field, with support from theory. Our work demonstrates that during photoexcitation strongly bound excitons are generated and their characteristics (mass, size, energy) can be modulated not only by the thickness of the 2D perovskites layers as in classic quantum-wells but also through structural distortions such as perovskite octahedra tilting induced by the organic spacer or crystal edge termination.[1] Similar effects are linked to local compositional changes or artificial interfaces, resulting in giant enhancement of photoemission at the 2DP and WS

H71.00287: Investigation of Spectral Diffusion due to Static and Dynamic Disorder in Perovskite Thin Films*  GEOFFREY DIEDERICH, ADAM HALAOUI (Presenter), AMANI H ALFAIFI, Univ of Denver, SEAN SHAHEEN, Electrical, Computer and Energy Engineering, University of Colorado Boulder, MARK SIEMENS, Univ of Denver — Multidimensional coherent spectroscopy (MDCS) is an ultrafast spectroscopy technique that spreads coherent information across multiple dimensions, resolving features that might overlap in one-dimensional measurements. Both coherent and incoherent transport, broadening mechanisms, and spectral diffusion can be separated and clearly measured with MDCS. Additionally, the phase sensitivity of MDCS measurements allows visualization of the full complex signal field. These attributes make MDCS ideal for studying complex material systems like perovskites thin films where cation mixing, ion migration, and inhomogeneous grain conditions can make spectra difficult to interpret.

Here, we present MDCS spectra from thin films of a mixed-cation perovskite at low temperature. The spectra show inhomogeneously broadened free and defect-bound excitons with a homogeneous dephasing time on the order of 1 ps. The excitons undergo spectral diffusion and relaxation on a much more rapid timescale than has been measured in GaAs quantum wells, increasing the resonance linewidth by a factor of ~3 over one picosecond.

*We acknowledge the financial support of the National Science Foundation

H71.00288: The evolution of ultrafast carrier dynamics in-situ perovskite optoelectronic devices  KANISHKA KOBBEKADUWA, PHYSICS, Clemson University, SHREETU SHRESTHA, LANL, PAN P ADHIKARI, EXIAN LIU, PHYSICS, Clemson University, WANYI NIE, LANL, JIANBO GAO (Presenter), PHYSICS, Clemson University — Although significant progresses have been made toward to optoelectronics application including solar cells, large color gamut LEDs, photodetectors, and X-ray detectors, the fundamental understanding of ultrafast carrier dynamics of organic-inorganic perovskite materials remains unclear. The ultrafast dynamics, which reveals some novel physical phenomena such as hot carrier cooling, phonon bottle-neck effect, and many-body problem was widely studied by ultrafast optical spectroscopies, which include pump-probe transient absorption (transmission, reflection, time-resolved THz, optical Kerr effect, and the most popular time-resolved photoluminescence(TRPL). However, it remains a challenge to study the perovskite optoelectronic devices in-situ in an ultrafast fashion.

In this talk, we use an ultrafast photocurrent spectroscopy with sub-25 picosecond time resolution to reveal the evolution of ultrafast carrier dynamics from sub-25 ps to microsecond in-situ perovskite solar cells and photoconductors. We address the basic questions of carrier photogeneration, recombination, transport, trapping, in addition to directly extracting carrier mobility, lifetime, and the property of trap states such as density, energy level, and capture cross-section.

H71.00289: WITHDRAWN ABSTRACT  —

H71.00290: WITHDRAWN ABSTRACT  —
H71.00291: Pentacene Thin Film Growth* BRADLEY LOCKHART (Presenter), Physics and Astronomy, Ohio Northern University, JESSICA BICKEL, Physics, Cleveland State University — Pentacene is a common organic semiconductor with a relatively high conductivity that increases when crystallized. In this experiment pentacene was studied by depositing it on highly ordered pyrolytic graphite (HOPG) using a thermal evaporator and characterizing it with scanning tunneling microscopy (STM). The daily pressure inside the evaporation chamber had small day-to-day variations, between 1 and 7x10^-5 torr, which caused significant variations in growth rates. We subsequently developed a method to measure the growth rate immediately before the deposition by opening the shutter of the thermal evaporator to a specific angle so that the growth rate could be measured with a quartz crystal monitor without depositing any material on the HOPG substrate. Examining the resulting depositions with STM, we find several images showing the deposited pentacene either forming into clumps, or into seemingly more ordered track-like patterns. These images were analyzed to find the dimensions of these structures and compared to previously gathered pentacene data from other groups.

*NSF REU Award # 1659541

H71.00292: Characterizing the Crystal Formation and Interdiffusion Mechanisms of PLA/PS/dSMMA Thin Films* SURAJ DHULIPALLA (Presenter), MUKIL SHANMUGAN, DORIS YANG, XIANGHAO ZUO, MIRIAM RAFAILOVICH, Stony Brook University — Polylactic Acid (PLA) thin films have emerged as an eco-friendly alternative for nonbiodegradable polymers in industrial coatings. As such, our investigation characterized the interfacial diffusion and crystal formation in thin films (PLA, polystyrene (PS), and deuterated styrene methyl methacrylate (dSMMA) blends) on different substrates. AFM data showed that larger molecular weight PS additives increased crystal size and roughness of PLA-PS annealed samples. In bilayer samples, we found a 32% roughness decrease in PS/dSMMA on PLA compared to PLA on PS/dSMMA samples. SIMS data showed that dSMMA was nearly absent in the PS layer and interfacial thickness increased with dSMMA concentration. Previous studies proved dSMMA's compatibilizing property in bulk[1]; we prove dSMMA retains this property under confinement without compromising crystallinity. This study shows that substrates influence the roughness and crystallinity of PLA thin films and that dSMMA is an effective compatibilizer of PLA and PS thin films which is a promising sign for future use in bioelectronics.


*Supported by the Garcia Center for Polymers at Engineered Interfaces
H71.00293: Quasi-static C-V Characterization of Traps in Sputtered Bismuth Selenide FET*
PROTYUSH SAHU (Presenter), JUNYANG CHEN, JIANPING WANG, University of Minnesota — Bismuth Selenide based devices have gained a lot of attention due to the highly conducting, spin-polarized, topologically protected surface states [1]. They have found a lot of promise in spintronics. Previous works have shown the existence of high charge to spin conversion in sputtered, polycrystalline Bi$_x$Se$_{1-x}$ [2-4]. This is attributed to the quantum confinement effect in the individual grains of the film. Characterizations have revealed non-idealities from this material due to charge trapping. In this work, we characterize charge traps in FET devices by quasi-static Capacitance-Voltage measurement. The experimental C-V curve shows a hysteretic behavior which is attributed to oxide and interfacial traps. We use the known charge trapping model to calculate the trap densities for different devices. To further understand the physics of random defects, we simulated the electric field in the FET device by 2D finite difference time domain technique (computational electrodynamics) to analyze the E-field uniformity near a defect edge and along the Bi$_x$Se$_{1-x}$/SiO$_2$ interface.


*This work was supported by ASCENT, a SRC program.

H71.00294: Investigation of phonon-mediated relaxation within the topological insulator Bismuth Tellurium*
CHAO-HONG LIN (Presenter), MENG-CHING LEE, JIN-WEI LI, TSUN-I CHEN, CHAO-KUEI LEE, Sun Yat-sen University — In this work, using double pulses excitation technique, the energy coupling ratio from excitation laser to coherent phonons of topological insulator bismuth tellurium(Bi$_2$Te$_3$) thin film was characterized. First of all, by analyzing excitation intensity dependent heating temperature of the thin film from the transmission pump probe results, the coherent phonon generation and the energy coupling from laser to phonons were confirmed. The coupling ratio was accordingly estimated and with decreasing nature as increasing temporal spacing between double pulses. Furthermore, the frequency and intensity of the phonon mode were investigated as well. Beside identification of the relaxation characteristic, we also find evidence of phonon-mediated relaxation of the energy density at the Bi$_2$Te$_3$ surface.

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H71.00295: Weak antilocalization in hexagonal Ca$TX$ ($T$ = Cu or Ag, $X$ = Sb or Bi) single crystal

SOUVIK SASMAL (Presenter), Condensed matter physics and Material science, Tata Institute of Fundamental Research, RAJIB MONDAL, Condensed matter physics, UGC-DAE Consortium for Scientific Research, RUTA KULKARNI, Condensed matter physics and Material science, Tata Institute of Fundamental Research, BAHADUR SINGH, Department of Physics, Northeastern University, A. THAMIZHA VEL, Condensed matter physics and Material science, Tata Institute of Fundamental Research — The hexagonal ABC-type topological semimetals Ca$TX$ ($T$ = Cu or Ag, $X$ = Sb or Bi) are currently drawing intense interest due to their intriguing properties. Specifically, the first-principles calculations have revealed that CaAgBi is a topological Dirac semimetal where the Dirac points are located on the rotational axis slightly above the Fermi level and are protected by $C_{6v}$ point-group symmetry [1].

We have grown the single crystals of these topological semimetals. We find that although ABC-type materials crystallize in the hexagonal structure, they adopt different space-groups depending on the $T$ (Cu/Ag) atom. The electrical resistivity shows metallic behaviour following Bloch-Gruneisen relation whereas the Hall resistivity measurements reveal a semimetallic nature with predominantly $p$ type charge carriers. The transverse magnetoresistance measurements reveal the weak antilocalization (WAL) behaviour for fields below 5 T and temperatures less than 100 K. The angular dependence of the magnetoconductance measurements show that CaCuSb and CaAgSb host topologically protected bulk and surface states. We find that WAL is specific to these type of topological semimetals single crystals.

H71.00296: Electronic transport properties of doped Bi$_2$X$_3$ (X = Se, Te) single crystals Shailja Sharma, C.S. Yadav School of Basic Sciences, Indian Institute of Technology Mandi-175005 (H.P.) India

SHAILJA SHARMA, CHADR YADAV (Presenter), School of Basic Sciences, Indian Institute of Technology Mandi — The observation of anomalous Hall effect and the occurrence of superconductivity in doped 3D topological insulators, are some of the very interesting phenomenon in these systems [1-3]. We have investigated the magneto-transport properties of Bi$_2$Se$_3$ and Bi$_2$Te$_3$ single crystals to explore the effect of intercalation and substitution of Fe, Ag, Au, Pt, Pd etc. on the electronic state of the systems. Magnetoresistance of the magnetically doped Bi$_2$Se$_3$ was found to follows Kohler’s rule, suggesting the single scattering rate at all the points on the Fermi surface. Hall effect measurements suggest the consistence doping of charge carriers in the system upon intercalation. Our findings on the weak antilocalization and weak localization cusps in the magnetoresistance and their evolution with dopant concentration bring out the effect of charge transfer or magnetic elements on the topological surface states of these compounds [4].

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*We acknowledge AMRC, IIT Mandi and DST-SERB for the experimental facility and financial support.

H71.00297: Tunable anomalous Hall effect in Dirac semimetal Cd$_3$As$_2$ nanowire SHUO WANG (Presenter), BENCHUAN LIN, Southern University of Science and Technology, YING LI, Peking University, DAPENG YU, Southern University of Science and Technology, ZHI-MIN LIAO, Peking University — Recent years, the combination of topology and physics has led to the rapid development of topological physics. Dirac semimetal Cd$_3$As$_2$, with a pair of symmetry-protected three-dimenisonal Dirac cones, has drawn a lot of attention. Here, we report the experimental observation of tunable anomalous Hall effect in Cd$_3$As$_2$ nanowire. The anomalous Hall signal maximizes near the Dirac point under an applied magnetic field. As the gate voltage is tuned away from the Dirac point, the anomalous Hall signal decreases and eventually disappears. Based on the detailed analysis of the anomalous signal with gate voltage, temperature and magnetic field direction, the observed anomalous Hall effect is attributed to the Berry curvature originated from the Weyl node.
H71.00298: Thermodynamic properties of non-trivial topological semimetal CaSn$_3$  
K A M HASAN SIDDIQUEE (Presenter), RIFFAT MUNIR, CHARUNI DISSANAYAKE, University of Central Florida, XINZHE HU, SWAPNIL YADAV, YASUMASA TAKANO, University of Florida, EUN SANG CHOI, Florida State University, TALAT RAHMAN, DUY LE, YASUYUKI NAKAJIMA, University of Central Florida — Topological semimetals, a group of gapless electronic phases with topologically stable energy band crossing, give pathways to observe new quantum phenomena. We will report torque magnetometry and heat capacity measurements on CaSn$_3$, which is theoretically proposed to be a non-trivial topological semimetal. We will present a detailed study of band structure for CaSn$_3$ single crystals via torque magnetometry in high magnetic fields up to 35T. We will also present the thermodynamics properties of this material.

H71.00299: Growth and transport measurements of nanowires of cubic B20 topological semimetals  
NITISH MATHUR (Presenter), ANDREW JACOB DERUITER, Department of Chemistry, 1101 University Avenue, Madison, WI-53706, University of Wisconsin Madison, ANASTASHIA GEORGE, Department of Chemistry, Durango, CO 81301, Fort Lewis College, MINGLIANG TIAN, High Magnetic Field Laboratory, Chinese Academy of Science, Hefei, Anhui 230026, China, SONG JIN, Department of Chemistry, 1101 University Avenue, Madison, WI-53706, University of Wisconsin Madison — Since the discovery of topological insulators and semimetals, topological materials are key research frontiers in the field of condensed matter physics. One of the examples of the topological material is a Weyl semimetal where two non-degenerate bands cross at a node in a momentum space and acquires a quantized topological charge known as the Chern number. Among them, cubic B20 material systems (such as CoSi, RhSi, AlPt) are found to possess unconventional chiral fermions with higher Chern number and long fermi arcs due to multiple point degeneracies at high symmetry Brillouin points. We have synthesized single-crystal cubic B20 topological semimetal nanowires (NWs) of CoSi and CrGe via chemical vapor deposition (CVD). We conducted magnetotransport measurements with different configuration of applied magnetic field (in-plane/out-of-plane) and current direction to connect quantum topological properties to electronic band structures. We are also performing physical property measurements under high magnetic field. These NW systems can act as the perfect prototypes to understand the impact of surface states and bulk Landau levels on the transport behaviors in finite size topological semimetals.
H71.00300: Measurements of cyclotron resonance of the interfacial states in strong-spin orbit coupled 2D electron gases proximitized with aluminum.*

PRASHANT CHAUHAN, Johns Hopkins University, CANDICE THOMAS, TYLER LINDEMAN, Department of Physics and Astronomy and Microsoft Quantum Purdue, Purdue University, West Lafayette, Indiana 47907 USA, GEOFF C GARDNER, SERGEI GRONIN, Microsoft Quantum Purdue, Purdue University, West Lafayette, Indiana 47907, USA, JAN GUKELBERGER, Quantum Architecture and Computation Group, Microsoft Research, Redmond, Washington 98052, USA, ROMAN LUTCHYN, Station Q, Microsoft Research, Santa Barbara, California 93106-6105, USA, MICHAEL MANFRA, Department of Physics and Astronomy and Microsoft Quantum Purdue, Purdue University, West Lafayette, Indiana 47907 USA, PETER ARMITAGE (Presenter), Johns Hopkins University — The two dimensional electron gas (2DEG) in InAs proximitized by aluminum (Al) is a promising platform for topological qubits based on Majorana zero modes. However, there are still substantial uncertainties associated with the nature of the electronic states at the interfaces of these system. In this work we have investigated a range of In$_{1-x}$Ga$_x$As heterostructures with Al overlayers using high precision time-domain THz spectroscopy. In magnetic field a prominent cyclotron resonance is observed that can be associated with the response of the interfacial states. Measurements of the THz range complex Faraday rotation allow the extraction of the sign and magnitude of the effective mass, density of charge carriers, and scattering times. We compare the results of measurements with numerical calculations.

*Funding support for work at The Johns Hopkins University and Purdue University is from Microsoft Quantum

H71.00301: Pressure-induced superconductivity and topological phase transitions in the topological nodal-line semimetal SrAs$_3$

ERJIAN CHENG (Presenter), SHIYAN LI, Fudan Univ — Topological nodal-line semimetals (TNLSMs) are materials whose conduction and valence bands cross each other, meeting a topologically-protected closed loop rather than discrete points in the Brillouin zone. TNLSMs have several anticipated properties, such as drumhead-like nearly flat surface states, the possibility of realizing high-temperature superconductivity and so on. Recently, SrAs$_3$ has been theoretically proposed and then experimentally confirmed to be a TNLSM. Here, we report high-pressure experiments on SrAs$_3$, identifying a Lifshitz transition below 1 GPa and a superconducting transition accompanied by a structural phase transition above 20 GPa. A topological crystalline insulator (TCI) state is revealed by means of density functional theory calculations on the emergent high-pressure phase. As the counterpart of topological insulators, TCIs possess metallic boundary states protected by crystal symmetry, rather than time reversal. In consideration of topological surface states and helical spin texture observed in the high-pressure state of SrAs$_3$, the superconducting state may be induced in the surface states, and is most likely topologically nontrivial, making pressurized SrAs$_3$ a strong candidate for topological superconductor.

H71.00302: MAGNETISM —

H71.00303: WITHDRAWN ABSTRACT —
Effect of Mn/Fe ratio on the Magnetic and Magnetocaloric Properties of Hexagonal Mn$_{2-x}$Fe$_{1+x}$Ge ($0 \leq x \leq 1$) Heusler Alloys*

ANIL ARYAL (Presenter), IGOR DUBENKO, Southern Illinois University Carbondale, JOSE LUIS SÁNCHEZ LLAMAZARES, JONATHAN ZAMORA, Instituto Potosino de Investigación Científica y Tecnológica A.C., Mexico, CESAR FIDEL SÁNCHEZ-VALDÉS, División Multidisciplinaria, Universidad Autónoma de Ciudad Juárez (UACJ), Mexico, DIPANJAN MAZUMDAR, SAIKAT TALAPATRA, Southern Illinois University Carbondale, SHANE STADLER, Department of Physics & Astronomy, Louisiana State University, Baton Rouge, USA, NAUSHAD ALI, Southern Illinois University Carbondale — In this work, we synthesized bulk Mn$_{2-x}$Fe$_{1+x}$Ge ($0 \leq x \leq 1$) by arc melting and Mn$_2$FeGe melt-spun ribbons by rapid solidification using the melt-spinning technique and investigated their structural, magnetic, and magnetocaloric properties. Room temperature X-ray diffraction analyses show that Mn$_2$FeGe crystallizes into the hexagonal DO$_{19}$ crystal structure with a small trace of a secondary phase. Mn$_2$FeGe was found to be ferrimagnetic (FIM) with saturation magnetization ($M_S$) values of ~1.7 µB/f.u. at ground state which is consistent with the value 2.0 µB/f.u. predicted by the Slater-Pauling rule. Substitution of Fe for Mn in bulk Mn$_{2-x}$Fe$_{1+x}$Ge resulted in a change of the magnetic ground state from FIM to ferromagnetic (FM) with a maximum $M_S$ value of 5.1 µB/f.u. for $x = 1.0$. A tunable Curie temperature ($T_C$) in a wide range of about 200 K, including the near room temperature ones, was found in Mn$_{2-x}$Fe$_{1+x}$Ge which may be important for practical applications. Maximum magnetic entropy changes of -3.1 Jkg$^{-1}$K$^{-1}$ (at $\mu_0\Delta H = 5$ T) was found at room temperature with a refrigerant capacity of 325 Jkg$^{-1}$ for $x = 0.4$.

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Characterization of ferrimagnetic and spin wave resonance for frequency selective limiting of iron garnet epitaxial films

SCOOTER JOHNSON (Presenter), HANS HAUCKE, CLIFFORD M KROWNE, SANGHOON SHIN, SYED B QADRI, United States Naval Research Laboratory — High-frequency devices, such as frequency selective limiters utilize magnetic materials such as yttrium iron garnet (YIG). The requirement of low loss to enable low-power limiting requires the material to be of high-quality single crystal. Unfortunately, the low magneto-crystalline anisotropy in YIG requires a bias magnet to generate the necessary field and frequency conditions for spin wave generation at higher frequency operation. Alternatively, the bismuth-substituted rare earth iron garnet (Bi-RIG) (BiGdLu)$_3$(Fe$_{1-x}$Ga$_x$)$_5$O$_{12}$ [1] has been found to show low loss (FMR linewidth ~50 Oe) with high anisotropy field (~2300 Oe), thus possibly avoiding the need for external bias [2]. In this study, we characterize and compare the magnetic properties and power dependences of single-crystal YIG and Bi-RIG grown using liquid phase epitaxy using a vibrating sample magnetometer and a coplanar waveguide configuration to assess dc and microwave magnetic properties for potential use in microwave device integration.

H71.00306: Antiferromagnetic characteristics in Sr- and Ba-doped phenanthrene superconductors LEI GAO (Presenter), Beijing Computational Science Res Ctr, GUO-HUA ZHONG, Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, HAI-QING LIN, Beijing Computational Science Res Ctr — It’s very important to clarify the competition between magnetism and superconductivity in alkaline earth metals doped phenanthrene. To achieve this, we have recently studied the crystal structures of Mg-, Ca-, Sr- and Ba- doped phenanthrene and found the most stable ones, which have the lowest energy by first-principles calculations. The result shows that only the most stable Sr\textsubscript{1.5}phenanthrene and Ba\textsubscript{1.5}phenanthrene show the weak AFM behavior and the others are non-magnetic. The Sr and Ba atoms intercalate the intralayer region and stay close to benzene-ring. By calculating the different charge density we found that the most stable Sr\textsubscript{1.5}phenanthrene and Ba\textsubscript{1.5}phenanthrene structures have charge redistribution and C atoms have gained electrons obviously. From the spin-charge density, we see inequitable phenanthrene molecules have opposite spin polarizations. The density of states (DOS) of the two structures shows that spin-up and spin-down electrons have the unsymmetrical distribution. Combining these results we conclude that the spin polarization of electrons transferring from metal atoms to C-2p orbitals atoms causes the local AFM behavior. This indicates that superconducting Sr\textsubscript{1.5}phenanthrene and Ba\textsubscript{1.5}phenanthrene are near the AFM ground state.

H71.00307: Magnetism in the honeycomb layers of Na\textsubscript{2}Ni\textsubscript{2}TeO\textsubscript{6} with chiral layers of Na\textsuperscript{*} NATHAN EPISCOPO (Presenter), KINLEY WANGMO, University of Texas, El Paso, NARAYAN POUDEL, KRZYSZTOF GOFRYK, Idaho National Laboratory, PO-HAO CHANG, RAJENDRA ZOPE, University of Texas, El Paso, RYAN KLEIN, National Renewable Energy Laboratory, CRAIG BROWN, NCNR, NIST, THOMAS HEITMANN, MURR, HARIKRISHNAN S NAIR, University of Texas, El Paso — Low dimensional magnetic lattices offer the possibility of realizing flatbands in the magnon spectrum which can then lead to dissipation-less spin transport and associated magnon Hall effect. One could expect to find a magnon insulator, similar to a topological insulator. In the present work we present a rather less-studied honeycomb material Na\textsubscript{2}Ni\textsubscript{2}TeO\textsubscript{6} where our preliminary density functional theory calculations of magnetic structure shows departures from reported structures. Our samples of Na\textsubscript{2}Ni\textsubscript{2}TeO\textsubscript{6} confirmed hexagonal \textit{P}6\textsubscript{3}/mcm space group with refined lattice parameters, a=5.2023(1)Å and c=11.1552(8)Å. The bulk magnetism for the present sample is characterized using magnetic susceptibility and specific heat, both of which confirm a phase transition at 28 K. Application of 8 T magnetic field only slightly polarizes the transition. We obtain a Curie-Weiss temperature of -9.7(2)K and effective paramagnetic moment of 2.24(4)\textit{m}_B/\textit{Ni}. This matches well with the spin-only moment of Ni\textsuperscript{2+}. Elastic and inelastic neutron scattering experiments are currently underway and reveal a rather flat spin wave excitation at 5 meV. Combining neutron diffraction with the DFT results, we would arrive at an accurate estimation of the exchange constants for Na\textsubscript{2}Ni\textsubscript{2}TeO\textsubscript{6}.

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H71.00308: Magnetism of stacked multilayered graphene nanostructures in carbon microspheres

ARMEN KOCHARIAN (Presenter), ARAM MANUKYAN, HARUTYUN GYULASARYAN, Physics Department, Russian-Armenian (Slavonic) University, Yerevan, EDUARD SHAROYAN, Institute of Physical Research, NAS of Armenia, Laboratory of Solid State Physics, Ashtarak, PAUL OYALA, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, OSCAR BERNAL, LUIS VALENCIA, CAL State University, Los Angeles — Morphology, structure and magnetic properties of synthesized by pyrolysis (using as precursors metal free phthalocyanine and polyethylene) samples with different concentration of nitrogen in multilayered graphene nanostructures with zigzag edges in carbon microspheres was investigated by XRD, XPS, Raman, HRTEM microscopy, magnetometry, EPR measurements. Studied magnetic characteristics depend on temperature, magnetic field and concentration of nitrogen impurity centers. Prepared sample at Tpyr=700 K demonstrates strong paramagnetism, ferromagnetism and temperature-independent diamagnetism with susceptibility $\chi^{Dia}=-10^{-6}$ emu/gOe at T=300K. Saturation magnetization vs temperature behavior with maximum magnetization $M_s$ saturation at 20 K closely resembles a spin glass behavior. The itinerant ferromagnetism of $\pi$-electrons in narrow impurity bands is interpreted using temperature dependence of spin correlations at zigzag edges in nanographenes. A magnetic hysteresis is also observed under variation of temperature at 100<T<300 K where magnetization displays diamagnetic character.

*This work supported by Russian-Armenian (Slavonic) University from Grant #SCS15T-1C249. The work at CSULA supported by the NSF CREST Grant #HRD-1547723 and PREM programs under Grant DMR-1523588.

H71.00309: Screening and Design of Novel 2D Ferromagnetic Materials with High Curie Temperature above Room Temperature

ZHOU JIANG (Presenter), PENG WANG, XUE JIANG, JIJUN ZHAO, Physics, Dalian University of Technology — Two-dimensional (2D) intrinsic ferromagnets with high Curie temperature ($T_C$) are desirable for spintronic applications. Using systematic first-principles calculations, we investigate the electronic and magnetic properties of 22 monolayer 2D materials with layered bulk phases. From these candidates, we screen out five ferromagnetic monolayer materials belonging to three types of structures: type i (ScCl, YCl, LaCl), type ii (LaBr$_2$), and type iii (CrSBr). Type i is a kind of metallic ferromagnetic material, whereas LaBr$_2$ and CrSBr of type ii and iii are small-bandgap ferromagnetic semiconductors with $T_C$ near room temperature. Moreover, the ferromagnetic CrSBr monolayer possesses a large magnetic moment of $\sim 3 \mu_B$ per Cr atom, originating from its distorted octahedron coordination. The robust ferromagnetism of the CrSBr monolayer is ascribed to the halogen-mediated (Cr-Br-Cr) and chalcogen-mediated (Cr-S-Cr) superexchange interactions; then, an isoelectronic substitution strategy is proposed to tailor the magnetic coupling strength. Hence, monolayer structures of CrSI, CrSCI, and CrSeBr with notably enhanced Curie temperature up to 500 K as well as favorable formation energy are designed.

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H71.00310: Griffiths-like phase in a Mn-Intercalated Dichalcogenide  PAUL SHAND
(Presenter), PAUL WHITE, Physics, Univ of Northern Iowa, EMILIA MOROSAN, Physics, Rice University — Static and dynamic magnetic measurements have been performed on polycrystalline Mn$_{0.23}$TaS$_2$. The measurements indicate the presence of a Griffiths-like phase preceding the paramagnetic to ferromagnetic transition at 57 K. The transition temperature in the clean limit, i.e., for single-crystalline Mn$_{0.25}$TaS$_2$, is known to be 80 K. dc magnetization measurements on Mn$_{0.23}$TaS$_2$ indicate a magnetic field-dependent downturn in the inverse susceptibility as a function of temperature below 105 K, a key indicator of the existence of a Griffiths phase. The magnetization also exhibited power law behavior as a function of both temperature and field in this regime. The power-law exponent for $M(H)$ varied with temperature in the Griffiths regime until the critical region was approached. At this point, a modified Arrott plot was necessary to describe the data, giving critical exponents close to the theoretical values for 3D Heisenberg magnets. The second-order ac susceptibility exhibited frequency-dependent peaks in the Griffiths region, which strongly suggests the formation of ordered clusters. The dc magnetization also exhibited logarithmic time decay. The evidence points to a robust Griffiths phase in Mn$_{0.23}$TaS$_2$.

H71.00311: X-ray absorption and magnetic circular dichroism studies of spin-orbital magnetism in the three-dimensional Kitaev honeycomb γ-Li$_2$IrO$_3$  ANNA SOPER (Presenter), KEWEI ZHOU, NICHOLAS BREZNAY, Harvey Mudd College, DANIEL HASKEL, YONGSEONG CHOI, Argonne National Lab, PHILIP MOLL, Ecole polytechnique federale de Lausanne, ALEJANDRO RUIZ, University of California, San Diego, JAMES ANALYTIS, University of California, Berkeley — Transition metal oxides are an exiting platform for exploring novel states of quantum matter. The choice of transition metal and its crystalline structure determine the magnitude of spin orbit coupling and electronic correlations, parameters that can be carefully tuned to create Mott insulators, topological insulators, superconductors and spin liquids. The 5d transition metal oxide lithium iridate γ-Li$_2$IrO$_3$, a Mott insulator and Kitaev spin liquid candidate, displays particularly strong spin orbit coupling, several honeycomb crystal structures, and magnetic ground states that can be tuned with applied pressure and magnetic fields; however, there are still open questions about its electronic structure. X-ray absorption spectroscopy was used to probe the γ-Li$_2$IrO$_3$ valence states and measure spin orbit coupling and crystal field splitting energy scales. In addition, X-ray Magnetic Circular Dichroism measurements were used to extract the spin and orbital content of the iridium magnetic moment. Evidence from these experiments will help to build a more accurate picture of the electronic states driving magnetism in this material.
H71.00312: Deviation from nonmagnetic \( J = 0 \) state in a pentavalent columnar iridate

\( \text{Sr}_3\text{NaIrO}_6 \)

ABHISEK BANDYOPADHYAY (Presenter), SUGATA RAY, School of Materials Science, Indian Association for the Cultivation of Science — Strong spin-orbit coupling (SOC) leads to the exotic properties in otherwise banal pool of 'paramagnetic' heavy ion oxides. The 5\( d^4 \) iridates eventually stirred up a controversy about the origin of magnetism in them. A nonmagnetic \( J = 0 \) ground state should be realized ideally for a pentavalent \( d^4 \) iridate in the \( jj \) coupling limit, which has never been achieved in any of the reported \( d^4 \) Ir oxides to date. Briefly introducing the previously handled (by our group) such \( 5d^4 \) cases with different Ir environments, we here pay serious focus on \( \text{Sr}_3\text{NaIrO}_6 \), a 5\( dt_2g^4 \) columnar iridate having well separated \( \text{Ir}^{5+} \) centers, which is expected to have a singlet \( J = 0 \) ground state with no net magnetic moment under strong SOC. However, stabilization of such state at moderate SOC is exceptionally fragile to minute external perturbation and enhanced magnetic responses appear. Moreover, the magnetic interaction between these developed magnetic moments becomes another important point. We, in this work, using detailed magnetic and thermodynamic measurements, refute any chance of nonmagnetic ground state in \( \text{Sr}_3\text{NaIrO}_6 \) compound. Instead, our experimental observations reveal the existence of quantum spin-orbital liquid state down to 40 mK atleast with sufficiently large magnetic moments on individual \( \text{Ir}^{5+} \).

H71.00313: Quantum spin liquid state in three dimensional metal-organic frameworks

CHARUNI DISSANAYAKE (Presenter), K A M HASAN SIDDIQUEE, RIFFATH MUNIR, Physics, University of Central Florida, WESLEY NEWSOME, FERNANDO URIBE-ROMO, Chemistry, University of Central Florida, XINZHE HU, SWAPNIL YADAV, YASUMASA TAKANO, Physics, University of Florida, EUN SANG CHOI, Florida State University, YASUYUKI NAKAJIMA, Physics, University of Central Florida — Quantum spin liquid (QSL) is a massive superposition state of spins, or highly entangled quantum matter in which electrons’ spins fluctuate and remain liquid-like, even at absolute zero temperature. Thus, they preserve spin-rotational symmetry but inhibit long range magnetic-ordering [1]. This novel state of matter attracted much attention in recent years due to the possibility of hosting fractionalized excitations, artificial gauge fields and exotic forms of superconductivity [2]. Here we attempt to uncover the QSL character of the hyperhoneycomb metal-organic framework (MOF) of \([\text{(C}_2\text{H}_5)_3\text{NH}]_2\text{Cu}_2(\text{C}_2\text{O}_4)_3\). We reveal the absence of magnetic transition in high magnetic fields up to 35T and magnetic anisotropy via torque magnetometry. Further, we will discuss the exotic nature of the spin liquid ground state and unusual excitations evidenced by the thermodynamic studies performed on candidate QSL \([\text{(C}_2\text{H}_5)_3\text{NH}]_2\text{Cu}_2(\text{C}_2\text{O}_4)_3\) down to 1.8K.

H71.00314: Structural Determination of Frustrated Double Perovskites $\text{Ba}_2\text{EuMoO}_6$ and $\text{Ba}_2\text{PrMoO}_6$°  JEREMY CARLO (Presenter), NICHOLAS LA MANNA, Villanova Univ — Geometric magnetic frustration occurs when magnetic order is inhibited by the arrangement of magnetic ions. In some materials with antiferromagnetic interactions, the moments are arranged in such a way that only certain interactions can be satisfied at once, and are said to be magnetically frustrated.

Double perovskites of composition $A_2BB'O_6$, with 'rock-salt' order of magnetic B' ions, potentially exhibit frustration. Double perovskites are of particular interest due to their chemical versatility, enabling the synthesis of compounds with divergent chemical and magnetic properties, providing great potential to yield new insights into frustration physics.

We have studied the structure of two double perovskites, $\text{Ba}_2\text{EuMoO}_6$ and $\text{Ba}_2\text{PrMoO}_6$, using X-ray diffraction. After encountering difficulties evidenced by peak splitting, a sample of $\text{Ba}_2\text{YMoO}_6$ was synthesized in order to test and refine the synthesis process. The Pr sample showed evidence of structural distortion while the Eu shows promise for future refinement.

°JPC acknowledges the Research Corporation for Science Advancement for financial support (CCSA #23314). NL acknowledges the Niedbala Family Fellowship and the Villanova Center for Research and Fellowships (CRF) for financial support.

H71.00315: Design and Synthesis of Novel Quantum Magnets  ERIC SEEWALD (Presenter), Department of Physics and Department of Chemistry, Duke University, LALIT YADAV, SACHITH DISSANAYAKE, RABINDRANATH BAG, Department of Physics, Duke University, SARA HARAVIFARD, Department of Physics and Department of Mechanical Engineering & Materials Science, Duke University — Due to recent advances in the field of topological quantum spin liquids, there is an increasing demand for high quality single crystals of frustrated magnets that host such exotic behavior. Here we present our recent results of such efforts. Solid-state reactions are used to synthesize polycrystalline samples of quasi-2D and 3D frustrated quantum magnets, whose purity is confirmed by powder x-ray diffraction analysis. With a pure polycrystalline sample, the optical floating zone and chemical vapor transport techniques are used to produce high quality large single crystal samples. We use an array of thermal and magnetic measurements as well as single crystal x-ray diffraction to characterize the samples, before performing advanced neutron and synchrotron x-ray scattering experiments at national user facilities.
Longitudinal spin fluctuations in complex ordered states with a Landau-Ising model

HARRY KEEN (Presenter), ANDREAS HERMANN, Univ of Edinburgh — Classical local-moment models, like the Heisenberg and Ising models, are often used in combination with ab initio calculations to predict the magnetic properties of real materials. These can often perform poorly for metals, where fluctuations in the magnitude of the moment are important. Modelling longitudinal spin fluctuations phenomenologically: by allowing spin magnitudes to vary constrained by a Landau-like on-site potential, has been applied frequently by other authors and tends to improve agreement with experiment.

We study a simple model of scalar spins with such an on-site potential, where the energy scale of the fluctuations is characterised by a single parameter: the rigidity of the magnetic moment. We explore the implications of these fluctuations on collinear magnetic states with Monte Carlo simulations. This is particularly challenging for the Metropolis algorithm, so we discuss the numerical implementation of an alternative method, the Heat-bath algorithm. We study a variety of ordered states on a stacked triangular lattice, including frustrated and modulated phases. The influence of fluctuations on the nature of these phases is discussed in depth, and we uncover interesting behaviour which is sensitively dependent on the configuration of interaction parameters.

Sign reversal of anomalous Hall effect in polycrystalline ultrathin Mn$_3$Pt films

JOYNARAYAN MUKHERJEE (Presenter), SATYAKI SASMAL, KARTHIK RAMAN, TIFR Centre for Interdisciplinary Sciences — The kagome structure of noncolinear antiferromagnet (NC-AFM) gives rise to finite Berry curvature which consequences many novel phenomena such as anomalous Hall effect (AHE), magneto optical Kerr effect and topological Hall effect$^1$. Although AHE has been reported in epitaxial thin films of NC-AFM, Mn$_3$Pt$^2$, here we present the sign reversal of AHE in polycrystalline Mn$_3$Pt films varying the thickness of the film and measurement temperature. Polycrystalline Mn$_3$Pt films of thickness 5-25 nm have been grown on SiO$_2$ substrate using co-sputtering technique. X-ray diffraction reveals the phase purity of our samples. Electrical transport has been carried out in Hall bar geometry prepared by optical lithography and Ar ion etching. We observe negative Hall resistivity ($\rho_{\text{AH}}$) at 300 K which changes sign ~ 10 K. In addition to that, we also observe nearly linear positive magnetoresistance (MR) at high temperature regime (300 to 15 K). Similar to the $\rho_{\text{AH}}$, MR becomes negative at the same temperature. We attribute this sign reversal due to the rotation of Mn moments confirmed from the temperature dependent of magnetization data$^3$.


*DAE, India
H71.00318: Magnetic anisotropy in the rare-earth honeycomb lattice YbCl₃*  HUIBO CAO
(Presenter), ERXI FENG, Oak Ridge National Lab, JIE XING, University of California Los Angeles, YAN WU, YAOHUA LIU, Oak Ridge National Lab, EVE EMMANOUILIDOU, CHAOWEI HU, TIANCI SONG, NI NI, University of California Los Angeles — The Kitaev quantum spin liquid (KQSL) is an exact solvable exotic state with bond-directional interactions in a honeycomb lattice [1]. Its potential applications in quantum information field attract a lot of attention. So far only a few KQSL candidates are available, such as honeycomb lattices α-RuCl₃ and Na₂IrO₃ with strong spin-orbital coupling 4d (Ru) and 5d (Ir) elements [2-4]. All these lattices show the long-range zig-zag magnetic order at low temperature instead of KQSL states. Recently we found a new Kitaev candidate, the rare-earth honeycomb lattice YbCl₃ with an effective spin-1/2, which presents a short-range magnetic order around 1.2 K and another kink at 0.6 K [7]. We investigated the magnetic ground state and magnetic anisotropy of YbCl₃ using unpolarized/polarized neutron diffraction techniques, which will be the focus of the presentation.


*The research was supported by the U.S. DOE, Office of Science, Early Career Research Program Award KC0402010 and used the DOE User Facility operated by the ORNL.
H71.00319: Phase transitions in novel Li-containing honeycombs, Li$_8$Cr$_2$(Te/Sb)$_2$O$_{12}$

HECTOR MANDUJANO (Presenter), SANDRA GONZALEZ, University of Texas, El Paso, NARAYAN POUDEL, KRZYSZTOF GOFRYK, Idaho National Laboratory, STUART CALDER, Oak Ridge National Laboratory, HARIKRISHNAN S NAIR, University of Texas, El Paso — Honeycomb frameworks of Li$_8$M$_2$(Te/Sb)$_2$O$_{12}$ ($M$ = transition metal), present interesting magnetic phenomena related to frustrated two-dimensional lattices of spins. In the present work, polycrystalline Li$_8$Cr$_2$(Te/Sb)$_2$O$_{12}$ were synthesized by standard solid-state route. Powder X ray diffraction patterns were recorded to check the phase formation and purity. C$_2$/m space group was confirmed using Rietveld analysis and lattice parameters are determined to be $a$=5.141Å, $b$=8.884Å, $c$=5.143Å, $\beta$=109.5Å for Li$_8$Cr$_2$Sb$_2$O$_{12}$, and $a$=5.128Å, $b$=8.850 Å, $c$=5.151Å, $\beta$=109.8Å for Li$_8$Cr$_2$Te$_2$O$_{12}$, presenting diminished unit cell sizes compared to that of Li$_8$Co$_2$Te$_2$O$_{12}$ are $a$=5.226Å, $b$=8.892Å, $c$=5.160Å, $\beta$=110.9Å. In the case of Li$_8$Cr$_2$Sb$_2$O$_{12}$ a magnetic phase transition is present at 7.4 K as determined from the derivative, $dCp/dT$. A similar transition is found in Li$_8$Co$_2$Te$_2$O$_{12}$ at 9.5 K. Neutron diffraction is underway for comprehending cationic ordering, crystal, and magnetic structure of Li$_8$Cr$_2$(Te/Sb)$_2$O$_{12}$ as well as its mixed occupancy of the 4g Wyckoff position in the C$_2$/m space group. Our experimental results will highlight the magnetism of the honeycomb layers of Cr and the ionic diffusion of inter-layer Lithium and will be of interest to magnetism as well as battery research.

*University of Texas at El Paso
The compound Cu$_9$O$_2$(SeO$_3$)$_4$Cl$_6$ is a new multiferroic material. Comprehensive studies on single and polycrystalline samples have revealed an anomaly at $T_N = 37$ K associated with long-range antiferromagnetic order. However, no signature of this phase transition is observed with the $H || b$-axis, indicating anisotropic magnetic properties. The magnetic structure derived from neutron scattering shows half of the Cu(5) ions carrying no moments. An anomaly in the dielectric constant near $T_E = 267$ K is identified with no measurable spontaneous polarization below $T_E$, suggesting an antiferroelectric order. A step-like anomaly seen in $c(T)$ at $T_E$ hints at weak spin-lattice coupling. High-resolution synchrotron x-ray diffraction experiments elucidate a local structural distortion at $T_E$.

H71.00321: Characterization of GaTa₄Se₈ single crystal with Jeff=3/2 ground state magnetic molecular*  
CHOONGJAE WON, Center for Complex Phase Materials, Max Planck POSTECH/Korea Research Initiative, SEUNGHWAN DO (Presenter), Oak Ridge National Lab, JAE-YOU KIM, JAE-HOON PARK, Pohang University of Science and Technology, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University — The geometrical spin frustration in the tetramer of lacunar spinel is a good subject for exploring the quantum spin liquid. In tantalum lacunar spinel, GaTa₄Se₈, there are molecular $J_{\text{eff}} = 3/2$ ground state and curious non-magnetic state with Jahn-Teller distortion [1]. Recently, we successfully grown the high quality of GaTa₄Se₈ single crystal, and studied by characterization of physical properties and inelastic neutron scattering. Temperature dependence of those characterization shows the difference between structure transition with orbital ordering, and indicates that gapped excitation already exists at higher temperature than orbital ordering temperature $T_S \sim 53 \text{K}$.


*This work was supported by the National Research Foundation of Korea(NRF) funded by the Ministry of Science and ICT(No. 2016K1A4A4A01922028)

H71.00322: First-principles study of the Ir-Ir dimerization effect on the magnetic phase diagram of honeycomb iridates  
KEVIN LUCHT (Presenter), Univ of Illinois - Chicago — Honeycomb lattice iridates have been a promising candidate for the realization of the Kitaev spin model. However, the addition of off-diagonal and Heisenberg interactions result in magnetic ordering at low temperatures, causing the quantum spin liquid (QSL) phase to remain elusive. The application of hydrostatic pressure to the system has shown the loss of magnetic ordering, and although indicative of a spin liquid phase, has been shown to be caused by dimerization between iridium ions. Using ab initio calculations, we intend to identify the pressure region in beta-Li₂IrO₃ and alpha-Na₂IrO₃ where the symmetry lowers in the systems, marking the onset of dimerization. Subsequently, using exact diagonalization (ED) and cluster mean field theory (CMFT) on a periodic cluster, we will identify the ground state of the dimerized system and explore its phase diagram and spin correlations.
H71.00323: Crystal structure and magnetic behavior of NdAlGe.* CHETAN DHITAL (Presenter), Kennesaw State Univ, RAMAKANTA CHAPAI, SUNIL KARNA, QIANG ZHANG, Physics, Louisiana State University, YAN WU, Oak Ridge National Laboratory, RONGYING JIN, Physics, Louisiana State University, HUIBO CAO, Oak Ridge National Laboratory, DAVID P YOUNG, JOHN DITUSA, Physics, Louisiana State University — Rare earth compounds are known to exhibit varieties of exciting electronic and magnetic properties arising from complex interplay of conducting charges, usually derived from s- or p-like bands and more localized f-electrons. Added variety of interesting states comes from differences in lattice symmetry, spin-orbit interactions, crystalline electric fields, and the related magneto-crystalline anisotropy. A recent addition to such exciting properties is the theoretical prediction and experimental verification magnetic Weyl fermion state in RAlGe (R=Rare earth) family of compounds. Previous investigations of this class of compounds were limited to R=La, Ce and Pr. In this work, we extend this line of inquiry to isostructural NdAlGe to explore how these electronic and magnetic properties vary as the size of the rare earth element and consequently the position of the f-electron states with respect to the Fermi level is varied. I will present the crystal structure and magnetic behavior of NdAlGe.

*U.S. Department of Energy under EPSCoR Grant No. DE-SC0012432, Kennesaw State University, High Flux Isotope Reactor, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

H71.00324: Raman Spectroscopy of layered magnetic systems MAINAK PALIT (Presenter), ANUDEEPA GHOSH, SUBHADEEP DATTA, Indian Association for the Cultivation of Science — Metal phosphorus trichalcogenides (MPX₃) have emerged as an exciting class of layered magnetic 2D materials for future spintronics. Retaining long range magnetic ordering even in the exfoliated few layers is the hallmark of 2D magnetism. Raman spectroscopy can be an effective probe to identify low-energy phonon modes and possible spin-phonon coupling in reduced dimension from bulk crystal. In this study, temperature dependent Raman Spectra of exfoliated iron phosphorous trichalcogenides (FePS₃) flakes reveal a distinct shift of the large wave number phonon peaks towards higher wavenumber as temperature decreases. A clear deviation from standard anharmonic behavior below characteristic Néel temperature (T_N) is also observed. Other low wave number symmetry modes exhibit temperature dependent non-anharmonic self-energy as a function of layer thickness below T_N, related to the strong spin-lattice interaction due to short-range magnetic order. Energies and symmetries of the observed Raman-active modes are in agreement with DFT calculations. Below T_N low wave number broad mode in the paramagnetic state(T>T_N) splits into multiple distinct modes and evolve further into a possible magnon mode. We believe these results will pave way for possible spintronic applications exploiting magnons.
H71.00325: Quantum magnetization reversal studied in S/F/S Josephson $\phi_0$ junction

GWANG-HEE KIM (Presenter), Sejong Univ — We study quantum tunneling of magnetization in the presence of the bias current and the magnetic field along the general direction in the Josephson $\phi_0$ junction. With account taken of the influence of the superconductivity on the ferromagnet in the kelvin or subkelvin range, we present the analytic formulas of the tunneling rate in the uniaxial and nonuniaxial symmetries, and find that the tunneling exponents depend on three parameters related to the current and the magnetic field. We demonstrate that the current is equivalent to the effect of the magnetic field along the easy axis and the tunneling rate can be shifted by the bias current in the presence of such an external magnetic field. These features are expected to be observable with existing experimental techniques.

H71.00326: Slowed relaxation of the magnetism through dilution into paramagnetic mediums

IAN MOSELEY (Presenter), JOSEPH ZADROZNY, Colorado State University — Single molecule magnets (SMMs) represent the smallest magnetic domains (a single molecule) and as such have potential applications in information storage, quantum computing, and spintronics. Extending the lifetime of the magnetic relaxation is critical to applications of these molecules. Dilution of SMMs is a common strategy employed to extend magnetic relaxation and is typically carried out by dilution into a solvent or cocrystallization with an isostructural diamagnetic species. Herein, we report the first known example of extended magnetic relaxation through dilution into a paramagnetic medium. Using the canonical SMM $[\text{PPh}_4]^2(\text{Co(SPh})_4)$, dilutions into the isostructural paramagnets $[\text{PPh}_4]^2(\text{M(SPh})_4)$ (where $M = \text{Ni, Fe, and Mn}$) were made by cocrystallization. We show that across a range of concentrations, both Fe and Ni perform like the diamagnetic Zn congener, whereas the Mn dilution results in an accelerated relaxation. Dipolar interactions between spin centers are considered and we hypothesize that the observed relaxation enhancement can be attributed to low temperature magnetism of the paramagnetic diluents.

*Magnetization experiments were performed at the CSU Central Instrument Facility, which is supported by an NIH-SIG award (1S10OD021814-01) and the CSU-CORES Program.
H71.00327: Charge Transfer in Single-Molecule Magnetic Complexes

[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CR})_{16}(\text{H}_2\text{O})_4]^* 

DMITRY SKACHKOV, JIA CHEN, GEORGE CHRISTOU, XIAOGUANG ZHANG, SAMUEL TRICKEY, HAI-PING CHENG (Presenter), University of Florida — Single-molecule magnetic (SMM) complexes [\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CR})_{16}(\text{H}_2\text{O})_4], with R=-H, -\text{CH}_3, -\text{CHCl}_2, -\text{C}_6\text{H}_5, have twelve Mn atoms in the core, eight of them are in 3+ charge state and located at peripheral ring of the molecule, while the four remaining Mn atoms in the center of the molecule are in 4+ charge state. When the SMM molecule is receiving the additional electron by excitation, this electron is localizing on one of the peripheral Mn atom, and the charge state of this atom is changing from Mn$^{3+}$ to Mn$^{2+}$, what is confirmed by experiment measuring the Mn-O bond lengths [Inorg. Chem. 2017, 56, 10706]. In order to develop the SMM with high catalytic activity, it is very important to know the energy barrier for electron transfer from Mn$^{2+}$ atom to another Mn$^{3+}$ atom located on diametral site of the molecule, in order to stimulate oxidation reaction. We calculated the minimum energy pathway for electron transfer in tunneling regime calculating the energy barrier for electron motion by plotting the profile of electrostatic potential along possible pathways. In the talk we will discuss the pathways for electron transfer in SMM for different ligands.

*US Department of Energy Basic Energy Sciences Energy Frontier Research Centers under Grant No. DE-SC0019330

H71.00328: WITHDRAWN ABSTRACT —

H71.00329: Electron Spin Resonance of Heisenberg Spin Chains of Four Ti Atoms

SOO-HYON PHARK (Presenter), Center for Quantum Nanoscience, Institute for Basic Science, KAI YANG, IBM Almaden Research Center, TANER ESAT, ANDREAS HEINRICH, Center for Quantum Nanoscience, Institute for Basic Science, CHRISTOPHER LUTZ, IBM Almaden Research Center — Heisenberg spin chain (HSC) is a one-dimensional circular array of spins, where the nearest neighbors are exchange-coupled. Quantum transitions between the energy eigenstates of such spin chains are well understood by the creation and annihilation of spin wave quanta. Using a low temperature (1.1K) scanning tunneling microscope (STM), we composed two circular spin chains of four hydrogenated Ti atoms, spin-$1/2$ atomic species, on MgO surface by atom manipulation techniques. The nearest neighbor couplings are antiferromagnetic and tuned to be 6 and 25 GHz by interatomic distance control. We performed electron spin resonance (ESR) combined with the STM on the spin chains. The measured ESR spectra show a remarkable consistency with the quantum transition probabilities calculated from the Heisenberg spin Hamiltonian, which identifies the energy eigenstates of the spin chains. We discuss the experimental data by employing the spin wave theories. This work suggests that our Ti spin chains deserve an ideal exchange-coupled quantum spin system. In addition, this work demonstrates an experimental approach plausible to creation and control of quantum phenomena in artificial spin structures.
H71.00330: Thermal spin-transfer torque driven by Chirality Induced Spin Selectivity effect in layered chiral hybrid perovskite*  KYUNGHOON KIM, ERIC VETTER, North Carolina State University, LIANG YAN, WEI YOU, University of North Carolina at Chapel Hill, DALI SUN, JUN LIU (Presenter), North Carolina State University — Thermal spin-transfer torque (STT), the transfer of the spin current mediated by heat current, provides a new way to control the orientation of nanomagnets. The recent discovery of the Chiral-Induced Spin Selectivity (CISS) effect offers an opportunity to create spin current in chiral materials without the need of ferromagnet elements, e.g., chiral (left- or right-handed) molecules. In the presence of electron transport mediated by heat current, the chiral materials would produce a spin current via CISS effect, of which the spin polarization determined by handedness of the material. Here we study the CISS effect in solution-processed, 2D-layered, hybrid perovskite materials incorporating chiral molecule ligands, sensed by the thermal STT signal using ultrafast Time-Resolved Magneto-Optical Kerr Effect (TR-MOKE) technique. The chirality-dependent precession of the magnetization in the ferromagnet layer on top of layered chiral hybrid perovskites were observed which is attributed to the CISS effect. Our work opens a new route for the use of layered chiral hybrid perovskite materials for novel STT devices. K.K., E.V., and L.Y. contributed to this work equally.

*We acknowledge funding from NC State-Nagoya Research Collaboration grant and the NSF award 1933324 and 1933297.

H71.00331: Electronic structure and magnetism of monolayer Janus transition metal dihalides*  CHASE HANSON (Presenter), ANTIA S. BOTANA, Arizona State Univ — Based on first-principles calculations, the evolution of the electronic and magnetic properties of transition metal Janus dihalides MXY (M= V, Mn, Fe, Co, Ni; X, Y = Cl, Br, I) is analyzed at the monolayer limit. A variety of magnetic ground states is obtained as a result of the competition between direct exchange and superexchange. We show how structural symmetry-breaking plays a crucial role in the magnetic and electronic properties of 2D magnetic materials.

*NASA Space Grant
H71.00332: Spinon-magnon interaction in an antiferromagnet with alternating antiferromagnetic and ferromagnetic quantum spin chains  
HEDA ZHANG (Presenter), Michigan State Univ, ZHIYING ZHAO, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Science, VASILE O GARLEA, TAO HONG, Oak Ridge National Lab, Neutron Scattering Division, DOMINIQUE M GAUTREAU, AMARTYAJYOTI SAHA, University of Minnesota, Department of Chemical Engineering and Materials Science, S D MAHANTI, Michigan State Univ, TURAN BIROL, University of Minnesota, Department of Chemical Engineering and Materials Science, XIANGLIN KE, Michigan State Univ

— The concepts of quasiparticles and collective modes have been successfully applied to describe low-energy excitations in physics. In conventional magnets low-energy excitations are carried by spin waves, represented by massless bosons called magnons with $S = 1$. However, in one-dimensional antiferromagnetic quantum spin ($S = 1/2$) systems, quantum fluctuations destroy LRO in the ground state and magnons do not exist. Instead, the low-energy excitations are known as spinons, with $S = 1/2$. Although both magnons and two-spinon continuum have been observed in several quasi-one-dimensional antiferromagnets, magnons and spinons do not coexist in the same energy range. Here, we report the observation of coexistence of magnon and spinon excitations in Cu$_2$(OH)$_3$Br, a quantum antiferromagnet consisting of nearly decoupled, alternating ferromagnetic and antiferromagnetic $S=1/2$ chains. Importantly, the excitation spectra of both the magnetic chains emerge in close energy range and cross over each other, enabling strong spinon-magnon interaction.

H71.00333: Synthesis of Amorphous Soft Magnet using the IR image furnace  
DEOK YOUNG LEE (Presenter), Agency for Defense Development, DAEHWAN PARK, JUN HAN LEE, YOON SEOK OH, Department of Physics, Ulsan National Institute of Science and Technology — Study of soft magnets has been an important research topic because of their various applications such as transformers, magnetic shielding, transducers, and large variety of apparatus. Amorphous soft magnets are conventionally synthesized by using melt-spinning method, in which molten metal is cast onto a fast-rotating copper wheel and could be cooled down with $10^5$-$10^6$ K/sec to form highly amorphous state. However, constitutionally, the melt-spinning method yields potential contamination from the copper wheel. An improved synthesis method is required to get highly pure and ultimate soft magnet. In order to avoid the potential copper contamination, we have synthesized soft magnet using the IR image furnace. The IR image furnace focuses high-power infrared light from two or four lamps in the middle of two ceramic rods with two or four mirrors and develops floating molten zone, where provides a crucible free environment. By control of lamp power, travelling speed, rotation speed of rods, and gas conditions, the amorphous alloy could be synthesized without copper contamination. Here we present morphology, chemical, and magnetic properties of amorphous soft magnet synthesized by the IR image furnace.
Synthesis and structural and magnetic properties of Sr$_{1-y}$Pr$_y$Fe$_{12-x}$Co$_x$O$_{19}$ nanocomposites prepared via auto combustion technique  

MRIDUL BHATTARAI (Presenter), JIBA NATH DAHAL, Department of Physics, Truman State University — Sr$_{1-y}$Pr$_y$Fe$_{12-x}$Co$_x$O$_{19}$ (x = 0.0 - 1.5 and y = 0.1 - 0.3) polycrystalline samples were prepared via auto combustion method and analyzed with respect to their structural and magnetic characteristics. The possibility of simultaneous substitution of Fe$^{3+}$ by Co$^{2+}$ was verified for low substitution degrees. At higher substitution of Co$^{2+}$, a secondary soft magnetic phase CoFe$_2$O$_4$ is observed. The room temperature magnetic parameters derived from hysteresis loops showed that the saturation magnetization of Sr$_{1-y}$Pr$_y$Fe$_{12-x}$Co$_x$O$_{19}$ increased with the increase in cobalt content, and a concomitant reduction in coercivity values is controlled by substituting Pr$^{3+}$ for Sr$^{2+}$. Mr value increases with increasing Co$^{2+}$ content indicating the presence of an exchange coupling between magnetic hard and soft phases of the composite. The highest magnetization 61.17emu/g and coercivity Hc 3.98 kOe is observed in y = 0.1, x = 1 content. The coercivity observed is about 11% higher than pure SrFe$_{12}$O$_{19}$. Therefore, the substitution of Pr$^{3+}$ and Co$^{2+}$ in SrFe$_{12}$O$_{19}$ can bring magnetization and coercivity enhancement, which is useful for the high-temperature magnetic application.

Permanent magnet properties of Fe$_5$C$_2$ from first principles*  
LI YIN (Presenter), DAVID PARKER, Oak Ridge National Lab — Iron carbides, such as Fe$_3$C, Fe$_2$C and the Hagg carbide Fe$_5$C$_2$ are commonly produced in steel-making and in fact often play an important role in strengthening such steel. Here we study the permanent magnet properties of Fe$_5$C$_2$ from first principles, focusing on the magnetization and magnetic anisotropy – two indispensable components of a permanent magnet material. We find a substantial magnetization exceeding 1.5 T, along with a significant magnetic anisotropy exceeding 1 MJ/m$^3$ (here defined as the energetic difference between the magnetically easiest and hardest directions). While the anisotropy for an intermediate direction is much smaller, likely precluding the use of Fe$_5$C$_2$ for permanent magnet applications, the 1 MJ/m$^3$ anisotropy value is rather significant for a material containing only relatively light elements such as Fe and C. It is in fact more than half again as large as the value for hcp Co. We discuss the implications of these results for permanent magnet applications.

*This research was supported by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.
**H71.00336: Detection of magnetic domain wall of YIG with scanning diamond NV center probe**

YUTA KAINUMA (Presenter), RUI WANG, KUNITAKA HAYASHI, KENICHI NAKASHITA, TOSHU AN, School of Materials science, Japan Advanced Institute of Science and Technology (JAIST) — Probing and imaging of the magnetic domain structure at the nanoscale are important to understand the basic physics of the magnetic interaction, and for the application in the spintronics field. The nitrogen-vacancy (NV) center; spin state of a defect structure in diamond, is attracting much attention for its novel spin sensing ability at nanoscale and room temperature conditions. We developed a scanning NV center spin sensing probe combined with atomic force microscopy (AFM) based on quartz tuning-fork resonator. Electron spin resonance (ESR) signal from the apex of the NV center probe can be detected optically (optically detected magnetic resonance, ODMR) via confocal microscope setup. A diamond probe (φ 4 µm, length 10 µm) hosting an ensemble of NV centers is glued at the end of the AFM probe enabling simultaneous measurements of the ESR and topographic images of the sample. Magnetic insulator of yttrium iron garnet (YIG) was used for the magnetic film sample that shows magnetic domain wall structures with a micrometer scale under zero external magnetic field. The stray magnetic field from magnetic domain walls was measured with the scanning NV center probe.

**H71.00337: A Low-Cost Vibrating Sample Magnetometry Based on Audio Components**

BABU SANKHI (Presenter), EMRAH TURGUT, Oklahoma State University-Stillwater — Measurement of magnetization is an important characterization step for magnetic materials to understand their fundamental properties and to utilize in industrial applications[1]. In this project, we construct a cheap and versatile vibration sample magnetometer (VSM) using the sound card. We tested our VSM for the hysteresis loops of three distinct magnetic samples: bulk Nickel piece, perm-alloy thin film with an easy- plane anisotropy, and Co/Pt multilayer with perpendicular magnetic anisotropy. The magnetizations of corresponding loops are analyzed at different frequencies and, the noises are also measured and compared for two methods. Although sound card performance is not very good for the frequencies below 20 Hz due to the cut-off frequency, its sensitivity is approximately 7 times better than that of lock-in amplifier at higher frequencies up to 60 Hz. The measured sensitivity of our sound card based VSM is of the order of emu, which is better than the sensitivities obtained in the previous similar experiments [2] at room temperature.

H71.00338: Resolution Increase and Faster Phase Identification for Electron Magnetic Imaging  MD MAZHARUL ISLAM (Presenter), EMRAH TURGUT, NATHANIEL BERRY, Oklahoma State University-Stillwater — A detailed imaging of magnetic skyrmion arrangement allows us to understand the interactions in them and their dynamics, which can pave the way to the low power spintronics device [1]. Lorentz Transmission Electron Microscopy is an effective way for imaging the internal magnetic properties of a material [2]. The phase shift of the electron beam has a relationship with the magnetization distribution of the nanostructure that is based on Aharonov-Bohm Effect. Here, we are using several methods to get the electron phase shift caused by the complex magnetization distribution. We then reconstructed the magnetization using a model based iterative algorithm [3]. For getting an accurate magnetization distribution, cost function minimization analysis was done. We then compared the accuracy of the reconstructed magnetization from the electron phase shift from different forward process. Here, our methods reduce the artifacts that are usually seen in magnetization reconstruction process.


H71.00339: Emerging Widefield Magnetic Microscopy Applications with Nitrogen-Vacancy centers in Diamond  PAULI KEHAYIAS (Presenter), TZU-MING LU, ANDREW M MOUCHE, Sandia National Laboratories — We will discuss using magnetically-sensitive nitrogen-vacancy (NV) color centers in diamond for widefield magnetic microscopy, a technique which offers sub-micron spatial resolution, high magnetic moment sensitivity, and parallel magnetic readout in ambient conditions. NV magnetic imaging is being used to study superconductivity, current flow in 2D materials, magnetic domain structures, and other condensed-matter physics applications. With the objective of exploiting the NV magnetic imaging advantages in a wider array of scientific problems, we will report on our recent progress using NV imaging for applications relating to synthetic micromagnets, magnetic materials, hardware security, and electronics fabrication.

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H71.00340: Tabletop EUV magnetic linear dichroism spectroscopy on thin-film antiferromagnetic chromium across the 3p absorption edge  PETER JOHNSEN, CHRISTIAN GENTRY, SINEAD RYAN (Presenter), MARGARET MURNANE, HENRY KAPTEYN, Department of Physics and JILA, University of Colorado, Boulder — We present the magnetic linear dichroism (MLD) reflection spectra measured on antiferromagnetic Chromium by use of a tabletop high harmonic generation (HHG) source across the 3p absorption edge. The spectra were obtained by rotating the field-cooled direction of the magnetization 90 degrees relative to the incident polarization angle. Furthermore, we investigate the effect as a function of both film thickness and angle of incidence.
**H71.00341: Tunneling Magneto Resistor Nano-columns**

DEREJE SEIFU (Presenter), Morgan State Univ — Nanowires inside carbon nanotubes (CNTs), nano-columns, and thin films of ferromagnet/insulator/ferromagnet (FM/I/FM) tunneling magnetoresistance (TMR) were synthesized using magnetron DC/RF sputtering [1]. Nanowires were synthesized inside CNTs using glancing angle deposition. The magnetic properties of nanowires, nano-columns and planar nano-metric thin films of FM/I/FM showed similarities including two-fold magnetic symmetry. Nanowires of Fe/MgO/Fe showed enhanced magnetic properties in particular a high increase in coercive field, 754% higher compared to planar thin films of Fe/MgO/Fe [1]. This could be due to shape anisotropy in nanowires, which play an important role in coherence. TMR of nano-columns and nano-metric thin films of FM/topological/FM are other examples studied. TMR is a macroscopic phenomenon that can only be explained by quantum mechanics, where electrical resistance varies when an external magnetic field is applied parallel to the tri-layer system.


*The corresponding author D.S acknowledges the support of ARL-W911NF-19-2-0222.

**H71.00342: Magneto Restrictive Sensor**

DEREJE SEIFU (Presenter), Morgan State Univ, ASHA J HALL, VTD, ARL — Magneto restrictive based sensors can be used for diagnosis and prognosis of cracks and creep in vital parts of several mechanical systems. One material studied extensively for this application is Tb$_{0.3}$Dy$_{0.7}$Fe$_2$ (TFD). We studied the structural and magnetic properties of micro-particles of TFD embedded inside reinforced carbon fiber polymer (RCFP) using VSM, TMM and MFM. Results show enhanced magnetic properties for TFM when embedded inside RCFP and a two-fold magnetic symmetry. To get a deeper understanding of the structural and magnetic properties of TFD, thin films were synthesized using magnetron DC/RF sputtering. Study of surface magnetism of films processed at a substrate temperature of 250 °C using MOKE revealed a four-fold magnetism. Results from magnetic and structural measurements will be presented.

**H71.00343: Structural, interface, and device properties of some Bi2Se3-based spintronic heterostructures.**

YUB RAJ SAPKOTA (Presenter), DUSTON WETZEL, DIPANJAN MAZUMDAR, Physics, Southern Illinois University Carbondale — Incorporating Topological Insulators in spintronic heterostructures and devices have gained interest due to several recent observations of greater spin-orbit torque compared to heavy metals. However, strong tunnel magnetoresistance (TMR) behavior has not been established with TIs compared to standard spintronics interfaces such as CoFeB-MgO. In this work, we have systematically investigated the structural, interface properties of prototypical a TI material (Bi2Se3) with normal Ferromagnets such as Co. Bilayer (Bi2Se3/Co) and TMR heterostructures (Co/Bi2Se3/Co) was fabricated using magnetron sputtering and their structure and interface investigated using X-ray diffraction and X-ray reflectivity method. Systematic thickness and substrate dependence studies with different growth and post-deposition annealing conditions have been carried out. We show that a sharp Bi2Se3/Co interface is possible, but annealing may lead to significant interdiffusion. Shadow mask techniques were incorporated to define micron-sized TMR devices. Detailed transport and magnetotransport and current-voltage characteristics will be discussed.

*NSF CAREER grant (ECCS: Award#1846829)

**H71.00344: Magnetic and Electronic Materials towards Realization of a FET based on Spin-Orbit Torques**

PHILLIP DANG (Presenter), ZEXUAN ZHANG, JOSEPH CASAMENTO, XIANG LI, JASHAN SINGHAL, DARRELL SCHLOM, DANIEL RALPH, HUILI XING, DEBDEEP JENA, Cornell University — The spin-orbit torque field effect transistor (SOTFET) is a recently proposed device that combines the spin-orbit-torque mechanism for writing magnetic memories with semiconductor transistors that are ubiquitous in logic. The SOTFET utilizes a magnetoelectric multiferroic to couple a SOT-controlled ferromagnet to the semiconducting channel. Therefore, this magnetic device may access the orders-of-magnitude on/off ratio of transistors, giving it the potential to combine memory and logic. It's realization, however, relies on the delicate interplay between topological insulating, ferro/ferrimagnetic, multiferroic, and semiconducting materials. In this talk, we discuss the material parameters and candidates that show promise for integration into a SOTFET and give an overview of the material advances towards realizing the device.

*The research was partially supported by the National Science Foundation under Grant Nos. E2CDA 1740286 and NewLAW EFRI 1741694 and partially supported by the Semiconductor Research Corporation as nCORE task 2758. P.D.’s support by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1650441 is acknowledged.
**H71.00345: Large Unidirectional Magnetoresistance in Topological Insulator/Ferromagnet Bilayers**

DUSTON WETZEL (Presenter), YUB RAJ SAPKOTA, DIPANJAN MAZUMDAR, Physics, Southern Illinois University Carbondale —

Strong spin-orbit coupling in topological insulators (TI) is expected to induce strong spin-orbit torque on proximal magnetic moments. This has motivated significant recent interest in topological insulator/ferromagnet (TI/FM) systems, with potential applications in spintronic memory and sensor technologies. We have thus carried out magnetotransport measurements on Bi$_2$Se$_3$/Co bilayers. Using standard four-probe methods, low-field, in-plane longitudinal and transverse (planar Hall) magnetoresistance (MR) has been measured, at room temperature, as well as angular-dependent MR at various field strengths. When current is passed predominantly through the Co layer, we observe typical AMR behavior. However, by promoting higher current near the TI/FM interface (verified by a two probe resistance value between that of Co and Bi$_2$Se$_3$), we observe unidirectional magnetoresistance orders of magnitude higher than Co alone, as well as an unusual cos(φ) angular dependence. The effects of current, sample angle, and sample thickness, along with comparison with standard Co/heavy metal systems will be discussed.

*NSF CAREER grant (ECCS: Award#1846829)

**H71.00346: Fabrication and characterization of CuO-doped Ni-Co-Zn ferrite composites for RF applications.**

POONAM LATHIYA (Presenter), JING WANG, Univ of South Florida — With the recent advancements related to imminent rollout of 5G and IoT technologies, there is a growing demand for soft magnetic materials for different applications such as antennas, circulators, inductors, interference suppressors and wireless power transfer etc. Ni-Co-Zn ferrites exhibit excellent soft magnetic properties such as high resistivity, high permeability and low magnetic loss for RF applications. To meet the performance specifications for aforementioned applications, Ni-Co-Zn sheets with a high permeability and low magnetic loss is desired. In this work, we present a novel method to prepare thin Ni-Co-Zn ferrite sheets with high permeability and low magnetic loss for RF antenna applications. Ni-Co-Zn ferrite powders were prepared by solid state synthesis. Different CuO wt% were doped in Ni-Co-Zn samples. Toroidal samples made from powders under different level of hydraulic force were sintered in air. Enhancement in the resonance frequency was achieved by doping of copper oxide (0 to 10 wt%) in Ni-Co-Zn ferrite. The permeability decreases from 7 (0 wt%) to 5.3 (10 wt%) along with increase in resonance frequency from 300 to 530 MHz. Magnetic loss of 0.04 achieved at 530 MHz frequency. Ni-Co-Zn sheets were prepared with same optimized conditions for RF antennas.
H71.00347: Effect of Demagnetization Method on Remnance Magnetization States in Metallic Ferromagnets  JENNIFER FREEDBERG (Presenter), E. DAN DAHLBERG, University of Minnesota — Parametric plots of the remagnetization versus demagnetization remnances, commonly called Henkel plots, were constructed for four metallic ferromagnets. These were compared to Wohlfarth's simple model for noninteracting particles [1]. Three different paths to a net zero magnetization state (AC and two types of DC demagnetization) were explored for all the samples and in addition two of the samples were thermally demagnetized. These results present a useful comparison between metallic and particulate ferromagnetic systems, and how fundamental differences in their magnetization processes affect subsequent measurements. While adherence of our data to Wohlfarth's model was poor for several paths to zero magnetization, many similarities between our data and models including magnetic interactions were found [2, 3].


*This work was funded by NSF grant DMR 1609782

H71.00348: Classical mechanism for the anomalous enhancement of Hall resistivity during magnetization reversal  CHRISTOPHER ARD (Presenter), HUA CHEN, OLIVIER PINAUD, Colorado State University — Certain bulk or synthetic ferromagnetic conductors with broken inversion symmetry show a characteristic hump in the hysteresis curve of the Hall resistivity, which is commonly ascribed to the topological Hall effect due to the formation of skyrmion lattice in finite fields. Here we argue that the hump could also be due to classical mechanisms associated with transport in random media. By modeling a 2D inhomogeneous ferromagnetic conductor using a random resistor network model, we are able to show that an anomalous enhancement of the Hall resistivity can arise before the ferromagnet is fully switched by a perpendicular magnetic field. The qualitative behavior is further analyzed by solving the diffusion equation with correlated disorder perturbatively.
H71.00349: Ferromagnetic Resonance Studies of MnZn Ferrites/Polymer Composite Materials. PAUL COUTURE (Presenter), ROBERT CAMLEY, KAREN LIVESEY, ZBIGNIEW J CELINSKI, University of Colorado, Colorado Springs — We characterize MnZn ferrite particles embedded in a polymer for use in low frequency EMF emissions shielding. The ferrites particles are approximately 1.2 µm in diameter and embedded in PVC resin in various concentrations: 10% - 70% by weight. The composite undergoes an extrusion process which creates a 0.6 mm thick slab and orders some of the particles along the extrusion direction. This creates an easy axis along the extrusion direction with an associated anisotropy. We characterized the ferromagnetic resonance absorption peaks with broad-band FMR, 1-30 GHz, and cavity based FMR systems. Comparing the results to the expected FMR peaks for measurements along the easy and hard axes, and normal to the slab, using the Landau-Lifshitz-Gilbert equation provides some interesting irregularities. Samples with high ferrite concentrations, Kittel's equation for thin film resonance can be used to describe the FMR frequency vs. field dependence. For low ferrite concentrations the resonance conditions have to be modified to account for an effective thickness beyond the normal filling factor correction associated with presence of a matrix. These results indicate the effective demagnetizing factors, determined by the spatial extend of the RF fields, can describe the observed FMR absorption.

H71.00351: Evolution of Skyrmion state from Helical state in Mn$_x$TaS$_2$*  RABILUL ISLAM (Presenter), Electrical & Computer Engineering, University of Waterloo, PENG LI, Institute of Quantum Computing, University of Waterloo, MARIJAN BEG, HANS FANGOHR, Faculty of Engineering and Physical Sciences, University of Southampton, GUOXING MIAO, Electrical & Computer Engineering, University of Waterloo — Skyrmion-based memory and logic devices are promising to overcome the limitations of the conventional data storage and information processing devices. However, the number of materials hosting magnetic skyrmions is very limited. Therefore, the discovery of new materials is an important avenue of research. In this work, we explore whether the skyrmion state can be an equilibrium state in Mn$_x$TaS$_2$ (MTD) as well as how does the skyrmion state emerges from the helical order with its helical length of 95 nm. By applying an external magnetic field, we were able to modulate the helical period and eventually obtain the skyrmion state. Our findings demonstrate the existence of the skyrmion state in MTD magnetic materials as well as the evolution path. 3D view of magnetic moments gives a picture of the Bloch-type skyrmion. Moreover, we measure the magnetoresistance as a function of the applied field for MTD materials. In the in-plane field dependence of magnetoresistance and magnetization, we saw the clear corresponding jumps when the skyrmion is formed.

*TQT

H71.00352: Nonmagnetic Zinc substitution on Cobalt Ferrites and measurement of their Structural, Dielectric and Magnetic Properties  TAMANNA MARIAM (Presenter), Univ of Toledo, KAZI HANIUM MARIA, Department of Physics, University of Dhaka, Dhaka, Bangladesh, NAZRUL ISLAM KHAN, Materials Science Division, Bangladesh Atomic energy Centre, Dhaka, Bangladesh, SHAMIMA CHOUDHURY, Department of Physics, University of Dhaka, Dhaka, Bangladesh — A series of Co$_{1-x}$Zn$_x$Fe$_2$O$_4$ ferrites with (x=0.0,0.1,0.2,0.3,0.4,0.5) compositions were synthesized by standard double sintering ceramic technique. Substituting nonmagnetic Zn in place of Co influenced the structural, dielectric and magnetic properties of the samples. The X-Ray diffraction pattern confirmed the single-phase cubic spinel structure. The lattice parameters were found to increase with Zn substitution. The grain size of the samples was reduced by enhancing the Zn concentration. The dielectric constant of the sample is found to decrease with increase in frequency exhibiting normal dielectric behavior. The variation of the resistivity versus temperature was also studied and the dielectric constant of the system has a variation quite similar to that of the resistivity. Saturation magnetization and coercivity were estimated with variation of Zn content by VSM measurement. These effects are due to facilitation of demagnetization by substitution of the non-magnetic Zn ions. Permeability was found to decrease with increasing in Zn content, which showed proportionality behavior with grain size. Low coercivity, moderate saturation magnetization and high anisotropy constant has made Cobalt Ferrite a good candidate to contribute in multiferroic materials and in storage devices
**H71.00353: Room-temperature ferromagnetism in oxidized-graphenic nanoplatelets induced by topographic defects**

JOHN PRIAS (Presenter), Doctoral Program in Physical Sciences, IIS and EITP, University of Quindío, KATHERINE GROSS, Department of Physics, University of Valle, HERNANDO ARIZA, Interdisciplinary Institute of sciences, University of Quindío, PEDRO PRIETO, University of Valle, CINZIA DI GIORGIO, FABRIZIO BOBBA, ANNAMARIA CUCOLO, Department of Physics, University of Salerno — Pyrolytic oxidized-graphenic nanoplatelets (OGNP) obtained from bamboo pyroligneous acid (BPA) by varying the density of extended defects, show room-temperature ferromagnetism. Topographic defects, created during the fabrication process, arise from a natural formation of clusters; such clusters drastically distort the graphitic basal plane, giving rise to abrupt surface curvatures. Topographic defects were found to be sources of the magnetic signal, as evidenced by bulk magnetization and MFM measurements. Increased defect density, which is tuned by carbonization temperature, results in enhanced magnetization.

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**H71.00354: Self-regulating magnetic hyperthermia (SrMH) of Ni$_x$Cu$_{1-x}$ nanoparticles**

BIANCA PAOLA MENESES BRASSEA (Presenter), MOHAMED F. SANAD, DAWN S. BLAZER, Physics, University of Texas at El Paso, SHIRIN POURMIRI, Physics and Astronomy, University of Delaware, AHMED A. EL-GENDY, Physics, University of Texas at El Paso — Ni$_x$Cu$_{1-x}$ ($x=0.2-0.5$) nanoparticles have been synthesized by reducing Ni and Cu from metal precursors using sol-gel route followed by annealing at different temperatures for controlled self-regulating magnetic hyperthermia applications (SrMH). SEM, TEM, and XRD reveal spherical 20-50 nm nanoparticles with FCC cubic structure for different compositions of Ni$_x$Cu$_{1-x}$. The magnetic properties exhibited ferromagnetic behavior with saturation magnetization ($M_s$) ranging from 8-20 emu/g at 300 K and Curie temperature ranging from 42-25 °C within the limit of the therapeutic temperature range of 42-46 °C. The feasibility of hyperthermia has been performed under the therapeutic limits of alternating magnetic field and frequency. The samples exhibited heating rate and a significant dissipated heating power or measured as specific absorption rate (SAR) ranging from 0.1-1.6 °C/min and 20-100 W/g, respectively. Results reveal nanoparticles' feasibility for self-regulating hyperthermia.

*AAE acknowledge the startup and rising stars funds by UTEP and UT-system respectively. Also, the research reported in this paper was partially supported by the National Institute of General Medical Sciences of the National Institutes of Health under linked award numbers RL5GM118969, TL4GM118971, and UL1GM118970.
H71.00355: Functionalized superparamagnetic Fe@Au Core/shell nanoparticles and their feasibility for magnetic hyperthermia*  BIANCA PAOLA MENESES BRASSEA (Presenter), MOHAMED F. SANAD, DAWN S. BLAZER, Physics, University of Texas at El Paso, SHIRIN POURMIRI, Physics and Astronomy, University of Delaware, AHMED A. EL-GENDY, Physics, University of Texas at El Paso — Superparamagnetic Fe@Au core/shell nanoparticles have been synthesized at ambient condition at different ratios of Fe:Au precursors using one-step wet chemistry method and functionalized with tween. SEM, TEM, and XRD reveal spherical FCC Fe core nanoparticles coated with Au shells. The particles sizes average 61, 71, 83 nm at Fe:Au precursor's ratio of 1:1, 2:1, 3:2 respectively. VSM reveals superparamagnetic behavior at 300 K. The saturation magnetization ($M_S$) of the samples amounts 79, 165 and 89 emu/g for 61, 71 and 83 nm respectively. Feasibility for hyperthermia treatment of cancer have been tested under applied magnetic fields and frequencies, heating power known as specific absorption rate (SAR) has been recorded. SAR dependence of magnetic field and frequency yields 35, 50, 25 W/g at therapeutic range of 400 Oe and 304 kHz for samples with $M_S$ of 79, 165 and 89 emu/g respectively. The samples show feasibility for future in vitro/in vivo studies for tumor cells.

*AAE acknowledge the startup and rising stars funds by UTEP and UT-system respectively. Also, the research reported in this paper was partially supported by the National Institute of General Medical Sciences of the National Institutes of Health under linked award numbers RL5GM118969, TL4GM118971, and UL1GM118970.

H71.00356: The evolution of electronic and magnetic states for transition-metal rings embedded in carbon nanotubes*  JOSEPH WARD (Presenter), RITHVI RAVICHANDRAN, JASON HARALDSEN, Univ of North Florida — We investigate the electronic and magnetic states for various sizes of transition metal rings that have been substituted into carbon nanotubes. Using density functional theory, we examine the electronic density of states, magnetic moment, and total energy for various transition metal atoms and magnetic configurations. After determining the structural and magnetic ground states, we show how the introduction of these metal atoms affect the electronic states and determine the ground state magnetic configuration with a variation of transition metal atom and onsite potential. Future work will look into the use of these magnetic systems in a device application setting as we work towards possible spintronic applications.

*This project is supported, in part, by the Institute for Materials Science at Los Alamos National Laboratory.
H71.00357: Effect of Structural Disorder on the Magnetic Properties of Melt-Spun Co$_{3+x}$V alloys

ONUR TOSUN (Presenter), Physics and Astronomy, University of Delaware, INCI RUZYBAYEV, Kinsley School of Engineering, Sciences and Technology, York College of Pennsylvania, FRANK M ABEL, Physics and Astronomy, University of Delaware, BALAMURUGAN BALASUBRAMANIAN, RALPH SKOMSKI, DAVID SELLMYER, Physics and Astronomy, University of Nebraska, Lincoln, GEORGE C HADJIPANAYIS, Physics and Astronomy, University of Delaware — We have investigated the structural and magnetic properties of melt-spun Co$_{3+x}$V alloys for x = 0, 0.2, 0.4 and 0.6 in order to study the effect of structural disorder on the magnetic properties of Co-V alloys. Bulk Co$_3$V exists in two phases: An ordered hexagonal (Al$_3$Pu-type) low-temperature phase (LTP) and a cubic $L1_2$ (Cu$_3$Au)-type high-temperature phase (HTP) [1, 2]. Both the LTP and HTP are paramagnetic down to 4.2 K. The as-spun samples have the HTP structure. However, when they are annealed at 1173 K, they transform into the LTP. Magnetic data suggest that the as-made ribbons are ferromagnetic with ordering temperatures of 10, 20, 30 and 75 K for x = 0, 0.2, 0.4 and 0.6, respectively. This behavior is attributed to a slight destruction of perfect order in the HTP and which can lead to an increase in the Co-Co exchange interaction. The magnetic properties of annealed samples are currently being measured and the results will be presented and discussed at the meeting.


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H71.00358: Structural and Magnetic Properties of Iodide-Mediated Synthesized L1$_2$ FePt$_3$ Nanoparticles

VIMAL DEEPCHAND (Presenter), Univ of Delaware, VASILEIOS TZITZIOS, Department of Chemical Engineering, Khalifa University of Science and Technology, Petroleum Institute, GEORGE C HADJIPANAYIS, Univ of Delaware — Halide ion-mediated synthesis of L1$_0$ FePt has previously been used to form magnetically hard L1$_0$-FePt phase without the need of any post-annealing or 3$^{rd}$ element addition [1,2]. In this work, we chemically synthesized L1$_2$ FePt$_3$ by the co-reduction of iron and platinum-based precursors in the presence of elemental iodine. Thermomagnetic data showed that the magnetic properties depend strongly on the degree of atomic ordering. The as-made structure showed the L1$_2$ phase but with a low degree of ordering. Magnetic measurements showed that the ordering temperature of the as-made sample is at 380 K. The chemical ordering increased to 0.71 when the samples were annealed at 700°C for 30 minutes. The annealed samples showed a different ordering temperature of 251 K. Our data agreed with those reported by Margeat et al [3]. Room temperature hysteresis loops showed that the coercivity of our samples increased with annealing temperatures, up to 0.23 kOe for samples annealed at 700°C. Thermomagnetic measurements from 50 K to 380 K also provide evidence of a phase transformation in the L1$_2$ FePt$_3$ nanoparticles, which we believe to be the transition from the AFM state to a FM state.

*DOE-FG02-90ER45413
Effect of Surfactants on the Shape of Iron Oxide Nanoparticles Synthesized by Thermal Decomposition

H71.00359

SHIRIN POURMIRI (Presenter), Physics and Astronomy, University of Delaware, VASILEIOS TZITZIOS, Institute of Nanoscience and Nanotechnology, NCSR “Demokritos, GEORGE C HADJIPANAYIS, Physics and Astronomy, University of Delaware — Superparamagnetic iron oxide nanoparticles are one of the most promising materials for biomedical applications. However, despite the large number of researches done on spherical nanoparticles, there is much less work on the effect of particle shape of these nanoparticles on their magnetic properties and biomedical applications. In this work, iron oxide nanoparticles were synthesized using thermal decomposition of iron acetylacetonate in the presence of a mixture of oleyl amine and oleic acid. The XRD measurements show that the nanoparticles have a pure Fe3O4 phase. TEM images show that by changing the ratio of oleic acid to oleyl amine from 0.6 to 1, 1.1 and 1.3 the nanoparticle’s shapes change from spheres to cubes, octopods and rods, respectively; when the ratio is increased to more than 1.3, the nanoparticles start to form spherical shape again. The size of each of these shapes can be precisely controlled by adjusting the time and temperature of the reaction. Magnetic properties and hyperthermia measurements of these samples will be presented and discussed in the meeting.

Characterization of NiFe/SiO2 multilayers for on-wafer inductors operating at radio and low GHz frequencies

H71.00360

SARA GOLDMAN (Presenter), Physics, UCCS — Magnetic layers surrounding copper core inductors are studied for use in circuits operating at radio and low GHz frequency ranges in order to address performance issues and quality losses normally observed in miniaturized inductors. Coating an inductor core in a magnetic material has the potential to increase the inductance proportional to the magnetic permeability of the coating. The objective of this research is to identify and construct an appropriate magnetic coating to improve the inductance and quality (Q-factor) of inductors. Permalloy (Py) was selected for these experiments due to its high relative permeability. Py layers, from 10nm to 1μm thick, were grown on silicon wafers using magnetron sputtering. These layers were characterized with SQUID magnetometer and broad-band FMR system. A specific issue we address is that inductor coatings have the potential to decrease the Q-factor due to eddy currents during high frequency operation. A method to reduce eddy current losses is to reduce layer thickness. Therefore, in addition to individual Py layers, multilayer coatings are developed: depositing 5 to 50 identical layers of Py (for total thickness from 150nm to 1.5μm) separated with 5nm layers of SiO2. Such structures are suitable for high frequency inductor operations.
H71.00361: Mn$_2$FeSi: Experimental realization of an antiferromagnetic inverse-Heusler alloy

DIPANJAN MAZUMDAR (Presenter), ANIL ARYAL, SAID A BAKKAR, HASSANA SAMASSEKOU, SUDIP PANDEY, IGOR DUBENKO, Physics, Southern Illinois University Carbondale, SHANE STADLER, Physics and Astronomy, Louisiana State University, NAUSHAD ALI, Physics, Southern Illinois University Carbondale — Search for low-moment magnetic materials with high spin-polarization is important for future spintronics applications. In this work, we have conducted detailed and varied materials growth and characterization along with complementary first-principles calculations to investigate the structure and magnetism of Mn$_2$FeSi, which is a prospective inverse-Heusler material identified by prior calculations. We show that Mn$_2$FeSi adopts a cubic structure that is in very good agreement with theoretical estimates while the magnetic and resistivity measurements show behavior consistent with antiferromagnetism which can be tuned to a very low-moment state under appropriate growth conditions. Supporting first-principles calculations show that compensated antiferromagnetic states are energetically feasible. Our work provides new evidence that the magnetic properties of Manganese-based inverse-Heuslers can be useful to explore new applications in the area of spintronics.

*NSF CAREER grant (ECCS 1846829); NSF DMREF grant No. 1235396; U. S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award No. DE-FG02-06ER46291 and DE-FG02-13ER46946

H71.00362: Emergent Topological Hall Effect in La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrIrO$_3$ Heterostructures

YAO LI (Presenter), Nanjing University, LUNYONG ZHANG, Max Planck Institute for Chemical Physics of Solids, QINGHUA ZHANG, Institute of Physics, Chinese Academy of Sciences, CHEN LI, Nanjing University, TIEYING YANG, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, YU DENG, Nanjing University, LIN GU, Institute of Physics, Chinese Academy of Sciences, DI WU, Nanjing University — Novel magnetic and electric phenomena could emerge in perovskite oxide heterostructures due to multiple and complex coupling at the hetero-interface. Here, we report that an emergent giant topological Hall effect (THE) can be induced in ferromagnetic La$_{0.7}$Sr$_{0.3}$MnO$_3$ thin films in a wide temperature range up to 200 K by constructing La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrIrO$_3$ epitaxial heterostructures. The observed THE indicates a non-coplanar spin texture, which also leads to strongly pinched field dependent magnetization (MH) loops in the out-of-plane direction. This THE and pinched MH loops are not observed in La$_{0.7}$Sr$_{0.3}$MnO$_3$ single layer films or La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrTiO$_3$/SrIrO$_3$ trilayer heterostructures, indicating the relevance of the La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrIrO$_3$ interface, where Dzyaloshinskii-Moriya interaction due to strong spin-orbital coupling in SrIrO$_3$ may play a crucial role. This work demonstrates the feasibility of using SrIrO$_3$ to modify magnetic and transport characteristics by interfacing with other correlated oxides, which might be useful to novel spintronic applications.
**H71.00363: Novel Magnon Transport Properties in Magnetic Oxides by Mesoscopic Boltzmann Approach**

YANXIA WANG, WEI WANG, YUHENG LI, JIANWEI ZHANG (Presenter), School of Physics Science and Engineering, Tongji University — The coherent transport properties of magnon in ferromagnetic insulator (FI) demand precise physical understanding of magnon scattering and relaxation processes. In this presentation, we invent a general magnon Boltzmann equation from full quantum magnon Hamiltonian[1]. By including N-process magnon-scattering due to dipole-dipole interaction, we demonstrated a novel collective decay dynamics of magnon group, which showed hydrodynamics transport properties of magnon. To conduct N-process scattering, a new spatial dependent magnon interaction field \( \lambda \) was introduced, which was describing collective local field in magnon. We also found N-process scattering is the physical origin that why coherence magnons can transfer to thermal magnons in FI relaxation process. Furthermore, our results showed magnon current can be manipulated by varying of anisotropy in magnetic oxides, especially in strong anisotropic energy materials, such as NiFe2O4 or CoFe2O4. In this framework, we also provide the methods to manipulate magnon transport by applying gradient magnetic field and gradient T field.


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**H71.00364: Two-dimensional magnetic monopole gas in an oxide heterostructure**

LUDI MIAO (Presenter), YONGHUN LEE, ANTONIO B MEI, MICHAEL J LAWLER, KYLE M SHEN, Cornell University — Magnetic monopoles have been proposed as emergent quasiparticles in magnetically frustrated pyrochlore spin ice compounds, such as R2Ti2O7 (RTO) (R = Ho, Dy). To date, all experimental investigations have been limited to the behaviour of large ensembles comprised of equal numbers of monopoles and antimonopoles in macroscopic bulk. Therefore, fundamental questions about the existence, properties, and dynamics of single, isolated monopoles, as well as the new phases of matter that these monopoles may form, remain unanswered or inaccessible. To address these issues, we propose the formation of a two-dimensional magnetic monopole gas (2DMG) with a net magnetic charge and whose monopole density can be controlled by an external field, at the interface between a spin ice and an isostructural antiferromagnetic (AFM) pyrochlore iridate (e.g. R2Ir2O7 (RIO)). Our proposal is based on a series of Monte Carlo simulations of the thermodynamic and transport properties, which also demonstrate the robustness of the 2DMG against long-range dipolar interactions. This proposed 2DMG should enable entirely new classes of experiments and devices which can be performed on magnetic monopoles, akin to two-dimensional electron gases in semiconductor heterostructures.
H71.00365: Magnetic Properties of MBE Grown La$_{1/3}$Y$_{1/3}$Sr$_{1/3}$MnO$_3$ thin films and Superlattices* THOMAS PEKAREK (Presenter), CAITLIN KENGLE, JAMES PAYNE, DAKOTA BROWN, MAITRI WARUSAWITHANA, Univ of North Florida — We have investigated the magnetic properties of thin films related to the standard CMR system La$_{2/3}$Sr$_{1/3}$MnO$_3$ where Y substituted for 50% of the La atoms. These La$_{1/3}$Y$_{1/3}$Sr$_{1/3}$MnO$_3$ films were grown as a random alloy where La, Y, and Sr atoms randomly occupied the A-site or as a superlattice where each unit-cell-thick layer stacked along the crystallographic (001) direction contained only one of the atoms La, Y, and Sr occupying the A-site. One key magnetic feature of La$_{2/3}$Sr$_{1/3}$MnO$_3$ is a prominent ferromagnetic transition near 350 K. We find the substitution of La with Y suppresses this ferromagnetic transition in both the random alloy and the superlattice samples. In the superlattice sample we find a magnetic transition that is coincident with a metal-to-insulator transition observed in electronic transport. In the random alloy sample, we see a similar magnetic transition but at lower temperatures, where we find the sample is too insulating to measure electronic transport. We will compare our measurements on these La$_{1/3}$Y$_{1/3}$Sr$_{1/3}$MnO$_3$ samples with CMR thin films of La$_{2/3}$Sr$_{1/3}$MnO$_3$.

*T.M.P. acknowledges support from the UNF Terry Presidential Professorship and the National Science Foundation Grant DMR-1626332. Some of the samples studied were grown at NSF funded PARADIM (DMR-1539918).

H71.00366: WITHDRAWN ABSTRACT —

H71.00367: Spin dynamics in a chain with three-spin interactions in a transverse magnetic field OSIEL BONFIM (Presenter), Physics, University of Portland, B BOECHAT, J. FLORENCIO, Physics, Fluminense Federal University — The quantum dynamics of a spin chain with three-spin interactions in the presence of a transverse magnetic field is investigated. We use both direct diagonalization and the method of recurrence relations to obtain the time-dependent correlation function and its corresponding frequency-dependent spectral density function. Although our calculations are done with chains up to 14 spins with periodic boundary conditions, the results are easily extended for infinite-size chains. We present the calculations for the behavior of these quantities as a function of the transverse magnetic field in the high-temperature limit.

H71.00368: Magnetic Properties and de Gennes Scaling of Quaternary Intermetallic Compounds WONCHOON LEE (Presenter), Physics, Sookmyung Women's Univ. — The interplay between antiferromagnetism and superconductivity has been studied for the quaternary intermetallic superconductor R$_{1-x}$R'$_x$Ni$_2$B$_2$C systems from the isothermal magnetization curves and temperature dependent magnetization measurements to determine the crystalline field effect such as low energy levels of singlet $\Gamma_4$ and excited $\Gamma_1$ and $\Gamma_5$ in theoretical group analysis of the energy scheme. In addition, by using the R$^{+3}$ ions Hund's rule, we have qualitative agreement between the de Gennes $T_N$ scaling behavior and crystalline electric effect scheme.
H71.00369: Reliable Electrical Switching of Tri-State Antiferromagnetic Néel Order in α-Fe₂O₃ Epitaxial Films* YANG CHENG (Presenter), SISHENG YU, MENGLIN ZHU, JINWOO HWANG, FENGYUAN YANG, Ohio State Univ - Columbus — Ability to manipulate antiferromagnetic (AF) moments is a key requirement for the emerging field of antiferromagnetic spintronics. Electrical switching of bi-state AF moments has been demonstrated in metallic AFs, CuMnAs and Mn₂Au. Recently, current-induced “saw-tooth” shaped Hall resistance was reported in Pt/NiO bilayers, while its mechanism is under debate. Here, we report the first demonstration of convincing, non-decaying, step-like electrical switching of tri-state Néel order in Pt/α-Fe₂O₃ bilayers. Our experimental data shows the switching behavior of α-Fe₂O₃ Néel order among three stable states, which can be detected by the change of Hall resistance $\Delta R_{xy}$ through spin Hall anomalous Hall effect (SH-AHE). We also show that the observed “saw-tooth” Hall resistance is due to an artifact of Pt, not AF switching, while the signature of AF switching is step-like Hall signals. Together with the Monte-Carlo simulations, we reveal the clear mechanism of AF Néel order switching and explain why only the first current pulse switches the Néel order. This demonstration of electrical control of magnetic moments in AF insulator (AFI) films will greatly expand the scope of AF spintronics by leveraging the large family of AFIs.

*This work is funded by the Department of Energy No.DE-SC0001304

H71.00370: Large magnetic anisotropy in hexagonal Fe₂MnSn alloy* YUNG HUH (Presenter), BISHNU DAHAL, ABDULLAH AL MARUF, Physics, South Dakota State University, SAM PROPHET, PAVEL LUKASHEV, Physics, University of Northern Iowa, PARASHU R. KHAREL, Physics, South Dakota State University — We performed combined theoretical and experimental studies of electronic, magnetic, and structural properties of Fe₂MnSn Heusler alloy. The density functional theory (DFT) calculations of bulk and thin-film Fe₂MnSn Heusler alloys predict that this compound crystallizes in energetically close hexagonal D0₁₉ and cubic L₂₁ phases due to their very similar equilibrium energies, which agrees well with the experimental results. Both the cubic and hexagonal phases are ferromagnetic with high $T_c$ of 325 K and 475 K, respectively. The high-field magnetizations measured at 100 K are 3.3 $\mu_B$/f.u. and 4.3 $\mu_B$/f.u) for the cubic and hexagonal phases, respectively. These values are smaller than the predicted values (6.0 $\mu_B$/f.u. for the cubic and 6.5 for the hexagonal phases) by the DFT calculations. The hexagonal phase shows high value of magnetic anisotropy of 5.1 Merg/cm³ at 100 K. The cubic phase has an energy gap in the minority-spin conduction band that vanishes in the hexagonal phase.

*This research is supported by Fishback Honors College at South Dakota State University, and Faculty Summer Fellowship at University of Northern Iowa. It is also supported by NSF ACI-1548562, and Pittsburgh Supercomputing Center through TG-DMR180059.
H71.00371: Study of magnetization dynamics in magnetic insulators for magnonic applications*  
RODRIGO VICTOR (Presenter), LUIZ SAMPAIO, FLAVIO GARCIA, Centro Brasileiro de Pesquisas Físicas —  
Electronics devices are based on semiconductors transistors, and their improvement is mostly due to reducing its size, which is reaching its limit. To overcome this problem magnonics have appeared as an alternative solution for electronics, with advantages such as lower energy cost, faster information exchange and lower heating due to the absence of Joule effect. Magnetic insulators, more specifically $Y_3Fe_5O_{12}$ (YIG), appear as a promising material for this application because it has low Gilbert damping and low coercivity, among other properties. In this work, YIG thin films were reproducibly grown on $Gd_3Ga_5O_{12}$ with 111 oriented substrates by magnetron sputtering furthermore an ex situ annealing with oxygen flow was performed. A systematic study of the magnetic dynamics using ferromagnetic resonance was carried out to optimize the growth conditions of YIG, seeking the lowest value of Gilbert damping aiming towards magnonic applications. After the optimization, non-magnetic metallic materials (bismuth-doped copper, which produces a giant spin Hall effect and Pt) were deposited on YIG to evaluate the applicability for the spin current generated by spin pumping and spin Hall effect via inverse spin Hall effect.  

*The authors thank Brazilian agencies CNPq and CAPES for financial support.
Heusler material via femtosecond laser excitation  CHRISTIAN GENTRY (Presenter), PHOEBE M TENG DIN, ADAM Z BLON SKY, DMITRIY ZUSIN, MICHAEL GERRITY, Physics and JILA, CU Boulder, LUKAS HELLBRUCK, MOR ITZ HOF HERR, University of Kaiserslautern, JUSTIN SHAW, Quantum Electromagnetics Division, National Institute of Standards and Technology, YAROSLAV KVASHNIN, ERNA DELCZE G-CZIRJAK, Physics and Astronomy, University Uppsala, MONIKA ARORA, HANS NEM BACH, TOM SILVA, Quantum Electromagnetics Division, National Institute of Standards and Technology, BENJAMIN STADTMULLER, University of Kaiserslautern, STEFAN MATHI AS, Physikalisches Institut, Georg-August-Universitat Gottingen, MARTIN AESCHLIMANN, University of Kaiserslautern, HENRY KAPTEYN, Physics and JILA, CU Boulder, DANNY THONIG, Physics and Astronomy, University Uppsala, KONSTANTINOS KOUMPOURAS, Engineering Sciences and Mathematics, Lulea University, OLLE ERIKSSON, Physics and Astronomy, University Uppsala, MARGARET MURNANE, Physics and JILA, CU Boulder — Heusler compounds are exciting materials for future spintronics applications because they display a wide range of tunable electronic and magnetic interactions such as metallicty, superconductivity, and giant magnetoresistance. We use a femtosecond light pulse to directly transfer spin polarization from one element to another in a half-metallic Heusler material, Co$_2$MnGe. This spin transfer initiates as soon as light is incident on the material, showing that we can transfer angular momentum between neighboring atomic sites on timescales less than 10 fs. The observation is made possible by the ability of ultrafast high harmonic pulses to simultaneously and independently probe the magnetic state at two atomic sites, Co and Mn, during laser excitation. We find that the magnetization of Co is enhanced by the laser pulse, while that of Mn rapidly quenches. By comparing our measurements to density functional theory, we show that the optical excitation *directly* transfers spin from one magnetic sub-lattice to another, via preferred spin-polarized excitation pathways. The enhancement of ferromagnetic order demonstrates direct manipulation of spins via light, thus providing a path towards spintronic devices such as switches that can operate on few femtosecond or faster timescales.
H71.00373: Finding Structural Phase Transitions in Barlowite and Claringbullite
ALYSSA HENDERSON, LIANYANG DONG, Florida State University, SANANDA BISWAS, Institut für Theoretische Physik Goethe Universität Frankfurt am Main, HANNAH REVELL (Presenter), YAN XIN, National High Magnetic Field Laboratory, JOHN A SCHLUETER, Division of Material Research, National Science Foundation, ROSER VALENTI, Institut für Theoretische Physik Goethe Universität Frankfurt am Main, THEO SIEGRIST, National High Magnetic Field Laboratory — Barlowite (Cu₄(OH)₆FBr) and claringbullite (Cu₄(OH)₆FCl) are minerals related to the quantum spin liquid candidate herbertsmithite ZnCu₃(OH)₆Cl₂, the popular S = ½ antiferromagnet with a geometrically perfect kagome lattice. The kagome lattices of claringbullite and barlowite are stacked perfectly on top of one another, separated by planes consisting of Cu²⁺ and halide ions, and show promise as QSL candidates. Both materials have a hexagonal crystal structure with P6₃/mmc symmetry and undergo temperature-dependent phase transitions to Pnma symmetry. Previously we examined the barlowite transitions at 276 K, but the claringbullite transition occurs much lower. To pinpoint the transition, equipment had to be modeled and aligned.

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H71.00374: Hanle effect in vertical Ohmic spin valves
YAROSLAW BAZALIY (Presenter), University of South Carolina — Hanle effect measurements in lateral spin valves provide valuable information on spin lifetimes and diffusion lengths in the transport channel. However, their interpretation is made difficult by the fact that current distribution near the injector substantially deviates from the assumptions of a simple 1D model. These difficulties can be partially alleviated by using the "three terminal" measurement method. A logical continuation of this line of thought is the usage of a “current perpendicular to plane” (vertical) F/N/F spin valve, where electric current distribution is strictly uniform. Additional advantage of the vertical valve is a better experimental control of the normal spacer thickness. The complication is the presence of two F/N interfaces, both contributing to the total voltage drop. Here we derive theoretical expressions for the valve magnetoresistance due to Hanle effect experienced by spins in the normal spacer. We assume diffusive regime, transparent boundaries with Ohmic conductivity, and allow for the back-action of spin accumulation in N on the injection process. Magnetoresistance is calculated for arbitrary angle between the magnetizations of the F-layers and any thickness of the N-spacer.
**H71.00375: Deterministic spin-orbit torque switching with a perpendicularly non-uniform magnet**  
SEYED ARMIN RAZAVI (Presenter), HAO WU, KANG-LUNG WANG, University of California, Los Angeles — Spin-orbit torque (SOT) switching of magnetization is a promising emerging technology for non-volatile memory and logic applications. However, deterministic switching of perpendicular magnetization with SOTs requires breaking of inversion-symmetry [1], usually provided by an external magnetic field, which is not suitable for practical applications. We experimentally realize deterministic SOT switching without any external magnetic fields by using a ferromagnet with non-uniform properties in the perpendicular direction (CoFe/CoFeB bilayer). In this structure, a heavy metal acts as the source of SOTs and all the layers have uniform thicknesses. We discuss the role of Dzyaloshinskii-Moriya interaction (DMI) as a possible cause of inversion-symmetry breaking. This method of symmetry breaking for SOT switching can be readily employed in current industrial processes and can pave the way for the practical application of SOT-based technology.


**H71.00376: Effect of interfacial intermixing on spin-orbit torque in Co/Pt bilayers**

GIOVANNI BAEZ FLORES (Presenter), KIRILL BELASHCHENKO, University of Nebraska - Lincoln — Using the first-principles non-equilibrium Green’s function technique [1] with supercell disorder averaging, we study the influence of interfacial intermixing on the spin-orbit torque in Co/Pt (111) bilayers. The interlayer distances are optimized, several models of intermixing are considered, and atomic potentials in the intermixed layers are obtained using the coherent potential approximation. The magnitude and thickness dependence of the damping-like torque are similar to earlier results for the Co/Pt (001) interface [1,2] and rather insensitive to intermixing. In contrast, the field-like torque, which is small in the case of an ideal interface, is dramatically enhanced by intermixing.


*This work was supported by NSF DMR-1609776.
H71.00377: Giant magnetoelectric effect in Pt/Co/Ta ultrathin films with perpendicular magnetic anisotropy on Pb(Mg$_{1/3}$Nb$_{2/3}$)$_{0.7}$Ti$_{0.3}$O$_3$ ferroelectric substrate  

AITIAN CHEN (Presenter), King Abdullah Univ of Sci & Tech (KAUST), HAOLIANG HUANG, University of Science and Technology of China, YAN WEN, SENFU ZHANG, JÜRGEN KOSEL, King Abdullah Univ of Sci & Tech (KAUST), YALIN LU, University of Science and Technology of China, XIXIANG ZHANG, King Abdullah Univ of Sci & Tech (KAUST) — Perpendicular magnetic anisotropy (PMA) is important for increasing the information storage density in the perpendicular magnetic recording media, and electric-field control of PMA is drawing much attraction due to its potential to lower energy consumption. Multiferroic heterostructures, hybrid ferromagnetic and ferroelectric, enable electric-field control of magnetism via strain-mediated magnetoelectric coupling, though most studies have focused on how to control ferromagnetic films with in-plane magnetization. Here, we deposited Pt/Co/Ta ultrathin films with PMA on PMN-PT ferroelectric substrate and investigate the effect of electric-field-induced piezostrain on its PMA. Through measuring anomalous Hall effect (AHE) under in situ electric fields, we observed a remarkable modulation of AHE curves by electric fields and achieved a giant converse magnetoelectric coefficient (approximately $-2.1 \times 10^{-6}$ s m$^{-1}$), which is comparable with the largest value in the multiferroic heterostructures with in-plane magnetization. Furthermore, the in situ polar Kerr image measurements with electric fields confirmed this giant magnetoelectric effect in PMN-PT/Pt/Co/Ta multiferroic heterostructure. These results pave a way to realize future energy-efficient PMA magnetoelectric and spintronic devices.

H71.00378: Magnetic field noise caused by surface paramagnetic impurities on nitrogen vacancy center diamonds*  

PHILIP CHROSTOSKI, Physics and Astronomy, University of Missouri - St. Louis, DEBORAH SANTAMORE (Presenter), Delaware State Univ — Noise is a detrimental issue for nitrogen vacancy (NV) center diamond sensing devices. The magnetic field noise is caused by both surface and bulk impurities. Here, we study the noise due to the interactions between the NV center electron spin and the surface impurity electron spins that are dissolved in a thin water layer on hydrogen (H-), oxygen (O-), or fluorine (F-) terminated surfaces. We apply the Langevin method to spin fluctuation theory to calculate and analyze the surface noise spectral density. Impurity hopping among the available sites determines the impurity relaxation time that controls the contribution of the noise either from the spin flip-flops noise only or additional spin precession noise. Our results show that O-terminated surface give a much lower surface noise than H- and F-terminated surfaces. This is because only spin flip-flop noise are present for O-terminated surface due to oxygen's picosecond electron spin-lattice relaxation time while both spin flip-flop noise and spin precession noise are present for H- and F-terminated surfaces. Comparing to the previous work on bulk impurity noise, we find that the surface impurities are indeed a greater source of magnetic field noise than the bulk impurities.

*This work is supported by NSF DMR-No.1505641.
H71.00379: Room temperature gate tunable spin-to-charge conversion in LaCrO₃/SrTiO₃ heterostructures

SHIJIA YANG (Presenter), North Carolina State University — The emergence of novel spintronics studies focuses on the generation, transmission, and control of a pure spin current through spin-orbit effects. The emergence of novel electronic and magnetic phenomena at the interfaces between polar and non-polar crystalline transition metal complex oxides such as high mobility two-dimensional electron gases (2DEG) provides an ideal platform for the design of spin-to-charge (StC) convertors. At these interfaces, an interface-driven spin-orbit coupling mechanism - the Rashba effect - shows great promise due to its unprecedented StC interconversion efficiency, called inverse Rashba-Edelstein effect (IREE). We report a new type of 2DEG formed at the interface between antiferromagnetic LaCrO₃ and insulating SrTiO₃ heterostructure with StC conversion efficiency. The measured IREE length is up to 0.3 nm which can be modulated by a gate voltage. The frequency and field orientation dependence of IREE response are both consistent with the spin pumping model, from which the spin relaxation time (~30ps) is derived. Our findings launch a new class of oxide-based 2DEGs for future spin orbitronic applications.

*Device preparation was partially supported by ECCS-1933297 and NC State-Nagoya Collaboration Grant. Sample growth was supported by NSF DMR-1751455.

H71.00380: Data-driven study of magnetic interactions of transition-metal based 2D materials

AYANA GHOSH (Presenter), Univ of Connecticut - Storrs, SHIZENG LIN, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory — Engineering magnetic interactions are critical to control magnetic behavior for device applications. Depending on the presence or absence of inversion symmetries, the magnetic interactions stabilize several exciting magnetic behaviors such as formation of chiral helimagnets, skyrmions, and even quantum spin liquid. Various exchange interactions and magnetic anisotropy within crystal lattices can be estimated using DFT-based simulations approaches, based on which an effective spin only Hamiltonian can be constructed. This multi-scale modeling allows one to predict magnetic properties for real materials. Here, we propose to use a data-driven approach to screen for suitable candidates exhibiting magnetic skyrmions, followed by evaluating their exchange interactions in transition-metal based 2D magnetic materials. This curated dataset of 2D magnetic materials and computed magnetic interactions can then be used to develop a combined protocol to search for similar compounds in a variety of materials space followed by constructing predictive machine learning models to understand magnetic behavior of such systems.

*This work was carried out under the auspices of the U.S. DOE NNSA under Contract No. 89233218CNA000001, and was supported by the LANL LDRD Program.
H71.00381: Study of Tunneling Magnetoresistance (TMR) in Twisted CrBr$_3$ Bilayers

ZHUANGEN FU (Presenter), PIUMI SAMARAWICKRAMA, JIFA TIAN, Univ of Wyoming — The recent discovery of two-dimensional (2D) magnetic materials (such as CrI$_3$ and Cr$_2$Ge$_2$Te$_6$) has opened new opportunities for novel electronics and spintronics [1][2]. By controlling the stacking angle between two monolayers, the twisted 2D bilayers have shown novel quantum states, such as unconventional superconductivity and ferromagnetism [3][4]. However, whether the magnetic ground states of twisted 2D magnetic bilayers can be tuned by the twisting angle is still an open question. In this work, we fabricated $h$-BN/Graphene/twisted CrBr$_3$ bilayer/Graphene/$h$-BN devices using a dry-transfer technique with the twisting angle well controlled. The tunneling magnetoresistances of the twisted CrBr$_3$ devices with different twisting angles will be measured at different temperatures and magnetic fields. We are aiming to establish a phase diagram of the magnetic ground states in the twisted CrBr$_3$ bilayers as a function of the twisting angle. Our study may pave a new way for manipulating magnetic orders in 2D magnetic materials and offer new opportunities in designing 2D material-based spin devices.


H71.00382: First-principles calculations for high-temperature ferromagnetic semiconductor (In,Fe)Sb

HIKARI SHINYA (Presenter), Tohoku University, TETSUYA FUKUSHIMA, The University of Tokyo, AKIRA MASAGO, KAZUNORI SATO, Osaka University, HIROSHI KATAYAMA-YOSHIDA, The University of Tokyo — Fe-doped semiconductors have been attracting much attention due to fascinating properties. In fact, Fe-doped InSb not only exhibits the high Curie temperature but can also be $n$-type doping [1]. Our previous calculations reveal that, (In,Fe)Sb has complex magnetic properties [2]. In the isoelectronic (In,Fe)Sb case, the Fe atoms show strong antiferromagnetic interactions due to the superexchange mechanism. We have demonstrated that by modulating the chemical potentials corresponding to $n$- or $p$-type doping, the magnetic property can be changed drastically from antiferromagnetism to ferromagnetism. This transition can be well understood in terms of the Alexander-Anderson-Moriya mechanism. However, we have obtained high Curie temperature in only $p$-type (In,Fe)Sb case. We suspect that there are the other ferromagnetic mechanisms in addition to the magnetic transition and spinodal nano-decomposition in (In,Fe)Sb. In this study, we have clarified the origin of high Curie temperature by the density functional theory calculations.


*The authors acknowledge the financial support from Japan Science and Technology agency (JST) CREST (Grant No. JPMJCR1777).
H71.00383: All-electron calculations of crystalline and amorphous phases in magnetic phase change materials by KKR Green's function method  
TETSUYA FUKUSHIMA (Presenter), The University of Tokyo, KAZUNORI SATO, Osaka University, HIROSHI KATAYAMA-YOSHIDA, The University of Tokyo, RUDOLF ZELLER, PETER DEDERICHS, Forschungszentrum Juelich — We perform large-scale density functional theory (DFT) calculations for crystalline and amorphous phases in magnetic phase change materials by all-electron full-potential screened Korringa-Kohn-Rostoker (KKR) Green's function method. Here, we choose transition metals doped Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} (GST) systems as the typical cases. We consider large unit cells containing 1000 sites for the crystalline phase and 1365 sites for the amorphous phase to model the configurational and structural disorders in the magnetic phase change materials. Such large-scale DFT calculations are performed using the program KKRnano, where a massively parallel linear scaling all-electron algorithm is implemented. We investigate the electronic structures and distance dependent magnetic exchange coupling constants in the crystalline and amorphous phases. It is found, in the crystalline phase, that ferromagnetic states are favorable in the cases of V and Cr doping, due to the double exchange mechanism, whereas antiferromagnetic superexchange interactions appear to be dominant for Fe- and Mn-doped GST. In particular, the Cr doped GST shows strong ferromagnetic interaction and high Curie temperature for both the crystalline and amorphous phases.

H71.00384: Interfacial Spin Conductance Behavior in Topologically Non-trivial Heterostructures*  
STEPHEN HOFER (Presenter), Physics, Southern Illinois University Carbondale, TRINANJAN DATTA, Chemistry and Physics, Augusta University, DIPANJAN MAZUMDAR, Physics, Southern Illinois University Carbondale — Spintronics is a paradigm that utilizes spin angular momentum as the fundamental logical bit for computing. Spin current is the means by which these bits can be altered to read and write digital information. Toward this end, topological magnon excitation offers a potentially alternative avenue to produce highly efficient topologically mediated spin currents in a device. Topological magnon excitations are hosted in 2D honeycomb topological magnon insulators (TMI) such as CrI\textsubscript{3}. We investigate the behavior of interfacial spin conductance at the boundary of TMIs, normal metals, and topologically trivial ferro- and anti-ferromagnets. The ensuing transport implications of the underlying topological heterostructure is discussed within the context of thermally driven spin conductivity.

*NSF CAREER grant (ECCS: Award#1846829).

H71.00385: WITHDRAWN ABSTRACT
H71.00386: Growth and characterization of magnetic van der Waals films  ALEXANDER BISHOP (Presenter), TIANCONG ZHU, DANTE J O’HARA, JAY A GUPTA, ROLAND KAWAKAMI, Ohio State Univ - Columbus — In the recent past, magnetic, two-dimensional (2D), van der Waals (vdW) systems have become an exciting class of materials to study. On their own, these materials can give insights to low-dimensional spin behavior, but they also have the potential to be integrated into vdW heterostructures. Both areas are rich in scientific novelty and potential spintronics applications. Here we present the synthesis and characterization of 2D vdW magnets 1T-MnSe$_2$ and MnBi$_2$Se$_4$. The materials were grown by molecular beam epitaxy (MBE) and studied with various techniques including X-ray diffraction (XRD), spin-polarized scanning tunneling microscopy (SPSTM), and superconducting quantum interference device (SQUID). The XRD measurements show that highly crystalline MnBi$_2$Se$_4$ films can be grown consistently and SQUID measurements indicate a layered antiferromagnetic structure. This material also exhibits ferromagnetism in the monolayer limit with a Curie temperature near 10K. Monolayer 1T-MnSe$_2$ exhibits room-temperature ferromagnetism when analyzed with SQUID measurements. The magnetic signal from this material was also directly observed using SPSTM with a chromium tip.

H71.00387: Magnetic phase transition of monolayer RuCl$_3$ induced by optical and electrostatic unipolar doping*  WEIWEI GAO (Presenter), University of Texas at Austin, YINGZHEN TIAN, ERIK HENRIKSEN, Washington University in St. Louis, JAMES CHELIKOWSKY, University of Texas at Austin, LI YANG, Washington University in St. Louis — RuCl$_3$ is a layered material showing signatures of a quantum spin liquid and strong magnetic frustration. Based on first-principles calculations, we predict that electrostatic doping with either electrons or holes and optical doping can both cause a phase transition of free-standing monolayer RuCl$_3$ from the spin-liquid phase to stable ferromagnetic ordering with a moderate carrier/e-h density, achievable with current experimental techniques. Increasing the electron-hole pair density by optical doping can further enhance ferromagnetism and also increases the Curie temperature significantly. The mechanisms for driving the magnetic phase transition of monolayer RuCl$_3$ are discussed based on orbital magnetism and itinerant magnetism. Our prediction of optically driving 2D ferromagnetism offers the possibility of non-contact tunability for exploring new physics and spintronic applications.

*Work at Texas is supported by a subaward from the Center for Computational Study of Excited-State Phenomena in Energy Materials, which is funded by the U.S. DOE under Contract No. DE-AC02-05CH11231. Work at St. Louis is supported by the National Science Foundation (NSF) CAREER Grant No. DMR-1455346, the Air Force Office of Scientific Research (AFOSR) grant No. FA9550-17-1-0304, and NSF DMR-1810305.
**H71.00388: Probing Chirality Induced Spin Selectivity in Chiral 2D Hybrid Perovskites Using Spin Hall Magnetoresistance**

ERIC VETTER (Presenter), Physics, North Carolina State University, YAN LIANG, Department of Chemistry, University of North Carolina at Chapel Hill, YUZAN XIONG, Department of Physics, Oakland University, SHULEI ZHANG, ZHIZHI ZHANG, Materials Science Division, Argonne National Laboratory, YI LI, Department of Physics, Oakland University, HONGWEI QU, Department of Electronic and Computer Engineering, Oakland University, VALENTYN NOVOSAD, AXEL HOFFMANN, Materials Science Division, Argonne National Laboratory, WEI YOU, Department of Chemistry, University of North Carolina at Chapel Hill, WEI ZHANG, Department of Physics, Oakland University, DALI SUN, Physics, North Carolina State University — The emergence of the Chirality Induced Spin Selectivity (CISS) effect, where electron transport through chiral materials is spin filtered, offers many new and exciting opportunities for the field of spintronics. However, many questions surrounding the exact nature of this physical phenomenon still remain. Here, we employ spin Hall magnetoresistance (SHMR) measurements and use pure spin currents for probing the effective magnetic fields native to the chiral two-dimensional hybrid perovskites as predicted by the CISS effect. Chiral 2D perovskites are spin coated on top of Pt Hall bars on a Si/SiO$_2$ substrate and the Pt resistance is measured using lock-in detection to separate the first and second harmonic dependencies as a function of magnetic field, field angle, and temperature. We find significant SHMR signals despite the lack of any ferromagnetic material, as well as exotic hysteretic behaviors that we attribute to a CISS-induced SHMR. This work helps to elucidate the mechanism of CISS and paves the way for the use of chiral hybrid perovskites for novel spintronic devices.

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**H71.00389: First-principles evaluation of four-fold symmetric component of anisotropic magnetoresistance in 3d transition metal alloys**

YOHEI KOTA (Presenter), National Institute of Technology, Fukushima College — Anisotropic magnetoresistance (AMR) is a conventional magnetotransport phenomenon, and its origin is understood based on the Campbell-Fert-Jaoul model. Recent experimental studies of AMR reported that the four-fold symmetric component of the electrical resistivity is not so small compared to the two-fold symmetric component in several material films. Theoretically, Kokado and Tsunoda proposed that the four-fold symmetric component of AMR is attributed to the degradation of the crystalline symmetry due to tetragonal distortion [1], whereas Yahagi, Miura, and Sakuma proposed that the four-fold symmetric component arises from the higher order contribution of spin-orbit interaction [2]. The both proposed mechanisms are possible, however, it is unclear which mechanism is more important to generate the four-fold symmetric component of AMR in a realistic material system. In this study, we simulate the magnetization angle dependence of the electrical resistivity in ferromagnets using first-principles calculations. We present the comparison of the two- and four-fold symmetric component of AMR in cubic and tetragonally distorted crystals.

H71.00390: Strain effects on the magnetotransport properties of transition metals*
RAFAEL GONZALEZ-HERNANDEZ (Presenter), JORGE AMELL, ALVARO GONZALEZ-GARCIA, WILLIAM LOPEZ-PEREZ, Departament of Physics, Universidad del Norte, Colombia., JAIRO SINOVA, Department of Physics, Johannes Gutenberg-Universität Mainz — The Anomalous Hall Effect (AHE) is a phenomenon which consists of an extra anomalous transverse voltage developing when current is passed through ferromagnetic material in a magnetic field. In this work, we studied the dependence of strain and magnetization effect on the intrinsic anomalous Hall conductivity (AHC) in 3d metal Fe-bcc, Co-fcc, Co-hcp, and FeCo structure. For the Fe-bcc case, the AHC shows a slightly decreasing with the increase of pressure, being this associate to the magnetization dependence with the lattice constant. However, the AHC for lattices constants above 2.95Å shows a downturn around 70%, even when the magnetization has increased. This decreasing seems to be related to a transition of d-states occupations above this lattice constant. The computation of the anomalous Hall conductivity was carried out using ab-initio calculations (included the effect of spin-orbit interaction for the ferromagnetic state) and the Wannier interpolation technique for the application of the Kubo-Greenwood formula.

*The authors gratefully acknowledge the computing time granted on the supercomputer Mogon at Johannes Gutenberg University Mainz (hpc.uni-mainz.de) and the support of the Alexander Von Humboldt Foundation.

H71.00391: Topological magnons in the checkerboard lattice*  ANTONIO PIRES (Presenter), Univ Fed de Minas Gerais — In analogy with topological insulators in electronic systems, one has the topological magnon insulators which are characterized by the existence of edge states modes in the presence of a gap. In these systems one has a transverse heat current mediated by magnons in response to thermal gradient, or a transverse spin current in response to a magnetic field gradient. Here we study topological magnon effects in a generalized ferromagnetic checkerboard lattice, also known as planar pyrochlore, with Dzyaloshinskii-Moryia interaction (DMI). The DMI breaks the inverse symmetry of the lattice, generates a magnetic flux and leads to non zero Chern numbers. We calculate the Berry curvature, the spin Hall conductivity, the spin Nerst coefficient and the Hall thermal conductivity as a function of temperature. We also analyze the effect of an applied magnetic fiels. Our study complements work done in the honeycomb, kagome, Lieb and pyrochlore lattices.

*Conselho Nacional de Desenvolvimento Cientifico e Tecnologico
**H71.00392: Hopfion Dynamics in Chiral Magnets**  
ZULFIDIN KHODZHAEV (Presenter), EMRAH TURGUT, Oklahoma State University-Stillwater — Resonant spin dynamics of topological spin textures are hugely correlated with their topological nature and can be employed to understand nature, which attracts interest in condensed matter physics and memory and storage technology [1]. Among topological spin textures, skyrmions and vortices have been heavily studied, but hopfions have been paid little attention thus far. In this study, we present a numerical resonant study of spin dynamics of a three-dimensional topological spin texture hopfion in a B20 chiral magnet. Recent studies proposed to use interfaces with strong perpendicular magnetic anisotropy adjacent to a B20 FeGe nanodisk to stabilize hopfions [2]. In our study, using micromagnetic simulations, we first identified the ground state spin configurations of a hopfion, effects of anisotropies, geometric confinements and demagnetizing fields. Then, we calculated the resonance frequencies and spin-wave modes of spin precession dynamics. Our work helps to guide experimental studies to identify 3-dimensional topological spin texture of hopfions in chiral magnets in a functioning device, where imaging is not possible.


**H71.00393: Transportation of Topological Spin Textures at Material Boundaries**  
JEFFREY MICHEL (Presenter), Department of Physics and Astronomy, Stony Brook University, EMRAH TURGUT, Department of Physics, Oklahoma State University — We examine the dynamics of topological spin textures, magnetic skyrmions and skyrmionium, at the boundaries where material properties vary. Using skyrmions or skyrmionium as information storage, e.g. race track memory, requires a basis of knowledge on how these topological spin structures react to changes in material parameters. Using micromagnetic simulations, we investigated the dependence of radius and Hall angle due to: exchange stiffness, magnetic saturation, Dzyaloshinskii-Moriya Interaction, damping constant, anisotropy, and non-adiabaticity of spin transfer torque. There is also a comparison made between the feasibility of skyrmionium as an alternative to skyrmions as a method of storing and transportation information.

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**H71.00394: Helimagnetism and Soliton Lattice in a Chiral Magnet**  
CHENHUI ZHANG (Presenter), JUNWEI ZHANG, PENG LI, YE YUAN, SENFU ZHANG, YAN WEN, DONGXING ZHENG, XIXIANG ZHANG, King Abdullah Univ of Sci & Tech (KAUST) — Herein, we report the observation of helimagnetism and soliton lattice in a chiral magnet. Below the Curie temperature, the in-plane field-dependent magnetization shows an abrupt increase as well as a narrow hysteresis just before saturation, which indicates a metamagnetic transition from soliton lattice to ferromagnetic state. Using Lorenz microscopy, we observed sinusoidal magnetic patterns in real space below the Curie temperature. In thin film samples, we also observed abrupt and hysteretic magnetoresistance jumps when sweeping the magnetic field.
H71.00395: A nonintrusive reduced order modelling of magnetic skyrmions  
MUHAMMET ANNAORAZOV (Presenter), SHADY AHMED, OMER SAN, EMRAH TURGUT, Oklahoma State University—Stillwater — We show that a nonintrusive reduced order modeling framework can predict the magnetic field dependent internal structures of magnetic skyrmions[1] and their density in thin films. After we train the framework using results of micromagnetic simulations, in which we vary the anisotropy, asymmetric exchange energy, and the external magnetic field, we were able to predict the ground state spin configurations for given anisotropy, asymmetric exchange energy, and external magnetic field. Besides, we implement PC[2] (principal component) manifold to interpolate multidimensional data more accurately compared to other methods. We then confirm these spin configurations by calculating micromagnetically[3] and found XX percent accuracy and XX orders of magnitude reduction in the simulation time. Our data-driven approach accelerates identifying the spin texture by eliminating the need of re-calculation of micromagnetic simulations for every material parameter in a functioning device.

H71.00396: Observation of skyrmion-like magnetism in multiferroic BiMnO3* 
ZONG-HENG YANG (Presenter), HUNG-CHENG WU, TING-WEI KUO, D. CHANDRA SEKHAR KAKARLA, Department of Physics, National Sun Yat-sen University, Kaohsiung 804, Taiwan, LIANGZI DENG, CHING (PAUL) W CHU, Texas Center for Superconductivity, University of Houston, Texas, 77204, USA, HUNG-DUEN YANG, Department of Physics, National Sun Yat-sen University, Kaohsiung 804, Taiwan — Polycrystalline sample BiMnO3 was synthesized at high-pressure and temperature and characterized by X-ray diffraction. In our previous reports [1, 2], the multiple magnetic anomalous transitions have been investigated under a hydrostatic pressure up to 11.9 kbar, where the interesting magnetic H-T phase diagrams were also established. In this study, we revisit the pressure effect on the magnetic properties in BiMnO3, particularly in low magnetic field region. Interestingly, a pressure induced skyrmion-like A phase was observed in low magnetic field. The striking and unexpected observation of skyrmion-like phase in BiMnO3 will be discussed.

References:

Transport in a Spintronic Device Using a Magnetic Skyrmion Lattice

DAVID KING (Presenter), JINKE TANG, Physics and Astronomy, University of Wyoming, JOHN ACKERMAN, Chemical Engineering, University of Wyoming — Magnetic skyrmions are a topologically protected state in certain magnetic systems. Their topological properties make skyrmions stable and thus a possible basis for memory or energy storage spintronic devices. We present results for a transport device that uses a skyrmion lattice in the magnetic insulator Cu$_2$OSeO$_3$ as a precursor to an energy storage device. Data from the transport device and its fabrication are presented. The transport data are then used to test the underlying elasticity theory for the skyrmion lattice.

*This work was supported by the National Science Foundation (DMR-1710512).

Effect of viscosity on propagation of MHD waves in astrophysical plasma

ALEMAYEHU CHERKOS (Presenter), Addis Ababa Univ — We determine the general dispersion relation for the propagation of magnetohydrodynamic (MHD) waves in an astrophysical plasma by considering the effect of viscosity with an anisotropic pressure tensor. Basic MHD equations have been derived and linearized by the method of perturbation to develop the general form of the dispersion relation equation. Our result indicates that an astrophysical plasma with an anisotropic pressure tensor is stable in the presence of viscosity and a strong magnetic field at considerable wavelength.

Unification of Gravity and Electromagnetism

MOHAMMED EL-LAKANY (Presenter), Physics, Faculty of Science, Cairo University — Gravity and electromagnetism are two sides of the same coin, which is the clue of this unification. Gravity and electromagnetism are represented by two mathematical structures, symmetric and antisymmetric respectively. Einstein gravitational field equation is the symmetric mathematical structure. Electrodynamics Lagrangian is three parts, for electromagnetic field, Dirac field and interaction term. The definition of canonical energy momentum tensor was used for each term in Electrodynamics Lagrangian to construct the antisymmetric mathematical structure; symmetric and antisymmetric gravitational field equations are two sides of the same Lagrangian.
H71.00401: Adding a Dynamic to Gravitation Reveals How Extra Gravity Halos are Projected from Galactic Cores*  JOHN HUENEFELD (Presenter), APS — It is unfortunate that the term *dark matter was used* to describe the extra gravity observed in galaxy clusters. The name presupposes a material answer, but the only thing *actually* observed is an Extra Gravity Halo (EGH). The mysterious source of this extra gravity remains unresolved. Or does it?

A new theory, sets GR in motion, predicting an ongoing space-time contraction within a gravitational field. Unlike Hubble expansion, this contraction field is non linear with distance from the source and projects more strongly with the increasing amount of concentrated matter generating the field. No assumed additional mass is needed to boost the orbital velocity of stars around a galactic core. The contraction field augments the acceleration of gravity to achieve galaxy rotation curves consistent with observation.

Dark matter is not a particle. EGHs are the result of relativity, and are an integral part of gravitation. The contraction field acts to scale up gravity. The scale factor, which falls easily from the math, has exactly the right mathematical shape to replicate assumed dark matter distributions. Not only do these contraction fields explain galaxy rotation curves, they also explain the Bullet Cluster, and Ultra Diffuse galaxies which have either a very strong EGH or none at all.

*N/A

H71.00402: Excess Surface Energy and Attraction of Matter: A New Vision to explain the Origin of Gravitation  PRITAM MANDAL (Presenter), Durgapur Women's College — This talk presents a model based on minimization of excess surface energy to better explain the origin of gravitation, which is more intuitive and coherent with other fundamental principles of the working of the physical world. Here’s a picture to imagine: If a big ball of liquid (say water or mercury) is broken into many pieces, and kept on a frictionless plane in vacuum (say in an enclosed glass-jar), the smaller balls would tend to merge back into a single ball (initial state). An observer watching the phenomena from outside the glass-jar would explain the phenomena in terms of some mysterious force (e.g. gravitation), but the merging of the smaller balls in this ideal experimental set-up is merely an outcome of the tendency of the universe to minimize free energy. Surface tension explains this phenomenon satisfactorily. For same reason, metallic surfaces touching in the vacuum can stick to each other and fuse, known as the cold welding. This model has the potential to lead us to the grand unification of the fundamental laws of nature. In our model, the concept of space-time curvature is replaced by the curved meniscus of “fluid” energy-field around a mass.

We strongly suggest designing a suitable experimental set-up to test the validity of the model.
H71.00403: Statistical Analysis of Low States in VY Scl Stars  KYLEE FORD (Presenter), FREDERICK A RINGWALD, California State University, Fresno — The first detailed statistics of the light curves of a class of cataclysmic variable binary star systems, known as the VY Sculptoris stars, was compiled. These light curves are time-series observations of these stars’ apparent magnitudes in visible light. These observations were made by the American Association of Variable Star Observers and were made available publicly on a server funded by the National Science Foundation. In every star in this sample, the presence of low states that define the VY Scl stars was confirmed. The VY Scl stars typically spend most of their time in a high state, and irregularly drop by between 0.4 and 7.6 magnitudes into low states. We have compiled tables of the depths and durations of the low states of each system. We discuss these statistics in the context of the explanation that the low states may be caused by concentrations of magnetism on the secondary star, namely starspots.

H71.00404: Sea water intrusion in coastal aquifers and sustainable solution to control the intrusion  LIBIA HAZRA (Presenter), N. SRINIVAS, CH. RAMAKRISHNA, Gandhi Institute of Technology and Management — Groundwater in coastal regions is often prone to degradation in quality due to sea water intrusion. Sea level rise, coastal geomorphology, the amplitude and frequency of water waves, the depth of water near the coast, changing precipitation regimes and changing groundwater recharge rates may all influence the incidence of saltwater intrusion. A systematic study has been carried out to evaluate salt water intrusion in the coastal aquifers of Visakhapatnam city, Andhra Pradesh, India. The study areas are alongside of the sea (Bay of Bengal) shore. Water samples from bore wells were analyzed to determine the physico-chemical parameters of groundwater. Presence of bromide in all samples and Cl/Br ratio confirms the seawater intrusion near seashore samples. This condition is attributed to anthropogenic activities of the respective area and also the influence of climate conditions over Bay of Bengal. We seek sustainable solution to control the intrusion and implement protective measures such as conservation of ground water resources along with coastal management practices i.e. green belt development and strengthening of bunds along the coastal areas.
We will report results for single crystals of Sm$_6$T$_4$Al$_{43}$ (T=Mo,W) that were synthesized using a molten Al flux. Powder X-Ray diffraction measurements show that both compounds crystallize in the hexagonal Ho$_6$Mo$_4$Al$_{43}$ structure with lattice constants near $a = 10.97$ Å and $c = 17.67$ Å, as reported previously [1]. As for other compounds in this structure, the electrical transport data exhibit a weak temperature dependence due to significant disorder scattering, likely associated with atomic site interchange. The temperature dependent magnetic susceptibility and heat capacity further show that ferromagnetic ordering emerges from a weakly paramagnetic state near $T_C = 15$ and 16 for the Mo and W variants, respectively. We will discuss these results in the context of other Sm-based intermetallics, where the $f$-state and the associated magnetism is strongly influenced by van Vleck physics.


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H71.00406: Au nanoparticle’s plasmonic nearfield induced photoluminescence enhancement of fluorophores  HASNA ALALI (Presenter), Western Michigan Univ — Gold nanoparticles in fused quartz substrates were synthesized with ion implantation using the Western Michigan University's particle accelerator lab. Localized Surface Plasmon Resonance with respect to ion fluence ($1 \times 10^{16}$ to $9 \times 10^{16}$ atoms/ cm$^2$) at fixed ion beam energy (70 keV) was studied. Rutherford Backscattering Spectrometry and UV/Vis techniques were used to quantify Au concentration and detect the formed nanoparticles respectively within the substrate. The investigation of enhanced electric fields of embedded nanoparticles with incident electromagnetic wave were used to amplify the photoluminescence intensity of dye and various perovskites nanocomposites. Steady state time resolved photoluminescence spectroscopy were used to investigate the emission enhancement and the energy transfer between the fluorophore and the metal nanoparticle. It was observed that the photoluminescence enhancement of perovskites in the vicinity of Au nanoparticles had a direct relationship with the ion implanted fluence. The photoluminescence intensity was quenched for C515 dye indicating the energy transfer from molecule to the Au nanoparticle. The photoluminescence enhancement was obtained for the lead halide perovskites and the maximum relative enhancement of $\sim 29$ times was obtained in CsPbI$_3$. 
H71.00407: Discovery of Faraday's law of self-induction*  JUNHO JEONG (Presenter), Dong-A University — Maxwell mathematically proved electromagnetic wave emission via his wave equations, and Hertz proved it experimentally. However, Hertz experimented on Henry's self-induction instead of mutual-induction. An oscillating electric dipole p(t) = Q(t)r with charge Q(t) emits electric dipole radiation because of the external energy, and Faraday's law shows the relationship between the two charges. Here, we have first discovered the existence of a new Faraday's law of self-induction, which only requires charge Q(t) and that an electromagnetic wave is a method of emitting the received external energy for Q(t) to return to the stable state according to Lenz's law. Second, when the inapplicability of relativistic electromagnetism to the Lorentz force was analysed based on the above facts, we additionally discovered that observers in different inertial systems could physically distinguish charges generating electric fields from those generating magnetic fields because the physical phenomena between the perspectives of mass and charge differ.

*I wish to thank SBN Science Ltd. for supporting funding.

H71.00408: Advances and possibilities of the Materials Innovation Platform with examples from Spin-ARPES  DANIEL BEATON (Presenter), M. LUNDWALL, T. WEILL, ScientaOmicron, Inc — The quest for device applications based on quantum materials, such as topological insulators or superconductors, requires strict control of the environments these materials are exposed to during production and while under investigation. It is therefore most straightforward to gather all parts of the experiment, from sample growth to analysis, in one connected UHV system - creating a so-called Materials Innovation Platform (MIP). This approach has proven to be extraordinarily valuable in recent years.

In this presentation, I will focus on a combination of MBE/ARPES, and also coupled spin detection. The advantages of this set-up will be explored, as well as highlighting some of the very recent electronic band structure research performed with such a system. Two specific examples will be reviewed: Yang et al.[1] investigation of the impact of photogenerated carriers on the superconducting transition temperature; and advances high efficiency spin-ARPES. The work by Yang et al. was enabled by the in-situ growth and analysis possibility and clearly demonstrates the possibility of making energy-efficient quantum optoelectronics devices. Future possibilities of Spin-ARPES and laser-ARPES in combination with MIP set-up will also be discussed.

**H71.00409: Probing Dark Matter Halos with Ultra-Faint Dwarf Galaxies: A Spectroscopic Analysis of Leo V**

SYDNEY JENKINS (Presenter), University of Chicago, TING LI, Carnegie Observatories, JOSHUA A FRIEMAN, University of Chicago — The nature of dark matter presents one of the most significant problems in astrophysics. Ultra-faint dwarf (UFD) galaxies may play a key role in solving this mystery, as they are the most dark-matter dominated systems known and they allow us to probe dark matter halos down to the scale of tens of parsecs. However, many UFDs have few known member stars, making it difficult to provide robust measurements of the galaxies’ key features. We are currently locating new members and providing refined, consistent measurements of physical parameters for 15 UFDs using publicly archived spectroscopic data from the Very Large Telescope. We present a representative analysis of Leo V, a UFD with twelve known non-variable member stars. We identify three new likely members in addition to five new plausible members that require further follow-up, and perform a comparative analysis of seven previously discovered members. Using our catalogue of member stars, we perform a search for binary stars within the galaxy and investigate the possibility that Leo V is tidally disrupted. Our analysis of Leo V and other UFDs will enhance our understanding of these enigmatic stellar populations and contribute to future dark matter studies.

**H71.00410: Casimir Energy For Perfect Electric Conductors Using the A-Phi Formulation**

CARLOS SALAZAR-LAZARO (Presenter), University of Illinois at Urbana-Champaign — Previous work by Reid, et.al. [1] calculated the Casimir energy for conducting geometries using the method of moments applied to the impedance matrix given by Electric Field Integral Equation (EFIE). His results were later extended by Atkins [2] by making use of the Argument Principle applied to the EFIE and transforming the calculation of the Casimir energy to one that used the Augmented EFIE (AEFIE) as its impedance matrix. We will use the same approach as Atkins but instead of using the AEFIE, we will propose using the A-Phi [3] formulation impedance matrix in order to calculate the Casimir energy for 2-D conducting geometries.

H71.00411: Tricritical physics in two-dimensional p-wave superfluids near resonance

FAN YANG (Presenter), FEI ZHOU, University of British Columbia — We study the effect of quantum fluctuations on the stability of two-dimensional \((p+ip)\)-wave superfluids near resonance. The system is a Bardeen-Cooper-Schrieffer superfluid on one side of the resonance and a Bose-Einstein condensate on the other side. When the quantum fluctuations are strong, the interactions between Cooper pairs or bosonic molecules are substantially renormalized. As a result, the interactions between bosonic fields can become attractive at low energy and destabilize the superfluid phase even if the mean-field interactions are repulsive. We find that in the strong coupling limit, there exists a finite region near resonance where the superfluids are unstable and the system undergoes a first order phase transition at its boundary. The size of this region scales as \(\exp(-c/g^2)\), where \(g\) is the \(p\)-wave interaction constant and \(c\) is a numerical factor. Using a simple renormalization group analysis, we identify the tri-critical points which separate the continuous phase transition from the first order phase transition.

H71.00412: Electron correlation Time-Dependent Density-Functional Theory for Higher Harmonic generation in solids

DIDARUL ALAM (Presenter), NASEEM UD DIN, SHIMA GHOLAM MIRZAEMOGHADAR, TAO JIANG, MICHAEL CHINI, VOLODYMYR TURKOWSKI, Univ of Central Florida — We present details of our Time-Dependent Density-Functional Theory (TDDFT) approach, which takes into account the effects of electron-electron correlations, to analyze high-order harmonic (HH) spectra in solids. The used TDDFT exchange-correlation kernel was obtained from the charge susceptibility for the effective Hubbard model for the system calculated by using Dynamical Mean-Field Theory. The corresponding system of the TDDFT equations for polarizations and state occupancies is a generalization of the semiconductor Bloch equations on the case of locally-interacting electrons. To establish the signs of the correlation effects in the HH spectrum, we solved the equations analytically in the limit of weak external laser-pulse perturbation and numerically for various field strengths in the case of one of the most studied system – ZnO. It was found that correlation effects significantly affect the HH spectrum, most notably by shifting the spectral weight to higher harmonics. We discuss possible extensions of the theory on the case of non-local electron-electron interactions.

*This work is supported in part by NSF Grant No. DMR-1809181
H71.00413: Hot electron noise in semiconductors from first principles* PEISHI CHENG (Presenter), ALEXANDER CHOI, AUSTIN MINNICH, Caltech — First principles calculations of the properties such as mobility in semiconductors are now routine owing to advances in the ab-initio treatment of the electron-phonon interaction. However, fluctuational properties like the spectral noise power of current fluctuations, which can be calculated from the same ab-initio inputs, are experimentally accessible but yet to be reported. Here, we report an ab initio calculation of the spectral noise power in GaAs using a Boltzmann-Green's function method. This approach expresses the noise spectral power using the current autocorrelation function computed from solutions of the Boltzmann transport equation with first principles electron-phonon interactions as input. The physical insights yielded by this description of fluctuational properties will help guide the design of semiconductor devices operating closer to the standard quantum limit of noise.

*AYC acknowledges support from the National Science Foundation Graduate Student Fellowship.

H71.00414: Consecutive Study Of Back Contact Barrier Height and CdS Layer Thickness And Their Effect On CdTe Solar Cell Efficiency* PATRICK MILAN (Presenter), MATTHEW MELFI, YUNIS YILMAZ, SADE SAMPSON, MEHMET ALPER SAHINER, PROF WEINING WANG, Seton Hall Univ — Favored for its low cost and relatively high efficiency (22.1% in 2016), Cadmium Telluride (CdTe) solar cells are popular among the thin film generation because they still have room for improvement. CdTe solar cells have a high electron affinity (about 4.5 eV) and as a result when metal contacts are used, a good ohmic contact is not created, and a Schottky barrier is formed at the back-contact junction. This barrier impedes current flow and lowers cell performance. The thickness ratio of Cadmium Sulfide (CdS) to CdTe is also important as increasing or decreasing the thickness of the [n-type] CdS layer will affect the production and recombination rate of charge carriers.

In this work, we show our studies on the effect of the back-contact barrier height and CdS layer thickness on the performance of CdTe solar cells. Using the turning point technique and a corresponding formula, we were able to obtain the barrier height at the back-contact junction of cells with different back-contact materials. We have also fabricated four CdTe samples using a pulsed-laser deposition process, each with a different CdS layer thickness, and have determined their efficiencies. Our results show us that barrier height and CdS layer thickness do have a direct effect on solar cell performance.

*NASA-NJSGC
H71.00415: Non-volatile nanosecond phase change in BiFeO$_3$ thin films induced by pulse laser

YI-DE LIOU, Natl Cheng Kung Univ, HAILI SONG, East China Normal University, WEN-YEN TZENG, National Chiao Tung Univ, RONG HUANG, East China Normal University, CHIH-WEI LUO, National Chiao Tung Univ, YI-CHUN CHEN, JAN-CHI YANG, YU CHEN LIU (Presenter), Natl Cheng Kung Univ — Nowadays, increasing technology interest has focused on the optical control of non-volatile functional units based on ferroic materials, especially those with ultrafast tunabilities. Despite the fact that various light sources can be used to alter the ferroelectricity and magnetization of ferromagnets via means of light, this usually requires low-temperature or high-energy flux to fulfill significant changes. In this work, we reveal nanosecond non-volatile phase alteration in multiferroic BiFeO$_3$ (BFO) thin films.

This approach utilizes the delicate combination of thermal effect and strain pulse triggered by pulsed laser illumination. Taking advantage of the low phase transition barrier in the mixed phase BFO, we successfully demonstrate an effective optical approach to alter the phase distribution and corresponding ferroic properties in BFO. The application of single laser pulse results in the preferred phase transition from mixed phase to tetragonal phase. The fast phase change is attributed to the martensitic phase transformation induced by laser pulse, as evidenced by HAADF-STEM. We further show that the changes results from laser illumination are reversible, demonstrating new pathways to control the ferroic systems in ultrafast time scale through optical stimulus.

H71.00416: Investigation of self-heating phenomena in high-electron mobility transistors (HEMTs) using millisecond-resolution Y-factor method*

ALEXANDER CHOI (Presenter), AUSTIN MINNICH, Caltech — Low noise microwave amplifiers are critical components in measurement systems with applications ranging from qubit readout in quantum computing to the detection of fast radio bursts in RF astronomy. Recent work has suggested that the noise floor in high electron mobility transistors (HEMTs), presently around a factor of 5 above the quantum limit, is in part set by the thermal noise from the gate metal corresponding to a temperature exceeding the cryostat temperature. This temperature differential originates from high thermal resistance associated with phonon blackbody radiation at cryogenic temperatures. In this talk, we report on experiments designed to examine self-heating phenomena in HEMTs at cryogenic temperatures using liquid helium cooling and a custom noise figure analyzer that measures noise temperature with millisecond resolution. Our results confirm that self-heating at cryogenic temperatures is key mechanism in setting the noise floor of transistor amplifiers. These findings help to identify a path for transistor microwave amplifiers operating closer to the standard quantum limit of noise.

*AYC wishes to acknowledge support from the National Science Foundation Graduate Research Fellowship.
**H71.00417: Design of Polyelectrolyte-based Materials using Molecular Modeling**

THOMAS OWEIDA (Presenter), IBRAHIM AHMAD, YAROSLAVA YINGLING, North Carolina State University —
Polyelectrolyte block copolymers have shown promise as carriers for drug and gene delivery due to their ability to self-assemble into a variety of responsive morphologies with tailored properties. Dissipative Particle Dynamics (DPD) is a computationally inexpensive, coarse-grained simulation technique that has previously been used to predict the resulting morphologies of polyelectrolyte block copolymers. However, the design space of these materials is still largely unexplored with the influence of most design parameters being poorly understood. This study utilizes DPD and machine learning methods to investigate a multi-dimensional, morphological phase diagram for polyelectrolyte block copolymers. A machine learning method, support vector machine (SVM), is trained and tested on DPD simulation data to handle the high dimension of features influencing the polyelectrolyte block copolymer morphology. The results are the development of a comprehensive and detailed morphological phase diagrams for block copolymer properties versus environmental conditions that can be used as a robust predictive tool. These results provide the fundamental basis for synthesizing polyelectrolyte block copolymers for materials with novel, desirable properties.

**H71.00418: Jammed solids held together with pins: structure and dynamics**

LIAM PACKER, BRIAN JENIKE, ARI LILOIA (Presenter), AMY GRAVES, Physics, Swarthmore College, SEAN RIDOUT, Physics, University of Pennsylvania — Currently, much is known about idealized grains like soft discs in the vicinity of the "Point J" threshold for jamming. However, an important unanswered question concerns the role that a scaffolding in the form of fixed particles, or "pins", plays in the structure and dynamics of a jammed solid. We model pins as tiny fixed particles organized in lattice shapes such as square, triangular, honeycomb, or randomly distributed lattices. We find a number of interesting results: While at low pin densities the jamming threshold, φj, does what one expects - decreases linearly with pin density and independently of pin geometry - this is not true in general. Instead, the behavior of φj with pin density depends on the type of lattice, and whether the particles are bi- or polydisperse. The distribution of contact forces is very different from the familiar gaussian shape in the absence of pins. The linear elastic response is significantly affected by pins, both in terms of the magnitudes of bulk and shear moduli and the Zener ratio, showing that pins can break the isotropy of jammed states.

*This work was supported by NSF DMR-1905474 and Swarthmore's Provost's Office, Div. of Natural Sciences, Individual Donors, and Sigma Xi. AG is grateful for a Michener Sabbatical Fellowship.*
H71.00419: Adsorption of Binary Gas Mixtures on Graphite*  
G.M DINUKA GALLABA  
(Presenter), ALDO DANTE MIGONE, Department of Physics, Southern Illinois University Carbondale — Determining how a binary gas mixture approaches equilibrium in the presence of a sorbent can have important implications for applications adsorption to gas separation. To understand the behavior of binary gas mixtures we are studying how adsorption equilibrium is reached on a well characterized planar sorbent, exfoliated graphite. We have conducted a series of adsorption measurements of methane and nitrogen mixtures on exfoliated graphite at low temperatures. We will present results for different initial mixture compositions and different temperatures. We will present results on the how the pressure approaches equilibrium, and, on the composition of the mixture at equilibrium for the different conditions explored.

*This work is supported through grant NSF DMR 1807094

H71.00420: Solving the Green's function as a single eigenstate in a boundary value problem  
JOSE HERNANDEZ (Presenter), LI GE, Physics and Astronomy, CUNY College of Staten Island — It is well known that the Green’s function of an operator $L(x)$ in a boundary value problem can be expressed as a bilinear expansion using the eigenstates of $L(x)$. Here we introduce an auxiliary eigenvalue problem, from which the Green’s function is uniquely determined by a single eigenstate. This approach is easy to implement numerically, and it becomes very helpful when the eigenstates of $L(x)$ are badly conditioned, for example, when $L(x)$ is non-Hermitian and at an exceptional point. We illustrate this approach in one-dimensional and two-dimensional Helmholtz equations, with a focus on non-Hermitian systems that are due to their openness as well as non-Hermitian potentials.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J01 DAMOP: Quantum Computing, Communication, and Information in AMO Systems 103 - Ruichao Ma, Purdue Univ

2:30PM J01.00001: Robust and high-fidelity quantum entangling gate with neutral Rydberg atoms*  
XIAO-FENG SHI (Presenter), Xidian University — In this talk, I will show some theoretical proposals of quantum entangling gate with neutral Rydberg atoms that have high intrinsic fidelity and are robust against dephasing from the atomic motion. With off-resonant transitions between ground and Rydberg states, it is possible to induce input-state-dependent phase to the two-qubit state, so that entanglement can be created with only one pulse efficiently. This talk also presents schemes for partially suppressing the motional dephasing of the transition between ground and Rydberg states for neutral atoms.

*This work was supported by the National Natural Science Foundation of China under Grant No. 11805146.
2:42PM J01.00002: Towards Trapping Electrons in Paul Traps for Quantum Computing  
JINEN GUO (Presenter), CLEMENS MATTHIESEN, HARTMUT HAEFFNER, University of California, Berkeley — Trapped-electron qubits provide an interesting alternative to trapped ions in quantum information processing. The operations on trapped electron systems can be all-electronic, making it easier to scale up, and the light mass of electrons enables faster two-qubit gates. In order to evaluate the feasibility of a trapped electron quantum computer, we simulate the electron dynamics inside Paul traps with a drive frequency of 1.5 GHz. From the simulations, we determine the trap depth and explore the validity of pseudopotential approximation. In addition to the electron dynamics in the trapping potential, we also explore how to deterministically eject electrons from the trapping potential towards a particle detector.

2:54PM J01.00003: Controlling entanglement sudden death in two coupled atoms interacting off-resonance with a radiation field*  
GEHAD SADIEK (Presenter), Applied Physics and Astronomy, University of Sharjah, WIAM AL-DRESS, Physics and Astronomy, King Saud University — We study a system of two coupled two-level atoms (qubits) interacting, at non-zero detuning, with a single mode radiation field. This system is of special interest in the field of quantum information processing (QIP) and can be realized in electron spin states in quantum dots or Rydberg atoms in optical cavities and superconducting qubits in linear resonators. We utilize our exact analytical solution for the time evolution of the system to show how entanglement sudden death (ESD), which represents a major threat to QIP, can be efficiently controlled by tuning atom-atom coupling and non-zero detuning. We demonstrate that while one of these two system parameters may not separately affect the ESD, combining the two can be very effective in reducing, eliminating or creating ESD depending crucially on the system initial state. A synchronization between the population inversion collapse-revival pattern and the entanglement dynamics is observed at all system parameter combinations. The variation of the radiation field intensity shows a clear impact on the duration of the ESD at any combination of the other system parameters.

*This work is supported by the University of Sharjah, Vice Chancellor of research office, grant No.1802143060-P.
3:06PM J01.00004: Realizing the Hayden-Preskill Protocol with Coupled Dicke Models*
YANTING CHENG (Presenter), CHANG LIU, Tsinghua University, JINKANG GUO, Department of Physics, Peking University, YU CHEN, Department of Physics, Capital Normal University, PENGFEI ZHANG, Institute for Quantum Information and Matter, California Institute of Technology, HUI ZHAI, Tsinghua University — Hayden and Preskill proposed a thought experiment that Bob can recover the information Alice throws into a black hole if he has a quantum computer entangled with the black hole, and Yoshida and Kitaev recently proposed a concrete decoding scheme. Here we propose to realize this decoding protocol in a physical system of two Dicke models, with two cavity fields prepared in a thermofield double state. We show that the Yoshida-Kitaev protocol allows us to read out the initial spin information after it is scrambled into the cavity. We show that the readout efficiency reaches a maximum when the model parameter is tuned to the regime where the system is the most chaotic, characterized by the shortest scrambling time in the out-of-time-ordered correlation function. Our proposal opens up the possibility of discussing this profound thought experiment in a realistic setting.

*This work is supported by Beijing Outstanding Young Scientist Program (HZ), MOST under Grant No. 2016YFA0301600 (HZ) and NSFC Grant No. 11734010 (HZ and YC), No. 11604225 (YC) and Beijing Natural Science Foundation (Z180013) (YC). PZ acknowledges support from the Walter Burke Institute for Theoretical Physics at Caltech.

3:18PM J01.00005: High-fidelity ground state preparation of single neutral atom in an optical tweezer* XIWANG LUO (Presenter), University of Texas at Dallas, MARK G RAIZEN, University of Texas at Austin, CHUANWEI ZHANG, University of Texas at Dallas — Arrays of neutral-atom qubits in optical tweezers are a promising platform for quantum computation. Despite experimental progress, a major roadblock for realizing neutral atom quantum computation is the qubit initialization. Here we propose that supersymmetry—a theoretical framework developed in particle physics—can be used for ultra-high fidelity initialization of neutral-atom qubits. We show that a single atom can be deterministically prepared in the vibrational ground state of an optical tweezer by adiabatically extracting all excited atoms to a supersymmetric auxiliary tweezer with the post-selection measurement of its atomic number. The scheme works for both bosonic and fermionic atom qubits trapped in realistic Gaussian optical tweezers and may pave the way for realizing large scale quantum computation, simulation and information processing with neutral atoms.

*AFOSR, NSF and ARO.
3:30PM J01.00006: A simple embedding scheme for quantum computer simulations of molecules
CHRISTINA DANIEL (Presenter), MANUEL WEBER, Georgetown University, DOMINIKA ZGID, University of Michigan, JAMES FREERICKS, Georgetown University — Current era noisy intermediate-scale quantum computers are limited in what they can accurately simulate. One of the most successful applications to date has been the variational quantum eigensolver, which uses the quantum computer to create a trial wavefunction and then employs a simple circuit to measure the expectation value of different pieces of the Hamiltonian. A classical computer is employed to accumulate all of the results and determine the energy; it also is employed to optimize the trial wavefunction, if desired. In this work, we focus on the question of whether one can easily improve the accuracy of this calculation via an embedding strategy. We take a classical Hartree-Fock (or similar) approximation for a large system and correct its energy using the correlation energy derived from the smaller quantum computer calculation. We illustrate this concept with calculations performed on some simple molecules.

*We acknowledge support from the National Science Foundation under grant number NSF-CHE-1836497.

3:42PM J01.00007: Memory-enhanced quantum communication using diamond quantum networks
CHRISTIAN NGUYEN (Presenter), MIHIR K BHASKAR, RALF RIEDINGER, BARTHOLOMEUS J MACHIELSE, DAVID LEVONIAN, ERIK KNALL, HONGKUN PARK, Harvard University, DIRK R. ENGLUND, Massachusetts Institute of Technology, MARKO LONCAR, DENIS D SUKACHEV, MIKHAIL LUKIN, Harvard University — The ability to communicate quantum information over long distances is of central importance in quantum science and engineering. For example, it enables secure quantum key distribution (QKD) relying on fundamental principles that prohibit the “cloning” of unknown quantum states. While QKD is being successfully deployed, its range is currently limited by photon losses and cannot be extended using straightforward measure-and-repeat strategies without compromising its unconditional security. Quantum repeaters, which utilize intermediate quantum memory nodes and error correction techniques, can extend the range of quantum channels. However, their implementation remains an outstanding challenge, requiring a combination of efficient and high-fidelity quantum memories, gate operations, and measurements. Here, we present our approach towards building a quantum repeater using silicon-vacancy color centers (a solid-state quantum memory) integrated into diamond nanophotonic cavities.

*This work was supported by the NSF, CUA, DoD/ARO DURIP, AFOSR MURI, ONR MURI, ARL, and a Vannevar Bush Faculty Fellowship. Devices were fabricated at Harvard CNS, NSF award no. 1541959
**3:54PM J01.00008: Continuous protection of a quantum state from inhomogeneous dephasing**

RAN FINKELSTEIN (Presenter), OHR LAHAD, OMRI DAVIDSON, EILON POEM, OFER FIRSTENBERG, Weizmann Institute of Science — Room-temperature atomic vapors are known for their simplicity and their potential scaling-up in applications. In spite of these benefits, laser-cooled atoms have evolved to be the prevalent systems for studying strong and coherent light-matter interactions, as the latter are unhindered by Doppler broadening. Here we present several methods to overcome the effective decrease of both atom-photon cross-section [1] and coherence time in vapors, and in fact in any inhomogeneously broadened atom-like system. The mechanism we study can be understood as the counteraction of the inhomogeneous dephasing of two coupled states, where one state has enhanced sensitivity to the source of dephasing. A far-detuned dressing field admixes a fraction \( \frac{\Omega^2}{\Delta^2} \) of this "sensor" state into the "protected" state, yielding a velocity-insensitive state and line-narrowing in two-color transitions [2]. Finally, we apply this method to extend the lifetime of collective excitations stored in a thermal atomic vapor. This method is continuous, in contrast to pulsed echo-based techniques.


**4:06PM J01.00009: Correlation spectroscopy as a tool for comparing optical clocks**

MAY KIM (Presenter), ETHAN R. CLEMENTS, KAIFENG CUI, AARON HANKIN, SAMUEL M BREWER, JWO-SY CHEN, DAVID B HUME, DAVID LEIBRANDT, National Institute of Standards and Technology Boulder — Highly accurate optical clocks are quantum sensors with fractional frequency uncertainty below one part in \( 10^{18} \) [1]. Comparisons between such clocks can lead to a better understanding of fundamental physics and potentially replace cesium microwave clocks to redefine the SI second. However, noise from the local oscillator often limits the measurement stability of these comparisons, requiring long averaging times to reduce statistical uncertainty. One way to overcome this limitation is by performing correlation spectroscopy in which a Ramsey pulse sequence derived from the same probe laser is applied to the clocks synchronously. The coherent differential frequency measurements between atomic systems permit interrogation times beyond the laser coherence time, which leads to a reduction in the quantum projection noise limit. As a result, the frequency comparison instability is significantly lower than is possible for incoherent comparisons using the same local oscillator. We demonstrate this technique using two Al+ quantum-logic clocks separated in space by a few meters.


*This work was supported by the Defense Advanced Research Projects Agency, the National Institute of Standards and Technology, and the Office of Naval Research.*
Correlation Spectroscopy Between Two $^{27}$Al$^+$ Quantum-Logic Clocks

ETHAN CLEMENTS (Presenter), MAY KIM, KAIFENG CUI, AARON HANKIN, SAMUEL M BREWER, JWOSY CHEN, DAVID LEIBRANDT, DAVID B HUME, National Institute of Standards and Technology Boulder — Correlation spectroscopy is a technique for performing coherent differential frequency measurements between two atomic clocks with an interrogation time beyond the coherence time of the local oscillator. This technique was initially demonstrated for two co-trapped ions [1-3]. Here, we present a demonstration of correlation spectroscopy between two independent $^{27}$Al$^+$ optical atomic clocks separated by a few meters. We discuss limitations caused by differential noise sources and techniques that can be used to mitigate these effects. Correlation spectroscopy allows us to extend the interrogation time to 8 seconds, beyond the capability of cavity stabilized lasers and approaching the lifetime limit of the Al$^+$ atomic transition. From this increase in the interrogation time we obtain a fractional measurement instability below $4 \times 10^{-16}$ at 1 s, a factor of $\sim 10$ improvement from previous Al$^+$ clock comparisons.


This work was supported by the Defense Advanced Research Projects Agency, the National Institute of Standards and Technology, and the Office of Naval Research.

Conversion of position correlation into polarization entanglement

CHITHRABHANU PERUMANGATT (Presenter), ALEXANDER LOHRMANN, ALEXANDER LING, Centre for Quantum Technologies — Photons entangled in polarization have been a prime tool for experiments in fundamental quantum physics. To generate polarization entanglement from spontaneous parametric down conversion (SPDC), it is necessary to impose coherent superposition of two pump-decay paths. There is a variety of techniques by which this coherent superposition can be achieved. Examples of previous entangled photon-pair sources have utilized momentum correlation, indistinguishable pump decay in two separate crystals, or two distinguishable pump beams. We present a method to convert position correlation of photon-pairs into polarization entanglement. This is achieved by individually manipulating the polarization state of photons generated in different parts of a non-linear medium and putting them in coherent superposition. This concept is experimentally demonstrated using photon-pairs produced by SPDC. The method was used to implement a compact source producing an observed photon-pair rate of 120,000/s/mW with an entanglement fidelity of 0.99. This method can be extended to any photon-pair generation process with initial position correlation.

This research is supported by National Research Foundation, and the Singapore Ministry of Education Research Centres of Excellence program.
4:42PM J01.00012: Toward quantum-logic spectroscopy of single molecular ions in a cryogenic ion trap* DALTON CHAFFEE (Presenter), ALEJANDRA L COLLOPY, DIETRICH LEIBFRIED, DAVID LEIBRANDT, CHIN-WEN CHOU, Time and Frequency Division, NIST, Boulder — Quantum state control of trapped and cooled atomic ions is an established technique with applications including precision metrology and quantum computing. Molecules provide even richer physics, but their additional degrees of freedom make such control more challenging. In our group, quantum-logic spectroscopy (QLS) of a single CaH⁺ ion has enabled preparation and coherent manipulation of pure molecular quantum states [1]. However, the currently used loading scheme is applicable only to certain hydrides, and background gas collisions and black-body radiation in the room-temperature apparatus eventually limit measurement precision and fidelity of quantum control. Here, we present progress of the design and construction of a cryogenic ion trap apparatus for more versatile loading of molecular ions and better control of their states. Molecules will be injected from an interchangeable gas source, ionized in a strong laser field, and co-trapped with an atomic ion for QLS. This device will be used to perform precision spectroscopy of molecules relevant for, e.g., tests of fundamental physics.


*This work was supported by the Army Research Office and the National Science Foundation.

4:54PM J01.00013: Towards quantum logic spectroscopy of multi-ion arrays* KAIFENG CUI (Presenter), KEVIN T BOYCE, DAVID LEIBRANDT, DAVID B HUME, PML, National Institute of Standards and Technology Boulder — We describe a new approach for precision spectroscopy of trapped ions using quantum logic. Our approach adapts method developed in the context of quantum information processing to non-destructive detection of the ¹S₀-³P₀ clock transition in ²⁷Al⁺. A state-dependent force is employed on the spectroscopy ion(s) to modulate the qubit state of the detection ion(s), similar to the techniques employed for high-fidelity quantum gates[1,2] and sensitive force detection experiments [3,4]. This method does not require ground state cooling and would enable scaling to large numbers of spectroscopy ions to improve ion clock stability.


*This work was supported by Argonne National Laboratory, the Defense Advanced Research Projects Agency, the National Institute of Standards and Technology, and the Office of Naval Research.
5:06PM J01.00014: Direct characteristic-function tomography of quantum states of the trapped-ion motional oscillator*  CHRISTA FLÜHMANN (Presenter), Institute for Quantum Electronics, ETH Zurich — Quantum state reconstruction is an important element enabling diagnosis and improvement of quantum control. As larger states come under experimental control the number of measurements required to perform state reconstruction becomes crucial. Here, significant gains can be found by choosing the appropriate basis in which to make measurements. In this talk I will present recent experiments analyzing direct phase-space tomography of the motion of a single trapped Ca$^+$ ion. The method, which is based on ion internal state rotations combined with state-dependent shifts of the oscillator, is used to reconstruct displaced squeezed oscillator states as well as a three-component superposition thereof. Such states have applications in quantum information, quantum sensing and fundamental studies. We find reductions in measurement times of a factor 20 compared to methods we used previously, which we anticipate to improve future ion motion state preparation and control.

*We acknowledge support from the Swiss National Science Foundation through the National Centre of Competence in Research for Quantum Science and Technology (QSIT) grant 51NF40-160591, and from the Swiss National Science Foundation under grant number 200020_165555/1.

5:18PM J01.00015: High dimensional entanglement between a photon and a multiplexed atomic quantum memory  CHANG LI (Presenter), YUKAI WU, WEI CHANG, SHENG ZHANG, LUMING DUAN, Center for Quantum Information, Tsinghua University — Multiplexed quantum memories and high-dimensional entanglement can improve the performance of quantum repeaters by promoting the entanglement generation rate and the quantum communication channel capacity. Here, we experimentally generate a high-dimensional entanglement between a photon and a collective spin wave excitation stored in the multiplexed atomic quantum memory. We verify the entanglement dimension by the quantum witness and the entanglement of formation. Then we use the high-dimensional entangled state to test the violation of Bell-type inequality. Our work provides a prominent method to generate multidimensional entanglement between the flying photonic qubits and the atomic quantum interfaces, a key step toward quantum networks.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J02 DQI DAMOP: Advances in AMO Quantum Information and Technologies 105 - Alejandra Collopy, National Institute of Standards and Technology Boulder
2:30PM J02.00001: Rydberg physics for quantum computing in arrays of neutral atom qubits  JONATHAN KING (Presenter), ALEXANDER PAPAGEORGE, SABRINA HONG, REMY NOTERMANS, BRIAN LESTER, STANIMIR KONDOV, KRISH KOTRU, MICKEY MCDONALD, ROBIN COXE, PRASAHNT SIVARAJAH, BENJAMIN BLOOM, Atom Computing, Inc — Ultracold neutral atoms have recently emerged as a scalable quantum computing platform. Their long coherence times and parallel coherent control portend the realization of high-fidelity quantum operations on large arrays of qubits. Interactions between neutral atoms in Rydberg states provide a means to 2-qubit and multi-qubit gates. Understanding the energy level structure of Rydberg atoms and their interactions are a necessary prerequisite to designing gate schemes. To this end we discuss Rydberg interactions for quantum computing with trapped single atoms, including simulations of the full Hilbert space relevant to 2-qubit gates.

2:42PM J02.00002: Robustness and sensitivity to imperfections in the dynamics of general observables within near-term quantum simulators*  PABLO POGGI (Presenter), University of New Mexico, NATHAN LYSNE, KEVIN KUPER, POUL STERNDORFF JESSEN, University of Arizona, IVAN DEUTSCH, University of New Mexico — We analyze the robustness of analog quantum simulators in the presence of weak perturbations. To this end, we focus on the dynamics of expectation values for generic observables and study the error arising from the imperfect operation of the device. We show that the properties of the error depend crucially on the observable considered as output of the simulator and we demostrate how even a low-fidelity quantum simulation is still able to reproduce the dynamics of other observables with a small relative error. To explain this, we define the observable purity, which characterizes the magnitude of the support of the observable in Hilbert space, and analytically show that these imperfect devices are able to reproduce the dynamics of low-purity observables (such as collective operators like the magnetization in a spin system) accurately, while the error in the expectation value of high-purity observables (such as projectors onto pure states) are much larger on average. We demonstrate our findings in a state-of-the-art 16-dimensional quantum simulator where, without assuming any particular error model, we observe this predicted behavior. This shows that these features are generic for a highly accurate device where we expect imperfections to be small.

*Support from NSF is acknowledged
A central goal for modern quantum information science is to demonstrate computational speedup for experimentally feasible architectures in the noisy intermediate-scale regime. In a previous work, we studied this problem in the context of simulating boson sampling by noninteracting bosonic atoms on a one-dimensional lattice [1]. We extend these results to include Bose-Hubbard-type interactions. In the presence of weak interactions, we show that the output-sampling distribution is close to that of a free-boson sampler in the total variational distance. We calculate the scaling of the interaction-strength such that this total variational distance is bounded by a constant, demonstrating a regime where the sampling complexity is equivalent to that of the corresponding boson sampler. We close with some outlook for the possibility of applying worst-to-average-case reduction tools to extend these results beyond the perturbative regime.


*Google Quantum Algorithms Focused Award.

Strong and precisely controlled interactions between quantum objects are essential for emerging technologies such as quantum information processing, simulation, and sensing. A well-established paradigm for coupling otherwise weakly interacting quantum objects is to use auxiliary quantum particles, typically bosons, to mediate interactions, for example photon-mediated interactions between atoms or superconducting qubits, and phonon-mediated interactions between trapped ions. General methods for amplifying these interactions through parametric driving of the boson channel have been proposed for a variety of quantum platforms, but an experimental demonstration has yet to be realized. Here we experimentally demonstrate the amplification of a boson-mediated interaction between two trapped-ion qubits by parametrically modulating the confining potential of the trap. The stronger interaction enables a 3.3-fold reduction in the time required to implement an entangling gate between the two qubits. Our method can be applied wherever parametric modulation of the boson channel is possible, enabling its use in a variety of quantum platforms to explore new parameter regimes and for enhanced quantum information processing.

*We acknowledge funding from the NIST Quantum Information Program
3:18PM J02.00005: TDDFT potential inversion applied to spin systems on noisy quantum computers*  JAMES BROWN (Presenter), JUN YANG, JAMES D WHITFIELD, Dartmouth Coll — One route to numerically propagating quantum systems is time-dependent density functional theory (TDDFT). We recently introduced a newly developed solver[arXiv:1904.10958] for the scalar time-dependent Kohn-Sham potential using a grid-like basis of Sinc functions. In this talk, we discuss the application of this method to describing interacting spin systems (which can be implemented readily on quantum computers) as a non-interacting Kohn-Sham system. The method's robustness when used in conjunction with current noisy quantum devices is discussed.

*This work was primarily supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, under the Quantum Computing Application Teams program (Award 1979657). JDW was also supported by Walter and Constance Burke award, the NSF (Grant 1820747) and additional funding from the DOE (Award A053685).

3:30PM J02.00006: Electric field in a two-dimensional time-multiplexed photonic quantum walk  HAMIDREZA CHALABI (Presenter), SABYASACHI BARIK, SUNIL MITTAL, THOMAS E. MURPHY, MOHAMMAD HAFEZI, EDO WAKS, University of Maryland, College Park — It is of fundamental importance to control the evolution of a photonic quantum walk for conducting various quantum simulations. However, due to the lack of charge, photons are indifferent to applied electric fields, which limits our ability to control photonic quantum walks. One approach to mimic the effect of electric fields is through the use of synthetic gauge fields. In this presentation, we show the creation of a uniform effective electric field using a linearly time-varying gauge field in a time-multiplexed two-dimensional quantum walk. In this platform, varied lengths of optical fibers create time delays and the gauge fields are implemented through phase modulations. We demonstrate that the generated electric field leads to Bloch oscillations that enable revival of the quantum walker state. By measuring the probability of the revival, we show good agreement between the observed values and the theoretically predicted results. We also demonstrate the possibility of waveguiding quantum walkers by applying an inhomogeneous electric field.
Experimental few-copy multipartite entanglement detection  

VALERIA SAGGIO (Presenter), Univ of Vienna, ALEKSANDRA DIMIĆ, University of Belgrade, CHIARA GREGANTI, VitreaLab GmbH, LEE ARTHUR ROZEMA, PHILIP WALThER, BORivoJE DAKiC, Univ of Vienna — The reliable verification of quantum entanglement is an essential task to scale up quantum technologies. Although progressively more efficient techniques have been developed, most of these focus solely on minimizing the number of measurement settings. Recently, a single-shot probabilistic method was proposed [1], wherein it was shown that even a single detection event can be sufficient to verify if a state exhibits entanglement. In our work [2] we extend this theoretical approach by showing that any entanglement witness can be translated into this probabilistic framework. To prove our findings, we report the experimental entanglement verification in a photonic six-qubit cluster state. We find that the presence of entanglement can be certified with at least 99.74% by using only 20 copies of the state, and that genuine six-qubit entanglement is verified with at least 99% confidence by using 112 copies of state. This novel method entails a significant reduction of resources, promising a great impact in future experiments where an efficient and resource saving approach will be essential for entanglement verification problems in multi-qubit states.


Deterministic Logic Gates for Photonic Qubits* 

MIKKEL HEUCK (Presenter), Massachusetts Institute of Technology MIT, KURT JACOBS, Computational and Information Sciences Directorate, U. S. Army Research Laboratory, DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — Quantum logic gates operating on qubits encoded in photons are highly desirable for processing quantum information as it is being transmitted through quantum networks. However, the difficulty of enabling sufficiently strong interactions between photons has hindered their experimental realization. Additionally, the multi-mode nature of finite-duration photon wave packets limits the gate fidelity if photons interact while travelling. We propose a method that converts travelling continuous-mode photons into quasi-single mode fields by absorbing them into cavities. This is enabled by strong classical control fields that perform the necessary re-distribution of photon frequency-modes. Letting the photons interact while occupying modes of a cavity with high quality factor and low mode-volume achieves a large interaction strength and simultaneously avoids gate fidelity degradations. We consider nonlinear interactions due to \( \chi^{(2)} \), \( \chi^{(3)} \), and atom-like emitters. Our numerical results show that high-fidelity gates are possible with near-term improvements in nanofabrication.

*This work was funded by the AFOSR program FA9550-16-1-039, the MITRE Quantum Moonshot Program, and the ARL DIRA ECI grant "Photonic Circuits for Compact (Room-temperature) Nodes for Quantum Networks".
4:06PM J02.00009: Accelerating quantum optics experiments using statistical learning*
Cristian Cortes (Presenter), Sushovit Adhikari, Xuedan Ma, Stephen K Gray, Argonne Natl Lab — Quantum optics experiments, involving the measurement of low-probability photon events, are known to be extremely time-consuming. In this talk, we present a new methodology for accelerating such experiments using simple statistical learning techniques such as Bayesian maximum a posteriori estimation based on few-shot data. We show it is possible to reconstruct time dependent data using a small number of detected photons, allowing for fast estimates in under a minute, and providing a one-to-two order of magnitude speed up in data acquisition time. We test our approach using real experimental data to retrieve the $G^2(\tau)$ time trace for thermal light emitted by a Neon light source as well as anti-bunched light emitted by a quantum dot driven with periodic laser pulses. We also show, through numerical simulations, that our approach can be used to accelerate sub-diffraction image reconstruction based on $G^2(\tau)$ coincidence measurements. The proposed methodology has the potential to impact the scientific discovery process across a multitude of domains.

*This work was performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, and supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

4:18PM J02.00010: Machine Learning Topological Phases with a Solid-State Quantum Simulator*
Wenqian Lian (Presenter), Center for Quantum Information, IIS, Tsinghua University, Shengtao Wang, Department of Physics, Harvard University, Sirui Lu, Wengang Zhang, Xiaolong Ouyang, Xin Wang, Xianzhi Huang, Dong-Ling Deng, Luming Duan, Center for Quantum Information, IIS, Tsinghua University — We report an experimental demonstration of a machine learning approach to identify exotic topological phases, with a focus on the three-dimensional chiral topological insulators. We show that the convolutional neural networks—a class of deep feed-forward artificial neural networks with widespread applications in machine learning—can be trained to successfully identify different topological phases protected by chiral symmetry from experimental raw data generated with a solid-state quantum simulator. Our results explicitly showcase the exceptional power of machine learning in the experimental detection of topological phases, which paves a way to study rich topological phenomena with the machine learning toolbox.

*This work was supported by the National key Research and Development Program of China (Grant No. 2016YFA0301902), Tsinghua University, and the Ministry of Education of China.
4:30PM J02.00011: Heralding High Fidelity Entanglement Between Imperfect Artificial Atoms*  
HYEONGRAK CHOI (Presenter), DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — Color centers in diamond have emerged as excellent candidates for quantum networks. However, despite their stable optical properties, residual spectral dephasing and diffusion still limit the achievable fidelity of heralded entanglement. Here, we address this problem through a new single-photon entanglement protocol that uses detuned optical coupling to spin-dependent optical transitions. Our calculations include entanglement distillation and are compared to other leading entanglement protocols. Estimates based on present-day technology indicate that this protocol enables entanglement fidelity in excess of 99% for leading diamond color centers.

*The authors acknowledge the support from the Air Force Office of Scientific Research MURI (FA9550-14-1-0052), the Army Research Laboratory (ARL) Center for Distributed Quantum Information (CDQI), the Defense Advanced Research Projects Agency (DARPA) DRINQS (HR001118S0024) and the National Science Foundation (NSF) RAISE TAQS (CHE1839155) and EFRI ACQUIRE (EFMA-1838911).

4:42PM J02.00012: A Dielectric Antenna for Quantum Emitter Interfaces*  
LINSEN LI (Presenter), HYEONGRAK CHOI, DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — Color centers in diamond have shown long spin coherence time and stable optical properties as a promising system for large scale quantum information processing. Collecting single photons from emitters with high efficiency can significantly boost the entanglement generation rate of remote quantum memories. Here, we propose a method to design a dielectric antenna for low numerical aperture optics systematically. Our simulation results show that the design is robust in the presence of fabrication imperfection. The dielectric antenna design enables efficient interfaces to closely packed arrays of quantum memories for multiplexed quantum repeaters, arrayed quantum sensors, and modular quantum computers.

*The authors acknowledge the support from the Defense Advanced Research Projects Agency (DARPA) DRINQS (HR001118S0024) and the Air Force Office of Scientific Research MURI (FA9550-14-1-0052). L. Li acknowledges the Analog Devices Fellowship.
4:54PM JO2.00013: Sub-kilohertz optical homogeneous linewidth in transparent Er$^{3+}$:Y$_2$O$_3$ ceramics*  RIKUTO FUKUMORI (Presenter), YIZHONG HUANG, University of Chicago, JUN YANG, HAITAO ZHANG, Corning Inc., TIAN ZHONG, University of Chicago — Global quantum networks require quantum memories with long coherence times to act as quantum repeaters connected by optical fibers. Erbium doped solid-state systems are good candidates for such memories, as they exhibit long coherence lifetimes and an optical transition in the low-loss telecom band. We measure an optical homogeneous linewidth of 580 Hz in transparent Er$^{3+}$:Y$_2$O$_3$ ceramics at millikelvin temperatures, the narrowest so far in rare-earth doped ceramics, and suppressed spectral diffusion at 300 Hz/decade. Temperature, field, and time dependence studies of homogeneous linewidth reveal the limiting dephasing mechanisms as tunneling two-level systems and superhyperfine interactions between the electronic spins of erbium and nuclear spins of yttrium. These spectroscopic results put Er$^{3+}$:Y$_2$O$_3$ ceramics as a promising candidate for telecommunication quantum memories.

*We acknowledge funding support from the National Science Foundation EAGER award No 1843044, Funder Id: http://dx.doi.org/10.13039/100000001

5:06PM JO2.00014: Cavity nano-optics with configurable interaction: room temperature strong coupling of single emitter  MOLLY A. MAY, University of Colorado, Boulder, DAVID FIALKOW, University of Maryland, Baltimore County, TONG WU, Institute d'Optique, CRNS, University of Bordeaux, KYOUNG-DUCK PARK, University of Colorado, Boulder, HAIXU LENG, JARON KROPP, THEODOSIA GOUGOUSI, University of Maryland, Baltimore County, PHILIPPE LALANNE, Institute d'Optique, CRNS, University of Bordeaux, MATTHEW A PELTON, University of Maryland, Baltimore County, MARKUS B. RASCHKE (Presenter), University of Colorado, Boulder — Quantum state control of two-level emitters is fundamental for many information processing, metrology, and sensing applications. However, quantum-coherent photonic control of solid-state emitters has traditionally been limited to cryogenic environments, which are not compatible with implementation in scalable, broadly distributed technologies. In contrast, plasmonic nanocavities with deep sub-wavelength mode volumes have recently emerged as a path towards room temperature quantum state hybridization and control. Here we establish plasmonic tip-enhanced strong coupling (TESC) with a configurable nano-tip cavity to modulate and control the cavity-emitter interaction with sub-nanometer precision, quantify coupling strength exceeding ~160 meV, at mode volumes of $< 10^{-6} \lambda^3$, augmented by theoretical modeling. Based on this work, we provide a perspective for nano-cavity optics as a promising tool for room temperature control of quantum coherent interactions that could spark new innovations in fields from quantum information and quantum sensing to quantum chemistry and molecular opto-mechanics.
5:18PM J02.00015: A cavity enhanced spin-photon interface for NV centers in a quantum network*  MATTHEW WEAVER (Presenter), MAXIMILIAN RUF, MATTEO PASINI, Delft University of Technology, MARTIN ESCHEN, TNO, RONALD HANSON, Delft University of Technology — Fast entanglement generation between remote nodes is the foundation for quantum networks. Experiments with Nitrogen Vacancy (NV) centers in bulk diamond have made promising progress towards such a network, because of their long spin coherence, narrow optical transitions and accessible nuclear spin memories. However, these demonstrations are currently limited by low emission into the zero phonon line and low collection efficiency. To boost emission and collection, we construct a tunable Fabry-Pérot cavity around NV centers in a diamond membrane. We verify the good optical properties of NV centers in membranes and observe the characteristic lifetime reduction from Purcell enhancement of the zero phonon line. These measurements progress towards an NV node for networks with two orders of magnitude faster entanglement rates.

*NWO, ERC, Quantum Flagship, QIA

Tuesday, March 3, 2020 2:30 PM - 5:06 PM

Session J03 GSCCM: Materials in Extremes: Novel Materials and Phenomena at Extreme Conditions 107 - Elissaios Stavrou, Lawrence Livermore Natl Lab -

Tag(s): Focus

2:30PM J03.00001: Novel experimental approaches toward metastable materials discovery under pressure [Invited]  JAMES WALSH (Presenter), Univ of Mass - Amherst — High pressure is a powerful synthetic tool that enables the discovery of novel materials with unprecedented bonding, crystal structure, and bulk properties. We are developing experimental methods that provide chemists with access to regions of high-pressure phase space that are currently difficult to explore. Examples include methods to target specific elemental compositions in ternary systems where competing binary phases are a complication, or techniques to kinetically stabilize high-pressure phases that do not survive traditional decompression routes. Our work is underpinned by state-of-the-art DFT packages that allow us to explore systems in search of candidate high-pressure phases and determine their formation conditions before even stepping into the lab. I will present recent results that highlight the growing synergy between cutting-edge computational methods and novel experimental approaches.
3:06PM J03.00002: New materials under extreme environments*  WENDY MAO (Presenter), Stanford Univ — The application of extreme environments (including variable pressure, temperature and irradiation) can induce dramatic changes in materials and give us a much broader field to discover new phases and explore novel phenomena. Improving our understanding of the modifications that occur can also provide guidance for designing improved materials with desirable properties that can be utilized for energy-related applications. I will presenting some examples which demonstrate the range of new materials that can be formed and properties which can be altered under extreme environments. In particular, I will focus on experimental work using high pressure as promising variable for tuning materials behavior.

*This work was supported by the Department of Energy (DOE) through the Stanford Institute for Materials & Energy Sciences DE-AC02-76SF00515.

3:18PM J03.00003: Detection of High-Pressure Electride Phases with X-ray Diffraction: A First Principles Analysis*  RAFI ULLAH (Presenter), STANIMIR BONEV, Lawrence Livermore Natl Lab — The direct experimental detection of high pressure electride phases of matter is a challenging problem. It was suggested that the interstitial localization of valence electrons - a signature of the electride phase - could be detected in the x-ray diffraction experiments. We have used first-principles calculations to quantify detectable changes in the x-ray scattering patterns of high pressure electrides. A comparison of the electron localization function and the first principles charge density to corroborate the nature and extent of interstitial electron localization will be discussed as well.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. The funding through LDRD Grant No. 17-ERD-025 is thankfully acknowledged. IM No. LLNL-ABS-795462.
**3:30PM J03.00004: High-pressure chemistry of transition metal polynitrides**

MAXIM BYKOV (Presenter), Howard University, STELLA CHARITON, Center for Advanced Radiation Sources, University of Chicago, ELENA BYKOVA, Geophysical Laboratory, Carnegie Institution of Washington, MOHAMMAD MAHMOOD, Howard University, ALEXANDER GONCHAROV, Geophysical Laboratory, Carnegie Institution of Washington, LEONID DUBROVINSKY, Bayerisches Geoinstitut, University of Bayreuth — The high-pressure chemistry of nitrogen and nitrogen-rich compounds have been in a focus of many studies in the recent years due to both fundamental and practical interest and due to the improvement of high-pressure synthetic and characterization techniques. Poly-nitrogen compounds are usually considered as potential high energy density materials (HEDM) due to the remarkable difference in the average bond energy between the single N–N bond, the double N≡N bond, and the triple N=N bond. Numerous polynitrogen compounds with various nitrogen polymeric networks were theoretically predicted, but there are only a very few experimental attempts to obtain such compounds.

In the present work we have systematically studied reactions between 5d transition metals and nitrogen at pressures up to 130 GPa in laser-heated diamond anvil cells. All 5d metals except Au react with nitrogen at these conditions resulting in the formation of polynitrides with various types of polynitrogen species. Here we will discuss current progress in high-pressure chemistry of nitrogen, methodological challenges and novel approaches to the high-pressure synthesis.

*Research was sponsored by the Army Research Office and was accomplished under the Cooperative Agreement Number W911NF-19-2-0172.

**3:42PM J03.00005: Formation of XeN$_4$ at high pressure-high temperature conditions**

MADDDURY SOMAYAZULU (Presenter), X-ray Science Division, Argonne Natl Lab, ALEXANDER GONCHAROV, Geophysical Laboratory, Carnegie Institution for Science, YUE MENG, JESSE SMITH, X-ray Science Division, Argonne Natl Lab, WATKINS B ERIK, DANA DATTELBAUM, M Division, Los Alamos National Laboratory, RUSSELL J HEMLEY, Department of Physics and Chemistry, University of Illinois at Chicago — Mixtures of xenon and nitrogen have been observed to form a cubic, van der Waals compound Xe(N$_2$)$_2$ at pressures above 2 GPa in concurrence with the study reported to pressures above 150 GPa [1,2]. The existence of the z phase of nitrogen [3] and hcp xenon [4] could be inferred from x-ray diffraction. The sample becomes opaque above 170 GPa and could be laser heated quite easily. In contrast to what is reported for pure N$_2$ [5], a new phase forms when the sample was laser heated above 2800 K and above 160 GPa. This phase is identified to be monoclinic and has distinctive Raman signatures that can be ascribed to the existence of N$_4$ units which are linear and double bonded. This is at variance to the theoretical prediction of cubic XeN$_6$ [6]. We will report the details of the spectroscopy (Raman and FTIR) as well as synchrotron powder diffraction analysis of this potentially energetic nitride of xenon.

3:54PM J03.00006: High Magnetic Field Probe of Hydride Superconductors*  FEDOR BALAKIREV (Presenter), DAN SUN, JONATHAN B BETTS, Los Alamos Natl Lab, SHIRIN MOZAFFARI, LUIS BALICAS, National High Magnetic Field Laboratory, MARI EINAGA, KATSUYA SHIMIZU, Osaka University, VASILY S MINKOV, PANPAN KONG, DMITRY KNYZAEV, ALEXANDER DROZDOV, MIKHAIL EREMETS, Max-Planck-Institut fur Chemie — High magnetic fields have proven to be an invaluable tool for exploring properties of novel superconductors. A combination of miniature diamond anvil cells and pulse magnets allows us to controllably tune and probe the superconducting order and the vortex matter in several recently discovered hydride superconductors at the extremes of pressure-field parameter envelope. Because of the larger superconducting energy scale, magnetic fields of the order of 100 T are required to establish key superconducting properties, including Cooper pair coherence length, the strength of the electron-phonon coupling, the role of the spin-orbit coupling, and the dominant mechanism breaking the Copper pairs. We find that the orbital effect suppresses superconductivity over the entire temperature range, while pronounced deviations from the Werthamer, Helfand, and Hohenberg theory predictions are observed at lower temperatures.

*The work at NHMFL was supported by the National Science foundation under cooperative Grant Nos. DMR-1157490 and DMR-1644779, the U.S. DOE, and the State of Florida, and DoE-BES DE-SC0002613.

4:06PM J03.00007: High-pressure studies of magnetism on EuAFe$_4$As$_4$ (A=Rb, Cs) via synchrotron Mössbauer spectroscopy*  WENLI BI (Presenter), Univ of Alabama - Birmingham, PHILIPP MATERNE, JIYONG ZHAO, ESEN E. ALP, JIN-KE BAO, Argonne National Laboratory, YI LIU, GUANG-HAN CAO, Zhejiang University — EuAFe$_4$As$_4$ (A=Rb, Cs) is a recent addition to the iron-based superconductors. EuAFe$_4$As$_4$ exhibits peculiar properties with coexistence of superconductivity ($T_C \sim 35$ K) and ferromagnetism from local moment in divalent Eu ($T_m \sim 15$ K) [1–4]. The application of pressure suppresses superconductivity and enhance magnetic ordering temperature [5,6] with a crossover of $T_C$ and $T_m$ around 7 GPa [5]. We have investigated the magnetic and valence state in Eu ions via synchrotron Mössbauer spectroscopy in $^{151}$Eu in diamond anvil cell. The detailed changes of Eu’s magnetism and local magnetic phase diagram will be discussed.


*The Experiments were carried out at beamline 3ID of the Advanced Photon Source, Argonne National Laboratory. Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
4:18PM J03.00008: Understanding EuD₄TEA and its Use as Impact or Radiation Sensors in Extreme Environments  JOHN MILLER (Presenter), WILLIAM A. HOLLERMAN, Physics, University of Louisiana at Lafayette, KARILI TOLGA, Chemistry, University of Louisiana at Lafayette, ALYSSA V. BIENVENU, Chemistry, Pennsylvania State University — If humans desire to leave the safety of Earth and explore extreme environments, cost effective and low mass health monitoring sensors will be essential to monitor impacts or incident ionizing radiation as they travel. To ensure the safety of the astronauts, a luminescent material-based sensor might be used to provide reliable in-situ impact detection or radiation monitoring for space vehicles. An extensive research program has been completed to date where many luminescent materials have been irradiated with protons and electrons. Results have generally shown that charged particle irradiation reduces the intensity of emitted luminescence by producing quenching centers. Related research has also shown that some of the same materials will emit copious light in the form of triboluminescence when crushed or struck. This paper investigates the effects of impacts or radiation on europium tetrakis dibenzoylmethide triethylammonium (EuD₄TEA). Special emphasis will be placed on our work to better understand the structure and composition of EuD₄TEA. This research can be used to help determine if luminescent materials can be used as an impact or radiation sensor in extreme environments like space.

4:30PM J03.00009: “Persistent” Insulator: Avoidance of Metallization at Megabar Pressures in Strongly Spin-Orbit-Coupled Sr₂IrO₄  ZHAORONG YANG (Presenter), CHUNHUA CHEN, YONGHUI ZHOU, High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei 230031, China, GANG CAO, Department of Physics, University of Colorado at Boulder — Here we report a rare insulating state that persists up to at least 185 GPa in the antiferromagnetic iridate Sr₂IrO₄, which is the archetype of a spin-orbit-driven Jₑₛₛ = 1/2 insulators. This study shows the electrical resistance of single-crystal Sr₂IrO₄ decreases initially with pressure, then reaches a minimum in the range, 32 - 38 GPa, and is followed by a rapid rise to fully recover the insulating state (~10⁷ W) with further pressure increases up to 185 GPa. The onset of the rapid increase in resistance is accompanied by a structural phase transition from the native tetragonal I₄₁/aₐcd phase to an orthorhombic Pbca phase (with much reduced symmetry) at 40.6 GPa, according to our synchrotron x-ray diffraction and Raman scattering data. This close correlation explains the existence of the rare insulating state at megabar pressures: the pressure-induced, severe structural distortions prevent expected metallization, despite a 26% volume compression in Sr₂IrO₄ at the highest pressure accessed in this experiment. It is striking that the high electrical resistance remains essentially unchanged with a tripling of very high pressure range from 61 GPa to 185 GPa.

4:42PM J03.00010: Pressure-Induced novel properties in Several Topological Materials.  XIANGANG WAN (Presenter), Nanjing Univ — Topological materials, exemplified by the topological insulators and nodal semimetals, showcase intriguing physical properties which could not emerge had electrons been classical particles. Recently the effect of high pressure on these materials has also attracted much attention. We will discuss our results in several topological materials.
4:54PM J03.00011: Hydrostatic pressure effect on several superconductors: 1T- & 2H-Ta(S,Se)₂ and (Ba, Sr)Bi₃  BOSEN WANG (Presenter), JINGUANG CHENG, Chinese Academy of Sciences, Institute of Physics, YUPING SUN, High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei, YOSHIYA UWATOKO, Institute for Solid State Physics, University of Tokyo — Under high hydrostatic pressure in Cubic Anvil Pressure Apparatus, we revealed the universal phase diagram of superconductivity and charge density wave (CDW) for 1T- and 2H-Ta(S,Se)₂ by electrical transport and ac susceptibility. For 1T-, CDWs and SC coexists in narrow pressure windows and superconducting transition temperature (T_c) increases monotonously, clarifying that the superconducting cooper-pairing is associated with CDW instability [1, 2]. For 2H-, CDWs and SC coexists in a real space and T_c tends to saturation at critical pressures. Possible physical mechanisms are proposed. Besides, we firstly reported pressured-induced crossover from Type-II to Type-I superconductivity in spin-orbit-coupled SCs (Ba, Sr)Bi₃ [3].

References:

J03.00012: High-pressure synthesis and pressure-induced spin, charge and lattice transitions of PbCoO₃  YOUWEN LONG (Presenter), Chinese Academy of Sciences — By using a peculiar high-pressure and high-temperature method, we for the first time prepared PbCoO₃ [1]. It crystallizes into an A-site and B-site ordered quadruple perovskite structure with space group of Pn-3. The charge combination is confirmed to be Pb²⁺Pb⁴⁺₃Co²⁺₂Co³⁺₃O₁₂, where the Co²⁺ is high spin while the Co³⁺ is low spin. Although only Co²⁺ is magnetic, the compound experiences two antiferromagnetic transitions. More interestingly, when external pressure is applied, the high spin Co²⁺ gradually changes to low spin with pressure up to 15 GPa. Between 15 and 30 GPa, the intermetallic charge transfer occurs between Pb⁴⁺ and Co²⁺. The accumulated charge-transfer effect triggers a metal-insulator transition as well as a first-order structural phase transition toward a Tetra.-I phase at ~20 GPa near room temperature. On further compression over 30 GPa, the charge transfer completes, leading to another first-order structural transformation toward a Tetra.-II phase and the reentrant electrical insulating behavior.

J03.00013: Computational prediction of correlated iron compounds at high pressure and experimental synthesis  DUCK YOUNG KIM (Presenter), HPSTAR (Beijing) — Iron is one of key elements in our contemporary technology and the backbone element of the Earth. Study on pure iron and iron-compounds in extreme conditions is important and finding new iron compounds is particularly of our interest. In this talk, I will present recent progress in finding new iron compounds at high pressure. Computationally we used ab initio structure searching strategies to predict the compositions and crystal structures based on density functional theory, which were successfully synthesized by experiments [1,2]. Dynamic mean field theory provides more precise description for the electronic structure of the predicted compounds by revealing metal-insulator transition, and spin transition induced by pressure [3, 4]. I will also discuss possible implications for geoscience of these studies [5].


Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J04 DCP DCOMP DBIO DSOFT: Water Dynamics in Different Environments: Experiment and Theory IV. Bulk Water and Solute Hydration 109 - Radha Boya, Univ of Manchester - Tag(s): Focus
2:30PM J04.00001: Systematic optimization of atomistic water models for molecular simulation using liquid/vapor surface tension data* [Invited] LEE-PING WANG (Presenter), YUDONG QIU, University of California, Davis, TERESA HEAD-GORDON, University of California, Berkeley, PAUL S NERENBERG, California State University, Los Angeles — The heat of vaporization is one of the most important experimental properties that is used to train the parameters of empirical potentials (force fields) commonly used to simulate molecular liquids. We investigated whether experimental surface tension measurements, which are less sensitive to quantum and self-polarization corrections, could replace the commonly used heat of vaporization data. To test this hypothesis we implemented new functionality into the automated ForceBalance optimization procedure for using surface tension data, and parameterized revised three-point and four-point rigid, fixed charge water models named TIP3P-ST and TIP4P-ST. The TIP3P-ST model reproduces the correct temperature of maximum density of water for the first time, but also leads to over-structuring of the liquid and less accurate transport properties. The TIP4P-ST model is highly accurate for a broad range of thermodynamic and kinetic properties, with similar performance compared to other recently developed four-point models. The results show surface tension to be a useful fitting property in general, especially when self-polarization corrections or nuclear quantum corrections for heat of vaporization are not readily available for molecular liquids of interest.

*PSN acknowledges the support of NASA Minority University Research and Education Project (MUREP) Institutional Research Opportunity grant NNX15AQ06A. THG acknowledges the support of grant CHE-1665315 from the U.S. National Science Foundation. LPW acknowledges the support of award 58158-DNI6 from the American Chemical Society Petroleum Research Fund.

3:06PM J04.00002: Kosmotrope and Chaotrope Salts Influence on Water Structural Relaxation and hydrogen Bond Dynamics Investigated by Coherent Quasielastic Neutron Scattering ANTONIO FARAONE (Presenter), Center for Neutron Research, National Institute of Standards and Technology, ERKAN SENSES, Department of Chemical and Biological Engineering, Koc University, EUGENE MAMONTOV, Neutron Scattering Division, Neutron Sciences Directorate, Oak Ridge National Laboratory — Salts can either increase or decrease the viscosity when dissolved in water. This phenomenon has been traditionally interpreted within the classification of the solutes as kosmotropes (structure makers) and chaotropes (structure breakers), with reference to their hypothesized property of enhancing or weakening the hydrogen bond network. However, at the molecular level the distinction is less clear as both kosmotropes and chaotropes affect the structure of the surrounding water molecules. Using coherent quasielastic neutron scattering, we have investigated the dynamics of NaCl/D O and KCl/D O, NaCl being a kosmotrope and KCl being a chaotrope, respectively. By probing the dynamics of these systems at the structure factor peak, we measured how different salts affect the structural relaxation of water. At the same time, by collecting data at the second peak in the deuterium intermolecular partial structure factor, the hydrogen bond dynamics was probed. Whereas the hydrogen bonding dynamics is largely unchanged by the presence of the salts, NaCl and KCl affect the structural relaxation differently: the former slows down the dynamics whereas the latter mostly leaves the relaxation unchanged.
3:18PM J04.00003: The SCAN330 dataset of first-principles molecular dynamics simulations of water*  MICHAEL D LACOUNT (Presenter), FRANCOIS GYGI, University of California, Davis — We present the SCAN330 dataset of first-principles molecular dynamics simulations of liquid water [1] obtained using the Qbox code [2] and the SCAN meta-GGA density functional [3] at a temperature of 330 K. The dataset consists of 16 independent simulations with a cumulative duration of 696 ps. Structural properties, polarizability, infrared and Raman spectra are compared with experiment and with previous results of PBE simulations carried out at 400 K, showing a substantial improvement in all computed properties. The availability of multiple independent trajectories provides a measure of the uncertainty associated with computed spectra. All simulation data and trajectories are available at http://quantum-simulation.org and provide uncorrelated configurations for use in further investigations of the electronic structure of water.


*Supported by the Midwest Integrated Center for Computational Materials (MICCoM), as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences.

3:30PM J04.00004: Sensitizing Hydration Shells of Ions by Analyzing Water Dynamics Using High Sensitive Dielectric Spectroscopy*  DJAMILA LOU (Presenter), LUAN DOAN, HENRY J. KESTING, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — A variety of measurement techniques have provided evidence that ions and other solute molecules affect the structure and dynamics of water directly surrounding them. Most experiments use infrared spectroscopy to study the vibrational relaxation of hydration shells, which observe intramolecular vibrations. In response, we have employed a highly sensitive, high-resolution, frequency domain, MHz to THz dielectric spectrometer that is sensitive to intermolecular dynamics. We have confirmed that water dynamics over this range are best described by three Debye relaxation processes with three-time constants of 8.56, 1.1ps and 179fs. Our argument is also supported by studies of dielectric relaxation of aqueous salt solutions, which produce the same three-time constants but amplitudes that vary with solute concentration. The amplitude of each process provides information about the structure of hydration shells. While the amplitude of the first process is related to the structure of the first hydration layer, the amplitude of the second and the third are linked to the second and/or the third hydration layers. Our results shed light on the dynamics of hydration shells around solute molecules in a biologically relevant environment.

*Supported by AFOSR (FA9550-18-1-0263) and NSF (CHE-1665157).
Spatio-temporal analysis of water molecules around DNA employing extended MHz-THz spectroscopy and MD simulations

ABHISHEK K SINGH (Presenter), LUAN DOAN, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — The molecular motion of water molecules within hydration shells around DNA strongly influences its functionality. However, the structure and dynamics of water molecules in their hydration shells are still controversially discussed among the research community. The understanding developed in this regard so far, is mostly due to computational/simulation studies, with far lesser experimental investigations. Here we present a temperature-dependent study for dynamics of water molecules around salmon testes DNA, employing extended megahertz-terahertz dielectric spectroscopic technique and Fourier transform infrared spectroscopy supported by MD simulations. We have observed that water molecules are heterogeneously distributed around DNA and they can be classified as “tightly” and “loosely” bound water molecules with the relaxation times of ~500 ps and ~70 ps, respectively. We are able to locate the successive hydration layers with respect to the DNA molecule. FTIR analysis of hydrogen bond fluctuations indicates that the DNA behaves like a “chaotropoc” solute and reduces the structural order of water molecules with respect to the bulk water.

*Air Force Office of Scientific Research under award number FA9550-18-1-0263 and National Science Foundation (CHE-1665157).
The solvation of molecules in water is pivotal for a myriad of molecular phenomena and is of crucial importance to understand diverse issues such as chemical reactivity and biomolecular function. It has been shown that laser techniques in the infrared (IR) and Terahertz (THz) frequency ranges offer fundamental insights into hydration from small solutes to proteins. In bulk liquid, motions of water molecules lead to ultrafast fluctuations at femto- to pico-second time scales. Underlying molecular processes range from diffusional motions spanning nanoseconds, rattling modes of anions and cations within their solvation shells on a ps time scale, the breaking and reformation of hydrogen bonds, and includes sub-100 fs librational motions. Here we report unprecedented non-linear THz experiments on water molecules in the liquid phase. This novel finding indicate that inducing anisotropy in bulk liquids is feasible.

*Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – EXC-2033 – Projektnummer 390677874, ERC Advanced Grant 695437. This work is part of the research programme of the Netherlands Organisation for Scientific Research (NWO) and supported by CALIPSOplus (grant agreement no. 730872, EU-H2020). T. H.-G. and L. R. P. thank the U.S. DOE under the Basic Energy Sciences program CPIMS, Contract No. DE-AC02-05CH11231. K. C. B. thanks the California Alliance Postdoctoral Fellowship. T. H.-G. appreciates the support received as a RESOLV Fellow while on sabbatical in Bochum Germany. This research used computational resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, under an ASCR Leadership Computing Challenge (ALCC) award.
Strong orbital interactions of the Zundel cation $\text{H}_5\text{O}_2^+$ with hydration shell water

MARIA EKIMOVA, CARLO KLEINE, JAN LUDWIG, Max Born Inst, MIGUEL OCHMANN, Institute for Nanostructure and Solid State Physics, University of Hamburg, THOMAS A. GUSTAFSSON, Department of Physics, Stockholm University, EVE KOZARI, EHUD PINES, Department of Chemistry, Ben Gurion University of the Negev, NILS HUSE, Institute for Nanostructure and Solid State Physics, University of Hamburg, PHILIPPE WERNET, Department of Physics and Astronomy, Uppsala University, MICHAEL ODELIUS, Department of Physics, Stockholm University, ERIK T. J. NIBBERING (Presenter), Max Born Inst

We use O K-edge X-ray absorption spectroscopy in transmission to determine the electronic structure and hydrogen bond characteristics of the Zundel cation $\text{H}_5\text{O}_2^+$ in solution. $\text{H}_5\text{O}_2^+$ plays a key role in water-mediated proton transport in bulk water, hydrogen fuel cells and transmembrane proteins. For this, we elucidate spectroscopic signatures of O 1s core excitations to O-H $\sigma^*$ anti-bonding orbitals of hydrated protons. By a dedicated and previously established sample preparation procedure, we can systematically tune the hydration degree of the protons, starting from the Zundel cation solvated by acetonitrile, and exchange solvation layers with water, thus altering the hydrogen bond characteristics of $\text{H}_5\text{O}_2^+$. The significant decrease of pre- and main-edge combined with a major increase of the post-edge transition cross sections point at strong interactions of the first hydration shell water molecules with the Zundel cation. With our flatjet system for x-ray absorption spectroscopy in transmission, now successfully operating for the polar acetonitrile solvent, and in combination with previously obtained laboratory infrared spectroscopic data, we can establish a systematic structural approach to hydrated proton structures in solution.
Molten hydrate clathrates as a new class of macromolecular fluids.*

CARLOS LOPEZ-BUENO (Presenter), CIQUS, Quimica-Fisica, University of Santiago de Compostela, CARLOS HERREROS-LUCAS, CIQUS, Quimica-Inorganica, University of Santiago de Compostela, MARIUS BITTERMANN, Van't Hoff Institute for Molecular Sciences, University of Amsterdam, ALFREDO AMIGO, Fisica-Aplicada, University of Santiago de Compostela, SANDER WOUTERSEN, Van't Hoff Institute for Molecular Sciences, University of Amsterdam, MARIA DEL CARMEN GIMÉNEZ-LÓPEZ, CIQUS, Quimica-Inorganica, University of Santiago de Compostela, FRANCISCO RIVADULLA, CIQUS, Quimica-Fisica, University of Santiago de Compostela — Despite water being the most prominent liquid and a common reaction media of biological processes, the effect of hydrophobic solutes on its properties is not completely understood. For instance, apolar chains of tetrabutyl ammonium salts promote the formation of clathrate hydrates at low temperatures or high pressures. Here we demonstrate the formation of a supramolecular liquid in ≈1.4-2.2m aqueous solutions of tetrabutyl ammonium bromide. Temperature and composition dependent compressibility, FTIR, thermal conductivity and heat capacity suggest that most of water molecules are locally ordered in a liquid clathrate-like structure. This completely rearranges the tetrahedral H-bond network characteristic of bulk water and affects dramatically to its thermodynamic and transport properties. Our results suggest a new way to design macromolecular solvents with different properties than its constituents.

*This work was supported by the Ministry of Science of Spain (Projects No. MAT2016-80762-R, RyC-2016-20258 and RTI2018-101097-A-I00), Xunta de Galicia (ED431F 2016/008, ED431B 2018/16, Centro singular de investigación de Galicia accreditation 2016-2019, ED431G/09 and ED481A-2018/013) the European Research Council (ERC) (StG-679124), the European Regional and Social Funds (ERDF and ESF).

A New Model for the Structure and Dynamics of the Hydrated Proton in Liquid Acetonitrile and Water

EVE KOZARI, MARK SIGALOV, DINA PINES, Ben-Gurion University of the Negev, BENJAMIN PHILIPP FINGERHUT, Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, EHUD PINES (Presenter), Ben-Gurion University of the Negev — A new proton-solvation and -transport model in aqueous solutions is proposed based on our combined NMR and IR experiments and theoretical quantum-classical-molecular-dynamics findings. The H$_7^{+}$O$_3$ solvate is at the center of the emerging model of the aqueous proton transport which is based on measurements made on protonated water solvates in liquid acetonitrile up to water-cluster size of at least 12 water molecules. The existence of structurally well-defined protonated water clusters in these solutions is unequivocally verified by NMR and FTIR spectroscopies of the hydrated proton. In contrast to the gas-phase where the H$_7^{+}$O$_3$ unit is symmetric, the core H$_7^{+}$O$_3$ unit in polar liquids is characterized by a chain of 3 water molecules with asymmetrically distorted oxygen-oxygen distances due the fluctuating solvent environment which does not allow a complete isotropic solvation of the proton. Such solvent-field-induced asymmetric distortion favors a Zundel-type, dimeric active proton solvation structure within the protonated water trimer unit. The dimeric solvation structure determines the (ultrafast) IR vibrational response of the genuine proton transfer mode in the ~ 1200 cm$^{-1}$ region putting the model in harmony with recent fs-resolved 2D-IR experiments.
5:06PM J04.00010: Determination of Ion–Water Correlated Motions in Aqueous Salt Solutions*  YUYA SHINOHARA (Presenter), Oak Ridge National Lab, RAY MATSUMOTO, MATTHEW THOMPSON, Vanderbilt University, WOJCIECH DMOWSKI, CHAE WOO RYU, University of Tennessee, Knoxville, TAKUYA IWASHITA, Oita University, DAISUKE ISHIKAWA, JASRI/SPring-8, ALFRED BARON, RIKEN SPring-8 Center, PETER THOMAS CUMMINGS, Vanderbilt University, TAKESHI EGAMI, University of Tennessee, Knoxville — We report on the real-space correlated motion of water molecules and ions in an aqueous salt solution. The Van Hove functions of aqueous salt solution were determined by high-resolution inelastic X-ray scattering (IXS) spectra and molecular dynamics simulation. (Pseudo-) Partial Van Hove function was determined to identify the element-specific correlated motions. Our results depict the distance-dependent correlated dynamics in the picosecond time-scale and identify the changes in the anion–water correlations. It is found that the anion–water correlations show a two-step relaxation. The fast term depends on the anion type, while the slow term is hardly dependent on the anion type. This result indicates that the process governing the molecular/ionic connectivity between the water molecules and the anions is almost independent of the type of anions.

*IXS was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Materials and Science and Engineering Division. High-energy X-ray diffraction work and MD simulation work were supported as part of the Fluid Interface Reactions, Structures and Transport Center, an Energy Frontier Research Center funded by the U.S. DOE, Office of Science, Office of Basic Energy Sciences.

5:18PM J04.00011: Lysozyme Solution-State Tertiary Structure Measured in Protic and Aprotic Ionic Liquid Aqueous Mixtures  IAN REYES (Presenter), JOSE L BANUELOS, University of Texas, El Paso —

Aqueous protic ionic liquid (PIL) mixtures are interesting solvent media for the stabilization of proteins over wide temperature ranges, which may help develop long term protein storage methods or high temperature catalysis applications. The stabilization and shift in the thermodynamics of hen egg white lysozyme (HWL) was previously demonstrated using differential scanning calorimetry (DSC). Understanding the relation between structure and function of HWL in PIL-based media will help design improved bioprotective solvents. The tertiary structure of HWL in mixtures of PIL ethylammonium nitrate (EAN), water, and an imidazolium-based aprotic ionic liquid (APIL) were measured using small-angle x-ray scattering (SAXS) over temperatures of 25-75 °C. APIL was introduced to confirm reports that APILs destabilize proteins, and to understand the role of aqueous solvation on all the dissolved species. A structural transition of HWL was observed between 50 and 55 °C. Results from models which delineate contributions due to protein unfolding from changes due to irreversible aggregation will be presented and compared with DSC results. The impact of water content on overall miscibility was studied using light scattering methods and the resulting protein structures will be discussed.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM
2:30PM J05.00001: Quantum cavities and Floquet materials engineering from first principles QEDFT* [Invited] ANGEL RUBIO (Presenter), Max Planck Inst Structure & Dynamics of Matter
— An appealing and challenging route towards engineering materials with specific properties is to find ways of designing or selectively manipulate materials, especially at the quantum level. We will provide an overview of how well-established concepts in the fields of quantum chemistry and materials have to be adapted when the quantum nature of light becomes important. We will pursue the question whether it is possible to create these new states of materials as groundstates of the system. To this end we will show how the emerging (vacuum) dressed states resembles Floquet states in driven systems. A particular appeal of light dressing is the possibility to engineer symmetry breaking which can lead to novel properties of materials, e.g. coupling to circularly polarized photons leads to local breaking of time-reversal symmetry enabling the control over a large variety of materials properties (e.g. topology). We show that the new quantum electrodynamics density-functional formalism (QEDFT) can account for those effects. We illustrate the realisation of those ideas in molecular complexes and 2D materials.

*This work was supported by the ERC (ERC-2015-AdG694097), Cluster of Excellence AIM and Grupos Consolidados (IT1249-19). The Flatiron Institute is a division of the Simons Foundation.

3:06PM J05.00002: Investigating New Reactivities Enabled by Polariton Photochemistry*
ARKAJIT MANDAL, PENGFEI HUO (Presenter), University of Rochester — We perform quantum dynamics simulations to investigate new chemical reactivities enabled by cavity quantum electrodynamics. With quantum dynamics simulations, we demonstrate that the selectivity of a model photo-isomerization reaction can be controlled by tuning the photon frequency of the cavity mode or the light-matter coupling strength, providing new ways to manipulate chemical reactions via light-matter interaction. We further investigate collective quantum effects enabled by coupling quantized radiation mode to multiple molecules. Our results suggest that in the resonance case, a photon is recycled among molecules to enable multiple excited state reactions, thus effectively functioning as a catalyst. In the non-resonance case, molecules emit and absorb virtual photons to initiate excited state reactions through fundamental quantum electrodynamics processes. These results from quantum dynamics simulations reveal basic principles of polariton photochemistry as well as promising reactivities that take advantage of intrinsic quantum behaviors of photons.

*This work was supported by the National Science Foundation under a Grant number CHE-1836546.
3:18PM J05.00003: Polariton Mediated Charge Transfer Reaction through Cavity-Quantum Electrodynamics*  ARKAJIT MANDAL (Presenter), PENGFEI HUO, University of Rochester — We study the polariton mediated electron transfer in a three-state model molecular system that describes the the photoinduced charge transfer process from an optically bright donor to an optically dark acceptor. With direct quantum dynamical simulations and analytical rate expressions, we demonstrate that coupling the molecular system to the quantized radiation field in an optical cavity can significantly enhance or suppress the photoinduced charge transfer process. Moreover, we also assess the accuracy of commonly used approximations in the field of polariton photochemistry such as the rotating wave approximation and the effect of ignoring the dipole self-energy term. We find that both terms are equally important to accurately describe the charge transfer process, especially in the ultra-strong coupling regime.

*National Science Foundation (NSF) “Enabling Quantum Leap in Chemistry” program under a Grant number CHE-1836546

3:30PM J05.00004: Polaronic effects on exciton-polaritons in two-dimensional metal-halide perovskite microcavities [Invited]  CARLOS SILVA (Presenter), Georgia Inst of Tech — While polarons --- charges bound to a lattice deformation induced by electron-phonon coupling --- are primary photoexcitations at room temperature in bulk metal-halide hybrid organic-inorganic perovskites (HOIP), excitons --- Coulomb-bound electron-hole pairs --- are the stable quasi-particles in their two-dimensional (2D) analogues. Here we address the fundamental question: are polaronic effects consequential for excitons in 2D-HIOPs? Based on our recent work, we argue that polaronic effects are manifested intrinsically in the exciton spectral structure, which is comprised of multiple non-degenerate resonances with constant inter-peak energy spacing. We highlight our own measurements of population and dephasing dynamics that point to the apparently deterministic role of polaronic effects in excitonic properties. We contend that an interplay of long-range and short-range exciton-lattice couplings give rise to exciton polarons, a character that fundamentally establishes their effective mass and radius, and consequently, their quantum dynamics. Finally, we consider how the exciton spectral struture and dynamics controls exciton-polaron properties in Fabry-Perot microcavities.
A variational approach for the dynamics of triplet harvesting in the polariton regime.* LUIS ANGEL MARTINEZ MARTINEZ (Presenter), University of California, San Diego, ELAD EIZNER, STEPHANE KENA-COHEN, Department of Engineering Physics, Ecole Polytechnique de Montreal, JOEL YUEN-ZHOU, University of California, San Diego — The recent interest on the manipulation of chemical processes within confined electromagnetic environments has opened up new directions on theoretical efforts to understand the emergent dynamics of organic molecules embedded in the former. Density-matrix, wave-packet propagation, and Langevin-based approaches, among other methodologies, have been developed to get insight on the interplay between the vibrational, electronic and photonic degrees of freedom in the dynamics of these hybrid light-matter (polariton) setups. Hereby, we extent the methodology toolbox to treat these systems by presenting a variational approach applicable to different regimes of vibronic and light-matter couplings for organic molecules. We use this method to understand the influence of coupling of molecular aggregates to photon fields on triplet harvesting. Furthermore, we elaborate on the role of the the so-called dark states, on generic electronic transitions featured by organic molecules, under the strong light-matter coupling regime.

*We acknowledge support of UC-Mexus CONACyT scholarship for doctoral studies, NSF EAGER Grant No. CHE-1836599, and the Canada Research Chairs program and NSERC Grant No. RGPIN-2014-06129.

Modifying reverse intersystem crossing with cavity polaritons* FRANCESCA FASSIOLI OLSEN (Presenter), COURTNEY DELPO, BRYAN J KUDISCH, KYU HYUNG PARK, Princeton University, DANIELE FAUSTI, University of Trieste, GREG SCHOLES, Princeton University — Strong light-matter coupling gives rise to a superposition of light and matter states called polaritons. In the molecular setting, strong light-matter coupling is usually achieved when a large number of molecules is coupled to the same mode of an optical cavity. In this case, the energy structure is normally described as consisting of two distinct polaritonic states together with a large set of intermediate molecular dark states, that due to their purely molecular nature are believed to exhibit dynamics that resemble those of the bare molecular states. In this work we investigate the nature of these intermediate states and how their dynamics and optical response deviate from those of molecules outside the cavity. We apply our framework to simulate linear and non-linear optical responses of an experimentally studied system, namely 4CzIPN, to gain insight into how these intermediate states are involved in and modify intersystem crossing and reverse intersystem crossing under the strong light matter coupling regime.

*FF acknowledges financial support from the European Union’s H2020 Marie Sklodowska-Curie actions, grant No 799408
4:30PM J05.00007: Multiscale Molecular Dynamics Simulations of Polaritonic Chemistry*
[Invited] GERRIT GROENHOF (Presenter), Department of Chemistry and NanoScience Center, University of Jyvaskyla, JOHANNES FEIST, Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center, Universidad Autónoma de Madrid, JUSSI TOPPARI, Department of Physics and NanoScience Center, University of Jyvaskyla — When photoactive molecules interact strongly with confined light modes in optical cavities new hybrid light-matter states form, the polaritons. These polaritons are coherent superpositions of excitations of the molecules and of the cavity mode. Because light-matter hybridization can change the potential energy surface with respect to the bare molecules, polaritons are considered a promising paradigm for controlling photochemical reactions. To gain insight into the effects of strong coupling on the reactivity of molecules, we have extended the Tavis-Jaynes-Cummings model into an all-atom hybrid quantum chemistry / molecular mechanics approach, capable of simulating thousands of molecules inside cavities. After presenting our model, we will discuss recent simulations that illustrate how the dynamics and reactivity of large ensembles of molecules are affected by their strong interaction with the confined light modes of the cavity.

*Academy of Finland

5:06PM J05.00008: Polariton assisted down-conversion of photons via nonadiabatic molecular dynamics: a molecular dynamical Casimir effect* JUAN PEREZ-SANCHEZ (Presenter), JOEL YUEN-ZHOU, University of California, San Diego — Recently it has been possible to reach new regimes in which the light-matter interaction energy is comparable to electronic or vibrational energies using optical microcavities or nanostructures, giving rise to new hybrid light-matter states called polaritons. Most recent works focus on using strong light-matter coupling to change molecular processes such as photodissociation and charge and energy transfer. Here, we focus on a less addressed complementary question: can the emergent molecular dynamics be harnessed for photonic applications? We calculate the quantum dynamics of the photoisomerization of a single molecule embedded in an optical microcavity. We found that for specific cavity frequencies and sufficiently strong couplings, molecular photoexcitation into an electronic excited state can be followed by the spontaneous emission of two photons of a lower frequency via the cavity after isomerization, thus offering a new mechanism for photonic down-conversion using molecular polaritons. We show how this mechanism occurs when the light-matter coupling is strong enough so the nuclear dynamics cannot be considered to be adiabatic with respect to the electronic and photonic degrees of freedom.

*NSF EAGER Award CHE 1836599.
5:18PM J05.00009: Cavity controlled inverse harmonic generation  DAVIS DAVE WELAKUH  (Presenter), MARY-LEENA MARTINE TCHENKOUE DJOUOM, MICHAEL RUGGENTHALER, HEIKO APPEL, ANGEL RUBIO, Max Planck Inst Structure & Dynamics of Matter — Interaction between quantized light and matter lies at the heart of a broad range of applications, such as frequency down-conversion in ultrastrong cavity QED [1]. Frequency down-conversion schemes are often treated with few-level approximations of the matter subsystem. In the present work, we consider the case of a semiconductor quantum ring described in real space coupled to more than one mode and investigate a down-conversion process. We show that the down-converted photons have unique features such as non-classicality and entanglement. In addition, we show shortcomings of few-level approximations and mean-field theory. An interesting outcome for down-conversion is that ultrastrong coupling is more efficient than just increasing the incoming field strength.


Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J06 DLS: Ultrafast Dynamics and Control of Quantum Materials 113 - Tag(s): Focus

2:30PM J06.00001: Terahertz through X-ray Control and Measurement of Quantum Material Dynamics [Invited]  KEITH NELSON (Presenter), Chemistry, MIT — This is for an APS-DLS FOCUS SESSION. The focus session is "Ultrafast Dynamics and Control of Quantum Materials"

This invited talk is to be given by Prof. Keith Nelson of MIT, who is a leader in the field of dynamics in complex materials.
3:06PM J06.00002: Magnetic symmetry breaking driven by photoinduced piezomagnetism*
ANKIT DISA (Presenter), MICHAEL FECHNER, BIAOLONG LIU, TOBIA NOVA, MICHAEL FOERST, Max Planck Institute for the Structure and Dynamics of Matter, PAOLO G. RADAELLI, Department of Physics, University of Oxford, ANDREA CAVALI, Max Planck Institute for the Structure and Dynamics of Matter — Symmetries govern the macroscopic behavior of solids and dictate how their properties can be controlled by external fields. Resonantly driving optical phonons offers the possibility to coherently manipulate symmetry and induce new functional properties away from equilibrium. Here, we demonstrate magnetic symmetry breaking by light leading to an induced ferrimagnetic phase in the classical antiferromagnet CoF$_2$. We utilize high-intensity terahertz pulses to simultaneously excite degenerate in-plane phonon modes and observe the resulting magnetization dynamics by optical Faraday rotation and circular dichroism. We find that the excitation generates a net c-axis magnetization on the picosecond time scale, evidencing an ultrafast magnetic phase transition. First-principles calculations show that the effect is driven by a novel photoinduced piezomagnetic effect, in which anharmonic phonon dynamics uncompensate the equilibrium antiferromagnetic order via a site-selective modulation of the crystal field. This rare example of photoinduced symmetry breaking provides a new mechanism for magnetic control, which could also be used for manipulating spins at heterointerfaces and engineering magnetoelectric phenomena by light.

*Research supported by the Alexander von Humboldt Foundation.

3:18PM J06.00003: Distinguishing Intrinsic from Extrinsic Effects in Time-resolved Photoemission*
PATRICK KIRCHMANN (Presenter), SIMES, SLAC - Natl Accelerator Lab, HEIKE PFAU, Lawrence Berkeley National Laboratory, JONATHAN A SOBOTA, SIMES, SLAC - Natl Accelerator Lab, HADAS SOIFER, School of Physics and Astronomy, Tel Aviv University, NICOLAS GAUTHIER, SIMES, SLAC - Natl Accelerator Lab, KEJUN XU, HONGYU XIONG, SHUJIE TANG, Geballe Laboratory for Advanced Materials, Stanford University, COSTEL R. ROTUNDU, ZHIXUN SHEN, SIMES, SLAC - Natl Accelerator Lab — Time- and angle-resolved photoemission is becoming established as a powerful tool for the study of nonequilibrium electron dynamics in quantum materials. With the proliferation of this technique it is important to develop a robust understanding of the method itself. I will discuss how electron dynamics that are intrinsic to the sample can be distinguished from generic electron dynamics that are extrinsic. This includes apparent binding energy shifts due to surface photovoltage, and shifts and broadening due to pump-induced vacuum space charge.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
3:30PM J06.00004: Tuning time and energy resolutions in time- and angle-resolved photoemission spectroscopy*  ALEXANDRE GAUTHIER (Presenter), Geballe Laboratory for Advanced Materials, Stanford University, JONATHAN A SOBOTA, NICOLAS GAUTHIER, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, KEJUN XU, Geballe Laboratory for Advanced Materials, Stanford University, HEIKE PFAU, Lawrence Berkeley National Laboratory, COSTEL R. ROTUNDU, ZHIXUN SHEN, PATRICK KIRCHMANN, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory — Time- and angle-resolved photoemission is a powerful probe of nonequilibrium band structures. Time and energy resolution are two important parameters which determine the range of possible measurements. We demonstrate tunable time and energy resolutions by adjusting the thickness of nonlinear BaB\textsubscript{2}O\textsubscript{4} crystals commonly used to generate 6 eV pulses from a 1.5 eV fundamental. We tune the time resolution between 58 and 103 fs and obtain corresponding energy resolutions of 55 to 27 meV, maintaining a time-bandwidth product under 150% of the Fourier limit. Calculations clarify the interactions between laser bandwidth and nonlinear crystal thickness which contribute to determining experimental resolutions.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. A.G. acknowledges support from the Stanford Graduate Fellowship and the National Defense Science and Engineering Graduate Fellowship.

3:42PM J06.00005: Time-resolved ARPES study on Ta\textsubscript{2}NiSe\textsubscript{5}  TAKESHI L. SUZUKI (Presenter), Univ of Tokyo-Kashiwanoha, YASUSHI SHINOHARA, School of Engineering, Univ. of Tokyo, YANGFAN LU, Dept. of Science, Univ of Tokyo, MARI WATANABE, JIADI XU, Univ of Tokyo-Kashiwanoha, KENICHI L. ISHIKAWA, School of Engineering, Univ. of Tokyo, HIDE TAKAGI, Dept. of Science, Univ of Tokyo, MINORU NOHARA, Research Institute for Interdisciplinary Science, Okayama University, NAOYUKI KATAYAMA, HIROSHI SAWA, Department of Applied Physics, Nagoya University, MASAMI FUJISAWA, TERUTO KANAI, NOBUHISA ISHII, JIRO ITATANI, Univ of Tokyo-Kashiwanoha, TAKASHI MIZOKAWA, School of Advanced Science and Engineering, Waseda University, SHIK SHIN, KOZO OKAZAKI, Univ of Tokyo-Kashiwanoha — Ta\textsubscript{2}NiSe\textsubscript{5} has been long proposed as an excitonic insulator, in which remarkable band flattening below the structural transition temperature at 328 K, as a result of the strong Coulomb attractive interactions between the conduction and valence bands. Recently, photo-excitation has been intensively used to explore non-equilibrium phases. Our previous result also confirms that Ta\textsubscript{2}NiSe\textsubscript{5} is an excitonic insulator from the characteristic dynamical behavior [1]. In this work, we have used time-resolved ARPES (TARPES) to investigate the photo-excited non-equilibrium phases in Ta\textsubscript{2}NiSe\textsubscript{5}. We have discovered that intense photo-excitation induce a transient semimetallic state, which could not be realized under equilibrium. In order to gain insight on the mechanism of this phase transition, we have pursued the TARPES measurements with better signal-to-noise ratio enabled by use of the higher repetition rate laser system. We have observed oscillating behaviors corresponding to the coherent phonons in the ARPES intensity maps, which allowed us to identify which phonon mode is relevant to the metallization.
3:54PM J06.00006: Light-driven ultrafast phonomagnetism* DMYTRO AFANASIEV, JORRIT HORTENSIIUS (Presenter), Delft University of Technology, BORIS IVANOV, National Academy of Sciences and Ministry of Education and Science, ALIREZA SASANI, ERIC BOUSQUET, University of Liège, YAROSLAV M. BLANTER, Delft University of Technology, ROSTISLAV MIKHAYLOVSKIY, Lancaster University, ALEXEY KIMEL, Radboud University Nijmegen, ANDREA CAVIGLIA, Delft University of Technology — Over the past few decades, ultrashort pulses of light have been widely employed to control the behavior of matter in its different phases. This is a particularly interesting challenge in magnetism, where the speed, dissipation and routes for ultimately fast switching of the spin orientation often lead to proposals for novel approaches in information processing and data recording. [1] In this work we control the magnetic state by resonantly pumping optical phonons, low-energy elementary vibrations of the crystalline lattice. We demonstrate that by exciting the crystal lattice of the prototypical antiferromagnetic DyFeO$_3$, it can be driven within picoseconds into a transient metastable magnetic state. The state is characterized by a change in the strength of magnetic anisotropy along different crystal axes. This is experimentally seen as a long-lived shift in the frequency of the spin precession driven along the corresponding axes. For sufficiently strong excitation, this promotes an instability of the initial magnetic structure and launches a spin reorientation transition within a few picoseconds.


*This work was partially supported by the EU through the European Research Council, grant No. 677458 (AlterMateria)

4:06PM J06.00007: Absence of amplitude mode softening of intermediate states in the charge density wave material 1T-TaSe$_2$ WENJING YOU (Presenter), XUN SHI, YINGCHAO ZHANG, YIGUI ZHONG, ZHENSHENG TAO, University of Colorado, Boulder, MICHAEL BAUER, KAI ROSSNAGEL, Kiel University, HENRY KAPTEYN, MARGARET MURNANE, University of Colorado, Boulder — Recently, we uncovered new long-lived metastable charge density wave (CDW) states in 1T-TaSe$_2$ that are launched by an ultrafast laser pulse [1]. Moreover, the transitions from CDW to metastable to normal phases exhibit second order phase transition behaviors with continuously tunable order parameters, although it is a first order transition under thermal-equilibrium conditions. Ultrafast light-induced phase transitions thus extend the phase diagram of strongly-coupled materials, allowing us to access new states which are unreachable by chemical doping or by varying the temperature. In order to further understand the nature of these new metastable intermediate states, a second weak pump pulse is applied to probe their properties. Surprisingly, the CDW amplitude mode frequency of all intermediate states (between the CDW and normal states) is the same as that of CDW state - and vanishes only when the material reaches the normal state. This abrupt change of phonon mode frequency, reveals an exotic interatomic potential that may be intrinsic to the first-order nature of the phase transition in equilibrium. Our results provide new insight in understanding the formation and nature of ultrafast laser- induced metastable states.

4:18PM J06.00008: Universal dynamics of order parameter fluctuations in pump-probe experiments  
PAVEL DOLGIREV (Presenter), MARIOS MICHAEL, Harvard University, ALFRED ZONG, NUH GEDIK, Physics, MIT, EUGENE DEMLER, Harvard University — Upon excitation by a laser pulse, broken-symmetry phases of a wide variety of solids demonstrate similar order parameter dynamics characterized by a dramatic slowing down of relaxation for stronger pump fluences. Motivated by this recurrent phenomenology, we develop a simple non-perturbative effective model of dynamics of collective bosonic excitations in pump-probe experiments. We find that as the system recovers after photoexcitation, it shows universal prethermalized dynamics manifesting a power-law, as opposed to exponential, relaxation, explaining the slowing down of the recovery process. For strong quenches, long-wavelength over-populated transverse modes dominate the long-time dynamics; their distribution function exhibits universal scaling in time and space, whose universal exponents can be computed analytically. Our model offers a unifying description of order parameter fluctuations in a regime far from equilibrium, and our predictions can be tested with available time-resolved techniques.

4:30PM J06.00009: Ultrafast nonlinear excitation of collective modes in iron pnictides by intense terahertz pulses  
CHIRAG VASWANI (Presenter), DIN HERATH MUDIYANSELAGE, Iowa State University, JONG-HOON KANG, University of Wisconsin - Madison, MARTIN MOOTZ, University of Alabama at Birmingham, XU YANG, Iowa State University, ILIAS PERAKIS, University of Alabama at Birmingham, CHANG-BEOM EOM, University of Wisconsin - Madison, JIGANG WANG, Iowa State University — Nonlinear terahertz (THz) spectroscopy has been a promising tool for the study of collective excitations in superconductors, as demonstrated by the observation of Higgs mode and Leggett mode in BCS superconductors with phonon-assisted pairing. The nonlinear nature of the excitation is essential as these modes arise from exotic symmetries and do not linearly couple to the electromagnetic field. Unconventional superconductors with strong inter-band pairing channels and multiple spin/charge fluctuations are expected to host new and rich collective excitations which have not yet been explored. Here we report the observation of collective modes in iron pnictides excited by intense THz pulses. The modes diminishes at both high temperatures and field strengths when there is strong quenching of the superconducting coherence. Our results clearly show out of equilibrium driving of multiband superconducting systems can induce nonlinear couplings between collective excitations of order parameters, leading to the formation of novel phase.
**4:42PM J06.00010: Experimental observation of phonon- and band-specific electron-phonon coupling in a topological semi-metal**

NICOLAS GAUTHIER (Presenter), Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, HADAS SOIFER, School of Physics and Astronomy, Tel Aviv University, ALEXANDRE GAUTHIER, Geballe Laboratory for Advanced Materials, Stanford University, EDBERT JARVIS SIE, AARON LINDENBERG, PATRICK KIRCHMANN, ZHIXUN SHEN, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory — Light excitation of quantum materials can drive phase transitions such as insulator-to-metal transitions or the melting of magnetic orders. It can also lead to ultrafast topological phase transitions, as it was demonstrated recently in the topological semi-metal WTe$_2$ using ultrafast electron diffraction [1]. The photoinduced transition in this system occurs when a shear phonon mode is driven sufficiently strongly to recover the inversion symmetry of the lattice. In this context we studied the electron dynamics of WTe$_2$ using time- and angle-resolved photoemission spectroscopy. We report the observation of band oscillations at four different frequencies that are due to $A_{1g}$ coherent phonon modes and include the shear mode causing the photoinduced topological transition. By isolating the effect of each phonon on the different electronic bands, we reveal the complexity of electron-phonon coupling in the electronic band structure.


*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. N.G. acknowledges support from the Swiss National Foundation (Fellowship No. P2EZP2 178542).*

**4:54PM J06.00011: Light-induced coherent modulation of the electrons and lattice in a charge density wave material**

XUN SHI (Presenter), WENJING YOU, YINGCHAO ZHANG, ZHESHENG TAO, YIGUI ZHONG, University of Colorado, Boulder, XIANXIN WU, RONNY THOMALE, University of Wurzburg, FAIROJA CHEENICODE KABEER, PABLO MALDONADO, PETER OPPENEER, Uppsala University, MICHAEL BAUER, KAI ROSSNAGEL, University of Kiel, HENRY KAPTEYN, MARGARET MURNANE, University of Colorado, Boulder — Ultrashort light pulses can selectively excite charges, spins and phonons in materials, providing a powerful approach for manipulating their properties. In this work, we use time- and angle-resolved photoemission spectroscopy to show that a femtosecond laser pulse can coherently modulate the electrons and lattice in the charge density wave (CDW) material $1T$-TaSe$_2$ [1, 2]. These intertwined electron-phonon dynamics are launched by displacive excitation of the CDW amplitude mode, and provide unique opportunities to capture mode-specific electron-phonon couplings, interatomic potentials, and hidden phases that are inaccessible using equilibrium excitation. Surprisingly, we observe a coherent modulation of the electron temperature/occupation at the amplitude mode frequency, that is synchronized to the modulation of the Ta $5d$ band (CDW order). Then, as we increase the laser fluence to drive the material into a metastable state mediated by mode-selective electron-phonon coupling, this oscillation exhibits a phase change of $\pi$, indicating a competition between different interactions. This approach can be extended to other complex materials, to steer strongly-coupled quantum materials towards a desired state using light.

5:06PM J06.00012: Towards a Many Body Theory for Fourier Transform Inelastic X-Ray Scattering Experiments in Correlated Materials*  RYAN NESSELRODT (Presenter), JAMES FREERICKS, Georgetown University — In recent years new ultrafast x-ray sources have enabled the probing of materials at previously inaccessible time and length scales, allowing for new insights into phonon populations and dynamics far from equilibrium through direct time domain measurements. As these experiments improve, classical descriptions of phonons, particularly in correlated materials, will be pushed to their limits. With this in mind we seek to develop a fully quantum mechanical, many-body theory for ultrafast pump-probe scattering experiments that accounts for electron-phonon coupling and electronic correlations that can inform and inspire experiments. A new theory could help us gain better insight into exotic nonequilibrium states in correlated materials, superconductivity, as well as lead to a better understanding of charge and heat transport under normal operating conditions in current and new devices.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under contract No. de-sc0019126.

5:18PM J06.00013: Ultrafast Nonlinear Optical Spectroscopy of the Charge Density Wave in 1T-TaS2  XIANGPENG LUO (Presenter), WENCAN JIN, Univ of Michigan - Ann Arbor, SANG-WOOK CHEONG, Physics & Astronomy, Rutgers University, LIUYAN ZHAO, Univ of Michigan - Ann Arbor — Nonlinear optics has recently emerged as an appealing symmetry-sensitive probe for revealing and investigating exotic quantum phases of matter, in addition to its more traditional application in determining crystalline structures. Here, we report using temperature-dependent and time-resolved nonlinear optical techniques to study the 1T polytype of TaS$_2$, an intensively-studied prototypical system hosting the charge density wave (CDW) order. We show that an enhancement of broken mirror symmetry is identified across the nearly commensurate to commensurate CDW transition by rotation anisotropy second harmonic generation (RA SHG). We then report the ultrafast responses of commensurate CDW to optical excitations, using both time-resolved reflectivity and time-resolved RA SHG. The excitation fluence dependence of the commensurate CDW phase will further be discussed.
2:30PM J07.00001: Design and Fabrication of Impedance Matched Parametric Amplifiers for Quantum Applications*  
JOEL GREBEL (Presenter), AUDREY BIENFAIT, HUNG-SHEN CHANG, MING-HAN CHOU, CHRISTOPHER R CONNER, Pritzker School of Molecular Engineering, University of Chicago, ETIENNE DUMUR, Argonne National Laboratory, GREGORY PEAIRS, Department of Physics, University of California, Santa Barbara, RHYS G POVEY, YOUPENG ZHONG, Pritzker School of Molecular Engineering, University of Chicago, ANDREW CLELAND, Pritzker School of Molecular Engineering, University of Chicago, Argonne National Laboratory — Josephson parametric amplifiers (JPAs) are an important resource for the single-shot readout of superconducting qubits. Being able to amplify signals at the quantum limit, with noise approaching 1/2-photon for phase-independent gain [1], enables high fidelity measurements of single as well as multiplexed qubits. We will describe the circuit designs and fabrication process for on-chip impedance matched lumped-element JPAs ([2], [3]) operated in both three-wave and four-wave mixing modes. We will present data on the devices’ gain, saturation power, and bandwidth. Key improvements from the previous year’s design will be discussed as well as practical advice for ensuring reliable performance in the cryogenic environment.


*This work supported by AFOSR MURI (FA9550-15-1-0029), UChicago MRSEC (NSF DMR-1420709), DOE, UChicago PNF via SHyNE (NNCI NSF -1542205), ARL (W911NF-15-2-0058), and ANL

2:42PM J07.00002: Josephson Array Mode Parametric Amplifier*  
VOLODYMYR SIVAK (Presenter), SHYAM SHANKAR, GANGQIANG LIU, Yale University, JOSE AUMENTADO, National Institute of Standards and Technology, MICHEL H. DEVORET, Yale University — We introduce a novel near-quantum-limited amplifier with a large tunable bandwidth and high dynamic range – the Josephson Array Mode Parametric Amplifier (JAMPA). The signal and idler modes involved in the amplification process are realized by the array modes of a chain of 1000 flux tunable, Josephson-junction-based, nonlinear elements. The frequency spacing between array modes is comparable to the flux tunability of the modes, ensuring that any desired frequency can be occupied by a resonant mode, which can further be pumped to produce high gain. We experimentally demonstrate that the device can be operated as a nearly quantum-limited parametric amplifier with 20dB of gain at almost any frequency within (4−12)GHz band. On average, it has a 3dB bandwidth of 11MHz and input 1dB compression power of −108dBm, which can go as high as −93dBm. We envision the application of such a device to the time- and frequency-multiplexed readout of multiple qubits, as well as to the generation of continuous-variable cluster states.

*This research is supported by: ARO, AFOSR, YINQE.
2:54PM J07.00003: Frequency Tunable Josephson Traveling Wave Parametric Amplifier with Nondegenerate Pump Phase Matching  Kaidaong Peng (Presenter), Mahdi Naghloo, Kevin O’Brien, Massachusetts Institute of Technology MIT — Resonantly phase-matched Josephson traveling wave parametric amplifiers (JTWPs) with gigahertz of bandwidth and near-quantum limited noise performance are now widely used in superconducting quantum computing experiments. For such conventional single-pump JTWPs, resonators are critical to cancel phase mismatch from both the normal group velocity dispersion and the nonlinear phase modulations. However, these resonators make up half of the device footprint, require high fabrication uniformity, and fix the device operating frequency. Here we develop a resonator-free, dual-pump JTWPA with a reduced footprint, wider bandwidth, but comparable gain, dynamic range, and noise performance. In contrast to the resonant phase matching technique, our dual-pump scheme generates a linear phase mismatch which naturally compensates the nonlinear phase mismatch. In addition to their larger fabrication tolerance, these dual-pump JTWPs have dynamically reconfigurable frequency bands controlled by the frequency detuning of the two pumps. These devices will open up new possibilities for tunable amplification, both phase sensitive and preserving, applicable to cQED and higher-frequency cosmological applications.

3:06PM J07.00004: Minimal manifestation of Kerr-mediated frequency combs in superconducting circuits*  Pinlei Lu (Presenter), Department of Physics and Astronomy, University of Pittsburgh, Saeed Khan, Department of Electrical Engineering, Princeton University, Tzu-Chiao Chien, Xi Cao, Department of Physics and Astronomy, University of Pittsburgh, Hakan Türeci, Department of Electrical Engineering, Princeton University, Michael Jonathan Hatridge, Department of Physics and Astronomy, University of Pittsburgh — In this presentation, we present an experimental realization of a coherently driven, Kerr-mediated, microwave frequency comb. Our device consists of two superconducting modes: a mode with modest Kerr-nonlinearity strongly coupled to a second, linear mode. We explore the phase space of the two-mode system, including the transition from a stable regime to a region where the system settles into limit cycle dynamics exhibiting a frequency comb [1]. Temporal correlation function measurements reveal it is highly coherent, with a phase coherence as 30 μs, significantly exceeding the bare mode decay times of 15 ns. Additionally, in contrast to standard optical comb devices the comb’s coherence is strongly influenced by quantum fluctuations due to the intrinsic Kerr nonlinearity of the system. This result is further supported by excellent agreement of comb coherence and dynamics measurements with a microscopic quantum theory of the two-mode system. The combination of strong and engineerable interactions in our system makes it a promising platform for engineering spectrally broader and denser microwave frequency combs, and also a good testbed for studying complex quantum nonlinear dynamics.


*Work supported by: Kaufman Foundation*
3:18PM J07.00005: Impedance-matched Josephson parametric amplifier using open stubs as shunt capacitance*  YOSHIRO URADE (Presenter), KUN ZUO, RIKEN, KUNIHIRO INOMATA, National Institute of Advanced Industrial Science and Technology, ZHIRONG LIN, Shanghai Institute of Microsystem and Information Technology, TSUYOSHI YAMAMOTO, NEC Corporation, YASUNOBU NAKAMURA, RIKEN — Broadband Josephson parametric amplifiers (JPAs) are essential devices for frequency-multiplexed readout of integrated superconducting qubits towards large-scale quantum computers. Lumped capacitors such as parallel-plate capacitors are often used for such broadband JPAs to bring LC resonance with Josephson inductances to the GHz frequency region. Fabricating insulating layers of the parallel-plate capacitors makes fabrication process complex and causes additional dielectric losses.

In this presentation, we show that open stubs (open-circuited transmission lines connected at one end) can be used as shunt capacitances for JPA resonators. Such distributed elements are implemented by planar structures and thus have advantages over parallel-plate capacitors in terms of fabrication simplicity and dielectric loss. Using the open-stub structure, we experimentally demonstrate a broadband flux-driven JPA device based on impedance-matching technique, which operates at around 10 GHz with an instantaneous bandwidth of 300 MHz and saturation input power of -110 dBm.

*This work was supported in part by JSPS KAKENHI (JP18J00874), NEDO, JST ERATO (JPMJER1601), and MEXT Q-LEAP (JPMXS0118068682).

3:30PM J07.00006: Four-port directional parametric amplifier*  VIDUL JOSHI (Presenter), GANGQIANG LIU, ANDREW LINGENFELTER, SHYAM SHANKAR, MICHEL H. DEVORET, Yale University — Quantum limited parametric amplifiers based on Josephson junctions are important for measurement of superconducting qubits. Traditionally, these are reflection amplifiers which need external non-reciprocal elements to separate the input from the output. It is possible however, to make multi-mode circuits and drive multiple parametric processes together to achieve non-reciprocity. Three-mode devices based on these techniques that have been made so far have either lacked output matching or provide unity reverse gain, thus relying on perfectly well matched and thermalized output lines. Adding a fourth mode can solve these issues and can help us build a fully directional parametric amplifier. We present the design and experimental progress towards realizing such a four-mode device which under appropriate drive conditions would act like an amplifier which has appreciable forward gain, has perfect isolation, is input- and output-matched and has an auxiliary port which acts as the cold load.

*Work supported by: ARO, ONR, AFOSR, and YINQE
3:42PM J07.00007: Pump-power-efficient 3-wave mixing Josephson parametric amplifier*  
WEI DAI (Presenter), VOLOYMDYR SIVAK, GANGQIANG LIU, SHYAM SHANKAR, MICHEL H. DEVORET,  
Yale University — Josephson Parametric Amplifiers (JPAs) are commonly used in superconducting  
quantum information processing. In linear amplification regime, a JPA typically requires pump  
that is orders of magnitude stronger than its output power. Larger signal power handling of a JPA  
would require application of even stronger pump. However, maximum pump power delivered to  
a JPA, which is proportional to power dissipated in attenuators, is limited by cooling power of  
dilution fridges. To address this limitation, we apply on-chip impedance engineering to enable  
strong coupling of the off-resonance pump to a 3-wave-mixing JPA. Compared to similar JPAs with  
a capacitively coupled pump port or mutual-inductively coupled flux-pumping, this design  
requires at least an order of magnitude less pump power, while achieving theoretically quantum-  
limited amplification with state-of-the-art dynamic range. Preliminary experimental results will be  
shown.  
*Work supported by: ARO, AFOSR, and YINQE

3:54PM J07.00008: Optimizing Josephson-Ring-Modulator-based Josephson Parametric  
Amplifiers via full Hamiltonian control*  
CHENXU LIU (Presenter), TZU-CHIAO CHIEN, MICHAEL  
JONATHAN HATRIDGE, DAVID PEKKER, Department of Physics and Astronomy, Univ of Pittsburgh — A  
Josephson Parametric Amplifier (JPA) with a large saturation power is an essential  
ingredient to achieve efficient quantum sensing and qubit readout in superconducting  
quantum computing circuits. In a previous work, we showed that the saturation power of  
JPAs is not limited by pump depletion, but instead by the strong nonlinearity of Josephson  
junctions, the nonlinear circuit elements that enables amplification in JPAs [1]. Here, we  
present a systematic study of the nonlinearities in JPAs, we show which nonlinearities  
limit the saturation power, and present a strategy for optimizing the circuit parameters  
for achieving the best possible JPA. For concreteness, we focus on JPAs that are  
constructed around a Josephson Ring Modulator (JRM). We show that by tuning the  
external and shunt inductors, we should be able to take the best experimentally available  
JPAs and improve their saturation power by ~ 15dB. Finally, we argue that our methods  
and qualitative results are applicable to a broad range of JPAs with few-Josephson  
junctions like SNAILs.  
*We acknowledge support from the ARO, LPS, and PQI
4:06PM J07.00009: Dependence of Kerr nonlinearity on junction array size in Josephson parametric amplifiers*  GANGQIANG LIU (Presenter), VOLODYMYR SIVAK, SHYAM SHANKAR, LUIGI FRUNZIO, MICHEL H. DEVORET, Yale University — Josephson parametric amplifiers have become indispensable components of superconducting quantum computing devices. However, their gain saturation power, which is limited by Kerr nonlinearity of Josephson junctions, is still too low for large scale readout. One way to suppress the Kerr nonlinearity, therefore improving the gain saturation power, is to replace the single Josephson element with an array of such elements. We investigate the dependence of Kerr nonlinearity on the array size under realistic fabrication constraints. We find the suppression of Kerr nonlinearity is sub-linear in array size for amplifiers with tens to hundreds Josephson element. We believe such a weak dependence accounts for the fact that arraying has not yet brought significant improvement of the dynamic range in Josephson parametric amplifiers.

*Work supported by ARO.

4:18PM J07.00010: A quantum state router based on parametrically driven photon exchange*  CHAO ZHOU (Presenter), PINLEI LU, Univ of Pittsburgh, MATTHIEU PRAQUIN, École Normale Supérieure (Paris), XI CAO, RYAN KAUFMAN, ROGER MONG, DAVID PEKKER, MICHAEL JONATHAN HATRIDGE, Univ of Pittsburgh — Precisely controlled couplings between qubits are a vital part of all quantum information processing. For superconducting qubits, most efforts seek to implement a “surface code” architecture, which only couples nearest-neighbor qubits. However, longer range couplings are very desirable as they reduce the overhead of interactions between distant qubits. We present a design that can realize long range couplings between qubits through a modular quantum router. The design contains a 3D superconducting waveguide ‘trunk’ of microwave modes and a Superconducting Nonlinear Asymmetric Inductive eElement (SNAIL) to generate parametric photon exchange couplings between each pair of modes. We couple individual modules via a communication cavity deliberately detuned from a corresponding waveguide mode, with resulting (weaker) parametric couplings directly from module to module. Quantum information is exchanged between modules by driving the SNAIL at the difference of the communication modes’ frequencies. We will present a theory treatment of our router’s performance, as well as experimental results from our realization in an aluminum waveguide prototype.

*This work is supported by the ARO, LPS, NSF and the Kauffman foundation.
4:30PM J07.00011: Superconducting Parametric Cavities as an “Optical” Quantum Computation Platform  JIMMY SHIH-CHUN HUNG (Presenter), CHUNG WAI SANDBO CHANG, A.M. VADIRAJ, IBRAHIM NSANZINEZA, C.M. WILSON, Institute for Quantum Computing and Electrical and Computer Engineering, University of Waterloo — Quantum information may be encoded into systems of discrete variables (DV) or continuous variables (CV). CV quantum computation has typically been studied at optical frequencies using linear quantum optics to realize Gaussian operations. To achieve universal computation, however, non-Gaussian resources such as the photon number measurements or the cubic phase state are necessary. In superconducting circuits, DV quantum computation is dominant. Here, we propose and study the superconducting parametric cavity for optical quantum computation using microwave photons. At optical frequencies, the qumodes are often separated spatial modes. Here we use the orthogonal frequency modes of the cavity. Gaussian operations between the modes are achieved via standard parametric interactions. In addition, the recent realization of three-photon spontaneous parametric downconversion in this system provides access to both a non-Gaussian gate and resource state, which provides a path to universality. We will present preliminary results towards the development of the parametric cavity for optical quantum computation starting with demonstrations of simple algorithms. One such algorithm is a quantum machine learning algorithm called Quantum Kitchen Sinks.

4:42PM J07.00012: In-cavity parametric amplification for qubit readout in 3D circuit QED architecture*  ZHIXIN WANG (Presenter), VOLODYMYR SIVAK, SHANTANU O MUNDHADA, SHYAM SHANKAR, MICHEL H. DEVORET, Yale University — High-efficiency qubit readout is essential for implementing quantum feedback and remote entanglement schemes as well as studying the basic physics related to quantum measurement processes. In circuit quantum electrodynamics (QED) systems, one typically reads out superconducting qubits by monitoring the qubit-state-dependent phase shift of a microwave tone, which is first amplified by a quantum-limited parametric amplifier before being processed by classical electronics. In this configuration, readout efficiency is mainly limited by the loss between the readout microwave resonator and the parametric amplifier. The optimized arrangement is therefore to place the latter inside the former. Here we introduce a design that uses two coupled transmon artificial atoms housed in a 3D readout cavity/waveguide to perform quantum-limited amplification within the circuit QED module. Compatible with 3D cold cavity attenuators, this layout minimizes the qubit dephasing induced by residual thermal photons and can potentially achieve the single-shot readout for qubits with long coherence times. Preliminary results will be presented.

*Work supported by: ARO, AFOSR, and YINQE
4:54PM J07.00013: Amplification with an array of lumped Josephson Parametric Converters*  
OLIVIA LANES (Presenter), TZU-CHIAO CHIEN, CHENXU LIU, Univ of Pittsburgh, ANJA METELMANN, Physics, Freie University of Berlin, DAVID PEKKER, MICHAEL JONATHAN HATRIDGE, Univ of Pittsburgh — Josephson Parametric Amplifiers, although nearly quantum-limited, suffer from lack of directionality, low saturation powers, and a fixed gain-bandwidth product. We have recently shown that when extremely strong, carefully imbalanced gain and conversion processes (GCI) are combined between a pair of modes, we produce an amplifier that has broadband, bi-directional gain in transmission and is matched at both ports. This latter feature opens the possibility of chaining GCI amplifiers together in series. We have realized an amplifier series array by chaining two Josephson Parametric Converters (JPCs) together in such a way that signal ports form the chain’s input and output and the two idlers are matched in frequency and capacitively coupled. The signal modes have deliberately different frequencies so that all parametric processes may be individually controlled. As the dynamic range of JPCs typically fall faster than linearly with gain, we can distribute gain unequally among the array elements to enhance the array’s overall saturation power. We will also use our array as a platform for studying new combinations of parametric couplings, with a particular focus on pump schemes which provide directional amplification.

*Work supported by: ARO, LPS, NSF, and the Kauffman foundation

5:06PM J07.00014: Experimental violation of the standard quantum limit for parametric amplification of broadband signals*  
MICHAEL RENGER (Presenter), KIRILL FEDOROV, STEFAN POGORZALEK, QI-MING CHEN, YUKI NOJIRI, MATTI PARTANEN, ACHIM MARX, FRANK DEPPE, RUDOLF GROSS, Walther-Meißner-Institut & Technische Universität München, Germany — Phase-preserving amplification of weak signals is a crucial part of many protocols in microwave quantum information processing, such as quantum teleportation, remote state preparation, or dispersive qubit readout. Flux-driven Josephson parametric amplifiers (JPAs) allow amplification close to the standard quantum limit (SQL), implying a fundamental bound of 1/2 for the maximal quantum efficiency $\eta$ for amplification of narrowband input signals. We demonstrate that the SQL does not hold for broadband input signals and experimentally find $\eta = 70\%$ with an amplification chain consisting of a JPA and a cryogenic HEMT amplifier. We show that $\eta$ can reach 100% and experimentally is limited by the Poissonian fluctuations in the JPA pump line. This result can be exploited for multiple applications such as high-efficiency parity measurements of superconducting qubits.

*We acknowledge support by Germany's Excellence Strategy EXC-2111-390814868, Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (GrantNo.820505)
5:18PM J07.00015: Nonreciprocal amplification via Hamiltonian Engineering* TZU-CHIAO CHIEN (Presenter), CHENXU LIU, PINLEI LU, OLIVIA LANES, XI CAO, RYAN KAUFMAN, DAVID PEKKER, MICHAEL JONATHAN HATRIDGE, Univ of Pittsburgh — In superconducting quantum information processing, we realize high fidelity measurements by using quantum-limited parametric processes. However, cavity-based amplifiers have limited bandwidth, saturation power, and operate in reflection, and so must be operated with external lossy microwave commercial components such as circulators. Many of these limitations can be circumvented by combining multiple parametric processes in a few-mode device. By combining multiple instances of imbalanced gain and conversion processes between three modes[1], we can realize an amplifier with non-reciprocal, transmission-only amplification, matched ports, and large, gain-independent bandwidth. We have realized this scheme in a Lumped, single-ended version of the Josephson Parametric Converter (LJPC) whose inductance is dominated by the central Josephson Ring Modulator. We avoid the use of hybrids by integrating the LJPC and superconducting bandpass filters on a single chip. The resulting device is small, relatively simple to fabricate and thus an excellent candidate for direct integration into superconducting quantum computers.


*Work supported by ARO, LPS, NSF, PQI, and the Kauffman foundation

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J08 DQI: NISQ: Quantum Chemistry and Quantum Simulation

II 104 - Abhinav Kandala, IBM TJ Watson Research Center

2:30PM J08.00001: Simulating quantum systems on quantum computers* SEAN A FISCHER, C STEPHEN HELLBERG, MARCO LANZAGORTA-SALDANA, DANIEL GUNLYCKE (Presenter), United States Naval Research Laboratory — In this presentation, we discuss a new mapping method—called symmetry configuration mapping (SCM)—that uses the symmetry of the physical system to isolate different parts of the computational space. As well as providing robustness against state leakage, this new approach allows the computation to be separated into a set of smaller independent calculations involving fewer quantum logic gate operations and fewer qubits. For a fluorine molecule, the numbers of quantum logic gate operations and qubits are reduced by factors of 3 and 4, respectively. These reductions have allowed us to solve for the full many-body ground state on the IBM Q “Poughkeepsie” quantum computer. As long as quantum computing resources remain limited, similar target-customized mappings are expected to be employed in quantum computing across all areas of application.

*This work has been supported by the U.S. Naval Research Laboratory through Base and Naval Innovative Science & Engineering (NISE) programs.
2:42PM J08.00002: Studying many-body localization on a universal quantum computer
SONIKA JOHRI (Presenter), Intel Corp - Santa Clara, DAIWEI ZHU, NHUNG NGUYEN, CINTHIA
ALDERETE, KEVIN LANDSMAN, NORBERT M LINKE, CHRISTOPHER ROY MONROE, Physics, University
of Maryland, ANNE MATSUURA, Intel Corp - Santa Clara — An interacting disordered system may
exhibit localized or thermal behavior depending on the ratio of the disorder to interaction
strength. The study of this phenomena has been proposed as an application of near-term
quantum computers. However, it is known that most diagnostics of localization such as many-
body level statistics and the failure of the eigenstate thermalization hypothesis do not survive
coupling to a bath. One robust diagnostic theoretically known to survive introduction of noise are
the spectral functions of local operators [1]. Signatures of localization in this diagnostic include a
discrete spectrum and a gap at low frequencies. Here, we design an algorithm to compute the
spectrum on a universal quantum computer using Trotterized time-evolution. Further, we
implement the technique on a three-qubit trapped ion system and find that we can clearly
discern the vanishing of the low-frequency response as the disorder increases. Thus, we show
that for near-term quantum computers, spectral functions of local operators provide a robust
and scalable diagnostic for distinguishing between localized and thermal phases.


2:54PM J08.00003: Towards material design applications in a quantum computer
PANAGIOTIS BARKOUTSOS (Presenter), IBM Research - Zurich, FOTIOS GKRITSIS, King's College London,
IGOR SOKOLOV, PAULINE JEANNE OLLITRAULT, STEFANWOERNER, IVANO TAVERNELLI, IBM
Research - Zurich — Developing new materials for specific applications is an active field of research
for both material science and quantum chemistry communities. The number of atomic
compositions of molecular structures scales combinatorically with the size of the molecules,
limiting the efficiency of classical algorithms. On the other hand, quantum computers can provide
an efficient solution to the sampling of the chemical compound space. In this talk we propose a
quantum algorithm with favorable scaling in resource requirements, allowing for the solution of
the material design problem in currently available noisy quantum processors. The proposed
scheme divides the problem into a classical optimization and a quantum search problem within a
hybrid quantum classical algorithm. We demonstrate both in simulations (with and without
noise) and in IBMQ quantum hardware the efficiency of our scheme and highlight the results in a
few test cases. These preliminary results can serve as a basis for the development of further
material design quantum algorithms for near term quantum computers.
3:06PM J08.00004: Simulating quantum field theory in the light-front formulation*
MICHAEL KRESHCHUK (Presenter), WILLIAM KIRBY, GARY R GOLDSTEIN, PIERRE-HUGUES BEAUCHEMIN, PETER LOVE, Tufts Univ — We explore the possibility of simulating relativistic field theories in the light-front (LF) formulation and argue that such a framework has numerous advantages as compared to both lattice and second-quantized equal-time approaches. These include a small number of physical degrees of freedom leading to reduced resource requirements, efficient encoding with model-independent asymptotics, and sparse Hamiltonians. Many quantities of physical interest are naturally defined in the LF, resulting in simple measurements.

The LF formulation allows one to trace the connection between relativistic field theories and quantum chemistry, allowing one to use numerous techniques developed in the last decade. It also provides a promising application for NISQ devices, since for certain calculations one may need of an order of hundred qubits. As an example, we provide a detailed algorithm for calculating analogues of QCD parton distribution functions in a simple 1+1-dimensional model. We also discuss the generalization to QCD, and provide estimates.

*William Kirby acknowledges support from the National Science Foundation, award number DGE-1842474.
Michael Kreshchuk was supported by the DOE HEP award DE-SC0019452.

3:18PM J08.00005: Simulating Dynamic Material Properties on Near-Term Quantum Computers*
LINDSAY BASSMAN (Presenter), KUANG LIU, YIFAN GENG, DANIEL SHEBIB, ARAVIND KRISHNAMOORTHY, Univ of Southern California, SHOGO FUKUSHIMA, FUYUKI SHIMOJO, Kumamoto University, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Univ of Southern California — Dynamic simulation of controllable electronic properties of materials offers insight into how to harness such tunability for use in myriad technologies. Recent successes have been achieved in computing static properties of small molecules on currently available quantum computers, however, simulating dynamical properties still remains a challenge. In this work, we demonstrate successful simulation of time-dependent magnetization in a simplified model of an atomically-thin two-dimensional material on IBM’s Q16 Melbourne quantum processor and Rigetti’s Aspen quantum processor. Near overlap between experimental results from the quantum computer and those theoretically derived from simulated noisy qubits indicates there is a good understanding of the largest sources of error currently faced on available quantum computers. This early proof-of-concept gives hope that near-future quantum computers, capable of simulating larger systems, may soon be able to give insights into the dynamic control of tunable electronic properties in material.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607.
3:30PM J08.00006: Robust Preparation of Many-body Ground States in Jaynes-Cummings Lattices

KANG CAI, PRABIN PARAJULI, Physics, University of California, Merced, CHEE WEI WONG, Electrical and Computer Engineering, University of California, Los Angeles, GUILU LONG, Physics, Tsinghua University, LIN TIAN (Presenter), Physics, University of California, Merced — Strongly-correlated polaritons in Jaynes-Cummings (JC) lattices can exhibit novel quantum phase transitions at integer fillings. However, it is often challenging to prepare such states with high fidelity, especially near the quantum critical points with a vanishing energy gap. Here we study the robust preparation of the many-body ground states of polaritons in a finite-sized JC lattice by combining the techniques of quantum state engineering and adiabatic evolution. In the deep Mott-insulating or deep superfluid regimes, the many-body ground states can be generated with high fidelity by applying quantum-engineered pulse sequences to the JC lattice. Using these states as the initial state and tuning the system parameters adiabatically, the many-body ground states in the intermediate regime can be reached. Our numerical result shows that the fidelity of the generated states can be significantly improved by employing a nonlinear ramping scheme during the adiabatic evolution. We derive the optimal nonlinear index analytically, which agrees well with the numerical result. This study gives insights into the preparation of many-body states in artificial quantum systems, such as quantum simulators.

*This work was supported by the UC LFRP under award # LFR-17-477237.

3:42PM J08.00007: Quantum Algorithm for Simulating a Driven Dissipative 3-site Hubbard Ring

BRIAN ROST (Presenter), LORENZO DEL RE, Georgetown University, MICHAEL C JOHNSON, Arizona State University, ALEXANDER F KEMPER, North Carolina State University, JAMES FREERICKS, Georgetown University — Much research has been done concerning the simulation of closed quantum systems on near term quantum computers. Considerably less focus has been given to the simulation of open quantum systems, despite their importance as realistic models of real world systems. We consider the simulation of a three site Hubbard model driven by an electric field, connected to a Fermionic bath. This is the simplest model capable of stabilizing a non-zero steady state current with the added benefit that the fermionic bath admits an analytic solution in the non-interacting limit. We simulate this model classically using a master equation approach and provide an implementation for simulating it on a quantum computer. Even this simple model shows rich steady state behavior and offers a promising approach for simulating a variety of time dependent, driven, dissipative, open quantum systems.

*This work was funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0019469. In addition, BR received supplemental support from the National Science Foundation under Award DMR-1747426 and JKF received supplemental support from the McDevitt bequest at Georgetown.
Simulation of quantum Hamiltonians is one of the most promising applications proposed for which quantum hardware may provide significant advances over classical methods. However, significant limitations on near-term hardware size and fidelity pose a significant challenge for implementing known methods for realistic applications in chemistry and material science. Finding realistic systems for which near-term hardware can produce a useful simulation remains an open question. In this work we demonstrate that downfolding Hamiltonians, a process by which real materials are mapped on to model Hamiltonians, can yield a Hamiltonian form and size that is suitable for simulation on near-term quantum hardware. We apply this approach to several example materials and show how to implement it on realistic hardware using generalized swap networks.


*We acknowledge support by the US NSF, DOD and DOE.
G. K.-L. Chan is a Simons Investigator in Physics and a member of the Simons Collaboration on the Many-Electron Problem.
Hardware simulations were made possible by a grant through Rigetti Quantum Cloud Services, supported by the CQIA-Rigetti Partnership Program.
4:18PM J08.00010: Quantum Computation of the Ground and Excited State Energies Using Quantum Imaginary Time Evolution and Quantum Lanczos Methods*  KUBRA YETER AYDENIZ (Presenter), RAPHAEL POOSER, Oak Ridge National Lab, GEORGE SIOPSIS, University of Tennessee, Knoxville — Various methods have been developed for quantum computation of the ground and excited states of physical systems, but many of them require either large numbers of ancilla or high dimensional optimization. The quantum imaginary time evolution (QITE) and quantum Lanczos (QLanczos) methods proposed in [1] eschew the aforementioned issues. In this study, we demonstrate the application of these algorithms on a nontrivial quantum computation, using the deuteron binding energy as an example. With the correct choice of initial and final states we showed that the number of time steps in QITE and QLanczos can be reduced significantly, which commensurately simplifies the required quantum circuit and improves compatibility with NISQ devices. We performed these calculations on cloud-accessible IBMQ quantum computers, and with the application of readout error mitigation and Richardson error extrapolation, we obtained ground and approximate excited state energies within 3% of the theory. These results show promise for using the algorithms in future field theory, scattering, and chemistry calculations.


*This work was supported by the QUANTISED program at ORNL under FWP number ERKAP61.

4:30PM J08.00011: Driven-dissipative quantum mechanics on a lattice: Describing a fermionic reservoir with the master equation*  LORENZO DEL RE (Presenter), BRIAN ROST, Georgetown University, ALEXANDER F KEMPER, North Carolina State University, JAMES FREERICKS, Georgetown University — The possibility of simulating dissipative processes with digital circuits and quantum simulators, and using dissipation as a resource for state preparation, have created a renewed interest on the driven-dissipative many body problem. Here, I address a tight binding model of electrons driven out-of-equilibrium by an electric field, where the system can exchange energy and number of particles with a fermionic reservoir. The problem is solved using the master equation formalism. I use the exact solution for the noninteracting driven-dissipative system to benchmark the accuracy of the results obtained with the master-equation, showing a very good quantitative agreement. Furthermore, to create a better link with the simulation of open quantum systems, I provide with the time dependent Kraus map that pumps the system to the non-equilibrium steady state. Generalizations of such a method to broken symmetry phases (like CDW) and their simulation on quantum computers are discussed too.

*This work was funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0019469
4:42PM J08.00012: Quantum synchronization on the IBM Q system  MARTIN KOPPENHOEFER (Presenter), CHRISTOPH BRUDER, ALEXANDRE ROULET, Department of Physics, University of Basel — We report the first experimental demonstration of quantum synchronization. This is achieved by performing a digital simulation of a spin-1 limit-cycle oscillator on the quantum processors of the IBM Q system. Applying an external signal to the oscillator, we verify typical features of quantum synchronization and demonstrate an interference-based quantum synchronization blockade. Our results show that state-of-the-art noisy intermediate-scale quantum processors are powerful enough to implement realistic open quantum systems. Finally, we discuss limitations of current quantum hardware and define requirements necessary to investigate more complex problems.

4:54PM J08.00013: Quantum Digital Cooling+ STEFANO POLLA (Presenter), YAROSLAV HERASYMENKO, THOMAS O'BRIEN, Lorentz Institute — We introduce a new method for digital preparation of ground states of a simulated Hamiltonians, inspired by cooling in nature and adapted to leverage the capabilities of digital quantum hardware. The cold bath is simulated by a single ancillary qubit, which is reset periodically and coupled to the system non-perturbatively. Studying this cooling method on a 1-qubit system toy model allows us to optimize two cooling protocols based on weak-coupling and strong-coupling approaches. Extending these, we develop two scalable protocols for larger systems. The LogSweep protocol extends the weak-coupling approach by sweeping energies to resonantly match any targeted transition, demonstrating preparation of an approximate ground state for ferromagnetic and critical Ising chain, with error that can be made polynomially small in time. The BangBang protocol extends the strong-coupling approach, and exploits a heuristics for local Hamiltonians to approximately match transition energies, allowing rapid cooling to an approximation of the ground state, which makes this protocol appealing for near-term simulation applications.

*This research was funded by the Netherlands Organization for Scientific Research (NWO/OCW) under the NanoFront and StartImpuls programs, and by Shell Global Solutions BV.

5:06PM J08.00014: Resource-Efficient Quantum Algorithm for Protein Folding IVANO TAVERNELLI (Presenter), ANTON ROBERT, PANAGIOTIS BARKOUTSOS, STEFAN WOERNER, IBM Research - Zurich — Due to the central role of proteins’ 3D structures in chemistry, biology and medicine applications (e.g., in drug discovery), protein folding has been intensively studied for over half a century. Although classical algorithms provide practical solutions for the conformation space sampling of small proteins, they cannot tackle the intrinsic NP-hard complexity of the problem, even reduced to its simplest Hydrophobic-Polar model. While fault-tolerant quantum computers are still beyond reach for state-of-the-art quantum technologies, there is evidence that quantum algorithms can be successfully used on Noisy Intermediate-Scale Quantum (NISQ) computers to accelerate energy optimization in frustrated systems. In this talk, I will present a folding algorithm that requires resources (number of qubits and gate operations) that scale polynomially with the number of amino acids (AA). In particular, we propose a robust and versatile optimisation scheme to simulate the folding of the 10 AA Angiotensin peptide on 22 qubits and a 7 AA neuropeptide model using 9 qubits on an IBM Q 20-qubit quantum computer.
5:18PM J08.00015: Digital quantum simulation of quantum vibrational dynamics and control*  ALICIA MAGANN (Presenter), Princeton University, MATTHEW D GRACE, Sandia National Laboratories, California, HERSCHEL A RABITZ, Princeton University, MOHAN SAROVAR, Sandia National Laboratories, California — Quantum computers are expected to offer speed-ups for solving certain scientific problems. One example is digital quantum simulation, where sequences of quantum gates can be used to simulate the dynamics of quantum systems in polynomial time. This could have applications in simulations of quantum optimal control, which aim to identify shaped fields to drive a quantum system towards a designated control objective. In this talk, I will explore how digital quantum simulation could be used to make quantum optimal control simulations more tractable. I will introduce a framework that utilizes a quantum computer to simulate the field-induced dynamics of a quantum system in combination with classical optimization to update the field. As a demonstration of this framework, a quantum vibrational control problem will be considered.

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Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J09 DQI: Open Quantum Systems II 106 - Peter Groszkowski, University of Chicago

2:30PM J09.00001: Master equation approach to study Non-Markovian dynamics of open quantum systems  YUSUI CHEN (Presenter), New York Inst of Tech — A full understanding of the decoherence dynamics of an open quantum system is of crucial importance for quantum information theory and quantum computing. In the last two decades, most theoretical and experimental research is replied on the Born-Markov approximation, a no-memory and quasi-static process. The associated Lindblad master equation has the great success in explaining some phenomena, e.g. the long-time limit steady state, quantum-classical transition. However, the recently achieved strong coupling between system and environment in many experiments breaks the Born-Markov approximation and forces one to study the decoherence in a strong non-Markovian and non-equilibrium regime. The major difficulty is raised up by lack of the technique to deal with the large number of degrees of freedom of the colored noisy environment. Starting from stochastic Schrödinger equations, we demonstrate a systematical method to derive the exact time convolution-less master equation for various open quantum systems, e.g. qubit systems, multi-level systems, and harmonic oscillator systems. Our methods can also be extended to the optomechanical systems and other non-linear coupling systems.
2:42PM J09.00002: Markovian Entanglement Dynamics under Locally Scrambled Quantum Evolution  
WEI-TING KUO (Presenter), AHMED AKHTAR, DANIEL AROVAS, YIZHUANG YOU, University of California, San Diego — We study the time evolution of quantum entanglement for a specific class of quantum dynamics, namely the locally scrambled quantum dynamics, where each step of the unitary evolution is drawn from a random ensemble that is invariant under on-site basis transformations. In this case, the average entanglement entropy follows Markovian dynamics that the entanglement property of the future state can be predicted solely based on the entanglement properties of the current state and the unitary operator at each step. We introduce the entanglement feature formulation to concisely organize the entanglement entropies over all subsystems into a many-body wave function, which allows us to describe the entanglement dynamics using an imaginary-time Schrodinger equation, such that various tools developed in quantum many-body physics can be applied. In addition to Haar random circuits and Brownian circuits, we also study a new type of circuit — fractional swap circuit in which the two local qudits are partially exchanged and partially staying on the same site. We further investigate the bipartite operator mutual information and tripartite operator mutual information of the fractional swap circuit and compare with different CFT results.

2:54PM J09.00003: Critical Properties of the Measurement-Induced Transition in Random Quantum Circuits*  
AIDAN ZABALO (Presenter), Rutgers University, New Brunswick, MICHAEL GULLANS, Princeton University, JUSTIN WILSON, Rutgers University, New Brunswick, SARANG GOPALAKRISHNAN, CUNY College of Staten Island, CUNY Graduate Center, DAVID HUSE, Princeton University, Institute for Advanced Study, JED PIXLEY, Rutgers University, New Brunswick — A transition was observed in random quantum circuits with local projective measurements where the entanglement entropy (EE) goes from volume law to area law scaling as the measurement rate, \( p \), is increased above a critical value, \( p_c \). Attempts to extract the critical properties through finite size scaling of the EE has proven difficult due to the logarithmic divergence at criticality. We study the tripartite mutual information (TMI) as an alternative diagnostic of the transition that is finite at criticality while maintaining a volume law for \( p<p_c \) and vanishing for \( p>p_c \). Our intuition for the Haar random circuit is guided by results on stabilizer circuits which can be simulated at much larger sizes. We find that the TMI has weaker finite size effects when compared to other quantities. Our numerics of the Haar random circuit suggests \( p_c=0.17 \) and the critical exponent \( \nu=1.3 \) for Renyi indices \( n\geq1 \), which are smaller than previously reported results. We also find a strong Renyi index dependence of the coefficient of the logarithmic divergence \( \alpha(n)=1.0(1)/n+0.7(1) \).

*RDI2 Fellowship (AZ), DARPA DRINQS program (MG,DH), NSF Grant No. DMR-1653271 (SG), Simons Fellowship (DH), United States-Israel BSF Grant No. 2018058 (JP)
3:06PM J09.00004: Boundary Theory of a Deformed AKLT Model on the Square Lattice  JOHN MARTYN (Presenter), University of Maryland, College Park, KOHTARO KATO, ANGELO LUCIA, Institute for Quantum Information and Matter, California Institute of Technology — The 1D AKLT model is a paradigm of antiferromagnetism initially devised as a modification to the Heisenberg model, and its ground state is a quintessential example of symmetry protected topological order. On a 2D lattice, the AKLT model is particularly interesting because it also exhibits symmetry protected topological order, and can act as a resource for universal quantum computation. In contrast to the 1D case, the existence of the spectral gap in 2D, which guarantees the robustness of the model, remains an open problem despite extensive analyses. Recently, it has been shown that one can deduce this spectral gap by analyzing its boundary theory via a tensor network representation of the ground state. In this work, we present a method to calculate the boundary state of the 2D AKLT model in terms of a classical loop model, where loops, vertices, and crossings are each given a weight. We use numerical techniques to sample configurations of loops and subsequently evaluate the boundary state and boundary Hamiltonian on a square lattice. As a result, we evidence a spectral gap, and also indicate the presence of several different phases by varying the weights of the model.

3:18PM J09.00005: Basic construction of a tensor network library*  THOMAS BAKER (Presenter), ALEXANDRE FOLEY, AGUSTIN DI PAOLO, MARTIN P THOMPSON, Département de Physique, Université de Sherbrooke — We present a template tensor network code written in the programming language julia. The code is simple, short, and is also is efficient, competing in speed with some implementations in lower-level languages. The code can provide an efficient means to learn tensor networks as it is well documented for users of all levels, and the code can be used to check other libraries in development. A large number of algorithms have been implemented. Given time, new algorithms developed while creating this library will be discussed.

*T.E.B. graciously thanks funding provided by the postdoctoral fellowship from Institut quantique and Institut Transdisciplinaire d'Information Quantique (INTRIQ). This research was undertaken in part to funding from the Canada First Research Excellence Fund (CFREF).

3:30PM J09.00006: Tree tensor network study of out-of-time-order correlators on a sparse graph  CHRISTOPHER WHITE (Presenter), BRIAN SWINGLE, University of Maryland, College Park — The SYK model, which consists of Majorana fermions with random few-fermion all-to-all interactions, is a paradigmatic model of a "fast scrambler". Recent work (Bentsen, Gu, and Lucas: PNAS 116, 6689) argued that all-to-all connectivity is not necessary: rather, interactions on a sparse connectivity graph are sufficient. Because many such graphs are locally treelike, they are amenable to treatment with tree tensor networks. In this talk I will describes a study of out-of-time-order correlators using tree tensor networks; I will also comment on some methodological subtleties.
3:42PM J09.00007: Sparsity of the stabilizer projector decomposition of a density matrix and robustness of magic*  
YIFEI HUANG (Presenter), PETER LOVE, Tufts Univ — We extend the stabilizer rank of state vectors to mixed states and define the rank(minimal $l_0$ norm) for stabilizer projector decomposition of a density matrix and show its advantage over the rank of Pauli decomposition. Both improvements on the scaling over standard orthonomal basis(computational basis for state vector and Pauli basis for density matrix) come from the fact that stabilizer states form a densely overcomplete basis. In comparison with Monte Carlo simulation that scales with Robustness of Magic(minimal $l_1$ norm), we analyse the strong simulation cost of noisy Clifford+T circuits with respect to the rank. Using results from compressed sensing, we explore the sparsity condition where the minimal $l_0$ and $l_1$ norm are reached at the same decomposition.

*This work was supported by NSF award number PHY 1720395 and from Google Inc.

3:54PM J09.00008: Single T gate in a Clifford circuit drives transition to universal entanglement spectrum statistics  
SHIYU ZHOU (Presenter), Boston Univ, ZHICHENG YANG, University of Maryland, ALIOSCIA HAMMA, University of Massachusetts Boston, CLAUDIO CHAMON, Boston Univ — Clifford circuits are insufficient for universal quantum computation or creating t-designs with t bigger than 4. While the entanglement entropy is not a telltale of this insufficiency, the entanglement spectrum is: the entanglement levels are Poisson-distributed for circuits restricted to the Clifford gate-set, while the levels follow Wigner-Dyson statistics when universal gates are used. In this paper we show, using finite-size scaling analysis of different measures of level spacing statistics, that in the thermodynamic limit, inserting a single T gate in the middle of a random Clifford circuit is sufficient to alter the entanglement spectrum from a Poisson to a Wigner-Dyson distribution.

4:06PM J09.00009: Recurrences in nonlinear few-body entanglement dynamics  
ALEXANDER KIRAL (Presenter), ARJENDU KISHORE PATTANAYAK, Carleton College — We study quantum tunneling for an initially pure coherent spin state in a many-body spin system. This manifests as dynamics which transforms it into a non-classical (in our case highly entangled) state that later recoheres. We develop a metric to determine the existence of tunneling as well as spectral techniques to predict rates of tunneling for an initial coherent state. We discover that the locations of tunneling reflect phase space structures that come from symmetries of the Hamiltonian. This can be visualized through the Husimi representation of stationary states which allows us to connect to other dynamical variables such as periodicity, entanglement, and chaos.
4:18PM J09.00010: Entanglement spectrum and entropy in non-Hermitian systems*  PO-YAO CHANG (Presenter), Department of Physics, National Tsing Hua University, JHIH-SHIH YOU, IFW Dresden, XUEDA WEN, Department of Physics, Massachusetts Institute of Technology, SHINSEI RYU, University of Chicago — In this talk, we study both the entanglement spectrum and the entanglement entropy by use of a biothogonal basis in non-Hermitian free fermion systems. We show the entanglement spectrum can characterize topological features in the non-Hermitian Su-Schrieffer-Heeger model with parity and time reversal symmetry. In addition, we find the entanglement entropy at the critical point of this model has a logarithmic scaling with corresponding central charge $c=-2$, which can be described by the non-unitary conformal field theory.

*P.-Y.C. was supported by the Young Scholar Fellowship Program by Ministry of Science and Technology (MOST) in Taiwan, under MOST Grant for the Einstein Program MOST 108-2636-M-007-004. X.W. is supported by the Gordon and Betty Moore Foundations EPIQS initiative through Grant No. GBMF 4303 at MIT. S.R. is supported in part by the National Science Foundation under Grant No. DMR-1455296, and by a Simons Investigator Grant from the Simons Foundation.

4:30PM J09.00011: GPU-accelerated simulations of realistic quantum systems with a focus on Quantum Information and Computation.*  ALEKSANDER LASEK (Presenter), HUGO V LEPAGE, CRISPIN H.W. BARNES, DAVID R M ARVIDSSON SHUKUR, Univ of Cambridge — In this talk we present our method of numerically simulating realistic quantum systems. With recent increases in GPU processing power, we are able to simulate two-particle 2D systems on thousands of spatial sites in a reasonable time. Even though today's quantum computers can manipulate multiple qubits, the long-term fidelity of many-qubit operations is still poor. Numerical simulations of quantum computers can help guide experiments towards better fidelities. We focus on simulating physical qubits, which leads to a better understanding of where the errors that are observed in quantum computers and experiments come from. We describe the techniques used to make our calculations possible, as well as present simulation results of realistic quantum experiments, including performing an entangling operation on two electron-spin qubits, controlling a charge qubit, and sound driven single electron transfer between quantum rails.

*A.L. acknowledges support from EPSRC and Hitachi via CASE studentships RG 94632.
4:42PM J09.00012: Unified Quantum Parallel Computing Theory and Discrete Time Crystals
CHENG-HSIAO WU (Presenter), Missouri Univ of Sci & Tech —
Quantum computing from general-purpose and birth-and-death biological types of computing, executed by a man-made quantum processor, to atom-as-processor type are formulated in a four-computational-state cellular automata architecture. When a chain of entangled atoms are employed as a computing machine in cellular automata, the computation results are the discrete time crystals with subharmonics value limited between $\frac{1}{2}$ and $\frac{1}{4}$. The four orthogonal states of each atom in the entangled environment requires that the transition rules for the four computational states be of equal probability and cyclic. Superposition of two transition rules in one cellular automaton is shown to exist and the quantum computing irreversibility will be presented.

4:54PM J09.00013: Error rates in interacting Kitaev chains at finite temperature
JOHN STENGER (Presenter), ROGER MONG, DAVID PEKKER, Univ of Pittsburgh — As proposed by Alexey Kitaev, a topological one-dimensional superconducting wire hosts Majorana zero modes, which could be used to store and process quantum information in a topologically protected manner. At finite temperatures (or quasi-particle densities), Kitaev's model remains topologically protected because it is integrable. However, in the presence of interactions and finite temperature, topological protection is lifted. We investigate how error rates depend on interactions and temperature using TEBD and perturbation theory. These results are significant to experimental efforts to build a Majorana zero mode qubit.

5:06PM J09.00014: Time dependent variational principle with ancillary global Krylov subspace
MINGRU YANG (Presenter), STEVEN ROBERT WHITE, University of California, Irvine — We propose an improved scheme to do the time dependent variational principle (TDVP) in finite matrix product states (MPS) for two-dimensional systems or one-dimensional systems with long range interactions. We present a method to represent the time-evolving state in a MPS with its bond dimension increased by state-averaging with global Krylov vectors. We show that the projection error is significantly reduced so that precise time evolution can still be obtained even if a larger time step is used.

Tuesday, March 3, 2020 2:30 PM - 4:42 PM

Session J10 GIMS: Advances in Scanned Probe Microscopy 4: Machine Learning for Correlative and Analytical Measurements in Scanning Probe Microscopy
108 - Neus Domingo, Institut Català de Nanociència i Nanotecnologia - Tag(s): Focus
2:30PM J10.00001: Surface Structure of α-Quartz(0001)  KRISTEN BURSON (Presenter), Physics Department, Hamilton College, GEORG H. SIMON, Fritz-Haber Institute of the Max Planck Society, CLARE M. MUNROE, Physics Department, Hamilton College, MARKUS HEYDE, H J FREUND, Fritz-Haber Institute of the Max Planck Society — Crystalline silica (SiO₂) surfaces play an important role in nature and technology, and are often used as substrates in scientific studies. Despite its importance, the atomic surface structure of quartz still remains poorly understood, especially on the experimental side. Here we present a real space structure study of α-quartz(0001) surfaces prepared at high temperature in air. The preparation approach is highly reproducible and leads to well-defined, flat, and clean terraces in ambient conditions. Using high-resolution atomic force microscopy (AFM), we observed a large scale surface termination with a reconstruction periodicity of 5 nm, consistent with previous literature [1,2]. By characterizing the samples with AFM in humid air, dry nitrogen, and water we establish insight into surface morphology and reconstruction. Using the enhanced resolution capabilities of atomic force microscopy in liquid water, we address the real space atomic scale structure of this surface and find that the lattice dimensions agree with the bulk crystal lattice constants for α-quartz.


*KMB thanks the Alexander von Humboldt foundation.

2:42PM J10.00002: Nonlinearity-induced frequency mixing in AFM: novel contrast imaging with machine learning  GREG HAUGSTAD (Presenter), Characterization Facility, University of Minnesota, ANDREW AVERY, Unilever Research, STEPHAN HUBIG, RACHEL RAHN, Ecolab, ALON MCCORMICK, Dept. of Chem. Eng. and Mat. Sci., University of Minnesota, BING LUO, HAN SEUNG LEE, Characterization Facility, University of Minnesota — On complex thin films pertinent to lubrication and superhydrophilicity, dynamic AFM methods were used to sense both the elastic and viscous response to an AFM tip. A novel strategy in "multifrequency" AFM -- vibrating the AFM microcantilever (to which the tip is attached) at two tones near the fundamental flexural resonance - - generates dozens of intermodulation tones of response due to nonlinear tip-sample interaction (a well-known concept in electrical engineering usually in the context of AC signal distortion). This method1 both expands contrast mechanisms -- with images of amplitude and phase at each mixing tone via 40 FPGA lock-in amplifiers -- and the ability to reconstruct the distance dependence of conservative and dissipative response at each image pixel via a 40-term discrete Fourier transform of tip motion. This reconstruction is an unprecedented capability in "force spectroscopy" (probing distance dependent interactions). Machine learning, to cluster force-spectroscopic fingerprints and thereby generate higher signal-to-noise images, is further discussed.

1Intermodulation Products AB, Stockholm.

*Equipment and effort funded by the Industrial Partnership for Research in Interfacial and Materials Engineering and the College of Science and Engineering, Univ. of Minnesota.
2:54PM J10.00003: Light Scattering and Localization by Dislocation Scattering Sites*  
FARBOD SHAFIEI (Presenter), University of Texas at Austin, TOMMASO ORZALI, ALEXEY VERT, SEMATECH, MOHAMMAD-ALI MIRI, CUNY, PY HUNG, MAN HOI WONG, SEMATECH, ANDREA ALU, CUNY, GENNADI BERSUKER, The Aerospace Corporation, MICHAEL C DOWNER, University of Texas at Austin — Lattice mismatch between epitaxially grown crystalline thin film over substrate introduce variety of subsurface defects including threading dislocations. Dislocations defects behave as an acceptor traps for electron and thus acting as Coulomb scattering sites. Multi-scattering and localization of the light from these atomic defects scattering sites was collected by a 50 nm aperture fiber based scanning probe microscope. The localized light appears as few to multiple hundreds of nm optical hotspots based on dislocation density of the film. The smaller hotspots correlated to higher defects density as the multi-scattering light is confined in smaller area. The optical collection was done in second harmonic regime to avoid the dominating surface reflection of fundamental light. We used this approach to introduces a noninvasive tabletop technique capable of optically detecting dislocation atomic defects in III-V materials thin films. New diagnosis and supporting simulation would be shown.

*Welch Foundation

3:06PM J10.00004: Native and induced surface charge-transfer doping of MoTe$_2$  
GHEORGHE STAN (Presenter), National Institute of Standards and Technology, CRISTIAN CIOBANU, SRI RANGA JAI LIKITH, Department of Mechanical Engineering and Materials Science Program, Colorado School of Mines, ASHA RANI, SIYUAN ZHANG, CHRISTINA HACKER, SERGIY KRYLYUK, ALBERT DAVYDOV, National Institute of Standards and Technology — In this work, the surface charge transfer doping (SCTD) of air-exposed MoTe$_2$ surfaces was investigated by means of Kelvin probe force microscopy (KPFM). The induced changes in the surface potential of MoTe$_2$ due to air adsorbates were detailed as a function of the thickness of exfoliated MoTe$_2$ flakes all the way down to a single atomic layer. It was found that the SCTD driven by adsorbates can be easily adjusted through thermal annealing and, in this way, have an effective modulation on the surface potential of MoTe$_2$. Furthermore, the SCTD was controlled locally at the nanoscale by using the probe of an electrostatic force microscope as a floating gate. Following either thermal annealing or contact electrification, the air-exposed MoTe$_2$ surfaces exhibited slow reversal processes of re-adsorption with the restoration of the original positively charged doping. The KPFM measurements were paired with X-ray photoelectron spectroscopy measurements and density functional theory calculations to assess the contribution of physisorbed molecules to the observed variations in the measured surface potential. The study emphasizes that, as a reversible and controllable nanoscale physisorption, the SCTD can add significant progress to the paradigm of emerging 2D-TMDC electronics.
3:18PM J10.00005: A traveling salesperson and sparse sampling boost to quasiparticle interference mapping*  JENS OPPLIGER, FABIAN NATTERER (Presenter), Department of Physics, University of Zurich — The serial nature of STM investigations render complex measurement tasks, such as QPI mapping, impractical. Conventionally, QPI is carried out by recording hundreds of thousands of point-spectra that capture LDOS modulations from which scattering-space is calculated via Fourier-transform. Yet, despite the efforts required, QPI is mapped extensively because it provides insight into band-structure details when measurement conditions prohibit the use of ARPES. However, in view of the large number of data-points, it is surprising that QPI patterns contain only little information. This motivates our use of compressed sensing (CS) to fundamentally speed-up QPI mapping [1]. From only a fraction of the usual LDOS measurements, we reliably recover the full QPI pattern. Since CS depends on incoherent measurements, we sparsely sample LDOS at randomly selected locations using constant and varying probability density. The STM tip is moved between LDOS measurements according to a traveling salesperson to achieve an overall 5-50 faster QPI throughput.


*Funding from the Swiss National Science Foundation under project number PP00P2_176866 is appreciated.

3:30PM J10.00006: Controlled Manipulation of Molecules: A New Pathway to Catalysis Research  OMUR DAGDEVIREN (Presenter), CHAO ZHOU, Yale University, MILICA TODOROVIC, Aalto University, ERIC ALTMAN, UDO DIETMAR SCHWARZ, Yale University — With the continued development of scanning probe microscopy techniques, the manipulation of single molecules has become possible. Thereby, the manipulation path can be chosen at will and energy barriers can be quantified, as can the energy landscape around the molecule [1]. The molecules were either pushed, pulled, jumped to the tip, or did not move depending on the chemical surrounding of the molecule and the chemical identity of the tip. To preserve the accuracy of recovered tip-sample interaction, we used oscillation amplitudes significantly larger than the decay length of the tip-sample interaction potential [1-3]. For further insight, we compared measured energy landscapes and manipulation outcomes with computational results obtained using a search protocol [4]. References: [1] O. E. Dagdeviren et al., Nanotechnology 27 (2016). [2] O.E. Dagdeviren et al., Phy. Rev. App. 9 (2018). [3] O. E. Dagdeviren et al., Rev. of Scien. Ins. 90 (2019). [4] M. Todorovic et al. npj Comp Mat. 5 (2019).
3:42PM J10.00007: Optimal Bayesian experimental design for everyday measurements*
ROBERT MCMICHAEL (Presenter), National Institute of Standards and Technology, SERGEY DUSHENKO, KAPILDEB AMBAL, University of Maryland and National Institute of Standards and Technology — This talk gives an overview of software that increases speed and precision of routine measurements. In experiments where one would traditionally fit data to extract parameters, the 'optbayesexpt' package recommends measurement settings “on the fly” based on analysis of accumulating data. The algorithm uses optimal Bayesian experimental design to predict settings with the best chance of reducing parameter uncertainty. In simulations and in tests, we demonstrate order-of-magnitude speedup in measurements of Lorentzian peaks and significant speedup of exponential decay measurements relative to measure-then-fit strategies. The package, written in Python, includes a server script that communicates with instrument control software in any popular instrument control language. Demonstrations include magnetic resonance spectra of NV centers in diamond, and simulations include calibration of π-pulses for spin control. See the manual at https://pages.nist.gov/optbayesexpt/ and software at https://github.com/usnistgov/optbayesexpt.

*S.D. and K.A. acknowledge support under the Cooperative Research Agreement between the University of Maryland and the National Institute of Standards and Technology, Award 70NANB14H209, through the University of Maryland.

3:54PM J10.00008: Defect Identification and Statistics Toolbox (DIST): A Tool for Automating Defect Analysis and Statistics Generation*
ALANA GUDINAS (Presenter), SHAWNA HOLLEN, Univ of New Hampshire, JASON P MOSCATELLO, Textron Systems, Wilmington, MA — Widely available scanning tunneling microscopy (STM) image analysis software do not automate the process of identifying and analyzing atomic defects in images. We present the Defect Identification and Statistics Toolbox (DIST) as a solution for automated defect analysis, based in MATLAB. DIST provides a graphical user interface for interactive image processing and background noise reduction to aid in defect identification. In DIST, topographical contour plots are generated in the image to isolate defects based on their brightness compared to the background. DIST implements an ant colony optimization (ACO) algorithm [1] to compare the shapes of individual defects defined by the contour plots. DIST also automatically compiles and outputs statistics of identified defects, such as apparent height, line profiles, and area. The novel automation techniques in DIST allow users to quickly and accurately analyze hundreds of defects at a time without relying on the user to manually identify each one.


*This research was supported by NSF-DMR #1709029 and the University of New Hampshire Hamel Undergraduate Research Center.
4:06PM J10.00009: Learning hidden structure of nanoscale spectroscopies with metric analysis* [Invited] PETRO MAKSYMOVYCH (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Lab — Scanning probe microscopy is routinely faced with analysis of heterogeneous datasets, largely without having reference analytical models. Ordered parts of probed materials, such as regular lattice structures or coherent scattering can often be effectively captured with integral transforms to reveal the atomic and electronic structure, sometimes with unprecedented resolution. However, the problem of capturing inhomogeneities and furthermore understanding of their physical significance demands further attention. Here we will demonstrate how an appropriately chosen metric, combined with analysis of its variability enables effective characterization of key and often hidden structures within hyperspectral datasets. We applied such methodology to three representative cases with remarkably strong inhomogeneity in the nanoscale properties — variability of superconducting gap and electronic structure in unconventional superconductors FeSe and Ba$_2$FeAs$_2$, measurement of individual defects in these systems and structural phase transitions in dipolar solids. In each case, metric analysis has revealed a wide-range of sometimes unexpected properties, such as log-normal distribution in tunneling spectroscopy and sub-surface location of atomic-scale defects, while also providing a robust approach to understand spectral weight transfer and spectral signatures of electronic defects and to detect phase transitions in dielectric solids from their hysteretic response to applied fields. Future extension of these methodologies to combine elements of machine and deep learning will also be discussed.

*We gratefully acknowledge materials and microscopy teams at Oak Ridge National Laboratory for their contribution in materials synthesis and nanoscale measurements. Support provided by U.S. DOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. Microscopy was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

Tuesday, March 3, 2020 2:30 PM - 4:54 PM

Session J15 DFD DSOFT: Active Colloids II 210/212 - Quentin Brosseau, University of Pennsylvania
Floor- or ceiling-sliding for chemically active, gyrotactic, sedimenting Janus particles

SAYAN DAS, Theory of Inhomogeneous Condensed Matter, Max Planck Institute for Intelligent Systems, Stuttgart, Germany, ZOHREH JALILVAND, Department of Chemical Engineering, City College of the City University of New York, MIHAIL POPESCU (Presenter), Theory of Inhomogeneous Condensed Matter, Max Planck Institute for Intelligent Systems, Stuttgart, Germany, WILLIAM E. USPAL, Department of Mechanical Engineering, University of Hawai'i at Manoa, SIEGFRIED DIETRICH, ILONA KRETZSCHMAR, Theory of Inhomogeneous Condensed Matter, Max Planck Institute for Intelligent Systems, Stuttgart, Germany — Chemically active particles achieve force- and torque-free motility via catalytic chemical reactions promoted on parts of their surface. These lead to inhomogeneity in the chemical composition of the solution (“chemical field”) and hydrodynamic flow of the solution. By means of coupling distortions of these fields back to its motion, a chemically active particle experiences effective interactions with boundaries; this can lead to the occurrence of, e.g., states of steady "sliding" along a wall.

The often employed Janus spherical particles are density mismatched with the solution and, additionally, gyrotactic ("bottom-heavy"); the latter promotes alignment of the axis orthogonal to a horizontal wall. It is thus unclear under which conditions sliding states for such particles may occur. Here we study this issue theoretically for model gyrotactic, self-phoretic Janus spheres near horizontal planar walls which are either below (“floor”) or above (“ceiling”) the particle. We construct "state diagrams" as a function of the sedimentation velocity and gyrotactic response of the particle. These show that in certain cases sliding states may emerge simultaneously at both the ceiling and the floor. The predictions are critically compared with experimental results.

Effects of Colloid Interactions on Active–Passive Collective Behavior

IAN MADDEN (Presenter), Northwestern University, LINLIN WANG, JULIANE SIMMCHEN, Technische Universität Dresden, ERIK LUIJTEN, Northwestern University — Active colloidal matter can exhibit different phases, such as flocking, rafting, and spinning, in response to changes in active particle properties (Soft Matter 14, 6969–6973 (2018)). The links between these phenomena and the catalytic, hydrodynamic, electrostatic, and phoretic properties of the colloids are disputed, in part because it is difficult to separate the impact of each force in experiment. Whereas current models can capture some aspects of a system's collective behavior, oversimplification can lead to incorrectly attributing a particular behavior to a specific interaction (The European Physical Journal E 41, 145–169 (2018)). Using experimentally informed models, we employ lattice-Boltzmann and molecular dynamics simulations to deconvolute these interactions and make direct connections between particle properties and observed collective phenomena.
RICARD ALERT (Presenter), Princeton University, JIE ZHANG, University of California, Santa Barbara, JING YAN, Yale University, NED WINGREEN, Princeton University, STEVE GRANICK, Ulsan National Institute of Science and Technology — At thermodynamic equilibrium, phase separation arises from attractive interparticle interactions. However, self-propelled particles can phase separate even if they have purely repulsive interactions. This phenomenon, called motility-induced phase separation (MIPS), has become a landmark of active matter physics. The conventional mechanism of MIPS is the decrease of particle speed due to repulsive interactions in high-density regions, which leads to further accumulation of particles. In this talk, I will demonstrate a new mechanism of MIPS, which instead of relying on a slowdown of particle motion with density, is based on interaction torques that reorient particles toward high-density regions. We show that such torques take place in suspensions of Janus colloids driven by an electric field. From the electrostatic interactions between the particles, we derive hydrodynamic equations that show how MIPS arises from orientational interactions in this system. Furthermore, we predict that, in contrast to the repulsion-based MIPS scenario, the phase diagram of torque-based MIPS exhibits reentrance, with the system reentering the uniform phase at high self-propulsion speed.

*R.A. acknowledges support from the Human Frontiers of Science Program (LT-000475/2018-C).

CHONG SHEN (Presenter), LANFANG LI, ZHIYU JIANG, JAMES F GILCHRIST, H DANIEL OU-YANG, Lehigh Univ — Active Brownian particles (ABPs), colloidal particles driven into persistent motions by external fields, can serve as a model for understanding the non-thermal behavior of biological systems. Non-thermal fluctuations of an ABP are expected to behave differently from thermal Brownian motions in distinctive manners, e.g., exhibiting different diffusivities, effective temperatures, and fluctuation power spectral densities. While the non-thermal fluctuations can be separated from the thermal ones in their power spectral densities, it is non-trivial to decouple the non-thermal from thermal changes in a fluctuation histogram, because the experimentally measured fluctuation histogram is a convolution of the two fluctuations. We hypothesize that the non-thermal fluctuation could be extracted from the overall noise histogram by standard deconvolution algorithms when thermal fluctuations can be determined independently. This presentation reports an experimental study using a model ABP in a quadratic potential well to test the hypothesis and its limitations.
3:42PM J15.00005: Transport phenomena and Green-Kubo relations in active media:
Theory* JEFFREY EPSTEIN (Presenter), KRANTHI MANDADAPU, University of California, Berkeley — We derive Green-Kubo relations for the several viscosity terms that appear in a constitutive theory of viscous active fluids with and without an internal spin degree of freedom, starting from an Onsager regression hypothesis on the non-equilibrium steady state. In particular, we focus on the connection between time-reversal symmetry breaking and the emergence of the non-dissipative component of viscosity known as odd viscosity. Our results allow measurement of this odd viscosity in molecular dynamics simulations (for details see the corresponding Simulation talk). Time permitting, extensions of our results to liquid crystals will be discussed, with possible relevance to the modeling of active fluids such as suspensions or colonies of bacteria.

REF: Epstein and Mandadapu, *Time reversal symmetry breaking in two-dimensional non-equilibrium viscous fluids*

*J.M.E. was supported by the Department of Defense (DoD) through the National Defense Science and Engineering Graduate Fellowship (NDSEG) Program. K.K.M was supported by Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under contract No. DEAC02- 05CH11231.

3:54PM J15.00006: Transport phenomena and Green-Kubo relations in active media:
Simulation CORY HARGUS (Presenter), University of California, Berkeley, KATHERINE KLYMKO, CCSE, Lawrence Berkeley National Laboratory, JEFFREY EPSTEIN, KRANTHI MANDADAPU, University of California, Berkeley — We compute the viscous transport coefficients of an active fluid composed of chirally rotated dumbbells with molecular dynamics simulations. We use recently obtained Green-Kubo relations to calculate the emergent viscous transport coefficients (for details see accompanying Theory talk), and find that odd viscosity arises due to the breaking of time-reversal symmetry at the level of stress correlations. We demonstrate agreement between viscosity coefficients obtained from Green-Kubo relations and non-equilibrium molecular dynamics simulations with imposed shear. This verifies the Green-Kubo relations derived using the application of Onsager’s regression hypothesis to non-equilibrium steady states of active systems, and provides an impetus for developing the theory of non-equilibrium thermodynamics of active media.

References:
Epstein, J. M., & Mandadapu, K. K.; *arXiv*; 2019
Klymko, K., Mandal, D., & Mandadapu, K. K.; *Journal of Chemical Physics*; 147, 194109, 2017
Nonlinear dynamics of chemically active microdrops grants an insight into interfacial chemistry

MATVEY MOROZOV (Presenter), LAURENCE RONGY, FABIAN BRAU, Universite libre de Bruxelles — Active emulsions are complex physicochemical systems that may provide a model for biological phenomena such as RNA polymerase clusters. Theoretical understanding of the physical chemistry of active emulsions is key for reliable modeling of these systems. We consider the simplest "building block" of an active emulsion: a microdroplet undergoing gradual micellar solubilization in the bulk of surfactant solution. In experiments, dissolving droplets may spontaneously induce a flow in the surrounding fluid. Our model links the features of the flow around the drop with the characteristics of nonlinear surfactant sorption kinetics and nonlinear chemical reaction at the droplet interface. We show that continuous assembly of micelles may act as a cleaning mechanism preventing the formation of a continuous monolayer of surfactant monomers even when bulk surfactant concentration exceeds CMC. Our asymptotics reveals that the Marangoni flow velocity depends heavily on the reaction rate and micelle size, while numerical simulations indicate that nonlinear kinetics of micelles production allows for multistability of flow regimes.

*This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 801505.

Revisiting the equation of state of active Brownian particles

STEWART MALLORY (Presenter), Caltech, AHMAD OMAR, University of California, Berkeley, JOHN F BRADY, Caltech — One of the unique feature of active systems is that they are able to phase separate without the presence of attractive interparticle interactions. Determining quantitatively the phase boundary for these fundamentally out-of-equilibrium systems is an on-going challenge within the community. The mechanically defined active pressure plays a central role in many of the recently proposed coexistence criteria. Using a combination of large-scale simulation and analytical theory, we reveal previously unknown features of this equation of state. Recognizing these features is essential when attempting to assess coexistence criteria by comparing the predicted phase diagram to simulation data. Upon using this refined equation of state, the predicted phase boundaries are qualitatively altered in comparison to previously work.

*Arnold & Mabel Beckman Foundation
4:30PM J15.00009: Three-body problem for Brownian particles at different temperatures*  
MICHAEL WANG (Presenter), ALEXANDER Y GROSBERG, New York Univ NYU — A mixture of Brownian particles at different temperatures has been a useful model for studying out-of-equilibrium systems of many components with differing levels of activity (e.g. phase separation of mixtures of passive and active particles). This model was previously studied analytically up to the second virial coefficients using pair distributions in the dilute limit. We are interested whether or not the two-particle results can be extended to understand the three-particle distributions. By considering the solvable case of pairwise quadratic interactions, we show that, unlike the two-particle distribution, the three-particle distribution takes on an interesting form that is not in general Boltzmann-like with an effective temperature. We summarize some of our results here and briefly discuss an interesting connection with the Newtonian three-body problem.

*This work was supported primarily by the MRSEC Program of the National Science Foundation under Award Number DMR-1420073.

4:42PM J15.00010: Microscopic Origins of the Swim Pressure and the Anomalous Surface Tension of Active Matter  
AHMAD OMAR (Presenter), University of California, Berkeley, ZHEN-GANG WANG, JOHN F BRADY, California Institute of Technology — The unique pressure exerted by active particles -- the "swim" pressure -- has proven to be a useful quantity in explaining many of the seemingly confounding behaviors of active particles. However, its use has also resulted in some puzzling findings including an extremely negative surface tension between phase separated active particles. Here, we demonstrate that this contradiction stems from the fact that the swim pressure is not a true pressure. At a boundary or interface, the reduction in particle swimming generates a net active force density despite no external fields or forcing -- it is an entirely self-generated body force. The pressure at the boundary, which was previously identified as the swim pressure, is in fact an elevated (relative to the bulk) value of the traditional particle pressure that is generated by this interfacial force density. Recognizing this unique mechanism for stress generation allows us to define a much more physically plausible surface tension. We clarify the utility of the swim pressure as an "equivalent pressure" (analogous to those defined from electrostatic and gravitational body forces) and the conditions in which this concept can be appropriately applied.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J16 DQI: Quantum Annealing and Optimization I  
201 - Rolando Somma, Los Alamos National Laboratory - Tag(s): Focus
2:30PM J16.00001: Toward integration of Kerr-nonlinear parametric oscillators for adiabatic quantum computation with Lechner-Hauke-Zoller scheme  TARO KANAO (Presenter), HAYATO GOTO, Toshiba Corp — Adiabatic quantum computation with networks of Kerr-nonlinear parametric oscillators (KPOs) has been proposed, which can solve combinatorial optimization problems (or Ising problems) by using quantum bifurcation [1, 2]. KPO networks integrated in two-dimensional plane can deal with all-to-all connected Ising problems by utilizing Lechner-Hauke-Zoller (LHZ) scheme [3], where KPOs are coupled by local four-body interactions [4, 5]. In the previous studies, however, the number of effective KPOs is limited within three. In this study, we investigate LHZ-scheme KPO networks with larger number of KPOs. Based on numerical simulations, we confirm that the LHZ scheme works for a wide range of the amplitude of the four-body interactions. Besides, we propose a method to improve the LHZ-scheme KPO networks, which is important for the case of larger number of KPOs.


2:42PM J16.00002: Long range coupling through a chain of RF-SQUIDs for superconducting flux qubit quantum annealers* ANTONIO JAVIER MARTINEZ (Presenter), DANIEL M TENNANT, XI DAI, DENIS MELANSON, ALI YURTALAN, SALIL BEDKIHAL, EDWARD TANG, University of Waterloo, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, RABINDRA DAS, DAVID K KIM, JONILYN YODER, STEVEN WEBER, ANDREW JAMES KERMAN, MIT Lincoln Laboratory, SERGEY NOVIKOV, STEVEN M DISSELER, JAMES I BASHAM, JEFFREY GROVER, Northrop Grumman Corporation, EVGENY MOZGUNOV, DANIEL A LIDAR, University of Southern California, ADRIAN LUPASCU, University of Waterloo — Increasing the degree of coupling in a quantum annealer can improve its computational power; however, each physical connection to a superconducting flux qubit increases its area and hence its susceptibility to noise. The coupler tree architecture is a proposed solution which allows increasing coupling degree without increasing qubit area. We report on a subgraph of the coupler tree consisting of 2 capacitively shunted flux qubits connected by 7 RF-SQUIDs. We experimentally demonstrate propagation of a magnetic flux signal through the chain, visible as a frequency step in the persistent current readouts attached to each qubit and coupler. Anticrossing spectroscopy is explored to confirm the quantum character of the coupling. Results are in agreement with full quantum circuit simulations. Prospects for measurement of entanglement and noise are discussed.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).
2:54PM J16.00003: Finding optimized anneal paths in capacitively shunted flux qubits

MOSTAFA KHEZRI (Presenter), Univ of Southern California, JEFFERY GROVER, Northrop Grumman, DANIEL A LIDAR, Univ of Southern California — Quantum annealers require accurate control and optimization of system parameters to reduce noise levels and ultimately demonstrate a computational advantage over classical algorithms. This requires a careful characterization of the system and its behavior in response to control biases.

In this work we study a capacitively shunted flux qubit (CSFQ), and use spectroscopy and dispersive readout to extract system parameters and model the qubit.

We confirm the multi-level structure of the circuit model of the CSFQ by annealing the qubit through small gaps and observing quantum signatures of level crossing between different eigenenergies.

We then use our model to mitigate the effect of noise by finding optimized anneal paths that minimize the transition width between the flux qubit's left and right wells.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) through the Army Research Office (ARO) Contract No. W911NF-17-C-0050.

3:06PM J16.00004: Quantum annealing with spin lock technique

HIDEAKI HAKOSHIMA (Presenter), YUICHIRO MATSUZAKI, YUYA SEKI, SHIRO KAWABATA, National Institute of Advanced Industrial Science and Technology (AIST) — Quantum annealing (QA) and adiabatic quantum computation (AQC) are attractive ways to tackle combinatorial optimization problems. However, the standard QA and AQC require strong interactions between qubits, and the coupling strength should be comparable with the resonant frequency of the qubits to solve practically useful problems. Such requirement prevents many systems from performing QA and AQC experimentally. Here, we propose an alternative way to implement a spin-lock based QA, which effectively tunes the qubit frequency by a continuous drive. Under the rotating-wave approximation, we show that our method is equivalent to the standard QA and AQC, and moreover we can analyze the deviation of the rotating-wave approximation systematically. Our method can be implemented by many systems such as superconducting transmon qubits, superconducting capacitive shunted flux qubits, and Si quantum-dots-based spin qubits. Since these systems have an advantage in scalability, our results pave the way to implement the practical QA and AQC.

*This work was supported by Leading Initiative for Excellent Young Researchers MEXT Japan, and is partially supported by MEXT KAKENHI (Grant No. 15H05870) and the New Energy and Industrial Technology Development Organization (NEDO), Japan.
3:18PM J16.00005: Assessing the potential of Rydberg atoms for adiabatic quantum computing of an NP-hard problem* BERTRAND MARCHAND (Presenter), FABRICE SERRET, THOMAS AYRAL, Atos Quantum Lab — When practically confronted with an NP-hard combinatorial optimization problem, the first question many computer scientists ask is whether a good approximation algorithm exists (i.e a tractable algorithm with provable guarantees on solution quality). We argue that the quality and potential of NISQ quantum annealers should therefore be assessed through the approximation ratio that they achieve on specific NP-hard problems. We put this methodology to practice for a platform consisting of neutral atoms trapped in optical arrays [1], which may be used to tackle an NP-hard problem called UD-MIS [2]. We present numerical estimates of the approximation ratio achieved by this approach under realistic noise conditions, on a class of experimentally-implementable random graphs. These results are then compared with the performances achieved by classical PTASs (Polynomial-Time Approximation Schemes) on the same problem.


*This work was supported by Atos and the European Union’s Horizon 2020 research and innovation program under grant agreement No. 817482 PasQuanS.

3:30PM J16.00006: A theoretical analysis of the power of pausing* HUO CHEN (Presenter), DANIEL A LIDAR, Univ of Southern California — Recent experimental results have shown that adding a pause during quantum annealing can significantly improve the success probability for certain hard optimization problems. An optimal pausing position, where the maximum performance improvement compared to the unpaused case is achieved, has also been observed. In this work, we present a theoretical analysis that explains these observations. We identify the key features of examples known empirically to benefit from pausing. Using these features as building blocks, we then construct a toy model with a simple analytic structure. Using this model, we derive, in an open quantum system setting, a set of sufficient conditions for which an optimal pausing position exists.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.
Quantum computation using Kerr-nonlinear parametric oscillators

HAYATO GOTO (Presenter), Toshiba Corp — In the past few years, the author and others have proposed quantum computation using Kerr-nonlinear parametric oscillators (KPOs). This approach opens new possibilities for adiabatic quantum computation [1-3], universal quantum computation [4,5], and physical implementations of qubits [6]. Since this idea is based on quantum bifurcations of KPOs [1], we refer to this kind of quantum computer as Quantum bifurcation Machine (QbM) [7]. Here we review the QbM with its recent progress.


Effectiveness of quantum annealing pause and partial gauges on embedded degree-bounded minimum spanning tree problems

SHON GRABBE (Presenter), NASA Ames Research Center, ZOE GONZALEZ IZQUIERDO, University of Southern California, STUART HADFIELD, JEFFREY MARSHALL, ZHIHUI WANG, ELEANOR RIEFFEL, NICHOLAS CRAMER, NASA Ames Research Center — Robust communication networks are essential to the growing use of small Unmanned Aerial Systems (sUAS) technologies. This work focused on evaluating the potential for harnessing quantum annealing to optimize communication routing in UAS communication networks subject to constraints. To support experimentation on early hardware, we consider as a surrogate problem finding the minimum degree-bounded spanning tree within a communication graph. While finding the minimum spanning tree is computationally tractable, with bounds on the degree the problem becomes NP hard. We provide a mapping of the degree-bounded minimum spanning tree problem to a Quantum Unconstrained Binary Optimization problem, and report on results demonstrating the effectiveness of an annealing pause on these embedded problem instances. Lastly, we demonstrate the effectiveness of partial gauge transformation for situations where asymmetric parameter ranges make standard gauge transformation infeasible.

*We are grateful for support from NASA Ames Research Center, from the AFRL Information Directorate under grant F4HBKC4162G001, and from the Office of the Director of National Intelligence (ODNI) and the Intelligence Advanced Research Projects Activity (IARPA), via IAA 145483.
4:30PM J16.00009: Quantum annealing with boundary canceling schedules* HUMBERTO MUNOZ-BAUZA (Presenter), LORENZO CAMPOS VENUTI, DANIEL A LIDAR, Univ of Southern California — The boundary cancellation theorem (BCT) for open systems bounds the distance between the final equilibrium state and the evolved state of an ergodic dissipative Liouvillian, where the scaling with anneal time depends on the number of vanishing derivatives of the annealing schedule at the end of the evolution. We test the thermal scaling of small gadgets up to 8 qubits on the D-Wave quantum annealer by controlling the vanishing derivatives of the schedule during the thermalization phase. While the theoretical BCT bounds are not accessible experimentally, we find that such schedules improve thermal scaling during the anneal and consequentially enhance the ground state probability of the gadgets.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.

4:42PM J16.00010: The Perils of Embedding for Sampling Problems* JEFFREY MARSHALL (Presenter), NASA Ames Research Center, and USRA, ANDREA DI GIOACCHINO, Dipartimento di Fisica, University of Milan and INFN, ELEANOR RIEFFEL, NASA Ames Research Center — Current quantum annealers impose constraints on the structure of the cost Hamiltonian due to the connectivity of the qubits. This means that in order to solve many problems of interest, one is required to embed the native graph into the hardware graph. The effect of embedding for sampling is more pronounced than for optimization, since one needs to consider states at all energies, and not just the ground states. We argue that as the problem size grows, the chance of a sample being in the logical subspace is exponentially suppressed. It is therefore necessary to construct post-processing techniques to evade this exponential sampling overhead, to project from the embedded distribution one is physically sampling from, back to the logical space. We observe that the simplest projection technique, majority vote, can fail quite spectacularly at preserving distribution properties. Furthermore, we show that even with care, one cannot avoid biasing the statistics. On the positive side, we demonstrate a new projection technique which substantially out-performs majority vote.

*We appreciate support from the AFRL Information Directorate under grant F4HBKC4162G001 and the Office of the Director of National Intelligence and the Intelligence Advanced Research Projects Activity, via IAA 145483.
4:54PM J16.00011: Reproducing the Performance Enhancement of Adiabatic Reverse Annealing

MATTHEW KOWALSKY (Presenter), Physics, University of Southern California, TAMMEM ALBASH, University of New Mexico — We propose a conventional (forward) quantum annealing protocol with a diagonal catalyst of programmable strength \( \lambda \). By adjusting \( \lambda \) we demonstrate an exponential improvement in the efficiency of quantum annealing for solving the p-spin model, reproducing the performance improvements of adiabatic reverse annealing\(^1\). Our protocol allows us to identify the enhancement mechanism of such approaches: balancing Hamiltonian terms in a way that mitigates discontinuous shifts in the global minimum of the semiclassical potential. This observation allows us to identify and solve other problems amenable to such protocols.


*The research is based upon work (partially) supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.

5:06PM J16.00012: Reverse quantum annealing with dissipation

GIANLUCA PASSARELLI, Dipartimento di Fisica "E. Pancini", Università di Napoli "Federico II", KA WA YIP (Presenter), Univ of Southern California, PROCOLO LUCIGNANO, Dipartimento di Fisica "E. Pancini", Università di Napoli "Federico II", DANIEL A LIDAR, Univ of Southern California, HIDETOSHI NISHIMORI, Tokyo Institute of Technology — Reverse annealing is a variant of quantum annealing where one initializes the system in a random classical state. The transverse field is first increased and then decreased at an inversion point, to find a better output state than the initial state of a given optimization problem. The procedure may be iterated with the last output state as the new input state.

[1] studied the unitary dynamics of reverse annealing of the fully-connected ferromagnetic p-spin model. Here we investigate the performance of reverse annealing for the p-spin model in a low-temperature open system setting. We study a system of qubits with collective and individual system-bath interaction models. We simulate the Markovian dynamics over a range of initial states and inversion points, and show that the relaxation mechanism gives an overall enhancement of performance over the closed-system setting. We also analyze the case of pausing at the inversion point, and show that prolonged relaxation near the avoided crossing can allow us to find the correct ground state solution with near certainty.


*Work supported by CINECA award under the ISCRA initiative, and by IARPA and ARO under Contract No. W911NF-17-C-0050.
Quantum annealing in a degenerate two-level system — SHOHEI WATABE (Presenter), Tokyo University of Science, YUYA SEKI, SHIRO KAWABATA, National Institute of Advanced Industrial Science and Technology — Quantum annealing is a method for avoiding the increase of the calculation cost of the combinatorial optimization problem. Since the combinatorial optimization problems are ubiquitous, quantum annealing machine with high efficiency and scalability will give an immeasurable impact on many fields. An idea for finding high success probability is one of the most important issues for quantum annealing. In this presentation, we show that a degenerate two-level system that is called quantum Wajnflasz-Pick model may provide the higher success probability than the conventional spin-1/2 model in a weak longitudinal magnetic field region. The origin of the higher success probability can be understood from the fact that the Hamiltonian in this model can be reduced into that of the spin-1/2 model. In the reduced Hamiltonian, the effective longitudinal magnetic field may open the energy gap, which suppresses the Landau–Zener tunneling providing leakage of the ground state.

*This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO), Japan. This work is also supported by Nanotech Career-up Alliance (Nanotech CUPAL), Japan Science and Technology Agency (JST).

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J17 DQI: Focus Silicon Spin Qubits in Double Quantum Dots — Susan Clark, Sandia National Laboratories - Tag(s): Focus

Si based quantum computer architecture and associated engineering challenges — MAUD VINET (Presenter), PIERRE-ANDRE MORTEMOUSQUE, LOUIS HUTIN, BENOIT BERTRAND, XAVIER JEHL, YANN-MICHEL NIQUET, GAËL PILLONNET, GÉRARD BILLIOT, MARC SANQUER, CEA Grenoble, BAPTISTE JADOT, EMMANUEL CHARION CHANRION, MATIAS URDAMPILLETA, TRISTAN MEUNIER, Néel Institute, CNRS — Si-based QC appears as a promising approach to build a quantum processor; thanks to the size of the qubits, the quality of the quantum gates and the VLSI ability to fabricate billions of closely identical objects. The quality of Si spin qubits has improved very fast with the introduction of isotopically purified 28Si. In this presentation, we will share our quantum accelerator architecture and will present progress made towards the actual demonstration of this architecture. We will show data ranging from material development to packaging with insights in device design. We will review the technological challenges that are still to be tackled. We will highlight how we leverage tight-binding simulations to develop a QCAD activity (quantum bit computer aided design).

*This work is partially funded by ERC Synergy grant QuCube and by French Agence Nationale de la Recherche and EU H2020 projects.
3:06PM J17.00002: A Valley Hot-Spot Driven Singlet-Triplet Qubit in a Silicon MOS DQD*
RYAN JOCK (Presenter), Sandia National Laboratories, NOAH T JACOBSON, Center for Computing Research, Sandia National Laboratories, MARTIN RUDOLPH, DAN R. WARD, MALCOLM S. CARROLL, DWIGHT R LUHM AN, Sandia National Laboratories — Electron spins in silicon quantum dots (QDs) have gained traction as a promising qubit platform due to the controllability of qubit-qubit interactions and the availability of mature silicon microelectronics fabrication techniques. However, confining electrons to QDs at the Si/SiO\textsubscript{2} interface has recently been shown to produce stronger than expected spin-orbit (SO) physics. Here, we present a novel operating mode of a singlet-triplet qubit that exploits an inter-valley SO interaction to drive high-orthogonality, electrical-only qubit control. We employ this interaction to produce a high-performance qubit with operational S-T\textsubscript{0} rotation frequencies exceeding 200 MHz and a quality factor, Q = f x T\textsubscript{2}*, near 20. Utilizing SO effects to drive qubits offers the advantage of all-electrical control, avoiding the need for micromagnets or on-chip microwave strip-lines, and allows for a characterization of the MOS platform without the added fabrication complexity of additional nano-fabricated metal layers.

*Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the DOE’s National Nuclear Security Administration under contract DE-NA0003525.
Learning the states of double quantum dot systems: A ray-based approach

JUSTYNA ZWOLAK (Presenter), National Institute of Standards and Technology, Gaithersburg, MD 20899, USA, THOMAS MCJUNKIN, Department of Physics, University of Wisconsin-Madison, Madison, WI 53706, USA, SANDESH KALANTRE, Joint Quantum Institute, University of Maryland, College Park, MD 20742, USA, SAMUEL NEYENS, EVAN R MACQUARRIE, Department of Physics, University of Wisconsin, Madison, WI 53706, USA, LISA F EDGE, HRL Laboratories LLC, 3011 Malibu Canyon Road, Malibu, California 90265, USA, MARK ALAN ERIKSSON, Department of Physics, University of Wisconsin-Madison, Madison, WI 53706, USA, JACOB TAYLOR, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

— Given the progress in the construction of multi-quantum dot (QD) arrays in both 1D and 2D [1,2], it is imperative to replace the current practice of manual tuning to a desirable electronic configuration with a standardized and automated method. Recently, we have experimentally realized an auto-tuning paradigm proposed by Kalantre et al. [3] that combines machine learning (ML) and optimization routines, with ConvNets used to characterize the state and charge configuration of single and double QD states from measurements via the conductance of a nearby charge sensor [4]. Now we expand on this work and propose a novel approach where we use 1D traces (“rays”) measured in multiple directions in the gate voltage space to describe the position of the features characterizing each state (i.e., to “fingerprint” the state space). Using these “fingerprints” instead of full-sized 2D scans we train an ML algorithm to differentiate between various state configurations. Here, we report the performance of the ray-based learning on experimental data and compare it with our image-based approach.

Spin shuttling in a silicon double quantum dot*  

FLORIAN GINZEL  
(Presenter), Department of Physics, University of Konstanz, D-78457 Konstanz, Germany, ADAM MILLS, JASON PETTA, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — Motivated by the demand[1] for long and intermediate range interaction in quantum information devices and recent developments[2,3] we theoretically analyze the dynamics of an electron during a detuning sweep in a silicon double quantum dot (DQD) occupied by one electron, and investigate possibilities and limitations of spin transport. Spin-orbit interaction and an inhomogeneous magnetic field which can introduce errors are included in our model. Interactions that couple the position, spin and valley degrees of freedom open a number of avoided crossings in the spectrum allowing for diabatic transitions and interfering paths. The outcome of a spin shuttling protocol is explored by means of numerical simulations and an approximate analytical model based on the solution to the Landau-Zener problem. We find that constructive interference can ensure a high transport fidelity even for a fast protocol. Exploiting destructive interference between different paths the DQD can also act as a spin or valley filter.


*This work has been supported by the ARO grant W911NF-15-1-0149.

Towards an electrically controlled spin-valley quantum dot qubit in silicon*  
NICHOLAS PENTHORN (Presenter), JOHN ROONEY, JOSHUA S SCHOENFIELD, California State University, Los Angeles, LISA F EDGE, HRL Laboratories, HONGWEN JIANG, California State University, Los Angeles — Electrical control of electron spins in semiconductor quantum dot qubits requires some form of spin-electric field interaction, typically as a micromagnet-induced field gradient. However, electron spins are known to couple to valley states in silicon [1], which could afford a new method for spin control without the need of a micromagnet or native spin-orbit interaction. Building on our recent result of electrical control of a valley qubit in a Si/SiGe double quantum dot [2], we show that the valley splitting can be tuned by 32 μeV with modest voltages on local gates. Using real-time spin relaxation measurements on a single electron in this device with a variable external field, we see evidence of spin-valley mixing signified by a “hot spot” with high spin relaxation below 500 mT. Additionally, we show our progress on implementing valley-mediated spin qubit operations.


*This work was supported by U.S. ARO through Grant. No. W911NF1410346.
3:54PM J17.00006: Charge noise induced spin decoherence in a double quantum dot: Effects of a micromagnet*  XINYU ZHAO (Presenter), XUEDONG HU, State Univ of NY - Buffalo — Charge noise is one of the most important error sources for quantum gates in semiconductor systems. We study the decoherence of an electron spin in a double quantum dot in the presence of an inhomogeneous magnetic field. An exact dynamical equation is derived directly from the microscopic Hamiltonian, which allows us to investigate the impact of the non-Markovian properties of the quantized bosonic environment. We show that non-Markovian dynamics could cause a notable correction when measuring spin relaxation time. Our results reduce to the one predicted by the traditional Redfield master equation when Born-Markov approximation is applied. The spin relaxation and dephasing caused by the charge noise is suppressed by certain factors since the noise is indirectly (through the artificial spin-orbit interaction from the micromagnet) coupled to spin. We show these factors strongly depend on the system parameters such as detuning, tunneling strength, field gradients in vertical or horizontal directions. Our results present a systematic approach to study decoherence processes caused by charge noise, particularly for quantum dots in an inhomogeneous magnetic field.

*We acknowledge financial support by US ARO via grant W911NF1710257.

4:06PM J17.00007: Universal quantum logic in hot silicon qubits  HARMEN EENINK (Presenter), LUCA PETIT, MAXIMILIAN RUSS, WILLIAM I.L. LAWRIE, NICO HENDRICKX, Delft University of Technology, JIM CLARKE, Components Research, Intel Corporation, LIEVEN M VANDERSYPEN, MENNO VELDHORST, Delft University of Technology — Large scale quantum computation can leverage significantly from semiconductor fabrication technology, to allow for quantum integrated circuits, hosting quantum hardware and control circuitry all on the same chip. However, leading qubit approaches operate at very low temperatures below 100 mK, where cooling power is extremely limited, and this severely impacts the perspective for practical quantum computation. Demonstrating qubit operation at elevated temperatures would therefore be a major breakthrough in the effort towards scalable quantum systems. Here, we study quantum operations in a silicon two-qubit system, operated at a temperature of 1.1 K. We perform readout using Pauli spin blockade and obtain coherent single-qubit control via electron-spin-resonance, with fidelities exceeding 99 %. We show tunability of the exchange interaction between the two spins from 0.5 up to 18 MHz and use this mechanism to execute coherent two-qubit controlled rotations (CROT). We additionally investigate the temperature dependence of the coherence times, which we find surprisingly robust against thermal noise. Our results mark an important step for the realization of quantum integrated circuits, a scalable approach towards practical quantum computation.
4:18PM J17.00008: Intel Spin Qubits: Automated low-temperature measurement and statistical data analysis for improved fabrication and device design  ROMAN CAUDILLO (Presenter), FLORIAN LUTHI, LESTER LAMPERT, THOMAS WATSON, DAVID J MICHALAK, ERIC HENRY, PAYAM AMIN, HUBERT C GEORGE, STEPHANIE BOJARSKI, BRENNEN MUELLER, RAVI PILLARISSETTY, JEANETTE MARIE ROBERTS, JIM CLARKE, Intel Corporation — Spin qubits in silicon are in many ways similar to state-of-the-art transistor devices, and they can both be manufactured with today's 300mm equipment and processes. The 300mm fab infrastructure is a powerful tool because of its excellent process control that results in high-quality devices with high reliability; however, it requires feedback from device performance grounded in statistical analysis of large data sets. Similarly, for quantum dots, automation and statistical data analysis of low-T measurements can be used to address challenges such as minimizing charge noise and TLS's in dielectrics and other on-chip materials, as well as eliminating spurious dots. Here we present an automated approach to tuning up quantum dots and extracting gate crosstalk, charging energy (E_c), leverarm, charge noise, and other device performance metrics, which are then fed back to device design and the fabrication process for iterative improvements in performance. Automation, and the large data sets that result, not only enable high-throughput measurements for rapid fabrication improvements, but also allow characterization of device limitations in new ways, including identifying regions of badness and the location of TLS's, and ultimately will point the way toward high-performance qubits.

4:30PM J17.00009: Intel Quantum Dot Devices: temperature dependence of electrical characteristics and correlating noise measurements for improved measurement turnaround  FLORIAN LUTHI (Presenter), ROMAN CAUDILLO, THOMAS WATSON, LESTER LAMPERT, OTTO ZIETZ, HUBERT C GEORGE, STEPHANIE BOJARSKI, BRENNEN MUELLER, PAYAM AMIN, ERIC HENRY, DAVID J MICHALAK, RAVI PILLARISSETTY, JEANETTE MARIE ROBERTS, JIM CLARKE, Intel Corporation — Quantum computing promises to tackle exciting and computationally difficult problems. Intel is leveraging 50 years of experience in semiconductor manufacturing to develop silicon-based spin qubits. One of the key challenges is the measurement bottleneck: Data acquisition at low temperatures (10 mK) is slow, and only few samples can be characterized per cooldown. Nonetheless, these measurements provide the ultimate feedback to device fabrication and design. At Intel, this problem is highlighted to the extreme: every week, thousands of SiMOS quantum dot devices are fabricated on 300 mm wafers, yet only a small fraction of these can be measured at mK temperatures. The need for low-temperature electrical characterization can be reduced by understanding the temperature dependence of device data, enabling learning from measurements at elevated temperatures. Furthermore, correlations between directly relevant quantities (such as quantum dot charge noise) and device properties which are measured more quickly (such as pinch-off noise) are investigated. These quick-turn monitors enable faster feedback to improve fab and pave the way to automated wafer-scale characterization of quantum dot devices at intermediate temperatures (2-4 K); this will help alleviate the measurement bottleneck.
4:42PM J17.00010: Fabrication process and failure analysis for robust quantum dots in silicon  JOHN DODSON ( Presenter), NATHAN HOLMAN, BRANDUR THORGRIMSSON, SAMUEL NEYENS, EVAN R MACQUARRIE, RYAN H FOOTE, THOMAS MCJUNKIN, University of Wisconsin - Madison, LISA F EDGE, HRL Laboratories, SUSAN NAN COPPERSMITH, MARK ALAN ERIKSSON, University of Wisconsin - Madison — We investigate several yield limiting steps in the fabrication of overlapping aluminum gate quantum dot devices in Si/SiGe. The thin, ~2 nm oxide that grows natively on aluminum and low thermal budget of aluminum devices presents a challenge for fabrication of quantum dot arrays with high yield. Gate-to-gate leakage from pinholing of the aluminum oxide, damage from electrostatic discharge (ESD), low breakdown voltages and gate geometry/morphology all present a significant risk of device failure in the active region. Additionally, dewetting of aluminum and formation of alloys during fabrication of interconnects from the active region of the device to the bond pads can result in failure of electrical signal transmission. We present low-temperature oxidation techniques for a thicker aluminum oxide with breakdown voltages of over 4 volts, reducing the risk of damage due to ESD and gate-to-gate leakage. TEM images of overlapping gate structures identify failure modes stemming from gate geometry/morphology. Finally, we investigate the fabrication of interconnects between the active region and device bond pads to introduce thermal anneals into the fabrication process, prevent damage due to ESD, and to identify the maximum processing temperature at different stages of device fabrication.

4:54PM J17.00011: Simplified MOS Quantum Dots for Materials Characterization  JOSHUA POMEROY (Presenter), ARUNA N RAMANAYAKA, YANXUE HONG, KE TANG, RYAN STEIN, MICHAEL DAVID STEWART, National Institute of Standards and Technology — Using single-layer metal gate patterns, metal-oxide-semiconductor (MOS) quantum dot devices with charge sensors are fabricated and measured as a simplified approach to developing more rigorous qualifying metrics than transport for materials and interfaces. Materials and interfaces are often identified as sources of charge traps and time instabilities difficult to assess with transport techniques, and the ability to form quantum dots and charge sense in these systems enables charge offset drift and, potentially, spin relaxation measurements to critically assess the feasibility of the materials and methods for use in qubit applications. Various multiple-dot designs with charge sensors have been fabricated, and the tunability and charge offset stability of these devices will be discussed in the context of developing tools for qualifying materials for quantum.
Development of simulator for silicon quantum dot devices based on semiclassical device modeling

Hidehiro Asai (Presenter), Shota Iizuka, Junichi Hattori, Tsutomu Ikegami, Koichi Fukuda, Takahiro Mori, AIST

Recently, the novel design for qubit integration has been vigorously investigated for the realization of fault-tolerant quantum computers and the noisy intermediate-scale quantum (NISQ) technology. Silicon qubits have attracted much attention as a promising candidate for a building block of integrated quantum circuits because they can utilize cutting edge nanofabrication facilities for conventional logic devices. In order to develop the qubit suitable for large-integrated quantum circuits and design whole picture of quantum circuits and its peripheral control circuits, the simulation tool for supporting the qubit design is strongly required, like technology computer aided design (TCAD) for conventional transistor design. In this presentation, we report our recent development of a prototype simulator which can simulate the basic characteristics of silicon quantum dot devices as a basis of spin qubit. We utilize semi-classical device simulation as solvers of Poisson equation and classical current continuity equation combined with newly-developed tunneling and Coulomb-blockade models to calculate transport in quantum dot devices. As a demonstration of the simulation, we are going to show calculation examples of charge stability diagrams for some quantum dot devices.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J18 DAMOP: Exploring Ergodicity-Breaking Through Nonequilibrium Order, Quantum Chaos and Integrability

205 - Bryce Gadway, University of Illinois at Urbana-Champaign - Tag(s): Invited
2:30PM J18.00001: Entanglement entropy of highly excited eigenstates of many-body lattice Hamiltonians* [Invited]  MARCOS RIGOL (Presenter), Pennsylvania State University — The average entanglement entropy of subsystems of random pure states is (nearly) maximal [1]. In this talk, we discuss how the average entanglement entropy of subsystems of highly excited eigenstates of integrable and nonintegrable many-body lattice Hamiltonians (with a conservation law) differ from that of random pure states. For translationally invariant quadratic models (or spin models mappable to them) we prove that, when the subsystem size is not a vanishing fraction of the entire system, the average eigenstate entanglement exhibits a leading volume-law term that is different from that of random pure states [2]. We argue that such a leading term is universal for translationally invariant quadratic models [3] and, likely, also for interacting integrable models [4]. For highly excited eigenstates of a particle-number-conserving quantum chaotic model away from half filling, we find that the deviation from the maximal value grows with the square root of the system's volume, when 1/2 of the system is traced out. Such a deviation is proved to occur in random pure states with a fixed particle number and normally distributed real coefficients [5].

References:

*This work was supported by the National Science Foundation under Grant No. PHY-1707482. The computations were carried out at the Institute for CyberScience at Penn State.

3:06PM J18.00002: Universal operator growth and emergent hydrodynamics in quantum systems* [Invited]  EHUD ALTMAN (Presenter), University of California, Berkeley — I will present a hypothesis on universal properties of operators evolving under many-body Hamiltonian dynamics. I will define a measure of operator complexity and argue that it generically grows exponentially in time, with an exponent α, measurable through the properties of a physical retarded correlation function. Furthermore, the complexity exponent places a sharp bound on Lyapunov exponents λ ≤ 2α characterizing chaos, generalizing the known universal low-temperature bound λ ≤ 2πT. In a sense the complexity growth exponent offers a measure of chaos that does not rely on having a nearby semiclassical limit. I will illustrate the results in paradigmatic examples such as non-integrable quantum spin chains, the Sachdev-Ye-Kitaev model, and classical models. Finally I will present applications of this approach to computation of Hydrodynamic transport coefficients and for characterizing the many-body localization transition in disordered systems.

*This work was supported in part by DOE Grant No. DE-SC0019380


4:18PM J18.00004: Matthias Weidemuller Invited Talk [Invited] —
4:54PM J18.00005: Kinetically constrained dynamics and electron-phonon interactions in Rydberg quantum simulators* [Invited] IGOR LESANOVSKY (Presenter), Institute for Theoretical Physics, University of Tuebingen — Rydberg quantum simulators, i.e. highly excited atoms held in optical tweezer arrays, are amongst the most advanced platforms for the implementation and study of strongly interacting spin systems. An interesting dynamical regime is reached when one atom that is brought to a Rydberg states facilitates the excitation of another nearby one. The resulting dynamics can be similar to that of epidemic spreading and also may form an ingredient for observing non-equilibrium phase transitions. In my talk I will discuss recent results concerning the analysis of constrained Rydberg spin dynamics in the presence of disorder which is caused by the coupling of electronic degrees of freedom and lattice vibrations. I will focus on incoherent and coherent regimes, discussing the breaking of ergodicity and the dressing of facilitated spins by phonons, respectively.

*The research leading to these results has received funding from the EPSRC Grants No. EP/M014266/1 and EP/R04340X/1 via the QuantERA project “ERyQSenS”. Support was also received from the Deutsche Forschungsgemeinschaft (DFG) within the SPP 1929 Giant interactions in Rydberg Systems (GiRyd) and The Leverhulme Trust [Grant number RPG-2018-181].

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J19 DMP: DMP Prize Session 207 - Antoinette Taylor, Los Alamos Natl Lab - Tag(s): Invited

2:30PM J19.00001: David Adler Lectureship Award Talk: Epitaxial Oxides: From Basic Science to Application [Invited] CHANG-BEOM EOM (Presenter), University of Wisconsin - Madison — Oxide materials are the most abundant compound in the earth’s crust and possess a wide range of electrical, optical, and magnetic properties. For instance, insulators, high quality metals, dielectrics, ferroelectrics, piezoelectrics, semiconductors, ferromagnetics, transparent conductors, ionic conductors, multiferroics superconductors, and nonlinear optical materials have all been produced using oxide materials. Oxide materials have enormous potential as the fundamental building block of new generations of electronic, magnetic, optical and electromechanical devices. We create these materials by artificially layering various atoms including oxygen at the single atom level, as well as stacking of epitaxial membranes. Our goal is to create new materials and heterostructures with novel properties likely to advance basic science and future applications. I will present advances in epitaxial oxide systems in general, and highlight several examples of how our research has played a role in understanding fundamental solid state phenomena at the atomic scale and in the discovery of new materials. Atomic layer control of novel oxide heterointerfaces may provide some of the answers that we need to continue the electronics revolution, particularly for frontier nanoscale devices. I will discuss the challenges and opportunities in this exciting field.
We studied the state of matter under extreme conditions and found new phenomena and materials, including polymeric nitrogen, transparent sodium, electrically conducting hydrogen, and superconductivity in various substances. Room-temperature superconductivity is becoming realistic given dramatic progress in conventional superconductivity: the critical temperature is $T_c = 203$ K in H3S under high pressures of about 150 GPa. We found even higher, nearly room temperature superconductivity in superhydride LaH10 with $T_c \approx 250$ K, following the theoretical predictions. This and yttrium and calcium superhydrides can be considered as a close realization of metallic hydrogen.

We will discuss prospects for further increase of $T_c$ to room temperature, which naturally is expecting for hydrides at high pressures. We will present recent studies on YHx and other compounds that are considered as potential room-temperature superconductors. We will consider various directions to explore high-temperature conventional superconductivity at low and ambient pressures.

3:42PM J19.00003: Edward A. Bouchet Award Talk: Controlling Dissipation in Superconductors: the Oxymoron that Leads to New Superconducting Phases and Transitions* [Invited] NADYA MASON (Presenter), University of Illinois at Urbana-Champaign — In this Bouchet Award talk, I will first briefly discuss why I feel that it is important to balance research, service, and outreach. I will then discuss my research on “dissipative” superconducting systems. In particular, superconductors are exciting materials for basic physics and applications because they conventionally exhibit zero-resistance and zero-dissipation. In contrast, unconventional superconductors—including high-temperature superconductors and hybrid superconductor-normal (S-N) systems relevant to quantum computation—combine superconductivity with dissipative normal metal-like states. Yet dissipation has been difficult to control and parametrize. Here, I will discuss electrical transport experiments on hybrid superconductor-normal metal systems where the dissipation is controlled, leading to new understanding of superconducting states and transitions. In particular, I will show how superconductivity is established in granular S-N systems, how metallic states appear in arrays of S-N systems as the normal metal fraction is increased, and how magnetic fields can be used to control a variety of dissipative phase transitions. The results are relevant to understanding the role of dissipation in superconducting systems, and in correlated materials in general.

*Work supported by the DOE under DE-FG02-07ER46453 and NSF under DMR-064467 & DMR-17-10437, and through the Illinois Materials Research Lab.
**4:18PM J19.00004: APS Medal for Exceptional Achievement in Research: The Metal-Insulator Transition in Strongly Interacting Electron Systems in Two Dimensions** [Invited]  MYRIAM SARACHIK (Presenter), Physics, City College of New York, CUNY — Over the course of my long career in physics my research has covered a variety of topics, including early measurements of the resistance minimum that provided the experimental key to the Kondo effect, metal-insulator transitions (MITs) and macroscopic quantum tunneling of the magnetization in molecular magnets. My work during the last few years has focused on the apparent metal-insulator transition that occurs in strongly interacting systems of electrons in two dimensions, where no metallic behavior and no metal-insulator transition were believed to be possible. In this talk I will give a thumbnail history of research on the 2D metal-insulator transition, the debate concerning whether a metallic phase exists in two dimensions, and whether this MIT is a quantum phase transition, as claimed by many (including me). I will report surprising results [1] that shed new light on the nature of the metal-insulator transition in 2D.


*My research has been supported over the years by City College (CCNY), the PSC (Professional Staff Conference) through CUNYFRAP (the CUNY Faculty Research Award Program) and grants from the Department of Energy, the National Science Foundation, the Air Force Office of Scientific Research, the Army Research Office and the US-Israel Binational Science Foundation.*

**4:54PM J19.00005: IUPAP Award Talk** [Invited]  ANDREA YOUNG (Presenter), University of California, Santa Barbara — TBD

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**Tuesday, March 3, 2020 2:30 PM - 5:30 PM**

**Session J20 DBIO: Physics of the Cytoskeleton Across Scales I: Mechanics and Rheology** 301 - Meredith Betterton, University of Colorado, Boulder - Tag(s): Focus
2:30PM J20.00001: A mechanistic view of collective filament motion in active nematic networks  MORITZ STRIEBEL, ISABELLA GRAF (Presenter), ERWIN A FREY, Ludwig Maximilian University of Munich — Protein filament networks are structures crucial for force generation and cell shape. A central open question is how collective filament dynamics emerges from interactions between individual network constituents. To address this question we study a minimal but generic model for a nematic network where filament sliding is driven by the action of motor proteins. Our theoretical analysis shows how the interplay between viscous drag on filaments and motor-induced forces governs force propagation through such interconnected filament networks. We find that the ratio between these antagonistic forces establishes the range of filament interaction, which determines how the local filament velocity depends on the polarity of the surrounding network. This force propagation mechanism implies that the polarity-independent sliding observed in Xenopus egg extracts, and in vitro experiments with purified components, is a consequence of a large force propagation length. We suggest how our predictions can be tested by tangible in vitro experiments whose feasibility is assessed with the help of simulations and an accompanying theoretical analysis.

2:42PM J20.00002: Time varying mechanical response of cytoskeletal networks [Invited] MOUMITA DAS (Presenter), Rochester Institute of Technology — Actin filaments and microtubules are critical components of the cytoskeleton, a composite network of filamentous polymers and regulatory proteins. The synergistic interplay of networks of actin filaments and microtubules and their continuous disassembly and reassembly via active de/re-polymerization play a crucial role in a wide range of mechanical properties and processes, including cell stiffness, shape change, and motility. While in-vitro actin networks have been intensely investigated over the past two decades due to their promise for understanding cell mechanics and designing smart materials, questions remain as to how the composite nature of the cytoskeleton and de/re-polymerization kinetics of individual filaments impact the collective, time-varying mechanics of cytoskeletal networks. This talk will discuss an integrated approach consisting of theory and experiments, that seeks to address these questions. In particular, we will describe the mechanical response of composites made of interconnected networks of semiflexible and stiff filaments, time-varying responses of these networks, and how they can be explained by mathematical models that couple the time-evolution of filament lengths with rigidity percolation theory. Our results provide insights into mechanisms that enable cells to exhibit a myriad of mechanical properties and can inform the general principles underlying the mechanics of a large class of dynamic systems and biomaterials of current interest.

*This research was funded in part by the Research Corporation and the Keck Foundation.
The cytoskeleton, composed of actin, microtubules, and associated motor and binding proteins, self-organizes into different structures and morphologies to drive diverse mechanical processes in eukaryotic cells. While in vitro actomyosin networks are well-characterized, few studies have examined how the structure and activity of these networks are altered by the presence of microtubules. We previously synthesized steady-state actin-microtubule networks, finding that mechanical properties, such as network elasticity, depend on molecular interactions between actin and microtubules, such as the degree of crosslinking and bundling. Here, we create active actin-microtubule networks by adding the motor protein myosin. Using confocal microscopy and microrheology, we characterize how the network structure evolves during motor activity, and connect how microscopic changes in network structure affect the mechanical properties of the network. Our results shed important new light on how actin-microtubule interactions influence the structure, mechanics and activity that motor-driven cytoskeleton networks exhibit.

*W.M. Keck Foundation Research Grant

3:30PM J20.00004: Probing length scale-dependent viscoelasticity from bending fluctuations of filaments  KENGO NISHI (Presenter), SUFI RAJA, Duke University, FRED C MACKINTOSH, Rice University, CHRISTOPH F. SCHMIDT, Duke University — Micron-sized beads are commonly used to perform microrheology in soft media. The size of the particles sets the length scale at which properties are probed. This can limit results when the properties of the medium vary with length scale. A typical example of such a system are living cells. Cells are constructed hierarchically, with structural elements ranging from nano- to mesoscopic scales. Here, we introduce the use of semi-flexible filaments/tubes to probe scale-dependent dynamics. We analyze shape fluctuations of semi-flexible filaments. We show that the bending dynamics of filaments can be used to probe the physical properties of such media at multiple scales, corresponding to the wavelengths of the modes analyzed.
3:42PM J20.00005: Triggering salt-induced contraction of cytoskeletal networks with microfluidics*  SHEA RICKETTS (Presenter), PAWAN KHANAL, CHRISTOPHER CURRIE, Univ of San Diego, MICHAEL RUST, Univ of Chicago, MOUMITA DAS, Rochester Institute of Technology, JENNIFER L ROSS, Syracuse, RAE M ROBERTSON-ANDERSON, Univ of San Diego — The mechanical tunability and morphology of the cytoskeleton is determined by interacting networks of semiflexible actin filaments and rigid microtubules. By altering the chemical environment of the cytoskeleton, actin and microtubule networks can dynamically change and rearrange to form entanglements, crosslinks and bundles. For example, increasing the concentration of divalent salt can induce crosslinking and bundling of actin filaments. Here, we use microfluidics and confocal fluorescence microscopy to show that increasing salt concentration triggers contraction of cytoskeleton networks in the absence of motor proteins. Specifically, we use microfluidics to cyclically vary the salt concentration over the course of minutes to hours while simultaneously visualizing the triggered structural changes to the networks and measuring the contraction velocity. Our measurements shed new light on how varying environmental conditions can dynamically tune the morphology of actin-microtubule networks and trigger active contraction without motor proteins.

*NIH Award #R15GM123420 and a W.M. Keck Foundation Research Grant.

3:54PM J20.00006: Slow stress relaxation of transient-crosslinked biopolymer networks  SIHAN CHEN (Presenter), TOMER MARKOVICH, FREDERICK COLIN MACKINTOSH, Rice Univ — It is well established that the unbinding of crosslinkers enables transient-crosslinked biopolymer networks to flow at long times. A recent experiment, however, shows that exerting prestress on such a network leads to near solid-like viscoelastic response. In this talk I will propose a microscopic theory for the rheology of transient networks under prestress. We show that the solid-like dynamics naturally appears as a result of the coupling between the strain-stiffening of semiflexible polymers and the transient nature of the crosslinkers. Our theory predicts the scaling behavior of shear modulus over the whole frequency regime and quantitatively fits the experimental data. This theory may also explain similar slow stress relaxation previously found in living cells.

4:06PM J20.00007: Electric Field Guidance of Actin Waves*  QIXIN YANG (Presenter), MATT HOURWITZ, LEONARD CAMPANELLO, University of Maryland, College Park, BEDRI SHARIF, PETER DEVREOTES, Department of cell biology, Johns Hopkins University, JOHN T FOURKAS, WOLFGANG LOSERT, University of Maryland, College Park — Directional cell migration induced by a DC electric field (DC EF) is an important physiological process involved in wound healing, development, and regeneration. This phenomenon is modulated by the self-generating waves of signaling molecules and actin traveling on cell membranes. It has been shown that chemical perturbations of wave components lead to changes in migratory behaviors. Here we first study how a DC EF provides a unidirectional perturbation of the actin wave patterns, then study the combined perturbation by a DC EF and nanotopography. By quantifying spatial-temporal actin wave patterns, we show that DC EFs can guide actin wave propagation, lead to inhomogeneous activities of actin waves, and alter cell migratory modes.

*This work is funded by the Air Force Office of Scientific Research grant FA9550-16-1-0052
**4:18PM J20.00008: Exploring the effects of actin-binding proteins on the percolation of actin networks using a mean field model**
CARLOS BUENO (Presenter), Systems, Synthetic and Physical Biology, Rice University, JAMES LIMAN, Department of Bioengineering, Rice University, NICHOLAS SCHAFER, Center for Theoretical Biological Physics, Rice University, MARGARET CHEUNG, Department of Physics, University of Houston, PETER G WOLYNES, Center for Theoretical Biological Physics, Rice University — The actin cytoskeleton is a dynamical system that can exert forces and transmit forces between the cell and its environment. The dynamical and rheological properties of the actin cytoskeleton are modulated by actin binding proteins (ABPs). Some ABPs, such as α-actinin or Arp2/3, connect different actin filaments thereby changing the topology of the network. Other ABPs, such as myosin, can also exert forces on the network thus altering its dynamic behavior. In this work we model an actin system and its interaction with α-actinin, myosin and Arp2/3 using ordinary differential equations and stochastic mechanochemical simulations. We then use a mean field approach to quantify how the concentrations of different ABPs affect the connectivity and rigidity of the network. We find that the presence of Arp2/3 increases the connectivity of the network. We also discuss the conditions needed for force exertion and transmission in this system. We expect that this result may provide a theoretical insight into how ABPs affect the ability of the actin cytoskeleton to exert and transmit forces.

*This work was supported by the National Institute of General Medical Sciences (R01 GM44557) and by the National Science Foundation (PHY 1427654, CHE 1743392)*

**4:30PM J20.00009: Mechanical stability of microtubule lattices under high crowdedness**
LUKASZ SZATKOWSKI (Presenter), ROHITH ANAND VARIKOTI, RUXANDRA I DIMA, Department of Chemistry, University of Cincinnati — Microtubules (MTs) are hollow cylindrical biopolymers of tubulin subunits that play key roles in cells. Understanding their functions in cilia or neurons is difficult because MTs associate in highly crowded bundled arrays. For example, it is unclear how this crowdedness or confinement and the mutual interaction between MTs chains relate to the anisotropy of MT lattices. Because of the large degree of confinement in MT bundles, the use of experimental techniques to answer such questions is not easy. In contrast, computational modeling methods do not exhibit the experimental limitations when studying MTs bundles. Still, most of the existing models treat MTs as an elastic polymer network, in which the anisotropy of the lattice is built in and which excludes the possibility of formation of cracks in the lattice during force application. Our coarse-grained molecular simulations of the response of MT lattices to applied forces allow us to study formation and propagation of cracks. We present a modified indentation protocol to determine the mechanical response of MT lattices under conditions which mimic high confinement. Our model shows that the strength of interactions between MT in bundles has substantial influence on the magnitude of the forces that induce cracks in MT lattices.
4:42PM J20.00010: Understanding the Topology of Microtubules  VARSHA SUBRAMANYAN (Presenter), KESAV SARANYAN KRISHNAN, KAY L KIRKPATRICK, University of Illinois at Urbana-Champaign, SARASWATHI VISHVESHWARA, Molecular Biophysics Unit, Indian Institute of Science, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign — The phenomenon of dynamical instability in microtubules is of immense importance in understanding transport within the cell. In recent times, these polymeric proteins have been studied as mechanical lattices possessing a topological edge mode (Phys. Rev. Lett. 103, 248101 (2009)). We extend this idea by modelling the microtubule as a cylindrical lattice of dimers, with interactions between dimers modelled by a hopping Hamiltonian. We show the emergence of topological edge modes, and propose the modelling of dynamic instability as a phase transition. We explicitly determine the conditions for the existence of these edge modes by setting up appropriate difference equations. We speculate on the biological implications of these results, by mapping the dynamic instability of microtubules to the propagation of lattice defects, and also discuss possible methods of computational/experimental verification via microscopic network models of microtubules.

4:54PM J20.00011: The role of multivalent actin-binding proteins in remodeling actomyosin networks*  YOSSI ELIAZ (Presenter), MARGARET CHEUNG, Physics, University of Houston; Center for Theoretical Biological Physics, Rice University — We explore the contribution of multivalent actin-binding proteins (ABPs) in remodeling actomyosin networks by using mesoscopic computer simulations. We model ABPs as junctions with varied multi-valencies that enable bundling or branching of actin filaments, which result in diverse morphologies of actomyosin networks. We developed network theory-based order parameters that quantify connectivity between graph nodes in order to analyze emergent morphologies in actomyosin networks. First, we show that ABPs, such as calmodulin-dependent kinase II (CaMKII), with multivalency greater than two not only increase the thickness of actin bundles, but also promote their arborization. Second, myosin motor proteins accelerate the arborization of actin filaments bundled by CaMKII. Because CaMKII is as abundant as actin filaments in neurons, it plays an important role in remodeling the morphology of actin filaments in actomyosin networks; CaMKII's chemical binding to actin filaments alters the mechanical properties of actomyosin networks that underpin the plasticity of dendritic spines.

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Mechanical properties of branched actin networks

MEHDI BOUZID
(Presenter), LPTMS, CNRS, CESAR VALENCE-GALLARDO, PMMH, ESPCI, LARA KOEHLER, LPTMS, CNRS, GIUSEPPE FOFFI, LPS-Orsay, University of Paris Sud, JULIEN HEUVINGH, OLIVIA DU ROURE, PMMH, ESPCI, MARTIN Lenz, LPTMS, CNRS — Gels of fibrous bio-polymers are ubiquitous within cells and their rigidity is crucial for their function. Our current understanding of their elastic response is usually understood as an interplay between the bending and stretching of their filaments. This point of view however fails when applied to the weakly coordinated branched actin networks found throughout the cell. Through experiments, simulations and theory, we show that their elasticity crucially involves reversible entanglements between their filaments. Additional entanglements may get locked in during network growth, setting the final properties of the network. These properties could be key to understanding how moving cells dynamically adapt their cytoskeleton to their environment.

Hydrodynamic effects on the motility of crawling eukaryotic cells*

MELISSA H MAI (Presenter), BRIAN CAMLEY, Johns Hopkins University — Eukaryotic cell motility is crucial during development, wound healing, the immune response, and cancer metastasis. Some eukaryotic cells can swim, but cells more commonly adhere to and crawl along the extracellular matrix. We study the relationship between hydrodynamics and adhesion that describe whether a cell is swimming, crawling, or combining these motions. Our simple model of a cell, based on the three-sphere swimmer, is capable of both swimming and crawling. As cell-matrix adhesion strength increases, the influence of hydrodynamics on migration diminish. Cells with significant adhesion crawl with speeds much larger than their nonadherent, swimming counterparts. We predict that, while most eukaryotic cells are in the strong-adhesion limit, increasing environment viscosity or decreasing cell-matrix adhesion could lead to hydrodynamic effects even in crawling cells. Signatures of hydrodynamic effects include dependence of cell speed on medium viscosity or the presence of a nearby substrate as well as interactions between noncontacting cells. These signatures are suppressed at large adhesion strengths, but even strongly adherent cells will generate fluid flows advecting passive particles and swimmers.

*We acknowledge the Provost's Undergraduate Research Award (PURA) of JHU.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J21 GERA: Photovoltaic Materials and Phenomena 302
2:30PM J21.00001: Role of defects in MAPbI₃ to modulate optical absorption, and solar efficiency

POOJA BASERA (Presenter), SASWATA BHATTACHARYA, Physics, Indian Institute of Technology, IIT Delhi — Methylammonium lead halide (MAPbI₃) perovskite has emerged as one of the frontier optoelectronic semiconductors. To avoid lead-toxicity, the role of Sn-substitution and Pb-vacancy (Pb-\(\bullet\)) is addressed in regulating the stability and solar cell efficiency of MAPb\(_{1-X-Y}\)Sn\(_X\)I\(_3\) perovskite using hybrid density functional theory (DFT). We find, to reduce the Pb-content from pristine MAPbI₃, Sn-substitution has favorable thermodynamic stability than Pb-\(\bullet\). High optical absorption coefficient (red shifted) and maximum solar cell efficiency are obtained in MAPb\(_{1-X-Y}\)Sn\(_X\)I\(_3\) for \(0 \leq X \leq 0.5\). The role of spin-orbit coupling (SOC) and electron self-interaction error are examined carefully. Despite SOC has a significant role in artificially shifting the electronic bands, it doesn't affect the relative hierarchy of formation energies of different defected configurations. However, electron self-interaction plays an important role in determining the same. We find a local/semi-local functional (e.g. PBE) gives a completely opposite trend to determine thermodynamic stability w.r.t HSE06+SOC.

*PB acknowledge UGC, India, for the senior research fellowship [grant no. 20/12/2015 (ii) EUV] and High Performance Computing (HPC) facility at IIT Delhi for computational resources.


YASHIKA GUPTA (Presenter), ANSHUMAN KUMAR, LOQM, Department of Physics, Indian Inst of Tech-Bombay — Organic-Inorganic Lead based perovskite solar cells offer a promising alternative to present day Si-solar cell, reaching an efficiency of almost 25% in a span of less than ten years. However, perovskite based cells still face stability and toxicity issues due to their constituents elements like organic molecules (Methylammonium, Butylammonium etc.) and heavy metal ions (Lead) thus limiting it's prospects towards commercialization. A lot of efforts have been made towards improving the stability of these lead base perovskites to improve their stability by introducing a heavy metal cation into conventional perovskite materials to generate a 2D structure, called Ruddlesden-Popper Perovskite with improved stability than the conventional 3D perovskites. But the issue of Lead toxicity remains. In this work, we propose use of plasmonics as an efficient method to improve the efficiency 2D Ruddlesden Popper perovskite solar cell. The use of plasmonic structures will result in improved light harvesting in the cell while keeping the perovskite layer thickness to minimum and hence reducing the toxic content of the cell giving it a fighting chance for practical applications.
2:54PM J21.00003: Scaling law for excitons in layered 2D perovskites systems: Dion-Jacobson (DJ) phases and Alternating Cation in the Interlayer space (ACI) phases  
Hao Zhang (Presenter), Siraj Sidhik, Wenbin Li, Rice Univ, Jacky Even, INSA Rennes, Jean-Christophe Blancon, Aditya Mohite, Rice Univ — Layered two-dimensional (2D) hybrid perovskites are emerging types of semiconductor quantum wells (QWs) with highly promising opto-electronic applications. These solution-processed materials offer tunability of opto-electronic properties, which can be achieved by varying quantum well thickness (n-value). For instance, our previous work has demonstrated the scaling behavior of excitons with different quantum well thickness in Ruddlesden-Popper (RP) Perovskites. Besides the well-studied RP perovskites, there’re other crystal structures such as Dion-Jacobson (DJ) and Alternating Cation in the Interlayer space (ACI) phases, whose intrinsic exciton and charge carrier properties still remain unrevealed. Here, using optical spectroscopy, we perform detailed studies of the optical and electronics properties on DJ and ACI systems, such as exciton fine structure, electron-phonon coupling and defect states, and demonstrate their scaling behavior with quantum well thickness. These results will bridge the gap between optical properties of 2D and 3D perovskite crystals, leading to better design of opto-electronics devices. The tendency of how different 2D perovskites phases merge into unique 3D perovskite will give us a deeper understanding of the fundamental physics of perovskite materials.

3:06PM J21.00004: Increasing open-circuit voltage in CdTe solar cells through passivation of the previously inaccessible front interface  
Deborah McGott (Presenter), Yegor Samoilenko, Colorado School of Mines, Brian Fluegel, National Renewable Energy Laboratory, Colin Wolden, Colorado School of Mines, Matthew Reese, National Renewable Energy Laboratory — Cadmium telluride (CdTe) is the leading commercialized thin-film photovoltaic (PV) technology with over 25-GW-scale annual production and record device efficiency of 22.1%. However, a major obstacle to achieving higher efficiencies in CdTe is a stubbornly low open-circuit voltage ($V_{OC}$) of ~800-900 mV despite having a near ideal bandgap of 1.45 eV. Surface passivation, particularly of the front interface, is thought to be critical to reduce electron-hole recombination and increase $V_{OC}$. The front interface, however, is buried under microns of material during standard growth of superstrate CdTe and made inaccessible. Here, we use a novel thermo-mechanical liftoff technique to expose the buried front interface, then passivate the surface to improve minority carrier lifetime measured using time-resolved photoluminescence (TRPL). We then complete the device by depositing a transparent front contact to correlate $V_{OC}$ changes in the front interface and minority carrier lifetime.
3:18PM J21.00005: Valley Photovoltaics: Experimental Evidence for a Practical Route towards the Realization of the Hot Carrier Solar Cell*  
KYLE R DORMAN (Presenter),  
HAMIDREZA ESMAIELPOUR, Homer L. Dodge Department of Physics & Astronomy, University of Oklahoma, DAVID K FERRY, School of Electrical, Computer, and Energy Engineering, Arizona State University, TETSUYA D MISHIMA, MICHAEL B SANTOS, VINCENT R. WHITESIDE, IAN R SELLERS, Homer L. Dodge Department of Physics & Astronomy, University of Oklahoma — Hot carrier solar cells offer the potential to increase the efficiency of single gap solar cells beyond 60%. Here a new and viable route is proposed where photoexcited electrons are scattered to and collected from the L and X valleys. We demonstrate proof-of-principle results for an InGaAs/AlInAs heterojunction solar cell that shows an operating voltage (~1.4 eV) in excess of the InGaAs absorber bandgap (0.75 eV) under 1-sun AM 1.5G. Hot carriers are confirmed in simultaneous monochromatic current–voltage and photoluminescence measurements. Hot carrier operation in this simple commercially mature system is driven by the transfer, storage, and extraction of hot carriers in the satellite valleys of InGaAs. Combining intervalley scattering and the Gunn Effect allows the majority of photoexcited electrons to be harnessed with voltages defined by the upper valley separation, and thus an optimized system would exceed the Shockley-Queisser limit for a single bandgap solar cell. A mismatch in the valley degeneracy across the n+-AlInAs/n-InGaAs interface currently limits the performance, but a clear route to the realization of such a device in traditional III-V technologies is presented.

*This work supported by the National Science Foundation ECCS program through Grant No. ECCS-1610062.

3:30PM J21.00006: PMEG and PMPG (plasmonic multi-electron and multi-photon generation) for PV  
LINDEN HAYES (Presenter), Physics, Boston College, LINGPENG LUO, CONG CHEN, South China Normal University, KRZYSZTOF KEMPA, Physics, Boston College, JINWEI GAO, South China Normal University, FRANK SHIH-YU TSUNG, MICHAEL NAUGHTON, Physics, Boston College — We have recently shown that by embedding nanoparticles possessing properly-tuned plasmonic resonances in the small gap semiconductor absorber of a solar cell that it is possible to achieve significant plasmonic multi-electron generation (PMEG)[1]. Synthesis efforts are underway to construct a perovskite-nanoparticle system in order to experimentally verify the viability of PMEG to increase the efficiency of the solar cell.

An additional method of using nanoparticles to enhance the efficiency of solar cells by utilizing the downconverting properties of nanoparticles, plasmonic multi-photon generation (PMPG) is also being investigated. In downconversion, high energy incident photons are converted into multiple lower energy photons that more closely correspond to the bandgap of a solar cell. This should simultaneously increase the efficiency of the cell and, in the case of perovskites, increase the long term stability, as these absorbers are negatively impacted by incident UV light. Synthesis of this system is also underway.

3:42PM J21.00007: Suppressing deep-trap formation in Cu$_2$ZnSnS$_4$-based solar cells  ROBERT WEXLER (Presenter), SAI GAUTAM GOPALAKRISHNAN, Princeton University, EMILY CARTER, UCLA — Cu$_2$ZnSnS$_4$ (CZTS) is a cheap, nontoxic, easy-to-synthesize, and stable solar cell absorber material. Despite these advantages over Si, GaAs, CdTe, CuIn$_x$Ga$_{1-x}$Se$_2$, and hybrid perovskites, CZTS-based solar cells are plagued by low efficiencies (12.6%) compared to the Shockley-Queisser limit (33.7%). This 21.1% efficiency deficit was suggested recently to be due to the formation of defect clusters involving the Sn$_Zn$ antisite, which induces deep-trap states and therefore promotes carrier recombination. In this talk, we present density functional theory calculations of defect thermodynamics to show that these deep-trap defect clusters can be suppressed in CZTS via Ge- and Se-codoping. Additionally, we will describe an electrostatic mechanism for the suppression of deep defects by Ge that can be readily applied to other kesterite-type absorber materials and therefore used to design next-generation CZTS-inspired solar cells.

3:54PM J21.00008: A low-temperature-low-intensity study of flexible CIGS solar cells*  HADI AFSHARI (Presenter), BRANDON DURANT, COLLIN BROWN, Univ of Oklahoma, KHALID HOSSAIN, Amethyst Research Incorporated, DMITRY POPLAVSKYY, MiaSolé Hi-Tech Corp, IAN R SELLERS, Univ of Oklahoma — Commercially available lightweight and flexible CIGS solar cells are investigated for their performance under low intensity low temperature (LILT) conditions governing outer planets Mars, Jupiter, and Saturn. Current density-voltage under varying temperatures and illumination intensities, including concentrated solar, as well as electroluminescence measurements is performed to investigate the effects of conditions in deep space. A barrier to minority carrier extraction is observed and attributed to the acceptor rich defect layer near the CIGS absorber/CdS buffer interface. The effect of this barrier on power generation is presented and shown to decrease after light soaking, due to a transition between the so-called relaxed to metastable states. The power conversion efficiencies are shown to be higher for LILT conditions compared to terrestrial application.

*The authors acknowledge funding through the Oklahoma Center for the Advancement of Science & Technology (OCAST) Program No. #AR18-052-2.
4:06PM J21.00009: Interfacial Properties of Solar Energy Materials from DFT: P3HT/ZnO and CdS/Graphene  LEAH BENDAVID (Presenter), Vassar College, LIAT H. KUGELMASS, Cornell University, AUSTIN ATSANGO, Stanford University, REID W. SMITH, Vassar College — We present two projects that demonstrate how computational quantum chemistry is used to better understand materials for solar energy applications. In the first project, we use density functional theory (DFT) to examine the P3HT/ZnO solar cell and the mechanism by which interfacial modification with PCBA and doping with Sr enhances photovoltaic efficiency. We find that the enhancement in photovoltaic efficiency is not due to changes in equilibrium structures or adhesion strengths. Rather, the impacts of Sr-doping and PCBA are linked to changes to the energy level alignments. In the second project, we focus on CdS/graphene photocatalytic interfaces. Using DFT calculations, we study the interfacial properties of CdS(0001)/graphene and a CdS/graphene bilayer, and examine whether doping with B/N can strengthen interfacial adhesion. The CdS/graphene bilayer is found to exhibit high interplanar distances and low adhesion energies, characteristic of dispersion-dominated interfacial adhesion. Doping graphene does not significantly modify the strength of adhesion, but it does enable modulation of the band edge and Fermi level alignments. The CdS(0001)/graphene interface is found to be similarly adhered via dispersion interactions, but here, doping with B strengthens interfacial adhesion.

4:18PM J21.00010: Polymer solar cell incorporating PEDOT:PSS films and MEH-PPV nanopillars*  ARCHANA KUMARI (Presenter), Slippery Rock Univ — Poly[2-methoxy-5-(2-ethylhexyloxy)-1.4-phenylenevinylene] (MEH-PPV) is an attractive polymer for organic solar cells which were fabricated with spin coating technique using capillary force through the pores in to the channels of the alumina templates on the Glass/ITO substrates. The nanopillars were studied using UV-Vis absorption spectroscopy and found an enhanced absorption as compared to same thickness of MEH-PPV films. Organic solar cells will be fabricated with structures as Glass/ITO/TiO₂/PEDOT:PSS/ MEH-PPV nanopillars/Al, where MEH-PPV acts as an electron donor and TiO₂ semiconductor material is used as an acceptor in polymer solar cell. PEDOT:PSS can improve performance by enhancement of hole collection, exciton diffusion and photocarrier transport. Surface morphology of the nanopillars in solar cell will be studied using Scanning Electron Microscopy, and various other characterization techniques such as UV-Vis spectroscopy, PL spectroscopy, energy dispersive X-ray spectroscopy and atomic force microscopy will be used. The performance of the solar cells will be determined by I-V characterization. Optimization of the dimensions of the nanopillars and thickness of the film will be done to obtain maximum efficiency of the devices.

*Slippery Rock University of Pennsylvania
4:30PM J21.00011: Hot carrier dynamics in Quantum Well Solar Cells (Thermal Photon Gain)  BRANDON DURANT (Presenter), Univ of Oklahoma, KEITH BARNHAM, Physics, Imperial College, VINCENT R. WHITESIDE, IAN R SELLERS, Univ of Oklahoma — Quantum well solar cells (QWSCs) have been shown to inhibit hot carrier thermalization relative to bulk materials and have therefore stimulated significant interest as a potential absorber region in third generation hot carrier solar cells. Investigations of high quality InGaAs/GaAsP QWs in GaAs p-i-n solar cells have recently alluded to the possibility of hot carrier extraction in device structures through the measurement of a diode ideality factor of $n < 1$. In order to prove the carriers extracted in these systems are in fact “hot,” simultaneous current density-voltage (JV) and photoluminescence (PL) measurements are performed to directly compare the carrier dynamics and photovoltaic performance in such devices. Several transitions complicate the PL spectra of QWs making determination of the carrier temperature via fitting of the high energy tail using simple Planck's law methods insufficient. Therefore, full spectral fitting is performed in order to extract the carrier temperature while considering the occupation of higher energy states in the QWs, which is then related to ideality factor determined in electrical measurements.

*The authors acknowledge support from the National Science Foundation ECCS Program Award No.# ECCS-1610062

4:42PM J21.00012: Giant Photovoltaic Effect in Magnetic Materials  OLES MATSYSHYN, INTI SODEMANN (Presenter), Max Planck Institute for the Physics of Complex Systems — We investigate a rectification process present in materials that break both inversion and time reversal symmetries. At second order in electric fields, this effect is inversely proportional to the relaxation rate, and, therefore, the rectified current would be infinity in a "naive" ideal clean and zero temperature limit. Employing Floquet theory, we show, however, that there is a non-perturbative correction in the electric field strength that regularises this divergence, but, which ultimately leads to a giant photo-current generation. Therefore, this effect offers a promising alternative paradigm for solar cell technologies.

4:54PM J21.00013: Thermodynamics of Photovoltaic Conversion with Nonreciprocal Processes  ANDREI SERGEEV (Presenter), US Army Rsch Lab - Adelphi, KIMBERLY SABLON, Office of the Deputy Assistant Secretary of the Army for Research and Technology — Nonreciprocal photon and electron processes can violate Kirchhoff's law, detailed balance, and chemical equilibrium in the system of electrons and phonons. As the fundamental Shockley – Queisser limit of photovoltaic conversion is directly based on detailed balance, nonreciprocal processes can improve the efficiency beyond the Shockley – Queisser limitation. We derived thermodynamic limits of efficiency of photovoltaic converters with nonreciprocal processes and consider various realization of nonreciprocal converters. We demonstrate that even dissipative nonreciprocal processes can increase the conversion efficiency beyond the Shockley – Queisser limit. The thermodynamic theory is applied to solar energy conversion, laser power beaming, and thermophotovoltaic conversion.

*The work is supported by the Army Research Laboratory. Research of AS was accomplished under Cooperative Agreement No. W911NF-18-2-0222.
Direct Observation of shift and ballistic photovoltaic currents

AARON BURGER (Presenter), Electrical and Computer Engineering, Drexel University, RADHE AGARWAL, Materials Science and Engineering, Drexel University, ALEXEY APRELEV, Physics, Drexel University, EDWARD SCHRUBA, Electrical and Computer Engineering, Drexel University, ALEJANDRO GUTIERREZ-PEREZ, VLADIMIR M. FRIDKIN, JONATHAN E SPANIER, Materials Science and Engineering, Drexel University — The quantum phenomenon of shift photovoltaic current was predicted decades ago, but this effect was never observed directly because shift and ballistic currents coexist. The atomic-scale relaxation time of shift, along with the absence of a photo-Hall behavior, has made decisive measurement of shift elusive. Here, we report a facile, direct-current, steady-state method for unambiguous determination of shift by means of the simultaneous measurements of linear and circular bulk photovoltaic currents under magnetic field, in a sillenite piezoelectric crystal. Comparison with theoretical predictions permits estimation of the signature length scale for shift. Remarkably, shift and ballistic photovoltaic currents under monochromatic illumination simultaneously flow in opposite directions. Disentangling the shift and ballistic contributions opens the way for quantitative, fundamental insight into and practical understanding of these radically different photovoltaic current mechanisms and their relationship.

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Bulk photovoltaic effect induced by elliptically-polarized light

LINGYUAN GAO (Presenter), ANDREW MARSHALL RAPPE, University of Pennsylvania — Shift current has been considered as one of the major origins for bulk photovoltaic effects. In this study, using time-dependent perturbation theory, we investigate the light polarization effect on shift current. We give a general formula for shift current induced by elliptically-polarized (EP) light, which represents the most general form of a polarized light. By using a two-band model widely applied in 2D materials, we calculate the EP shift current quantitatively, and compare it with the linearly-polarized shift current and circularly-polarized injection current.

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J22 DBIO DCP DMP DPOLY: Biomaterials II: Paleo and Modern Structure and Function in Animals 303 - Pupa Gilbert, University of Wisconsin - Madison - Tag(s): Focus
2:30PM J22.00001: Building with melanin: Low complexity Glycera jaw protein is master of multitasking* [Invited] J HERBERT WAITE (Presenter), University of California, Santa Barbara — In protein structure-function relationships, there is a widely held view that complex functions require complex structures. Recent studies with a low complexity protein from the jaws of Glycera, a benthic marine polychaete, appear to challenge this. Used for grasping and injecting venom, the jaws are stiff, sharp, durable and wear resistant. Proteins (50 wt %) are one of three jaw components including melanin (40 wt %) and copper (10 wt %) present as a copper mineral (atacamite) and Cu$^{2+}$ ions. Although jaw stiffness is correlated with melanin not mineral, little was known about the protein contribution until its recent characterization and recombinant expression. The Glycera jaw protein has an extremely low complexity sequence in which GGH repeats represent 80% of the composition. Notwithstanding such monotony, GJP exhibits the following distinct properties: 1) it binds 26 equivalents of Cu per protein, 2) catalyzes oxidation of Dopa to Dopa-quinone en route to melanin, 3) templates a sheet-like assembly (32 nm thick) of melanin at the air-water interface, and 4) forms a structural network with melanin and Cu in the stacked sheets of higher order architecture.

*We thank NSF grant DMR 1720256 for partial support.

3:06PM J22.00002: Memory and learning in biomolecular soft materials CHARLES COLLIER (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Lab, JOSEPH NAJEM, Mechanical Engineering, Penn State, STAN WILLIAMS, Electrical and Computer Engineering, Texas A&M University, GRAHAM TAYLOR, T&T Scientific Corporation, CATHERINE SCHUMAN, Computer Science Division, Oak Ridge National Laboratory, ALEX BELIANINOV, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, BENJAMIN DOUGHTY, Chemical Sciences Division, Oak Ridge National Laboratory, RYAN WEISS, MD SAKIB HASAN, GARRETT ROSE, Electrical Engineering and Computer Sciences, University of Tennessee, STEPHEN SARLES, Mechanical Aerospace and Biomedical Engineering, University of Tennessee — Neuromorphic elements have been predominantly solid-state devices which simulate the resistive and capacitive behaviors needed for neural networks and brain-inspired computing, but in non-brain-like ways. We are integrating lipid and polymer bilayer membranes with micro- and nanofabrication to develop fundamentally new types of neuromorphic elements that have the composition (biomolecules), structure (biomembranes), and switching mechanism (voltage-sensitive ion channels) of real biological synapses, and operate at lower power than the current state-of-the-art. Our devices consist of insulating, nm-thick lipid or polymer-based bilayer membranes that assemble at the interfaces of two or more aqueous droplets in oil, and that have demonstrated both memristive and memcapacitive behaviors, including memory resistance and capacitance, synaptic functions such as paired-pulse facilitation and depression, spike rate dependent plasticity, voltage-dependent inactivation and recovery, and charging hysteresis. These behaviors are linked to electrostriction, an electromechanical phenomenon that encompasses both electrowetting and electrocompression in the membrane, which are changes in membrane area and thickness due to charging in the presence of electric fields.
3:18PM J22.00003: Formation temperature of biomaterials through geologic time* [Invited]
KRISTIN BERGMANN (Presenter), SAM GOLDBERG, NOAH ANDERSON, ADAM JOST, Massachusetts Institute of Technology MIT, PUPA GILBERT, Physics, University of Wisconsin, Madison, CORINNE MYERS, University of New Mexico — The well-known secular increase in δ^{18}O values of both calcitic and phosphatic marine fossils through early Phanerozoic time suggests three end-member hypotheses 1) early Paleozoic surface temperatures were high, in excess of 40°C (tropical MAT), 2) the δ^{18}O value of seawater has increased by up to 7–8‰ VSMOW over Paleozoic time, or 3) early Paleozoic samples are more significantly altered than younger materials, with the secular trend reflecting these differences in post-depositional processes. Carbonate clumped isotope analysis, in combination with petrographic and elemental analysis, has the capacity to deconvolve fluid composition from temperature effects and therefore to determine which of these hypotheses is best supported. A sample suite including calcitic, aragonitic and phosphatic marine fossils from the last 500 million years indicate surface temperatures in tropical seas were similar to slightly warmer than today (avg. 26-38°C) in the early Paleozoic, while the oxygen isotope budget of seawater appears to be similar to that of today.

*Packard Foundation

3:54PM J22.00004: Nano-optical characterization of photosynthetic bacteria-2D material coupled system
SHARAD AMBARDAR (Presenter), ZACHARY FREY, DMITRI V VORONINE, Univ of South Florida — Atomically thin 2D materials especially TMDs grown laterally, on combining with other TMDs form heterostructures with atomically sharp interfaces. We use conventional far-field (FF) photoluminescence (PL) and near-field (NF) tip-enhanced photoluminescence (TEPL) to investigate the bio-sensing applications of TMD materials by depositing photosynthetic cyanobacteria on MoS_2-WS_2 heterostructure grown on SiO_2/Si substrate. The energy transfer between the 2D materials and the photosynthetic bacteria leads to formation of an energy funnel at the pole of the bacteria. Due to this, the photoluminescence at the pole is high and is enhanced due to the cyanobacteria. The coupling between the photosynthetic bacteria and 2D material can be used for production of sustainable energy resources.
4:06PM J22.00005: African Elephant Sensing Capabilities through Skin and Hair* ANDREW SCHULZ (Presenter), Mechanical Engineering, Georgia Institute of Technology, COLIN J BOYLE, Mechanical Engineering, Imperial College London, CLAIRE A HIGGINS, Bioengineering, Imperial College London, DAVID HU, Mechanical Engineering, Georgia Institute of Technology — The mouse and the elephant share a common sensing mechanism, vibrissae, or whiskers. In this study, we dissect an African elephant trunk and perform histology and measurement of the mechanical properties of the skin. We observe both long and short vibrissal hairs, ranging from 1 cm at the base of the trunk to 8 cm at the base. The length of hairs is likely associated with the different requirements at each position. Skin surrounding the vibrissae is stiffer, which may help the vibrissae better receive information. The dorsal part of the trunk is also stiffer than the ventral side, which may help the trunk grasp objects using the ventral portion. Through experiments conducted with histological and tensile test we report the different characteristics of the dermis. Heterogeneous properties of the skin in the elephant may give inspiration to designing of new flexible surfaces for biologically inspired soft robotic manipulators.

*N/A

4:18PM J22.00006: The role of residual stresses in biomineral morphogenesis revealed by 3D dark-field x-ray microscopy* [Invited] VANESSA SCHÖPPLER (Presenter), IGOR ZLOTNIKOV, BCUBE, TU Dresden — Residual stresses occur in numerous synthetic, geological and biogenic crystals having desirable or undesirable effects on materials performance. Recent studies have shown the significance of residual stresses in the mechanical functionality of a number of biomineralized tissues. However, the role of these forces in biomineral morphogenesis was never previously examined, mainly due to the lack of an appropriate multiscale characterization approach. Most of the state-of-the-art methods are either surface techniques yielding 2D information or allow limited 3D analysis of very small sample volumes. In this work, we employed the recently developed technique—dark-field x-ray microscopy—to study the relationship between residual stresses and crystallographic properties of biogenic calcite in the prismatic ultrastructure in the bivalves Pinna nobilis and Pinctada nigra in 3D. This method, developed at the European Synchrotron Radiation Facility, utilizes magnifying refractive lenses to map lattice distortions with an angular resolution of 0.001° and allows to analyze millimeter sized samples with a spatial resolution of 50 nm. Whereas the prisms in P. nobilis have an almost perfect single crystalline character, the prisms in P. nigra gradually change their crystallographic orientation and split into sub-prismatic domains. Due to the high angular resolution of the method, we were able to obtain unprecedented detail on the mosaicity of prisms in the two organisms and to demonstrate a correlation between internal lattice strains and local crystallographic properties of biogenic calcite in 3D. By comparing the experimental data from the two species, we not only shed a new light on the relationship between structure and texture during biomineralized tissues formation, but also demonstrate the role of internal stresses in biomineral morphogenesis.

*This work was financially supported by Bundesministerium für Bildung und Forschung through Grant 03Z22EN11.
4:54PM J22.00007: Effect of Sea Water pH on the Maturation of Marine Mussel Plaques
JUSTIN BERNSTEIN (Presenter), University of California, Santa Barbara, EMMANOUELA FILIPPIDI, Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, J HERBERT WAITE, MEGAN VALENTINE, University of California, Santa Barbara — Marine mussel plaques are an exceptional model for wet adhesives. Despite understanding their protein composition, we do not know how soluble proteins are rapidly processed into load-bearing structures. Here, we examine the effects of seawater pH on the time evolution of the internal microstructures in Mytilus californianus plaques. Experimentally, plaques deposited by mussels on glass surfaces are immediately collected, placed into pH-controlled artificial seawater for varying times, and characterized using scanning electron microscopy and tensile testing. We found a pH dependent transition from a liquid-like state to a porous solid within 30 minutes for pH ≥ 6.7; these plaques are load-bearing. By contrast, samples maintained at pH 3.0 showed no porosity and no measurable strength. Interestingly, we found no differences in cuticle thickness, suggesting that cuticle mechanics may be compromised at low pH. Our results suggest that sea water infusion after deposition is critical to the rapid formation of internal structures, which in turn plays an important role in the plaques’ mechanical performance.

*This work was supported by the MRSEC Program of the National Science Foundation under Award No. DMR 1720256, and an Otis Williams Postdoctoral fellowship (to EF).

5:06PM J22.00008: Mechanics and Adhesive Performance of Mussels on Roughness- and Geometry-controlled 3D printed Substrates
YOUNGHOON KWON (Presenter), JUSTIN BERNSTEIN, MEGAN VALENTINE, University of California, Santa Barbara, NOY COHEN, Israel institute of technology — Marine mussels have the remarkable ability to adhere to a variety of natural and artificial surfaces under hostile environmental conditions. Although the molecular composition of mussel adhesives has been well studied, a mechanistic understanding the physical origins of mussels' impressive adhesive strength remains elusive. Here, we investigated the role of substrate roughness and geometry in the adhesive performance of mussels. Using 3D printing, sandblasting, and laser texturing we created substrates with differing surface treatments and introduced these to mussels, which in turn adhered to the engineered surfaces via plaque-thread byssal structures. Tensile testing with in situ imaging was used to determine the adhesion strength and mechanical properties of the mussel adhesive plaques under various conditions. Our results inform the relationships between adhesive performance and substrate properties, give insight into the physical governing factors of mussel adhesion, and provide design criteria for development of synthetic adhesives for use on complex, textured surfaces.

*This work was supported by the MRSEC Program of the National Science Foundation under Award No. DMR 1720256.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J23 DBIO GSNP: Evolutionary and Ecological Dynamics II: Communities and Networks 304 - Mikhail Tikhonov, Washington University, St. Louis - Tag(s): Focus
2:30PM J23.00001: Resource-rich environments can reduce stability and diversity in microbial communities by strengthening interspecies interactions  CHRISTOPH RATZKE, JULIENE BARRERE, JEFFREY GORE (Presenter), Massachusetts Institute of Technology MIT — Organisms – especially microbes – tend to live in complex communities. While some of these ecosystems are very bio-diverse, others aren’t, and while some are very stable over time others undergo strong temporal fluctuations. Despite a long history of research and a plethora of data it is not fully understood what sets biodiversity and stability of ecosystems. Theory as well as experiments suggest a connection between species interaction, biodiversity, and stability of ecosystems, where an increase of ecosystem stability with biodiversity is often observed. However, what causes these connections remains unclear. Here we show in microbial ecosystems in the lab that the concentrations of available nutrients can set the strength of interactions between bacteria. At high nutrient concentrations, extensive microbial growth leads to strong chemical modifications of the environment, causing more negative interactions between species. These stronger interactions exclude more species from the community – resulting in a loss of biodiversity. At the same time, these stronger interactions also decrease the stability of the microbial communities, providing a mechanistic link between species interaction, biodiversity and stability.

2:42PM J23.00002: Niche-Neutral Transition in a Lotka-Volterra Model of Diverse Ecosystems  JIM WU (Presenter), Princeton University, DAVID J. SCHWAB, City University of New York, PANKAJ MEHTA, Boston University — Niche and neutral theory are two prevailing, yet much debated, ideas in ecology proposed to explain the patterns of biodiversity. Whereas niche theory emphasizes selective differences between species and interspecific interactions in shaping the community, neutral theory supposes functional equivalence between species and points to stochasticity as the primary driver of ecological dynamics. In this work, we draw a bridge between these two opposing theories. Starting from a Lotka-Volterra (LV) model with demographic noise and random symmetric interactions, we analytically derive the stationary species abundance distribution and extract the population statistics. Using these results, we demonstrate the existence of a phase transition between niche and neutral regimes, thus reconciling how neutral-like statistics may arise from a diverse community of species with different traits.
2:54PM J23.00003: Competition-driven strategies for controlling multistable microbial communities  VERONIKA DUBINKINA (Presenter), University of Illinois at Urbana-Champaign, AKSHIT GOYAL, The Simons Centre for the Study of Living Machines, NCBS, YULIA FRIDMAN, National Research Center “Kurchatov Institute”, PARTH PRATIM PANDEY, SERGEI MASLOV, University of Illinois at Urbana-Champaign — Microbial communities often need particular species compositions, or community states, to perform a certain function. Because these communities play crucial roles in human health and industry, we need to maintain them in particular desirable states, and prevent them from reaching undesirable ones. What makes this task especially challenging is that microbial communities are often multistable; both desirable and undesirable states may be possible in the same environmental conditions. Due to these complications, we still lack pragmatic and reliable strategies to fulfill this task. Here, we propose two strategies to control multistable microbial communities: that of controlling the colonization order in which species are introduced into a community, and that of controlling the supply of nutrients to a community. Both strategies are driven by competition for nutrients between microbial species. As a proof of concept, we illustrate their implementation in a resource-explicit model. Our proposed strategies have the potential to greatly improve existing methods to engineer and manipulate real microbial communities, such as in industrial bioreactors and the human gut.

3:06PM J23.00004: Long-range patterns of activity shaped by signaling interactions within bacterial communities*  JAMES BOEDICKER (Presenter), KALINGA PAVAN T SILVA, Tahir YUSUFALY, Univ of Southern California — Bacteria communicate to coordinate macro-scale patterns of gene expression and associated group behaviors such as biofilm formation. Cells secrete, sense, and respond to small chemical signals in a process known as quorum sensing. Within diverse bacterial communities, signal exchange is modulated by signaling interactions between different cell types, including interference through signal crosstalk and signal destruction. Our work explored how signaling interactions between multiple cell types shape global patterns of gene expression. We examined how community composition modulated signal-dependent gene expression using both experiments and reaction-diffusion models. In some communities, the pattern of gene expression followed a 2D percolation transition, controlled by the ratio of signal producing and signal destroying strains in the community. At a critical amount of interference, signal exchange was disrupted and long-range communication was suppressed. We explored the limitations of diffusive communication and strategies cells could use to coordinate behavior at length scales exceeding distances over which diffusion is effective.

*Army Research Office MURI Award W911NF1910269, ONR Award N00014-18-1-2632, and NSF Award PHY-1753268.
3:18PM J23.00005: Ecological interactions constrain the coexistence of generalists and specialists during coevolution in microbial communities  
AKSHIT GOYAL (Presenter), Massachusetts Institute of Technology MIT — Natural microbial communities are complex ecosystems in which species with different metabolic strategies—both generalists and specialists—stably coexist. We do not understand how coevolution within a community can both lead to, and stabilize, such coexistence, and how generic we expect it to be. Here, we propose and study a minimal model of a co-evolving microbial community shaped by ecological interactions. Our model combines competition and cooperation for nutrients with evolutionary game theory. In doing so, it makes three broad and surprising predictions about co-evolved microbial communities. First, we find that generalists and specialists coexist only in a narrow range of ecological interactions; in all other regimes, specialists dominate. Second, we find that co-evolving with others makes it strikingly difficult for generalists to evolve a correlation between their nutrient preferences and growth rates; such a correlation is often observed in experiments. Finally, we find that communities with a greater fraction of generalists are also likely to have more stable states, which can be tested. This model provides a simple framework through which to quantify and make testable predictions about coevolution in microbial communities.

3:30PM J23.00006: Criticality on topologically disordered systems and the Harris criterion*  
HATEM BARGHATHI (Presenter), THOMAS VOJTA, Missouri Univ of Sci & Tech — To test the stability of clean critical points against quenched spatial disorder, Harris introduced the criterion \( d\nu > 2 \). Its predictions are in agreement with the vast majority of analytical and numerical results on phase transition in disordered systems. However, in systems where disorder arises from random connectivity, a number of violations of the Harris criterion have been reported. We recently introduced \([1]\) a modified stability criterion, \( (d+1)\nu > 2 \), for systems in which the presence of topological constraints suppresses disorder fluctuations, resulting in a violation of the usual Harris criterion. However, some recent results on topologically disordered systems appear to violate even the modified criterion. To uncover the source of such apparent violations we perform a detailed statistical analysis of such systems together with large-scale Monte Carlo simulations.


*This work was supported by the NSF under Grant No. DMR-1828489.
**3:42PM J23.00007: The Emergence of Spatial Patterns in Tree Yield: A New Model for the Masting Phenomenon**  
SHADISADAT ESMAEILI (Presenter), University of California at Davis, ALAN HASTINGS, University of California at Davis, Santa Fe Institute, KAREN ABBOTT, Case Western Reserve University, JONATHAN MACHTA, University of Massachusetts Amherst, Santa Fe Institute, VAHINI REDDY NAREDDY, University of Massachusetts Amherst — The emergence of patterns of synchrony is ubiquitous across many fields, including ecological systems in which synchrony can be both favorable and detrimental. The prevalence of synchrony creates the expectation of the existence of detail-independent principles that can explain and predict this phenomenon and its emergence. A notable example of synchrony is the “masting” phenomenon observed in many plant species in which individual plants show variable annual production (bearing), which is spatially correlated. External forces and local dynamics can lead to the emergence of spatial patterns or full synchrony in such systems. Currently, existing models for masting phenomenon, while proposing a mechanism for alternate bearing, do not address the spatial patterns observed in real data. In this talk, we introduce a new model to emulate the observed spatial patterns and study the effects of local coupling and external forces on the dynamics of the system.

*This work is supported by NSF grant DMS-1840221*

**3:54PM J23.00008: Binary Decisions of Large Cliques of Evidence Accumulators**  
BHARGAV KARAMCHED (Presenter), Univ of Houston, ZACHARY KILPATRICK, Applied Mathematics, University of Colorado - Boulder, KRESIMIR JOSIC, MEGAN STICKLER, WILL OTT, Univ of Houston, BENJAMIN LINDNER, Physics, Humboldt University — We consider cliques of N evidence accumulators making a binary decision based on noisy observations. Each agent's evidence is a drift-diffusion process on a symmetric, bounded domain with absorbing boundaries. An agent makes an immutable decision when their evidence reaches one of the boundaries (thresholds). Prior to a decision, each agent's evidence is an independent stochastic process. Following a decision, each agent's evidence receives a bump equal to the value of the threshold corresponding to the decision. In large cliques, such a decision can induce a large fraction of the agents to agree with the initial decider. If the first decider is correct, this bodes well for the overall performance of the clique. However, if the initial decider is incorrect, the overall performance of the clique can be disastrous. We derive asymptotic results conveying what fraction of agents agree with the initial decider upon observing their decision and how the remaining agents decide thereafter to agree with the initial decider or collectively disagree with them. We also show how the framework of the evidence accumulation in cliques can be modified so that it is self-correcting and, even if the first decision is wrong, have the majority of the clique choose the correct decision.
4:06PM J23.00009: Identifying Suspicious Users and Products to Predict New Opinions
SUKHWAN CHUNG (Presenter), Physics, University of Notre Dame — An opinion network describes how a person values an object, which can be another person or product. This type of network is ubiquitous because humans constantly evaluate their surroundings. Analyzing an opinion network can bring deeper understanding of what and how people are thinking, but at the same time, a malicious attempt to influence such network can be harmful to the public. One problem naturally arising while studying opinion networks is identifying users leaving intentionally fake opinions to influence the opinions of others. Another question that can be asked is how to predict a person's opinion towards another. In this work, a solution to those issues is suggested using the Rev2 algorithm (developed by S. Kumar, et al) and the principle of maximum entropy. The Rev2 algorithm is used to assign a suspiciousness score to users based on how much the user's action deviates from the rest. Also, a quality index will be assigned to products based on reliable opinions. Using this information, the principle of maximum entropy is invoked to produce the most unbiased prediction of new opinions. The proposed solution is tested against public network data including a user-to-user trust network of Bitcoin platform users and a user-to-product rating network of Netflix users.

4:18PM J23.00010: Optimal evidence accumulation on social networks* BHARGAV KARAMCHED, SIMON STOLARCZYK, KRESIMIR JOSIC, University of Houston, ZACHARY KILPATRICK (Presenter), University of Colorado, Boulder — To make decisions we are guided by the evidence we collect, as well as the opinions of friends and neighbors. How do we integrate our private beliefs with information we obtain from our social network? To understand the strategies humans use to do so, it is useful to compare them to observers that optimally integrate all evidence. Here we derive network models of rational agents who accumulate private measurements and observe decisions of their neighbors to choose between two options. The resulting information exchange dynamics has interesting properties: When one option is preferred, the absence of a decision can be increasingly informative over time. In recurrent networks an absence of a decision can lead to a sequence of belief updates akin to those in the literature on common knowledge. In large networks, a single decision can trigger a cascade of agreements and disagreements that depend on the private information agents have gathered. Our approach provides a bridge between social decision making models in the economics literature, which largely ignore the temporal dynamics of decisions, and the single-observer evidence accumulator models used widely in neuroscience and psychology.

*NIH R01MH115557; NSF DMS-1517629; NSF DMS-1662305; NSF DBI-1707400
4:30PM J23.00011: Sensitivity of collective outcomes identifies pivotal components*
EDWARD LEE (Presenter), Cornell University, DANIEL M KATZ, MICHAEL J BOMMARITO, Chicago-Kent School of Law, Illinois Institute of Technology, PAUL GINSPARG, Cornell University — The relation between collective outcomes and individual behavior is a central question in social science, biology, and statistical physics. Using the information geometry of minimal models from statistical physics, we develop a general approach for identifying key "pivotal" components on which aggregate statistics depend most sensitively. For political voting, pivotal blocs are like swing voters on whom the distribution of majority-minority divisions depends most sensitively. Analogously, collective market movement may be characterized by a few important stock indices, or the identity of a community on Twitter may hinge on a few individuals. In neural networks, pivotal components may be important for determining collective states. Our approach may help evaluate how political bodies change with membership or analyze the robustness of social institutions and biological networks to targeted perturbation.

*Dirksen Congressional Research Center, NSF GRFP (DGE-1650441), Omega Miller Program at the Santa Fe Institute, Cornell University, Illinois Tech - Chicago Kent College of Law

4:42PM J23.00012: Community optimization and ruggedness of ecological landscapes*
ASHISH B. GEORGE (Presenter), KIRILL S KOROLEV, Boston University — Many applications require the assembly of an optimal microbial community that maximizes biofuel production, crop yield, or remediation potential. The number of combinations in which these communities can be assembled grows exponentially with the number of species. Therefore, optimization strategies have to rely on heuristic algorithms that iteratively select the best community from a small set of trial communities. The success of such strategies depends on the ruggedness of the landscape of community function. We show that consumer-resource models with and without cross-feeding have unique steady states that depend only on the presence or absence of species in the community. Thus, community selection is a search on an ecological landscape in close analogy with evolution on fitness landscapes in population genetics. We report typical ruggednesses of such landscapes, and discuss how they depend on inter-specific interactions and environmental conditions. We also determine the conditions under which landscape ruggedness can be estimated from incomplete data.

*Simons Foundation Grant #409704, Research Corporation for Science Advancement through Cottrell Scholar Award #24010 and the Scialog grant #26119, and Moore foundation grant #6790.08 ro Kirill S. Korolev
4:54PM J23.00013: History-dependent tradeoffs in changing environments* [Invited] MIKHAIL TIKHONOV (Presenter), Washington University, St. Louis — Performance tradeoffs, which simple models typically postulate, are known to themselves evolve. This leads to a curious feedback loop: evolutionary history shapes tradeoff strength, which, in turn, shapes evolutionary future. Using a simple model, I will show that this feedback can lead to counterintuitive consequences in the context of multiple or changing environments: specifically, a direct exposure to some environment of interest will, in general, no longer be the most effective way of achieving highest fitness in it. I will demonstrate three different mechanisms for how alternate exposure strategies can prove more effective: inducing a more evolvable architecture, counteracting a form of “use it or lose it”, or relying on horizontal gene transfer; and will discuss the prospects of linking these theoretical expectations to experiments.

*This work was supported in part by National Science Foundation grants PHY-1607606, PHY-1545840, and PHY-1720397.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J24 GSNP DFD: Crystallization, Jamming, and Glassy Behavior

2:30PM J24.00001: Nucleation in Granular Media Undergoing Cyclic Shear [Invited] WEIWEI JIN (Presenter), COREY SHANE O'HERN, Yale University, CHARLES RADIN, Department of Mathematics, University of Texas at Austin, MARK SHATTUCK, The City College of New York, HARRY L SWINNEY, University of Texas at Austin — Recent experiments have found that homogeneous nucleation occurs in dense granular materials undergoing cyclic shear from an initially disordered state. In the experiments, the mm-sized grains are under gravitational loading and interact via frictional contact forces. In this work, we carry out discrete element method simulations to determine the contributions of friction and gravity to crystallization of granular materials during cyclic shear. We show that cyclic shear of frictionless granular materials in the absence of gravity gives rise to a first-order-like phase transition from a disordered state to a polycrystalline state with domains of face-centered cubic and hexagonal close packed positional order. The polycrystalline ordering develops through homogeneous nucleation, i.e., spontaneous formation of crystalline clusters far from the boundaries of the system. The small crystalline clusters typically shrink before they reach a critical size, above which crystallites with no preferred orientation grow to reach the system size. Thus, gravitational loading and frictional forces are not necessary to induce crystallization in driven granular media.
3:06PM J24.00002: Structural and Mechanical Characteristics of the Disordered-Ordered Transition in Mechanically Stable Sphere Packings  HIDEYUKI MIZUNO, The University of Tokyo, KUNIYASU SAITO, Tohoku University, LEO SILBERT (Presenter), Central New Mexico Community College — Using the discrete element method, we generate mechanically stable sphere packings in three dimensions that span a wide range in structural order, ranging from fully amorphous through to (quasi) ordered structures, as characterized by the globally averaged bond orientational order parameter. While amorphous systems exhibit features consistent with hyperuniformity – suppressed density fluctuations in the long-wavelength limit – as the packing structure becomes more ordered, the low-wavenumber limit of the static structure factor grows with increasing order. As the packing pressure, $p$, is varied from the marginally rigidity ($p \sim 0$) to more robust systems ($p >> 0$), the packing coordination number, $z$, follows a familiar scaling relation with pressure, $\Delta z = z - z_0 \sim p^{1/2}$, where $z_0 = z(p=0)$. While it has previously been noted that $\Delta z$ is the control parameter that determines packing properties, here we show how packing structure plays an influential role on the mechanical properties of the packings. Specifically, we find that the elastic (bulk and shear) moduli, generically referred to as $M$, become functions of both $\Delta z$ and structure, to the extent that, $M - M_0 \sim \Delta z$. Here, $M_0$ are the values of the elastic moduli in the zero-pressure limit, whose values depend on the structure of the packing.

3:18PM J24.00003: Isostatic, ordered disk packings  PHILIP TUCKMAN (Presenter), KYLE VANDERWERF, Yale University, MARK SHATTUCK, The City College of New York, COREY SHANE O’HERN, Yale University — Numerous studies have shown that disordered, jammed disk packings are isostatic (with the same number of contacts as the number of degrees of freedom) and can occur over a wide range of packing fractions, $\varphi_{\text{min}} < \varphi_j < \varphi_{\text{max}}$. For systems composed of 2D bidisperse disks with half large and half small particles, and diameter ratio $r = 1.4$, $\varphi_{\text{min}} \approx 0.84$ and $\varphi_{\text{max}} \approx 0.855$. Further, these disordered, isostatic packings display similar structural and mechanical properties, such as the power-law scaling of the excess contact number $\Delta z$ and shear modulus $G$ with pressure $p$. In this work, we show that isostatic, ordered jammed packings of nearly monodisperse disks also occur over a range of packing fractions, $\varphi_{\text{O,min}} < \varphi_j < \varphi_{\text{xtal}}$, where $\varphi_{\text{xtal}} \approx 0.907$ is the packing fraction for a triangular lattice. These packings are achieved by first generating packings of monodisperse disks, then changing the sizes of a fraction of the disks by a small amount, then finding the nearest jammed packing. Here, we characterize the structural and mechanical properties of these isostatic, ordered jammed packings.
3:30PM J24.00004: Athermal fluctuations in disordered crystals  PAPPU ACHARYA (Presenter), SURAJIT SENGUPTA, TCIS, TIFR, BULBUL CHAKRABORTY, Brandeis University, KABIR RAMOLA, TCIS, TIFR — We analyze the fluctuations in particle positions and inter-particle forces in disordered jammed crystals in the limit of the weak disorder. We demonstrate that such athermal systems are fundamentally different from their thermal counterparts, characterized by constrained fluctuations of forces perpendicular to the lattice directions. We develop a disorder perturbation expansion in polydispersity about the crystalline state, which we use to derive exact results to linear order. We show that constrained fluctuations result as a consequence of local force balance conditions, and are characterized by non-Gaussian distributions which we derive exactly. We analytically predict several properties of such systems, including the scaling of the average coordination with polydispersity and packing fraction, which we verify with numerical simulations using soft disks with one-sided harmonic interactions.

3:42PM J24.00005: Mechanically stable sphere packings at arbitrarily low densities  ROBERT DENNIS (Presenter), ERIC CORWIN, Univ of Oregon — Lightweight materials can be formed by creating mechanically rigid structures with a combination of compressive and tensile forces. By considering purely compressive forces in sphere packings, we determine the limits on creating low density rigid systems. An Apollonian packing proves that a rigid packing can completely fill space, but proof for the existence of a lowest density rigid packing was unknown. The previously known lowest density packings are constructed by diluting simple crystals, but we present a new construction based on rigid bridges. This new construction not only demonstrates that lower density packings can be achieved, but it can be used to create rigid packings with densities arbitrarily close to zero. We demonstrate the rigidity of these low density packings using both established and novel procedures and we explore the properties of these configurations to gain a deeper understanding of the limits of rigidity in repulsive systems. Such constructions not only lay an old puzzle to rest, but enable the development of new lightweight materials.

3:54PM J24.00006: Real-space renormalization of randomly vacated lattices: a renormalization group for jamming?  ABE CLARK (Presenter), US Naval Postgraduate School — Jamming occurs in granular materials, as well as in emulsions, dense suspensions, and other amorphous, particulate systems. When the packing fraction $\varphi$, defined as the ratio of particle volume to system volume, is increased past a critical value $\varphi_c$, a liquid-solid phase transition occurs, and grains are no longer able to rearrange. Previous studies have shown evidence of spatial correlations that diverge near $\varphi = \varphi_c$, but there has been no explicit spatial renormalization group (RG) scheme that has captured this transition. Here, I present a candidate for such a scheme, using a block-spin-like transformation of a randomly vacated lattice of grains. I define a real-space RG transformation based on local mechanical stability. This model displays a critical packing fraction $\varphi_c$ and gives estimates of critical exponents in two and three dimensions.
Critical scaling for yield is independent of distance to isostaticity

Granular materials, suspensions, foams, and emulsions can form amorphous jammed states. These states can yield when subjected to a shear stress $\tau$. When $\mu = \tau/p$, where $p$ is the system pressure, exceeds a critical value $\mu_c$, jammed states become inaccessible and flow persists indefinitely. Near $\mu = \mu_c$, long-range cooperative effects become dominant, as shown by the success of recent nonlocal rheological models. Long-range cooperativity in these systems is often framed in terms of the isostatic jamming point, which occurs at $p = 0$. The relationship between isostatic jamming and yielding is not fully understood. Here, using simulations of quasi-statically sheared soft sphere packings, we observe critical behavior near $\mu = \mu_c$, with a diverging length scale $\xi \sim |\mu - \mu_c|^{-\nu}$, that is independent of distance to isostaticity over a wide range of $p$. The critical scaling functions and values of the scaling exponents are nearly independent of distance to isostaticity despite the large range of $p$. Our results demonstrate that yielding of jammed systems represents a critical transition that is distinct from the isostatic point. Our results may also be useful in deriving and improving nonlocal rheological models.

The Influence of the Wall on Confined Random Packing of Rods

We experimentally study the random packing of rods into small containers, and in particular, examine the influence of the container surface on the packing. Our experiments use cylindrical containers of different radii, and rods of aspect ratio 8. As previously seen, rods packed into smaller cylindrical containers yielded lower volume fractions than in larger containers. In this current work, we coat the inner vertical surface of the containers with sandpaper to change the enhancement of friction between the wall and the rods. We find a linear relationship between the volume fraction $f$ and $1/R$ (using the radius $R$ of the container). The intercept gives the infinite-radius container extrapolated volume fraction, and the slope quantifies how strongly the walls affect the packing. As might be expected, rougher sandpaper results in a stronger influence from the walls. Surprisingly, sandpaper also influences the infinite-radius extrapolation volume fraction.

Two-stage jamming in semiflexible polymers and fibers

We find that jamming in model freely rotating polymers with bond angle $\theta_0$ occurs in two stages. The first, precursor stage occurs when the average number of unique interchain contacts $Z_{\text{chain}}$ jumps discontinuously as chains “entangle” at a packing fraction $\varphi_e(\theta_0)$. Entanglement is a necessary but not a sufficient condition for mechanical rigidity; systems rigidify (i.e. jam) at $\varphi_j(\theta_0) > \varphi_e(\theta_0)$, and $Z_{\text{chain}}$ jumps discontinuously again at $\varphi_j(\theta_0)$. These discontinuities become sharper as polymers stiffen (as $\theta_0$ decreases). We find that $\varphi_e(\theta_0) \sim 0.8 \varphi_j(\theta_0)$ despite the fact that both decrease by a factor of nearly two as polymers stiffen. Our results for small $\theta_0$ may also describe jamming phenomena in fiber networks.

Support from NSF Grant No. DMR-1555242 is gratefully acknowledged.
4:42PM J24.00010: Low frequency vibrations of deformable particles  
DONG WANG  
(Presenter), ARMAN BOROMAND, MICHAEL MURRELL, Yale University, MARK SHATTUCK, The City College of the City University of New York, COREY SHANE O’HERN, Yale University — Disk packings at jamming onset exhibit an excess of low-frequency vibrational modes compared to the number predicted by Debye scaling. The excess number of modes, which controls the mechanical response of packings, decreases as the packings are compressed above jamming onset. In this work, we calculate the spectrum of vibrational modes from the eigenvalues of the dynamical matrix for truly deformable particles at jamming onset as a function of the shape parameter $A = p^2/(4\pi a)$, where $p$ is the perimeter and $a$ is the area of the particle. We show that there is an excess number of low frequency, collective modes in the density of vibrational modes for jammed packings of deformable particles over a wide range of particle shape both above and below the characteristic value $A \approx 1.15$ at which the system is confluent.

4:54PM J24.00011: Structure and dynamics during training of memory in jammed packings  
IAN GRAHAM  
(Presenter), ANDREA JO-WEI LIU, University of Pennsylvania — Jammed packings can be trained by intermediate-amplitude quasistatic oscillatory shear to fall into periodic trajectories in which the same multiple local minima are explored in each period. Here we ask how the rearrangement dynamics and stroboscopic snapshots of packing structure evolve during the training process. We use persistent homology to characterize the structure. We characterize rearrangements in terms of T1 events and classify them as reversible if they return to their initial configuration and irreversible if they do not. At the end of the training process, irreversible T1 events must vanish when the system falls into a periodic trajectory (develops a memory). We find that the structure varies continuously during the training, but that the nature and number of T1 events remains nearly constant until the last cycle or two before the system develops memory. Thus, observable changes in structure have relatively little effect on dynamics until near the end of the training process, in contrast with glassy dynamics, in which extremely subtle changes in structure lead to enormous changes in dynamics.

5:06PM J24.00012: Measuring the Granular Density of Modes in 3D via Impact  
ELI OWENS  
(Presenter), SYDNEY BLUE, SALEM C WRIGHT, Presbyterian College — The jamming transition is an important feature of granular materials, with prior work showing an excess of low frequency modes in the granular density of states (or modes). In this work, we present an experimental method for acoustically measuring the granular density of modes using a single impact event to excite vibrational modes in the granular material. We test three different granular materials, all of which are composed of spherical plastic beads. The first two systems are monodisperse collections of either 6 mm or 8 mm diameter beads. The third system is a bidisperse mixture of the previous two bead sizes. During data collection, the particles are confined to a 30x30x20 cm box; on top of this box, and resting on the granular material is a light, rigid sheet onto which weights can be placed. To excite the material, an impactor is dropped on top of the system. The response of the granular material to the impact pulse is recorded by piezoelectric sensors buried throughout the material, and the density of modes is computed from the spectrum of the velocity autocorrelation of these sensors. Our initial measurements of the density of modes differentiate between the three different systems and between different pressure states.
5:18PM J24.00013: Quenching to field-stabilized magnetization plateaus in the unfrustrated Ising antiferromagnet*  ADAM IAIZZI (Presenter), YING-JER KAO, Natl Taiwan Univ — We study the square-lattice Ising antiferromagnet in a uniform field using single spin flip Metropolis algorithm dynamics. Starting from an infinite temperature state, we perform an instantaneous quench to finite $T$. Under this protocol, the field stabilizes two magnetization plateaus in a regime where the equilibrium magnetization is zero. This occurs despite the absence of intrinsic disorder or frustration. These metastable plateau states are extremely stable, even for small sizes and moderate temperatures. Ergodicity is restored near the edges of the plateaus. The plateaus can be understood as ‘tilings’ of stable local configurations. Once the system reaches one of these tiled states, the probability of flipping even a single spin is exponentially suppressed. Although the details of the plateaus will depend on the update scheme, the underlying principle causing the breakdown of ergodicity is quite general. This simple case can thus provide a paradigm for understanding ergodicity breakdown in Monte Carlo dynamics more generally.


Tuesday, March 3, 2020 2:30 PM - 5:06 PM

Session J25 GSNP DSOFT DCP: Physics of Liquids II 402 - Yang Zhang, University of Illinois at Urbana-Champaign - Tag(s): Focus

2:30PM J25.00001: Using Algebraic and Geometric Topology to Characterize Hierarchical Organization in Complex Solutions and Their Interfaces* [Invited]  AURORA CLARK (Presenter), Washington State Univ — Complex, multicomponent, solutions are often characterized by multiple length and timescale correlations that challenge chemical intuition. Recently developed tools are leveraging graph-theoretical interpretations of the intermolecular networks of interactions in such systems, supporting topological data analysis as a means to characterize organizational patterns, from the identification of molecular species and solvation environments, to new interpretations of fluid phase transformation. One may interpret these topological descriptors as high-dimensional order parameters that can also be used to enhance sampling of the energy landscape. Complementary geometric topological methods of liquid surfaces have also emerged as a powerful tool for the identification of interfacial structures responsible for transport. Ongoing work is combining both the algebraic and geometric topology formalism to create a holistic approach that relates hierarchical organizational patterns to structure and even function within complex solutions and their interfaces.

*This work was funded by the Department of Energy Basic Energy Sciences Separations program grant DE-SC0001815.
3:06PM J25.00002: Hanging droplets from liquid surfaces  GANHUA XIE (Presenter), JOE FORTH, Lawrence Berkeley National Laboratory, SHIPEI ZHU, Department of Mechanical Engineering, The University of Hong Kong, BRETT HELMS, PAUL ASHBY, Lawrence Berkeley National Laboratory, HO CHUENG SHUM, Department of Mechanical Engineering, The University of Hong Kong, THOMAS RUSSELL, Polymer Science and Engineering Department, UMass — Nature uses surface tension to support dense objects on liquid surfaces, from water striders to insect larvae for mating and survival, which has inspired fabrication of man-made robotic systems for transport across water. These systems present hydrophobic surface to prevent sinking. Here, we show that a droplet of a denser aqueous solution, containing a polyelectrolyte can hang on the surface of a less dense aqueous solution containing an oppositely charged polyelectrolyte. The magnitude of the interfacial forces acting on the droplet and the shapes of the hanging droplets can be controlled by releasing heights of the droplet and the polyelectrolyte concentrations. Coacervate sacs with homogeneous and heterogeneous surfaces can be produced that hang from the surface and, by capillary forces, form well-ordered arrays. Controlled locomotion and rotation can be achieved by functionalizing the hanging droplets with magnetic microparticles. The suspended droplets are in direct contact with air enabling in situ manipulation of the droplets and using the encapsulated aqueous phases for compartmentalized cascading chemical reactions with selective transport. These hanging droplets have potential applications in functional micro-reactors, micro-motors and biomimetic micro-robots.

3:18PM J25.00003: Dipolar dimer liquid  JUNYI ZHANG (Presenter), Princeton University — A lattice liquid model, dipolar dimer liquid (DDL), is proposed motivated by the water. The DDL on the bipartite lattice may be exactly mapped to the annealed Ising model on random graphs. We showed that there exists a phase transition of the DDL when the density is not too small. In the low temperature phase, which we called glacia phase, the polar charges are ordered while the dimers are still free to move and rotate. On two-dimensional square lattice and honeycomb lattice, we may bound the critical temperature $T_G$ by comparing the Ising model on random graphs to the exactly-solved Ising models.

3:30PM J25.00004: Extended equation of state for non-ideal mixtures near the consolute critical point.  YEYGENII RUDNIKOV (Presenter), MYKOLA POTOMKIN, Taras Shevchenko National University of Kyiv — The problem of constructing the equations of state and calculating the thermodynamic parameters of mixtures near the liquid-liquid critical point using the parameters of their components remains an urgent task of the condensed matter physics. To solve it, the new method of choosing the countdown start for calorific values is founded, in which the corresponding states law for liquids is satisfied. An analysis of thermodynamic consistency conditions in the dissolution of solution components allow concluding that a consistent calculations of the mixture parameters for variable values are approximate due to excessive non-additive contributions to them; similar calculations are exact for values which remain constant for components. Using the proposed approach for liquid components of obtained and literature data for mixtures C4H8O2 - H2O, CH4O – C6H14, C6H7N – D2O, the constant combinations of thermodynamic parameters have been found. It allowed using the consistent rules for calculating the calorific parameters of mixture and obtaining the parameters of the theory of critical mixtures.
3:42PM J25.00005: Numerical Modeling of Room Temperature Ionic Liquids*  
KATHERINE KLYMKO (Presenter), JOHN BELL, Lawrence Berkeley National Laboratory, ALEJANDRO GARCIA, Physics, San Jose State University, SEAN CARNEY, Math, UT Austin, ANDY NONAKA, Lawrence Berkeley National Laboratory — We present a mesoscale numerical model for room temperature ionic liquids. The model uses a fluctuating low Mach number formulation based on a thermodynamically consistent formulation. Repulsion effects between the different ions are represented by an excess free energy. We first investigate the structure of the fluid to quantify the interplay between electrostatic forces and repulsion of the different ions. We then investigate the structure of the electric double layer that forms at a solid surface at fixed potential as a function of the applied voltage. Finally, we investigate the effect of composition dependence of the electric permittivity in the presence of an external field.

*Center for Computational Sciences and Engineering
Lawrence Berkeley National Laboratory

3:54PM J25.00006: Evaporation of Lennard-Jones Monomer-Dimer Mixtures*  
BINGHAN LIU, SHENGFENG CHENG (Presenter), Virginia Tech — Evaporation and condensation are important physicochemical processes for the conversion between liquids and gases. We use Lennard-Jones (LJ) liquids as model systems to study the nonequilibrium physics of evaporation. The evaporation of pure LJ fluids has been studied extensively. However, the studies on evaporating liquid mixtures are limited and the relevant physics is poorly understood. Here we employ molecular dynamics simulations to study the evaporation behavior of LJ monomer-dimer mixtures. During fast evaporation, the concentration of LJ dimers, which are less volatile, increases significantly from the bulk of the mixture to the evaporating liquid-vapor interface. Correspondingly, the concentration of LJ monomers exhibits a negative gradient in the same region. In other words, the LJ monomers and dimers stratify in the region below the evaporating interface. Furthermore, the degree of stratification is stronger at higher evaporation rates. The effect of evaporative cooling on stratification is also clarified on the basis of thermophoresis. This stratification phenomena may be utilized to separate suspended particles interacting differently with the components of an evaporating liquid mixture.

*Supported by a competitive research grant from the 4-VA Consortium.
Decomposing thermal fluctuations in fluids with hydrodynamic modes

XIAOHUI DENG (Presenter), China / Hong Kong University of Science and Technology — Presenter: Xiaohui Deng

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Abstract
Thermal fluctuations are usually manifest as tiny displacement velocity variations or as molecular self diffusion. We report the analytic solution of the complete set of 2D hydrodynamic modes in a channel geometry, under the Navier slip boundary condition. By using this complete set, thermal fluctuations and their consequences can be expressed in terms of the hydrodynamic modes. In particular, the fluctuation dissipation theorem can be written in terms of the eigenvalues of the hydrodynamic modes as an expression for the diffusion constant $D$. Our work offers a new perspective on fluid system’s inherent thermal fluctuations and its reliance on the boundary condition. In particular, it offers a way to spatially tune the thermal fluctuations by modulating the hydrodynamic boundary condition

*sponsored by RGC(The Research Grants Council)

Correlation between local viscosity and the atomic-level stresses in liquids

TAKUYA IWASHITA (Presenter), Oita University — Liquids are ubiquitous, but the atomic origin of the viscosity remains unknown because of structural disorder. To study the relationship between viscosity and local structures we performed molecular dynamics simulations on various metallic liquids. Here the local structures of the liquids are characterized by the atomic-level stresses which describe the local mechanical states. We showed strong correlation between local viscosity and atomic-level stress in the liquids; for example, the atomic sites under compression are more unstable against shear than those under tension. The results indicate a universal structure-dynamics relationship in liquids.

*The work is supported by JPSj KAKENHI Grant Number JP19K03771.
4:30PM J25.00009: Importance of nuclear quantum effects on the hydration of chloride ion*

JIANHANG XU (Presenter), ZHAORU SUN, FUJIE TANG, Department of Physics, Temple University, DEYU LU, Center for Functional Nanomaterials, Brookhaven National Laboratory, XIFAN WU, Department of Physics, Temple University — The solvation structure of Cl\(^{-}\) ion in aqueous solution is determined by the H-bonding between the solvated ion and surrounding water molecules, which is in competition with the water-water H-bonds in the solvent. We performed \textit{ab initio} path-integral molecular dynamics simulations based on the SCAN functional. We find that quantum nuclei tilt the above balance compared to conventional classical simulations. Nuclear quantum effects (NQE) weaken the ion-water H-bonding strengths as shown by the increased first-peak position in the ion-oxygen pair distribution function. In turn, the H-bond interactions among water molecules in the solvent become effectively strengthened. As a result, the population of interstitial water molecules increases in the first coordination shell, which are non-bonded to Cl- ion, however, are H-bonded to other water molecules in a tetrahedral network. By including NQEs, our local dielectric response function calculations suggest that the surrounding water molecules electronically screen the charge of Cl\(^{-}\) more effectively than the classical counterpart. Our resulting solvation structures are in excellent agreement with the recent neutron scattering experiments by Soper \textit{et al}.

*This work is supported by the U.S. Department of Energy under Grant No. DE-SC0012575.

4:42PM J25.00010: Connectedness of the configuration space of hard disk systems*

OZAN ERIK OK (Presenter), JEREMY KYLE MASON, Materials Science and Engineering, University of California, Davis — Hard disk systems are often regarded as prototypes for simple fluids, and can offer valuable insight into the origins of phase transitions and glass transitions in general. A phase transition is usually believed to occur when averages of thermodynamic quantities over the accessible part of the configuration space change discontinuously. A phase transition could then be driven by a discontinuous change in the accessible region, and this depends on the connectedness of the configuration space as a function of disk radius. A regularized potential energy function is defined on the configuration space, the critical points of which correspond to configurations where the topology of the configuration space changes, and are extensively sampled for small numbers of disks. Knowledge of the critical points allows the configuration space to be decomposed into regions that are homeomorphic to spheres of known dimensions, but does not indicate how these regions are attached to one other. Preliminary attaching maps are then found using the zero-temperature string method, resulting in a complete characterization of the topology of the configuration space of hard disk systems for small numbers of disks.

*O.B.E. and J.K.M. were supported by the National Science Foundation under Grant No.1839370.
The stability-limit conjecture revisited

PHEERAWICH CHITNELAWONG (Presenter), Queen's University, FRANCESCO SCIORTINO, Sapienza University of Rome, PETER POOLE, St. Francis Xavier University — The stability-limit conjecture (SLC) proposes that the liquid spinodal of water returns to positive pressure in the supercooled region, and that the apparent divergence of water’s thermodynamic response functions as temperature decreases are explained by the approach to this reentrant spinodal. Subsequently, it has been argued that the predictions of the SLC are inconsistent with general thermodynamic principles. Here we reconsider the thermodynamic viability of the SLC by examining a model equation of state for water first studied to clarify the relationship of the SLC to the proposed liquid-liquid phase transition in supercooled water. By demonstrating that a binodal may terminate on a spinodal at a point that is not a critical point, we show that the SLC is thermodynamically permissible in a system that has both a liquid-gas and a liquid-liquid phase transition. We also describe and clarify other unusual thermodynamic behavior that may arise in such a system, particularly that associated with the so-called “critical-point-free” scenario for a liquid-liquid phase transition, which may apply to the case of liquid Si.

NSERC Canada

Tuesday, March 3, 2020 2:30 PM - 5:06 PM

Session J26 DBIO DSOFT: Multimodal Optical Trapping/Microscopy/Spectroscopy of Living Matter 403 - Minjoung Kyoung, University of Maryland Baltimore County (UMBC) - Tag(s): Focus

Development and Application of Three-Dimensional Multi-Resolution Imaging* [Invited] HAW YANG (Presenter), Princeton University — A complex system contains dynamics that span several orders of time scales over several length scales that are spatially non-homogeneous. Examples include virus (or nanoscale drug delivery vehicle) uptake by a living cell and particle percolation through a dynamically reconfiguring medium. The spatial heterogeneity and the lack of separation of time scales are such that ensemble-averaged experimental approaches tend to miss the mechanism-defining steps in such processes. In this presentation, we explain how a multi-resolution approach helps to elucidate dynamics in complex systems. We then describe the basic ideas and implementations for these types of instrument. Applications to biological and materials systems will also be discussed.

The U.S. Department of Energy and the Princeton University Schmidt Transformative Technology Fund are grateful acknowledged for their financial support.
3:06PM J26.00002: Avalanching Upconverting Nanoparticles for Super Resolution Imaging*
EMMA XU (Presenter), CHANGHwan LEE, KAIYUAN YAO, Columbia University, BRUCE COHEN, EMORY CHAN, Lawrence Berkeley National Laboratory, YUNG DOUG SUH, Korea Research Institute of Chemical Technology, P. JAMES SCHUCK, Columbia University — Photon avalanche (PA) is a photon energy upconversion excitation mechanism. It enables nonlinear dependence on excitation power, which is a key factor for various applications in photon science. One exciting application is that it suggests a possible approach to super-resolution imaging with a simple confocal microscope system. Here, we introduce avalanching upconverting nanoparticles (AUCNPs), NaYF₄ nanocrystals doped with Thulium ions. The presence of PA was verified by time-resolved photoluminescence measurement. Upon the exitation of 1064nm laser, the resolution of 2-dimensional photoluminescence map was resolved to 90nm as a result of high nonlinearity, more than 4 times of diffraction-limited imaging resolution. AUCNPs are thus a promising new method for super resolution bioimaging.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship (NSF GRFP) under Grant No.DGE - 1644869. Portions of this research were supported by the Global Research Laboratory (GRL) Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (no. 2016911815).

3:18PM J26.00003: Mechanical unzipping of DNA molecules in parallel using nanophotonic tweezers
FAN YE (Presenter), JAMES T. INMAN, MICHELLE D. WANG, Physics, Cornell University / HHMI — Optical trapping is a valuable technique widely used in biological and materials sciences, covering size scales ranging from the single molecule to the cellular level, and force scales from sub piconewton (pN) to tens of pN. In the past decades, the rapid development of nano techniques has bolstered the emergence of nanophotonic tweezers. The ability of nanostructures to direct and confine light beyond the diffraction limit enables miniaturized, on-chip devices with abilities beyond microscope-based optical traps. Our lab has developed and implemented such an on-chip device - the nanophotonic standing-wave array trap (nSWAT) [1,2]. The nSWAT is based on Si or Si₃N₄ waveguides and allows for controlled and precise manipulation of trapped single biomolecule (such as DNA) arrays via microparticle handles. Here, we present an nSWAT that achieves manipulation forces large enough to mechanically unzip an array of DNA molecules at room temperature. This benchmark achievement is another step closer to the full realization of nanophotonic tweezers’ capabilities, promising increased accessibility and expansion of these platforms to a wide range of biological and biomedical research topics.

A Simple Approach to Optical Trapping Analysis*  
JAVIER E HASBUN, JAMES HOWARD, ZACHARY PATTERSON-GOSS, SUVRANTA KUMAR TRIPATHY (Presenter), Univ of West Georgia — Optical tweezers provide a noninvasive approach for detecting pico-newton forces with nanometer level spatial resolutions [1]. We have developed a simplified model of an optically trapped micron-sized particle using a modified version of a numerical approach [2]. The equations of motion associated with the model assume a low Reynolds number and the stochastically simulated bead behavior is carried out in two dimensions. The passive power spectrum analysis and equipartition theorem analysis confirm the agreement between simulated and experimental data. Based on the experimental and simulation analysis this simple approach can be used to gain information about bead's confining environment such as local temperature and viscosity.


Bacterial proteomes are predictable from cellular Raman spectra*  
KENICHIRO F KAMEI (Presenter), Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, KOSEKI J KOBAYASHI-KIRSCHVINK, Klarman Cell Observatory, Broad Institute of MIT and Harvard, HIDENORI NAKAOKA, YUICHI WAKAMOTO, Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo — Whole-cell Raman spectra reflect its molecular composition and allow us to distinguish cellular states in a label-free and non-destructive manner. Previously, we showed that in S. pombe and E. coli, cellular Raman spectra and transcriptomes were linked quantitatively and that the transcriptomes could be inferred from Raman spectra (Kobayashi-Kirschvink et al., Cell Systems, 2018). We now ask whether Raman spectra could also be connected to other types of omics information. Using quantitative proteome data of E. coli cultured under various conditions (Schmidt et al., Nature Biotechnology, 2016), we show that proteomes can be linked to and reconstructed from cellular Raman spectra. These results suggest that cellular Raman spectra have the potential to unravel and integrate multi-omic states of cells non-destructively, and therefore show great promise in establishing live-cell omics.

*JSPS KAKENHI Grant Number JP19J22448, JP15H05746
JST CREST Grant Number JPMJCR1927
3:54PM J26.00006: Live measurements of transcriptional bursting and dynamic gene regulation in early fly embryos*  
PO-TA CHEN (Presenter), BENJAMIN ZOLLER, MICHAL LEVO, THOMAS GREGOR, Princeton University — Gene regulation is intrinsically dynamic: from the microscopic molecular events underlying transcriptional bursting, to genes cross-regulating each other in the context of a genetic network during cellular fate specification. However, knowledge about the transcriptional dynamics of individual genes and the coordinated dynamics of multiple genes in their endogenous context is largely missing. We have developed an optimized 2-photon microscope to measure realtime gene activity in early fly embryos. Our data is highly quantitative making higher-order noise and cross-correlation analysis between multiple simultaneously measured genes possible. Focusing on the gap gene network, we measure endogenous transcriptional activity of individual and multiple genes simultaneously to test a novel time-dependent mathematical framework for transcriptional bursting dynamics and link these to transcriptional states at the network level. We are addressing two questions in particular: What are the dynamics of transcriptional bursting for individual genes, and how are they related to fluctuations of a key regulator? And how do the complex out-of-equilibrium dynamics of individual genes affect the dynamics of the gene regulatory network as a whole?

*Funding: NSF Center PHY–1734030, NIH R01 GM097275

4:06PM J26.00007: The Origin of Enhanced Enzyme Motility Probed with Optical Tweezers  
TIAN HUANG (Presenter), JIN TAE PARK, HYUK KYU PAK, STEVE GRANICK, Institute of Basic Sciences — Ingenious prior observations show that enzymes in solution display enhanced diffusivity when they catalyze chemical reactions but too little is known about the mechanism. A serious impediment to understanding is that the forces generated during enzyme catalysis are not known. In this talk, we will discuss our effort to measure these forces by using optical tweezers. The displacement probability distribution is enhanced as if the temperature were increased, but the reasons are different.

4:18PM J26.00008: Multimodal microscopy through optimal integration of wide-field and focused-beam laser illumination*  
SANG-HYUK LEE (Presenter), Physics and Astronomy, Rutgers University — Microscopy can be largely classified into two groups according to how light illuminates specimen: 'wide-field' or 'focused-beam' illumination microscopy. The two microscopy modalities are often integrated into the same instrument, especially for the purpose of combining optical tweezers and fluorescence imaging, with typically employing separate lasers for the two illumination schemes. We have developed a new microscope platform that enables operation of the same laser for the both modalities interchangeably or simultaneously in a way scalable to multiple lasers. In this talk, I will describe the design of the instrument and its application to the multimodal imaging and spectroscopy of biological systems.

*This research is supported by grants from DOE (DE-SC0019313) and NSF (1825433).
4:54PM J26.00009: Near-field optical interferometer for refractive index sensing*  ABBAS GHAFFARI (Presenter), KEVIN GIA DO, ROBERT RIEHN, North Carolina State University — Single-molecule sensing for biological physics predominantly uses fluorescence sensing due to the high signal to volume ratio. However, it is far from an ideal detection mode since fluorescence sensing requires the chemical modification of biological molecules. A better alternative is the sensing of refractive index changes due the introduction of a biomacromolecule. Here we introduce a near-field optical interferometer that detects the presence of nanoparticles and proteins by measuring the deflection of a light, and not transmission as commonly performed.

*We acknowledge funding from the National Institutes of Health (GM126887).

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J27 FIAP DMP GIMS: Experimental optical spectroscopic measurements of 2D materials 404 - Ying Wang, University of California, Berkeley

2:30PM J27.00001: Giant nonlinear optical modulation based on layered materials beyond EFISH  YING WANG (Presenter), JUN XIAO, SUI YANG, XIANG ZHANG, University of California, Berkeley — The efficient modulation of optical signals is central to communication and computing, the key in emerging data science revolution. Towards the realization of on-chip nonlinear optical applications such as on-demand nonlinear optical sources and neutral network, electrical-field-induced second harmonic generation (EFISH) dominates the development because of its ubiquitous presence in different material systems. However, its third order nature grinds itself to be a weak and inefficient process. A new mechanism that directly controlling second-order electric susceptibility to realize efficient nonlinear tunability is on demand. We report an electrically controlled new strategy to achieve giant and broadband modulation of second-order optical nonlinearities with an ultra-large modulation strength as well as efficiency. This demonstration will have a profound impact to optical communication and photonic computation.
2:42PM J27.00002: Probing the Influence of Dielectric Environment upon Volume-confined Hyperbolic phonon Polaritons  ALIREZA FALI (Presenter), University of Georgia, SAMUEL T WHITE, Department of Physics and Astronom, Vanderbilt University, THOMAS G FOLLAND, Department of Mechanical Engineering, Vanderbilt University,, NEDA AGHAMIRI, University of Georgia, JOSHUA D CALDWELL, Department of Mechanical Engineering, Vanderbilt University,, RICHARD F HAGLUND, Department of Physics and Astronom, Vanderbilt University, YOHANNES ABATE, University of Georgia — The unique ability of hyperbolic phonon polaritons (HPhPs) to confine long-wavelength light to nanoscale volumes in low-loss, naturally hyperbolic materials – such as hexagonal boron nitride (hBN) – has generated immense interest. We employ nano-scale imaging and spectroscopy techniques to elucidate the characteristics of HPhPs to elucidate polariton characteristics as a function of the complex refractive index of the substrate, including the impact of both the real and imaginary contributions. Although higher-order polariton modes exhibit wavelengths weakly sensitive to the environment, the principal mode strongly depends on the substrate dielectric constant. Furthermore, we demonstrate a reconfigurable hyperbolic metasurface comprised of a heterostructure of hBN in direct contact with the phase-change material (PCM) single-crystal vanadium dioxide (VO2). Metallic and dielectric domains in VO2 provide spatially localized changes in the local dielectric environment, enabling launching, reflection, and transmission of hyperbolic phonon polaritons (HPhPs) at the PCM domain boundaries, and tuning the wavelength of HPhPs propagating in hBN over these domains.

2:54PM J27.00003: Polarized Raman spectroscopy in monolayer ReSe2*  GEOVANI CARVALHO DE RESENDE (Presenter), Univ Fed de Minas Gerais, BRUNO CARVALHO, Física Teórica e Experimental, Universidade Federal do Rio Grande do Norte, MARCOS PIMENTA, Univ Fed de Minas Gerais — Raman spectroscopy is a powerful tool to study two-dimensional compounds and has been widely used to obtain important information of their electronic and vibrational structures. In the case of graphene and MoS2-type compounds, the Raman spectrum is isotropic when the light polarization lies in the layer plane. However, for low-symmetry materials such as black phosphorus and triclinic transition metal dichalcogenides, the spectra are polarized dependent and polarized Raman spectroscopy should be used. By changing the angle between the light polarization and the crystallographic axes, the elements of the Raman tensors for the different phonon modes can be determined. Previous studies in black phosphorus showed that Raman tensor elements are complex numbers, but the physical origin of the phase differences are not yet well understood. In this work, polarized Raman spectroscopy is used to investigate the anisotropic behavior in monolayer ReSe2. The angular dependence of the polarized Raman spectra using different polarization configurations is obtained for the 18 Raman active modes as well as the Raman tensor elements for each mode. It was also observed that the principal axes of those Raman tensors are not along the crystallographic axes.

*CNPq, CAPES, FAPEMIG and INCT-Nanocarbono.
JIAN MAO (Presenter), STEPHANE KENA-COHEN, Engineering Physics, Polytechnique Montreal — Black phosphorus (BP) emerges as a promising optoelectronic material because of its outstanding electrical and optical properties. [Proc. Natl. Acad. Sci. USA 2015, 112 (15), 4523-30.]. Like graphite, BP has a layered structure and can be exfoliated into nanosheets from its bulk form through mechanical and liquid exfoliation. Mechanical exfoliation (the scotch-tape method) has been predominantly used for proof-of-concept devices [Nat. Nanotechnol. 2014, 9 (5), 372-7], but it is inherently unscalable and typically produces BP sheets with lateral size below ten micrometers. For practical applications, scalable approaches for the fabrication of BP large-area films are essential. We will present our results on the development of a Langmuir-Blodgett (LB) protocol which is well suitable for assembling BP nanosheets into thin films. Through functionalization, we achieve large-area (centimeters), homogenous, and smooth BP thin films. With ZnO as an electron transport layer and 1,1-Bis[(di-4-tolylamino)phenyl]cyclohexane (TAPC) as a hole transport layer, the BP films are fabricated into photodiodes, which show responsivity from visible to infrared region. Our work highlights the great potential of BP for applications in near- and mid-infrared detection and imaging.

3:18PM J27.00005: Photocurrent Spectroscopy of Titanium Trisulfide Nanoflakes* ZHEN LIAN (Presenter), TIANMENG WANG, ZHIPENG LI, SUFEI SHI, Rensselaer Polytechnic Institute — Titanium trisulfide (TiS3) is an emerging 2D semiconductor which possesses a direct bandgap in the near-infrared regime, along with strong polarization-dependent electronic and optical properties, making it a promising material for various optoelectronic applications. However, constrained by the infrared response, it is challenging to characterize the bandstructure of TiS3 via optical spectroscopy, especially for devices based on thin layer TiS3, which often exist in the form of ribbon due to their quasi-1D atomic structure. In this work, we carry out low-temperature polarization-dependent photocurrent spectroscopy characterization of TiS3 ribbons. We clearly resolve the bandgap of TiS3 for both thick and thin flakes, and the results are consistent with the theoretical expectation. Our findings are crucial to the understanding of the electronic structure of TiS3 and lay the foundation for future device applications.

* This work is supported by the NY State Empire State Development's Division of Science, Technology and Innovation (NYSTAR) through Focus Center-NY–RPI Contract C150117.
3:30PM J27.00006: Substrate-Mediated Hyperbolic Phonon Polaritons in MoO$_3$  JEFFREY J. SCHWARTZ (Presenter), NIST & University of Maryland, SON LE, NIST & Theiss Research, SERGIY KRYLYUK, ALBERT DAVYDOV, ANDREA CENTRONE, NIST — Hyperbolic phonon polaritons (HPhPs) are hybrid excitations of light and coherent charge oscillations that exist in strongly optically anisotropic 2D materials (e.g., MoO$_3$). These polaritons propagate through the material's volume with long lifetimes, enabling novel mid-infrared nanophotonic applications by compressing light to sub-diffraction dimensions. Here, the dispersion relations and HPhP lifetimes (up to $\approx 2$ ps) in single-crystal $\alpha$-MoO$_3$ are determined by Fourier analysis of real-space, nanoscale-resolution polariton images obtained with the photothermal induced resonance (PTIR) technique. Measurements of MoO$_3$ crystals deposited on periodic gratings showed longer HPhP propagation lengths ($\approx 2 \times$) and lower optical compressions in suspended regions compared to regions in direct contact with the substrate. Additionally, PTIR data reveal polymeric contaminants, resulting from sample preparation, localized under parts of the MoO$_3$ crystals. This work enhances the ability to engineer nanophotonic devices by leveraging substrate morphology to control polariton propagation.

3:42PM J27.00007: Giant second harmonic generation from polar van der Waals Bismuth tellurohalide semiconductors  PRASHANT PADMANABHAN (Presenter), Center for Integrated Nanotechnologies, Los Alamos National Laboratory, SAMUEL GILINSKY, Department of Physics, Northern Arizona University, KEVIN KWOCK, Columbia Univ, NICHOLAS SIRICA, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, JAEGOOK KIM, SANG-WOOK CHEONG, Department of Physics, Rutgers University, ROHIT P PRASANKUMAR, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — Rashba materials from the Bismuth tellurohalide family of polar layered van der Waals (vdW) semiconductors hold great promise for nonlinear optical (NLO) applications, since their broken spatial inversion symmetry leads to a large second-order nonlinear optical polarizability, $\chi^{(2)}$. Here, we report the first second harmonic generation (SHG) studies of the bulk polar semiconductors BiTeBr and BiTeI. Our results reveal that BiTeBr, in particular, hosts a large SHG response, comparable to that of archetypal semiconductors and larger than other vdW materials. In contrast to BiTeBr, the response of BiTeI is substantially smaller, suggesting that their relative halide polarity plays a key role in the dramatically different nonlinear optical response. Furthermore, we compared our results to the nonlinear optical response of the Weyl semimetal TaAs, which has previously been shown to produce extremely large SHG, under identical conditions and observe that BiTeBr has nearly half the nonlinear conversion efficiency of TaAs, despite the absence of any known topological properties. This suggests that the BiTeX family of compounds, particularly the BiTeBr compound, are ideal candidates for NLO applications.
3:54PM J27.00008: Nanoscale imaging and spectroscopy of charge carrier distribution with terahertz and mid infrared near-field nanoscopy  NEDA AGHAMIRI (Presenter), University of Georgia, FLORIAN HUTH, ANDREAS J HUBER, neaspec GmbH, ALIREZA FALI, University of Georgia, RAINER HILLENBRAND, CIC nanoGUNE, YOHANNES ABATE, University of Georgia — We perform terahertz (THz) and mid infrared nanoscopy to probe and quantify charge carriers in doped semiconductor surfaces and doped Si nanowires at the nanoscale. We introduce hyperspectral THz nano-imaging by combining scattering-type scanning near-field optical microscopy (s-SNOM) with THz time-domain spectroscopy (TDS). We describe the technical implementations that enabled this achievement and demonstrate its performance. Combination of nanoscale spectroscopy and Drude model allows for measuring—noninvasively and without the need for Ohmic contacts—the local mobile carrier concentration of the differently doped semiconductor areas.

4:06PM J27.00009: Raman Studies on Polytypism in Layered Gallium Selenide  SOO YEON LIM (Presenter), JAE-UNG LEE, Physics, Sogang University, JUNG HWA KIM, Materials Science and Engineering, UNIST, LIANGBO LIANG, Xiangru Kong, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, THANH-HUONG THI NGUYEN, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, ZONGBHOON LEE, Materials Science and Engineering, UNIST, SUNGLAE CHO, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, HYEONSIK M CHEONG, Physics, Sogang University — Gallium selenide (GaSe) is one of layered group-III metal monochalcogenides, which has an indirect bandgap of 3.0 eV in monolayer and a direct bandgap of 2.0 eV in bulk phase unlike other conventional transition metal dichalcogenides (TMDs) such as MoX$_2$ and WX$_2$ (X=S and Se). Since GaSe has high photo-responsivity and external quantum efficiency (EQE) in the UV-range, it can be used as a photodevice such as a photodetector [1]. In bulk phase, four polytypes designated as $\beta$-, $\epsilon$-, $\gamma$-, and $\delta$-GaSe have been reported. Since different polytypes result in different optical and electrical properties even for the same thickness, identifying the polytype is essential in utilizing this material for various optoelectronic applications. We found different ultra-low-frequency Raman spectra of inter-layer vibrational modes even for the same thickness due to GaSe polytypism. By comparing the ultra-low-frequency Raman spectra with theoretical calculations and high-resolution electron microscopy measurements, we established the correlation between the ultra-low-frequency Raman spectra and the polytypes for trilayer GaSe. We further found that the AB-type stacking is more stable than the AA'-type stacking in GaSe.

4:18PM J27.00010: Ultrafast Carrier Recombination from Quantum Pillars in Black Silicon*  
SEREF KALEM (Presenter), Department of Electronics, Bahcesehir University — We report on ultrafast photoluminescence (PL) phenomena from black silicon produced by ion etching using chlorine plasma. An ultrafast blue PL component competing with non-radiative recombination at surface defects was quantified as originating from the no-phonon transition. This component involves two decay processes with a peak energy at 480 nm: a fast component of 6 ps followed by a component of 48 ps decay time constant. It exhibits also a slow component in the red spectral region with a time constant of about 2.5 ns. When it is oxidized, slow band at around 600 nm is enhanced in intensity to the detriment of blue emission band. This process results in a much slower states assuming 3-components exponential decay. Ultrafast PL decay leads to transfer of carriers to long-lived defect states as evidenced from red emission at around 2 eV. Time-correlated single photon counting revealed a life-time of about 5 ns for these states. The results are discussed in terms of electronic band structure modification at reduced sizes and surface point defects.

*This work was funded by European Commission LASERLAB-EUROPE program (LLC001765).

4:30PM J27.00011: Anisotropic optical and structural properties of hexagonal boron nitride epilayers probed by optical ellipsometry*  
MICHAEL MCKAY (Presenter), JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech Univ — Hexagonal boron nitride (h-BN) is a 2D layered material that has gained increasing attention in recent years due to its unique physical properties that make h-BN a promising material for DUV optoelectronics and solid-state neutron detectors. There are many material properties still uncertain, including h-BN's optical constants. The anisotropic index of refraction of h-BN free-standing epilayers grown by metal organic chemical vapor deposition were measured using spectroscopic ellipsometry in the UV spectral range. It was found that the index of refraction for $E_{\perp c}$-axis (ordinary) is much higher than $E_{\parallel c}$-axis (extraordinary). The scattered data for the index of refraction of h-BN reported earlier for various h-BN materials can be explained by including the inclination of turbostratic (t-) phase layers or the change of the c-plane orientation of individual layers. Our results show that ellipsometry can be used to characterize the crystalline quality of h-BN epilayers by determining the average inclined angle of t-phase layers within the sample while being non-invasive and highly sensitive.

*This research was supported by DOE ARPA-E (No. DEAR0000964). H. X. Jiang and J. Y. Lin are grateful to the AT&T Foundation for the support of Ed Whitacre and Linda Whitacre endowed chairs.
4:42PM J27.00012: Unraveling nonlinear formation and relaxation of excitons in atomically thin 2D semiconductors  MATTHEW STRASBOURG (Presenter), CORY JOHNS, Montana State University, Bozeman, THOMAS DARLINGTON, JIM SCHUCK, JAMES C HONE, Mechanical Engineering, Columbia University, NICHOLAS J BORYS, Montana State University, Bozeman — Transition metal dichalcogenide semiconductors are layered van der Walls materials that exhibit exceptional optoelectronic properties in monolayer form. Their atomically thin nature and reduced long-range dielectric screening make them ideal systems in which to study many-body electronic states. Here, the dynamics of several higher-order exciton states in monolayer-WSe$_2$ are probed using temperature-, energy-, and power-dependent time-resolved optical spectroscopy. These studies reveal a complex interplay between multiexciton states and single-exciton states in 2D materials that depends on both the density and excitation energy of the initial exciton population. In addition, the presence of defect-bound excitons is found to drastically alter the formation of multiexciton states. This competition between exciton trapping and multiexciton formation highlights the need for high-quality materials to enhance multiexciton physics. Understanding these formation and relaxation dynamics of the rich manifold of exciton states is critical for leveraging this new class of 2D semiconductors for advanced technologies.

4:54PM J27.00013: Dipole Orientation Shift of Ga$_2$Se$_2$ by Quantum Confinement* KE XIAO (Presenter), TENGFEI YAN, XIAODONG CUI, The University of Hong Kong — In the family of III-VI monochalcogenides M$_2$X$_2$ (M = Gallium, Indium; X = Sulfur, Selenide, etc), the interlayer interaction and the electronic band edges share the contribution of the same chalcogenide atomic orbits. This makes quantum confinement and interlayer interaction play a subtle role in 2 dimensional (2D) monochalcogenides crystals. In this report we study the direction-resolved photoluminescence of 2D Ga$_2$Se$_2$ at various thickness. We observe that the in-plane dipole radiation survives but out-of-plane dipole radiation fades at 2D limit.

*The work was supported by GRF17317316, CRF7036 of Hong Kong research council and Croucher Foundation.
**5:06PM J27.00014: Valley Phonons and Exciton Complexes in a Monolayer Semiconductor**
MINHAO HE (Presenter), PASQUAL RIVERA, University of Washington, DINH VAN TUAN, University of Rochester, NATHAN P WILSON, University of Washington, MIN YANG, University of Rochester, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, JIAQIANG YAN, DAVID MANDRUS, Oak Ridge National Laboratory, HONGYI YU, University of Hong Kong, HANAN DERY, University of Rochester, WANG YAO, University of Hong Kong, XIAODONG XU, University of Washington — The coupling between spin, charge, and lattice degrees of freedom plays an important role in a wide range of fundamental phenomena. Monolayer semiconducting transitional metal dichalcogenides have emerged as an outstanding platform for studying these coupling effects because they possess unique spin-valley locking physics for hosting rich excitonic species and the reduced screening for strong Coulomb interactions. Here, we report the observation of multiple valley phonons – phonons with momentum vectors pointing to the corners of the hexagonal Brillouin zone, in monolayer WSe$_2$. We find that these valley phonons lead to efficient intervalley scattering of quasi particles in both exciton formation and relaxation. This leads to a series of photoluminescence peaks as valley phonon replicas of dark trions, and the identification of intervalley exciton near charge neutrality.

**5:18PM J27.00015: Microcavity Organic Light Emitting Diodes with Higher Order Resonance Modes**
EKRAJ DAHAL (Presenter), BENJAMIN ISENHART, DAVID ALLEMEIER, Univ of Vermont, KAREN CIANCIULLI, Asheville School, MATTHEW WHITE, Univ of Vermont — Organic light emitting diodes (OLED) have a characteristic broad spectral width. The output emission characteristic of the light source can be controlled by the use of a microcavity. A microcavity OLED has metal electrodes encasing the organic layer which allow for the unique bandwidth narrowing and angle resolved spectral emission. We investigate the emission spectrum through the fundamental and higher order resonant modes using a single organic emitter molecule, just by designing the microcavity structure alone. We use Tris(8-hydroxyquinolinato)aluminium, Alq3, as the emissive layer (EML) with the electron transport layers (ETL) and hole transport layers (HTL) added in between the metal electrodes. The output characteristic (spectral bandwidth and viewing angle) of the microcavity is affected by its optical path length. The desired design is achieved by varying the thickness of the ETL, EML, and HTL layers which make up the microcavity. We generate the full visible spectrum at the forward emission and the angle resolved emission spectrum for various order resonance modes.

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**Tuesday, March 3, 2020 2:30 PM - 5:30 PM**

**Session J28 FIAP GDS: New Ways of Seeing with Data Science**

**2:30PM J28.00001: Data science and video games**
SPENCER STIRLING (Presenter), Activision — A video game is a microcosm combining tracking capabilities (movement, attack, defense, scoring), marketplace data (microtransactions), and social networking (chat, user-generated content, friend networks). We use machine learning to touch each of these facets, hoping to improve engagement, profitability, and fun! Projects include cheat detection, churn mitigation, marketing optimization, and toxicity detection.
3:06PM J28.00002: Modeling complex physical systems with big data and machine-learning
[Invited] HENDRIK HAMANN (Presenter), SIYUAN LU, IBM TJ Watson Research Center — Modeling complex physical systems continues to be a major challenge in many fields of science and technology. In this talk we present a general framework, which advances such endeavor. Specifically, we describe the development of a machine-learning based model blending architecture for statistically combining multiple models for improving the accuracy of an application-specific forecast or prediction. Most importantly, we demonstrate that in addition to parameters to be predicted or forecasted, including additional state parameters which collectively define a situation as machine learning input provides enhanced accuracy for the blended result. ANOVA (analysis of variance) shows that the error of individual models can have a substantial dependence on the situation. The machine-learning architecture effectively reduces such situation dependence error and thus produces more accurate results compared to conventional multi-model ensemble approaches based on simplistic equally or unequally weighted model averaging. The framework is first illustrated in the context of weather forecasting, which is arguably one of the hardest problems in physics, not only because of the complexity and scale of the problem but also given the additional complication that predictions/forecasts have to be made using limited observation at sparse locations. We will also demonstrate that the framework is applicable to other applications.

3:42PM J28.00003: Machine learning for seeing and hearing more [Invited] PATRICK F RILEY (Presenter), Google Accelerated Science, Google — Modern machine learning has had some of its greatest successes in perceptual problems like image and sound understanding. Extracting relevant information from such high dimensional input is frequently the challenge in scientific data understanding as well. I'll survey some exciting results from the Google Accelerated Science team in the areas of cellular imaging for biomedical research, extracting surprising results from human clinical imaging, and disease staging from auditory signals. Collectively these show the promise of further machine assistance in making sense of scientific data, with a great deal of exciting work still to come.
In this talk, I will discuss how SPM can be greatly enhanced via careful and tailored use of machine/statistical learning methodologies in every aspect, from data acquisition to real-time analytics to model comparison and selection. I will show that Gaussian process regression and active learning schemes can enable increases in sampling efficiency in large dimensional spaces, enabling new experiments that were previously unfeasible. Moreover, complete information acquisition in conjunction with statistical learning methodologies can enable new SPM techniques with enhanced spectral and spatial resolution that are orders of magnitude faster than existing state of the art techniques [2]. Finally, the use of Bayesian methodologies for model fitting and model selection can enable a rigorous uncertainty-quantified answer regarding the appropriate cantilever dynamics model to employ in analyzing dynamic atomic force microscopy data. These methods that are developed point towards an autonomous future of ‘self-exploring’ SPM systems for physics knowledge generation.

References

*This research was conducted at and supported by the Center for Nanophase Materials Sciences, which is a US DOE Office of Science User Facility.
**Immunotherapy Modeling: Molecular Interaction and Recognition of MHC/peptide/TCR Complexes** [Invited] RUHONG ZHOU (Presenter), IBM Thomas J. Watson Research Center — Cancer immunotherapy has been among the most promising breakthroughs in oncology, particularly in the case of immune check point inhibitors, however, the effective response rate remains quite low, only about 20-30%. In this talk, I will talk about our recent collaborative work which solves one mystery behind this low response rate with molecular modeling and machine learning techniques. We found that patients with certain HLA genotype (HLA-B44) have consistently higher survival rate, while patients with some other type (HLA-B15) have much poorer survival rates. It's also shown that patients harboring tumors with very high mutation rates responded disproportionately well to these immune checkpoint inhibitor treatments. Large scale molecular dynamics simulations further reveal that HLA-B15 proteins with poorer therapeutic outcomes had structural appendages (HLA bridges with residues Arg62, Ile66, and Leu163) that closed over the cancer neoantigens with much less flexibility. The same techniques have also been applied to the design and development of vaccines for HIV and T1D, which has been of great interest as well in recent years. With a combined in silico and in vivo approach, we studied the TCR/peptide/HLA interactions from multiple clonotypes specific for a well-defined HIV-1 epitope, and found that effective and ineffective clonotypes bind to the terminal portions of the peptide-HLA through similar salt bridges, but their hydrophobic side-chain packings can be very different, which accounts for the major part of the differences among these clonotypes. Meanwhile, a novel super potent autoantigen has been identified for T1D, which opens new door for potential T1D vaccine. Together with state-of-the-art free energy perturbation calculations for point mutations on antigens, our results clearly indicate a direct structural basis for heterogeneous T cell function.

Tuesday, March 3, 2020 2:30 PM - 4:54 PM

Session J29 DSOFT GSNP: Emergent Mechanics of Active, Robotic, and Living Materials II 501 - Corentin Coulais, Univ of Amsterdam - Tag(s): Focus

2:30PM J29.00001: Rectification of energy and motion in non-equilibrium parity violating metamaterials [Invited] ZHENGHAN LIAO, WILLIAM THOMAS MARK IRVINE, SURIYANARAYANAN VAIKUNTANATHAN (Presenter), University of Chicago — Uncovering new mechanisms for rectification of stochastic fluctuations has been a longstanding problem in non-equilibrium statistical mechanics. Here, using a model parity violating metamaterial that is allowed to interact with a bath of active energy consuming particles, we uncover new mechanisms for rectification of energy and motion. Our model active metamaterial can generate energy flows through an object in the absence of any temperature gradient. The nonreciprocal microscopic fluctuations responsible for generating the energy flows can further be used to power locomotion in, or exert forces on, a viscous fluid. Taken together, our analytical and numerical results elucidate how the geometry and inter-particle interactions of the parity violating material can couple with the non-equilibrium fluctuations of an active bath and enable rectification of energy and motion.
3:06PM J29.00002: Robotic swarms as adaptive active matter  WEERAPAT PITTAYAKANCHIT (Presenter), MARTIN FALK, JIAYI WU, ARVIND MURUGAN, HEINRICH M. JAEGER, University of Chicago — The field of active matter has been closely tied to swarming behaviors from its origins. However, a key feature of natural swarms, feedback regulation of activity in space and time, is usually absent in active matter models. Here, we study a model of active matter with adaptive activity inspired by recent experiments on mechanically coupled robotic swarms. We allow for self-propulsion to be modulated over space and time based on local stresses and strains and study how such self-regulated activity modifies transport and the jamming phase diagram.

3:18PM J29.00003: Rheology of Active Polymer-like T. Tubifex Worms  ANTOINE DEBLAIS (Presenter), SANDER WOUTERSEN, DANIEL BONN, Univ of Amsterdam — Of all complex fluids, it is probably the rheology of polymers we understand best. In-depth insight into the entanglement and reptation of individual polymers allows us to predict for instance the shear-thinning rheology and the behaviour in virtually any flow situation of practical importance. The situation is markedly different when we move from passive to active polymers where the coupling of filament activity, hydrodynamic interactions, and conformations open the way to a plethora of novel structural and dynamical features. Here we experimentally study the rheology of long, slender and entangled living worms (Tubifex tubifex) and propose this system as a new type of active polymer. Its level of activity can be controlled by changing the temperature or by adding small amounts of alcohol to make the worms temporarily inactive. This allow us to unlock existing experimental limitations and to unravel the recent fundamental questions on the mechanical and flow properties of such assembly.

* A.D acknowledges the funding from the European Union’s Horizon 2020 research and innovation program under the Individual Marie Sklodowska-Curie fellowship grant agreement number 798455.

3:30PM J29.00004: Collective Behavior of Worm Blobs  YASEMIN OZKAN-AYDIN (Presenter), DANIEL I GOLDMAN, SAAD BHAMLA, Georgia Inst of Tech — We study the aggregation of blackworms (Lumbriculus variegatus) into large ensembles of entangled, living “blobs” composed of thousands of slender bodies knotted together. To understand the mechanism and advantages of aggregation in these worm blobs, we systematically expose them to various environmental stresses including light and temperature. The diameter of the worm blob can be controlled by both light stimulus history and light intensity. At low light intensity, the blob dilates; conversely, increasing the light intensity contracts the blob and leads to a more entangled and tightly packed state. This behavior also affects the collective movement under thermal stress. Under high light intensity (>1500 Lux) we find that a 5 g (~600 hundred) worm blob placed under a linear temperature gradient between 15 to 50°C stays as a blob and moves collectively to the cold side with a speed of 0.35± 0.01 cm/min. In contrast, if the light intensity is reduced to 400 lux, the worm blob dissipates and individual worms crawl to the cold side with a speed of 0.21± 0.03 cm/min. We find that the number of surviving worms increases when they move as a blob.
3:42PM J29.00005: Predicting Crowd Dynamics Using Local Structure* JULIA GIANNINI (Presenter), ETHAN STANIFER, M. LISA MANNING, Syracuse University — Unstable and active disordered materials exhibit interesting collective properties and nontrivial dynamics. While the behavior of amorphous solids under shear is relatively well-understood, the instabilities in active systems remain difficult to characterize and predict. In the context of dense crowd dynamics, existing work has analyzed position fluctuations in a self-propelled particle (SPP) model to identify Goldstone modes and soft spots in models for human crowds. This analysis requires time-resolved trajectory information in order to form predictions for collective behavior, which can be cumbersome. To address this issue, we have developed a novel method to generate static packings in an artificial potential that reproduce the packing structures in a class of point-of-interest active SPP crowd simulations. These static packings then allow us to precisely identify local structural defects that govern dynamical group behavior, so that we can predict the locations of material-like failures in dense, active SPP models. Unlike previous methods, these predictions can be derived from a single snapshot and could be relevant to preventing dangerous emergent phenomena in real crowd systems.

*Simons Foundation MMLS grant #446222

3:54PM J29.00006: The dynamics of in-silico active filamentous elastic swimmers explored using Brownian dynamics simulations DENIZ AKPINAROGLU (Presenter), ARVIND GOPINATH, University of California, Merced — Slender elastic filaments when continuously deformed by active or actuating forces fields can move persistently. In filament-motor assays for instance, animating forces act directionally along the filament; forces thus follow the ensuing filament motion thereby driving and sustaining the deformation. Here, we study the spatiotemporal dynamics of a computationally minimal swimmer - an active elastic filament attached to a viscous cargo that can move in a plane. Locomotion is achieved via competition between activity, elasticity, dissipation and boundary constraints. Examination of the emergent phase space allows us to identify three distinct stable locomoting forms attained by the filament-cargo complex - straight, rotation, and oscillatory flutter. We show that transitions between these states may be triggered by ramping or dampening noise, by tuning global elasticity and by adjusting the type or softness of the connection between the cargo (head) and the filament (tail). Furthermore, these in-silico swimmers move as soft blobs with effective spatial extent primarily determined by a combination of activity and elasticity. Our results allow for a nuanced understanding of the patterns seen in assays and also offer rules that may guide the design of synthetic soft microswimmers.
**4:06PM J29.00007: Controlled reversal of vortex chirality in populations of colloidal rollers**

BO ZHANG (Presenter), ANDREY SOKOLOV, OLEKSIY SNEZHKO, Argonne Natl Lab — Chiral active liquids composed of spinning individual units represent a new class of active materials where both energy and angular momentum is injected at the microscopic level. Spontaneous emergence of particle flocks and global polar states are prime examples of remarkable collective dynamics and self-organization recently observed in active chiral liquids. Formation of the globally correlated polar states in such systems proceeds through an emergence of a macroscopic steadily rotating vortex that spontaneously selects a clockwise or counterclockwise global chiral state. We demonstrate in experiments and simulations that active chiral liquids in a collective vortex state exhibit memory and the subsequent formation of the polar states is not random. Our results provide new fundamental insights into mechanisms of formation of collective polar states in active systems.

*The research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

**4:18PM J29.00008: Mechanics of ultrasonically levitated active granular membranes**

MELODY LIM (Presenter), University of Chicago, ANTON SOUSLOV, University of Bath, VINCENZO VITELLI, HEINRICH M. JAEGER, University of Chicago — We explore granular rafts in an acoustic trap consisting of hundreds of macroscopic particles. These close-packed rafts are self-assembled by a sonic depletion force mediated by scattering, which establishes short-range attractions between the constituent particles [1,2]. We show that droplets of this granular fluid display emergent surface tension and elasticity. These droplets interact with the acoustic field, inducing forces and torques that drive coalescence, deformations, and break-up. We use a persistent torque in the acoustic field to extract the droplet surface tension. At the same time, active fluctuations in the acoustic field act as an effective temperature, driving the droplet to explore its configurational space. Microstructural measurements, and the fluctuation spectra of the droplet perimeter, reveal the far-from-equilibrium dynamics of this granular active membrane.

References:
4:30PM J29.00009: Impact of wall constraint on the dynamics of self-propelled particles*
RYOICHI YAMAMOTO (Presenter), FEDERICO FADDA, JOHN J. MOLINA, Kyoto Univ — The presence of wall constraint strongly affects the motions of dispersed particles in a fluid. A striking example can be seen in the dynamics of self-propelled particles near fluid/solid boundaries where the single (collective) motion of such particle(s) depend sensitively on the detailed flow profile around them. In the present study, we investigate the dynamics of two popular types of self-propelled particles, i.e., spherical micro-swimmers (squirmers) and rolling spheres (Quincke rollers) on a flat plate and by means of direct numerical simulation of fluid/particle composite systems with fully resolving the hydrodynamics.

*We acknowledge support by the Japan Society for the Promotion of Science (JSPS) KAKENHI Grants No.17H01083.

4:42PM J29.00010: Construction of non-equilibrium structures by insect aggregations: the case of fire ants  
ROBERT WAGNER (Presenter), TONG SHEN, FRANCK J VERNEREY, KRISTEN SUCH, ETHAN HOBBBS, University of Colorado, Boulder — Active matter networks are ubiquitous in nature and synthetic materials, ranging from molecular-scale polymers to macroscale swarms of social insects. These materials are characterized by their transient, reversible crosslinks and non-equilibrium state. Due to these reversible bonds and non-equilibrium states, active matter networks can exhibit directed viscous flow and morphogenesis. One such set of active matter networks is the aggregations formed by the bodies of red imported fire ant (Solenopsis invicta). These ants aggregate into floating rafts when placed in water, and will form steady-state, convective towers if given vertical rods around which to nucleate. In this presentation, we explore the mechanical rules individual fire ants follow on the surfaces of these towers by measuring their statistical velocity distribution, parking rates, and unparking rates, through imaging analysis. We then present and numerically employ a theoretical framework, that bridges these physical rules to the emergent behavior, to replicate the global morphologies observed. Thus, verifying that the postulated physical rules explain the global morphological response of this active matter system and generally informing our understanding of what drives these collective mechanical phenomena.

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J30 DSOFT GSNP DBIO: Composite Active Materials 502 - John Berezney, Brandeis Univ - Tag(s): Focus
2:30PM J30.00001: Comparison of different approaches to single particle tracking of enzymes displaying enhanced diffusion
MENGQI XU (Presenter), JENNIFER L ROSS, Physics, Syracuse University — Enzymes have been shown to perform faster diffusion with the presence of their substrate. Recently, we have revealed new insights of this emergent enzyme activity using single particle tracking (SPT). We found that while the overall mobility of enzyme is improved by 2-3 folds at saturated substrate concentration, the mode of diffusion remains Brownian. Meanwhile, in order to achieve long trajectories, a polymer brush coated surface and a large viscous polymer was utilized to slow down the diffusion, raising questions as to the effect of these additives. Here, we investigate the effect of the surface coating by replacing the polymer brush with a lipid bilayer; we also replace the crowding polymers with a smaller viscous molecule, glycerol. We make the same diffusion measurements and compare the results from both methods. We found a faster diffusion together with an artificial anomalous exponent for enzymes diffusing on lipid bilayer. Also, the presence of high percentage of glycerol, leads to the failure in reproducing enhanced diffusion due to the low enzymatic reaction rate in such a high viscous environment. Our results indicate the critical responsibility of the polymer brush in slowing the diffusion and enabling the direct reporting on single enzyme enhanced diffusion.

2:42PM J30.00002: Vortices, space-time braids and loops in the membrane of a living cell.
JINGHUI LIU (Presenter), PEARSON MILLER, Physics, Massachusetts Institute of Technology, JÖRN DUNKEL, Mathematics, Massachusetts Institute of Technology, NIKTA FAKHRI, Physics, Massachusetts Institute of Technology — Topological defects determine the structure and function of matter over a wide range of scales. Many advances have been made in understanding and controlling the defect dynamics in active and passive non-equilibrium fluids. Yet, it remains unknown whether the statistical laws which govern the dynamics of defects in classical or quantum fluids extend to active living matter. Here, we show a defect-mediated turbulence underlies the complex wave propagation patterns of Rho-GTP signaling proteins on the membrane of starfish oocytes. Our experiments reveal that the phase-velocity field extracted from Rho-GTP concentration patterns exhibits vortical defect motions and annihilation dynamics reminiscent of those seen in quantum systems. Space-time analyses of defect trajectories reveal the existence of two characteristic types of braids: loops braided by multiple pairwise creation and annihilation events, and long-lived defect pairs that wiggle and form braid groups. Several key statistics and scaling laws of the defect dynamics, braids and loops can be captured by a generic complex Landau-Ginzburg continuum theory, suggesting space-time braids and loops are useful topological measures for unraveling information scrambling and transmission in dissipative living systems.
2:54PM J30.00003: Creation and evolution of defects in composite biopolymer nematics
KIMBERLY WEIRICH (Presenter), RUI ZHANG, JUAN DE PABLO, University of Chicago — Structured soft materials have internal order that give rise to unusual mechanical properties and emergent organization of inclusions. Here we present a composite structured liquid formed from biopolymers of distinct rigidities, actin and DNA. Actin filaments, well below their persistence length, behave as rigid rods while long polymers of DNA, well above their persistence length, form globular molecules. Crowded into a thin layer, actin filaments form a nematic liquid crystal phase within the DNA domains. As these nematic phases grow and coalesce, defects in the actin nematic filled with DNA are created. We investigate the evolution of these soft, polymer filled defects and compare the dynamics to a continuum model of lyotropic liquid crystal. From the model, we use the defect shape to extract material properties of the liquid crystal. Our results suggest a novel structured soft composite, potentially informing physical mechanisms of controlling material properties and templating functional polymeric materials.

3:06PM J30.00004: Microtubule based composite active matter [Invited] ZVONIMIR DOGIC (Presenter), University of California, Santa Barbara — Active matter dynamics is determined by the balance between active stresses generated by the motile component, and the passive viscous or elastic stresses that arise due to deformation of the background material. In many current formulations of active matter Independent control of active and reactive stresses is not possible. For example, in microtubule-based 2D active nematics, decreasing ATP concentration simultaneously decreases the magnitude of the active stresses and increases the elasticity of the liquid crystalline materials. This limits the range of accessible dynamical states, while also impeding quantitative tests of theoretical models. Recent advances in formulation of microtubule based active matter has enabled dispersion of these motile elements in various passive soft materials including phase separated suspensions, viscoelastic networks and 3D colloidal liquid crystals. These new model systems of composite active matter exhibit diverse dynamical states that are not accessible in previous one components systems.
**3:42PM J30.00005: Information and motility exchange in collectives of active particles**

MATTEO PAOLUZZI (Presenter), CNR-ISC Inst for Complex Systems, MARCO LEONI, University Paris Sud, M CRISTINA MARCHETTI, University of California Santa Barbara — Active systems exploit the interplay of autonomous motility and mechanical interactions to spontaneously organize in complex patterns. In many situations, the collective behavior of active agents is driven by the exchange of information that can change the state of the agents. In a minimal model of information exchange, we have studied numerically run-and-tumble runners with an additional two-state internal variable that specifies their motile or nonmotile state. Motile particles change irreversibly into nonmotile ones upon collision with a nonmotile particle. Once turned non-motile, they can reacquire their motility or "reawaken" at a rate \( m \). When \( m=0 \), the system relaxes to an absorbing fractal aggregate of non-motile particles, with fractal dimension controlled by density and tumbling rate [1]. For finite reawakening, we find motile, non-motile and mixed states that can organize in complex spatial patterns. We characterize the kinetics of approach to the steady state and its structure in terms of tumbling and reawakening rates.


* MCM was supported by NSF grants DMR-1609208 and DMR-1938187.
MP was supported by Regione Lazio, Grant Prot. N. 85-2017-15257.

**3:54PM J30.00006: Corralling Active Brownian Particles With "Active Billiard" Particles**

ALEXANDRA NILLES (Presenter), Computer Science, University of Illinois at Urbana-Champaign, ANA PERVAN, THOMAS BERRUETA, TODD MURPHEY, Mechanical Engineering, Northwestern University — We examine the role of boundary conditions in a heterogenous active matter system in a bounded domain. The system consists of two types of particles: active Brownian particles, such as Janus particles, and "active billiard" particles, inspired by microorganisms that move in straight paths until they bounce off boundaries at a specific angle determined by their body morphology. This model has been of recent interest in robotics but also applies to microscale active matter systems. Here, we develop a parameterized model of particle type mixtures and characterize how "corralling" behavior emerges. We define corralling as system configurations where the billiard particles converge to a stable periodic orbit with a greater density of active Brownian particles within the convex hull of the orbit than its complement. We confirm that corralling behavior occurs in our model active matter system, in simulation. In previous work, we analytically determined the conditions guaranteeing such stable orbits, as a function of environment geometry and billiard departure angle. We will present extensions of this theoretical approach to statistical models of our example active matter system, with a focus on developing strategies for control.

* NSF 1328018, NSF DGE-1842165, ARO MURI #W911NF1910233
4:06PM J30.00007: Spontaneous demixing of mixed active-passive suspensions.  MARCO POLIN (Presenter), STEVEN WILLIAMS, Univ of Warwick, RAPHAËL JEANNERET, Ecole Normale Superieure Paris — Understanding the properties of active matter is currently driving a rapid growth in soft- and bio-physics. Some of the most important examples of active matter are at the microscale, and include active colloids and suspensions of microorganisms, both as a simple active fluid and as mixed suspensions of active and passive elements. In these systems, recent work has started to provide a window into new phenomena including activity-induced depletion interactions, phase separation, and the possibility to extract net work from active suspensions. Building on current research in our group exploring the physics of colloid-microswimmer interactions we are interested in understanding how external control of the dynamics of the active component can be used to alter the transport of passive cargo. Here we report on new experiments studying the behaviour of active-passive systems under spatial confinement. We show that the spatial inhomogeneity in swimmers’ distribution and orientation resulting from confinement has a dramatic effect on the spatial distribution of passive particles, with the colloids accumulating either towards the boundaries or towards the bulk of the sample depending on the size of the container. We show that this can be used to induce the system to de-mix spontaneously.

4:18PM J30.00008: Unifying descriptions of phase separation in multi-component driven, steady-state systems.*  GARRETT WATSON (Presenter), ERIK LUIJTEN, Northwestern University — Combined experimental and computational work has shown that a nonequilibrium driven system of Janus particles exhibits phase behavior that is accurately described by the standard Ising model. This suggests that certain steady-state, yet nonequilibrium systems may be described by thermodynamic equilibrium universality classes. Such a description would allow precise control over the phase behavior of active particles, enabling us to design the next generation of active materials analogous to the widespread application of phase separation in creating conventional materials. We examine the generality of this proposition by considering multi-component systems of composite active particles that may belong to other universality classes.

*NSF GFRP
4:30PM J30.00009: Phase Diagram of a 2D system of Granular Self-propelled Particles*
ZHEJUN SHEN (Presenter), NARAYANAN MENON, Univ of Mass - Amherst — We report experiments on the phase behaviour of granular squares as a function of number density and activity. The granular particles are energized by vibrating them on a horizontal plane and are designed to have polar activity along a body diagonal. The activity of particles (quantified by the persistence length of motion along the mobility direction) can be controlled by varying the gap between top cover and bottom base. We find that adding activity to the particles qualitatively modifies their phase diagram. At large enough activity, particles always migrate to the boundary and form a high-density ordered state. At smaller values of activity, different phases are seen as a function of density. At low density, the particles form an isotropic liquid. As the density is increased, particles separate into a high-density ordered region while the remaining particles remain in the fluid state. Above a finite density, the phase coexistence curve terminates and all particles freeze into an ordered state. The start and end density of the coexistence region is found to be a function of density. We also discuss dynamics within the dense, ordered state.

*Acknowledge NSF DMR1905698

4:42PM J30.00010: Irreversibility in biological active matter [Invited]  NIKTA FAKHRI (Presenter), Massachusetts Institute of Technology MIT — Cellular structures constantly consume and dissipate energy on a variety of spatiotemporal scales in order to function. While progress has been made in elucidating their organizing principles, much of their thermodynamics remains unknown. In this talk, I will address the question: why measure dissipation in such nonequilibrium systems? I will show that by measuring a multi-scale irreversibility (time-reversal asymmetry) one can extract model-independent estimates of the time-scales of energy dissipation based on time series data collected in an experimental biological system. I further demonstrate that the irreversibility measure maintains a monotonic relationship with the underlying biological nonequilibrium activity. The basic idea of estimating irreversibility for various levels of coarse-graining is quite general; we expect it to lead to important inferences whenever there is a well-defined notion of dissipative scale.

Tuesday, March 3, 2020 2:30 PM - 5:42 PM

Session J31 DSOFT: Workshop: Grand Challenges in Soft Matter and Opportunities for Microgravity Research 503 - Paul Chaikin, New York University - Tag(s): Focus
2:30PM J31.00001: Hot topics and lukewarm opportunities for soft matter science up in the sky* [Invited] ROBERTO PIAZZA (Presenter), Politecnico di Milano Univ — I will first discuss some topics in soft matter that truly deserve to be investigated in microgravity conditions, focusing in particular on spontaneous restructuring processes in colloidal gels, referring to our recent experience with the NASA ACE T10 mission too, and on thermal forces in complex fluids. I shall then present the new opportunities given by the ESA COLIS facility for optical correlation spectroscopy to be installed on the ISS in a couple of years. Finally, however, I shall also point out some limiting factors that tend to cool my enthusiasm towards space experiments in our field.

*PRIN Project ID 2017Z55KCW, “Soft Adaptive Networks” by the Italian Ministry for Education, University and Research
ESA Topical Team "Colloids in microgravity"

3:06PM J31.00002: Non-equilibrium behaviour of colloidal systems.* [Invited] DAAN FRENKEL (Presenter), Univ of Cambridge — There is an explosion of interest in the collective properties of active matter. This interest is understandable because it is exciting to step outside the confines of the classical statistical mechanics that was developed to describe systems at or near equilibrium.

However, many puzzles remain about the way in which active matter is propelled. In my talk, I shall discuss some of these problems and indicate how the study of colloidal systems in the presence or absence of gravity might help us gain a better understanding of the physical processes that drive active matter.

*This work was partially funded by the Horizon 2020 program through 766972-FET-OPEN-NANOPHLOW.
3:42PM J31.00003: Squeezing order out of disorder* [Invited] STEFANO MARTINIANI (Presenter), Chemical Engineering & Materials Science, University of Minnesota, BUMING GUO, Physics, New York University, YUVAL LEMBERG, Physics, Technion - IIT, PAUL M CHAIKIN, Physics, New York University, DOV LEVINE, Physics, Technion - IIT — Computable Information Density (CID), the ratio of the length of a losslessly compressed data file to that of the uncompressed file, is a measure of order and correlation in both equilibrium and nonequilibrium systems. I will show that correlation lengths can be obtained by decimation, thinning a configuration by sampling data at increasing intervals and recalculating the CID. When the sampling interval increases above the system's correlation length, correlations vanish and the data becomes incompressible. The correlation length critical exponents are thus accessible with no a-priori knowledge of an order parameter or even the nature of the ordering. The critical scalings for the length scales obtained by CID agree well with those from the decay of two-point correlation functions \( g_2(r) \) when they exist. But CID also reveals a correlation length with the right scaling when \( g_2(r) = 0 \), as we demonstrate by “cloaking” the data with a Rudin-Shapiro sequence. Finally, I will show how CID revealed previously unknown ordering phenomena, such as a cascade of phase transitions in the BML traffic model, and a "checkerboard" dynamical instability in the parallel update Manna sandpile model.

*This work was primarily supported by the National Science Foundation Physics of Living Systems Grant No. 1504867.

4:18PM J31.00004: ESA microgravity program for Soft Matter research MARCO BRAIBANTI (Presenter), European Space Agency — The International Space Station offers a unique environment to study Soft Matter systems, which are susceptible to the effect of gravity. For instance, gravitational stresses are known to influence the structure of colloidal crystals and gels and even the glass transition. Moreover, in microgravity the absence of drainage affects the stability of foams and emulsion stability and offer the possibility to study "wet" foams and low viscosity emulsions which cannot be stabilized on ground. Finally, granular matter quickly sediment under gravity. Under microgravity conditions the process of cooling (the loss of energy due to collisions between particles) can be studied disentangled by sedimentation.

For this purpose, the European Space Agency is developing non-conventional scattering methods like Depolarized Dynamic Light Scattering (DDLS), Time Resolved Correlation (TRC), Diffusing Wave Spectroscopy (DWS) and Shadowgraph that will be implemented in different experiments using different instruments. This will enable the systematic study of Soft Matter systems which covers the entire range of particle sizes from colloids to granular materials.
4:30PM J31.00005: Electric field driven aggregation of negatively and positively polarized particles in dilute suspensions* BORIS KHUSID (Presenter), QIAN LEI, EZINWA ELELE, Chemical and Materials Engineering, New Jersey Institute of Technology — A variety of colloidal structures observed in terrestrial experiments could also have been influenced by gravity effects (particle sedimentation, convection, etc.) It is often assumed that weightlessness simulated in a time-averaged sense by slowly rotating a specimen in a clinostat about an axis perpendicular to the gravity direction that is widely used in biological tests would reduce the effect of gravity on suspensions. Experiments on a non-buoyancy-matched suspension in flights in NASA Zero-gravity aircraft revealed that particle patterns formed in a clinostat and under normal gravity are actually similar. A requirement for matching densities between particles and a solvent severely limits possibilities to study the field-induced structuring in colloids in terrestrial experiments. Long-term microgravity in ISS offers unique opportunity to employ not density matched suspensions to explore a wide range of the mismatch of electric characteristics between particles and a solvent. We will report experimental data on the field driven structure formation in suspensions and present our approach to the development of ISS experiments. The aim is to understand mechanisms of structure formation and suggest novel routes for creating functional materials.

*NASA NNX13AQ53G, NSF1832260.

4:42PM J31.00006: Structure and dynamics of a two-dimensional colloid of liquid droplets* CHRISTOPH KLOPP (Presenter), Department of Nonlinear Physics, Otto von Guericke University Germany — Free-standing liquid crystal bubbles were prepared in microgravity on the International Space Station (ISS) in order to study the hydrodynamics of inclusions in quasi 2D fluid systems [1]. The layered structure in in of smectic A and C phases allows the preparation of thin and homogeneous films. Arrays of droplets of molten film material can be formed near the clearing point when the inner layers of the film melt and the film undergoes thinning transitions. The droplets interact repulsively with each other, they spontaneously forming nearly approximately regular triangular lattices in smectic A films, with short range positional order. Local lattice cell parameters depend on droplet sizes. These structures can be considered as genuine, two-dimensional (2D) colloidal crystals. We investigate the internal dynamics in these lattices [2]. The mobility of each droplet in its six-neighbor cage is determined by the ratio of cage and droplet sizes, rather than by the droplet size as in isolated droplets.


*This work was supported by DLR OASIS-Co 50WM1744, 50WM1430 and DFG Grant STA 425/40, by NASA Grant No. NNX-13AQ81G, and by NSF MRSEC Grants No. DMR-0820579 and DMR-1420736.
Anisotropic 2D colloids can show a plethora of liquid crystalline phases including nematic, columnar and smectic. Due to the ability to control the shape and forms, zirconium phosphate nanoplates have been utilized as a model system. We will discuss the challenges for controlling the size, shape and forms of 2D materials in general. We also present results on control of their self-assembly using external fields including shear, electromagnetic, optical, temperature gradient and gravity.

We acknowledge financially supported by NASA (NASA-NNX13AQ60G).

Model hard ellipsoids: the practical matter of producing them

Model hard colloids have a great deal of relevance to physics and in particular the study of their phase behavior which can mimic that of simple atomic liquids and solids. "Nearly hard colloidal sphere" suspensions were formulated 35 years ago by the Ottewill group (Univ. of Bristol) and Imperial Chemical Industries Ltd., which were used by Pusey and van Megen in their seminal study of the phase behavior of hard-sphere colloids. We report on our efforts to reproduce and refine this benchmark polymer colloid, including the recent synthesis of hard ellipsoids for random and ordered packing studies in microgravity*. The custom-made samples are composed of linear polymer chains of poly(methyl methacrylate), functionalized with photo-crosslinkable moieties and fluorescent molecules. The resulting ellipsoidal shapes are about 1 micron in size and stabilized with surface-grafted poly(12-hydroxystearic acid) chains. The particles are dispersed in a refractive index matching fluid and particle aspect ratios vary from 1 to 4.

* Launched March 2020 aboard SpaceX CRS-20 resupply service mission to the International Space Station.

*NASA NNX13AR67G (NYU); NSF GOALI 1832291 (NYU); NSF GOALI 1832260 (NJIT)
5:18PM J31.00009: Coarsening of two-dimensional island emulsions on smectic liquid crystal bubbles in microgravity*  CHEOL PARK (Presenter), ERIC MINOR, JOSEPH E MACLENNAN, MATTHEW GLASER, NOEL ANTHONY CLARK, Physics and Soft Materials Research Center, University of Colorado Boulder, CHRISTOPH KLOPP, TORSTEN TRITTEL, RALF STANNARIUS, Institute of Solid State Physics, Otto von Guericke University — Two-dimensional island emulsions in molecularly thin, tethered smectic liquid crystal bubbles in microgravity are observed to coarsen via coalescence and Ostwald ripening in both the smectic A and smectic C phases. We report here on the observed dynamics of island growth and disappearance in the absence of coalescence at locations in the island emulsion far from the meniscus around the bubble inflation needle. This Ostwald ripening occurs as a result of the system’s tendency to reduce its energy through a decrease in the total length of the island boundaries, a process that is generally dependent on the surface and line tensions and the disjoining pressure of the islands. Smaller islands generally have a higher disjoining pressure than their larger neighbors, which results in permeative flow from the smaller to the larger islands. We will also describe emulsion coarsening by island coalescence and compare the experimentally observed coarsening dynamics with simulations.

*Work supported by NASA Grant No. NNX-13AQ81G and by NSF MRSEC Grants No. DMR-0820579 and DMR-1420736. The German group was supported by DLR OASIS-Co 50WM1744, 50WM1430 and DFG Grant STA 425/40.

5:30PM J31.00010: Temperature-gradient-induced thermomigration in smectic liquid crystal bubbles and freely suspended films in microgravity*  NOEL ANTHONY CLARK (Presenter), CHEOL PARK, ERIC MINOR, JOSEPH E MACLENNAN, Physics and Soft Materials Research Center, University of Colorado Boulder, MATTHEW GLASER, TORSTEN TRITTEL, ALEXEY EREMIN, KIRSTEN HARTH, RALF STANNARIUS, Institute of Solid State Physics, Otto von Guericke University — In-plane temperature gradients were applied to tethered smectic bubbles on the ISS during the OASIS mission and to thin freely-suspended smectic films during suborbital rocket flights in order to study the Marangoni effect in a 2D fluid in microgravity. Tethered bubbles of smectic A liquid crystal were inflated in a temperature-controlled chamber. An emulsion of islands subsequently generated on the bubble with an air jet was initially homogeneously distributed over the entire bubble surface. When the inflation syringe was heated, however, the islands moved away from the point of heating, with the island velocity decreasing as they migrated away from the syringe. The islands appear to be moving with the background film, not as a direct consequence of the thermal gradient. In flat films, on the other hand, in-plane temperature gradients were observed to cause two specific Marangoni effects, directed flow and convection patterns.


*This work was supported by NASA Grant No. NNX-13AQ81G and by the Soft Materials Research Center under NSF MRSEC Grant No. DMR-1420736, and by DLR Grants OASIS-Co 50WM1430 and 50WM1744 and DFG Grant STA 425/40.
3:06PM J32.00002: Mobility Gradient of Polymer Chains near a Solid Interface* [Invited] KEIJI TANAKA (Presenter), HUNG K. NGUYEN, DAISUKE KAWAGUCHI, Kyushu Univ — Polymer composites have been widely used in a variety of engineering fields. The performance and functionality of the composites are closely related to the quality of the interface between polymer and filler. Thus, it is important to study polymer behavior at the filler interface. The local conformation of rubbery chains in direct contact with a quartz substrate was here examined by interface-sensitive sum-frequency generation (SFG) spectroscopy. SFG signals, which could be obtained from functional groups only oriented at the interface, were clearly observed for the rubber polymer in a film at room temperature which was much higher than the bulk glass transition temperature ($T_g$). When the film was thermally annealed, rubbery chains at the quartz interface changed their conformation to one with a lower energy state, accompanied by the randomization of both the main and side chain parts. The characteristic temperature, at which interfacial chains started to lose their orientations, was much higher than the bulk $T_g$. Also, the extent found to be more remarkable for the spin-coated film than for the solvent-cast one. This implies that the stress accumulated at the interface, which resulted from the centrifugal force during the spin-coating process, accelerates the mobility of chains there. Then, the relaxation dynamics of rubbery chains at the quartz interface were directly probed as a function of distance from the quartz surface using time-resolved evanescent wave-induced fluorescence anisotropy (TRFA), dielectric relaxation spectroscopy (DRS) and SFG spectroscopy. We found the presence of the dynamics gradient of chains in the interfacial region with the quartz surface. The segmental relaxation of chains in the strongly adsorbed layer at the interface could be slower than that of bulk chains by more than 10 orders.

*This research was partially supported by the JST-Mirai Program (JPMJMI18A2).
3:42PM J32.00003: Direct observation of mobility of thin polymer layers via asymmetric interdiffusion using neutron reflectivity measurements* KOJI FUKAO (Presenter), MEGUMI OOE, KAIRI MIYATA, JUN YOSHIOKA, Department of Physics, Ritsumeikan University, NORIFUMI L. YAMADA, KEK — In this study, we investigated the diffusion dynamics at the interface between deuterated poly(methyl methacrylate) (d-PMMA) and protonated PMMA (h-PMMA) in two-layered thin films of d- and h-PMMA layers via neutron reflectivity (NR) measurements during annealing above the glass transition temperature $T_g$. When $T_g$ of d-PMMA was higher than that of h-PMMA, the d-PMMA layer thickness increased with annealing time $t_a$, and simultaneously the h-PMMA layer thickness decreased. However, the opposite $t_a$ dependence of the layer thicknesses was observed, if the $T_g$ of d-PMMA was decreased. This change in the $t_a$ dependence of the layer thickness was related to the change in the mobility of the d-PMMA layer. With the decrease in the d-PMMA layer thickness when the h-PMMA layer thickness was maintained, the $t_a$ dependence of the layer thickness changed, and the mobility of the d-PMMA layer dramatically increased. Hence, the $T_g$ of the d-PMMA layer decreased with the decrease in the d-PMMA layer thickness. These results suggest that the mobility and $T_g$ of thin polymer films can be determined by interfacial dynamics via NR measurements.

*This work was in part supported by the Grant-in-Aid for Scientific Research (B) (No. 19H01865) and Exploratory Research (No. 18K18740) from the JSPS.

3:54PM J32.00004: Reconciling Computational and Experimental Trends in the Temperature Dependence of Interfacial Mobility in Polymer Films* JACK DOUGLAS (Presenter), WENGANG ZHANG, National Institute of Standards and Technology, FRANCIS STARR, Department of Physics, Wesleyan University — Many measurements have indicated that thin supported polymer films in their glass state exhibit an interfacial layer of enhanced mobility whose thickness grows upon heating, as found also in crystalline materials approaching their melting temperature $T_m$, while simulations and limited measurements of such films above their glass transition temperature $T_g$ instead exhibit a region of enhanced mobility whose thickness $\xi$ grows upon cooling. To better understand these contradictory trends, we performed MD simulations over a $T$ range over which our simulated polymer films enters a glassy state, and found that the relaxation time $\tau_\alpha$ within the film interior, relative to the polymer-air interfacial region, exhibits a maximum near the observed computational glass transition temperature, $T_{g,c}$, reconciling previous measurements and simulations of supported polymer films in their glass and liquid states. Correspondingly, we also observe that the interfacial mobility scale exhibits a maximum near $T_{g,c}$ but the scale of collective polymer segment exchange motion increases monotonically upon cooling below $T_{g,c}$ so that the interfacial mobility scale is no longer linked to the scale of collective motion in the non-equilibrium glass state.

*This work was supported in part by NIST award 70NANB15H282.
4:06PM J32.00005: Ellipsometry Modeling with Gradient in Refractive Index Resolves Unrealistic Density Increases in Thin Polymer Films and Demonstrates Inhomogeneous Film Structure Decoupled from Dynamics  YIXUAN HAN (Presenter), CONNIE ROTH, Emory University — We show polystyrene (PS), poly(methyl methacrylate) (PMMA), and poly(2-vinylpyridine) (P2VP) all exhibit similar large increases in refractive index with decreasing film thickness for ellipsometry data modeled by a homogeneous Cauchy layer. Such increases in refractive index have been interpreted by others recently as large increases in density (~25%) via the Lorentz-Lorenz relation, despite being physically unrealistic. We demonstrate that an ellipsometric layer model with a gradient in refractive index provides more physically realistic parameters for very thin films, retaining a bulk-like refractive index for much of the film’s interior, while exhibiting a sharp gradient in index near the free surface whose breadth grows from 4 to 9 nm with decreasing film thickness from 50 to 30 nm. Such an inhomogeneous film structure would invalidate the use of homogeneous Cauchy layers and the Lorentz-Lorenz relation whose derivation is based on assuming an isotropic distribution of dipoles. Surprisingly the refractive index gradient has an opposite trend to that based on a simple density correlation to dynamics. A higher refractive index near the free surface could reflect more optimized molecular packing from surface mobility, similar to vapor deposited stable molecular glasses.

4:18PM J32.00006: Density Measurements of Thin Polymeric Films using Magnetic Levitation*  SAMUEL ROOT (Presenter), RUI GAO, SHENCHENG GE, GEORGE M. WHITESIDES, Harvard University — When a polymeric film—supported by a sacrificial release layer—is placed in a paramagnetic solution between two magnets, it lifts off and levitates to a height that is linearly dependent upon the mass density. Using the principle of magnetic levitation, we construct a simple metrology for directly measuring the mass density of polymeric films down to 3 nm thick—an important quantity for understanding the glassy dynamics of such films. We validate the technique with several polymer films with a range of densities (1-1.4 g cm$^{-3}$) and by measuring density variations as a function of thickness in polystyrene and polymethylmethacrylate films. Our results are in agreement with existing data obtained by reflectometry experiments and confirm the trends previously observed in PS and PMMA, with important implications for understanding the dynamics of such glassy systems. Moreover, we demonstrate the potential utility of our technique for studying crystallization in ultrathin films of polymers using polyethylene as a model system. MagLev of thin polymeric films provides a simple, accessible metrology that will be useful for polymer scientists and engineers to study and optimize the properties of thin films for electronics, barriers, and separation membranes.

*Department of Energy
**4:30PM J32.00007: Polymeric Liquid Layer Densified by Surface Acoustic Wave**

TIANHAO HOU, JINGFA YANG, Institute of Chemistry, Chinese Academy of Sciences, WEN WANG, Institute of Acoustics, Chinese Academy of Sciences, JIANG ZHAO (Presenter), Institute of Chemistry, Chinese Academy of Sciences — With the application of surface acoustic wave (SAW) of 39.5 MHz to a model polymer liquid film, polyisobutylene, deposited on the solid substrates, the liquid film is densified, proved by the decrease of film thickness and the increase of refractive index, measured by ellipsometry. Rotational motion of fluorescent probes doped inside the liquid film, measured by polarization-resolved single molecule fluorescence microscopy, is retarded and the dynamical heterogeneity is reduced. It is demonstrated that the application of SAW of high frequency makes the thin polymeric liquid film densified and more dynamically homogeneous.

*This study is supported by National Natural Science Foundation of China (21774137).*

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**4:42PM J32.00008: Investigating molecular origins of mechanical stress during deformation of polymer glasses: in-situ birefringence measurements**

DA HUANG (Presenter), MASOUD RAZAVI, SHIQING WANG, Univ of Akron — In absence of microscopic experimental tools to investigate molecular deformation due to macroscopic deformation of glassy polymers, we monitor in real time the emergence of birefringence at different temperatures during ongoing uniaxial tensile deformation, stress relaxation and creep. By comparing the stress-optical behavior among PS, PMMA and bisphenol A PC where the optical anisotropy arises from either side group (PS) or backbone (PMMA and PC), we can learn about the intermolecular and intramolecular contributions to mechanical stress and obtain more insights into the stress-optical relationship identified in the mechanical deformation of these glassy polymers.

*This work is supported by NSF (DMR-1609977).*
**4:54PM J32.00009: Light-facilitated dewetting in amorphous selenium thin films**

AIXI ZHANG (Presenter), University of Pennsylvania, DANIXA RODRIGUEZ, Department of Chemistry, University Of Puerto Rico at Cayey, RICHARD B STEPHENS, ZAHRA FAKHRAAI, University of Pennsylvania

— Properties of glass thin films deviate from bulk for various materials, such as polymers, molecular glasses, and metallic glasses. When the film thickness is below a certain threshold, fast surface dynamics plays a strong role. Here, we study dewetting and glass transition temperature ($T_g$) of amorphous selenium (a-Se) thin films. A unique property of a-Se is that it forms random chain length and exhibits structural flexibility through bond breakage and formation of new bonds or over-coordinated sites upon above bandgap light irradiation. We investigate light-induced fluidity in a-Se and its effect on the length scale and the magnitude of enhancement in surface dynamics. Isothermal dewetting experiments are performed on a-Se films of different thicknesses below and above $T_g$. The hole-growth rate satisfies non-slip dewetting conditions. Thus, the growth velocity is directly related to the film's viscosity. Both the viscosity and activation energy in thin films are enhanced compared to the bulk. Films that start to deviate from bulk can be as thick as 100 nm, while this length scale turned out to be about 30 nm in most organic glasses. By applying various illumination condition, we study the relationship between the film structure and enhanced surface dynamics.

*NSF-MRSEC DMR-1720530*

**5:06PM J32.00010: Geometry-Dictated Wrinkle Patterns in Vapor-Deposited Thin Films on Liquid Substrates**

ROBERT ENRIGHT (Presenter), LAURA BRADLEY, Polymer Science and Engineering, Univ of Mass - Amherst

— Surface patterns and wrinkles in thin films are of fundamental and technological interest for their use in tuning morphological, mechanical, optical, and surface properties. Here, we use initiated chemical vapor deposition (iCVD) to generate polymer films with controlled wrinkle patterns and geometries. The iCVD technique is a solvent-free method to produce functional polymer coatings by free-radical polymerization of surface adsorbed monomers. Previously, iCVD has been used to produce parallel and herringbone wrinkles by deposition onto pre-strained elastomers and random wrinkles by deposition onto compliant amorphous substrates. We examine wrinkle formation in thin films on liquid substrates. The resulting wrinkle patterns are dictated by the topography and boundaries of the liquid surface pinned in micropost arrays with various post sizes, spacings, and shapes. Properties of the wrinkled films also depend on the iCVD deposition conditions. This presentation will demonstrate control of the wrinkle patterns and elucidate the mechanism of wrinkle formation in thin films grown on liquid surfaces.

*This work is supported by the National Science Foundation Graduate Research Fellowship under Grant No. 1451512.*
In situ Molecular Aggregation Structure Analyses on Glassy Polymers during Mechanical Deformation* KEN KOJIO (Presenter), AYA FUJIMOTO, TOMOKO KAJIWARA, CHAO-HUNG CHENG, SHIORI MASUDA, NATTANEE DECHNARONG, KENTO FUKADA, KAZUTAKA KAMITANI, ATSUSHI TAKAHA, Kyushu Univ — Poly (methyl methacrylate) (PMMA) and polycarbonate (PC) were chosen as a glassy polymer. Molecular aggregation structure and stretching properties of these glassy films were investigated by polarized high-speed camera observation and synchrotron X-ray wide-angle and small-angle scattering techniques during uniaxial and bulge deformation processes. 

$M_n$ of PC was 30k. $M_n$ of PMMAs were 70k and 1.2M. During both uniaxial and bulge deformation processes, PMMA-70k showed brittle nature, and PC and PMMA-1.2 M showed ductile property. In situ wide-angle X-ray scattering measurement revealed that increase in interchain distance during bulge deformation. Also, polarized high-speed camera observation revealed that PMMA-1.2M showed a wrinkle structure. This structure must be related to emergence of ductile property of PMMA-1.2M.

*This work was supported by the Impulsing Paradigm Change through Disruptive Technology (ImPACT) Program from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J33 DPOLY: Thermodynamics and Structures of Microstructured Polymers 505 - Sangwoo Lee, Rensselaer Polytechnic Institute - Tag(s): Focus

2:30PM J33.00001: BREAK —
3:06PM J33.00002: Packing Frustration in Block Copolymer Double Gyroids: Is it really all about the tubular domains?*  
ABHIRAM REDDY (Presenter), University of Massachusetts - Amherst, XUEYAN FENG, EDWIN THOMAS, Rice University, GREGORY GRASON, University of Massachusetts - Amherst — Understanding the molecular-scale mechanisms that lead to self-assembly of complex 3D morphologies remains an active area of research in soft matter systems. Block copolymers (BCPs) provide an exciting avenue to probe these mechanisms due to advancements in theory, synthesis and characterization tools. In this talk, we will revisit the thermodynamic connection between stability of triply-periodic network (TPN) phases, such as the Double Gyroid (DG), and packing frustration, or the variation in chain extension required by space filling constraint. We propose Medial Thickness (MT) analysis which provides a generic and practical measure of domain thickness of BCP morphologies of any arbitrary topology. Based on MT analysis of both theoretical models and experimental measurements of inter-block dividing surfaces of DG, we argue that previous measures of domain thickness severely overestimate both magnitude and dispersity of chain extension required to fill the tubular domains of TPN, belying the heuristic picture that their dominant thermodynamic costs arise from the stretching to reach the center of tubular interconnects. These insights also lead us to revisit longstanding question about absence of DG in the equilibrium phase diagram of strongly-segregated BCPs.

*DOE-BES(DE-SC0014599)

3:18PM J33.00003: Effects of Tacticity on the Formation of Bicontinuous Phases in Diblock Copolymers  
CHI TO LAI (Presenter), AN-CHANG SHI, McMaster Univ — The most prominent feature of block copolymers is their ability to self-assemble into ordered structures with periods typically on the scale of 10-100 nm. The symmetry of these ordered structures can depend on a number of factors, including block composition, strength of interactions, conformational asymmetry and tacticity. Tacticity is defined as the order of neighboring dangling groups along a polymer backbone, and influences many properties, ranging from thermal to rheological to conformational. In particular, block copolymers of the same composition with different tacticities could form different microphases. Recent experiments on stereoregular diblock copolymers have also observed the existence of the bicontinuous double-diamond phase, which is not found in neat atactic diblock copolymers. On the other hand, the effects of tacticity on self-assembly is yet to be completely understood. We develop a toy model to incorporate the effects of tacticity within the theoretical framework of self-consistent field theory. We then examine how the formation of bicontinuous phases in diblock copolymers is affected by the inclusion of tacticity effects.
3:30PM J33.00004: Cylindrical to Lamellar Microdomain Order to Order Transition upon Heating for Upper Critical Ordering Transition Block Copolymer* SEONGHYEON AHN (Presenter), YESEONG SEO, Department of Chemical Engineering, Pohang Univ of Sci & Tech, CHAO DUAN, LIXUN ZHANG, WEI-HUA LI, Department of Macromolecular Science, Fudan University, JINKON KIM, Department of Chemical Engineering, Pohang Univ of Sci & Tech — For block copolymers with upper critical ordering transition (UCOT) where $\chi$ decreases with increasing temperature, the sequence of order to order transition (OOT) upon heating of AB diblock and $A_1BA_2$ triblock copolymers with UCOT is as follows: lamellae to gyroids to cylinders to spheres before order to disorder transition. However, the opposite direction OOT is impossible in UCOT block copolymers.

Here, we investigated the OOT of polystyrene-block-polyisoprene-block-polystyrene-block-polyisoprene ($S_1I_1S_2I_2$) linear tetrablock copolymer. Very interestingly, this block copolymer showed cylindrical to lamellar microdomains transition upon heating. This behaviour is the exactly opposite to commonly observed OOT for linear AB diblock and $A_1BA_2$ triblock copolymers with upper critical ordering transition, where lamellar microdomains have been transformed to cylindrical microdomains upon heating. This interesting transition sequence is due to the chain architecture of linear tetrablock copolymer with two PS and two PI blocks.

*This work was supported by the National Creative Research Initiative Program, the National Research Foundation of Korea (2013R1A3A2042196), and the National Natural Science Foundation of China (Grants Nos 21574026 and 21774025).

3:42PM J33.00005: Unique self-assembly behaviors of ABCA tetrablock copolymer* QIONG XIE (Presenter), WEI-HUA LI, Department of Macromolecular Science, State Key Laboratory of Molecular Engineering of Polymers, Fudan University, Shanghai, China. — The self-assembly behavior of linear ABCA tetrablock copolymers is investigated using self-consistent field theory (SCFT). Although the general mechanism of block copolymer self-assembly has been well established, the self-assembly behaviors of some block copolymers are still hard to be understood and are even quite counterintuitive. Here we focus on the self-assembly of symmetric ABCA linear tetrablock copolymer. Our results indicate that the Janus-like superspherical phase can exist stably when the Flory-Huggins interaction between B and C blocks is much larger than the other two interactions. Moreover, a helical-Janus spherical phase is predicted to compete with the Janus phase. Meanwhile, the Janus-like supercylinder is predicted to be only metastable, and instead supercylinders composed of B/C-helices and B/C-stacked-disks are predicted to be stable. The stability of these novel structures is mainly dictated by the competition between the stretching energy and interfacial energy.

*This work was supported by the National Natural Science Foundation of China (NSFC) (Grants No. 21774025)
3:54PM J33.00006: Tuning Helical Structures via Designed Block Copolymer Systems*  
MEI-JIAO LIU (Presenter), Department of Chemistry, Zhejiang Sci-Tech University, Hangzhou, China, WEI-HUA LI, Department of Macromolecular Science, Fudan University, Shanghai, China — Block copolymers confined in nanopores provide unique achiral systems for the formation of helical structures. With AB diblock copolymers, stable single and double helical structures are observed. Aiming to obtain more different helical structures, we replace AB diblock copolymer with linear ABC triblock copolymers. We speculate that a core-shell superstructure is formed within the nanopore, which is composed of a C-core cylinder wrapped by B-helices within the A-shell. A number of helical structures with strands ranging from 1 to 5 are predicted by self-consistent field theory (SCFT), and in general, the number of strands decreases as the volume fraction of C-block increases in a given nanopore. More surprisingly, the variation of helical strand in the confined system is in an opposite trend to that in the bulk, which is mainly resulted by the constraint of the cylindrical confinement on the change of the curvature between the outer A-layer and the inner B/C-superdomain. Furthermore, adding C homopolymers to ABC triblock copolymers, the helical structures with more strands are predicted. Our work demonstrates a facile way to fabricate different helical superstructures.

*This work was supported by the National Natural Science Foundation of China (NSFC) (Grants No. 21704091)

4:06PM J33.00007: Miscibility Enhancement in Polyisoprene-Polyolefin Block Copolymers via Styrene Incorporation*  
SRAVYA JANGAREDDY (Presenter), RICHARD REGISTER, Princeton University — Polydienes like polyisoprene (PI) and polyolefins like hydrogenated mid-vinyl polybutadiene (hPB) generally show limited compatibility (high interaction energy density, X). Both the regular mixing model and the copolymer equation suggest that styrene units (S) should boost inter-block miscibility when incorporated in small amounts into hPB, up to 40 wt% S, via random copolymerization. Mixing thermodynamics in symmetric polydiene-polyolefin block-random copolymers composed of PI and a selectively saturated random copolymer of mid-vinyl polybutadiene and styrene (hSBR) were investigated via location of the order-disorder transition (ODT) temperatures. Block and “block-random” copolymers were prepared by anionic polymerization, followed by selective saturation of the butadiene units. ODT measurements show that X is 0.74 MPa at 0 wt% S, and exhibits the predicted parabolic variation with wt% S, with a minimum in X near 40 wt% S. Near the minimum, one-phase and two-phase blends of an hSBR with PIs of two different molecular weights, revealed that 0.10 < X < 0.16 MPa, indicating that the copolymer equation provides a better description of the mixing thermodynamics than the regular mixing model (for which X = 0 at the minimum).

*ExxonMobil Research and Engineering (EMRE)

4:18PM J33.00008: WITHDRAWN ABSTRACT
4:30PM J33.00009: Pattern Imprinted Polyacrylonitrile Thin Films Using an Ionic Liquid

CHUQING YUAN (Presenter), REBECCA BARRY, Department of Chemical and Biomolecular Engineering, Univ of Houston, KATHRYN BEERS, Materials Science & Engineering Division, National Institute of Standards & Technology, ALAMGIR KARIM, Department of Chemical and Biomolecular Engineering, Univ of Houston — Polyacrylonitrile (PAN)-based conductive graphitic microstructures have tremendous potential for a variety of applications such as patterned electrodes, and anisotropic conductive films in the electronics industry due to its high carbonization yield. However, because of the crystallinity and high melting point of pristine PAN, thin films are difficult to get patterned at routine temperatures and pressures via methods such as capillary force lithography (CFL), a straightforward lithographic technique. We demonstrate that adding ionic liquid (IL) can greatly improve the imprintability of PAN by decelerating the crystallization rate and providing the needed mobility at accessible temperatures for efficient mold filling. The effect of IL additives concentration, annealing temperature and hold time of patterned PDMS elastomer on the imprintability of PAN are well-correlated in a balancing act. The resulting patterned films demonstrate extraordinary IL removal ability at the end of the process, and thermal stability of final patterned structures, promising results on easy patterning route to create graphitic structures after carbonization for multitude of applications ranging from sensors to membranes.

*NSF-DMR 1905996
NSF-DMR 1659763

4:42PM J33.00010: Glass Transitions in PS-TiO\textsubscript{2} Nanocomposites

MIRCEA CHIPARA (Presenter), ELVIA CURIEL IZAGUIRRE, DORINA CHIPARA, MATAZ ALCOUTLABI, University of Texas Rio Grande Valley — Atactic polystyrene is considered a fully amorphous polymer. Homogeneous solutions of atactic polystyrene in chloroform were obtained by adding the two components and stirring the mixture for 4 hours. After homogenization, the polystyrene-chloroform solutions were moved in a larger beaker and sonicated for about 1 hour. Then, deionized water was suddenly added to the polymer solution, without interrupting the sonication process. The added volume of water was typical twice the volume of the polymer solution. The sonication was stopped after 15 minutes and the polymer was collected and then dried in an oven at 90°C, for about 12 h. Full water evaporation was confirmed by TGA. Nanocomposites of PS-TiO\textsubscript{2}, containing various amounts of TiO\textsubscript{2}, have been obtained by using this procedure. It was expected that the rapid collapse of the polymeric chain (as the nonsolvent was added) would trap the nanofiller within the polymeric matrix.

The as-obtained nanocomposites were investigated by using a TA Instruments Q 50 DSC at various heating and cooling cycles ranging between 5 °C/min to 30 °C/min. The research is focused on the effect of heating/cooling rates (ranging between 5 °C/min to 30°C/min) and of the concentration of TiO\textsubscript{2} on the glass transition temperature of PS-TiO\textsubscript{2} nanocomposites.
The pliable morphology of block copolymer crystals [Invited] EDWIN THOMAS (Presenter), XUEYAN FENG, Materials Science, Rice Univ, CHRISTOPHER BURKE, Polymer Science, University of Massachusetts, MUJIN ZHUO, HUA GUO, KAIQI YANG, AMANDA SUAREZ, WENPENG SHAN, Materials Science, Rice Univ, ABHIRAM REDDY, ISHAN PRASAD, Polymer Science, University of Massachusetts, RONG-MING HO, National Tsing Hua University, APOSTOLOS AVGEROPOULOS, Ioannina University, GREGORY GRASON, Polymer Science, University of Massachusetts — Block copolymers form soft crystals of ‘mesoatomic’ building blocks comprised of many thousands of molecules, whose sub-unit-cell configurations couple strongly to sub- and super-strate boundary conditions and symmetries. High-fidelity 3D tomographic structural information from both the near-surface as well as interior regions is key to understanding the properties of a given polymer structure. BCPs having a tubular network morphology are particularly attractive for applications ranging from photonic crystals to 3D batteries. Additionally, such complex 3D structures are quite sensitive to confinement by interfaces. We study the 3D domain morphology of a solution-cast block copolymer double gyroid. Analysis reveals that the morphology reconstructs in the near surface regions as well as with non-affine deformation of the sub-unit-cell symmetry in the interior region. Such strongly pliable morphological behavior has strong implications for properties, raising the question as to whether highly perfect cubic self assembled BCP structures are possible.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J34 DPOLY: Dillon Medal Symposium 506 - Richard Register, Princeton University

Structured Polymer Colloids by Flash NanoPrecipitation [Invited] RODNEY PRIESTLEY (Presenter), Princeton University — Colloids with internal and external structure have shown great promise in applications ranging from biosensors to optics to drug delivery, where the overall particle structure is paramount to performance. The growing demand for such nanomaterials motivates the development of a scalable processing platform for their production. Here, we demonstrate that Flash NanoPrecipitation (FNP), a rapid and inherently scalable colloid precipitation technology, can be used to prepare structured colloids from homopolymers, polymer mixtures and block copolymers. As revealed by a combination of experiments and simulations, by varying key process parameters and functional groups within the polymers, a range of structured colloids can be produced without any modification to the FNP process. Finally, in one application, we demonstrate how ionomer-based Janus colloids can be used to stabilize Pickering emulsions.
3:06PM J34.00002: Exploiting supramolecular associations in interpenetrating networks and elastomers* LASHANDA KORLEY (Presenter), University of Delaware — Supramolecular interactions may hold the key to the development of network systems with tunable mechanics and modulated architecture, such as observed in the muscle protein titin. It is the dynamic nature of these physical associations that we have exploited in the design of tough supramolecular materials that super-impose covalent and non-covalent interactions to tailor tensile response. We have developed supramolecular elastomers and interpenetrating network (IPN) systems that probe the interplay of non-covalent and covalent interactions in structural organization and mechanical response. By tailoring physical associations via control of self-assembly and composition, we have demonstrated enhanced supramolecular dynamics driven by architecture and toughness enhancements due to phase behavior. Recently, non-covalent interaction strength, network regularity, and chemoresponsiveness have been utilized as handles to derive gradient materials and to induce actuation behavior.

*This work was supported by the National Science Foundation (NSF, DMR 1608441; NSF, OISE 1844463).

3:18PM J34.00003: Droplet aggregates as model systems for connecting granular systems to continuum mechanics: how few is too few?* KARI DALNOKI-VERESS (Presenter), JEAN-CHRISTOPHE ONO-DIT-BIOT, JOHNATHAN HOGGARTH, McMaster Univ — In recent years we have developed a method to produce microscopic monodisperse oil droplets in an aqueous environment. With an attractive interaction between the droplets, monodisperse droplets form perfect crystalline aggregates, while a blend of small and large droplets allows us to prepare a disordered glass. By carefully tuning the adhesion forces between the droplets, the aggregates provide model systems for studying various physical phenomena that are not accessible by investigating molecular systems. Here I will provide a brief overview of experiments we have carried out to address two fundamental questions. How does a system transition from crystal to glass, when blending large and small droplets? And secondly, how does a system transition from a few particles, to many particles, where continuum models are valid. These experiments enable us to study the transition from few-to-many, and crystal-to-glass.

*Financial support was provided by the National Sciences and Engineering Research Council of Canada (NSERC).
3:30PM J34.00004: Evolution of polymer conformation during droplet-to-particle formation
JOAO CABRAL (Presenter), Imperial College London — Motivated by ubiquitous spray drying approaches in the manufacturing of polymer particles and composites, we experimentally investigate the mechanism and kinetics of particle formation by controlled solvent extraction and evaporation of polymer solution droplets. We employ microfluidics and acoustic levitation to precisely handle the polymer droplets in controlled environments. We then couple our experimental platforms with small angle neutron scattering (SANS) to elucidate chain conformation under equilibrium conditions and along the particle formation pathway, supplemented by optical and electron microscopies that characterise overall external and internal particle morphologies. We examine three model systems: two water-soluble polymers, poly(vinyl alcohol) and semi-flexible polyelectrolyte sodium carboxymethyl cellulose, and high-glass transition, semicrystalline poly(2, 6-diphenyl-p-phenylene oxide). We investigate the roles of composition (with respect to c* and c**), molecular mass, viscosity, and salt addition. Equipped with this knowledge, we then predictively design and fabricate polymer particles and capsules with prescribed dimensions, shape, porosity, microstructure and dissolution profile, and discuss complementarity with ‘flash nanoprecipitation’ methods.

3:42PM J34.00005: Gelation of Methylcellulose Chains Versus Methylcellulose Fibers
TIMOTHY LODGE (Presenter), SVETA MOROZOVA, S. PIRIL ERTEM, MCKENZIE COUGHLIN, FRANK S BATES, University of Minnesota — Upon heating in aqueous solutions, MC reversibly self-assembles into ~ 7-10 nm fibrils that percolate, resulting in physical gelation. We have chemically crosslinked both MC solutions at room temperature, and MC physical fibril gels at 80 °C, and compare the swelling and shear modulus properties. Hydroxyl moieties on MC were substituted with allyl groups, with a degree of substitution of about one pendant double bond per nine anhydroglucose repeat units. The allyl groups undergo crosslinking in the presence of a photo-initiator and UV light. Chemically crosslinking MC fibril gels at 80 °C results in opaque solid materials, and locks in the fibril structure, which persists even on cooling to room temperature. The shear modulus $G'$ increases modestly with temperature, and the volume fraction scaling is consistent with previous results for fibril gels. On the other hand, chemically crosslinking MC solutions at room temperature leads to clear, solid hydrogels which no longer form fibrils. Instead, swelling measurements show that the MC gels shrink by an order of magnitude when the temperature is increased from 25 °C to 80 °C. The equilibrium polymer volume fraction and $G_c$ are consistent with established theories for crosslinked polymer chains.

*NSF MRSEC Program, DMR-1420013

3:54PM J34.00006: Non-linear Deformation of Polymer Grafted Nanoparticles
RAMANAN KRISHNAMOORTI (Presenter), Chemical and Biomolecular Engineering, Univ of Houston — Linear viscoelastic properties of polymer grafted nanoparticles indicate that the systems behave like elastic solids with elastic moduli that scale with concentration of the nanoparticles and with the molecular weight of the polymer chains grafted to the particles. We studied the non-linear viscoelastic properties of such polymer grafted nanoparticle melts through a systematic examination of steady shear behavior and the recovery after cessation of flow. The local re-arrangement of particles and the formation of slip-planes and the regenearation of local order upon cessation of flow dominate the flow and recovery properties of these nanocomposites.
Harnessing nanoparticle vibrations to probe surface mobility and glass transition

EUNSOO KANG, BARTLOMIEJ GRACZYKOWSKI, GEORGE FYTAS (Presenter), Max Planck Institute for Polymer Research, KATELYN RANDAZZO, RODNEY PRIESTLEY, Princeton University — Advances in polymer nanoparticle synthesis and assembly techniques have enabled new applications, from drug delivery carriers to novel coatings. However, the polymer dynamics, especially at the particle surfaces of architected colloids, must be understood in order to realize their potential. Brillouin light spectroscopy as a direct probe of the particle surface mobility via nanoparticle vibrations, reveal the correlation between the glass transition behavior and surface dynamics and the presence of a low frequency mode extremely sensitive to particle-particle interactions. These are enabled by the surface mobility which can be engineered by different shell architecture layers. We demonstrate that a thin shell layer is able to eliminate the effect of enhanced particle surface mobility and drastically modify the structure of nanoparticle assembly. Surface mobility is strongly affected by the application of pressure modifies enabling a facile soldering of the colloidal film.

Non-Equilibrium Effects in Polymer Nanocomposites

SANAT KUMAR (Presenter), Columbia Univ — We have previously shown that the polymer nanocomposites, especially those that involve pure polymer-grafted nanoparticles, have a solid-like mechanical response with extraordinarily long relaxation times. In parallel with these efforts here we show that the structure and dynamics of these materials (and apparently for all nanocomposites) relax over similarly long times. The implications of these results for our understanding of this class of hybrid materials will be explored.

Programming surface energy driven Marangoni convection to pattern polymer films*

CHRISTOPHER ELLISON (Presenter), University of Minnesota — The Marangoni effect describes how fluid flows in response to gradients in surface energy. We recently developed a method for photochemically preprogramming surface energy patterns in glassy polystyrene (PS) thin films. Patterned UV irradiation through a mask selectively dehydrogenates PS, increasing surface energy in the UV exposed regions compared to the unexposed regions. After heating the film to the liquid state, transport of polymer occurs from regions of low surface energy to regions of high surface energy. This method can be harnessed to rapidly manufacture polymer films possessing prescribed three-dimensional topographies reflective of the original light exposure pattern without solvent washes or etching procedures. To better understand this phenomenon, a theoretical model will be presented that reveals the physics of this process, its limits and ways to apply it efficiently for various target metrics.


*We would like to acknowledge partial financial support from the National Science Foundation, grant# DMR-1053293.
4:42PM J34.00010: Influence of Pore Morphology on the Diffusion of Water in Triblock Copolymer Membranes

DIPAK ARYAL, MICHAEL P HOWARD, RITUPARNA SAMANTA, University of Texas at Austin, SEGOLENE ANTOINE, RACHEL A SEGALMAN, University of California at Santa Barbara, THOMAS TRUSKETT, VENKATRAGHAVAN GANESAN (Presenter), University of Texas at Austin — Understanding the transport properties of water in self-assembled block copolymer morphologies is important for furthering the use of such materials as water-purifying membranes. In this study, we used coarse-grained dissipative-particle-dynamics (DPD) simulations to clarify the influence of pore morphology on the self-diffusion of water in linear-triblock-copolymer membranes. We considered representative lamellar, cylindrical, and gyroid morphologies and present results for both the global and local diffusivities, as well as the structural characteristics of water in the pores. Our results suggest that the diffusivity of water in the confined, polymer-coated pores differs from that in the unconfined bulk. Explicitly, in confinement, the mobility of water is reduced by the hydrodynamic friction arising from the hydrophilic blocks coating the pore walls. We demonstrate that in lamella and cylindrical morphologies, the latter effects can be rendered as a universal function of the pore size relative to the brush height of the hydrophilic blocks.

*Center for Materials for Water and Energy Systems, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0019272.

4:54PM J34.00011: Enhanced Conductivity via Homopolymer-Rich Pathways in Block Polymer Composite Electrolytes

THOMAS EPPS (Presenter), MELODY A MORRIS, Univ of Delaware — The BP electrolyte polystyrene-block-poly(oligo-oxyethylene methacrylate) [PS-b-POEM] was blended with POEM homopolymers of varying molecular weights to explore the impact of polymer additives on ion conductivity. The incorporation of a higher molecular weight homopolymer additive promoted a ‘dry brush-like’ homopolymer distribution within the BP self-assembly and led to higher lithium salt concentrations in the more mobile homopolymer-rich region, increasing overall ionic conductivity relative to the ‘wet brush-like’ and unblended composites. Furthermore, using $^7$Li solid-state nuclear magnetic resonance spectroscopy, we found a temperature corresponding to a transition in lithium mobility ($T_{Li\ mobility}$) that was a function of blend-type. $T_{Li\ mobility}$ was found to be 39 °C above $T_g$ in all cases. Interestingly, the ionic conductivity of the blended BPs was highest in the ‘dry brush-like’ composites even though these composites had higher $T_g$s than the ‘wet brush-like’ composites, suggesting that homopolymer-rich conducting pathways formed in the ‘dry brush-like’ assemblies had a larger influence on conductivity than the greater lithium ion mobility in the ‘wet brush-like’ blends.

*Department of Energy, Basic Energy Sciences
5:06PM J34.00012: Comparison of macroscopic and microscopic measurements of segmental dynamics in aging polymer glasses

MARK EDIGER (Presenter), JOSH RICCI, TREVOR BENNIN, ENRAN XING, University of Wisconsin - Madison — Optical probe reorientation experiments and mechanical stress relaxation measurements in the linear response regime were performed during aging of glasses of poly(methyl methacrylate) (PMMA) and poly(D,L-lactide) (PLA). For each polymer, across all aging times and temperatures, an excellent correlation is observed between the relaxation times for mechanical and optical experiments with the two observables showing a power law relationship with an exponent near one. For PMMA, relaxation times for the two observables in crosslinked and uncrosslinked materials follow the same correlation. The probe reorientation method has previously been utilized to track changes in segmental dynamics during nonlinear deformations. Our new experiments validate the conclusion that probe reorientation is a good reporter of segmental dynamics in the glass, in the linear response regime. The strong agreement between macroscopic and microscopic measurements of mobility in the aging polymer glasses contrasts to recent work on colloidal and metallic glasses.

*Supported by NSF DMR 1708248

5:18PM J34.00013: Confinement Effects on Dye Diffusivity in Polymer Films Depend on Polymer Molecular Weight: Relation to Fragility-Confinement Effects

JOHN TORKELSON (Presenter), TONG WEI, TIAN LAN, Northwestern University — We studied the translational diffusivity of 9,10-bis(phenylethynyl)anthracene ($D_{dye}$) in supported, polystyrene (PS) films. Relative to bulk films and near $T_g$, $D_{dye}$ is reduced by 80 - 90% in 100-nm-thick, high molecular weight (MW) PS (400 kg/mol) films. These results are associated with fragility-confinement effects, with fragility decreasing in films with decreasing thickness below ~ 200 nm. Fragility reflects the breadth of the cooperative segmental relaxation distribution: that breadth narrows with confinement. The thickness dependence of $D_{dye}$ reflects the time scales associated with the fast relaxation tail of that distribution. At thickness below ~200 nm, the distribution narrows, with the shortest relaxation times shifting to longer times, leading to a reduction in $D_{dye}$. We also studied $D_{dye}$ in low MW PS (6 kg/mol). Because 6 kg/mol PS exhibits much lower bulk fragility than high MW PS, confinement has a much-reduced effect on low MW PS fragility: both fragility and $D_{dye}$ in 100-nm-thick low MW PS films are unchanged from bulk. Thus, for thicknesses where fragility-confinement effects are observed (high MW PS), $D_{dye}$ also exhibits confinement effects. By suppressing fragility-confinement effects by using very low MW PS, confinement effects on $D_{dye}$ are also suppressed.

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J35 GMED: Physics of Medical Imaging, Measurement, and Tissue Characterization 110 - Wojciech Zbijewski, Johns Hopkins University
2:30PM J35.00001: Imaging the brain across scales using light, magnetic fields, and models*

MICHÈLE DESJARDINS (Presenter), Univ of Laval — Functional Magnetic Resonance Imaging (fMRI) is a powerful tool to map brain activity non-invasively and is the foundation of tens of thousands of published neuroscience studies. However, fMRI does not measure neurons directly. Instead, in the most common form of fMRI called Blood Oxygen Level Dependent (BOLD), changes in the concentration of paramagnetic deoxyhemoglobin in the blood are detected. Although BOLD is correlated with neural activity, its interpretation in healthy and diseased brain remains limited. Animal models provide invaluable insight for studying the cellular origin of fMRI. In mice, state-of-the-art optical technologies have been developed to probe neuronal activity, blood flow and oxygenation while manipulating cell-type-specific neuronal activity.

A framework for imaging the brain of awake behaving mice across scales, from two-photon microscopy at the micrometer scale to macroscopic fMRI, will be demonstrated. High-resolution 3D images of cerebral vasculature measured in mice can be graphed into a connected network to model blood circulation and oxygen diffusion. In this model, the physics of magnetic resonance are leveraged to predict human brain imaging signals. Applications in neuroscience and fundamental cancer research will be discussed.

*NSERC; FRQNT.

2:42PM J35.00002: Calculation of carbon-ion beam's range in different media used for radiation therapy

PANAGIOTA GALANAKOU (Presenter), THEODORA LEVENTOURI, WAZIR MUHAMMAD, Florida Atlantic University — Carbon-ion radiotherapy (CIRT) is a new radiation modality with significant physical and biological advantages over photon irradiation. Range assessment is a major challenge and it is considered the key for using the full potential of carbon ion therapies. The purpose of this research is to develop a novel and practical method for monitoring accurately the carbon ion range in different types of tissue during treatment. The proposed method is based on the Doppler Shift Effect of Prompt Gammas (PGs), which give real-time information due to the instantaneous nuclear de-excitation, and thus PG shifted energy can quantify the mean carbon energy with respect to PG spectrum, and then the predicted range can be calibrated. We develop a mathematical model with initial carbon ion energies within the range of 100MeV/u-450 MeV/u for different detection angles of 0°-90°, and different target materials including water, air, and soft tissue. The results of our calculations are verified by Monte Carlo simulations.
2:54PM J35.00003: MRI Mapping of Heat Dissipation from Polydopamine Particles under Infra-Red Irradiation  JANUSZ HANKIEWICZ, JOHN STROUD, ZBIGNIEW J CELINSKI, BioFrontiers, University of Colorado, Colorado Springs, YURIY GARBOVSKIY, Physics, Connecticut State Colleges & Universities, AIMING LU, KRZYSZTOF GORNY, DAVID WOODRUM, Radiology, Mayo Clinic College of Medicine, STEFAN JURGA, KOSMA SZUTKOWSKI, RADOSLAW MROWCZYNSKI (Presenter), NanoBioMedical Center, Adam Mickiewicz University — Polydopamine (PDA) is a new nanomaterial with promising properties for photothermal therapies. We investigated heating of phantoms made of agar gel with different concentrations (from 1 to 200 mg/ml) of PDA 100 nm particles. Spectrophotometry measurements show significant absorption in near-infrared range with increases below 300 nm. The laser beam (808 nm, 5W) was guided through a fiberglass guide and dispersed by a diffuser. A 25 ml phantom was placed in styrofoam thermal insulation. The temperature of the phantom after 5 minutes of continuous laser irradiation increased dramatically for concentrations above 100 mg/ml. For concentration of 200 mg/ml, an increase of 41 ºC was achieved, about 14 times higher than for the control pure agar gel. Larger phantoms were studied in MRI settings to obtain heat dissipation maps, i.e. relative change of temperature in the phantom volume for different laser irradiation time and power. Temperature maps were obtained by analyzing the phase change due to proton resonance frequency shift (PRF). PRF results were compared to measurements using four miniature MRI compatible temperature sensors. Results allowed us to determine thermal gradients produced by single point heating which may be useful in MRI guided laser ablations of cancers.

3:06PM J35.00004: Multi-Regularization Reconstruction of One-Dimensional $T_2$ Distributions in Magnetic Resonance Relaxometry*  CHUAN BI, National Institutes of Health - NIH, YVONNE M. OU, Mathematical Sciences, University of Delaware, WENSHU QIAN, YOU ZHUO, RICHARD SPENCER (Presenter), National Institutes of Health - NIH — Measurements of $T_2$ relaxation time distributions in magnetic resonance relaxometry are increasingly used to probe microstructural details of materials or tissues. However, extracting the model from the acquired data is a severely ill-conditioned problem. Tikhonov regularization and related methods are widely used to address this. Methods such as the L-curve and generalized cross-validation (GCV) select a single regularizer to obtain an optimal approximation to the underlying distribution. However, this procedure does not make use of the information content of the non-selected regularized results; given the lack of definitive criteria for regularization parameter selection, this represents a potential loss of substantial information. In contrast, we propose a new reconstruction method, Multi-Reg, incorporating a range of calculated regularized solutions. Multi-Reg is based on a dictionary of noise-corrupted regularized reconstructions of distribution basis functions. We demonstrate that Multi-Reg can out-perform the L-curve or GCV methods in simulation analyses of Gaussian distribution components, and present experimental results on mouse spinal cord and human muscle tissue.

*Supported by the Intramural Research Program, National Institute on Aging, National Institutes of Health.
3:18PM J35.00005: Hidden Dangers in MRI: Investigating Heating of Metallic Objects from Switching Gradient Fields*  JOHN STROUD (Presenter), University of Colorado, Colorado Springs, KARL STUPIC, NIST, TUCKER WALSH, TIM READ, ZBIGNIEW J CELINSKI, JANUSZ HANKIEWICZ, University of Colorado, Colorado Springs — With the number of medical implants increasing every year it is inevitable that some patients with implants will at some time undergo an MRI procedure. Investigating the safety of implants during an MRI scan is vital as with current medical record keeping it can be difficult to track implants, which may put patients in possible danger. It is known in MRI oscillating magnetic fields produced by an MRI scanner have the potential to induce eddy currents in metallic implants in turn these eddy currents can heat surrounding tissue and may potentially cause damage to healthy tissue. However, much of the research evaluating the safety risks that are associated with imaging around metallic implants has focused mainly on the magnetic component of RF radiation present in the MRI scanner, and not much attention has been paid to switching gradient fields in MRI which oscillate at much lower frequencies. We investigate local heating of conductive materials within an MRI scanner producing quantitative data on the position dependence of induced EMF and heating, as well as the interaction between different gradients within the scanner. This work will assist in evaluating any dangers that may be present to patients with a metallic implants.

*Funded by the Undergraduate Research Academy at UCCS

3:30PM J35.00006: Superparamagnetic particles as MRI temperature contrast agent JANUSZ HANKIEWICZ (Presenter), JOHN STROUD, BioFrontiers, University of Colorado, Colorado Springs, STEPHEN RUSSEK, National Institute of Standards and Technology Boulder, KAREN LIVESEY, CASEY CHALIFOUR, Physics, University Colorado Colorado Springs, GIACOMO PARIGI, Magnetic Resonance Center, University of Florence, Italy, ZBIGNIEW J CELINSKI, ROBERT CAMLEY, BioFrontiers, University of Colorado, Colorado Springs, DOROTA LACHOWICZ, ANGELIKA KMITA, MARTA GAJEWSKA, ELA TRYNKIEWICZ, ROMA WIRECKA, MAREK PRZYBYLSKI, Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology, Krakow, Poland — A method of MRI temperature contrast developed by our group, which employs temperature dependent local field inhomogeneities due to a presence of micrometer sized magnetic particles and corresponding changes in image intensity (T2* contrast), faces limitations due to particle size. For human applications, large particles cannot be used as they face problems with delivery and secretion. Smaller particles are required. However, spin transverse relaxation process for such particles is no longer governed by a static dephasing regime and T2* temperature dependent inhomogeneity contributions vanish due to averaging by spin motion. We hypothesize that superparamagnetic particles may provide contrast mechanisms only if nuclear relaxation is temperature dependent. To test this hypothesis, we used Mn-Zn ferrite superparamagnetic particles with an average size of 7.8 ± 2.1 nm. Particles with a 2 mM concentration were embeded in agar gel for NMR and MRI measurements at temperature 5 - 50 °C. At 3.0 T, NMR results show that T1 is temperature independent, while observed NMR linewidth drops from 130 Hz to 70 Hz and T2 increases from 1.3 ms to 2.8 ms. Intensity of T2 weighted MR images depends linearly on temperature, providing the contrasting mechanism necessary for temperature determination.
3:42PM J35.00007: Modeling of human body tissue compositions for Monte Carlo algorithm of Proton therapy dose computation with the Single Energy Computed Tomography Calibration Curve  MARYAM GHASEMI GHONCHEHNAZI (Presenter), Florida Atlantic University, GRANT EVANS, CHARLES SHANG, South Florida Proton Therapy Institute — Proton dose computation with most planning systems rely on single energy computed tomography (CT) images in which the relative proton stopping-power ratio (SPR), mass density and the relative electron density are derived from CT Hounsfield units (HU). Using a proton Monte Carlo dose calculation algorithm in treatment planning system (TPS), a CT number of each pixel in patient CT image is converted to mass density; then the proton stopping power ratio is computed. The accuracy of proton dose computation in Monte Carlo algorithm relies on conversion from HU to mass density. We explore the potential improvement in determining mass density to reduce the uncertainty in predicting the proton range in patients. The Stoichiometric method is used to calculate the CT scanner specific parameters related to the photoelectric effect, coherent scattering, and Compton interactions, in order to model the CT number of human body tissue compositions. In the stoichiometric calibration curve, elemental compositions and densities of 34 “standard” human biological tissues have been taken from the ICRU report 44. Our results demonstrate that a more accurate prediction of HU to mass density can be achieved by the stoichiometric calibration curve for proton therapy dose computation (rms error 0.81%).

3:54PM J35.00008: Method, Mechanism, and Metrology for Measurement of Multi-Dimensional MTF in Medical Imaging  PENGWEI WU (Presenter), MAHADEVAPPA MAHESH, Johns Hopkins University, JOHN BOONE, University of California, Davis, JEFFREY H SIEWERDSEN, Johns Hopkins University — The spatial resolution characteristics of CT and cone-beam CT (CBCT) systems is well characterized by the spatial-frequency-dependent modulation transfer function (MTF). Emerging scanner technologies and reconstruction algorithms challenge conventional methods for MTF assessment, including the degree to which the system / image exhibits 3D resolution characteristics that are isotropic (vary in direction), stationary (vary with location), and linear (vary with contrast). We report an angled-edge test tool and oversampling method to measure the MTF in any direction in 3D image data, with extension to a spherical test tool for measurement in all directions. One particular direction (45° relative to the axial plane) is shown to avoid null space effects in cone-beam geometries and provide useful 1D quantitation of the fully 3D resolution characteristics. This method was tested using a mobile C-arm CBCT system and a high-resolution diagnostic CT scanner and shown to reveal underlying sources of non-isotropic resolution characteristics – for example, asymmetric apodization filters, detector binning modes, and focal spot size. The angled-edge or spherical test tools provide a practical means for quantitative characterization of 3D MTF characteristics for medical imaging systems.
4:06PM J35.00009: A novel approach to lead concentration measurements in bone using the L-shell x-ray fluorescence and strontium Kβ/Kα ratio.* MIHAI GHERASE (Presenter), JOSH JARDENIL, SARAH KROEKER, California State University, Fresno — Lead (Pb) is a well-known toxic element which accumulates in the bone after years or decades of exposure. Long-term Pb exposure is, therefore, assessed by in vivo bone Pb concentration measurements. In vivo bone Pb x-ray fluorescence (XRF) measurements are typically done in tibia bone to minimize the soft tissue (ST) x-ray attenuation. Bone Pb L-shell XRF (LXRF) can use compact XRF systems – a useful feature for potential bone Pb surveys. An optimal grazing-incidence position (OGIP) method was developed in our lab to enhance Pb detection by mitigating the x-ray scatter. The obstacle to in vivo applications is the unknown ST x-ray attenuation. The average ST x-ray linear attenuation coefficient and ultrasound-measured thickness past approach gave inaccurate results. In our method, the measured Kβ/Kα ratio of strontium (an essential trace element in the bone) was used to estimate the ST attenuation of the Pb x-rays. Plaster-of-Paris (poP) bone phantoms made with known Pb and Sr concentrations and polyoxymethylene (POM) ST phantoms of varying thickness were measured. The concordance correlation coefficients between the computed and the known Pb concentrations were in the -0.444 to 0.998 range.

*Research was supported by an NIH award #SC2GM121187.

4:18PM J35.00010: Quantifying Macroscopic and Microscopic Radiation Dose Enhancement with Gold Nanoparticles for a Range of Therapeutic Energies* TARA GRAY (Presenter), University of Texas at San Antonio, NEMA BASSIRI, Radiation Oncology, University of Texas Health Mays Cancer Center, SHAQUAN DAVID, DEVANSHI PATEL, University of Texas at San Antonio, NEIL KIRBY, Radiation Oncology, University of Texas Health Mays Cancer Center, KATHRYN MAYER, University of Texas at San Antonio — The purpose of this study is to computationally quantify the macroscopic and microscopic radiation dose enhancement effects of different sizes and shapes of gold nanoparticles. A MicroSelectron HDR Ir-192 brachytherapy seed and a Varian 600C gantry head with 6 MV and 18 MV photon energies were modeled using Monte Carlo N-Particle radiation transport software (MCNP 6.2, Los Alamos National Laboratory). The repeating structures capability of MCNP6.2 was utilized to simulate nanoparticles of varying sizes inside a tumor with a diameter of 1 x 1 x 1 cm³. Additionally, a phase space file was created to compute dose deposited from secondary electrons around single nanoparticles of varying shapes (nanocubes, nanoprisms and nanospheres). Macroscopic simulations show an increase in dose enhancement generally with increasing mass percentage of gold and compare well with experimental results. Microscopic simulations show an increased dose enhancement of 20% - 50% due to secondary electrons up to 1 µm from the nanoparticle and is highest for nanoprisms due to a larger surface area to volume ratio. This work indicates the potential for gold nanoparticles to provide significant dose enhancement and more effective tumor cell killing in radiation oncology practice.

*San Antonio Medical Foundation
4:30PM J35.00011: Dependence of deep learning-based whole organ segmentation on training dataset size in computed tomography (CT) images  DANIEL HUFF (Presenter), AMY J WEISMAN, ROBERT JERAJ, Medical Physics, University of Wisconsin - Madison — A significant drawback of deep learning-based medical image segmentation is its reliance on large amounts of labeled training data. However, little literature has characterized the dependence of model performance on the amount of training data provided. Here, we examine this dependence in the application of abdominal organ segmentation on patient CT images.

Two public datasets, BTCV (N=30) and VISCERAL.eu (N=20), were used for training. A third dataset, pancreasCT (N=43) was used as an independent test set. Segmentation was performed for five abdominal organs: liver, spleen, kidneys, stomach, and pancreas. Instances of the same CNN were trained on a varying number of randomly selected training scans (N=5-50). The architecture used was DeepMedic, a 3D patch-based CNN. Performance was measured with Dice coefficient, average surface distance, and 95% Hausdorff distance.

We observe that segmentation performance improves with increasing training dataset size, but in some cases plateaus before the whole training set is used. Absolute performance of our model is comparable to literature while minimizing the amount of labelled data required. This work has implications for optimizing deep learning-based image segmentation pipelines by minimizing time spent on unnecessary dataset labelling.

4:42PM J35.00012: Monte-Carlo simulation of X-ray energy spectrum for single and dual-energy radiography  NASTARAN KHAMOOSHI (Presenter), Physics and energy engineering, Amirkabir university of technology — Single-energy radiography is one of the most everyday nondestructive/noninvasive image methods that generate detailed images of tumors, nodules, cracks, defects, and discontinuities inside the human body or an object. Dual-energy X-ray is a novel technique which uses two X-ray spectrums for imaging. It can produce much higher contrast for radiographs for when two different subjects with different atomic numbers are close to each other. In this study, X-ray beam geometry has been precisely implemented in the code. Tungsten target anode material and the angle of 20 degrees is used as typical X-ray source’s anode. Electron-photon transformation cross-sections have been taken from ENDF data libraries. Photon energy distribution finally calculated exactly after inherent and/or additional filters. Effects of filtering materials with different thicknesses on HE and LE have been investigated. Excellent agreement results obtained in the spectrums generated by our Monte-Carlo simulation by IPEM software and experimental data. In this study filter quality effect has been conducted as well. The results of this investigation are very important in optimizing dose calculation, image quality consideration and a lot of other parameters in the area of the medical and industrial imaging field.
Complex impedance quantification of cell migration for the physics of cancer*   

MICHAEL J. MIMLITZ (Presenter), ANDREW J. WALThER, MICHAEL MERRICK, CATHERINE WEEDER, JOE BAMESBERGER, HARIs AKHTER, HONOUR DJAM, ANDREW EKPENYONG, Creighton University — Cell migration is a crucial step in cancer metastasis, the complex process which accounts for over 90% of cancer-related deaths. There is emerging evidence that radiotherapeutic doses meant to kill cancer cells can promote metastasis by enhancing cell migration. Here we quantify radiation-induced changes in cell migration as part of the physics of cancer: a novel research frontier unraveling the roles of physical properties of cells in cancer. We used a standard laboratory irradiator to irradiate both non-cancer (HCN2 neurons) and cancer cells (T98G glioblastoma) with 2 Gy, 10 Gy and 20 Gy of X-rays. To assess cell migration post-irradiation, we used a commercially available device, ECIS Z-Theta, which non-invasively measures and converts complex cell-substrate electric impedance into series resistance and capacitance in real time. We also used CdSe/ZnS core-shell quantum dots to quantify molecular changes in cells following radiotherapy. Both irradiated cell lines showed significantly (p <0.01) enhanced migration compared to non-irradiated cells, within the first 40 hours following irradiation with 20 Gy. Our results suggest cell migration as a new therapeutic target in antimetastasis strategies for improved radiotherapy outcomes.

*Creighton University Startup Grant (to AEE).

Test-retest Reproducibility for Resting State Networks in fMRI

MARGARITA LOPEZ (Presenter), Univ Veracruzana, BRENDA BEDolla-MoCTezuma, Psicología, Universidad del Valle de México — Resting state networks (rsN) are important to assess the neural connectivity in the brain in repose. The assessment of the rsN could help to the diagnosis and treatment of different psychological and psychiatric disorders, for example different studies have found that the DMN is affected in patients with major depression. The BOLD signal could be affected and change by technical and physiological factors as: movement, cardiac function, different potioning of the subject in the scan, the hour of the day, etc. for that reason is important to evaluate the rsN reproducibility between subjects and sessions. In the present study we obtain the rsN for 36 volunteer healthy subjects (18-60 years old) in three different sessions separated by 15 days each one, we acquired two different BOLD rsfMRI sequences (eyes open) with different spatial resolution in a 3T scanner with a 32 head sense channel coil, the FE-EPI sequences have the following parameters TE/TR = 30/ 2000 ms, FA = 75, FOV= 240 mm x 240 mm x 123 mm, matrix 80x 78 x 35, with isometric spatial resolution of 3 mm and other with anisotropic resolution. The Intraclass Correlation Coefficient (ICC) was calculated and we found the ICC between first and second sessions less than the ICC between second and third sessions.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J36 DQI: DQI Invited Session: Quantum Memories for Superconducting Qubits 601/603 - Anja Metelmann, Princeton University - Tag(s): Invited
ALEXANDER GRIMM (Presenter), Yale University — Superpositions of two opposite-phase coherent states in an oscillator, so-called Schrödinger-cat states, can be used to encode a qubit protected against phase-flip errors. Such a protected “cat qubit” has the potential to significantly reduce the overhead associated with quantum error correction. However, the practical operation of a cat qubit faces several challenges: Its basis states are highly excited states of the oscillator and need to be stabilized in order to maintain the protection. At the same time, the system has to be compatible with fast gates on the encoded qubit and a quantum non-demolition (QND) readout of the encoded information.

In this talk, we will present our recent experimental results on the stabilization of an error-protected cat qubit through the interplay between Kerr nonlinearity and single-mode squeezing in a superconducting microwave resonator. Our experiment demonstrates a full set of single-qubit gates and QND-readout on timescales significantly shorter than the relevant decoherence times.

*Work supported by: ARO, ONR, NSF, AFOSR, YQI, and YINQE

JEREMIE GUILLAUD (Presenter), MAZYAR MIRRAHIMI, Quantic, Inria Paris — Quantum error correcting codes provide, when operated below the threshold, an arbitrary good protection against noise, thus solving the decoherence problem for quantum information processing. However, the actual implementation of the most promising ones, such as the surface code, comes at the price of tremendous physical resources to reach a sufficient level of protection. We present a 1D repetition code based on the so-called cat-qubits as a viable candidate for a massive reduction in the hardware requirements for universal and fault-tolerant quantum computation. The cat-qubits that are stabilized by a two-photon driven dissipative process, exhibit a tunable noise bias where the effective bit-flips are exponentially suppressed with the average number of photons. Exploiting this noise bias, we build, at the level of the repetition cat-qubit, a universal set of fully protected logical gates. Remarkably, this construction avoids the costly magic states preparation, distillation and injection, even for non-Clifford gates.

*Work supported by ARO and DIM SIRTEQ.
3:42PM J36.00003: Detection of optical photons from a superconducting qubit* [Invited] ALP SIPAHIGIL (Presenter), Caltech — The ability to convert a superconducting qubit excitation to an optical photon would enable the incorporation of superconducting quantum processors in optical quantum networks. In this talk, we present an integrated device platform for converting a qubit excitation to an optical photon via piezo-optomechanical transduction. We first describe the design and fabrication of a nanomechanical resonator with strong piezoelectric coupling to a transmon qubit and a large optomechanical coupling rate. We then discuss experiments using this mechanical mode as an intermediary to convert a qubit excitation to an optical photon in two steps. First, we dynamically tune the qubit frequency to perform a swap operation between the qubit and the mechanical mode. This is followed by an optical pulse that upconverts the phonon to an optical photon via the optomechanical interaction. We detect the resulting photons and demonstrate optical photon generation from a transmon qubit. We measure qubit Rabi oscillations using single optical photon detection to characterize the transducer’s noise and efficiency. Finally, we discuss prospects for optically mediated entanglement generation between remote superconducting circuits using this platform.

In collaboration with: Alp Sipahigil, Mohammad Mirhosseini, Mahmoud Kalaee, Oskar Painter, Caltech

*This work was supported by ARO/LPS CQTS, AFOSR MURI, and IQIM.

4:18PM J36.00004: Quantum information processing using multimode cavities* [Invited] SRIVATSAN CHAKRAM (Presenter), University of Chicago — Multimode superconducting microwave cavities provide a hardware efficient means of engineering a large Hilbert space with high coherence, suitable for quantum simulations and information processing. Coupling to a superconducting transmon circuit results in random access control [1], with logic gates possible between arbitrary pairs of cavity modes. I will present our progress towards realizing such a processor using the quantum flute - a seamless rectangular 3D multimode cavity, with a tailored mode dispersion and lifetimes approaching a millisecond for ~10 modes. We present various schemes for controlling the cavity states using interactions mediated by the dispersively coupled transmon. 4-wave mixing processes induced by the non-linearity of the transmon can be used to exchange quantum states between the transmon and the cavity modes in a few hundred nanoseconds. When driven off-resonantly, these sideband drives can be used to controllably dress the cavity states, and engineer novel multimode interactions that are useful for quantum simulations. These interactions can also be used to compensate multimode-state-dependent Stark shifts, and perform generalized parity measurements, crucial for high fidelity gate operations and quantum error correction.


*This research was supported by Samsung Advanced Institute of Technology Global Research Partnership.
Encoding a qubit in logical quantum states with wavefunctions characterized by disjoint support and robust energies can offer simultaneous protection against relaxation and pure dephasing. Using a two-dimensional circuit-quantum-electrodynamics architecture, we experimentally realize a superconducting 0-π qubit, which hosts protected states suitable for quantum-information processing. Our multi-tone spectroscopy measurements reveal the energy level structure of the system, which can be precisely described by a simple two-mode Hamiltonian. We find that the circuit realizes an effective one-dimensional crystal with two sub-lattices, where the geometrical phase difference between Wannier states localized at adjacent phase unit cells leads to interference effects associated with tunneling of pairs of Cooper pairs. The parity symmetry of the qubit results in charge-insensitive levels connecting the protected states, allowing for logical operations. The measured relaxation (1.6 ms) and dephasing times (25 μs) demonstrate that our implementation of the 0-π circuit not only broadens the family of superconducting qubits but also represents a promising candidate for the building block of a fault-tolerant quantum computer.

*Work was supported by Army Research Office Grant No. W911NF-1910016, NSERC and the Canada First Research Excellence Fund.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

2:30PM J37.00001: Circuit QED theory and experiment: Encoding quantum information in harmonic oscillators* [Invited] STEVEN GIRVIN (Presenter), Yale Quantum Institute, Yale University — ‘Circuit quantum electrodynamics’ is the theory of non-linear quantum optics extended to the study of microwave photons strongly interacting with ‘artificial atoms’ (Josephson junction qubits) embedded in superconducting electrical circuits. Recent remarkable theoretical and experimental progress in our ability to measure and manipulate the quantum states of individual microwave photons is leading to novel applications ranging from accelerating dark matter searches to quantum error correction using bosonic codes that have successfully extended the lifetime of quantum information. This talk will present an elementary introduction to the basic concepts underlying circuit QED and describe several recent novel experiments demonstrating these new found capabilities.

*This work was supported by the Army Research Office under Grant Number W911NF-18-1-0212, by the National Science Foundation under Grant Number DMR-1609326 and by the Yale Quantum Institute.

3:06PM J37.00002: Phase-Controlled Topological Superconductivity* [Invited] CHARLES MARCUS (Presenter), Microsoft Corp — This talk will explore alternative routes to generating Majorana zero modes, finding similarities between Majorana modes in vortex cores of 2D and 3D topological superconductors and schemes based on one-dimensional semiconductor-superconductor hybrids in a strong Zeeman field. Phase winding in vortices and full-shell nanowires has a 2D analog as well, which is phase control across an SNS junction, which in the presence of spin-orbit coupling and Zeeman field, also generates leads to topological superconductivity. Results from recent experiments will be discussed in the context of this unified picture.

*We thank Microsoft and the Danish National Research Foundation for support. Materials provided by Microsoft Quantum Materials Labs in Copenhagen and Purdue.

3:42PM J37.00003: Mechanics and applications of bio-conformable electronics* [Invited] NANSHU LU (Presenter), University of Texas at Austin — Seamlessly merging human body with electronics can not only digitize our body for internet of health and human-computer interaction, but also deliver therapeutics or even augment our capabilities. As human organs are soft and curvilinear, it is important to understand and rationally design the conformability of soft electronics to human tissue. This talk will present 2D and 3D analytical and numerical models along with experimental validations for the conformability of flexible and stretchable electronics on rigid and soft curvilinear surfaces. It will also introduce reversible physical adhesives based on cratered surfaces that can attach securely on bio-tissue but easy to remove and reuse. Noninvasive and invasive bio-conformable electronics will be demonstrated in this talk.

*National Science Foundation Grants CMMI-1301335, CMMI-1663551, ECCS-1509767, and CNS-1738293.
4:18PM J37.00004: Supersolidity in the ultracold: when atoms behave as solid and superfluid at the same time [invited] FRANCESCA FERALINO (Presenter), Univ of Innsbruck —

Ultracold quantum gases are both an ideal test-bed platform to address key questions in quantum physics and a powerful resource to realize novel paradigms and novel phases of quantum matter. Moreover, the potential of such systems is becoming ever more enabling as scientists acquire an increasingly fine control over optical manipulation and inter-particle interactions.

Recently, a novel class of atomic species, possessing an exceptionally strong magnetic character is entering the stage, offering a new conceptual twist for the field. In our laboratories in Innsbruck, we have realized the first dipolar Bose-Einstein condensate and Fermi gas of the highly magnetic Erbium species and the first dipolar quantum mixture of Erbium and Dysprosium.

I will report on our recent observations of the elusive and paradoxical supersolid state of quantum matter, using both Erbium and Dysprosium ultracold gases. Such paradoxical phase, in which crystal rigidity and superfluid flow coexist, has intrigued scientists across different disciplines for decades. It now became possible to create supersolidity in the ultracold thanks to the unique interplay between long-range dipolar interactions, contact interactions, and a powerful stabilization mechanism based on quantum fluctuations.

4:54PM J37.00005: Strange Metals and Black Holes* [Invited] SUBIR SACHDEV (Presenter), Harvard University — The ‘strange metal’, a state of matter formed by electrons in many modern materials, including the compounds which exhibit high temperature superconductivity. In this state, electrons quantum entangle with each other and conduct electric current collectively (rather than one-by-one, as in an ordinary metal like copper). Quantum entanglement also has remarkable effects near the horizon of a black hole, leading to the Bekenstein-Hawking black hole entropy, and the Hawking temperature. Surprisingly, there is a deep connection between the nature of quantum entanglement in strange metals and black holes, and this has led to mutually beneficial insights. This connection is simply described by the Sachdev-Ye-Kitaev model, which leads to a common set of equations describing the quantum dynamics of certain strange metals and black holes. I will describe recent progress in developing a theory of strange metals building on the solvable SYK model.

*U.S. Department of Energy Grant DE-SC0019030; National Science Foundation Grant DMR-1664842

Tuesday, March 3, 2020 2:30 PM - 4:18 PM

Session J38 FOEP FPS: Outreach and Public Science Communication 607 -
James Kakalios, University of Minnesota - Tag(s): Invited, Outreach, Undergrad Friendly
MATTHEW J O’DOWD (Presenter), Lehman College — Traditional efforts to engage the public with science have led to a growing science fandom, and yet these broad positive feelings don’t seem to correlate with improving scientific literacy. It seems our approach to science communication need an overhaul, however methods employed by traditional media are heavily constrained by institutional wisdom and the profit motive. But new forms of media such as YouTube are allowing the next generation of science communicators to test old wisdom and experiment with new methods.

PBS Space Time has been at the forefront of this experiment, having spent the last five years communicating unusually complex topics in physics and astronomy to a lay audience. In this talk we share some of the unintuitive insights that we and other YouTubers have gained, and discuss how these can be implemented by anyone to help close the science communication gap.

JEANNA BRYNER (Presenter), Live Science — Science communication — Why is it so important? Science plays a vital role in the world, from the discovery of new drugs to futuristic technologies that promise to help support human life on Mars. But if that science is not communicated clearly, the people who rely on scientific knowledge are left confused and perhaps less likely to trust scientists and science in general. In addition to bolstering trust in science, your words could inspire a person to enter a scientific field or give them a deeper understanding of the world and their place in it. Explaining the beauty of quantum physics, the wonders being created inside a particle accelerator or the mind-boggling energy of a supernova can open another’s eyes to the boundless nature of science.

In this talk, I will describe what good science communication looks like and the many avenues it can take, from social media posts to full features in digital and print news publications. Whether you’re interested in dipping your toe into the waters of communicating science to the public or hope to dive right in, this talk will give you tips and resources to get you started.

FRANCIS SLAKEY (Presenter), American Physical Society — How many constituent requests does a typical congressional office get every day? How much time do staff have to process a request, before they have to move on to the next one? What approach makes it easiest for staff to respond? We’ll explore the answers to each of those question and consider the resulting boundary conditions for effective communication with policymakers: keep it tight, make it compelling, have a crystal clear ask. We’ll see what we can learn from a related format – the evening local 1/2 hour news broadcast -- where time is precious, and information is conveyed quickly and efficiently. We'll then have audience volunteers tackle some real-world cases to see how effective communication with policymakers works in practice.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM
Ground and excited states of open-shell systems from a spin-flip Bethe-Salpeter approach* [Invited] DAVID STRUBBE (Presenter), Physics, University of California, Merced — Open-shell systems, including molecules and defects, are interesting platforms for spin physics and quantum information. Their multi-determinantal states are difficult to handle with conventional first-principles calculations. A solution from quantum chemistry is the spin-flip (SF) approach: the ground and excited states are considered as spin-flipping excitations of a single-determinant high-spin reference state. The SF approach was originally used with wavefunction-based approaches such as configuration interaction, then later extended to time-dependent density-functional theory (TDDFT), showing some successes. Standard TDDFT approximations, however, have well-known deficiencies including treatment of charge-transfer excitations and condensed phases. Therefore, we introduce a spin-flip approach to the GW/Bethe-Salpeter approach (GW/BSE), taking advantage of a similar structure of the equations to TDDFT, but with an \textit{ab initio} long-ranged and non-local interaction kernel, which enables more accurate calculations of excited states. I will discuss the theory of the spin-flip BSE method and our implementation with the Octopus and BerkeleyGW codes, and show our investigation of the critical issues of spin contamination and convergence with number of states in BSE. We have demonstrated success of SF-BSE on some simple problems. In the torsion of the ethylene molecule (C_2H_4), which transitions between singlet and triplet ground states, we found excellent agreement with higher-level and more expensive calculation methods, and a consistency at the equilibrium geometry with standard BSE calculations. We find good results also for the Si atom’s singlet-triplet splitting, which has been problematic for TDDFT. Given these successes on small systems, I will discuss prospects for application of our approach to problems in condensed phases.

*U.S. Department of Energy, Office of Science, Basic Energy Sciences, CTC and CPIMS Programs, Award DE-SC0019053.
All-electron Implementation of Bethe-Salpeter Equation Method: Development and Application

YI YAO (Presenter), Department of Chemistry, University of North Carolina at Chapel Hill, DOROTHEA GOLZE, Department of Applied Physics, Aalto University, CHI LIU, Department of Mechanical Engineering and Materials Science, Duke University, PATRICK RINKE, Department of Applied Physics, Aalto University, VOLKER BLUM, Department of Mechanical Engineering and Materials Science, Duke University, YOSUKE KANAI, Department of Chemistry, University of North Carolina at Chapel Hill — A new all-electron implementation of the Bethe-Salpeter Equation (BSE) method for optical excitations is presented. We benchmarked the accuracy of our implementation on low lying optical excitations of organic molecules in the Thiel benchmark set for validation, and the basis-set dependence is carefully analyzed. We then integrated the core-GW approach by Golze et al. into our BSE implementation for X-ray absorption spectroscopy (XAS). We compare our results for K-edge XAS spectra of small organic molecules to earlier EOM-CCSD work by Peng et al. We found the accuracy of our BSE approach is comparable to or better than EOM-CCSD, which gives the errors within 0.5 eV of experimental value for the test set. The implementation for extended periodic systems is discussed lastly with examples of liquid water and crystalline silicon.


Efficient Construction of 4-point Green’s Function in Real-Space Representation using Permutation Sampling Monte Carlo method

NICOLE SPANEDDA (Presenter), PETER MCLAUGHLIN, ARINDAM CHAKRABORTY, Syracuse University — A principle challenge in constructing the 1-particle Green's function is the steep scaling of computational cost with increasing system size. We address this problem by transforming the Green's function into real-space representation and calculating all required integrals using the Permutation Sampling Monte Carlo method (PSMC). We started with the frequency-domain representation of the self-energy and performed Laplace transformation to obtain a 4-point representation of the self-energy in position basis. The main benefit of PSMC is that it avoids the steep scaling associated with the traditional methods of constructing the self-energy. Specifically, we avoided AO-to-MO integral transformation and explicit representation of the self-energy in particle-hole basis. In this work we demonstrated the linear scaling of computational cost with the number of molecular-orbital basis functions that was achieved by the PSMC method. Consequently, PSMC can be applied to systems that are computationally impractical using conventional methods. We used PSMC to calculate the ionization potentials of PbS quantum dots (Pb4S4-P140S140).
**3:30PM J39.00004: Equation of motion coupled-cluster approach for multi-electron excitations in x-ray spectra**

JOHN REHR (Presenter), FERNANDO VILA, JOSHUA KAS, University of Washington, KAROL KOWALSKI, BO PENG, Pacific Northwest National Laboratory — We present a real-time equation of motion coupled cluster approach [1] for calculations of multi-electron excitations in core-level x-ray absorption and emission spectra. Integration of the equations to leading order in particle-hole excitations yields a cumulant representation of the core-hole spectral function. Absorption and emission spectra are then calculated in terms of a convolution of an effective one-body x-ray spectrum and the core-hole spectral function. Comparisons with determinantal approaches and with the Delta-SCF approximation are also discussed. Illustrative calculations are discussed separately [2].


*Supported by the Center for Scalable, Predictive methods for Excitation and Correlated phenomena (SPEC) which is funded by the U.S. DOE, Office of Science, Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences.

**3:42PM J39.00005: Real-time EOM-CCS Green's function method for the core spectral functions**

FERNANDO VILA (Presenter), JOHN REHR, University of Washington, BO PENG, KAROL KOWALSKI, PNNL — X-ray photoemission spectra (XPS) typically exhibit satellite peaks associated with many-body excitations that have proved difficult to simulate from first principles. We address this problem using a real-time equation-of-motion coupled-cluster-singles (RT-EOM-CCS) approach for the core spectral function. RT methods provide a versatile approach to electronic response, but have not been widely applied using CC theory. In RT-EOM-CCS, the Green's function (GF) for an \( N \)-electron system is computed from the overlap between the initial core-excited \(|N-1>\) wavefunction and its time-propagated form \(|N-1,t>\). The latter is approximated using a CC ansatz with time-dependent amplitudes. The EOM of the overlap is solved using a centered predictor-corrector approach. We show that the form of the overlap is analogous to that in the static CC equations, and that the form of the GF is related to that in the cumulant approach. Finally, we present results for low \( N \) systems.


*Supported by the Center for Scalable, Predictive methods for Excitation and Correlated phenomena (SPEC), funded by the U.S. DOE, Office of Science, BES, Division of Chemical Sciences, Geosciences, and Biosciences, with computer support from DOE-NERSC.
3:54PM J39.00006: Neutral Excitation Energies of Crystalline Solids from Periodic Equation-of-Motion Coupled-Cluster Theory  

XIAO WANG (Presenter), Center for Computational Quantum Physics, Flatiron Institute, TIMOTHY BERKELBACH, Department of Chemistry, Columbia University — There have been increasing interests in the development of high-accuracy, wavefunction-based quantum chemistry methods, such as coupled-cluster theory, with periodic boundary conditions for electronic structure problems of crystalline solids. We present an ab initio study on electronically excited states of solids using Gaussian-based periodic equation-of-motion coupled-cluster theory with single and double excitations (EE-EOM-CCSD). EE-EOM-CCSD provides a quantitative treatment of singly excited states, such as excitons and plasmons, and a qualitative treatment of doubly excited states, such as biexcitons. Results of optical band gaps, exciton binding energies, and exciton dispersions will be presented for a variety of inorganic insulators and semiconductors.

4:06PM J39.00007: Fingerprints of dynamical correlation in electron spectroscopies [Invited]  

MATTEO GATTI (Presenter), LSI, CNRS, Ecole Polytechnique — One of the great challenges of condensed-matter physics is the description, understanding, and prediction of the effects of the Coulomb interaction on materials properties. In electronic spectra, the Coulomb interaction causes a renormalization of excitation energies and a transfer of spectral weight. Most importantly, it can lead to qualitatively new structures, such as satellites in photoemission or double-plasmon resonances in energy-loss spectra. Being a genuine signature of dynamical correlation, they are absent in a non-interacting picture but can be understood in terms of the coupling between different elementary excitations.

In this framework, a key physical ingredient is the dynamical screening of the Coulomb interaction, containing charge excitations such as plasmons and excitons. It can be accurately calculated within time-dependent density-functional theory (including double plasmons [1]) or by solving the Bethe-Salpeter equation. Its microscopic picture can be obtained from the mixed dynamic structure factor that is measured by coherent inelastic X-ray scattering spectroscopy [2]. Building upon a detailed knowledge of dynamical screening, the cumulant expansion of the Green's function can efficiently explain plasmon and exciton satellites in the photoemission spectra of several materials, ranging from simple metals to correlated transition-metal oxides [3]. Finally, the combined effect of many-body interactions and experimental conditions can lead to novel signatures in the measured spectra [4], underlining the need to bridge the gap between theory and experiments.

4:42PM J39.00008: Biexcitons and exciton dynamics in low-dimensional systems from an *ab initio* interacting Green's function formalism*  

FELIPE DA JORNADA (Presenter), Materials Science and Engineering, Stanford University, ANDREA CEPELLOTTI, Materials Science & Mechanical Engineering, Harvard University, STEVEN LOUIE, Department of Physics, UC Berkeley — The synthesis of quasi low-dimensional materials, such as the monolayer transition metal dichalcogenides (TMDs), opened the door to studying new classes of systems with nanoscale dimensionality confinement and weak electronic screening, leading to strongly enhanced electron interactions. Many of these systems host a variety of charged and neutral multiparticle excitations – such as excitons, trions, and biexcitons. We present here a first-principles formalism based on the interacting Green’s function to compute and understand these excitations and their dynamics. We apply our formalism and its associated code on high performing computers to the monolayer TMDs, predicting a diversity of multiparticle excitations with large binding energies (~20 meV) and complex valley and spin textures. We also show how this formalism can be employed to investigate other exciton-exciton interactions to understand challenging phenomena involving dynamics from first principles.

*This work was supported by the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) at LBNL, funded by the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources provided by NERSC and XSEDE.

4:54PM J39.00009: Electron-hole attraction effect under time-dependent electric field within a generalized Landau-Zener model  

YASUSHI SHINOHARA (Presenter), School of Engineering, The Univ of Tokyo — The exchange term is a crucial term for first-principles electronic structure theories, leading to accurate prediction within hybrid-functional for density-functional theory and the most simple many-body effect as a term in the Hartree-Fock (HF) equation. This term is also crucial for the description of the electronically excited state, namely excitonic influence on dielectric function either due to bound- or unbound-excitons. In spite of its importance in photoabsorption spectra, the effect of the (screened) exchange term for nonlinear phenomena has not been investigated well because of severe calculation cost. Higher energetic electron-hole pairs in high-order harmonic generation spectra are reported by using one-dimensional HF simulation, compared with an independent particle system[1]. The effect is totally from modulation of the mean-field via a density-matrix change to a self-consistent solution of the HF equation. We develop a much simpler model that has an electron-hole attraction term imitating the exchange term on the top of the Landau-Zener model to investigate the dynamical effect of electron-hole attraction. We have observed a pronounced gap renormalization by increasing the field strength.

5:06PM J39.00010: First principle excited state calculations using a frequency–dependent geminal–screened electron–hole interaction kernel  
PETER MCLAUGHLIN (Presenter), ARINDAM CHAKRABORTY, Syracuse University — A primary computational limitation for excited state methods is the inclusion of virtual or unoccupied states in the calculations. The inclusion of these states increases the calculation cost for excited state calculations. We present the frequency–dependent geminal–screened electron–hole interaction kernel (FD–GSIK) method for describing electron–hole correlation in electronically excited many–electron systems. FD–GSIK avoids using unoccupied orbitals for kernel construction by performing infinite–order summation of particle–hole excitation and representing it as a compact real–space operator. The central idea of our approach is to use Löwdin partitioning technique to construct a frequency–dependent and r12–explicitly correlated operator for treating electron–hole correlation for the excited state wave function that is derived from first principles and is parameter–free. Evaluation of all integrals were performed in real space using stratified Monte Carlo, which avoided the steep computational cost of evaluation, storage and transformation of the atomic orbitals to molecular orbitals. The FD–GSIK was applied to large nanoparticles including Pb$_{140}$S$_{140}$, Pb$_{140}$Se$_{140}$, and Cd$_{144}$Se$_{144}$, to obtain excitation and electron–hole binding energies.

5:18PM J39.00011: Atomic relativistic approximation for $ab$ initio prediction of excited-state potential energy surfaces and X-ray spectra*  
TIANYUAN ZHANG (Presenter), JOSEPH M KASPER, XIAOSONG LI, University of Washington — The atomic relativistic approach is a formally simple and linear scaling ansatz that exploits the locality of the relativistic effect. Studies have shown that this approximation introduces moderate error on ground state absolute energy in the presence of short bonds between heavy nuclei. However, scientists have not investigated its accuracy on computing excited states for absorption spectra and excited-state potential energy surfaces. In this work, we demonstrate atomic exact two-component (X2C) predictions of the L$_{2,3}$-edge X-ray absorption spectra of five representative heavy-atom-centered molecules and the excited-state potential energy curves of the platinum dimer (Pt$_2$). Surprisingly, not only the errors to full X2C results in core excitation energies are negligible on the order of 0.01 eV, but the oscillator strengths also agree well with those from full X2C computations. Meanwhile, the atomic X2C potential energy curves and crossings of Pt$_2$ are almost indistinguishable from the full X2C ones.

*The development of the two-component electronic structure method is funded by the US Department of Energy (DE-SC0006863). The development of non-perturbative spectroscopic methods is supported by the National Science Foundation (CHE-1856210).

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J40 DCOMP DMP: Matter in Extreme Environments II: Liquids, Geological, and Complex Materials 705 - Tiange Bi - Tag(s): Focus
2:30PM J40.00001: Using liquid informed searches to predict high pressure and finite temperature phase transitions* [Invited] STANIMIR BONEV (Presenter), Lawrence Livermore Natl Lab — Recent developments in computational algorithms have enabled crystal structure prediction at high pressure conditions, leading the way to the discovery of materials with unexpected and fascinating properties. However, structure prediction at finite temperature remains a challenge, while advances in experimental platforms and measurement techniques have opened up access to the properties of matter via a wide range of pressure-temperature pathways. In this talk, I will discuss the use of structural information and/or sampling from liquid simulations to predict high pressure phase transitions and crystal structures at finite temperature conditions. The techniques will be illustrated with examples of successful applications on several systems, including magnesium, nitrous oxide, and nitrogen.

*This work was performed at LLNL under the auspices of the U.S. DOE under Contract DE-AC52-07NA27344.

3:06PM J40.00002: Ab initio investigation of post-PPV transitions in $\text{MgGeO}_3$ and $\text{NaMgF}_3$* KOICHIRO UMEMOTO (Presenter), ELSI, Tokyo Institute of Technology, RENATA WENTZCOVITCH, Columbia University — We present an ab initio investigation of the pressure induced behavior of $\text{MgGeO}_3$ and $\text{NaMgF}_3$, traditional low-pressure analogs (LPAs) of $\text{MgSiO}_3$. The latter undergoes post-post-perovskite (post-PPV) transitions which are exceedingly important in planetary sciences, but at very high pressures of $>\sim500$ GPa [1-3]. Although neither $\text{MgGeO}_3$ nor $\text{NaMgF}_3$ are perfect LPAs of $\text{MgSiO}_3$, in overall both display similar dissociation and recombination transitions and the novel types of phases displayed by $\text{MgSiO}_3$ but at much lower pressures easily achievable in diamond anvil cells. Both systems also confirm the ultimate tendency of $\text{MgSiO}_3$ toward the dissociation into its elementary binaries, i.e., $\text{AX}$ and $\text{BX}_2$. We also predict potential metastable phase transitions that may occur more easily than dissociation/recombination reactions under insufficiently heated compression.


*This research was supported by JSPS-Kakenhi and MEXT as “Exploratory Challenge on Post-K computer”.
Ronald Cohen (Presenter), Carnegie Inst of Washington — Using density functional theory and the QUANTUM ESPRESSO code, first-principles molecular dynamics simulations have been performed over a wide range of pressures and temperatures, for pure Fe, pure H, and Fe-H solutions. Pressures range from 0 to 100 MB (10 TPa) and temperatures from 2000-40000 K. From these results the equations of state are fit for extreme conditions in planetary core from Earth to Jupiter and beyond. Transport properties are also being computed from snapshots of the MD runs. Good agreement is found with new experiments and results are consistent with a thermally driven dynamo over Earth history.


This work is supported by NSF CSEDl grant EAR-1901813 and the Carnegie Institution for Science. It was funded previously by the ERC Advanced Grant ToMCaT. The author gratefully acknowledges the Gauss Centre for Supercomputing e.V. (www.gauss-centre.eu) for funding this project by providing computing time on the GCS Supercomputer SuperMUC-NG at the Leibniz Supercomputing Centre (www.lrz.de).

Renata Wentzcovitch (Presenter), Department of Applied Physics and Applied Mathematics, Columbia University, Juan J Valencia-Cardona, Chemical Engineering and Materials Science, University of Minnesota, Gaurav Shukla, Department of Earth Sciences, Indian Institute of Science Education and Research Kolkata, Kanchan Sarkar, Department of Applied Physics and Applied Mathematics, Columbia University — The major mineral phase of the Earth’s lower mantle, (Al,Fe)-bearing bridgmanite, transitions to a seemingly layered structure known as post-perovskite at Earth’s deep lower mantle conditions. Despite extensive investigations, there are still important aspects of this transformation that need clarification. Here, we address this transition in (Al$^{3+}$, Fe$^{3+}$), (Al$^{3+}$), (Fe$^{2+}$) and (Fe$^{3+}$)-bearing bridgmanite using ab initio calculations, particularly the phase boundary dependence on the chemistry and acoustic velocity changes across this transformation. These results help us to constrain possible seismic signatures of this phase transition, which is necessary for a better understanding of the nature of the D” region. While our results are consistent with previous mineral physics studies, we find that the seismic features produced by the post-perovskite transition depend on the chemical composition of bridgmanite. Therefore, the absence of a D” seismic discontinuity or signature of a double-crossing of the post-perovskite phase boundary has clear implications for the local aggregate chemistry and/or temperature.

Research supported by NSF awards EAR-1502594 and EAR-1918126.
Life in Extreme Environments: Material Properties of the Enzymes

TOSHIKO ICHIYE (Presenter), Georgetown University — Life on Earth has been found in many extremes of pressure $P$ and temperature $T$. Understanding how life works at high $P$ and high $T$ has implications for the origin of life on Earth and for the search for extraterrestrial life. In addition, extremes of $P$ and $T$ are used in sterilization and food preservation. To understand how the proteins necessary for life can function at extremes, we use a combination of molecular dynamics simulations of enzymes in aqueous solution, combined with experimental data, to understand how their material properties affect their biochemical activity. We will discuss the effects of $P$ and $T$ on enzymes, evolutionary timescale adaptations in the material properties of enzymes for extremes, and rapid response changes in the intracellular environment to protect enzymes against extremes.

*Funding from the National Science Foundation, Grant No. CHE-1464766; the National Institutes of Health, Grant No. R01-GM122441; and the McGowan Foundation. Computational resources from the LoBoS cluster at the Laboratory for Computational Biology, NHLBI, NIH; XSEDE granted via MCB990010 from NSF Grant No. OCI-1053575; and the Medusa cluster maintained by University Information Services at Georgetown University.

Express: nonstop calculations with the Quantum ESPRESSO

QI ZHANG (Presenter), Department of Applied Physics and Mathematics, Columbia University, MICHEL MARCONDES, Department of Earth and Environmental Sciences, Columbia University, HONGJIN WANG, Department of Computer Science, Columbia University, JINGYI ZHUANG, Department of Earth and Environmental Sciences, Columbia University, PEDRO DA SILVEIRA, RENATA WENTZCOVITCH, Department of Applied Physics and Mathematics, Columbia University — The intrinsic complexity of ab initio mineral physics studies inspired the development of workflows to automate long and extensive sequences of ab initio calculations [1]. This complexity emerges from the need to sample thermodynamic and chemical phase space for useful geophysical applications. Here we introduce Express, a new generation of Python and Julia workflows designed to facilitate calculations of thermoelastic and thermochemical properties of materials.

Various materials properties can be computed, e.g., static equation of state, phonon density of states, static elasticity, thermal equation of state, and thermodynamic properties. They work either separately or jointly. Each workflow consists of three steps: 1) pre-processing: dynamic generation and validation of input files for the target software; 2) processing: submission, supervision of jobs, and retrieval of results; 3) post-processing: analyses of outputs and error handling.

Express codes are concise and come with user-friendly APIs to be integrated into other codes. It currently supports Quantum ESPRESSO, but other ab initio software is expected to be supported in the future.


*Research supported by DOE award DE-SC0019759.
Ab initio simulation of heat and charge transport in water at planetary pT conditions

FEDERICO GRASSELLI (Presenter), SISSA - Scuola Internazionale Superiore di Studi Avanzati, Trieste, LARS PETER STIXRUDE, Earth, Planetary, and Space Sciences, University of California at Los Angeles, STEFANO BARONI, SISSA - Scuola Internazionale Superiore di Studi Avanzati, Trieste — The transport properties of water at extreme pT conditions govern the evolution of icy planets, such as Uranus and Neptune, and moons, such as Europa or Encelado. New theoretical and data-analysis methods have been recently developed to estimate accurate transport coefficients of electronically gapped materials from ab initio equilibrium molecular dynamics and the Green-Kubo theory of linear response [1-3]. In this talk we report on recent results of the application of these methods to heat and charge transport in water at the extreme pT conditions occurring in the interior of icy giants, in all the different relevant phases (partially dissociated liquid, solid, and super-ionic) [4]. These results are finally employed to build a model of the thermal evolution of Uranus, which accounts for its hitherto poorly understood very low luminosity.


First-principles predictions of electrical and thermal conductivity of liquid and solid iron at Earth core conditions

KAI LUO (Presenter), RONALD COHEN, Geophysical Laboratory, Carnegie Institution of Science — Transport properties such as thermal and electrical conductivities of the liquid iron alloy are critical in understanding the dynamic history of Earth's outer core and the evolution of the geomagnetic field. These conditions (beyond ~200 GPa) pose great challenges to experimental measurement. In contrast, first-principles simulation is not subject to this limitation and allows explorations of a wider range of conditions.

We use Kubo theory to compute transport properties from first-principles molecular dynamics (FPMD) simulations, incorporating scattering of electrons by disorder and thermal vibrations using density functional theory, and by other electrons using dynamical mean field theory. Studying pure liquid and solid iron at such conditions, we address the saturation effects and calibrate the violation of the Wiedemann-Franz law.

KL and REC are supported by U.S. NSF CSEDI grant EAR-1901813 and the Carnegie Institution for Science. REC was supported by ERC Advanced Grant ToMCaT.
4:30PM J40.00009: Anomalous structural behaviour near a Mott transition in compressed Ca$_2$RuO$_4$  
HARRY KEEN (Presenter), Univ of Edinburgh, STEPHEN R JULIAN, University of Toronto, ANDREAS HERMANN, Univ of Edinburgh — Ca$_2$RuO$_4$ has a rich phase diagram, featuring a metal-insulator transition with a structural distortion upon cooling, antiferromagnetic ordering upon further cooling, and metallisation and ferromagnetic order, followed by a further structural transition, under pressure. It is one end member of the Ca$(2-x)$Sr$(x)$RuO$_4$ series that includes the proposed triplet superconductor Sr$_2$RuO$_4$ at the other end. Ca$_2$RuO$_4$ shows intriguing collective phenomena in its own right, several of which are intricately linked to structural distortions of the RuO$_6$ octahedra, which in turn are susceptible to pressure-induced changes. In fact, Ca$_2$RuO$_4$ shows an unusual c-lattice expansion under hydrostatic compression. However, the structural and electronic properties of Ca$_2$RuO$_4$ under pressure have not been investigated in detail before. Here, we study the high-pressure phase evolution of Ca$_2$RuO$_4$ using density functional theory (DFT) and DFT+U calculations. We show that the c-lattice expansion in the metallic high-pressure phase as well as details of the octahedral arrangements can be described if the on-site repulsion U is fine-tuned appropriately. The sensitivity to the size of U highlights how close the metallic phase remains to the Mott insulating phase.

4:42PM J40.00010: Theoretical Prediction of Novel Materials with the XtalOpt Evolutionary Algorithm  
XIAOYU WANG (Presenter), PATRICK AVERY, State University of New York at Buffalo, DAVIDE M. PROSERPIO, Università degli Studi di Milano, CORMAC TOHER, STEFANO CURTAROLO, Duke University, EVA ZUREK, State University of New York at Buffalo — The XtalOpt evolutionary algorithm for crystal structure prediction has been extended to enable the prediction of materials with specific properties. A fitness function has been implemented wherein the user can denote the percent contribution that enthalpy and the property (e.g. Vickers hardness obtained via a macroscopic hardness model and the shear modulus as determined via machine learning, percentage of hydrogen atoms that do not form H-H bonds, or density of states at the Fermi level) have on the fitness function. We have used XtalOpt to search for hard and stable carbon allotropes. Several novel carbon allotropes that are superconducting or possess super-long sp$^3$-sp$^3$ bonds were found. We also discovered novel hydrides that could potentially be conventional superconductors.
4:54PM J40.00011: Ab initio investigation of hydrogen-bond disorder in δ-AlOOH*

CHENXING LUO (Presenter), TIANQI WAN, ZIYU CAI, Department of Applied Physics and Applied Mathematics, Columbia University, KOICHIRO UMEMOTO, Earth-Life Science Institute, Tokyo Institute of Technology, RENATA WENTZCOVITCH, Department of Applied Physics and Applied Mathematics, Columbia University — δ-AlOOH (δ) is an important carrier of water in the lower mantle. Attempts to resolve the structure of δ revealed that hydrogen bonds (H-bond) “symmetrize” under compression in a process similar to the high-pressure ice VII- or ice VIII-X transition. Like H₂O-ice, δ has its own “ice-disorder rules” and disorder is also observed experimentally prior to H-bond symmetrization [1]. H-bond disorder in δ had been suggested by an ab initio study as a possibility based on its broad band of Raman active OH-stretching modes [2].

In this ab initio study, we address the H-bond disordering process that precedes its symmetrization from several perspectives, including a) the accuracy of standard DFT functionals to address the structural properties of δ, b) vibrational stability and the pressure-range of validity of the quasiharmonic approximation (QHA), and c) order-disorder transition using a multi-configuration QHA calculation at 300 K. With these results, we reproduce the structural behavior and the neutron diffraction peculiarities under pressure.

[1] A. Sano-Furukawa et al., DOI: 10.1038/s41598-018-33598-2

*Research supported by DOE award DE-SC0019759.

5:06PM J40.00012: Thermal Conductivity of CaSiO₃ Perovskite at Lower Mantle Conditions*

ZHENG ZHANG (Presenter), Columbia Univ, KOTARO ONGA, Tokyo Institute of Technology, DONG-BO ZHANG, Beijing Normal University, KENJI OHTA, Tokyo Institute of Technology, TAO SUN, University of the Chinese Academy of Sciences, KEI HIROSE, The University of Tokyo, RENATA WENTZCOVITCH, Columbia Univ — Thermal conductivity (κ) of mantle minerals modulates strongly both the style of mantle convection and the time scale of the mantle and core cooling. It is therefore a fundamental parameter for geodynamic modeling. Cubic CaSiO₃ perovskite (CaPv) is believed to be the third most abundant mineral in the lower mantle (LM) (6 – 10 wt%). However, despite its importance, investigations of its properties are challenging because of its strong anharmonicity, particularly κ since prevailing theoretical approaches encounter difficulties in dealing with its strong anharmonicity. Experimental measurements at relevant high pressures and temperatures are equally challenging. Therefore, no previous estimate of CaPv’s κ exists at mantle conditions, experimental or theoretical. Here we present ab initio quantum mechanical results of this property obtained using an established phonon quasiparticle approach that can address the strongly anharmonic situation in CaPv. These results are substantiated by direct experimental measurements of this property at LM conditions. These results and data agree very well and reveal a surprisingly large κ of cubic CaPv compared to MgSiO₃-perovskite, which is only weakly anharmonic.

*This research was supported primarily by the Department of Energy Grant DE-SC001975.
5:18PM J40.00013: Determination of Diffusion Constants and Partial Pressures in the Adsorption of Methane-Propane and Methane-Ethane Mixtures  VALLE ROY ZACHARY (Presenter), Univ of Missouri - Columbia, GONZALO DOS SANTOS, Universidad de Mendoza, TODD LOMBARDI, CARLOS WEXLER, Univ of Missouri - Columbia — Natural gas (NG) has advantages vs. gasoline/diesel: lower CO$_2$ emissions per unit energy, less emission of NOx's, particulate matter and unburned hydrocarbons. However, storing NG is problematic due to its low density, requiring very high pressures, costly compression and storage systems. A solution is storage by adsorption in porous media such as activated carbon (AC). NG is comprised mainly of methane, thus most studies have focused on adsorption of pure methane. Here we investigate the influence of heavier alkanes commonly found in NG (propane, ethane) on the adsorption process.

We performed extensive molecular dynamics simulations of mixtures of methane-propane and methane-ethane at $T=300$-$400$K and $P=0$-$600$atm. The system considered were AC's comprised of slit-shaped pores with interlayer spacings $H=8$-$20$Å. We observed that heavier hydrocarbons adsorb preferentially, but remain mobile, promising for the intended application. We also solved a common problem with simulations of molecules with high adsorption affinity: the difficulty to determine their partial pressure. We developed an Arrhenius-type relationship allowing the calculation of these partial pressures from relationships between energy distributions of the different molecules in the simulations.

Tuesday, March 3, 2020 2:30 PM - 5:06 PM

Session J41 GMAG: Spin, Charge, Thermal Interactions, and Conversion 707 - Jiahao Han, Massachusetts Institute of Technology MIT
2:30PM J41.00001: Spin pumping under magnetic field gradient  HIROKI ARISAWA (Presenter), Institute for Materials Research, Tohoku University, SHUNSUKE DAIMON, Department of Applied Physics, The University of Tokyo, YASUYUKI OIKAWA, Advanced Institute for Materials Research, Tohoku University, TAKASHI KIKKAWA, Institute for Materials Research, Tohoku University, EIJI SAITO, Department of Applied Physics, The University of Tokyo — The spin pumping effect is the generation of a spin current by spin waves in a ferromagnet. Its properties have enthusiastically been investigated mainly in uniform magnetic fields, but they are yet to be explored well in nonuniform magnetic fields. Meanwhile, a recent study reported an interesting behavior of spin waves that the wave number of spin waves is converted to another value during its propagation under inhomogeneous magnetic fields. This fact indicates that spin current emission via the spin pumping effect can be spatially tuned taking advantage of the spin-wave wave number conversion in nonuniform magnetic fields. In this talk, we report spatially nonuniform spin current generation by the spin pumping effect under a magnetic field gradient in a Pt/Y₃Fe₅O₁₂ bilayer system. We found that a spin current generated by spin waves is nonlocally enhanced depending on the magnetic field gradient. We explain the result on the basis of the wave number conversion of spin waves, considering its dispersion relation spatially varying with the magnetic field gradient. Our results offer a new insight of spin current generation utilizing nonuniform magnetic fields.

2:42PM J41.00002: Drag induced giant anomalous Nernst effect in Ferromagnetic MnBi  BIN HE (Presenter), Solid State Chemistry, Max Planck Institute for Chemical Physics of Solids, CUNEYT SAHIN, Department of Physics and Astronomy, The University of Iowa, STEPHEN R BOONA, The Ohio State University, BRIAN SALES, Oak Ridge National Lab, JOSEPH P C HEREMANS, The Ohio State University, MICHAEL FLATTÉ, Department of Physics and Astronomy, The University of Iowa, CLAUDIA FELSER, Max Planck Inst — Anomalous Nernst effect (ANE) is the thermal equivalent to the Anomalous Hall effect (AHE). It has been observed in various materials and attributed to the Berry curvature of topological materials. In this talk, we present the observation of giant anomalous Nernst effect in MnBi single crystals. In addition to intrinsic contribution from the band structure, magnon drag also contributes to the anomalous Nernst signal in MnBi crystals, resulting in a giant anomalous Nernst thermopower of 18 μV/K at 0.6 T. At the same time, we also observe a magnon drag thermopower and positive magnetothermal conductivity. This magnon drag induce anomalous Nernst effect can be viewed as a self-spin Seebeck effect, which provides alternative path of understanding the electron magnon interaction.
Electrically-induced ferromagnetism in diamagnetic FeS$_2$*  

JEFF WALTER (Presenter), Department of Physics, Augsburg University, BRYAN VOIGT, Department of Chemical Engineering and Materials Science, University of Minnesota, EZRA DAY-ROBERTS, School of Physics and Astronomy, University of Minnesota, KEI HELTEMES, Department of Physics, Augsburg University, TURAN BIROL, Department of Chemical Engineering and Materials Science, University of Minnesota, RAFAEL FERNANDES, School of Physics and Astronomy, University of Minnesota, CHRIS LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota — Recent years have seen increasingly impressive demonstrations of all-electrical control of magnetism, including electrolyte-gating-induced ferromagnetism in non-ferromagnetic materials. These demonstrations, however, involve induction of ferromagnetism from some other finite-spin magnetic state, e.g., antiferromagnetic, paramagnetic, etc. In this work we use ionic liquid gating, which can induce electron densities >10$^{14}$ cm$^{-2}$, to achieve voltage-induced ferromagnetism in diamagnetic (i.e., zero-spin) FeS$_2$ single crystals. Temperature-dependent transport measurements establish a remarkably reversible positive-bias-induced insulator-metal transition, accompanied by inversion of the FeS$_2$ surface conduction channel to $n$-type. Anomalous Hall effect measurements then reveal an accompanying onset of voltage-induced soft 2D ferromagnetism, with Curie temperature up to ~20 K. These results are supported by DFT-based tight-binding modelling that indicates induction of Stoner FM by gate-controlled band filling.

*Work supported by the NSF MRSEC under DMR-1420013 (UMN) and by a Margaret A. Cargill Philanthropies grant (Augsburg).

Spin to charge and charge to spin conversion in a Dirac semimetal*  

WILSON YANEZ (Presenter), RUN XIAO, Physics, Pennsylvania State University, JACOB T HELD, Chemical Engineering and Materials Science, University of Minnesota, DI XIAO, JEFFREY G RABLE, Physics, Pennsylvania State University, ENRIQUE GONZÁLEZ, Physics and Electronics, University of Puerto Rico at Humacao, YONGXI OU, ANTHONY R. RICHARDELLA, Physics, Pennsylvania State University, K. ANDRE MKHOYAN, Chemical Engineering and Materials Science, University of Minnesota, NITIN SAMARTH, Physics, Pennsylvania State University — We report evidence of spin to charge and charge to spin conversion at room temperature in thin films of the archetypal three-dimensional Dirac semimetal Cd$_3$As$_2$ grown by molecular beam epitaxy. This has been detected by means of ferromagnetic driven spin pumping (SP) and spin torque ferromagnetic resonance (ST-FMR) in NiFe/Cd$_3$As$_2$ heterostructures. Analysis of the frequency and power dependence of the SP signal and of the symmetric and antisymmetric contributions to the mixing voltage in ST-FMR show that the behavior of these processes is consistent with previously reported spin to charge conversion mechanisms in heavy metals and topological insulators. Finally, we compare the efficiency of these phenomena with the one due to the inverse spin Hall effect in NiFe/Platinum bilayers.

*This work is supported by SMART/nCORE/SRC/NIST, the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331, 2DCC-MIP/NSF DMR-1539916 and the Office of Graduate Educational Equity Programs and Eberly College of Science at The Pennsylvania State University.
3:18PM J41.00005: Spin Seebeck effect in Pt/SrMnO$_3$ heterostructures  ESWARA PHANINDRA VALLABHANENI (Presenter), ARJIT DAS, TAMALIKA BANERJEE, physics, univ of Groningen — Spin Seebeck effect (SSE) is one of the effective ways of generating pure spin currents driven by thermal gradients and has been extensively explored in spin caloritronics, an active branch in spintronics. In recent years, the focus has shifted to antiferromagnetic insulators (AFM-I), where spin currents created by a thermal gradient has been studied. Thermal gradients across the AFM-I film produce pure spin currents in an adjacent heavy metal layer such as platinum (Pt) due to non-equilibrium distribution of thermal magnons. These spin currents can be detected as a transverse charge current across the Pt layer via inverse spin Hall effect. Here, we have performed systematic investigations of SSE employing two measurement geometries, local and non-local configurations, on oxygen (non-)stoichiometric-SrMnO$_3$ thin films, which exhibit weak-ferromagnetic, insulating behavior down to low temperatures. Controlled experiments as a function of the applied dc bias, magnitude and orientation of applied magnetic field were used to disentangle the role of possible magnetic proximity effects. We observe a quadratic dependence of the SSE signal in Pt/SrMnO$_3$ with the applied current density. SSE is an important tool to detect and study magnon transport in hitherto unexplored complex oxides.

3:30PM J41.00006: Longitudinal Spin Seebeck effect in Pyrochlore Iridates with Bulk and Interfacial Dzyaloshinskii-Moriya interaction*  BOWEN MA (Presenter), University of Texas at Austin, BENEDETTA FLEBUS, University of California, Los Angeles, GREGORY A FIETE, Northeastern University — The longitudinal spin-Seebeck effect (SSE) in magnetic insulator|non-magnetic metal heterostructures has been theoretically studied primarily with the assumption of an isotropic interfacial exchange coupling. Here, we present a general theory of the SSE in the case of an antisymmetric Dzyaloshinskii-Moriya interaction (DMI) at the interface, in addition to the usual Heisenberg form. We numerically evaluate the dependence of the spin current on the temperature and bulk DMI using a pyrochlore iridate as a model insulator with all-in all-out (AIAO) ground state configuration. We also compare the results of different crystalline surfaces arising from different crystalline orientations and conclude that the relative angles between the interfacial moments and DM vectors play a significant role in the spin transfer. Our work extends the theory of the SSE by including the anisotropic nature of the interfacial DMI in magnetic insulator|non-magnetic metal heterostructures and can suggest possible materials to optimize the interfacial spin transfer in spintronic devices.

*NSF Grant No. DMR-1729588, NSF Materials Research Science and Engineering Center Grant No. DMR-1720595, the Simons Foundation, and a QuantEmX grant GBMF5305 from ICAM and the Gordon and Betty Moore Foundation.
3:42PM J41.00007: Spin Seebeck effect in Vanadium Tetracyanoethylene  
YUANHUA ZHENG (Presenter), SETH KURFMAN, ANDREW FRANSON, EZEKIEL JOHNSTON-HALPERIN, JOSEPH P C HEREMANS, Ohio State Univ - Columbus — Vanadium tetracyanoethylene (V(TCNE)$_x$, $x \sim 2$) is an organic based ferrimagnetic coordination compound, with extremely low Gilbert damping which is comparable to yttrium iron garnet. Due to its non-crystalline nature, it is interesting to investigate how spin waves propagate in the material. One possible way is through thermally driven spin pumping, namely spin Seebeck effect (SSE). Here, we present a systematic study on the temperature and thickness dependence of SSE in V(TCNE)$_x$. The thin films (thickness on the order of 100 nm) are grown via chemical vapor deposition on a platinum layer on sapphire substrate. By applying a temperature gradient perpendicular to the V(TCNE)$_x$/Pt, a large SSE signal is collected. Further analysis on the temperature and thickness dependence helps us understand the length scales of the propagation of spin waves.

*YZ and JPH acknowledge CEM, an NSF-MRSEC under grant number DMR-1420451. SK, AF and EJH acknowledge NSF Award under award number 1808704.

3:54PM J41.00008: Temperature Dependence of the Anomalous Nernst Coefficient for Ni$_{80}$Fe$_{20}$ Determined with Metallic Nonlocal Spin Valves  
RACHEL BENNET ( Presenter), Univ of Denver, ALEX HOJEM, Physics, University of California San Diego, BARRY L ZINK, Univ of Denver — The anomalous Nernst effect, which generates an out-of-plane charge voltage in response to a thermal gradient perpendicular to the magnetization of a ferromagnet, can play a significant role in any spintronic device where large thermal gradients exist.[1] Since they typically include features deep within the submicron regime, nonlocal spin valves can be made very sensitive to this effect by lowering the substrate thermal conductance.[2] Thus, material parameters are extremely important to the performance of these devices. Although studies have been conducted into the thickness dependence of the anomalous Hall coefficient for permalloy, little is known about the temperature dependence of the anomalous Nernst coefficient.[3,4]

Here, we use nonlocal spin valves suspended on thin silicon nitride membranes to determine the temperature dependence of the anomalous Nernst coefficient of 35 nm thick permalloy (the NiFe alloy with 80% Ni) from 78 K to 300 K.


*NSF grant ECCS-1610904
4:06PM J41.00009: Magneto-thermoelectric effect in lanthanum orthoferrite with Pt overlayer*  WEIWEI LIN (Presenter), Department of Physics and Astronomy, Johns Hopkins University, JIAMING HE, JIANSHI ZHOU, Department of Mechanical Engineering, University of Texas at Austin, BOWEN MA, Department of Physics, University of Texas at Austin, GREGORY A FIETE, Department of Physics, Northeastern University, CHIA-LING CHIEN, Department of Physics and Astronomy, Johns Hopkins University — Spin caloritronic phenomena, utilizing heat flow to transport spin signals with minimal or no charge current, are of fundamental interest with important applications. We have observed nontrivial magneto-thermoelectric effects in lanthanum orthoferrite (LaFeO$_3$) perovskite single crystals with Pt overlayer at room temperature. The LaFeO$_3$ is a canted antiferromagnetic insulator with weak magnetization of about 0.04 $\mu_B$ per Fe atom along the c-axis, which is only 1% of that of the common ferromagnet iron. The amplitude of magneto-thermovoltage in the Pt/LaFeO$_3$ with an in-plane temperature gradient is comparable to those of the longitudinal spin Seebeck effect and inverse spin Hall effect in Pt/yttrium iron garnet. It provides a sensitive probe of very weak magnetization in the insulator, which can be manipulated by a magnetic field of the order of 10 mT. However, from the thermoelectric measurement configurations and the angular dependence on the applied magnetic field, our results are distinctly different from those of the anomalous Nernst effect and longitudinal spin Seebeck effect. We attribute our results to a thermal magnon transport at the Pt/LaFeO$_3$ interface.

*This work was supported by National Science Foundation DMREF, Grants No. 1729555 and 1729588, and DMR-1949701.

4:18PM J41.00010: Effects of CoFeAl Alloy Composition on Magnetization Dynamics and Magnetic Thermal Transport*  RAMYA MOHAN (Presenter), YIWEI SUN, SUVEEN MATHAUDHU, SINISA COH, RICHARD WILSON, University of California, Riverside — The lifetime of magnetic excitations in metals is governed by scattering rates between magnons and electrons. Recent investigations [1, 2] document how electronic band structure engineering in magnetic alloys allows for suppression of magnon scattering rates; e.g. Co$_{0.25}$Fe$_{0.75}$ thin-films display low magnetic damping ($\alpha \sim 10^{-4}$). My talk will focus on experimental measurements that demonstrate how ultrafast magnetization dynamics and transport properties of CoFeAl magnetic alloys depend on alloy composition. To explore the magnetization dynamics, I use a time-resolved MOKE set-up to observe ultrafast demagnetization in a few hundred femtoseconds followed by precessional dynamics. Through TDTR measurements, I check if lower electron-magnon scattering rates lead to improved thermal transport. My investigation sheds light on how magnon-electron scattering rates govern dynamics on femtosecond (ultrafast demagnetization), nanosecond (magnetic precession and damping), and microsecond time-scales (thermal transport of energy).


*This work was supported by the U.S. Army Research Laboratory and the U.S. Army Research Office under grant # W911NF-18-1-0364.
Investigation of thermal Hall conductivity in hexagonal LuFeO$_3$ type multiferroics

HENA DAS (Presenter), SERGEY NIKOLAEV, Laboratory for Materials and Structures, Tokyo Tech World Research Hub Initiative (WRHI), Institute of Innovative Research, Tokyo Institute of Technology — Materials those exhibit electric and magnetic ordering simultaneously in their ground states and show electric field control of magnetism, may also exhibit novel/enhanced thermal Hall transport phenomena [Nat. Mater. 16, 797 (2017)] that have immense utilitarian worth in various device applications. In this study, we have investigated topology of the magnonic bands and the magnon-mediated thermal transport of the LuFeO$_3$ type novel multiferroics, in which the geometric origin of the ferroelectricity induced not only a net magnetization but also non-trivial magnetoelectric couplings [Nature Communications 5, 2998 (2014), Nature Materials 13, 163-167 (2014)]. We have employed the framework of linearized spin wave and linear response theories to study thermal conductivity as a function of the ferroelectric trimer lattice distortion. The calculated thermal Hall conductivity shows a non-trivial dependence on the ferroelectric distortion. We have also discussed the thermal transport in multiferroic LuFeO$_3$ and LuMnO$_3$ as case studies involving real materials.

Phase transitions and magnetocaloric effects in the Heusler compounds Ni$_2$Mn$_{0.70}$Cu$_{0.30}$Ga and Ni$_2$Mn$_{0.70}$Cu$_{0.25}$Cr$_{0.05}$Ga

SUNDAY AGBO (Presenter), MAHMUD KHAN, Miami University — The structural, magnetic and magnetocaloric properties of Ni$_2$Mn$_{0.70}$Cu$_{0.25}$Cr$_{0.05}$Ga and Ni$_2$Mn$_{0.70}$Cu$_{0.30}$Ga Heusler alloys have been investigated by x-ray diffraction, magnetization, transport, and DSC measurements. For the Ni$_2$Mn$_{0.70}$Cu$_{0.25}$Cr$_{0.05}$Ga alloy, a first order coupled magnetostructural phase transformation near room temperature with a thermal hysteresis of ~1 K was observed. In the vicinity of the transition, large magnetic entropy changes of ~39 J/kg K (while warming) and ~17 J/kg K (while cooling) was observed for a field change of 50 kOe. For the Ni$_2$Mn$_{0.70}$Cu$_{0.30}$Ga material, the first order phase transition with a thermal hysteresis of ~7 K was observed near 345 K. For a field change of 50 kOe, peak magnetic entropy changes of -17 J/kg K and -33 J/kg K were observed for warming and cooling, respectively. The electrical resistivity data showed interesting behavior near the phase transitions. The experimental results will be presented and discussed considering the coupling and de-coupling of the first order structural and second order magnetic phase transitions in the materials.
4:54PM J41.00013: Theory of spin magnetic quadrupole moment and temperature-gradient-induced magnetization*  ATSUO SHITADE (Presenter), AKITO DAIDO, YOUICHI YANASE, Kyoto Univ. — We formulate what we call gravitomagnetoelectric (gravito-ME) effect, in which the magnetization is induced by a temperature gradient. Although the Kubo formula for the gravito-ME effect provides an unphysical divergence at zero temperature, we prove that the correct susceptibility is obtained by subtracting the spin magnetic quadrupole moment from the Kubo formula. It vanishes at zero temperature and is related to the ME susceptibility by the Mott relation. We explicitly calculate the gravito-ME susceptibility in a Rashba ferromagnet and show its experimental feasibility.


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J41.00014: Oscillatory spin pumping in Nb/NiFe/Nb junctions*  YUNYAN YAO (Presenter), RANRAN CAI, ICQM, Peking Univ. Beijing 100871, P. R. China., YASUMASA TSUTSUMI, RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan., YANG MA, WENYU XING, YUAN JI, CHEN XIE, ICQM, Peking Univ. Beijing 100871, P. R. China., SEE-HUN YANG, IBM Research - Almaden, San Jose, California 95120, USA., SADAMICHI MAEKAWA, RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan., WEI HAN, ICQM, Peking Univ. Beijing 100871, P. R. China. — The quantum size-induced oscillating physical phenomena has attracted a lot of interest in condensed matter physics and materials science. In this talk, I will discuss the oscillatory spin pumping in the Nb(100nm)/NiFe/Nb(100nm) trilayer structure. In the normal state of Nb, via systematical varying the thickness of NiFe from 5nm to 20nm, an oscillating Gilbert damping is observed. This oscillating behavior can be attributed to the quantum-interference effect of angular momentum transfer between the local precessing magnetic moment and conduction electrons in thin NiFe that was theoretically predicted by Mills [1]. As the NiFe layer is thin and coupled to nonmagnetic Nb layers, quantum-interference effect of the spin-polarized electrons shows up, which gives rise to the oscillating spin-transfer torque to the NiFe. This oscillating feature is observed to be largely enhanced below the superconducting critical temperatures in the Nb/NiFe/Nb Junctions.


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Tuesday, March 3, 2020 2:30 PM - 5:30 PM
2:30PM J42.00001: Ultra-low-power switching of IrMn/CoFeB/MgO structure with voltage-controlled spin-orbit torque  SHOUZHONG PENG (Presenter), JIAQI LU, WEIXIANG LI, LEZHI WANG, HE ZHANG, WANG KANG, ZHAOHAO WANG, Fert Beijing Institute, BDBC, School of Microelectronics, Hefei Innovation Research Institute, Beihang University, XIANG LI, KANG-LUNG WANG, Department of Electrical Engineering, University of California, Los Angeles — How to efficiently manipulate magnetization remains one of the key challenges for spintronic devices and magnetic random-access memories[1-3]. Here we experimentally demonstrate the ultra-low-power and field-free switching of perpendicular magnetization by a combination of spin-orbit torque (SOT) and voltage-controlled magnetic anisotropy effect. Firstly, field-free SOT switching is achieved with the aid of an in-plane exchange bias (EB) generated in the perpendicularly magnetized IrMn/CoFeB/MgO structure. Then we explore the VCMA effect and observed a clear reduction of perpendicular magnetic anisotropy (PMA) when a gate voltage is applied. A VCMA coefficient of 35 fJ/Vm is obtained in this structure, comparable to that of the Ta/CoFeB/MgO structure. By applying a gate voltage of 0.6 V on this film, the SOT switching current can be significantly reduced, resulting in a critical switching current of 6.2 MA/cm². Finally, an ultra-low-power and high-density spintronic memory array based on voltage-controlled SOT is proposed and demonstrated by both experiments and hybrid CMOS/MTJ simulations.

2:42PM J42.00002: Electrical noise in magnetic tunnel junctions due to magneto-structural transitions of CoFeB/MgO interfaces*  AREZOO ETESAMIRAD (Presenter), DAVID NELSON, KEANUHEA DAILEY, Physics and Astronomy, University of California, Riverside, JORDAN A KATINE, Western Digital, San Jose, ILYA KRIVOROTOV, Physics and Astronomy, University of California, Irvine, IGOR BARSUKOV, Physics and Astronomy, University of California, Riverside — Magnetic tunnel junctions (MTJs) play a central role in spintronics research as memory elements, nanoscale microwave oscillators, local magnetic sensors, and neuromorphic network components. Understanding and controlling electric noise in MTJs is a prerequisite for employing them in next-generation applications. Here, we study MTJ nanopillars of 50 nm diameter consisting of CoFeB free layer, MgO tunnel barrier, and CoFe based synthetic antiferromagnet. We observe random telegraph noise which is frequently found in MTJs and yet not fully understood. Varying the temperature in the range of 80-300 K for an MTJ in the parallel state, we encounter anomalous device resistance (steps) attributed [1,2] to magneto-structural phase transitions of iron oxide clusters at the CoFeB/MgO interface. At temperatures of these anomalies, telegraph noise shows a significant increase. This correlation suggests that the oxide clusters have a significant impact on MTJ noise characteristics.

*Supported by DoE EFRC SHINES DE-SC0012670 and NSF ECCS-1810541.
2:54PM J42.00003: Finite-size Kosterlitz-Thouless transition in Fe/W(001) ultrathin films*

DAVID VENUS (Presenter), JORDAN ATCHISON, AMANJOT BHULLAR, BRYCE NORMAN, McMaster Univ — The Kosterlitz-Thouless (KT) transition involves the unbinding of topological excitations (vortex-antivortex pairs) in an infinite, isotropic, 2DXY system. In real 2D ferromagnetic films, it is not clear that such a transition occurs in the presence of crystalline anisotropy and finite size effects. We report MOKE magnetic susceptibility measurements $\chi(T)$ of 4-fold in-plane ultrathin Fe/W(001) films, where a prominent peak is observed. Above the peak temperature, the paramagnetic susceptibility is in excellent agreement with the form expected for a vortex-antivortex gas: $\chi(T) = \chi_0 \exp[B/(T/T_{KT} - 1)]^a$, with $a = 0.50\pm0.03$ and $B = 3.48\pm0.16$. In accord with finite size KT theory, the KT transition temperature, $T_{KT}$, is tens of K below the susceptibility peak, giving a “finite size” consistent with $\mu$m magnetic domains. Fitting instead to a power law, as would be consistent with a 2nd order transition, gives unphysical parameters $\gamma_{eff} = 3.7\pm0.7$ and a Curie temperature $T_{\gamma}$ far below the peak temperature. Below the peak, the measured susceptibility has a complicated behaviour qualitatively consistent with the re-emergence of 4-fold anisotropy and magnetic domains.

*This work is funded by the Natural Science and Engineering Research Council of Canada (NSERC), under the Discovery Program.

3:06PM J42.00004: Spin-Orbit-Torque Field-Effect Transistor (SOTFET): A New Magnetolectric Memory*

XIANG LI (Presenter), PHILLIP DANG, JOSEPH CASAMENTO, ZEXUAN ZHANG, OLALEKAN AFUYE, ALYSSA B. APSEL, DARRELL SCHLOM, DEBDEEP JENA, DANIEL C. RALPH, HUILI XING, Cornell University — Spin-based memories are attractive for their non-volatility and high durability but provide modest resistance changes, whereas semiconductor logic transistors are capable of large resistance changes but lack memory function with high durability. The recent availability of multiferroic materials provides an opportunity to directly couple the change in spin states of a magnetic memory to a charge change in a semiconductor transistor. In this work, we propose and analyze the spin-orbit-torque field-effect transistor (SOTFET), a device with the potential to significantly boost the energy efficiency of spin-based memories, and to simultaneously offer a palette of new functionalities. Analysis of the memory aspect indicates that the SOTFET can offer orders of magnitude increase in the on-off resistance ratio compared to existing magnetic memories, which can potentially lower the operation energy significantly. We establish a quantitative model of the operations of the SOTFET. From the model, the materials needs for the successful operation are identified and the feasibility of the SOTFET is proved in a properly designed CoFe/BiFeO$_3$ gate stack.

*This work was supported by SRC as nCORE task 2758.001 and NSF under the E2CDA program (ECCS 1740286).
3:18PM J42.00005: Pulsed or Microwave Currents Induced Random Telegraph Signal in a Magnetic Tunnel Junction*  RAJAPKASYALAGE RAJAPAKSE (Presenter), NICHOLAS PENTHORN, Physics and Astronomy, University of California, XIAOJIE HAO, ZIHUI WANG, YIMING HUAI, Avalanche Technology, HONGWEN JIANG, Physics and Astronomy, University of California — Recent work has shown creation and dynamics of magnetic skyrmions, without the Dzyaloshinskii-Moriya interaction, in the free layer of a magnetic tunnel junction (MTJ) at a temperature of 4K [1]. In order to study how skyrmions, the topological excitations, can be protected against disorders and temperature fluctuations, we have extended our experimental investigation to higher temperatures, up to 200K, for various device sizes. For the intermediate resistance state, initiated by pulse or microwave currents, we have observed stochastic switching between two resistance states, commonly referred as the random telegraph signal (RTS). Statistics of the observed RTS depends on device temperature and microwave stimulation while the corresponding relations have been studied. In conjunction with micro-magnetic simulations, we discuss the interplay of the topological skyrmion and disorder-induced domains in MTJs.


*The work was supported by National Science Foundation (NSF under Grant No. DMR-1809155).

3:30PM J42.00006: Controlling long-range skyrmion lattices using field and temperature in Fe/Gd multilayers*  LISA DEBEER-SCHMITT (Presenter), Oak Ridge National Lab, RYAN DESAUTELS, Seagate Technology, NAN TANG, Material Science Department, University of Tennessee, SERGIO MONTOYA, CMRR, University of California San Diego, W L. N. C. LIYANAGE, Material Science Department, University of Tennessee, SHEENA PATEL, Physics, University of California San Diego, MICHAEL FITZSIMMONS, Oak Ridge National Lab, ERIC FULLERTON, CMRR, University of California San Diego, JULIE ANN BORCHERS, NIST Center for Neutron Research, National Institute of Standards and Technology, DUSTIN GILBERT, Material Science Department, University of Tennessee — Ordered magnetic skyrmion lattices presents a playground of new and interesting physics to explore. This opportunity is provided by the topological nature of the skyrmion. We have recently fabricated thin-films of amorphous Fe and Gd multilayers that support skyrmions and skyrmion lattices at room temperature and zero applied magnetic field. These skyrmions are stabilized by dipolar interactions, rather than the Dzyaloshinskii–Moriya interaction (DMI). By varying the film thickness and alloy composition we can alter the dipole interactions relative to the exchange and anisotropy and thus control the skyrmion size, pitch, and stability. Using small angle neutron scattering (SANS), we demonstrated that once formed these dipole skyrmions are stable over a large field and temperature range including zero field and room temperature. We observe temperature and field dependent changes in the scattering vector (Q) for peak scattering related to the skyrmion lattice spacing. The origin of this change has led us to identify a key requirement necessary for the range of stability that we have observed in these amorphous thin films.

*Work at UCSD supported by DOE award No. DE-SC0003678. Neutron work was done at HFIR at ORNL supported by DOE BES and NCNR at NIST supported by DOC.
Multi-probe, laser-scanning optical microscopy for investigation of novel magnetic domain structures and boundaries  
AUSTIN KACZMAREK (Presenter), LIUYAN ZHAO, Univ of Michigan - Ann Arbor — Spin ordering in a magnetic material leads to the breaking of time-reversal symmetry along with some crystallographic symmetries, defining the magnetic symmetry group of the magnetic phase. Multiple degenerate ground states always exist, related through these broken symmetries, leading to interesting magnetic domain structures in macroscopic samples, which potentially host novel low-dimensional phases at the domain boundaries. In this talk, I will present our development of a spatially resolved, diffraction limited, ultrafast laser-based optical scanning microscope, which includes measurement capabilities of the magneto-optic Kerr effect (MOKE), a direct measure of broken time-reversal symmetry, and the optical second harmonic generation rotational anisotropy (SHG RA), a sensitive probe to broken spatial symmetries. I will present a comparison between this scanning-based microscope and a more traditional wide-field microscope. I will then discuss our experimental results on resolving magnetic domain structures in two types of antiferromagnetism, Ising and Heisenberg, on a honeycomb and a triangle lattice respectively. Finally, I will discuss the possibility of incorporating time-resolution into the aforementioned static probes.

Chirality-driven growth of stripe domains in Co/Ni/Pt-based multilayers*  
JEFFREY BROCK (Presenter), RAJASEKHAR MEDAPALLI, ERIC FULLERTON, Center for Memory and Recording Research, University of California, San Diego — The interfacial Dzyaloshinskii-Moriya interaction (iDMI) arising from inversion asymmetry at interfaces between magnetic materials and heavy metals with large spin-orbit coupling can transform DWs from Bloch to chiral Néel, leading to asymmetric DW propagation in the presence of a symmetry-breaking in-plane magnetic field. However, stripe domain growth in systems with iDMI is not yet well understood. Here we present an experimental study of [Co(0.7 nm)/Ni(0.5 nm)/Pt(0.7 nm)]N (1 ≤ N ≤ 5) multilayers designed to have asymmetric Pt/Co and Ni/Pt interfaces and perpendicular anisotropy. Kerr microscopy reveals that for N ≥ 3, reversal occurs via stripe domains and that when a static in-plane magnetic field is applied, the growth directionality is strongly linked to the field strength. For low fields, the domains grow roughly perpendicular to the field – a directionality not predicted by current understanding of the iDMI. The propagation direction becomes strongly collinear to the field at higher field magnitudes, as expected from the iDMI. Possible explanations in terms of a mixed domain wall with a mixed chiral Neel and chiral Bloch character will be discussed.

*This work was supported by US DOE Grant DE-FOA-0001810.
4:06PM J42.00009: High tunability of synthetic antiferromagnets applied in magnetic field sensing and memory devices*  
KANG WANG (Presenter), YIOU ZHANG, GANG XIAO, Department of Physics, Brown University — We investigated magnetic configurations in synthetic antiferromagnets (SAFs) of CoFeB/Ta/CoFeB by tuning interlayer exchange coupling (IEC, the energy density is denoted by $J_{ex}$) and perpendicular magnetic anisotropy (PMA, $K_u$). Two magnetic layers are either ferromagnetic or antiferromagnetic coupling, depending on both the non-magnetic layer thickness ($d_{NM}$) and the ferromagnetic layer thickness. Besides spin-flip transitions in SAFs with large PMA, we observed the canted magnetic configurations and spin-flop transitions when $K_u < J_{ex}/d_{NM}$. Most interestingly, the transfer curve of anomalous Hall resistance (magnetizations) becomes linear when tuning IEC and PMA to moderate values. This allows for applications in anomalous Hall effect (AHE) sensors with ultrahigh magnetic field detectability. Noise spectra reveal the magnetic field detectability reaches 100 nT/√Hz (at 1 Hz) at room temperature and decreases to sub-µT/√Hz (at 1 Hz) at 150 K. The studies indicate that the synthetic antiferromagnets are good candidates for both the magnetic memory devices and ultra-detectable magnetic field sensors with high thermal stability.

*We acknowledge the financial support by the US National Science Foundation through Grant No. DMR-1307056.

4:18PM J42.00010: Dynamic Skyrmion-Mediated Switching of Perpendicular MTJs: Scaling to 20 nm with Thermal Noise*  
MD MAHADI RAJIB (Presenter), WALID AL MISBA, DHRITIMAN BHATTACHARYA, JAYASIMHA ATULASIMHA, Virginia Commonwealth Univ — One method of creating and annihilating skyrmions in confined geometries is to use Voltage-Controlled Magnetic Anisotropy (VCMA) [1, 2, 3]. Previous study shows that robust voltage controlled ferromagnetic reversal from “up” to “down” state in the soft layer of a p-MTJ can be achieved by creating and subsequently annihilating an intermediate skyrmion state [4] in the presence of room temperature thermal noise and anisotropy variation across grains [4]. However, when scaling to 20 nm, thermal noise can annihilate the skyrmions, for example, by randomly moving the core towards the boundary of the nanostructure. Thus, a region of different anisotropy in the skyrmion core may be needed to stabilize the skyrmion state allowing competitive scaling. Here, we will investigate the extent to which the skyrmion mediated switching scheme can scale to lateral dimensions ~ 20 nm in ferromagnets.

References:

*NSF SHF Small Grant #1909030
4:30PM J42.00011: Skyrmion Breathing Modes in Synthetic Ferri- and Antiferromagnets*

MARTIN LONSKY (Presenter), AXEL HOFFMANN, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Magnetic multilayers that combine strong spin-orbit interaction with lacking inversion symmetry can give rise to the presence of topologically nontrivial spin textures, so-called magnetic skyrmions. Recent studies have indicated strongly enhanced propagation velocities of skyrmions in antiferromagnets and compensated ferrimagnets [1]. At the same time, it is unclear how magnetic compensation may affect dynamic excitations of magnetic skyrmions, such as breathing modes which entail an oscillation of the skyrmion size at GHz frequencies [2]. Here, we present micromagnetic simulations of these excitations in synthetic ferri- and antiferromagnets. The observed features in the calculated power spectra show a systematic dependence on the coupling strength between the individual layers and are related to pure breathing modes as well as to hybridizations of breathing and spin wave modes that are characteristic for the considered geometry. Based on these simulations, we then discuss the impact of these results for potential skyrmion sensing.


*This work is supported by the Deutsche Forschungsgemeinschaft (DFG) through the research fellowship LO 2584/1-1.

4:42PM J42.00012: Voltage Control of magnetic Skyrmions in patterned nanodots*

DHRITIMAN BHATTACHARYA (Presenter), Virginia Commonwealth Univ, SEYED ARMIN RAZAVI, HAO WU, BINGQIAN DAI, KANG-LUNG WANG, University of California, Los angeles, JAYASIMHA ATULASIMHA, Virginia Commonwealth Univ — Manipulation of magnetic skyrmions that are fixed in space can lead to the implementation of computing devices with smaller footprint. Moreover, if the control is achieved solely via applying an electric field, additional advantage of energy efficiency can be obtained. We have previously shown the feasibility of such a scheme by annihilating and creating skyrmions in a thin film of IrMn/CoFeB/MgO using Voltage Control of Magnetic Anisotropy (VCMA) [1]. However, in patterned structures, due to the confinement effect, complete reversal of skyrmion polarity as well as skyrmion mediated ferromagnetic reversal can be achieved using only voltage pulses [2, 3]. Here we propose to show this behavior in patterned nanodots of CoFeB sandwiched between an oxide and a heavy metal layer. We will also study the intermediate magnetic states during the reversal by performing magnetic force microscopy (MFM) imaging under in situ voltage. Finally, micromagnetic simulations will be presented that corroborate our experimental observations.


*NSF SHF Small Grant #1909030
The Dzyaloshinskii-Moriya Interaction (DMI) gives rise to chiral magnetic structures, which include chiral spin-chains and skyrmions. DMI requires broken inversion symmetry and can exist in the bulk as well as at interfaces. We use Brillouin Light Scattering spectroscopy (BLS) to determine the DMI from the non-reciprocal frequency-shift of Damon-Eshbach spin-waves [1]. In order to gain deeper insight into the underlying physics of DMI and explore ways, on how to tune the DMI through interface modifications, we prepared multiple sample series to study different aspects of the DMI, examples are: 1.) A Cu/Co\textsubscript{90}Fe\textsubscript{10} and a Pt/Co\textsubscript{90}Fe\textsubscript{10} sample series were in-situ oxidized for different times and subsequently capped to prevent any further oxidation. Density functional theory (DFT) calculations have demonstrated that the hybridization and the associated charge transfer is important for DMI at oxide interfaces. We determined that the spectroscopic splitting factor $g$ is correlated to the DMI. This is an indirect confirmation of the theory predictions. [2] 2.) We introduced a Cu dusting layer at the interface between CoFeB and Pt to disrupt the Heisenberg exchange directly at the interface. SQUID magnetometry shows that the Cu dusting layer reduces the proximity magnetization in the Pt as well. The proximity magnetization is a direct result of the exchange coupling and can be seen as a measure for its strength. 3.) So far, most work on DMI has been carried out for highly symmetric interfaces. Low symmetry systems can have anisotropic DMI. We prepared a Pt/Fe(110) sample and found that the DMI is anisotropic with the strongest DMI along the [001] direction, which coincides with the magnetic easy axis. We compared the results for the DMI with DFT calculations.


Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J43 DCOMP DAMOP DCMP: Precision Many-Body Physics V: Dynamics and Finite Temperature Properties 702 - Thomas Schaefer, Ecole Polytechnique - Tag(s): Focus
2:30PM J43.00001: T-linear resistivity and spectroscopy of hot metals and cold atoms: DMFT, SYK and beyond [Invited] ANTOINE GEORGES (Presenter), Collège de France, Paris and Flatiron Institute, New York — Many materials with strong electronic correlations display metallic-like resistivity up to very high temperature, with values exceeding the Mott-Ioffe-Regel (MIR) criterion (‘bad metals’). Understanding transport in this regime, in relation to spectroscopic probes such as optical conductivity and ARPES, raises the fundamental question of transport in regimes where long-lived quasiparticles may not exist. Recently, cold atomic gases in optical lattices have offered a beautiful experimental platform to investigate this question without the intervening effect of phonons. Even more challenging is the crossover into a ‘strange metal’ regime at lower temperatures, in which resistivity becomes smaller than the MIR value while still departing from Fermi liquid behaviour.

I will review recent work on these questions in the context of Dynamical Mean Field Theory and the Sachdev-Ye-Kitaev models, as well as high-temperature series expansions and several computational approaches. I will emphasize some commonalities between these approaches, and assess what is established at this point and which questions are still open.

3:06PM J43.00002: SYK non-Fermi-liquid solution of the Hubbard model* AARAM J. KIM (Presenter), Department of Physics, King’s College London, PHILIPP WERNER, Department of Physics, University of Fribourg, EVGENY KOZIK, Department of Physics, King’s College London — The bold-line diagrammatic technique solution of the Hubbard model in the strong coupling regime is of an SYK non-Fermi-liquid (nFL) type, obtained in a controlled way by the numerically exact diagrammatic Monte Carlo method. In the atomic (zero-hopping) limit, the solution corresponds to the unphysical branch of the Luttinger-Ward functional, for which the SYK model is the exact solution at the second order. Interestingly, the Green’s function retains its scaling form at higher orders. The solution for the doped 2d Hubbard model features an SYK-type nFL regime in a wide intermediate temperature range enclosed by the low-temperature Fermi-liquid and the high-temperature atomic limit. The possibility of SYK physics taking place in the Hubbard model is discussed.

*EPSRC grant EP/P003052/1

3:18PM J43.00003: Variational Schrieffer-Wolff Transformations for Quantum Many-body Dynamics* JONATHAN WURTZ (Presenter), PIETER W CLAEYS, ANATOLI S POLKOVNIKOV, Boston Univ — Building on recent results for adiabatic gauge potentials, we propose a variational approach for computing the generator of Schrieffer-Wolff transformations, and demonstrate its accuracy in spin chains and fermionic systems. Because of their variational nature, the generator goes beyond standard perturbative regimes and has accuracy controlled by the locality of the ansatz. This allows for precision non-equilibrium many-body dynamics far from integrable regimes, and can be considered as improvements to the Truncated Spectrum Approach.

*NSF DMR-1813499 and AFOSR FA9550-16-1-0334
3:30PM J43.00004: Investigating non-integrable quantum many-body systems with sub-exponential computational effort  PAVAN HOSUR (Presenter), Univ of Houston — Non-integrable quantum systems - systems with no or few conserved quantities - are generically exponentially hard to solve. Recent developments have proven, at least for small system sizes, that these systems satisfy the eigenstate thermalization hypothesis (ETH). Specifically, their physical properties such as expectation values of simple observables and few-point correlation functions, depend smoothly on macroscopic variables such as the energy density, particle density etc. This behavior explains, qualitatively, how statistical mechanics and ergodicity emerges from quantum mechanical laws for such systems. In this talk, an algorithm will be presented that enables quantitative predictions based on the ETH. In particular, it can simulate finite temperature properties of non-integrable systems with sub-exponential effort by exploiting the ETH. By expressing an eigenstate density matrix as truncatable series of orthogonal polynomials of the Hamiltonian, it will require only sparse matrix multiplication instead of matrix diagonalization. Moreover, it will store sparse matrices as vectors in the Fock space of operators, which reduces storage requirements from exponential to polynomial. Benchmarks between the algorithm and exact diagonalization on prototypical models will be shown.

3:42PM J43.00005: Space- and time-crystallization effects in multicomponent superfluids  BORIS SVISTUNOV (Presenter), NIKOLAI PROKOF'EV, Univ of Mass - Amherst — We observe that space- and time-crystallization effects in multicomponent superfluids—while having the same physical origin and mathematical description as in the single-component case—are conceptually much more straightforward. Specifically, the values of the temporal and spatial periods are absolute rather than relative, and the broken translation symmetry in space and/or time can be revealed with experiments involving only one equilibrium sample. We discuss two realistic setups—one with cold atoms and another one with bilayer superconductors—or observation of space and time crystallization in two-component counterflow
3:54PM J43.00006: A generic quantum Monte Carlo approach for electronic correlations in out-of-equilibrium systems.  CORENTIN BERTRAND (Presenter), Simons Foundation, SERGE FLORENS, Univ. Grenoble Alpes, CNRS, Institut Néel, F-38000 Grenoble, France, OLIVIER PARCOLLET, Simons Foundation, XAVIER WAINITAL, Univ. Grenoble Alpes, CEA, IRIG-PHELIQS, GT F-38000 Grenoble, France — We propose a systematic approach to the non-equilibrium dynamics of strongly interacting many-body quantum systems, building upon the standard perturbative expansion in the Coulomb interaction. High order series are derived from a determinantal diagrammatic Quantum Monte Carlo in the real time Keldysh formalism.

Such an algorithm was already designed by Profumo at al. (PRB, 91 245154 (2015)) and can compute perturbation series for single quantities after an arbitrary long (real) time evolution. We improved it to compute an entire time-dependent function in a single run. With a similar sampling method and computation time, the new algorithm gather much more information and give access to dynamical quantities directly in real frequencies.

The algorithm has been tested on the Anderson impurity model at equilibrium, and applied to the same system driven out of equilibrium by a bias voltage. In these systems, we obtained 10 orders of the Green's function perturbation series. To reach the non-perturbative regime, we developed a robust resummation scheme based on conformal transforms of the complex plane in the perturbation parameter.

4:06PM J43.00007: Dynamic Behavior of Strongly Coupled Quantum Dots  PHILIPP DUMITRESCU (Presenter), Simons Foundation, MARJAN MAČEK, Univ. Grenoble Alpes, CORENTIN BERTRAND, Simons Foundation, XAVIER WAINITAL, Univ. Grenoble Alpes, OLIVIER PARCOLLET, Simons Foundation — We study a system of strongly correlated quantum dots, using a recently developed diagrammatic quantum Monte Carlo approach. Here, one calculates high orders of Schwinger-Keldysh perturbation theory and uses numerical resummation to obtain spectral functions directly in real time. We show that even non-Fermi liquid behavior of strongly coupled quantum dots can be revealed. We study this behavior in both equilibrium and in situations where the dots are driven by an external current.
4:18PM J43.00008: Dynamical properties of the spin-boson model using real-time quantum Monte Carlo*  OLGA GOULKO (Presenter), Boise State University, GUY COHEN, MOSHE GOLDSTEIN, Tel Aviv University, HSING-TA CHEN, University of Pennsylvania — We present results for the real-time dynamics of the spin-boson model (a two-state system coupled to a bath of non-interacting harmonic modes) using the inchworm Monte Carlo algorithm. In particular, we study the population difference between the two states at strong system-bath coupling. We focus on sub-Ohmic spectral densities of the bosonic bath, where the system exhibits a second order quantum phase transition between localized and delocalized regimes. The inchworm algorithm is efficient over a wide range of temperatures (including low, intermediate, and high temperatures) and thus allows us to examine the changes in dynamics as the temperature is increased above zero and the emergence of a quantum critical fan.

*US-Israel Binational Science Foundation (Grants No. 2014262 and No. 2016087), The Chaoul Center for Nanoscale Systems

4:30PM J43.00009: Reconstructing Nonequilibrium Regimes of Quantum Many-Body Systems from the Analytical Structure of Perturbative Expansions  CORENTIN BERTRAND, Simons Foundation, SERGE FLORENS, CNRS, OLIVIER PARCOLLET (Presenter), Simons Foundation, XAVIER WAINTAL, CEA-Grenoble — We present a systematic approach to the nonequilibrium dynamics of strongly interacting many-body quantum systems, building upon the standard perturbative expansion in the Coulomb interaction. High-order series are derived from the Keldysh version of the determinantal diagrammatic quantum Monte Carlo algorithm. The reconstruction of physical quantities beyond the weak-coupling regime is obtained using a conformal change of variable, based on the approximate location of the singularities of these functions in the complex U plane, and a Bayesian inference technique, that takes into account additional non-perturbative relations, in order to control the amplification of noise occurring at large interaction. The approach is then applied to the Anderson quantum impurity model in the quantum dot geometry in and out of equilibrium.

4:42PM J43.00010: Time-symmetric stochastic action in curved phase-space  

PETER DRUMMOND (Presenter), MARGARET REID, RIA RUSHIN JOSEPH, Swinburne Univ of Tech — Quantum field dynamics is equivalent to a forward-backward stochastic process in both time directions, and can be calculated from an equilibration in a fifth space-time dimension [1]. Stochastic time-symmetric action principles in a curved phase-space are central to these results. They can be used to compute a stochastic bridge, the probability for random paths between two states, with any positive or negative diffusion. Such bridges have other precision applications, in fields ranging from many-body quantum dynamics to cell biology, control theory and finance.

Numerical methods and examples of solutions to the resulting stochastic partial differential equations in a higher time-dimension are obtained. These give agreement with exact solutions for bosonic quantum field dynamics, including entangled systems. This novel approach may lead to useful computational techniques, as the action principle is real. Of more fundamental significance is that it provides an ontological model of reality [2] in cosmological models, and allows an interpretation of objective measurement without wave-function collapse.

(1) P. D. Drummond, arXiv:1910.00001
(2) P. D. Drummond, M.D. Reid, arXiv:1909.01798

4:54PM J43.00011: Bounding the finite-size error for simulations of quantum many-body systems  

ZHIYUAN WANG (Presenter), KADEN HAZZARD, Rice Univ, MICHAEL FEIG, Honeywell Intl — Finite size errors are ubiquitous in numerical simulations of quantum many body systems, and an estimation of these errors is crucial to the assessment of the reliability of their results. In this talk I present rigorous upper bounds on finite size error of local observables measured in gapped ground states of locally-interacting systems, as well as in real time quench dynamics simulations initiated from a product state. The key step of our method relies on the well-known Lieb-Robinson (LR) bound, which is a direct consequence of locality. We show that the error bounds are practically useful, enabled by the recent tightening of the LR bounds [1]. For example, in a ground state simulation of the transverse field Ising model with J=1, h=2 and L=25 sites, the relative error for a center site observable is less than 2% and decays exponentially with system size. In a quench dynamics simulation of the same model, the relative error bound remains to be within 1% up to the time at which the system equilibrates, and decays superexponentially with system size at fixed time.

References:
5:06PM J43.00012: Thermofield theory for finite-temperature many-body physics*  
Gaurav Harsha (Presenter), Thomas M Henderson, Gustavo E Scuseria, Rice Univ — Wave function methods are widely used to study ground-state properties of many-electron systems in condensed matter physics and chemistry, and have therefore seen tremendous development over the last fifty years or so. But standard wave function techniques cannot easily be used to compute thermal properties, because doing so requires the entire spectrum and the problem becomes computationally intractable. Thermofield dynamics, which has seen widespread application as a field-theoretical tool to study non-equilibrium properties, provides a wave function representation for the thermal density matrix. In this talk, I will present our recently developed framework (arXiv:1901.06753 and 1907.11286) which shows how the thermofield theory can be utilized to construct finite-temperature generalizations of ground-state wave function methods. I will provide an example of thermal coupled cluster theory and present results for its performance on standard electronic and spin systems.

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5:18PM J43.00013: Analytical continuation of transport functions with deep neural networks*  
Simon Verret (Presenter), Mila, Université de Montreal & IQ, Université de Sherbrooke, Reza Nourafkan, Samuel Desrosiers, André-Marie Tremblay, Université de Sherbrooke — In the last few years, deep neural networks have proved to be highly efficient tools to address the problem of analytical continuation of the Matsubara Green’s function [1,2,3,4]. Extending these tools to reconstruct spectral representation of correlation function for transport quantities would be very beneficial because for several of transport quantities, such as Hall conductivity and Seebeck effect [5,6], the spectral weight is not strictly positive, restricting the use of the maximum entropy method. In this work, we extend the use of deep neural networks to the case of the longitudinal conductivity, in particular the DC-conductivity. We explore various modern architectures of neural network and various tailored-made loss functions for this problem.


*CFREF - Institut Quantique, CFREF - IVADO (postdoctoral sclarships program), Research Chair in the Theory of Quantum Materials, Canadian Foundation for Innovation, Ministere de l'Education des Loisirs et du Sport (Quebec), Calcul Quebec, Compute Canada

Tuesday, March 3, 2020 2:30 PM - 5:30 PM
2:30PM J44.00001: Quantifying Uncertainty in First-Principles Predictions of Phonon Properties and Thermal Conductivity [Invited]

ALAN MCGAUGHEY (Presenter), HOLDEN LOW PARKS, VENKAT VISWANATHAN, Carnegie Mellon Univ — We present a robust method for quantifying the uncertainty in phonon properties and thermal conductivity predicted from density functional theory calculations using the BEEF-vdW exchange-correlation (XC) functional. The procedure starts by displacing atoms in an equilibrium structure and using the energies of the perturbed structures to determine harmonic and anharmonic force constants. BEEF-vdW generates an ensemble of energies for each perturbed structure as a computationally efficient post-processing step by perturbing the XC functional and solving for the energy non-self consistently. Thus, each perturbed structure yields an ensemble of energies. This energy ensemble is then used to determine an ensemble of force constants, which is then used as input to lattice dynamics calculations and a solution of the Boltzmann transport equation. This procedure results in ensembles for the phonon frequencies, group velocities, and lifetimes, and overall heat capacity and thermal conductivity, whose spreads can be used to quantify uncertainty. Results for silicon, graphene, and graphite are presented and compared to predictions from the PBE, RPBE, and PBEsol XC functionals.

3:06PM J44.00002: From Coherent State Statistics to the Frozen Phonon Model*

CHRISTOPHER FECHISIN (Presenter), ERIC JOHNSON HELLER, Harvard University — We present a formalism for employing the basis of coherent states for analytical and numerical computations involving systems at thermal equilibrium. We identify an integration measure on the complex plane which may be understood as the weight function for a thermal distribution of coherent states. When applied to phonons in a thermally occupied harmonic crystal, this method yields an intuitive and rigorously quantum mechanical justification of the frozen phonon model of thermal diffuse scattering. In this and many other applications, the semiclassical dynamics of coherent states can mediate the application of classical reasoning to otherwise intractable quantum problems, including those involving anharmonic potentials. We also discuss and refine the concept of “quasi-elastic” scattering.

*This project was funded in part by the Harvard College Herchel Smith Undergraduate Research Fellowship.
**3:18PM J44.00003: Anomalous elasticity of 2D materials beyond self-consistent approximation**

DAVID SAYKIN (Presenter), Department of Physics, Stanford University, IGOR BURMISTROV, Landau Institute for Theoretical Physics, VALENTIN KACHOROVSKIĬ, Ioffe Physico-Technical Institute, IGOR GORNYI, Karlsruhe Institute of Technology — We study elastic properties of two-dimensional crystalline materials, such as graphene. It is known that in 2D membranes strong thermal fluctuations of flexural phonons lead to dramatic change of phonon spectrum and, as a result, in anomalous material-independent elastic properties, such as non-linear Hooke’s law under the low stress and auxetic behavior.

We compute elastic moduli \( \eta \) and Poisson ratio \( \nu \) of 2D membrane in the approximation of high embedded dimensionality \( d_c = 2 + d \). We go beyond one-loop approximation and find that famous self-consistent screening approximation is only as good as first-order approximation. Most remarkably, we analyze a case of disordered membrane and find new disorder-dominant phase, where all the critical exponents are different from the clean case. We find that phase transition happens at finite temperature in contrast to the prediction given by self-consistent screening approximation, that transition is only possible at absolute zero.

Presented work is a continuation of the results reported in papers PhysRevB.97.125402, PhysRevB.92.155428.

**3:30PM J44.00004: Continuity of phonon dispersion curves in layered ionic crystals**

NATALIE A HOLZWARTH (Presenter), YAN LI, WILLIAM KERR, Wake Forest Univ — We investigate in detail the origin of apparent discontinuities and mode disappearances in phonon band diagrams of ionic materials having hexagonal and other anisotropic structures. The phenomenon is due to the coupling of some of the vibrational modes to long wavelength electromagnetic waves within the material as described in 1951 by Huang. Modern analyses by Giannozzi, Gonze, Baroni, and others, based on density functional theory and density functional perturbation theory, have been implemented in several first principles code packages such as ABINIT and QUANTUM ESPRESSO. These use the so-called non-analytic correction to the dynamical matrix to correctly represent the modified longitudinal optical vibrational modes. In this work, we extend the analysis to include the transverse phonon-photon modes as well. The combination of the longitudinal and transverse phonon-photon mode dispersions are continuous functions of the wavevector \( \mathbf{q} \). These effects are demonstrated for cubic and hexagonal BN.

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1. https://doi.org/10.1088/1361-648X/ab4cc1

*Supported by NSF grant DMR-1507942.*
3:42PM J44.00005: Theoretical Analysis of Vibrational Lineshapes from Molecular Dynamics

ANDREW CUPO (Presenter), DAMIEN TRISTANT, KYLE REGO, VINCENT MEUNIER, Rensselaer Polytechnic Institute — The conventional spectral method for extracting anharmonic phonon properties from molecular dynamics (MD) requires prohibitively long simulations as the fitting function relies on the infinite time approximation. To that end, we derived the spectral lineshapes for arbitrary simulation lengths, while retaining the frequency shift and lifetime as fitting parameters. The theory was illustrated for graphene, hexagonal boron nitride, and silicon at the density functional theory (DFT) level, with up to nearly a factor of nine reduction in the required simulation time to reach convergence in the vibrational properties as compared to the standard approach. Such improvement in the convergence is expected in general provided the phonon anharmonicity is sufficiently weak, resulting in well-defined renormalized phonon quasiparticles. Application of the proposed approach has the potential to be far reaching as the theory applies equally well to ab initio MD based on DFT, time-dependent DFT dynamics, and parameterized force-fields and is thus expected to have important impact on topics ranging from strongly-correlated materials with sophisticated treatment of electron-electron interactions to biological systems.

3:54PM J44.00006: Influence of spin-orbit coupling and Rashba interaction on the electron-phonon renormalized electronic energy levels

VÉRONIQUE BROUSSEAU-COUTURE (Presenter), Département de physique, Université de Montréal and RQMP, Montréal, Québec, Canada, XAVIER GONZE, Institute of Condensed Matter and Nanosciences, UCLouvain, Louvain-la-Neuve, Belgium and Skolkovo Institute of Science and Technology, Moscow, Russia, MICHEL COTE, Département de physique, Université de Montréal and RQMP, Montréal, Québec, Canada — Electron-phonon (e-p) interaction calculations from first-principles are well documented in the literature. The predominance of non-adiabatic effects in the zero-point renormalization (ZPR) of the band gap for polar materials has been recently assessed in the light of the Fröhlich interaction. Yet, even for benchmark materials, spin-orbit coupling (SOC) is frequently neglected to reduce the numerical cost of calculations. SOC manifests itself in the electronic structure through the split-off energy and by lifting band degeneracies away from time-reversal invariant momenta (TRIM). This modification of the energy levels will affect both e-p coupling energies and ZPR. Materials lacking inversion symmetry also exhibit an in-plane shift of the band extrema away from the TRIM, known as Rashba splitting. This could lead to resonant couplings at finite phonon wavevectors, which will strengthen the EP coupling energies.

We explicitly compute e-p coupling energies and ZPR for binary semiconductors, using density-functional perturbation theory (DFPT), with and without SOC. We also investigate Rashba semiconductor BiTeI. We finally analyze our results in the light of a three-dimensional Fröhlich Hamiltonian, including both SOC and Rashba interaction.

*NSERC BESC-D and Grant No. RGPIN-2016-06666
4:06PM J44.00007: Anharmonicity in Zirconium Hydrides: a first-principles study combined with inelastic neutron scattering  
JIAYONG ZHANG (Presenter), North Carolina State University, YONGQIANG CHENG, ALEXANDER KOLESNIKOV, Oak Ridge National Laboratory, JERRY BERNHOLC, WENCHANG LU, North Carolina State University, ANIBAL J. RAMIREZ-CUESTA, Oak Ridge National Laboratory — Zirconium Hydrides and Deuterides are candidates for neutron moderators and fuel-rod cladding materials. We investigate anharmonic phenomena in these materials using inelastic neutron scattering (INS) and lattice dynamics calculations within the framework of density functional theory (DFT). We observe multiple sharp peaks below harmonic (free) multi-phonon bands in the experimental spectra, which do not show up in the simulated INS spectra based on the harmonic approximation. We have thus carried out a detailed study of the anharmonicity by exploring the 2D potential energy surface with DFT calculations and solving the corresponding 2D single-particle Schrödinger equation of the H/D atom in zirconium hydrides/deuterides to get the eigenfrequencies. The results describe well the experimental INS spectra, showing harmonic behavior of the fundamental modes and strong anharmonicity at higher energies. The DFT calculations were carried out with the real-space multigrid (RMG) and VASP codes, and the experimental INS spectra were measured with the VISION spectrometer at the Spallation Neutron Source, Oak Ridge National Laboratory.

4:18PM J44.00008: Phonon-induced topological phase transition in SnTe*  
JOSE D. QUERALES-FLORES (Presenter), Tyndall National Institute, Cork, Ireland, PABLO AGUADO-PUENTE, Queen's University Belfast, Belfast, UK, DORDE DANGIC, Tyndall National Institute, Cork, Ireland, JIANG CAO, Nanjing University of Science and Technology, Nanjing, China, TCHAVDAR TODOROV, MYRTA GRÜNING, Queen's University Belfast, Belfast, UK, STEPHEN B FAHY, IVANA SAVIC, Tyndall National Institute, Cork, Ireland — Unlike the topologically trivial semiconductor PbTe, SnTe has an inverted band gap at the L point that gives rise to a topological crystalline insulating phase protected by mirror symmetry [1]. In this work, we calculate the temperature renormalization of the electronic band structure of SnTe. We account for the energy shift of the electronic states due to thermal expansion, and electron-phonon interaction using the nonadiabatic Allen-Heine-Cardona formalism within density functional perturbation theory [2,3]. Corrections to the electronic band structure due to electron-electron interaction are obtained using many-body perturbation theory (GW). We capture the decrease of the direct gap with temperature yielding a temperature-induced phase transition to a topologically trivial phase at ~800 K. We find that both thermal expansion and electron-phonon interaction have a considerable effect on these temperature variations. We also analyze the temperature dependence of the electron-phonon self-energy.


*This work is supported by Science Foundation Ireland under Investigators Programme No. 15/IA/3160.
Phonon renormalization and four-phonon scattering in semiconductors and insulators

NAVANEETHA KRISHNAN RAVICHANDRAN (Presenter), DAVID BROIDO, Boston College —

In semiconductors and insulators, heat is carried by phonons. Conventional ab initio methods for thermal conductivity ($k$) of materials assume that the lowest order theory of 3-phonon scattering sufficiently describes thermal transport. Here we show that this is not the case for several materials where higher-order 4-phonon scattering can significantly affect $k$. Furthermore, we show that for many naturally occurring materials, phonon scattering is so strong that not only is 4-phonon scattering important, but the underlying phonon quasiparticle picture itself can break down. To address this issue, we present a novel ab initio method that features an anharmonic many-body renormalization scheme to create well-defined phonon quasiparticles with weakened interactions, and includes both 3-phonon and 4-phonon scattering to obtain $k$ [1]. We demonstrate the method's success by comparing with experimental data of $k$ for many common semiconductors and insulators. Our work presents a unified ab initio framework to accurately predict the thermal properties of solids with varying bond strengths.


*This work was funded by ONR MURI [No. N00014-16-1-2436]

Ab-initio calculation of Seebeck coefficient of transition-metal elements

HISAZUMI AKAI (Presenter), Univ of Tokyo, SONJU KO, Tokyo Institute of Technology — Ab-initio calculation of the Seebeck coefficient $S$ of transition metal elements are performed within the framework of Kubo–Greenwood formula. The difficult points of calculating $S$ are that, firstly, at $T = 0K$, the conductivity of pure metal diverges. Second, the Fermi surfaces of transition metals composed of many different states where the constant relaxation time approximation breaks down. To overcome the difficulties, we included the effects of electron-phonon scattering in the calculation of $S$. We exploited the Korringa–Kohn–Rostoker (KKR) Green's function method combined with the Kubo–Greenwood formula. The electron-phonon scattering was taken into account through ab-initio phonon calculations and an alloy analogy applied to the local static phonons. The KKR coherent potential approximation (KKR–CPA) was used for the latter. The calculated Cu resistivity and the Seebeck coefficients for various transition-metal elements at finite temperature show reasonable overall agreements with experiments. The present approach provides us with a framework applicable to a wide range of materials, including pure metals, compounds, ordered and disordered alloys.

*This work is partly supported by Grants-in-Aid for Scientific Research (MEXT 23654133, 26400330, and 17K05566).
4:54PM J44.00011: Understanding the Restoring Force From a Local Bonding Perspective: A First-Principles Picture of Phonons and Elasticity* ETHAN RITZ (Presenter), GURU BAHADUR KHALSA, HSIN-YU KO, ROBERT DISTASIO, NICOLE A BENEDek, Cornell University — Though the calculation of bulk elastic quantities and phonon frequencies using modern ab-initio techniques is now routine, understanding the crystal chemical origins of these properties is still an open question. How do we relate the value of a specific bulk elastic constant or vibrational mode to chemically intuitive ideas about local structure and bonding, especially when our calculations are often done in a spatially delocalized Bloch basis? Using a basis of maximally localized Wannier functions, we partition the total electronic energy onto real space representations of occupied states, as well of the curvature of that energy with respect to mechanical deformations and phonon distortions. By understanding how the energy of each individual bond changes with these distortions, we can obtain orbitally decomposed, chemically specific understanding of bulk properties. We use this approach to explore various perovskite oxides, exploring the chemical origins of elasticity, structural phase transitions, Grüneisen parameters, and thermal expansion properties, and discuss the possibility of enhancing or controlling these properties.

*This work was supported by the National Science Foundation (DMR-1550347)

5:06PM J44.00012: Finite temperature electronic properties of diamond and diamondoids* ARPAN KUNDU (Presenter), Pritzker School of Molecular Engineering, University of Chicago, MARCO GOVONI, Argonne National Laboratory, MICHELE CERIOTTI, Ecole polytechnique federale de Lausanne, FRANCOIS GYGI, University of California, Davis, GIULIA GALLI, Pritzker School of Molecular Engineering, University of Chicago — Accurate calculations of electron-phonon coupling are essential to predict the finite temperature (T) properties of materials and molecules, especially those containing light-atoms. We present an approach to compute electron-phonon coupling which treats the motion of ions quantum mechanically, through the use of path-integral calculations, and the electronic states at the DFT or many-body-perturbation theory (MBPT) level. In particular, we carried out simulations for diamond and diamondoids by coupling the first-principle molecular dynamics code Qbox (http://qboxcode.org) with i-PI (http://ipi-code.org), a path integral simulation package, and we obtained single-particle energy levels within MBPT using the WEST code (http://west-code.org). We present results for different cluster sizes and surface terminations and we compare the zero-temperature limit of our simulations with results recently reported for electron-phonon coupling at T=0 [1].


*Supported by the Midwest Integrated Center for Computational Materials (MICCoM) as part of the Computational Materials Sciences Program funded by DOE/BES.
The FeTi system is amenable to computational investigations due to its simple crystal structure and minimalist Fermi surface. A thermally-driven electronic topological transition that results in anomalous phonon softening was recently reported to occur in FeTi at elevated temperatures as new features appear in the Fermi surface and new spanning vectors increase electronic screening of particular phonon modes. We investigated the pressure dependence of the electronic structure and the phonon dispersions using density functional theory and uncovered an octahedral splitting with an energy difference that increases with pressure and a Kohn anomaly with a wavevector that decreases with pressure. The calculated Fe partial phonon density of states are in agreement with nuclear-resonant inelastic x-ray scattering measurements and show that the phonons stiffen at different rates.

Session J45 DCOMP GDS DSOFT DPOLY: Emerging Trends in Molecular Dynamics Simulations and Machine Learning I

Pankaj Rajak (Presenter), LCF, Argonne National Laboratory — In recent years, machine learning models based on supervised learning has shown tremendous success in materials property prediction such as band gap, elastic modules, thermo-electric properties that has accelerated the discovery of new materials. However, applicability of these supervised learning-based ML models is limited, and they cannot be used for complex tasks such as inverse design of materials structure, where the input to the ML model is desired property and the output is structure of the material. Deep leaning models based on reinforcement learning and deep generative model can be used for inverse design of materials. In particular, in this talk we will discuss about (1) designing MoS$_2$ kirigami structure with desired stretchability, (2) computational synthesis of layered materials using reinforcement learning and (3) a generative model based on graph convolution to design polymer structure with desired dielectric properties.

This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0014607. An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.
3:06PM J45.00002: Unbiasing machine learning for molecular dynamics: emphasising out-of-equilibrium geometries using clustering

GRÉGORY CORDEIRO FONSECA (Presenter), IGOR POLTAVSKYI, ALEXANDRE TKATCHENKO, University of Luxembourg — Machine learning (ML) force-fields (FF) became an increasingly popular tool in computational physics due to their speed and accuracy. By construction, ML models are often biased towards more abundant "close-to-equilibrium" states. A small mean error does not guarantee accurate prediction for rare "out-of-equilibrium" configurations, which are typically underrepresented in reference datasets.

We propose a method to train unbiased ML FF, which leads to equally accurate predictions independently of the density of training data. To achieve this, we divide datasets into smaller subsets (clusters) based on data similarities. Then, the quality of a ML model is evaluated for each individual cluster, thereby revealing problematic cases. Representative data for each problematic cluster is added to the training set, and the ML model is retrained. The improved learning process results in a flattening of the prediction errors throughout the reference data. The method is applied to molecular trajectory datasets, decreasing the largest errors of the obtained ML FF up to an order of magnitude.

3:18PM J45.00003: Challenges in developing an extremely accurate many-body force field

ELIZABETH DECOLVENAERE (Presenter), RIAN CORT KORMOS, ALEXANDER DONCHEV, JOHN L KLEPEIS, DAVID E. SHAW, D. E. Shaw Research — Our group has been working to develop a physics-motivated, generalizable model fit only to quantum chemical data that reproduces experimental values of condensed phase properties across a wide range of conditions. Developing such a model is challenging and requires better physical models and higher accuracy quantum chemical reference data than are typically used when developing force fields for molecular dynamics simulations. I will describe some of our recent work that leverages machine learning ideas to generate high-accuracy quantum chemical reference data for the fitting of two-body and many-body models. I will also outline some theoretical and practical challenges in modeling many-body interactions and show a few preliminary results on small molecules of biochemical interest.

3:30PM J45.00004: Uncertainty quantification in molecular simulations with dropout neural network potentials

MINGJIAN WEN (Presenter), University of California, Berkeley, ELLAD B. TADMOR, University of Minnesota, Twin Cities — Machine learning interatomic potentials (IPs) can provide accuracy close to that of first-principles methods, such as density functional theory (DFT), at a fraction of the computational cost. This greatly extends the scope of accurate molecular simulations, providing opportunities for quantitative design of materials and devices on scales hitherto unreachable by DFT methods. However, machine learning IPs have a basic limitation in that they lack a physical model for the phenomena being predicted and therefore have unknown accuracy when extrapolating outside of their training set. In this paper, we propose a new class of Dropout Uncertainty Neural Network (DUNN) potentials, which provide rigorous uncertainty estimates that can be understood from both Bayesian and frequentist statistics perspectives. As an example, we develop a DUNN potential for carbon and show how it can be used to predict uncertainty for static and dynamical properties including stress and phonon dispersion in graphene. In addition, we show that DUNN uncertainty estimates can be used to detect configurations outside the training set, and in some cases, can serve as a predictor for the accuracy of a calculation.
3:42PM J45.00005: Improving Fidelity and Transferability of Machine-Learned Reactive Interatomic Models Through Active Learning  REBECCA LINDSEY (Presenter), LAURENCE FRIED, NIR GOLDMAN, SORIN BASTEA, Lawrence Livermore Natl Lab — Force fields of machine-learned (ML) topography are ideal for describing complex phenomena including condensed phase chemistry, but parameterization is often challenging due to the proclivity for overfitting exhibited by high-flexibility models. Active learning provides an alternative route to robust ML model development, however there is no “one-size-fits” all solution. In this work, we present the Chebyshev Interaction Model for Efficient Simulation (ChIMES), a ML force field targeting chemistry in condensed phase systems. ChIMES models are comprised of linear combinations of Chebyshev polynomials explicitly describing many-body interactions and thus can also exhibit overfitting. We discuss development of a ChIMES active learning scheme leveraging physical intuition and Shannon information theory for systematic improvements in fidelity and transferability of resulting models.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

3:54PM J45.00006: Uncertainty quantification of classical interatomic potentials in OpenKIM database*  YONATAN KURNIAWAN (Presenter), CODY PETRIE, KINAMO JAHALI WILLIAMS, MARK TRANSTRUM, Brigham Young Univ - Provo — Interatomic models (IMs) are used in molecular modeling to predict material properties of interest. The development of a single IM can take anywhere from several months to years and relies on expert intuition, and yet these potentials are usually only valid for a particular application of interest. Extending existing IMs to new applications is an active area of research. Quantifying the uncertainty of an IM can tell us how much we can trust the predictions it makes. I compare Bayesian (Markov Chain Monte Carlo) and Frequentist (profile likelihood) methods to quantify uncertainty of IM parameters. I demonstrate these methods on Lennard-Jones and Morse potentials fit to triclinic crystal configurations from the OpenKIM database. Results indicate that these models are "sloppy" in some of their parameters, i.e., likelihood surfaces have long, narrow canyons and broad, flat plateaus. I discuss the relative strenghts and weaknesses of each approach.

*This work is supported by the NSF under award CMMT-1834332.

4:06PM J45.00007: Molecular dynamics density and viscosity simulations of alkanes  PAVAO SANTAK (Presenter), GARETH CONDUIT, Univ of Cambridge — We use molecular dynamics to study liquid density of small branched alkanes and kinematic viscosity of linear alkanes. The density models compare well to experimental values, with an average absolute deviation of 3.38 g/l. We run non-equilibrium molecular dynamics simulations for viscosity to explore its shear rate profile, which is used to extrapolate Newtonian viscosity. We develop a new method to systematically identify the range of shear rates at which the simulations are performed. We compare our models of linear alkanes as a function of temperature and pressure with experimental values, obtaining an average percent error of -1.1%.
Study of the microstructure of amorphous silicon and its effect on Li transportation with neural network potential*  

WENWEN LI (Presenter), YASUNOBU ANDO, AIST — The machine learning-based simulation methods have attracted much attention recently. In this talk, neural network (NN) potential is used to study Li diffusion mechanism in amorphous silicon (α-Si).

The structure and property of the experimental α-Si sample are significantly affected by the experimental fabrication method. In this work, the NN potential was used to generate a series of atomic structures of α-Si with different degrees of disorder. By systematically comparing various structural and vibrational properties with experiments, we can determine the corresponding theoretical model for experimental samples prepared with a certain method.[1]

The kinetics of Li diffusion in α-Si is one of the most important issues for its performance as the anode of lithium-ion battery. The effect of structural order on Li diffusion behavior is investigated with NN potential. We found that Li transportation needs higher activation energy in the highly disordered α-Si matrix. The result can be explained with the “trap” mechanism.


*Our works presented in this talk were supported by a project (No. P16010) commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

Relative entropy indicates an ideal concentration for structure-based coarse graining of binary mixtures*  

DAVID ROSENBERGER (Presenter), Los Alamos National Laboratory, NICO F. A. VAN DER VEGT, Chemistry, TU Darmstadt — Many methodological approaches have been proposed to improve systematic or bottom-up coarse-graining techniques to enhance the representability and transferability of the derived interaction potentials. Here, we shift the focus away from methodological aspects and rather raise the question whether we can overcome the disadvantages of a given method in terms of representability and transferability by systematically selecting the state point at which the CG model gets parametrized. We answer this question by applying the inverse Monte Carlo (IMC) approach—a structure-based coarse-graining method—to derive effective interactions for binary mixtures of simple Lennard-Jones (LJ) particles, which are different in size. For such simple systems we indeed can identify a concentration where the derived potentials show the best performance in terms of structural representability and transferability. This specific concentration is identified by computing the relative entropy which quantifies the information loss between different IMC models and the reference LJ model at varying mixture compositions.

*Financial support is granted by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through Project No.233630050-TRR 146.
4:42PM J45.00010: Exploring, fitting, and characterizing the configuration space of materials with multiscale universal descriptors  NOAM BERNSTEIN (Presenter), United States Naval Research Laboratory, VOLKER L DERINGER, Department of Chemistry, University of Oxford, GÁBOR CSÁNYI, Department of Engineering, University of Cambridge — Descriptors of the environment of an atom in a material give a similarity metric between different structures. We present a universal set of multiscale Smooth Overlaps of Atomic Position (SOAP) parameters that can be used for a wide range of purposes. For each atom type these consist of two or more SOAP expansions of the smoothed atomic neighbour density with cutoffs (and proportionately scaled smoothness parameters) related by a constant factor, covering bond lengths from the shortest to the longest expected for that species in the system. These descriptors can be used as part of an automatic interatomic potential generation process by combining iterated random structure search (RSS) with Gaussian Approximation Potential (GAP) fitting. We show results from the GAP-RSS process for elemental and multicomponent systems, as the procedure simultaneously explores and fits a wide range of structures. The descriptors can also be used in the context of characterization of large sets of configurations. As an example, we show the results of large scale and long time simulations such as quenching of a liquid into an amorphous structure, and the relation between the fitting data set of a potential and the configurations that occur in tests of physically meaningful material properties.

4:54PM J45.00011: Predictive Atomistic Simulations of Materials using SNAP Data-Driven Potentials  AIDAN THOMPSON (Presenter), MITCHELL WOOD, MARY ALICE CUSENTINO, JULIEN TRANCHIDA, Computational Multiscale, Sandia National Laboratories, NICHOLAS LUBBERS, Computer Computational Statistical Sciences, Los Alamos National Laboratory, STAN MOORE, Computational Multiscale, Sandia National Laboratories, RAHUL GAYATRI, Application Performance, NERSC, Lawrence Berkeley National Laboratory — Molecular dynamics (MD) is a powerful materials simulation method whose accuracy is limited by the interatomic potential (IAP). SNAP is an automated methodology for generating accurate and robust application-specific IAPs. SNAP is formulated in terms of a set of general four-body geometric invariants that characterize the local neighborhood of each atom. This approach has been used to develop potentials for diverse materials, including metals (Ta, W), metal alloys (AlNbTi), III-V semiconductors (InP), and plasma-facing materials (W/Be/He/H/N). Each SNAP IAP is trained on DFT calculations of energy, force, and stress for many small configurations of atoms. Cross-validation analysis and evaluation on test problems are used to further improve IAP fidelity and robustness. Varying the number of geometric descriptors allows a continuous tradeoff between computational cost and accuracy. The resultant potentials enable high-fidelity MD simulations of these materials, yielding insight into their behavior on lengthscales and timescales unreachable by other methods. The relatively large computational cost of SNAP is offset by combining LAMMPS' spatial parallel algorithms with Kokkos-based hierarchical multithreading, enabling the efficient use of Peta- to Exa-scale CPU and GPU platforms.
5:06PM J45.00012: Accurate and Data-Efficient Machine Learning Force Fields for Periodic Systems  
LUIS GÁLVEZ-GONZÁLEZ (Presenter), Programa de Doctorado en Ciencias (Física), Universidad de Sonora, HUZIEL SAUCEDA, STEFAN CHMIELA, Machine Learning Group, Technische Universität Berlin, ALVARO POSADA-AMARILLAS, Departamento de Investigación en Física, Universidad de Sonora, LAURO OLIVER PAZ-BORBÓN, Instituto de Física, Universidad Nacional Autónoma de México, KLAUS-ROBERT MÜLLER, Machine Learning Group, Technische Universität Berlin, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, University of Luxembourg — It remains a substantial challenge to develop machine learning force fields that combine accuracy, efficiency, and physical interpretability, especially for complex periodic systems. In this work, we present an extension of the symmetrized gradient-domain machine learning (sGDML) framework [1][2] for periodic systems, which allows the construction of accurate molecular force fields with high data efficiency. We test this implementation in a variety of systems, including 2D materials, bulk materials and surfaces, for which we achieved errors of less than 1 kcal/mol/Å for atomic forces using less than 100 training points. Furthermore, in the particular case of graphene this error was achieved training on 20 samples. The low errors from sGDML calculations on phonon dispersion relations and thermodynamic properties compared to those obtained directly from DFT further confirm the predictive power of the model. These results extend the applicability of machine learning to increasingly complex periodic materials.


5:18PM J45.00013: Phase diagrams of nuclear pasta phases in neutron star matter  
JORGE MUNOZ (Presenter), JORGE ALBERTO LOPEZ, University of Texas, El Paso — Neutron stars are the remnants of the supernova explosion of a massive stars and gravitational collapse and have densities that approach that of atomic nuclei. Nuclear pasta is a theoretical type of nuclear matter that is hypothesized to exist within their core. We performed classical molecular dynamics simulations with modified Pandharipande potentials at temperatures from 0.2 to 4 MeV, densities from 0.04 to 0.08 nucleons/fm3, and proton fraction from 0.1 to 0.5. We built a dataset of configurations by selecting 9,600 uncorrelated instants from the simulations and calculated the Minkowski functionals (volume, surface, integral mean curvature, and Euler characteristic) from which the phase of the nuclear pasta at each instant can be determined. We then used the dataset to train a neural network that allowed us to build phase diagrams for nuclear pasta phase similar to those that are used in traditional materials research.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J46 GMAG: Single Molecule Magnets  
708 - Selvan Demir, Michigan State Univ -  
Tag(s): Focus
2:30PM J46.00001: The power of typicality applied to magnetic molecules and low-dimensional quantum spin systems* [Invited] JUERGEN SCHNACK (Presenter), Univ Bielefeld — Molecular or low-dimensional quantum spin systems often prevent an exact calculation of their magnetic properties due to a prohibitively large size of the related Hilbert spaces. Typicality-based approaches such as the finite-temperature Lanczos method allow to investigate rather large systems with unprecedented accuracy. This way quantum critical as well as magnetocaloric properties of large cyclic clusters could be elucidated. For the kagome lattice antiferromagnet it became possible to model a lattice of size N=42 (!) quasi exactly. This enabled us to study in particular that the low-lying density of singlet states moves up in energy contrary to common believe. In addition, we could demonstrate for lattices up to 72 sites that magnon crystallization occurs slightly below the saturation field, an effect driven by the existence of flat energy bands.


*Computing time at the Leibniz Center in Garching (Germany) is gratefully acknowledged.

3:06PM J46.00002: Effect of substrate on characteristics of the Mn₃ dimer* ZAHRA HOOSHMAND (Presenter), RAINIER BERKLEY, TALAT S. RAHMAN, Department of Physics, University of Central Florida — Single-molecule magnets (SMMs) are considered candidates for next generation information technology. These molecules possess high spin and their ground states can be tuned. The Mn₃ dimer is such an example in which the Mn₃ triangles are connected via linkers to form either the ferromagnetic (FM) or the antiferromagnetic (AFM) ground state. One challenge for SMMs is finding a suitable substrate that keeps their magnetic properties intact. We present results of our spin-polarized density functional theory calculations of the adsorption and interactions of Mn₃ dimers on graphene and monolayer hexagonal boron nitride (h-BN). We show that while graphene is benign, h-BN has interesting interaction with the SMMs. We compare the effect of these two substrate on the magnetic properties and electronic structure of the Mn₃ dimers. We also show that charge corrections need to be accounted for in the calculations for reliable description of the isolated as well as supported Mn₃ dimers. Results will be compared with available and ongoing experimental results.

*This work is supported by DOE-DE-SC0019330.
A DFT Study of Single-Molecule Magnets (Mn$_3$ Dimers)*

RAINIER BERKLEY
(Presenter), ZAHRA HOOSHMAND, Physics, Univ of Central Florida, JIE-XIANG YU, HAI-PING CHENG, Physics, University of FL, TALAT RAHMAN, Physics, Univ of Central Florida — Single-molecule magnets (SMMs) have become of increasing interest for magnetic technology. This is due to their many quantum phenomena and the ability to modify their structure and magnetic properties. It is thus important that SMM properties be characterized; thus, two configurations of the Mn$_3$ dimer ferromagnetic (FM) and antiferromagnetic (AFM) have been studied via Density Functional Theory (DFT). Our calculations for the total spin of the FM (S = 12) and AFM (S = 0) configurations of the isolated dimers, agrees with the experimental spin results per monomer (S = 6)\(^1\) only when the dimers are charged (+2) (similar to molecules in solvent). This charge issue brings about long range jellium effects which have to be corrected in DFT. Our results shed insight into the differences between the magnetic anisotropy, magnetic coupling constants and the spin for both the neutral and the charged (+2) versions of the FM and AFM dimer as a comparison. The application of the Makov-Payne method, for charge corrections, results in very small changes to the magnetic anisotropy and the magnetic coupling constants for both charged version of the Mn$_3$ dimers.

\(^1\) Nguyen et al. J. Am. Chem. Soc. 2015, 137, 7160−7168.

*This work is supported by DOE-DE-SC0019330

Atomic-clock transition behavior in a Cr$_7$Mn molecular nanomagnet*

GAJADHAR JOSHI, ILIJA NIKOLOV, GUANCHU CHEN, Amherst College, DANIEL SAVA, GRIGORE TIMCO, RICHARD WINPENNY, Department of Chemistry, University of Manchester, JONATHAN FRIEDMAN (Presenter), Amherst College — A clock transition (CT) occurs at an avoided level crossing where the transition frequency is independent on the magnetic field. Enhancement of $T_2$ has been observed at clock transitions in some molecular nanomagnets, suggesting these systems as viable spin qubits [1,2]. The study of such systems can elucidate the mechanisms of decoherence since spin-spin interactions are suppressed at CT. A CT is observed in the $S = 1$ molecular magnet Cr$_7$Mn with pulsed electron-spin resonance. The Carr-Purcell Meiboom-Gill (CPMG) pulse sequence in dilute samples of Cr$_7$Mn increases $T_2$ more than an order of magnitude over that obtained with a Hahn echo sequence, indicating that a significant decoherence mechanism arises from fluctuations that are slower than the delay between the CPMG pulses (~1 us). We also observe electron spin echo envelope modulation (ESEEM) at fields slightly away from the zero-field avoided crossing. Remarkably, CPMG provides a significant enhancement to $T_2$ when the pulse period matches the ESEEM period, suggesting that CPMG dynamically decouples the molecular and the nuclear spins.


*Work supported by NSF under Grant No. DMR-1708692, and by the Amherst College Dean of Faculty.
Chemical Approaches to Quantum Information Science

Stephen Von Kugelgen, Daniel Laorenza, Northwestern University, Joseph Zadrozny, Chemistry, Colorado State University, Chung-Jui Yu, Danna Freedman (Presenter), Northwestern University — Synthetic chemistry enables us to build up systems from the bottom up with angstrom scale precision. We harness this precise synthetic control towards the emerging challenge of quantum information science (QIS), in which we are creating and understanding qubits, the smallest unit of a QIS system. Our approach enables fundamental insight into the factors that contribute to electronic spin decoherence, the creation of qubits with millisecond coherence times, and the creation of arrays of qubits. These results and others will be described.

The muon-fluorine interaction: a model quantum system for exploring decoherence

Stephen Blundell (Presenter), John Wilkinson, Physics, University of Oxford, Franz Lang, ISIS, STFC, Tom Lancaster, Physics, University of Durham — In non-magnetic fluorides, an implanted muon will stop very close to the highly electronegative fluoride ion, or very often stop between two of them. The dipolar interaction between the fluorine nuclei spins and the muon spin gives rise to a characteristic signature which characterises the state. The remaining fluorine nuclei are more distant and usually ignored, since their coupling to the muon is weaker. We show that taking them properly into account allows one to model the data in greater quantitative detail, understand the stopping site more accurately, and explore how the quantum information held by the state decoheres into its environment.

We thank EPSRC (UK) for funding.

Decoherence of Molecular Qubits: Insights From Quantum Many-Body Simulations

Jia Chen, University of Florida, Cong Hu, University of Connecticut, John Stanton, Hai-Ping Cheng, Xiaoguang Zhang (Presenter), University of Florida — Quantum properties of magnetic molecules will drive their applications in quantum information science. Electron spin decoherence time in such molecules depends strongly on molecular structure. A synthetic study of a series of vanadyl molecular qubits by Danna Freedman’s group found that the decoherence time decreases as size of molecule increases. To explain this counterintuitive experimental result and provide insights for decoherence in molecular qubits in general, we combine ab-initio electronic structure calculations and quantum many-body simulation to study hyperfine interactions between electron and hydrogen nuclear spins and their effects on electron spin decoherence. We show that, for an isolated molecule, decoherence is always incomplete, but the residual coherence decreases as the size of the molecule increases. This result explains the experimentally observed diffusion barrier for decoherence, also suggests a quantitative approach to connect molecular structure and diffusion barrier.


This work was supported as part of the Center for Molecular Magnetic Quantum Materials (M2QM), an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0019330.
Counterintuitive Control of Molecular Magnetic Relaxation via Chemically Tunable Electron-Spin Baths  
IAN MOSELEY, JOSEPH ZADROZNY (Presenter), Colorado State Univ — Magnetic molecules are critical components in current and next generation applications in molecular imaging and information processing. Toward functionality in these applications, long spin-lattice and spin-spin relaxation times are desired. However, most magnetic molecules display fast relaxation times when in the presence of a magnetic environment. Bioimaging and information storage environments are nuclear and electron spin-rich. Hence, we need to understand how to design long relaxation times in highly magnetic environments. This presentation will detail our efforts toward that knowledge by studying the spin-bath-to-molecule interaction via molecular chemistry and magnetic analysis. Specifically, we will discuss the response of the relaxation times in a set of cobalt-containing molecules to a chemically tunable magnetic environment as determined by electron spin resonance and alternating current magnetic susceptibility. In the long term, these fundamental studies will deliver design principles for molecules with long relaxation times in magnetically chaotic environments.

Investigating the Magnetic Properties of the Giant Mn$_{84}$ Torus*  
DIAN-TENG CHEN (Presenter), Department of Physics and Quantum Theory Project, University of Florida, ASHLYN HALE, GEORGE CHRISTOU, Department of Chemistry, University of Florida, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — The giant single-molecule magnet Mn$_{84}$ has a shape of torus of eighty-four Mn$^{3+}$ ions ($S=2$). As the manganese atoms in Mn$_{84}$ are all bridged by O$_2^-$ or MeO$^-$ groups, strong pairwise exchange interactions between these manganese atoms are expected. Even though the magnetic susceptibility of this system has been measured experimentally, its electronic-magnetic structure and spin-spin couplings remain unknown. In this work, we investigate these interactions using first-principles calculations, from which a Heisenberg model is developed. The exchange coupling constants are extracted by fitting to the total energies of different spin configurations of Mn$_{84}$. In addition, we compute the magnetic anisotropy energy by including spin-orbital couplings.

*This work was supported by the US Department of Energy's EFRC program under Grant No. DE-SC0019330.
5:06PM J46.00010: Adjustable coupling and in-situ variable frequency probe with loop-gap resonators for cw and pulse electron paramagnetic resonance spectroscopy up to X-band*

GAJADHAR JOSHI (Presenter), JAMES KUBASEK, ILIJA NIKOLOV, BRENDAN SHEEHAN, Amherst College, THOMAZ DE ANDRADE COSTA, R. A. ALLÃO CASSARO, Instituto de Quimica, Universidade Federal do Rio de Janeiro, JONATHAN FRIEDMAN, Amherst College — In standard electron paramagnetic resonance (EPR) spectroscopy, the frequency of an experiment is set and the spectrum is acquired using magnetic field as the independent variable. There are cases in which it is desirable instead to fix the field and tune the frequency such as when studying atomic-clock transitions at avoided level crossings in molecular nanomagnets and other spin qubits [1,2,3]. We have designed and tested an adjustable frequency and variable coupling EPR probe with loop-gap resonators (LGRs) that works at a temperature down to 1.8 K [4]. The frequency is tuned by adjusting the height of a dielectric piece of sapphire inserted into the gap of an LGR; coupling of the microwave antenna is varied with the height of the antenna above the LGR. We demonstrate the operation of our probe with continuous wave EPR by mapping out avoided crossings for the Ni₄ single-molecule magnet to determine the tunnel splittings with high precision.


*Supported by NSF under Grant No. DMR-1708692, and by the Amherst College Dean of Faculty. R. A. Allão Cassaro thanks FAPERJ and CNPq for support.

5:18PM J46.00011: A Very-Low-Cost Flexible Electron Spin Resonance Spectrometer for Molecular Nanomagnet Experiments*

CHARLES COLLETT (Presenter), Department of Physics, Muhlenberg College, Allentown, PA 18104, USA, JONATHAN FRIEDMAN, Department of Physics & Astronomy, Amherst College, Amherst, MA 01002, USA — Electron spin resonance (ESR) spectroscopy is a useful tool for exploring and manipulating a wide variety of systems, including molecular nanomagnets. Commercial spectrometers offer high sensitivity in specific frequency bands, but are both expensive and limited in their experimental flexibility. We have developed an ESR spectrometer based on a cheap and readily-available field-programmable gate array (FPGA), which, when combined with loop-gap resonators (LGRs), enables spectroscopy on a budget at a wide range of frequencies. I will present the spectrometer design along with benchmark results demonstrating its sensitivity and flexibility with two different combinations of cryostat and magnet, and discuss future experiments on molecular nanomagnets.

*Work supported by U. S. National Science Foundation under Grant Nos. DMR-1310135 and DMR-1708692, and the Muhlenberg College and Amherst College Deans of Faculty.
2:30PM J47.00001: Understanding the Magnetic-Field Anisotropy of Kitaev Materials
AHMED RAYYAN (Presenter), JACOB GORDON, HAE-YOUNG KEE, Univ of Toronto — The Kitaev spin liquid remains the most theoretically well-understood quantum spin liquid due to the exact solvability of the Kitaev model. However, other interactions such as the off-diagonal spin interactions render the model non-integrable, but give rise to the magnetic order seen at low temperatures in candidate materials. Recently it was shown that when a magnetic field is applied along a certain direction, the magnetic order melts into an intermediate-field phase before the spins are fully polarized. A thorough understanding of the interplay between field and spin exchange anisotropy is required to understand field-induced phases. To this end, we present the classical and quantum phase diagrams of the extended anisotropic Kitaev model under different magnetic field directions.

2:42PM J47.00002: Majorana-magnon crossover by a magnetic field in the Kitaev model*
YUKITOSHI MOTOME (Presenter), JUNKI YOSHITAKE, Department of Applied Physics, The University of Tokyo, JOJI NASU, Department of Physics, Yokohama National University, YASUYUKI KATO, Department of Applied Physics, The University of Tokyo — Kitaev quantum spin liquids host Majorana fermions via the fractionalization of spins. In a magnetic field, the Majorana fermions were predicted to comprise a topological state with anionic excitations, which has attracted great attention by the recent discovery of the half-quantized thermal Hall conductivity. Nevertheless, a reliable theory remains elusive for the field effect, especially at finite temperature. Here we present unbiased large-scale numerical results for the Kitaev model in a wide range of magnetic field and temperature, obtained by continuous-time quantum Monte Carlo simulations. We find that the unconventional paramagnetic region showing fractional spin dynamics extends at finite temperature, far beyond the field range where the topological state is expected at zero temperature. Our results show the confinement-deconfinement behavior between the fractional Majorana excitations and the conventional magnons.

*This work is supported by Grant-in-Aid for Scientific Research under Grant No. JP16H02206, JP18H04223, JP18K03447, and JP19K03742, and by JST CREST (JP-MJCR18T2).

2:54PM J47.00003: Spin-one Kitaev model, same but different?
ILIA KHAIT (Presenter), HAE-YOUNG KEE, YONG-BAEK KIM, Univ of Toronto — We study various properties of the spin-one Kitaev model on honeycomb lattices consisting of two and three-leg ladder geometries using density matrix renormalization group. We discuss similarities to the spin-half model, and outline differences. Our results suggest that the spin-one model is a bona fide spin liquid candidate.
3:06PM J47.00004: Vacancy-induced Low-energy States in the Kitaev Model* WEN-HAN KAO (Presenter), School of Physics and Astronomy, University of Minnesota, JOHANNES KNOLLE, Department of Physics, Technical University of Munich, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, NATALIA PERKINS, School of Physics and Astronomy, University of Minnesota — Since 2006, the Kitaev honeycomb model has attracted significant attention due to the exactly solvable spin-liquid ground state with fractionalized Majorana excitations [1] and the possible materialization in magnetic Mott insulators with strong spin-orbit couplings [2]. Recently, the 5d-electron compound H$_3$LiIr$_2$O$_6$ has shown to be a strong candidate of Kitaev physics considering the absence of long-range ordered magnetic state [3]. In this work, we demonstrate that a finite density of random vacancies gives rise to a remarkable pile up of low-energy states and possibly explains the experimental findings in H$_3$LiIr$_2$O$_6$. We study both the free-flux and the vacancy-induced bound-flux background and their responses to additional time-reversal symmetry-breaking term, which imitates the magnetic field in real experiments.


*We acknowledge the US Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0018056.

3:18PM J47.00005: Field induced phases of the Kitaev-Γ ladder* ERIK SORENSEN (Presenter), Physics, McMaster University, ANDREI CATUNEANU, JACOB GORDON, HAE-YOUNG KEE, Physics, University of Toronto — The Kitaev spin model on honeycomb lattice has attracted significant attention since the emergence of α-RuCl$_3$ as a promising Kitaev spin liquid candidate in the presence of a magnetic field. While the mechanism of such a field-induced Kitaev spin liquid is not yet fully understood, theoretical studies have shown that the bond-dependent Γ and Kitaev interactions are equally significant in α-RuCl$_3$ leading to a minimal spin-$\frac{1}{2}$ Kitaev-Γ (KG) model. In the pure antiferromagnetic Kitaev limit, previous numerical studies have shown gapless states for a range of intermediate field strengths, leading to the suggestion of a U(1) spin liquid phase. However, a possibility of incommensurate magnetic orderings cannot be excluded. Employing large-scale numerical techniques, we study the KG model in a two-leg ladder system in the presence of a magnetic field for the entire phase space of the KG model, finding both disordered and incommensurate ordered phases near the antiferromagnetic Kitaev region. We discuss the models limitations and relation to the two-dimensional honeycomb lattice.

*Supported by NSERC of Canada, SHARCNET (www.sharcnet.ca) and Compute Canada (www.computecanada.ca)
3:30PM J47.00006: Field-Driven Phenomena in 2-d and 3-d Kitaev Magnets*  CIARAN HICKEY (Presenter), SIMON TREBST, University of Cologne, MATTHIAS GOHLKE, Okinawa Institute of Science and Technology, CHRISTOPH BERKE, University of Cologne — Kitaev's honeycomb model is an exactly solvable spin model that realises a quantum spin liquid ground state, with fractionalised excitations in the form of Majorana fermions and plaquette flux excitations. Recent studies have shown that applying an external magnetic field can give rise to a rich set of field-driven phenomena, including the appearance of a gapless U(1) spin liquid. However, the Kitaev model is not unique to the honeycomb lattice, the model can in fact be defined, and exactly solved, on a range of tri-coordinated lattices in two and three dimensions. This naturally provides an enormous playground within which to study field-driven phenomena in quantum spin liquids. We will discuss a number of examples and construct a generic phase diagram for the Kitaev model in the presence of a magnetic field.

*We acknowledge support from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), Projektnummer 277101999 – TRR 183 (project B01).

3:42PM J47.00007: Magnetic Field Induced Competing Phases in Spin-Orbital Entangled Kitaev Magnets*  LI ERN CHERN (Presenter), Univ of Toronto, RYUI KANEKO, HYUN-YONG LEE, Institute for Solid State Physics, University of Tokyo, YONG-BAEK KIM, Univ of Toronto — There has been a great interest in magnetic field induced quantum spin liquids in Kitaev magnets after the discovery of neutron scattering continuum and half quantized thermal Hall conductivity in the material $\alpha$-RuCl$_3$. In this work, we provide a semiclassical analysis of the relevant theoretical models, which enable us to treat large system sizes approximating the thermodynamic limit. We find a series of competing magnetic orders with fairly large unit cells at intermediate magnetic fields, which are mostly missed by previous studies. We show that quantum fluctuations are typically strong in these large unit cell orders, while the spin wave dispersion resembles a scattering continuum. The huge quantity of magnon bands with finite Chern numbers also gives rise to an unusually large thermal Hall conductivity. Given the highly frustrated nature of the spin model, the large unit cell orders are likely to melt into the putative spin liquid in the quantum limit. Our work provides an important basis for a thorough investigation of emergent spin liquids and competing phases in Kitaev magnets. [arXiv:1905.11408]

*This work was supported by MEXT of Japan, the Killam Research Fellowship, the NSERC of Canada and the Center for Quantum Materials at the University of Toronto.
Numerical Studies of the Kitaev-Gamma Model Under a Magnetic Field

Recently, there has been excitement generated around α-RuCl$_3$ as a candidate for the material realization of the Kitaev spin liquid (KSL). Beyond the dominant ferromagnetic (FM) Kitaev interaction, subleading spin interactions are required to explain the zig-zag (ZZ) magnetic ordering and behaviour of α-RuCl$_3$ under a magnetic field. On the basis of exact diagonalization (ED) and DMRG, an antiferromagnetic (AFM) Gamma interaction was found to be essential for stabilizing the KSL under tilted magnetic fields. A subsequent classical study of the Kitaev-Gamma model found a multitude of large unit cell magnetic orders due to the competition between Gamma and the applied field. Furthermore, an infinite tensor product state (iTPS) study found that these classical orders are melted by quantum fluctuations, giving way to two nematic paramagnetic states. The topological nature of these nematic phases and their relation to the KSL remain unknown. Here we present results obtained with ED to address these open questions.

This work was supported by the Natural Sciences and Engineering Research Council of Canada, and the Center for Quantum Materials at the University of Toronto.

Vison crystals in an extended Kitaev model on the Honeycomb lattice

I will introduce an extension of the Kitaev honeycomb model by including four-spin interactions that preserve the local gauge structure and hence the integrability of the original model. This extended model emerges naturally from generic time reversal invariant perturbations to the Kitaev honeycomb model. The model has a rich phase diagram containing five distinct vison crystals, as well as a symmetric -flux spin liquid with a Fermi surface of Majorana fermions and a sequence of Lifshitz transitions. We will discuss possible experimental signatures of the different phases, including finite-temperature Monte Carlo calculations of the specific heat and the static vison structure factor. Finally, we will see how different topologically ordered Z$_2$ quantum spin liquids with abelian and non-abelian anyons emerge naturally from this model, complementing the liquids with Chern numbers equal to 0, 1 and -1 that appear in the Kitaev honeycomb model.

Partitioning the phase diagram of pyrochlore and Kitaev magnets using graph theory

Highly frustrated magnets host rich exotic states of matter such as spin liquids and hidden orders. Those phases can occur in various forms and are notoriously difficult to identify. In this talk, I will show that the combination of a kernel method and graph partitioning theory provides an efficient framework to unravel the complex phase diagram of frustrated magnets. It delimits regimes of both classical spin liquids and broken symmetry phases, including hidden orders, and provides the analytical order parameters and/or characteristic local constraints. The method is demonstrated by examples of pyrochlore and Kitaev magnets but applies to general (semi-)classical spin systems.
4:54PM J47.00011: Quantum Spin Liquid and Proximate Magnetic Orders in Magnets with Spin-Orbit Coupling*  ANIMESH NANDA (Presenter), International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bangalore, India, KUSUM DHUCHAR, Department of Physics, Indian Institute of Technology Palakkad, India, SUBHRO BHATTACHARJEE, International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bangalore, India — Quantum phase transitions out of magnetic orders in quantum spin liquid (QSL) phases have gained much recent attention in the context of several spin-orbit coupled magnets such as α-RuCl$_3$, Yb$_2$Ti$_2$O$_7$ etc. In this talk, I shall report our theoretical calculations about the nature of such unconventional phase transition in a class of experimentally relevant Hamiltonians in the honeycomb magnets. In particular, we shall show how such deconfined quantum phase transitions are naturally captured in terms of the condensation of the fractionalised excitations of the QSL. In addition, we shall show how to think about such transitions in terms of the domain walls of the magnetically ordered phases.

*We acknowledge MPG for funding through the Max Planck Partner Group on strongly correlated systems at ICTS and SERB-DST (India) for funding through project grant No. ECR/2017/000504.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J48 DCMP: Superconductivity: Nickelates  Mile High Ballroom 1A - Bing Lv, University of Texas at Dallas

2:30PM J48.00001: The Superconducting Phase Diagram of the Infinite-Layer Nickelates*  DANFENG LI (Presenter), BAI YANG WANG, KYUHO LEE, MOTOKI OSADA, Stanford University, BERIT GOODGE, LENA FITTING KOURKOUTIS, Cornell University, HAROLD HWANG, Stanford University — The recently discovered superconducting infinite-layer nickelate, Nd$_{0.8}$Sr$_{0.2}$NiO$_2$ [1], provides an additional platform of studying the physics of the high-$T_c$ superconductors in a cuprate-like system. The possible similarities and differences in the electronic structure to cuprates have been debated and attracted a lot of interest. One particular question among them is whether there is a “dome-shape” in the superconducting phase diagram of this new superconductor upon varying the Sr doping, analogous to that of cuprates. Here, we present a first study of such doping dependence of transition temperatures, lattice spacings as well as transport properties, to which controlling the crystallinity and nickel oxidation state across different dopings by our approaches to materials synthesis appears to be essential.

References:

*Supported by DOE BES MSD (DE-AC02-76SF00515), the Moore Foundation (GBMF4415) and DOD AFOSR (FA 9550-16-1-0305)
2:42PM J48.00002: Efforts to Synthesize Bulk Superconducting Infinite-Layer Nickelates: R$_3$Ni$_3$O$_7$ and Other Phases Prepared by Hydrogen Reduction of RNiO$_3$**

GREGORIO PONTI (Presenter), QUINN D. B. TIMMERS, ZACHARY P. KUKLINSKI, JOHN MARKERT, Department of Physics, University of Texas at Austin — Recently, superconductivity in a nickelate was reported$^1$ in an apparently hole-doped RNiO$_2$ (“infinite-layer”) film (with $R \approx$ Nd$_{0.8}$Sr$_{0.2}$), after CaH$_2$ reduction. We have prepared both parent and electron- and hole-doped specimens of the bulk, nearly simple-perovskite RNiO$_3$ structures: $R_{1-x}A_x$NiO$_3$ [$R = \text{Nd, Pr, (La,Y)}; A = \text{Sr, Ce, Th}$] using high oxygen pressure (200 bar) at high temperatures ($T \approx$1000°C). We reduced these phases in several ways in an effort to produce bulk infinite-layer materials. For reduction in 5% H$_2$ in Ar, and for $T >$ 400°C, we find excess reduction to pure metal(s) or elemental oxides. But for temperatures in the range 300–375°C (reduction times of hours), we have synthesized a number of nickelate structures in bulk, dense form, suitable for transport and other measurements. One product is the “337” structure: R$_3$Ni$_3$O$_7$. X-ray diffraction, electrical resistivity, magnetic, and other data indicate that $n$-doping (Ce$^{4+}$) induces structural and electronic changes in the 337 material, and thus may provide an alternative path to “Ni$^{2+}$/Ni$^{1+}$” superconductivity. We also report other product phases and, thus, a rich reduced-nickelate phase diagram.

$^1$D. Li et al., Nature 572, 624 (2019).

**Support: University of Texas, College of Natural Sciences Freshman Research Initiative
Superconductivity was recently discovered in the infinite-layer nickelate Nd$_{0.8}$Sr$_{0.2}$NiO$_2$.\textsuperscript{1} To proceed with further systematic studies in the superconducting properties of this material, it is important to establish a reproducible method to synthesize single-phase, single-crystalline Nd$_{0.8}$Sr$_{0.2}$NiO$_2$. The synthetic route to this infinite-layer nickelate structure poses two major challenges. First, the precursor perovskite phase is difficult to stabilize due to the unusually high formal nickel valence of Ni$^{+3.2}$ and the structural instability induced by chemical doping. Second, topochemical reduction on perovskite nickelates have shown limitations in coherent transition to the infinite-layer phase.\textsuperscript{2}

After careful optimization, we have successfully established a reproducible method to stabilize Nd$_{0.8}$Sr$_{0.2}$NiO$_2$ (001) epitaxial thin films on SrTiO$_3$ (001) substrate by pulsed-laser deposition and CaH$_2$-assisted topochemical reduction. The details of the optimization process and the dependence of structural and superconducting properties on growth conditions will be discussed.

\textsuperscript{1} Li, D. \textit{et al.}, \textit{Nature} \textbf{572}, 624 (2019).

\textsuperscript{*}Supported by DOE BES MSD (DE-AC02-76SF00515), the Moore Foundation (GBMF4415), and DOD AFOSR (FA 9550-16-1-0305).
3:06PM J48.00004: A superconducting praseodymium nickel oxide with infinite-layer structure*  
MOTOKI OSADA (Presenter), BAI YANG WANG, DANFENG LI, KYUHO LEE, Stanford University, BERIT GOODGE, LENA FITTING KOURKOUTIS, Cornell University, HAROLD HWANG, Stanford University — Nickel oxide compounds, which are analogous to copper oxides, have been intensively investigated in the past decades since the discovery of high-$T_c$ superconductivity in copper oxides. The recent discovery of superconductivity in a neodymium nickel oxide of infinite-layer structure suggests the possible existence of a family of superconducting nickel oxide. Here, we present the synthesis of an infinite-layer praseodymium nickel oxide by topochemical reduction of the precursor perovskite thin films using calcium hydride as reagent. We report the observation of superconductivity with $T_c$ of 9-12 K in such compound upon doping with strontium, Pr$_{0.8}$Sr$_{0.2}$NiO$_2$. Details of the materials synthesis of the infinite-layer structure, measurements on temperature-dependence of resistivity and Hall coefficient will be discussed in this presentation.


*Supported by DOE BES MSD (DE-AC02-76SF00515), the Moore Foundation (GBMF4415), and DOD AFOSR (FA 9550-16-1-0305).

3:18PM J48.00005: Atomic Lattice and Electronic Structure of Superconducting Nickelate Thin Films*  
BERIT GOODGE (Presenter), Cornell University, DANFENG LI, KYUHO LEE, MOTOKI OSADA, BAI YANG WANG, HAROLD HWANG, Stanford University, LENA FITTING KOURKOUTIS, Cornell University — The recent discovery of superconductivity in Sr-doped NdNiO$_2$ is an important development for condensed matter physics [1]. Nominally similar in structure to the infinite-layer cuprate superconductors, the nickelates present a complementary platform for investigating the underlying physical mechanisms driving superconductivity in these systems. The stabilization of superconducting samples is, however, as yet limited to thin film geometries, raising the importance of spatially localized characterization techniques capable of probing only the regions of interest without contributions from the substrate. Here, we harness the high spatial and energy resolution achieved with scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) to explore both the lattice and electronic structure of these superconducting thin films. Structurally, the effects of different growth parameters are explored across several films within the nickelate series. Electronically, we investigate possible similarities to the cuprate superconductors.


*This work is supported by DOD AFOSR (FA 9550-16-1-0305), DOE BES MSD (DE-AC02-76SF00515), and the Moore Foundation (GBMF4415).
3:30PM J48.00006: In Situ Synchrotron X-ray Studies of Nickelate Growth and Reduction*

YAN LI (Presenter), XI YAN, Materials Science Division, Argonne National Laboratory, ZHAN ZHANG, Advanced Photon Source, Argonne National Laboratory, HUA HUAN WANG, Institute of High Energy Physics, Chinese Academy of Sciences, HUA ZHOU, Advanced Photon Source, Argonne National Laboratory, DILLON FONG, Materials Science Division, Argonne National Laboratory —

Long-sought non-cuprate superconductivity has recently been discovered in epitaxial thin films of alloyed neodymium nickelate (Nd$_{0.8}$Sr$_{0.2}$NiO$_2$) [1]. Interestingly, the superconducting phase is only observed in the infinite layer A$_1$B$_1$O$_2$ or ‘112’ phase, and not the more typical A$_1$B$_1$O$_3$ (‘113’) perovskite phase. Reduction of the 113 to the 112 phase generally requires use of a strong reducing agent like hydrides. However, the topotactic transition process involving significant oxygen loss is intrinsically non-trivial and remains elusive for precise synthesis control. Here we present the results of in situ synchrotron X-ray studies on the growth of nickelate heterostructures by pulsed laser deposition (PLD). We employ a Nd$_{0.8}$Sr$_{0.2}$NiO$_3$ target for the growth of Nd$_{0.8}$Sr$_{0.2}$NiO$_3$/SrTiO$_3$ (001) heterostructures and NdNiO$_3$ and SrNiO$_x$ targets for the growth of nickelate superlattices. We will discuss the relationships between phase stability and the oxygen concentration for different deposition parameters prior to CaH$_2$ reduction. The results of in situ studies of the reduction process to realize square-planar nickelates will also be described.

*Work supported by the Department of Energy, Office of Science, Basic Energy Sciences under contract no. DE-AC02-06CH11357.

3:42PM J48.00007: Transport Characterization of Infinite Layer Nickelate Superconductor*

BAI YANG WANG (Presenter), DANFENG LI, KYUHO LEE, Physics, Stanford University, BERIT GOODGE, Applied and Engineering Physics, Cornell University, MOTOKI OSADA, Physics, Stanford University, LENA FITTING KOURKOUTIS, Applied and Engineering Physics, Cornell University, HAROLD HWANG, Physics, Stanford University —

The recently discovered infinite layer nickelate superconductor presents a potential new family of unconventional superconductors [1]. While sharing similar crystal structure with infinite layer cuprates, the electronic properties can be non-trivially distinct due to the relatively extreme valence state of Ni$^{1+}$. DFT calculations have also pointed out potential involvement of multiple bands [2]. In this sense, a careful comparison against the cuprate system is imperative in obtaining a proper and unbiased view of the nickelate superconductivity. Furthermore, detailed characterization of the difference between the two systems may provide new insights into the ingredients of superconductivity in layered oxide systems. As a step in this direction, we investigate and report the magnetotransport properties of nickelates in both the normal and superconducting state.


*Supported by the Moore Foundation (GBMF4415) and DOD AFOSR (FA 9550-16-1-0305).
Electronic structure of the parent compound of superconducting infinite-layer nickelates

MATTHIAS HEPTING, DANFENG LI, CHUNJING JIA, SLAC National Accelerator Lab., HAIYU LU, Stanford University, E. PAIRS, YI TSENG, Paul Scherrer Institute, X. FENG, SLAC National Accelerator Lab., MOTOKI OSADA, EMILY BEEN, Stanford University, YASUYUKI HIKITA, SLAC National Accelerator Lab., Y. CHUANG, ZAHID HUSSAIN, Lawrence Berkeley Lab., KEJIN ZHOU, A. NAG, MIRIAN GARCIA-FERNANDEZ, Diamond Light Source, MATTEO ROSSI, SLAC National Accelerator Lab., HSIAO-YU HUANG, DI-JING HUANG, Taiwan Photon Source, ZHIXUN SHEN, Stanford University, THORSTEN SCHMITT, Paul Scherrer Institute, HAROLD HWANG, B. MORITZ, SLAC National Accelerator Lab., JAN ZAANEN, Leiden University, THOMAS DEVEREAUX, WEI-SHENG LEE (Presenter), SLAC National Accelerator Lab. — Very recently, the first superconducting nickelate has been discovered, opening a new field of research. The novel superconductor is a Sr-doped infinite layer nickelate NdNiO$_2$, which is isostructural to the infinite-layer cuprates and possesses the same nominal 3d electron count. Yet, it is important to experimentally characterize the electronic state of the parent compound from which the superconductivity emerges. In this presentation, we will present data of soft x-ray spectroscopy (XAS and RIXS) near the Ni L-edge and O K-edge on parent compound RNiO$_2$ (R = La, Nd). Together with LDA + U calculations, the gross feature of the electronic structure and a low energy effective model for the infinite layer nickelate will be discussed.

Doping evolution of the electronic structure of Sr-doped NdNiO$_2$

MATTEO ROSSI (Presenter), HAIYU LU, DANFENG LI, CHUNJING JIA, EMILY BEEN, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA, Y. CHUANG, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, KEJIN ZHOU, Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom, ZHIXUN SHEN, BRIAN MORITZ, THOMAS DEVEREAUX, HAROLD HWANG, WEI-SHENG LEE, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — Since the discovery of high-temperature superconductivity in cuprates, many efforts have been devoted to reproduce their electronic structure by proper material engineering. Nickel oxides occupy a prominent place since they are theoretically proposed to host superconductivity. After intense research, superconductivity has been recently discovered in Sr-doped NdNiO$_2$. Theory and experiments have been conducted to understand the electronic structure of the parent compound NdNiO$_2$. Yet, spectroscopic information about how Sr-doping affects the electronic states is still lacking. In this presentation, I will discuss the doping evolution of the electronic structure, as revealed by our recent experimental results from x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS).
**4:18PM J48.00010: Exotic electronic structure in cuprate-like trilayer nickelate Pr$_4$Ni$_3$O$_8$**

HAOXIANG LI, PEIPEI HAO (Presenter), KYLE GORDON, Physics, University of Colorado-Boulder, HONG ZHENG, JUNJIE ZHANG, Material Science Division, Argonne National Lab, XIAOQING ZHOU, Physics, University of Colorado-Boulder, JOHN MITCHELL, Material Science Division, Argonne National Lab, DANIEL DESSAU, Physics, University of Colorado-Boulder — As sharing similar layered structure and close electron configuration with the high-Tc cuprate superconductors, various series of nickel oxides have naturally become potential candidates for cuprate analogues. A previous study found a rare metallic state lying in the trilayer nickelate Pr$_4$Ni$_3$O$_8$ (Pr438) with a quasi-2D lattice structure, which together with similar d-electron counting to the overly hole-doped cuprates and strong orbital polarization near the Fermi energy has drawn more attention to this compound[1]. Here we present a more direct and detailed study of the electronic structure of Pr438, with a combination of the Angle-resolved photoemission spectroscopy and Density-functional-theory calculations. Our spectroscopy data shows a non-gapped Fermi surface resembling the heavily hole-doped cuprates residing in the Fermi-liquid regime, bearing both electron- and hole-pockets, as has been corroborated by DFT calculations. These combine the predominant d$_{x^2-y^2}$ feature and strong hybridization between the Ni-3d and O-2p states, rendering Pr438 an extraordinary analogue to cuprates, making it a promising host for superconductivity.


**4:30PM J48.00011: Electronic Correlations in Nickelate Analogues of Cuprate Superconductors**

JONATHAN KARP (Presenter), Department of Applied Physics and Applied Math, Columbia University, MANUEL ZINGL, Center For Computational Quantum Physics, Flatiron Institute, ANTIA S. BOTANA, Department of Physics, Arizona State University, MICHAEL NORMAN, Materials Science Division, Argonne National Laboratory, ANDREW MILLIS, Department of Physics, Columbia University — Motivated by recent experiments on tri-layer (Pr4Ni3O8) and infinite layer (NdNiO2) analogues of cuprate superconductors, we use a combination of density functional and dynamical mean field (DFT+DMFT) methods to perform a comparative study of the metal-insulator and magnetic phase diagrams, many body electronic structure, and conduction band many-body mass enhancements of cuprate and nickelate materials. In the Ni materials the transition metal d-bands are more widely separated in energy from the O-p bands than in the cuprates, suggesting that the nickelates are more accurately modelled by a Hubbard model than are the cuprates. The role of Nd-derived d-bands in the physics of the nickelates is discussed and the possibility that in the nickelate case other Ni-d orbitals may be relevant is analyzed. Preliminary results on superconductivity within the DMFT approximation will be presented.

*US Dept. of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division*
Electronic Structure across the Rare-Earth Series in Superconducting Infinite Layer Nickelates

EMILY BEEN (Presenter), Physics, Stanford, WEI-SHENG LEE, HAROLD HWANG, SIMES, SLAC, JAN ZAANEN, Leiden Institute of Physics, Leiden University, THOMAS DEVEREAUX, BRIAN MORITZ, CHUNJING JIA, SIMES, SLAC — The exciting discovery of superconductivity in oxygen-reduced monovalent nickelates has raised a new platform for the study of unconventional superconductivity, with similarities and differences to the cuprate high temperature superconductors. General trends appear in the infinite nickelates RNiO2 with rare-earths R spanning across the Lanthanides. The role of oxygen charge transfer diminishes in comparison to the cuprates, with an increased and prominent role played by rare-earth 5d electrons near the Fermi level when traversing from La to Lu. A decrease in lattice volume indicates that the magnetic exchange additionally grows, which may be favorable for superconductivity. However, compensation effects from the itinerant 5d electrons presents a close analogy to Kondo or Anderson lattices, indicating a more complex interplay between charge transfer, bandwidth renormalization, compensation, and magnetic exchange.

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under contract DE-AC02-76SF00515.

Hybridization and correlation effects in the electronic structure of infinite-layer nickelates

YUHAO GU, Institute of Physics, Chinese Academy of Science, SICHEN ZHU, XIAOXUAN WANG, Department of Physics, New York University Shanghai, JIANGPING HU, Institute of Physics, Chinese Academy of Science, HANGHUI CHEN (Presenter), Department of Physics, New York University Shanghai — We combine density functional theory and dynamical mean field theory to study the electronic structure of infinite-layer nickelate NdNiO2. Without considering correlation effects on Ni, we find adjacent NiO2 planes are coupled by a metallic Nd spacer layer. However, the largest hybridization between Ni-\(d_{x^2-y^2}\) state and itinerant electrons origins from an interstitial-s orbital instead of Nd-\(d\) orbitals. Correlation effects on Ni reduces the hybridization between Ni-\(d_{x^2-y^2}\) state and itinerant electrons and when sufficiently strong, they can open a Mott gap, which is separated by the lower Hubbard band of Ni-\(d_{x^2-y^2}\) state and hybridization states (interstitial-s and Nd-\(d\) orbitals). With correlation strength increasing, antiferromagnetic ordering occurs before the metal-insulator transition. Experimentally long-range magnetic order has not been observed in NdNiO2. This places NdNiO2 in a paramagnetic metallic phase in which the hybridization between Ni-\(d_{x^2-y^2}\) and itinerant electrons is non-negligible and Ni correlation strength is moderate.

H.C. acknowledges the funding of National Natural Science Foundation of China (Grant No. 11774236) and NYU University Research Challenge Fund.
KWAN-WOO LEE (Presenter), Division of Display and Semiconductor Physics, Korea University, Sejong, MI-YOUNG CHOI, Department of Applied Physics, Korea University, Sejong, WARREN PICKETT, Department of Physics, University of California, Davis — For a long time, condensed matter physicists have a question whether there may be nickelates that can host a cuprate-type superconductor. Very recently, NdNiO$_2$ by 20%-Sr doping leads to superconducting up to $T_c=15$ K, while another most promising candidate LaNiO$_2$ has never been superconducting. These discovery has been rejuvenated the long standing issue. In this presentation, we will focus on a primary distinction between NdNiO$_2$ and LaNiO$_2$. An obvious difference is that La$^{3+}$ is closed shell and nonmagnetic, while Nd$^{3+}$ with Hund’ rule ground state $S=3/2$, $L=6$, $J=9/2$ has a Curie-Weiss moment of about $3\mu_B$. Our results indicate that this magnetic interaction in Nd$_{0.8}$Sr$_{0.2}$NiO$_2$ causes spin-disorder broadening of the $\Gamma$-centered Nd-driven electron Fermi surfaces and should be included in models of normal and superconducting states of Nd$_{0.8}$Sr$_{0.2}$NiO$_2$.

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SIHEON RYEE, HONGKEE YOON, TAEKJUNG KIM, MIN YONG JEONG, MYUNG JOON HAN (Presenter), KAIST — To understand the superconductivity recently discovered in Nd$_{1-x}$Sr$_x$NiO$_2$, we carried out LDA+DMFT (local density approximation plus dynamical mean-field theory) and magnetic force response calculations. The on-site correlation in Ni-3$d$ orbitals causes notable changes in the electronic structure. The calculated temperature-dependent susceptibility indicates the localized character of its spin moment. We also analyzed the low-frequency behavior of self-energy and resulting correlation strength. Remarkable new finding is that magnetic interactions in this material become two-dimensional by hole doping. While the undoped NdNiO$_2$ has the sizable out-of-plane interaction, hole dopings strongly suppress it. This two-dimensionality is maximized at the hole concentration of $\delta \approx 0.25$. Further analysis as well as the implications of our new findings are presented.
2:30 PM J49.00001: Coulomb correlation in noncollinear antiferromagnetic α-Mn

AKI PULKKINEN (Presenter), LUT University, BERNARDO BARBIELLINI, LUT University and Northeastern University, JOHANNES SAMULI NOKELAINEN, LUT University, VLADIMIR SOKOLOVSKIY, DANIL BAIGUTLIN, OLGA MIROSHKINA, MIKHAIL ZAGREBIN, VASILIY BUCHELNIKOV, Chelyabinsk State University, CHRISTOPHER LANE, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern University, JIANWEI SUN, Tulane University, KATARIINA PUSSI, ERKKI LAHDERANTA, LUT University — We discuss the interplay between magnetic and structural degrees of freedom in elemental Mn. The equilibrium volume is shown to depend critically on the magnetic interactions between the Mn atoms. While the standard generalized-gradient-approximation underestimates the equilibrium volume, a more accurate treatment of the effects of electronic localization and magnetism is found to solve this longstanding problem. Our calculations reveal the presence of a magnetic phase in strained α-Mn that has been reported previously in experiments. This new phase of strained α-Mn is found to exhibit a noncollinear spin structure with large magnetic moments.

2:42 PM J49.00002: Magnetic and electronic properties of tetragonal GeNFe3

MARI TSUMURAYA (Presenter), DAVID SINGH, Physics, The University of Missouri — GeNFe3 has a tetragonal symmetry at room temperature with a space group I4/mcm. Previous studies unveiled its physical properties, such as a spin-glass behavior and anomalous Hall effect. Through first-principles calculations, we report magnetic and electronic properties of GeNFe3 with tetragonal structure.

*Work at the University of Missouri was supported by the Department of Energy, Award number DE-SC0019114

2:54 PM J49.00003: The effect of Si substitution on the magnetocaloric properties of Al1.2-xSi_xFe_2B_2 intermetallic system

MD SAKHAWAT HOSSAIN HIMEL (Presenter), MAHMUD KHAN, Department of Physics, Miami University — The AlFe2B2 material has drawn considerable attention recently due to its magnetocaloric properties near room temperature. Here, we have investigated the magnetic and magnetocaloric properties of a series of Si-doped Al1.2-xSi_xFe_2B_2 (0 ≤ x ≤ 0.25) compounds by x-ray diffraction, scanning electron microscopy (SEM), and dc magnetization measurements. The samples were prepared by arc-melting followed by drop-casting and annealing. The x-ray diffraction patterns confirmed that all samples exhibited the single-phase Cmmm-type orthorhombic crystal structure. SEM micrographs confirmed the homogeneity of the samples. A second-order ferromagnetic phase transition was observed near room temperature for all samples. While the Curie temperature (Tc) was minutely effected due to Si doping, the magnetocaloric properties were significantly enhanced. A peak magnetic entropy change of 7.39 Jkg⁻¹K⁻¹ was observed in the doped samples for a field change of 50 kOe. The experimental results and related discussion will be presented in detail.
**3:06PM J49.00004: A first-principles study of the impact of paramagnetism on grain boundary segregation in FeMn alloys**

OMKAR GOPALKRISHNA HEGDE (Presenter), TILMANN HICKEL, CHRISTOPH FREYSOLDT, JOERG NEUGEBAUER, Max Planck Inst fuer Eisenforschung GmbH — To understand the impact of paramagnetism on defect energetics and kinetics is, though conceptually and computationally challenging, important for designing Fe-based alloys. Since magnetic degrees of freedom change faster than atomic degrees of freedom in the high-temperature paramagnetic state, the atoms move according to an averaged force instead of instantaneous forces attained from each spin configuration.

Therefore, a new computationally efficient method based on spin-space averaging [1] has been developed to handle magnetic disorder next to defects, which uses the spin constraint tool developed in the DFT code S/PHI/nX. First, we focus on vacancies in the FeMn system, for which we demonstrate that paramagnetism significantly affects atomic relaxations as well as vacancy diffusion barriers and thereby explain why Mn diffusion shows a different temperature dependence than Fe-self diffusion in α-Fe. Next, we expand our method to extended defects and show that paramagnetism has a significant effect on the grain boundary segregation of Mn. Finally, we combine our results to reveal the chemo-magneto-structural coupling underlying Mn segregation to grain boundaries in Fe alloys.


*Funding from IMPRS-SurMat is acknowledged.

**3:18PM J49.00005: Tuning of the collapsed tetragonal phase transition in the SrTM$_2$P$_2$ (TM = transition metal) system**

GUILHERME GORGON LESSEUX (Presenter), RAQUEL RIBEIRO, SERGEY L. BUD'KO, PAUL C CANFIELD, Iowa State University and Ames Laboratory — The tetragonal to collapsed tetragonal phase transition$^1$ combines dramatic changes in structural, electronic, and (sometimes) magnetic states. This phase transformation can be controlled by application of hydrostatic pressure or uniaxial stress and offers the possibility of achieving shape memory behavior combined with remarkable super-elastic properties in intermetallic compounds.$^2$ For the SrTM$_2$P$_2$ system, given that the collapse occurs when P-P bonding takes place across Sr plane, TM substitution is the least perturbative substitution that can be made. As part of our effort to broaden our understanding and control of this transition, we have studied the effects of transition metal substitution on SrNi$_2$P$_2$. Here we report on solution growth and transport measurements on single crystals of SrTM$_2$P$_2$ (TM = Ni, Rh, Pd, Cu) which are potential hosts for the tetragonal collapse transition. Particularly, the effects of Rh-doping on SrNi$_2$P$_2$ will be discussed.

$^1$Kreyssig et al., PRB 78, 184517 (2008).

$^2$Sypek et al., Nat. Commun. 8, 1083 (2017).

*This work was carried out at Iowa State University and supported by Ames Laboratory, US DOE, under Contract No. DE-AC02-07CH11358. GGL and RAR were supported by the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant No. GBMF4411.
3:30PM J49.00006: First Principles study of enhanced stability of Au@Pt nanoparticles on MoS₂ support through alloying kinetics

TIMOTHY T YANG, Department of Materials Science and Engineering, University of Pittsburgh, BOAO SONG (Presenter), Department of Mechanical and industrial Engineering, University of Illinois at Chicago, WISSAM A SAIDI, Department of Materials Science and Engineering, University of Pittsburgh, REZA SHAHBAZIAN-YASSAR, Department of Mechanical and industrial Engineering, University of Illinois at Chicago — Two-dimensional MoS₂ supported Pt and Au@Pt nanoparticles (NPs) have received great attention for various catalysis applications. Deep understanding on the NPs migration and coalescence under different service conditions is crucial to enhance their stability. Herein, we employ first-principles density functional theory calculations to study the stabilities and diffusion kinetics of supported Au@Pt NPs at room temperature up to 400 °C in atmospheric hydrogen and vacuum environments. We show that Pt at the bottom layer of the NP interacts strongly with the MoS₂ substrate resulting in a strong adhesion energy. However, the adhesion energy is reduced in hydrogen environment due to strong Pt-H interactions. Further, we show that smaller NPs are more favored in alloy form rather than core/shell due to the facile diffusion kinetics at the edges. Our results are validated using transmission electron microscopy, showing that small size Au@Pt alloy NPs are more stable than the larger ones with the Au core in contact with MoS₂ substrate and Pt shell in contact with hydrogen. The present work gives insights to the degradation mechanisms of the NPs supported on substrates and offers strategies to enhance their stability.

3:42PM J49.00007: Quantum Quench and f-Sum Rules on Linear and Non-linear Conductivities*

HARUKI WATANABE (Presenter), MASAKI OSHIKAWA, Univ of Tokyo — Electric conductivity is one of the most important response properties of materials. The "frequency sum rule" is a non-perturbative constraint on the conductivity integrated over all frequency. In this talk, we give a new derivation to the f-sum rule for general quantum many-particle systems by considering a quench process. We then extend the discussion to higher order responses and derive various types of new sum rules on nonlinear conductivities.

*The work of M.O. was supported in part by MEXT/JSPS KAKENHI Grant Nos. JP19H01808 and JP17H06462.

The work of H.W. is supported by JST PRESTO Grant No. JPMJPR18LA.
3:54PM J49.00008: Binary and ternary metallic compounds with soft magnetic properties: predictions from density functional theory calculations  
AKANSHA SINGH (Presenter), AARON P. STEBNER, CRISTIAN CIOBANU, Colorado School of Mines — Nanocrystalline magnetic materials have fundamental and technological importance, due to their soft magnetic properties. These materials have a two-phase microstructure, a nanocrystalline ferromagnetic phase with $D0_3$ structure and a residual amorphous alloy phase. FINEMET (Fe$_{73.5}$Si$_{13.5}$Nb$_3$B$_9$Cu$_1$, with the nanocrystalline phase Fe$_3$Si) is one such material, having large saturation magnetization, low magnetocrystalline anisotropy, and coercivity. Still, it has some disadvantages related to its brittleness and power dissipation. With the aim of finding better soft magnetic alloys, we performed a systematic computational search across binary ($D0_3$, formula $X_3Z$) and ternary ($L_{21}$, $XY_2Z$) compounds, using generalized gradient approximation calculations. We choose the 3d-transition metals (Sc, Ti, V, Cr, Mn, Fe, Co and Ni) as $X$ or $Y$ element, and Al, Si, P, Ga, Ge, As, In, Sn and Sb as $Z$, for a total of 576 alloy combinations. We have filtered the best candidates based on their magnetization, crystalline anisotropy, heat of formation, and ductility. We have thus found 12 compounds (including, e.g., Fe$_3$Sn, Fe$_3$Ga, Fe$_3$Sb, MnCo$_2$As) that can have properties superior to Fe$_3$Si. Our results may offer guidance for future synthesis efforts aimed at discovering new and superior soft magnetic materials.

4:06PM J49.00009: Ab initio thermodynamics of carbides in high Mn steels  
LEKSHMI SREEKALA (Presenter), Computational Materials Design, Max Planck Inst fuer Eisenforschung GmbH, POULUMI DEY, Materials Science and Engineering, Technische Universiteit Delft, TILMANN HICKEL, JOERG NEUGEBAUER, Computational Materials Design, Max Planck Inst fuer Eisenforschung GmbH — The addition of Cr to high-Mn steels improves their corrosion resistance. At the same time, it has been experimentally reported that the alloying with Cr yields a substantial increase in the number of carbides, like cementite and Fe$_{23}$C$_6$. They can contribute to a precipitation hardening of the material, but also provide interfaces that might be critical for hydrogen embrittlement. In the present work, we therefore use density functional theory to determine the thermodynamic driving force for the formation of carbides as a function of the chemical composition of the alloy. These investigations are performed at finite temperatures considering the vibrational, electronic and magnetic contributions to the free energy of formation. We analyze the critical role of Cr by determining the partitioning of Cr and Mn into the carbides. At the same time, the role of these alloying elements for the solution enthalpy of H in the carbides is determined. We report that the chemical trends for the carbides show surprising differences from the behavior in the Fe-Mn matrix.
4:18PM J49.00010: Atomic-level defect formation mechanism in high-entropy alloys  CHI-HUAN TUNG (Presenter), Natl Tsing Hua Univ, GUAN-RONG HUANG, WEI-REN CHEN, Oak Ridge National Lab, SHOU-YI CHANG, Natl Tsing Hua Univ —
With the aid of atomistic simulations, we found that in solid solution alloys the soft spots detected by the the spatial distributions of low frequency vibration modes served as precursors of atomic level rearrangement. In high-entropy alloys, the successive defect growth has a chain-like manner which relied on the coupling of local shear transformations and vortex like atomic motion. This mechanism resembles the reported nucleation mechanism of shear transformation zone in metallic glasses, which is different from the dislocation slip induced planer fault growth in dilute solution alloy. In addition to the distinct defect formation mechanism, the extremely short correlation length of mechanical heterogeneity in high-entropy alloys also suppressed the synchronized motions of the dislocation line. This effect impeded the long-ranged dislocation slip and contributed to strong strain hardening ability. Our study reveals the critical defect formation mechanism at the atomic level and provides the theoretical description of various signature mechanical properties of high-entropy alloys.

4:30PM J49.00011: Drag viscosity of metals and its connection to Coulomb drag  YUNXIANG LIAO (Presenter), VICTOR GALITSKI, University of Maryland, College Park — Shear viscosity is a key parameter in the hydrodynamic description of fluids, including electronic matter - an interdisciplinary subject that has attracted an increasing amount of interest recently. Related to the rate of momentum transport, viscosity is given by the retarded correlation function of the momentum current, i.e., the stress tensor, in the linear response theory. In this work, we find that there exists a previously overlooked contribution to viscosity, which originate from the interacting part of the stress tensor. This new contribution, which we name drag viscosity, is connected to the frictional drag forces induced by the long-range interactions. A related phenomenon is the Coulomb drag of a double-layers electronic system, which measures the rate of charge transport originating from scattering between quasiparticles in different layers in the presence of Coulomb interactions. Using the diagrammatic approach in the Keldysh formalism, we derive the drag viscosity of the 2D and 3D electronic systems as well as the drag resistivity of the 2D double-layers systems. At low enough temperatures, both the drag viscosity and resistivity exhibit quadratic temperature dependence which becomes linear as temperature increases.
4:42PM J49.00012: Local structure analysis of carbon in ferritic steel by C K-edge X-ray absorption fine structure and multiple scattering calculations  
KAKERU NINOMIYA  
(Presenter), Kyushu University, YUSUKE TAMENORI, KAZUKI TSURUTA, Japan Synchrotron Radiation Research Institute, MAIKO NISHIBORI, Kyushu University — The ferritic steel with supersaturated solid solution carbon remarkable increase in hardness by heat treatment (so-called aging) at low temperature. This has been considered to cause by the formation of the carbon cluster in ferritic steel. In this study, we aimed to understand the local structure changes of solid solution carbon in ferritic steel with aging by soft X-ray absorption spectroscopy. In the C K-edge X-ray absorption near edge structure (XANES) spectrum, extended X-ray absorption fine structure (EXAFS) analysis by peak fitting is difficult due to parameter restrictions based on the sampling theorem. Therefore, we proposed the analysis method of C-Fe bond length ratio based on Natoli’s law. Because solid solution carbon in bcc-Fe is a $D_{4h}$ point group symmetry, it is expected that the peak position of C-Fe $\sigma^*$ state splits in the xy and z directions. We found that the C-Fe bond length ratio, $l_{xy}/l_z$, began to decrease with the formation of carbon clusters. Therefore, it suggests that the C-Fe$z$ bond was expanded by the increase of local carbon concentration due to the formation of carbon clusters, and structure transition of bcc to bct occurred.


4:54PM J49.00013: Accelerating Materials Discovery through Bezier Interpolation of Electronic Band Structure*  
NATHAN FOULK  
(Presenter), JEREMY JORGENSEN, GUS HART, Department of Physics and Astronomy, Brigham Young University — One important part of DFT calculations is the numerical integral of the electronic band structure. Unfortunately, this critical step of DFT simulation is the most computationally expensive, because each k-point requires solving the Kohn-Sham equations, an eigenproblem, in a large basis set. Almost all of the error in the band energy integral comes from misrepresenting the Fermi surface, so the most important part of any integration technique is approximating the Fermi surface correctly. Current DFT codes approximate the bands using three-dimensional Riemann sums, which represent the Fermi surface very poorly. We present an integration technique of interpolating the bands using Bezier surfaces in order to more accurately represent the Fermi surface, and thereby achieve the same accuracy with fewer k-points. We also explore further improvement by using an adaptive mesh refinement technique in those integration regions which contain the Fermi surface. Preliminary results suggest that 1 meV accuracy can be achieved using ~10× fewer k-points.

*We thank the Office of Naval Research for generously funding a major portion of this project through grant MURI N00014-13-1-0635.
5:06PM J49.00014: Exploring band topology of engineered materials using deep neural networks  VITTORIO PEANO (Presenter), FLORIAN SAPPER, FLORIAN MARQUARDT, Max Planck Inst for Sci Light — This talk focuses on the first applications of our deep Neural Network (NN) based approach to band structure calculations. A distinctive feature of our approach is that our NN does not predict the band structure directly but rather learns to predict the parameters of an auxiliary Tight-Binding (TB) model. This TB model gives then access not only to the band structure but also to the topological properties of the Bloch waves.

The applications we consider are geared towards engineered materials such as photonic and phononic crystals in that we use as an input of our neural network the unit cell geometry. We demonstrate the use of our NN to perform efficiently the statistical analysis of the topological properties of selected distributions of potentials. Our analysis is based on recent break-throughs in the understanding of band structure topology and ties to the the systematic classification of all natural materials based on their electronic topological properties (sometimes known as Topological Quantum Chemistry). Moreover, we demonstrate the use of our NN for optimization (random or gradient based) of band structures in the design of (i) band inversions, (ii) physical implementations of fragile topology, (iii) physical implementations of selected topological TB models.

5:18PM J49.00015: Micro-Structure and Transport Mechanism in Graphene Copper Composites  RAJU GHIMIRE (Presenter), Nanoscience and Microsystems Engineering, University of New Mexico — The addition of nanocarbons to copper (Cu), specifically in the form of graphene (GN), has shown to enhance copper's physical properties. GN-Cu nanocomposites can potentially achieve a higher current carrying capacity and a lower temperature-sensitivity of electrical resistivity compared with copper. These characteristics make GN-Cu materials interesting for several applications including but not limited to interconnects, high current power lines, and elevated-temperature rotating machines. Charge conduction in these materials is controlled by microstructural features as well as nanoscale interfacial phenomena between the GN and Cu. In this work, we analytically investigated the possibilities for an improved electrical conductivity in GN-Cu composites. Subsequently, GN-Cu samples were prepared by the consolidation of CVD Cu-graphene films under high pressures and temperatures. The effects of processing time, temperature, and pressure on both the structure and physical properties of the GN-Cu composite films were investigated. Finally, in-situ conductivity measurements of the Cu-GN interfaces were carried out. These measurements provide insights into transport mechanisms in nanocarbon-metal composites.

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J50 DCMP: Quantum Criticality and Phase Transitions  Mile High
Ballroom 1C - Emilian Nica, Arizona State Univ
2:30PM J50.00001: Superconductivity from quantum fluctuations of itinerant quantum critical points  YUNCHAO HAO (Presenter), YANG QI, Fudan Univ, KAI SUN, University of Michigan — In the vicinity of a quantum critical point, critical fluctuations can often act as glue for the formation of BCS pairs, which is one important path way towards unconventional superconductivity. Recently, thanks to the development in quantum numerical techniques, such as sign-problem-free quantum Monte Carlo simulations, new insights and unbiased numerical understanding about this phenomenon become accessible. In particular, the numerical results suggest superconductivity emerged from these quantum critical points are highly diversified and are highly sensitive microscopic details. In this study, we investigate these systems utilizing analytic approach. By exploring different model systems and compare with numerical results, we aim at understanding universal properties behind these diversified behaviors.

2:42PM J50.00002: Critical properties of antiferromagnetic and valence-bond-solid transitions in lattice quantum electrodynamics  NIKOLAI ZERF, Humboldt-Universität zu Berlin, RUFUS BOYACK, University of Alberta, PETER MARQUARD, DESY, Zeuthen, JOHN A GRACEY, University of Liverpool, JOSEPH MACIEJKO (Presenter), University of Alberta — Lattice gauge theories underlie the effective low-energy description of many strongly correlated electron systems, such as frustrated magnets and high-temperature superconductors, but can now also be simulated directly in cold atom experiments. Elucidating the phase diagram of lattice gauge theories is thus an important problem with a wide range of applications to condensed matter physics. Recent sign-problem-free quantum Monte Carlo simulations of lattice quantum electrodynamics (QED) with $N$ flavors of fermions on the square lattice have found evidence of continuous quantum phase transitions between a critical deconfined phase at small gauge coupling and confined antiferromagnetic (for $N=2$) or valence-bond-solid (for $N=4,6,8$) phases at large gauge coupling. We derive Landau-Ginzburg-Wilson theories of the QED-Gross-Neveu(-Yukawa) type for these transitions, find stable renormalization-group fixed points corresponding to the observed quantum critical points, and compute their critical exponents using epsilon and large-$N$ expansions.

2:54PM J50.00003: Structure of Quantum Entanglement at a Finite Temperature Critical Point*  TARUN GROVER (Presenter), TSUNG-CHENG LU, University of California, San Diego — We propose a scheme to characterize long-range quantum entanglement close to a finite temperature critical point using tripartite entanglement negativity. Across a conventional order-disorder transition, tripartite negativity does not exhibit any singularity in the thermodynamic limit, in contrast to the short-range component of negativity, which is singular. This indicates that the long-distance critical fluctuations are completely classical, allowing one to define a ‘quantum correlation length' that remains finite at the transition despite a divergent physical correlation length.

*This project is supported by an Alfred P. Sloan Research Fellowship.
Universal Prethermal Dynamics in Gross-Neveu-Yukawa Criticality

SHAOKAI JIAN (Presenter), University of Maryland, College Park, SHUAI YIN, Sun Yat-Sen University, BRIAN SWINGLE, University of Maryland, College Park — We study the prethermal dynamics of the Gross-Neveu-Yukawa quantum field theory, suddenly quenched in the vicinity of a critical point. We find that the universal prethermal dynamics is controlled by two fixed points depending on the size of the quench. Besides the usual equilibrium chiral Ising fixed point for a shallow quench, a dynamical chiral Ising fixed point is identified for a deep quench. Intriguingly, the latter is a nonthermal fixed point without any equilibrium counterpart due to the participation of gapless fermionic fields. We also find that in the scaling regime controlled by the equilibrium fixed point, the initial slip exponent is rendered negative if there are enough flavors of fermions, thus providing a unique signature of fermionic prethermal dynamics. We then explore the temporal crossover between the universal scaling regimes governed by the two universality classes. Possible experimental realizations are also discussed.

Critical behavior near the many-body localization transition in driven open systems

ZALA LENARCIC (Presenter), University of California, Berkeley, ORI ALBERTON, ACHIM ROSCH, University of Cologne, EHUD ALTMAN, University of California, Berkeley — In a many-body localized (MBL) system, the coupling to an external bath typically breaks local integrals of motion. Thus the system relaxes to a unique thermal steady state. When the bath is non-thermal or when the system is weakly driven out of equilibrium, local conservation laws can be excited far from any thermal equilibrium value. I will show how this property can be used to study the MBL phase transition in weakly open systems. Here, the strength of the coupling to the non-thermal bath plays a similar role as a finite temperature in a T=0 quantum phase transition. By tuning this parameter, we can detect key features of the MBL transition: the divergence of dynamical exponent due to Griffiths effects and the critical disorder strength.

We propose a new order parameter, based on the fluctuations in local temperatures. For vanishing strength of coupling to the bath, fluctuations vanish on the ergodic side, while they are large on the MBL side. By increasing the coupling strength, fluctuations grow with a fractional exponent related to the inverse dynamical exponent on the ergodic side, while they decrease monotonically on the MBL side. This paves the way for studies of the MBL transition with new numerical approaches and, importantly, also with solid-state experiments.
3:30PM J50.00006: B$_{1g}$ Raman response near an Ising-nematic quantum critical point: properties of a quasielastic peak*  
XIAOYU WANG (Presenter), Natl High Magnetic Field Lab, EREZ BERG, Weizmann Institute of Science — Raman scattering has long been used to probe dynamical electronic correlations in various condensed matter systems. Here we present a theoretical study of the B$_{1g}$ channel Raman response in the vicinity of an Ising-nematic quantum critical point (QCP) in two space dimensions. We show the appearance of a “quasi-elastic peak” as the QCP is approached. The peak frequency is related to the relaxation rate of the deformation of the Fermi surface in the angular momentum l=2 channel, while the peak intensity is directly proportional to the Ising-nematic thermodynamic susceptibility. We discuss our results in the context of iron selenide materials which host such a quantum critical point.

*XW acknowledge support from National MagLab, which is funded by the National Science Foundation (DMR-1644779) and the state of Florida making all taxpayers stakeholders in our science.

3:42PM J50.00007: Nematic fluctuations in the Hubbard models*  
TIANYI LIU (Presenter), Stanford University, EDWIN HUANG, University of Illinois at Urbana-Champaign, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford University — An electron nematic is an electronic phase with translation symmetry, but broken rotational symmetry. Signatures of nematic fluctuations have been observed in strongly correlated materials such as cuprates, iron pnictide, and iron chalcogenide superconductors, and may be related with other sorts of broken symmetries such as charge or spin density waves. Here we report calculations of the nematic susceptibilities from determinant quantum Monte Carlo (DQMC) simulations of the Hubbard models, for various model parameters, doping levels, and temperatures. We draw possible connections between these susceptibilities to other phenomena observed in the Hubbard model.

*Supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract DE-AC02-76SF00515. Computational work is performed on the Sherlock cluster at Stanford University.
3:54PM J50.00008: Direct Measurement of the Soft Mode Driving a Quantum Phase Transition*

MATTHEW LIBERSKY (Presenter), Caltech, RYAN D MCKENZIE, University of British Columbia, DANIEL SILEVITCH, Caltech, PHILIP STAMP, University of British Columbia, THOMAS F ROSENBAUM, Caltech — Understanding the excitations, fluctuations, and dynamics at a quantum phase transition is an important research thrust in pure condensed matter and atomic physics. An important question remains of whether critical excitations remain in the presence of an external spin bath, as is the case for many real-world implementations of quantum systems. Addressing this issue is necessary for connecting theory and modeling to observations and device design. Here, we directly measure the low energy excitation modes of a well-known realization of the quantum Ising model in transverse field, LiHoF$_4$, using microwave spectroscopy techniques to probe energies below what is accessible via neutron scattering experiments. Instead of the single excitation expected for a simple quantum Ising system, we find and characterize a remarkable array of modes arising from coupling of the spin-$1/2$ Ising electronic spins to a bath of spin-$7/2$ Ho nuclear spins, the lowest of which indeed softens at the quantum critical point. These results suggest that quantum criticality persists in the presence of a spin bath and that similar modes may exist in other quantum Ising systems, including adiabatic quantum computers.

*The work at Caltech was supported by DOE Basic Energy Sciences.

4:06PM J50.00009: Duality Web on a 3D Euclidean Lattice and Manifestation of Hidden Symmetries

JUN HO SON (Presenter), JING-YUAN CHEN, SRINIVAS RAGHU, Stanford Univ — We generalize our previous lattice construction of the abelian bosonization duality in 2+1 dimensions to the entire web of dualities as well as the $N_f=2$ self-duality, via the lattice implementation of a set of modular transformations in the theory space. The microscopic construction provides explicit operator mappings, and allows the manifestation of some hidden symmetries. It also exposes certain caveats and implicit assumptions beneath the usual application of the modular transformations to generate the web of dualities. Finally, we make brief comments on the non-relativistic limit of the dualities.

4:18PM J50.00010: London penetration depth in disordered unconventional superconductors with competing interactions*

MAXIM KHODAS (Presenter), Hebrew University - Jerusalem, MAXIM DZERO, Kent State Univ - Kent, ALEX LEVCHENKO, University of Wisconsin-Madison — A topic of an interplay between disorder and competing electronic phases in multiband superconductors have recently got renewed interest in the context of iron-based superconductors. In my talk I will present a theory of disordered unconventional superconductor with competing magnetic order. Our discussion will be based on the results obtained for on a two-band model with quasi-two-dimensional Fermi surfaces, which allows for the coexistence region in the phase diagram between magnetic and superconducting states in the presence of intraband and interband scattering induced by doping. We will demonstrate that disorder has a crucial effect on the magnetic field penetration depth as a function of disorder scattering rates.

*The work of M.D. was financially supported by NSF-DMR Grant No. 1506547. The work of A.L. was financially supported by DOE-BES Grant No. DESC0017888
4:30PM J50.00011: Magnetic phase transitions in quantum spin-orbital liquids*  SHI FENG (Presenter), NIRA KirkumAR PATEL, Department of Physics, The Ohio State University, PANJIN KIM, National Security Research Institute, Korea, JUNG HOON HAN, Department of Physics, Sungkyunkwan University, NANDINI TRIVEDI, Department of Physics, The Ohio State University — We investigate the spin and orbital correlations of a superexchange model with spin S=1 and orbital L=1 relevant for 5d^4 transition metal Mott insulators, using exact diagonalization and density matrix renormalization group (DMRG). For spin-orbit coupling λ=0, the orbitals are in an entangled state that is decoupled from the spins, leading to emergent spin-orbital separation within spin-orbital interacting system. We find two phases with increasing λ: (I) the S2 phase with two peaks in the structure factor for λ < λ_{c1} ≈ 0.34 J, where J is the ferromagnetic exchange, and (II) the S1 phase λ_{c1} < λ < λ_{c2} ≈ 1.2 J with antiferromagnetic correlations. The λ = 0, S2 and S1 phases are shown to exhibit power law correlations, indicative of a gapless phase. Increasing λ > λ_{c2} leads to a product state of local spin-orbital singlets that exhibits exponential decay of correlations, indicative of a gapped phase. Using mean-field like approximation, we demonstrate that our model can be approximated with the well-known Uimin-Lai-Sutherland (ULS) model with an external field.

* S.F., N. D.P. and N. T. acknowledge support from DOE grant DE-FG02-07ER46423. P. K and J. H. H. acknowledge support from Samsung Science and Technology Foundation under Project Number SSTFBA1701-07

4:42PM J50.00012: Universal quantum glass transition on the Bethe lattice  IZABELLA LOVAS (Presenter), TU Munich, CATALIN PASCU MOCA, GERGELY ZARAND, Budapest University of Technology and Economics — We study the Coulomb glass behavior emerging from the interplay of interactions and disorder, by examining a model of spinless fermions at half filling on the Bethe lattice [1,2]. We consider the limit of infinite coordination number, where we combine dynamical mean field theory with a Hartree-Fock approximation to investigate the glass transition and the properties of the glassy phase in the presence of full replica symmetry breaking. This approach allows us to study the opening of the Efros-Shklovskii pseudogap in the glassy phase, and grants us access to the spectral function. In particular, we demonstrate the universal scaling collapse of the pseudogap and the spectral function at close to zero temperatures, where the melting of the glass is governed by the quantum fluctuations induced by the hopping of fermions. We show that this quantum scaling function differs from the classical scaling function of the thermal transition of the spin glass limit. Our results should be relevant for the glassy dynamics observed in Si inversion layers, persisting in the metallic phase [3].

4:54PM J50.00013: Atomic-scale fragmentation and collapse of antiferromagnetic order in a
doped Mott insulator*  HE ZHAO (Presenter), Boston College, SUJIT MANNA, Indian Institute of
Technology Delhi, ZACH PORTER, XIANG CHEN, University of California, Santa Barbara, ANDREW
UZDEJCZYK, Boston College, JAGADEESH MOODERA, Massachusetts Institute of Technology, ZIQIANG
WANG, Boston College, STEPHEN WILSON, University of California, Santa Barbara, ILIJA ZELJKOVIC,
Boston College — Measuring magnetic and electronic properties at atomic length scales would
provide crucial insight into the physics of doped antiferromagnetic Mott insulators, but this has
been difficult to achieve. We use spin-polarized scanning tunneling microscopy (SP-STM) to
visualize the periodic spin-resolved modulations originating from the antiferromagnetic order in
a \( J_{\text{eff}} = \frac{1}{2} \) strongly spin-orbit coupled Mott insulator \( \text{Sr}_2\text{IrO}_4 \). We discover that near insulator-to-
metal transition (IMT), the long-range antiferromagnetic order melts into a spatially fragmented
state with short-range correlations. Importantly, we find that the short-range antiferromagnetic
order is locally uncorrelated with the observed spectral gap magnitude. This suggests that static
short-range antiferromagnetic correlations are unlikely to be the cause of the inhomogeneous
closing of the spectral gap and the emergence of pseudogap regions near the IMT in doped
\( \text{Sr}_2\text{IrO}_4 \). Our work establishes SP-STM as a powerful tool for revealing atomic-scale magnetic
information in complex oxides.

*We gratefully acknowledge the support from the US Department of Energy Early Career Award
DE-SC0020130.

5:06PM J50.00014: Phase Structure of Isotropic and Anisotropic Ising Models at Complex
Couplings*  SANKHYA BASU (Presenter), VADIM OGANESYAN, Department of Physics, GC and CSI,
CUNY, CHRIS A HOOLEY, SUPA, School of Physics and Astronomy, University of St Andrews — In this
work, we study the phase structures and phase transitions that arise in both the Isotropic and the
Anisotropic Ising Models by analytically continuing away from real coupling – both temperature
and field. In particular, we observe that away from real temperatures, Yang-Lee circle theorem
indeed breaks down, even for the Isotropic Ising Model. We also observe symmetry breaking of
the global minima of the free energy away from real temperatures in the high temperature
phase. We use both analytical as well as numerical techniques based on Tensor Network
formulations (Tensor Renormalization Group(TrG), Higher Order Tensor Renormalization
Group(HOTRG)) to access these novel regimes in the phase space that is out of reach of standard
Monte Carlo techniques.

*NSF DMR Grant No. 1508538 and NSF DMR Grant No. 1653271

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J51 DCMP: Optoelectronic Properties of 2D Materials Mile High
Ballroom 1D - Shaowei Li, University of California, Berkeley
2:30PM J51.00001: van der Waals photothermoelectric effect in atomic layer heterojunctions*  
YUNQIU (KELLY) LUO (Presenter), Cornell University, TONG ZHOU, Physics, University at Buffalo, State University of New York, MAHESH R NEUPANE, Sensors and Electron Devices Directorate, U.S. Army Research Laboratory, ALEX MATOS ABIAGUE, Physics and Astronomy, Wayne State University, RYAN BAILEY-CRANDELL, MICHAEL J NEWBURGER, IGOR LYALIN, Physics, Ohio State University, IGOR ZUTIC, Physics, University at Buffalo, State University of New York, ROLAND KAWAKAMI, Physics, Ohio State University — Two-dimensional (2D) van der Waals (vdW) heterostructures provide exceptional opportunities for new physics and devices due to their unprecedented ability to tune the electronic, optical, magnetic and spintronic properties by atomic layer stacking and electrostatic gating. Harnessing this versatility requires a fundamental understanding of light-matter interactions and establishing new functionalities for photon-charge and photon-spin conversions. Here, we report the first observation of a highly-tunable vdW photothermoelectric effect in dual-gated MoS$_2$/graphene junctions with a striking multiple-polarity switching of photocurrent as a function of junction bias and carrier density. In stark contrast to photovoltaic effects arising from excitonic absorption in MoS$_2$, the vdW photothermoelectric effect originates from photoexcitation of hot electrons in graphene and thermoelectric transport across the vdW junction. Systematic studies of photoconductance as a function of photon energy and intensity reveal vdW photothermoelectric effect as the dominant mechanism for photocurrent generation at room temperature, as opposed to excitonic absorption. These findings provide an important step for understanding and control of vdW-interface devices.

*NSF MRSEC DMR-1420451

2:42PM J51.00002: Realizing precise charge neutrality in van der Waals heterostructure p-n junctions through data intensive photoresponse imaging  
TREVOR ARP (Presenter), Physics and Astronomy, University of California, Riverside, FATEMEH BARATI, Physics, New York University, SHANSHAN SU, ROGER LAKE, University of California, Riverside, NATHANIEL GABOR, Physics and Astronomy, University of California, Riverside — In atomically thin materials, the narrow phase space for exciton–phonon interactions could be used to engineer unusual devices that mimic molecular optical transitions. A van der Waals heterostructure tuned to a charge neutral state allows for the formation of excitons where the electron and hole are localized in different materials. Such interlayer excitons have a well-defined dipole moment making them sensitive to the interlayer electric field and out-of-plane vibrations. To isolate the behavior of interlayer excitons and explore their dynamics, we employ Multi-Parameter Dynamic Photoresponse Microscopy on encapsulated heterostructures composed of monolayer MoSe$_2$ and bilayer WSe$_2$. Gathering a large set of spatial photocurrent images as a function of source-drain and gate voltages, we unambiguously identify the charge neutrality condition. We observe that the system can be tuned to exhibit clear rectification with highly uniform spatial dependence in the heterojunction consistent with the formation of a two-dimensional distributed p-n junction at charge neutrality. Under these precise charge neutrality conditions, we observe striking spectroscopic features that reveal highly unusual exciton-phonon interactions.
Enhanced intrinsic photovoltaic effect in tungsten disulphide nanotubes

YIJIN ZHANG (Presenter), Max Planck Institute for Solid State Research, TOSHIYA IDEUE, MASARU ONGA, FENG QIN, RYUJI SUZUKI, Univ of Tokyo, ALLA ZAK, HIT-Holon Institute of Technology, RESHEF TENNE, Weizmann Institute of Science, JURGEN HUBERT SMET, Max Planck Institute for Solid State Research, YOSHIHIRO IWASA, Univ of Tokyo — Transition metal dichalcogenides (TMDs) are representative 2D materials. Group VI-B TMDs in 2H-type crystal structure have a semiconducting band structure. One of their unique features is the controllability of the crystal symmetry. The inversion symmetry inherent in bulk TMDs can be broken by isolating a monolayer. Various optoelectronic functionalities have been demonstrated by breaking this inversion symmetry. A further reduction of crystal symmetry can be achieved by rolling up 2D sheets to form a tubular structure. In such TMD nanotubes, not only the inversion symmetry but also mirror and rotation symmetries can be broken simultaneously, leading to a polar structure. We have investigated the photovoltaic effect in intrinsic WS\textsubscript{2} with different crystal symmetries and observed a sizable photovoltaic effect from TMD nanotubes without \textit{p-n} junction. Such a phenomenon is called bulk photovoltaic effect (BPVE). In our study BPVE was observed in WS\textsubscript{2} nanotubes only, indicating a importance of the polar structure to enhance BPVE.

Carrier transport dynamics in 2D semiconductors optoelectronic devices

PAN P ADHIKARI, PHYSICS, Clemson University, PEIJIAN WANG, Physics, University at Buffalo, KANISHKA KOBBEKADUWA, EXIAN LIU, PHYSICS, Clemson University, HAO ZENG, Physics, University at Buffalo, JIANBO GAO (Presenter), PHYSICS, Clemson University — Despite that 2D semiconductors have promising optoelectronic and electronic applications, our fundamental understanding of its carrier transport dynamics is still in its infancy. In general, it remains challenging to unravel the carrier transport properties in devices since they are altered in the presence of defects/impurities or trap states. An ultrafast probe or high quantum efficiency device (the ratio between electrons collected to photon number), or both, are required to elicit carrier transport properties before significant carrier trapping into trap states and recombination occur.

In this work, we integrate black phosphorus and WS\textsubscript{2} in an ultra-high-speed photodetector structure with sub-25 ps response time to study the carrier transport dynamics. We elucidate the nature of transport mechanisms in different temporal regimes: pre-trapping and band-like transport in early time up to nanoseconds, followed by multiple trapping and release (MTR) hopping transport. In addition to demonstrating visible and infrared high-speed photodetectors, our study reveals the fundamental device physics, leading to device performance manipulation.
3:18PM J51.00005: Nanoscale Mapping of Photoconductivity Enhanced by Localized Charge Traps in the Grain Structures of MoS$_2$ Monolayer  HYESONG JEON (Presenter), Department of Materials Science and Engineering, Seoul National University, Seoul, 08826, Korea, MYUNGJAE YANG, TAEYOUNG KIM, TAKHEE LEE, Department of Physics and Astronomy, Seoul National University, Seoul, 08826, Korea, SEUNGHUN HONG, Department of Physics and Astronomy, and Institute of Applied Physics, Seoul National University, Seoul, 08826, Korea — We present a method for the nanoscale mapping of photoconductivity and charge trap density in the grain structures of a monolayer molybdenum disulfide (MoS$_2$). In this method, the lateral current and noise maps were measured by scanning the MoS$_2$ surface with a nanoscale conducting contact probe. The measured data were analyzed to obtain the sheet resistance and charge trap density maps in the MoS$_2$ grain structures. Interestingly, the sheet resistance was found inversely proportional to the charge trap density in the grains. It was explained by the sulfur vacancies working as both charge hopping sites and traps in the MoS$_2$ monolayer. When illuminated with a light, the regions with a relatively high trap density showed a high photoconductivity. These results indicate that high photoconductivity was enhanced by charge traps. This method can be a powerful tool for the basic research about noises and the device applications based on two-dimensional materials.

3:30PM J51.00006: Effect of light-matter interaction on the ballistic conductance of an irradiated dice material  DIPENDRA DAHAL (Presenter), The Graduate Center, City University of New York, GODFREY GUMBS, Physics and Astronomy, Hunter college, City University of New York — We derived closed-form analytic expressions for the transmission coefficient of quasiparticles impinging on a square electrostatic potential barrier and step formed by split gates on a dice material which is irradiated by circularly polarized light. A consequence of modifying the states by the dressing field is to suppress Klein tunneling for head-on collision. Our results for transmission are employed in the Landauer-Buttiker formalism to examine the ballistic transport properties for varying barrier widths, incident quasiparticle energy, and light intensity. A comparison is made between our results for dressed and undressed states.
3:42PM J51.00007: Spatially resolved photoconductivity mapping of MoS$_2$ / WS$_2$ lateral heterostructures  
SAMUEL BERWEGER (Presenter), National Institute of Standards and Technology, Boulder, CO, HANYU ZHANG, National Renewable Energy Laboratory, Golden, CO, PRASANA K SAHOO, Indian Institute of Technology, Kharagpur, BENJAMIN M KUPP, Pennsylvania State University, State College, PA, JEFFREY L BLACKBURN, ELISA M MILLER, National Renewable Energy Laboratory, Golden, CO, DIMITRI VORONINE, University of South Florida, Tampa, FL, THOMAS M WALLIS, PAVEL KABOS, National Institute of Standards and Technology Boulder, CO, SANJINI U NANAYAKKARA, National Renewable Energy Laboratory, Golden, CO — The presence of free carriers directly affects the optical properties of transition metal dichalcogenides. For instance, free carriers directly underpin the competition between neutral excitons and carrier-bound trions and they strongly affect radiative and nonradiative decay pathways. However, despite their fundamental importance for TMDs, spatially resolved studies of the carrier distribution and the associated photoresponse remain challenging. Here we use scanning microwave microscopy (SMM, also called microwave impedance microscopy, MIM) to study the spatial carrier distribution in MoS$_2$/WS$_2$ lateral heterostructures under dark conditions as well as under illumination with photon energy-resolved narrowband illumination. We find strong spatial variations in the photoconductive response throughout the flakes studied. We further find significant long-term dynamics in the optically generated free carriers that manifest themselves in persistent charging and discharging and are strongly correlated with observed spatial variations in the steady-state photoconductive response. A comparison with spatially resolved photoluminescence mapping reveals excellent agreement between the local conductivity determined by SMM and the interplay between trion and exciton emission characteristics.

3:54PM J51.00008: Controllable beam slicing through fractional phase shifts accumulated at an atomically-thin interface*  
MYUNGJAE LEE (Presenter), James Frank Institute, University of Chicago, FAUZIA MUJID, Department of Chemistry, University of Chicago, ANDREW YE, Pritzker School of Molecular Engineering, University of Chicago, JIWOONG PARK, Department of Chemistry, University of Chicago — The interface between different media has been one of the crucial sources of light-matter interactions where properties of light, such as intensity, phase, or polarization, may change. One previously unexplored regime is when light propagates parallel to and bisected by the interface. Here, we realized an optically suspended and atomically-thin interface based on wafer-scale monolayer MoS$_2$ on fused silica that is immersed inside index-matching liquid. With this system we observed that a beam propagating along the interface is sliced into two sub-beams leaving a node at the interface. We quantified the upper and lower bounds of absorption and concluded that the atomically-thin interface behaves like a partial mirror that reflects light with an additional phase shift, which results in self-interference with the incident beam. In addition, we found that the degree of interference can be tuned by using interfaces with different number of MoS$_2$ layers. Our results indicate that the value of phase shift by a monolayer is a fraction of $\pi$, not an integer of $\pi$, which is unexpected from classical interfaces.

*This work was primarily supported by the Air Force Office of Scientific Research (FA9550-16-1-0347).
4:06PM J51.00009: Engineering the exciton spontaneous emission time in MoSe$_2$ monolayer

BO HAN (Presenter), CÉDRIC ROBERT, HONGHUA FANG, Institut National des Sciences Appliquées de Toulouse, MARINA SEMINA, Ioffe institute, DELPHINE LAGARDE, EMMANUEL COURTADE, Institut National des Sciences Appliquées de Toulouse, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan, THIERRY AMAND, BERNHARD URBASZEK, Institut National des Sciences Appliquées de Toulouse, MIKHAIL GLAZOV, Ioffe institute, XAVIER MARIE, Institut National des Sciences Appliquées de Toulouse — Encapsulation of monolayers such as MoSe$_2$ in hexagonal boron nitride (hBN) yields narrow optical transitions approaching the homogenous exciton linewidth. In time-resolved photoluminescence measurements we demonstrate that the exciton radiative lifetime in the MoSe$_2$ monolayer can be tuned by a factor 10 (typically from 1 to 10 ps) as a function of the hBN thickness. This variation is a consequence of the Purcell effect and it is in very good agreement with the calculated dependence using transfer matrix techniques [1]. We show that the exciton linewidth measured in cw photoluminescence can be controlled as well. The variation of the charged exciton lifetime due to cavity-like effects will also be discussed.


4:18PM J51.00010: Optical Switching Based on a Single Layer of WSe$_2$* ZHENG SUN

(Presenter), Astronomy and Physics, University of Pittsburgh, KE XU, Chemical and Petroleum Engineering, University of Pittsburgh, JONATHAN BEAUMARIAGE, Astronomy and Physics, University of Pittsburgh, JIERUI LIANG, SUSAN FULLERTON-SHIREY, Chemical and Petroleum Engineering, University of Pittsburgh, DAVID WAYNE SNOKE, Astronomy and Physics, University of Pittsburgh — Two-dimensional materials are an emerging class of new materials with a wide range of electrical and optical properties and potential practical applications. Single layers materials such as semiconducting transition metal dichalcogenides with MX$_2$ stoichiometry, where M is a transition metal element from group VI (M=Mo, W) and X is a chalcogen (X=S, Se, Te) are gaining increasing attention as promising gate insulators and channel materials for field-effect transistors. Here, we report a type of optical switching based on a single-layer WSe$_2$ transistor. A side gate controls the polarization of the ions in PEO:CsClO$_4$, after which we can turn on and off the photoluminescence using a back gate. An on-off ratio of 90 is observed under constant pump light intensity. We believe the “off” and “on” states originate from the net electric field produced by the polarized ions and the back-gate, which aligns the dipole within the WSe$_2$ either in the same way or in the opposite way.

*We acknowledge the U.S. Army Research Office under MURI Award No. W911NF-17-1-0312. K.X., J.L., and S.K.F.-S. acknowledge funding from the National Science Foundation, Grant No. 1607935.
Excitonic Complexes in a Charge Tunable WSe2 Monolayer Device
CEDRIC ROBERT, EMMANUEL COURTADE, DELPHINE LAGARDE, LPCNO, University of Toulouse, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS Tsukuba, BERNHARD URBASZEK, THIERRY AMAND, XAVIER MARIE (Presenter), LPCNO, University of Toulouse — Transition Metal Dichalcogenides (TMD) monolayers have emerged as exciting 2D materials for optoelectronics and spintronics. Due to the large exciton binding energies and strong spin-orbit coupling, these materials can host various and robust excitonic complexes. The encapsulation of TMD monolayers into hBN combined with the constant improvement of the material quality now enable to reproducibly observe and control these excitonic complexes in the optical spectra.
In this work, we study a WSe2 monolayer embedded into a charge tunable device made of graphite electrodes and hBN. This allows us to study excitonic complexes in different doping regimes (neutral, n or p). We systematically performed magneto-photoluminescence/reflectivity and time resolved photoluminescence as a function of doping to identify the nature of the excitonic transitions based on their characteristic Landé g-factor and their temporal dynamics. The fine structure of the trion (intervalley, intravalley, dark trion) will first be discussed. Phonon assisted transitions (momentum mismatch dark exciton and spin forbidden dark exciton) are also identified. Finally the origin of more complex transitions observed under high n type doping will be discussed.

Widely Tunable Mid-Infrared Light Emission in Thin-Film Black Phosphorus
*CHEN CHEN (Presenter), Yale University, XIAOBO LU, Washington University in St. Louis, BINGCHEN DENG, XIAOLONG CHEN, QIUSHI GUO, CHENG LI, CHAO MA, SHAOFAN YUAN, ERIC SUNG, Yale University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, LI YANG, Washington University in St. Louis, FENGNIAN XIA, Yale University — In this work, we report the widely tunable mid-infrared light emission from dual-gate hexagonal boron nitride (hBN)/Black Phosphorus (BP)/hBN heterostructure devices. The photoluminescence (PL) from a ~20-layer BP flake can be continuously tuned from 3.7 to 7.7 μm with a moderate displacement field of 0.48 V/nm, spanning 4 μm in mid-infrared. The PL emission remains perfectly linear-polarized regardless of the bias field due to the preservation of the optical transition rule. We further performed first-principles calculation to investigate the gate dependence of the band structure and optical conductivity in BP. Moreover, together with theoretical analysis we show that the radiative decay probably dominates over other nonradiative decay channels in the PL experiments. Our results reveal the great potential of thin-film BP in widely tunable, mid-infrared light emitting and lasing applications.

*We acknowledge the financial support from the National Science Foundation (NSF) EFRI-2DARE program (1542815). K.W. and T.T. acknowledge support from the Elemental Strategy Initiative conducted by the MEXT, Japan and the CREST (JPMJCR15F3), JST. X.L. acknowledges the financial support from the NSF CAREER program (DMR-1455346).

WOOJOO LEE (Presenter), Physics, University of Texas at Austin, LI-SYUAN LU, WEN-HAO CHANG, Department of Electrophysics, National Chiao Tung University, CHIH-KANG SHIH, Physics, University of Texas at Austin — The emergence of van der Waals (vdW) 2D electronic materials and their heterostructures, especially the semiconducting family of transition metal dichalcogenides (TMD), has opened a new frontier of science and technology. Although interesting novel devices have been created using these 2D electronic materials and heterostructure, they are created only as discrete single devices. Namely, they are not scalable. A scalable material platform must satisfy the following conditions: (a) the ability to create single continuous layer of a continuous area of the same orientation, (b) the ability to stack dissimilar semiconducting layers to form wafer size heterostructures that are laterally homogeneous. Here we report successful development of a wafer size monolayer, quasi continuous and single orientation (but containing twins) platform of TMD that can be exfoliated and transferred to create wafer size TMD semiconducting heterostructures (in this case, monolayer MoS$_2$ on multilayer MoSe$_2$) with atomically clean interface. We use angle resolved photoemission to probe the electronic structure of such heterostructure and their respective constituents, revealing evidence of strong hybridization near the zone center.


5:06PM J51.00014: Emergent optical properties in crystalline, semiconducting 2D covalent organic framework / TMD heterostructures  

HALLEH BALCH (Presenter), Physics, University of California, Berkeley, AUSTIN EVANS, Chemistry, Northwestern University, RAGHUNATH DASARI, Chemistry, Georgia Tech, RUOFAN LI, Physics, Cornell, SIMIL THOMAS, HONG LI, Chemistry, Georgia Tech, DANQING WANG, Physics, University of California, Berkeley, JEAN-LUC E BREDAS, SETH R. MARDER, Chemistry, Georgia Tech, DANIEL C. RALPH, Physics, Cornell, WILLIAM DICHTEL, Chemistry, Northwestern University, FENG WANG, Physics, University of California, Berkeley — Two dimensional covalent organic frameworks are a new class of Van der Waals materials formed of periodic, covalently-bound lattices of planar organic molecules. The symmetry, lattice constant, optical, and electronic properties of 2D COFs can be controlled via choice of molecular constituents, which give rise to lattice properties not present in the component parts. To date, 2D COFs have been limited by large bandgaps, low coupling, and poor control of material morphology. Here, we present results on a new semiconducting 2D covalent organic framework and the unusual optical properties that emerge in COF / TMD heterostructures and when exfoliated to few-layer sheets. We characterize the structure by X-ray scattering, TEM, AFM, transport, and optical spectroscopy, and demonstrate facile manipulation onto arbitrary experimental platforms. Our data demonstrates that the formation of a highly crystalline and semiconducting 2D COF permits thickness-dependent optical properties not previously observed in 2D covalent organic frameworks. We further demonstrate thickness-dependent energy transfer dynamics in semiconducting COF / TMD heterostructures and outline directions of future research.
J51.00015: Sub-picosecond hot electron transfer in WS\textsubscript{2}/hBN/p-Si hybrid structure revealed by energy- and time-resolved photoemission electron microscopy*  
YAOLONG LI (Presenter), YUNAN GAO, XIAOYONG HU, QIHUANG GONG, Peking Univ — Carrier transfer plays a central role in all optoelectronic applications. It can occur much faster in low dimensional materials than in conventional bulk materials, which can be exploited in developing ultrafast and high-efficient optoelectronic devices. Here, we report an ultrafast hot electron transfer study in a hybrid structure of monolayer WS\textsubscript{2} on p-type silicon substrate separated by thin layer of hexagonal boron nitride (hBN). We studied the ultrafast electron transfer dynamics by an energy- and time-resolved photoemission electron microscopy, and determined that photoexcited electrons transfer to p-type silicon via two paths of a direct hot-electron transfer on a sub-picosecond timescale and another one of intra-band carrier cooling and subsequent electron transfer on a timescale of a few picoseconds. The transfer rate and the relative weight of the two paths can be quantitatively determined, which depends on excitation wavelength and the thickness of the hBN layer.

*This work was supported by the National Key Research and Development Program of China under Grant No. 2018YFB2200403, and the National Natural Science Foundation of China under Grant Nos. 61775003, 11734001, 11527901, 91850111, and Beijing Municipal Science & Technology Commission No. Z191100007219001.

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J52 DCMP: Oxide Films, Surfaces, and Interfaces  Mile High Ballroom 1E -
Wennie Wang, University of Chicago

2:30PM J52.00001: Microstructure structure of air-grown UN\textsubscript{x}O\textsubscript{y} on nitrogen-rich uranium nitride*  
XIAOFANG WANG (Presenter), ZHONG LONG, RONGGUANG ZENG, YIN HU, KEZHAO LIU, Institute of Materials, China Academy of Engineering Physics — Uranium nitrides have aroused great attention for their important application in the corrosion protection of metallic uranium, due to formation of a nanoscale surface oxide layer when exposed to air or an oxygen-including atmosphere that slows or protects against further oxidation, but direct observations on the microstructure of oxide layer and the relationship of the crystal structure between the oxide layer and the underlying uranium nitride remain unresolved. In this work, oxide formation on surface of nitrogen-rich uranium nitride was investigated using X-ray photoelectron spectroscopy (XPS), auger electron spectroscopy (AES), aberration-corrected transmission electron microscopy (TEM), and high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) coupled with electron energy-loss spectroscopy (EELS). XPS and AES studies indicated that the oxidized layer on UN\textsubscript{2-x} film is ternary compound uranium oxynitride (UN\textsubscript{x}O\textsubscript{y}) in about 10 nm thickness. TEM/HAADF-STEM and EELS studies revealed the UN\textsubscript{x}O\textsubscript{y} crystallizes in the FCC CaF\textsubscript{2}-type structure with the lattice parameter close to the CaF\textsubscript{2}-type UN\textsubscript{2-x} matrix. The work can provide further information to the oxidation mechanism of uranium nitride.

*NSAF Foundation of China [grant number U1630250]
Segregation Effects and Charge Transport in Yttria-Stabilized Zirconia Thin Films on Langasite Substrates

FIRAS MAHYOB (Presenter), GEORGE BERNHARDT, ROBERT LAD, Univ of Maine — Yttria-stabilized zirconia (YSZ) is widely used as a bulk ceramic in solid-state oxygen sensors due to its high ionic conductivity, chemical inertness, and stability up to 1500°C. In thin film form, YSZ is an attractive component for use in wireless microwave acoustic sensors to monitor conditions within harsh industrial environments. In this work, RF-magnetron sputter deposition was used to synthesize YSZ (8%Y2O3-92%ZrO2) films with thicknesses from 15nm to 200nm on piezoelectric langasite (La3Ga5SiO14) substrates at growth temperatures from 25-600°C. X-ray diffraction indicated that the cubic YSZ films grow with preferred (111) out-of-plane texture on the langasite substrate with random in-plane orientation. Scanning electron microscopy revealed the presence of stress hillocks at the YSZ/langasite interface, and this was minimized at a 400°C deposition temperature where extremely smooth films were obtained as determined by x-ray reflectivity. Post-deposition air annealing caused yttria segregation to the film surface region as evidenced by increases in the Y3d/Zr3d photoelectron peak area ratio upon annealing up to 1000°C. This segregation is accompanied by an increase in film ionic conductivity and larger YSZ grain size as measured by high temperature impedance spectroscopy.

Surface reconstruction of TiO2 nanocrystals

ARAM YOON, XIAO ZHANG, ANDRE SCHLEIFE, JIAN-MIN ZUO (Presenter), University of Illinois at Urbana-Champaign — One of the best studied photocatalysts is TiO2. As chemical reactions occur on surfaces, the surface of TiO2 has been extensively investigated [1]. However, focus has largely been on 2D surfaces of bulk crystals, while real catalysts are nanocrystals or nanoparticles. Surface reconstruction on a nanocrystal is expected to be different with multiple facets. Here, we report on reconstructed surfaces on rutile nanocrystals studied by environmental transmission electron microscopy [2]. The reconstruction is imaged using an electron direct detection detector (DDD). The DDD provides significantly improved signal/noise ratio and high spatial resolution. Using these new approaches [3], we observed the surfaces of {110}, {210}, and {100} on TiO2 nanocrystals at atomic resolution and compared with previous models and with DFT calculations of atomic positions and total energies. Most importantly, the results allow an examination of surface reconstruction dependence on nanocrystal sizes.


*The development of ETEM is supported by NSF MRI-1229454.
3:06PM J52.00004: Epitaxial Growth of Sr$_3$Al$_2$O$_6$ by Pulsed Laser Deposition as a Water-Soluble Sacrificial Layer for GaAs Deposition  IMRAN KHAN (Presenter), BILL MCMAHON, ANDREW NORMAN, ANDRIY ZAKUTAYEV, National Renewable Energy Laboratory — Despite the record high efficiency for GaAs solar cells, its terrestrial application is limited due to both the particularly high costs related to the required single crystal substrates and the epitaxial growth. A water-soluble lift off layer could reduce costs by avoiding the need for toxic etchants, substrate re-polishing and expensive process steps.

Sr$_3$Al$_2$O$_6$ (SAO) is a water soluble, cubic oxide with lattice constant 15.84Å. This is close to $(2\sqrt{2})a_{GaAs}$, giving a close lattice match after 45° lattice rotation. We investigated the epitaxial growth of high structural quality SAO on single crystal SrTiO$_3$ (STO) substrates by pulsed laser deposition, and the feasibility of subsequently growing GaAs epitaxially on top of it. We identified that the SAO film quality is strongly dependent on the growth temperature and O$_2$ partial pressure. An STO capping layer was grown on the SAO to protect from moisture induced degradation. XRD spectra for the films with optimized deposition parameters showed epitaxial SAO aligned to the STO (100) substrate. TEM analysis revealed that the grown SAO films are epitaxially crystalline throughout the thickness. The epitaxial growth of the STO capping layer is a qualitative indication for the high quality of the SAO surface.
3:18PM J52.00005: Surface and Interface Energetics of Pyrite-type Materials* JOSEPH
MINNICH (Presenter), Department of Physics, American University, ANDREW O’HARA, SOKRATES T
PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — Materials with the pyrite
crystal structure, such as iron and cobalt sulfide, are composed of earth-abundant
elements with potential applications in photovoltaics, catalysis, and spintronics. While the surface
properties of FeS$_2$ have received significant attention in the literature, less is known about the
surface
properties of other pyrite-type materials like CoS$_2$ as well as the interfaces between these
materials. In this
work, we perform calculations using density functional theory (DFT) to gain insight into the
surface and
interface energetics of these pyrite materials. Specifically, we compute the energies for several
low-index
surface orientations with different surface terminations (i.e., sulfur-rich to sulfur-poor). We
compare the
minimal surface energy and interface energy between the two materials along these directions.
Extending
the basic surface characterization, we also include the effects of ligands bound to these surfaces.
The
results provide insights concerning the observed epitaxy of these materials in hybrid
nanoparticle
experiments and provide guidance for additional experiments regarding the growth of structures
utilizing
these materials.

*J. M. was supported by NSF REU grant 1852158. A.O. and S.T.P. were supported by DOE grant
DE-FG02-09ER46554.

3:30PM J52.00006: Atomic scale dynamic process of oxide growth during copper oxidation* MENG LI, MATTHEW T CURNAN, WISSAM A SAIDI, JUDITH YANG (Presenter), Univ of Pittsburgh —
Understanding oxide growth mechanism during metal oxidation is essential for rational design
and control of oxides for applications in catalysts, sensors, as well as corrosion protection.
Despite ample research on bulk oxidation, little is known on the initial oxide growth process. In
this work, we use correlated in situ Environmental Transmission Electron Microscope, DFT
simulation, quantitative data extraction and statistical analysis to investigate the dynamic atomic
process of initial oxide growth. An unusual layer-by-layer growth of Cu$_2$O island along Cu$_2$O(110)
plane is observed, instead of along the previously assumed Cu$_2$O(100) plane that is parallel to the
Cu surface. Statistical analysis of growth dynamics indicates a diffusion limited monolayer growth
process. DFT results showed Cu$_2$O(110) has lower surface energy, favorable Cu and O diffusion
barriers and adsorption energies during oxidation, leading to easier Cu$_2$O monolayer formation
along Cu$_2$O(110). These results shed new light on surface oxidation process.

*NSF-DMR grants 1410055, 1508417, 1410335.
3:42PM J52.00007: Structure and electro-optical properties of Sr$_x$Ba$_{1-x}$Nb$_2$O$_6$ films grown by molecular beam epitaxy.* ILYA BESKIN (Presenter), JACQUELINE GELER KREMER, AGHAM POSADAS, ALEXANDER DEMKOV, University of Texas at Austin — With the rise of processor speed, optical fibers are replacing copper wires in carrying data between computer boards. Silicon photonics has applications in not only chip interconnects, but also neuromorphic and quantum computing. The Pockels effect offers a way to build fast, low power modulators of optical signals. The Pockels effect uses an electric field to change the index of refraction in a material. One can make devices that encode or alter information using the phase of light. Sr$_x$Ba$_{1-x}$Nb$_2$O$_6$ (SBN) has been shown to have one of the highest available Pockels coefficients (~850pm/V). SBN was grown by molecular beam epitaxy on SrTiO$_3$ (STO) substrates and STO can be used to integrate materials on Si. The growth was monitored with Reflective High Energy Electron Diffraction. Composition and oxidation states were measured in-situ by X-Ray Photoemission Spectroscopy. X-Ray Diffraction was used to verify the crystal phase and orientation of the SBN crystal.

*The work is supported by the Air Force Office of Scientific Research under grant FA9550-18-1-0053

3:54PM J52.00008: Probing TiO$_2$ as a potential filter material for adsorption and destruction of chemical warfare agents* ROMAN TSYSHEVSKIY (Presenter), University of Maryland, College Park, MONICA MCENTEE, ERIN DURKE, CCDC Chemical Biological Center, TIANYU LI, MATTHEW LEONARD, EFRAIN RODRIGUEZ, University of Maryland, College Park, CHRISTOPHER KARWACKI, CCDC Chemical Biological Center, MAIJA M KUKLA, University of Maryland, College Park — An atomistic level understanding of mechanisms of adsorption and decomposition of chemical agents on components of filtration materials is required for improvements of existing and design of new materials for chemical protection. Here, we present a comprehensive study of sarin interactions with TiO$_2$ performed by means of quantum chemical calculations and a combination of IR and XPS measurements. Computational modeling was used to reveal mechanisms of sarin adsorption and decomposition on an ideal (defect free) and hydroxylated TiO$_2$ rutile (110) and anatase (101) surfaces, whereas experimental measurements were performed for TiO$_2$ nanoparticles and synthesized mesoporous materials. Calculations revealed strong adsorption of sarin on both the ideal rutile and anatase surfaces, although high activation barriers preclude a decomposition of sarin. The presence of water, on the other hand, reduces binding strength of sarin to rutile and anatase, but promotes the decomposition of sarin. Results of computational modeling were found in good agreement with experimental measurements.

*This work was supported by US DOD through DTRA (HDTRA11910001). R.T. and M.M.K acknowledge support from XSEDE (DMR-130077), NERSC (Contract DE-AC02-05CH11231), MARCC and UMD supercomputing resources.
Thin films of Hf-based oxides gained importance after the discovery of the ferroelectricity in these materials\textsuperscript{1}. One of the ways to achieve ferroelectricity in HfO\textsubscript{2} is doping with metals such as Zr and Al to modify the crystal structure towards orthorhombic symmetry. In Hf based oxide thin films prepared by doping, multiple crystal phases could emerge. In this work, we theoretically investigated the stability of the possible structures that could be present in Al doped HfO\textsubscript{2} using quantum mechanical methods. Specifically, using plane wave density functional theory, the monoclinic, tetragonal, orthorhombic, and rhombohedral phases of aluminum doped hafnia were geometrically optimized. The resulting equilibrium structures for 3\%, 6\%, and 7\% Al doped hafnia structures will be used as theoretical reference structures for EXAFS spectra obtained Al doped HfO\textsubscript{2} thin films.

Keywords: Density functional theory, ferroelectricity, doped hafnia

Investigation of the thickness-dependent optical properties of ZnO films on Si and SiO$_2$ substrates from the Mid-infrared to the Vacuum-ultraviolet using UV and FTIR spectroscopic ellipsometry

NUWANJULA SAMARASINGHA ARACHCHIGE (Presenter), STEFAN ZOLLNER, New Mexico State University, Las Cruces, NM, United States., DIPAYAN PAL, AAKASH MATHUR, AJAIB SINGH, RINKI SINGH, SUDESHNA CHATTOPADHYAY, IIT Indore, Indore, India. — The conventional approach to describe the dielectric function $\varepsilon$ as a sum of oscillators sometimes fails because each term only has a single broadening parameter. Instead, we find it more convenient to describe $\varepsilon$ as a product of Drude, TO/LO phonon, and electronic interband transition factors. Specifically, we explore the behavior of phonon and excitonic absorption in bulk zinc oxide (ZnO) and ZnO thin films grown on Si and SiO$_2$ using UV/VIS and FTIR spectroscopic ellipsometry. We characterized the structural properties of our ZnO films with x-ray diffraction, x-ray reflectivity, and atomic force microscopy.

We find that the real and imaginary parts of $\varepsilon$ in ZnO films on Si and SiO$_2$ are much smaller than in bulk. Excitonic enhancement, absorption coefficient, and refractive index decrease monotonically with decreasing film thickness. The impact of the excitonic contribution to $\varepsilon$ was described by Tanguy [1]. We also fit our ellipsometric spectra by describing the dielectric function of ZnO using the Tanguy model. Also, we investigate the thickness dependence of the Born effective charge, high-frequency and static dielectric constant, and exciton parameters.

References

Supported by NSF (DMR - 1505172)

Surface structure and electronic properties of $a$, $b$, and $e$ polymorphs of Ga$_2$O$_3$

TENGFEI CAO (Presenter), ROHAN MISHRA, Mechanical Engineering & Materials Science, Washington University in St. Louis — Ga$_2$O$_3$ is an emerging wide-band-gap semiconductor that exhibits diverse phases with varying electronic properties. $\varepsilon$-Ga$_2$O$_3$, a metastable polymorph, has recently been reported to be a ferroelectric semiconductor with potential application in power and high-frequency electronics [1]. Although there have been numerous attempts to grow $\varepsilon$-Ga$_2$O$_3$ on various substrates, single-phase $\varepsilon$-Ga$_2$O$_3$ thin films have not been reported. An investigation of the stability of the surface of $a$, $b$, and $e$ polymorphs of Ga$_2$O$_3$ can facilitate the synthesis of phase-pure thin films. Results of first-principles calculations of the surface stability of the three Ga$_2$O$_3$ polymorphs as a function of the chemical potential along with their electronic properties will be presented. The stability of its (001) polar surface of Ga$_2$O$_3$ as a function of polarization and thickness will be presented. Moreover, electronic structure calculations indicate a lack of quantum confinement in $\alpha$-Ga$_2$O$_3$ thin-films. Finally, different substrate effects on the stability of the three Ga$_2$O$_3$ polymorphs will be talked.


This work was supported by NSF DMR-1931610.
Atomistic determination of the surface structure of Cu$_2$O (111) and Cu$_2$O (110): experiment and theory*  

JEFFREY GUEST (Presenter), Center for Nanoscale Materials, Argonne National Laboratory, RUI ZHANG, Department of Physical and Material Sciences, Anhui University, LIANG LI, Center for Nanoscale Materials, Argonne National Laboratory, LASZLO FRAZER, Centre of Excellence in Exciton Science, University of New South Wales, KELVIN B. CHANG, KENNETH R POEPPELMEIER, Department of Chemistry, Northwestern University, MARIA CHAN, Center for Nanoscale Materials, Argonne National Laboratory — Photocatalytic reactions on the surface of cuprous oxide (Cu$_2$O) hinge on atomic scale structure of the defected Cu$_2$O surfaces; however, to date, the atomic morphologies of these surfaces have not been unambiguously characterized. In this work, high-resolution ultrahigh vacuum (UHV) scanning tunneling microscopy (STM) and density functional theory (DFT) calculations combined with STM simulations have been used to determine the structure of the defected (111) and (110) surfaces of a Cu$_2$O bulk crystal. Under STM, the imaged Cu$_2$O (111) surface is dominated by coordinatively unsaturated copper atoms, and atomic-scale defects including the Cu vacancy and the O-vacancy-induced local surface restructuring [1,2] are identified. The Cu$_2$O(110) surface reveals aggregation of defects and periodic distortions of the atomic rows.


*Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
4:54PM J52.00013: Structural and Electrical Properties of Pulsed Laser Deposited Yttrium Doped Zirconium Oxide Thin Film Stabilization* MATTHEW MELFI (Presenter), SARAH TUTTLE, SAMANTHA DALLI, KELLEN MURPHY, MEHMET ALPER SAHINER, Seton Hall Univ — Solid Oxide Fuel Cells (SOFC) are devices that use electrochemical reactions to convert chemical energy from fuel to electricity. In comparison with coal power plants, a SOFC produces a higher electrical conversion efficiency. SOFC is a possible candidate for energy production. However, at higher temperatures (800-1000°C) it creates a lower ionic conductivity, which limits the SOFC. When lowering the temperature, the ohmic resistance increases, as a thin film. In our research a YSZ, layer will be produced from a fine dimple grain structure allowing high flow of O\textsubscript{2} mobility. This mobility increases ionic conductivity and decreases ohmic loss. The goal of our research is to determine if the YSZ thin film synthesis lead to minimum ohmic resistance of the films at optimum film thickness. The method that is used is to test different molecular ratios of the YSZ and deposit the ratios with different energy levels onto different substrates, including conductors, semi-conductors, and insulators, and compare the properties of the YSZ layer. The thin films will be characterized through electrical measurements such as 4-Point Probe Resistivity measurements as well as AFM, SEM, and EDX Spectroscopy for the structural and compositional characterization.

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5:06PM J52.00014: Time-resolved Nanosecond-Laser Recrystallization of Amorphous FeDy-O Thin Films in the (S)TEM* KRISHNA KOIRALA (Presenter), CHENZE LIU, University of Tennessee, Knoxville, TATIANA ALLEN, University of Tennessee-Chattanooga, RAMKI KALYANARAMAN, GERD DUSCHER, University of Tennessee, Knoxville — Iron-Dysprosium oxide thin film can be an amorphous semiconductor with unusual magneto-optic properties. The properties of amorphous materials are often governed by local structure and recrystallization mechanism is important for the stability of the materials system as well as engineering of properties. To investigate the structure and chemical composition of this material, we employed laser processing inside the (S)TEM with simultaneous High-Resolution Transmission Electron Microscopy (HRTEM) imaging, Electron Diffraction, and Electron Energy Loss Spectroscopy (EELS) measurements. It shows that the structural change in amorphous FeDy-O can be seen as early as with 100 ns single laser pulse at the laser fluency of 1.49E6 J/cm\textsuperscript{2} as indicated by the emergence of sharp diffraction rings from initial broad and diffuse diffraction ring. The pulsed laser-induced changes were studied up to 10,000 pulses where intense Brag's spots were visible. Our results provide insight on unique way of understanding the local structure evolution and time resolution of the recrystallization process with laser pulses and allow us to conclude back onto the amorphous atomic arrangement of this material system.

*The authors acknowledge support by the National Science Foundation and the Department of Energy.
J52.00015: Ionic liquid gate induced modifications of oxides surface

YUECHEN ZHUANG

(Presenter), BIN CUI, HAO YANG, FANG GAO, STUART PARKIN, Max Planck Institute of Microstructure Physics — Intense electric fields developed during gating at the interface between an ionic liquid (IL) and an oxide layer have been shown to lead to significant structural and electronic phase transitions in the entire oxide layer. An archetypical example is the reversible transformation between the brownmillerite SrCoO$_{2.5}$ and the perovskite SrCoO$_3$ engendered by ionic liquid gating. In this presentation, we show using in-situ atomic force microscopy studies, with photothermal excitation that allows for high quality measurements in the viscous environment of the ionic liquid, that the edges of atomically smooth terraces at the surface of SrCoO$_{2.5}$ films are significantly modified by IL gating but that the terraces themselves remain smooth. The edges develop ridges that we show, using complementary X-ray photo emission spectroscopy studies, result from the adsorption of hydroxyl groups. Our findings open up opportunities for electrically controlled surface modifications in emergent ionitronic applications.

*This research was supported by the DFG through SFB 762 and EU H2020 program “Phase Change Switch”.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J53 DCMP: Scanning Tunneling Microscopy of 2D Materials and Hall Effect in 2D Materials

Mile High Ballroom 1F - Geng Li

2:30PM J53.00001: Atomic-scale spectroscopy of 2D Transition metal dichalcogenide heterostructures

SARA SHABANI (Presenter), ABHAY PASUPATHY, Columbia Univ — Bilayers of 2H-WSe2 and 2H-MoSe2 form a type-II semiconductor heterostructure. A number of interesting optoelectronic phenomena have been observed in such heterostructures including charge transfer excitons, photovoltaic and photothermal effects, and Mott transitions at high exciton density. In this talk, we will describe complementary single-particle measurements of the electronic structure of these heterostructures using scanning tunneling microscopy (STM) and spectroscopy. Using a large-area exfoliation technique, coupled with pre-patterned electrodes to make ohmic contact to these bilayers, we have succeeded in fabricating devices that are compatible with surface-sensitive probes such as STM and angle resolved photoemission. We will describe the spatial structure of the bilayers including the effect of lattice mismatch on the electronic properties, as well as spectroscopic measurements performed under optical illumination both below and above the Mott threshold.
2:42PM J53.00002: Unraveling the Tunneling Spectrum of Bernal Stacked Bilayer Graphene*  
JOHN DAVENPORT (Presenter), ZHEHAO GE, FREDERIC JOUCKEN, EBERTH A QUEZADA, Physics Dept., University of California: Santa Cruz, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS Japan, JAIRO VELASCO JR., Physics Dept., University of California: Santa Cruz — Scanning tunneling spectroscopy (STS) has recently provided important insight on the symmetry breaking effects and correlated states in magic angle twisted bilayer graphene (MATBLG). Conventional STS, however, can unintentionally change the dynamic band structure of MATBLG sheets due to the unavoidable and prominent electric field from the STS probe tip. Such an effect can obscure the intrinsic nature of correlated electron states present in MATBLG. We will discuss our latest experimental progress towards using a simpler tunneling system—planar tunneling spectroscopy nanodevices—to controllably probe the dynamic band structure of Bernal-stacked bilayer graphene. Our methods can be applied to MATBLG as well as other two-dimensional material systems that have a dynamical band structure.

*US Army Research Office  
Department of Education GAANN Fellowship

2:54PM J53.00003: Proximity-induced superconducting gap in the quantum spin Hall edge state of monolayer WTe$_2$*  
FELIX LUEPKÉ (Presenter), DACEN WATERS, Carnegie Mellon University, SERGIO DE LA BARRERA, Massachusetts Institute of Technology, MICHAEL WIDOM, Carnegie Mellon University, DAVID MANDRUS, University of Tennessee, Knoxville, JIAQIANG YAN, Oak Ridge National Lab, RANDALL M FEENSTRA, BENJAMIN HUNT, Carnegie Mellon University — Van der Waals heterostructures allow the combination of different material properties, e.g. non-trivial topology and superconductivity in order to create a topological superconducting state. In my talk, I demonstrate a novel dry-transfer flip technique which allows to place atomically-thin layers of WTe$_2$, a quantum spin hall system, on NbSe$_2$, a van der Waals superconductor. Using scanning tunneling microscopy and spectroscopy (STM/STS), we demonstrate atomically clean surfaces and interfaces and the presence of a proximity-induced superconducting gap in the WTe$_2$ for thicknesses from a monolayer up to 7 crystalline layers. At the edge of the WTe$_2$ monolayer, we show that the superconducting gap coexists with the characteristic spectroscopic signature of the QSH edge state [1]. Taken together, these observations provide conclusive evidence for proximity-induced superconductivity in the QSH edge state in WTe$_2$, a crucial step towards realizing 1D topological superconductivity and Majorana states in this van der Waals material platform.


*This research was funded by DOE DE-SC0018115, DOE DE-SC0014506, NSF DMR-1539916, NSF DMR-1809145, NSF DMR-1626099.
3:06PM J53.00004: Observation of Deep In-gap States of Line and Point defects in Monolayer WS₂ via Scanning Tunneling Microscopy and Spectroscopy*  MADISEN HOLBROOK (Presenter), WEI-TING HSU, CHIH-KANG SHIH, University of Texas at Austin — Atomic defects in crystalline semiconductors strongly affect their electronic properties, such as electron transport and optical response. Defects in two dimensional (2D) semiconductors, such as transition metal dichalcogenides (TMD’s), have a more dramatic impact than bulk counterparts due to less screening and increased substrate interactions. In particular, different atomic vacancies have been reported, but their role in the electronic structure must be established. Deep in-gap states were predicted for different defect structures in 2D TMD’s, but direct experimental observation of defect structure and electronic properties is necessary to tailor TMD’s for device design. Here we report the creation of point and line defects in WS₂ monolayers by vacuum annealing. The electronic properties and structure of these defects was probed using scanning tunneling microscopy and spectroscopy. We find these defects have a rich variety of deep in-gap states, shedding light on the role of defects in TMD electronic properties.

*This work was supported by NSF MRSEC (DMR-1720595) and DMR-EPM (DMR-1808751) as well as contributions from the US Airforce (FA2386-18-1-4097) and the Welch Foundation (F-1672).

3:18PM J53.00005: Determination of the trigonal warping orientation in Bernal-stacked bilayer graphene via quasiparticle interference imaging*  FREDERIC JOUCKEN (Presenter), ZHEHAO GE, EBERTH A QUEZADA, Physics, University of California, Santa Cruz, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan, JAIRO VELASCO JR., Physics, University of California, Santa Cruz — The existence of strong trigonal warping around the K point for the low energy electronic states in multilayer graphene films and graphite is well established. It is responsible for phenomena such as Lifshitz transitions and anisotropic ballistic transport. The absolute orientation of the trigonal warping with respect to the center of the Brillouin zone is however not agreed upon. Here, we use quasiparticle scattering experiments on a gated bilayer graphene/hexagonal boron nitride heterostructure to resolve this disagreement. We compare Fourier transforms of scattering interference maps acquired at various energies away from the charge neutrality point with joint density of states simulations. This comparison permits unambiguous determination of the trigonal warping orientation for bilayer graphene at low energy. Our experimental technique is promising for studying quasi-directly fine features of the band structure of two-dimensional materials such as band topologies and Lifshitz transitions.

*Funding for this research was provided by an NSF CAREER award under award number DMR-1753367 and we acknowledge partial support from UCOP and the Army Research Office under contract W911NF-17-1-0473.
3:30PM J53.00006: Charge/spin density waves at the edges and mirror twin boundaries of Transition Metal Di-Chalcogenides*  
SRIDEVI KRISHNAMURTHI (Presenter), Univ of Twente —  
Grain boundaries and edges of two-dimensional semiconducting TMDCs MX₂ (M=Mo,W; X=S,Se,Te) exhibit metallicity, which is remarkably robust against variations in structure or stoichiometry. The origin of these metallic boundary states lies in the lattice polarization and the states are topologically protected by the D₃h symmetry of the TMDC lattice. From first-principles (DFT+U) calculations we show, however, that symmetry breaking at edges or boundaries leads to one-dimensional charge and spin density wave (C/SDW) instabilities. Such C/SDWs are commensurable with a period of three lattice sites, dictated by the lattice symmetry, and open up a band gap. The resulting electronic structure agrees well with experimental measurements on, for instance, the mirror twin boundary.

*Computational Sciences Energy Research joint initiative by NWO-i and Shell.

3:42PM J53.00007: Quantum spin Hall effect in twisted bilayer WTe₂ measured with STM*  
DACEN WATERS (Presenter), FELIX LUKAS LÜPKE, BENJAMIN HUNT, RANDALL M FEENSTRA, Physics Department, Carnegie Mellon University —  
Tungsten telluride is a two-dimensional (2D) material that exhibits a range of properties, depending on the number of layers. Bilayers are reported to be a topologically trivial semimetal that exhibit a ferroelectric effect¹. In the monolayer (ML) limit, WTe₂ has been shown to be a quantum spin Hall (QSH) insulator², resulting in topologically protected edge modes. In this work, we report scanning tunneling microscopy and spectroscopy (STM/STS) studies of twisted bilayers of WTe₂ for a variety of configurations. We find that tunneling spectra of the twisted bilayers resemble that of decoupled monolayers for twist angles ≥5°, and observe edge states to exist at the boundaries of the twisted bilayer regions, in contrast to the case of the trivial bilayer. To study exfoliated WTe₂ in STM, which is air sensitive, we utilize a novel transfer technique³ that enables stacking in an inert gas environment but maintains an atomically pristine surface available for surface probe measurements.


*The authors would like to thank the US Department of Energy (DE-SC0018115, SC0014506) and the National Science Foundation (DMR-1539916, 1626099, 1809145) for their support.
Disorder-induced nonlinear Hall effect with time-reversal symmetry

ZONGZHENG DU, Southern University of Science and Technology, CHUNMING WANG, Shanghai Normal University, SHUAI LI, HAIZHOU LU (Presenter), Southern University of Science and Technology, XINCHENG XIE, Peking University — The nonlinear Hall effect has opened the door towards deeper understanding of topological states of matter. It can be observed as the double-frequency Hall voltage response to an ac longitudinal current in the presence of time-reversal symmetry. Disorder plays indispensable roles in various linear Hall effects, such as the localization in the quantized Hall effects and the extrinsic mechanisms of the anomalous, spin, and valley Hall effects. Unlike in the linear Hall effects, disorder enters the nonlinear Hall effect even in the leading order. Here, we derive the formulas of the nonlinear Hall conductivity in the presence of disorder scattering. We apply the formulas to calculate the nonlinear Hall response of the tilted 2D Dirac model, which is the symmetry-allowed minimal model for the nonlinear Hall effect and can serve as a building block in realistic band structures. More importantly, we construct the general scaling law of the nonlinear Hall effect, which may help in experiments to distinguish disorder-induced contributions to the nonlinear Hall effect in the future. This work will be insightful for studying the disorder effects in the nonlinear Hall effect.


Intrinsic orbital moment and prediction of a large orbital Hall effect in the 2D transition metal dichalcogenides

SAYANTIKA BHOWAL (Presenter), SASHI SEKHAR SATPATHY, Univ of Missouri - Columbia — Orbital Hall effect (OHE) is the phenomenon of transverse flow of orbital angular momentum caused by an applied longitudinal electric field. From density-functional and tight-binding model studies, we predict the existence of a large OHE in the 2D transition metal dichalcogenides (TMDC) due to the intrinsic orbital moment induced by the broken inversion symmetry of the system. We show that monolayer TMDC, the prototypical example of broken inversion symmetric 2D material, have a hitherto-unknown intrinsic orbital moment in the momentum space, which in turn leads to a large OHE with possible applications in the newly emerging field of orbitronics. The orbital moment and the OHE appear even in absence of the spin-orbit coupling (SOC) and give rise to “valley dependent spin splitting” and spin Hall effect in presence of SOC. We show that the OHE can also be tuned by a transverse electric field due to the orbital Rashba coupling, that produces an additional orbital texture which in turn modifies the OHE.

*We thank the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering for financial support under Grant No. DE-FG02-00ER45818.
4:18PM J53.00010: Magnus Hall effect*  MICHAL PAPAJ (Presenter), LIANG FU, Massachusetts Institute of Technology MIT — A new type of a linear response Hall effect is predicted in time-reversal-invariant systems with built-in electric field at zero magnetic field. The Hall response results from a quantum Magnus effect where a self-rotating Bloch electron wavepacket moving under electric field develops an anomalous velocity in the transverse direction. We show that in the ballistic limit the Magnus Hall conductance measures the distribution of the Berry curvature on the Fermi surface.

*This work was supported by DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0018945.

4:30PM J53.00011: The Curious Magnetic Properties of Orbital Chern Insulators  JIHANG ZHU (Presenter), ALLAN MACDONALD, University of Texas at Austin — Chern insulator ferromagnets are characterized by a quantized anomalous Hall effect, and have so far been identified experimentally in magnetically-doped topological insulator (MTI) thin films and in bilayer graphene moiré superlattices. We classify Chern insulator ferromagnets as either spin or orbital, depending on whether the orbital magnetization results from spontaneous spin-polarization combined with spin-orbit interactions, as in the MTI case, or directly from spontaneous orbital currents, as in the moiré superlattice case. We argue that in a given magnetic state, characterized for example by the sign of the anomalous Hall effect, the magnetization of an orbital Chern insulator will often have opposite signs for weak n and weak p electrostatic or chemical doping. This property enables pure electrical switching of a magnetic state in the presence of a fixed magnetic field.

4:42PM J53.00012: Hall Conductivity of Two-Dimensional Electrons in an Abrikosov Magnetic Flux Lattice*  JONATHAN SCHIRMER (Presenter), Pennsylvania State University, RAVI KHANDELWAL, Physics, Indian Institute of Science, Bangalore, KENJI WATANABE, NIRM, TAKASHI TANIGUCHI, Kyoto Univ, PRATAP RAYCHAUDHURI, Tata Institute of Fundamental Research, JAINENDRA JAIN, CHAOXING LIU, Pennsylvania State University, ANINDYA DAS, Physics, Indian Institute of Science, Bangalore — We study, both theoretically and experimentally, the Hall transport of two-dimensional electrons exposed to a magnetic field produced by an Abrikosov flux lattice. Our experiments on monolayer graphene-hBN-NbSe2 heterostructure demonstrate a substantial reduction in the Hall conductivity as the temperature is reduced from above the superconducting critical temperature of NbSe2, when the magnetic field is uniform, to below, where the magnetic field bunches into an Abrikosov flux lattice. We provide a quantitative explanation of this phenomenon by evaluating the cumulative Berry curvature of occupied states using a lattice model, while also taking account of disorder, and extrapolating to the continuum limit. A fundamental role is played by a correlation between the Berry curvature and the energy within Landau levels broadened by the non-uniform magnetic field.

*U.S. Department of Energy, Office of Basic Energy Sciences, Grant No. desc0005042
4:54PM J53.00013: Energy gaps of low filling factor quantum Hall states in two-dimensional Indium Selenide. DMITRY SHCHERBAKOV (Presenter), PETR STEPANOV, JIAWEI YANG, Ohio State Univ - Columbus, SHAHRIAR MEMARAN, WENKAI ZHENG, National High Magnetic Field Lab, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Namiki Tsukuba Ibaraki, Japan, LUIS BALICAS, National High Magnetic Field Lab, CHUN NING LAU, Ohio State Univ - Columbus — Indium selenide is a promising two-dimensional semiconductor with thickness-dependent bandgap and high electron mobility. We have fabricated high mobility few-layer InSe devices and studied them in quantum Hall regime. Landau levels at filling factors between 1 and 10 are resolved. Energy gaps at different magnetic fields, gate voltage and temperatures will be discussed.

5:06PM J53.00014: Non-perturbative valley Hall effect in graphenes* WEI-YUAN TU (Presenter), CI LI, HONGYI YU, WANG YAO, The University of Hong Kong — Valley Hall currents can be induced in graphene by breaking its version symmetry that opens a gap which is usually very small. A finite electric field can easily exceed the adiabatic limit on which the standard semiclassical theory for the valley Hall effect is based. Here we provide a non-perturbative formulation for valley Hall effect. We show that the non-perturbation effects of the electric field directly lead to an oscillating anomalous velocity in the coherent evolution of an electron, in contrast to the stationary one inherited to the adiabatic limit. By properly taking into account the decoherence effect, we obtain a steady-state valley Hall current that is in all orders of the electric field. It clearly shows nonlinearity in the Hall conductivity to high electric-field values and still retains the intrinsic role of the Berry curvature. Through the inspection of the non-perturbative effect of the electric field, it becomes obvious that the valley Hall conduction in gapped graphene is mediated by the interference between the electric field induced electron-hole excitations and the fermi sea.

*The work is supported by the Research Grant Council of HKSAR (17306819, C7036-17W).
5:18PM J53.00015: Edge channels in graphene with proximity-induced Spin-Orbit Interaction
TARO WAKAMURA, SOPHIE GUERON (Presenter), NIANTHENG WU, MEYDI FERRIER, HÉLÈNE BOUCHIAT, Laboratoire de Physique des Solides Orsay, U. Paris Sud, U. Paris Saclay, CNRS, France, CECILIA MATTEVI, PAWEL PALCZYNSKI, MAURO OCH, Imperial College London, UK, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, Japan — Enhancing spin-orbit interaction (SOI) in graphene may lead to new properties, including a possible Quantum Spin Hall state, characterized by counterpropagating, spin-polarized channels at the edges of graphene. We previously demonstrated how graphene coupled to Transition Metal Dichalcogenides (TMDs) acquires a strong and mirror-symmetric spin-orbit interaction, especially with monolayers of WSe2 and WS2. The signature of induced spin-orbit was weak antilocalization (positive magnetoresistance) in mesoscopic samples with normal contacts at low temperature [1, 2]. In this talk I will present our recent measurements of supercurrents induced through graphene/WS2 heterostructures connected to high-critical-field superconductors. I will discuss how signatures of edge conduction are detected for both graphene coupled to hBN and graphene coupled to WS2 in short Josephson junctions, but how the edge channels are far more dominant in long junctions of graphene coupled to WS2, and visible also at high magnetic fields applied perpendicularly to the graphene plane.

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J54 DCMP: Bulk-Boundary Correspondence and Classification of Topological Phases Mile High Ballroom 2A

2:30PM J54.00001: Realizing the bulk-boundary correspondence for anomalous symmetry-enriched topological phases DANIEL BULMASH (Presenter), MAISSAM BARKESHLI, University of Maryland, College Park — We construct models of anomalous 2+1D symmetry-enriched topological phases (SETs) on the surfaces of 3+1D symmetry-protected topological phases, providing an explicit realization of the bulk-boundary correspondence for SETs. Our construction takes as input the symmetry fractionalization data and does not require a priori knowledge of the SET’s anomaly. Our method works for both non-permuting and anyon-permuting symmetry actions on both Abelian and non-Abelian topological orders. We discuss the extraction of the absolute anomaly using our construction.
2:42PM J54.00002: Bulk-boundary correspondence for (2+1)D symmetry protected topological phases*  KYLE KAWAGOE (Presenter), MICHAEL LEVIN, University of Chicago — A universal property of symmetry protected topological (SPT) phases is that they have low energy boundary modes that are protected under the symmetry. This fact inspires an important problem in the theory of SPT phases: How does one identify a bulk SPT phase given a low energy theory of its boundary? This question is particularly challenging in the case of interacting SPT phases where band theory approaches are inapplicable. In this talk, we present a general method for solving this problem in the case of (2+1)D interacting bosonic systems with internal (non-spatial) symmetries.

*This work was supported by the Simons Foundation through the "Ultra-Quantum Matter" Simons Collaboration.

2:54PM J54.00003: Correlated bulk-boundary correspondence of the higher-order topological insulator*  KOJI KUDO (Presenter), TSUNEYA YOSHIDA, YASUHIRO HATSUGAI, Univ of Tsukuba — In this talk, we propose a novel topological state which we call “higher-order topological Mott insulator” (HOTMI) [1]. It gives a distinct bulk-boundary correspondence from a conventional higher-order topological insulator; $d$-dimensional bulk topology of the HOTMI predicts the emergence of gapless states not in charge excitations but in spin excitations around $(d-n)$-dimensional boundaries with $n = 2, \ldots, d$. We numerically demonstrate that the Hubbard model on the kagome lattice gives the 2nd-order HOTMI states for $d = 2$. Specifically, the corner-Mott states appearing in the system under the open boundary condition, which is gapless only in the spin excitations, are predicted by the $Z_3$ spin Berry phase calculated in the bulk system.


*The work is supported by JSPS KAKENHI Grant Numbers JP16K13845 (Y.H.), JP17H06138, JP18H05842 (T.Y.), and JP19J12317 (K.K.).

3:06PM J54.00004: Anomaly and symmetry fractionalization of mirror-symmetric fermionic topological orders  BINBIN MAO (Presenter), CHENJIE WANG, The University of Hong Kong — We study symmetry fractionalization and quantum anomaly in general 2D fermionic topological orders with the mirror reflection symmetry. A set of constraints on mirror fractionalization and an explicit anomaly indicator formula are derived. Our derivation is based on the recently developed folding approach, which was originally proposed in bosonic topological orders. The anomalous mirror-symmetric topological orders can only live on the surface of 3D topological crystalline superconductors, and we establish a direct bulk-boundary correspondence.
3:18PM J54.00005: Computing the Classification of Fermionic Symmetry-Protected Topological States  
YUNQING OUYANG (Presenter), Department of Physics, Fudan University, QING-RUI WANG, ZHENGCHENG GU, Department of Physics, The Chinese University of Hong Kong, YANG QI, Department of Physics, Fudan University — The bosonic symmetry protected topological (SPT) states are classified by the cohomology groups of the symmetry group. However, for interacting fermionic systems, the classification is much more complicated. It was until very recent that a breakthrough was made on the classification and construction of fermionic SPT states based on the concept of equivalence class under finite-depth symmetric fermionic local transformations. However, though layers of data for classification and construction can be obtained theoretically, the formalism based on the bar resolution of symmetry groups (also known as the inhomogeneous cochains) makes it impossible for realistic computation due to high computational costs. To solve these problems, we first design reduced resolutions for general groups by group extension, then we apply the chain maps between the bar resolution and reduced resolution to solve the obstruction function to get the unobstructed layers of data. Meanwhile, to simplify the computation, we apply the technique of spectral sequence. Finally, we give a classification of fermionic SPTs protected by 2D wallpaper-group symmetries.

3:30PM J54.00006: Non-Abelian reciprocal braiding of Weyl nodes and fragile topology  
ADRIEN BOUHON (Presenter), NORDITA, QUANSHENG WU, Physics, EPF Lausanne, ROBERT-JAN SLAGER, Physics, Harvard University, TOMAS BZDUSEK, LSM, Paul Scherrer Institut — Weyl nodes trapped within $C_2T$ symmetric planes (i.e. -crystalline rotation combined with time reversal) acquire a non-Abelian topological charge on top of their chirality. E.g. three-level systems realize the quaternion group [1]. The non-Abelian nature of Weyl nodes can alternatively be captured by the Euler class [2,3], which itself can be efficiently computed through the Wilson loop as the winding number of a Pfaffian [3]. These tools allow us (i) to design minimal experimental setups, and (ii) to search for material candidates. Furthermore, we show that additional crystalline symmetries can lead to the obstruction of the Euler class which naturally gives rise to nontrivial fragile topology.

3:42PM J54.00007: Topology of SO(5) monopoles and three dimensional Dirac semimetals
PALLAB GOSWAMI (Presenter), ALEXANDER TYNER, SHOUVIK SUR, Northwestern University — The topological properties of Kramers degenerate band structures generally emerge from non-trivial textures of underlying SO(5) Berry's vector potential. The linear touching between a pair of Kramers degenerate energy bands at isolated points of momentum space along an n-fold axis of rotation gives rise to three dimensional Dirac semimetals, where the Dirac points act as singularities of SO(5) gauge fields. Even though considerable progress has been made in recent years toward understanding the stability of Dirac points in the presence of parity, time reversal and discrete rotational symmetries, as of now there is no clear definition of topological invariants for Dirac points and any arbitrary momentum plane that is perpendicular to the direction of nodal separation. We will show how the implementation of global rotational symmetry causes an U(1) x U(1) abelian gauge fixing of SO(5) vector potential, allowing us to define monopole invariants and quantized "spin Chern" numbers respectively for the Dirac points and the two dimensional planes perpendicular to the direction of nodal separation. We also demonstrate that generic form of Kramers degenerate Dirac semimetals do not support protected helical Fermi arcs.

*NSF DMR-1720139

3:54PM J54.00008: Duality between supercohomology fermionic SPT (symmetry-protected-topological) phases and higher-group bosonic SPT phases
YU-AN CHEN (Presenter), Physics, Caltech, TYLER ELLISON, Physics, University of Washington, NATHANAN TANTIVASADAKARN, Physics, Harvard — The first part of this talk will introduce generalized Jordan–Wigner transformation on arbitrary triangulation of any simply connected manifold in arbitrary dimensions. This gives a duality between any fermionic systems and a new class of $\mathbb{Z}_2$ lattice gauge theories. This map preserves the locality and has an explicit dependence on the second Stiefel–Whitney class and a choice of spin structure on the manifold. In the Euclidean picture, this mapping is exactly equivalent to adding topological terms, Steenrod square, to the spacetime action. The second part of the talk is the application of this boson-fermion duality on SPT phases. By the boson-fermion duality, we are able to show the equivalent between any supercohomology fermionic SPT and some higher-group bosonic SPT phase in arbitrary dimensions. Particularly in (3+1)D, we will show a unitary quantum circuit for any supercohomology fermionic SPT state with gapped boundary construction.
Non-Abelian anomalies in multi-Weyl semimetals

RENATO M. A. DANTAS (Presenter), FRANCISCO PENÁ-BENÍTEZ, Max Planck Inst, BITAN ROY, Lehigh University, PIOTR SUROWKA, Max Planck Inst — We construct the effective field theory for time-reversal symmetry breaking multi-Weyl semimetals (mWSMs), composed of a single pair of Weyl nodes of (anti-)monopole charge $n$, with $n = 1, 2, 3$ in crystalline environment. From both the continuum and lattice models, we show that a mWSM with $n > 1$ can be constructed by placing $n$ flavors of linearly dispersing simple Weyl fermions in a bath of an $SU(2)$ non-Abelian static background gauge field. Such an $SU(2)$ field preserves certain crystalline symmetry (four-fold rotational or $C_4$ in our construction), but breaks the Lorentz symmetry, resulting in nonlinear band spectra. Consequently, the effective field theory displays $U(1) \times SU(2)$ non-Abelian anomaly, yielding anomalous Hall effect, its non-Abelian generalization, which we further substantiate by numerically computing the regular and "isospin" densities from the lattice models of mWSMs. Altogether our findings unify the field theoretic descriptions of mWSMs of arbitrary monopole charge $n$ (featuring $n$ copies of the Fermi arc surface states), predict signatures of non-Abelian anomaly in table-top experiments, and pave the route to explore anomaly structures for multi-fold fermions, transforming under arbitrary half-integer or integer spin representations.

Entanglement Entropy of Generalized Moore-Read Fractional Quantum Hall State Interfaces

RAMANJIT SOHAL (Presenter), Physics, University of Illinois at Urbana-Champaign, BO HAN, Physics, University of Cambridge, LUIZ SANTOS, Physics, Emory University, CHI YAN JEFFREY TEO, Physics, University of Virginia — Topologically ordered phases of matter can be characterized by the presence of a universal, constant contribution to the entanglement entropy known as the topological entanglement entropy (TEE). The TEE can been calculated for Abelian phases via a "cut-and-glue" approach by treating the entanglement cut as a physical cut, coupling the resulting gapless edges with explicit tunneling terms, and computing the entanglement between the two edges. We provide a first step towards extending this methodology to non-Abelian topological phases, focusing on the generalized Moore-Read (MR) fractional quantum Hall states at filling fractions $\nu=1/q$. We consider interfaces between different MR states and write down explicit tunneling terms, which we motivate using an anyon condensation picture. We compute the entanglement entropy for an entanglement cut lying along the interface. Our work provides new insight towards understanding the connections between anyon condensation, gapped interfaces of non-Abelian phases, and TEE.

*We acknowledge support from NSERC of Canada, NSF, and ERC.
4:30PM J54.00011: Majorana zero modes in the presence of many-body interactions

MACIEJ MASKA (Presenter), ANDRZEJ WIECKOWSKI, MARCIN MIERZEJEWSKI, Department of Theoretical Physics, Wroclaw University of Science and Technology — Recently, there has been substantial progress in methods of identifying local integrals of motion in interacting integrable models or in systems with many-body localization [1]. We show that one of these approaches can be utilized for constructing local, conserved, Majorana fermions in systems with an arbitrary many-body interaction [2]. Then, we discuss how the many-body interactions influence the spatial structure and the lifetime of the Majorana modes. Finally, we determine the regime for which the information stored in the Majorana correlators is also retained for arbitrarily long times at high temperatures. We show that it is included in the regime with topologically protected soft Majorana modes, but in some cases is significantly smaller.

References:

*This work was supported by the National Science Centre, Poland via Projects No. 2016/23/B/ST3/00647 and 2013/11/B/ST3/00824.

4:42PM J54.00012: The Nieh-Yan Anomaly: Torsional Landau Levels, Central Charge and Anomalous Thermal Hall Effect

ZE-MIN HUANG (Presenter), University of Illinois at Urbana-Champaign, BO HAN, University of Cambridge, MICHAEL STONE, University of Illinois at Urbana-Champaign — The Nieh-Yan anomaly is the anomalous breakdown of the chiral U(1) symmetry caused by the interaction between torsion and fermions. We study this anomaly from the point of view of torsional Landau levels. It was found that the torsional Landau levels are gapless, while their contributions to the chiral anomaly are canceled, except those from the lowest torsional Landau levels. Hence, the dimension is effectively reduced from (3+1)d to (1+1)d. We further show that the coefficient of the Nieh-Yan anomaly is the free energy density in (1+1)d. Especially, at finite temperature, the thermal Nieh-Yan anomaly is proportional to the central charge. The anomalous thermal Hall conductance in Weyl semimetals is then shown to be proportional to the central charge, which is the experimental fingerprint of the thermal Nieh-Yan anomaly.
4:54PM J54.00013: Bulk-edge and bulk-hinge correspondence in inversion-symmetric insulators*  
RYO TAKAHASHI (Presenter), YUTARO TANAKA, SHUICHI MURAKAMI, Tokyo Inst of Tech - Tokyo — We show that a slab of a three-dimensional inversion-symmetric higher-order topological insulator (HOTI) in class A is a 2D Chern insulator, and that in class AII is a 2D $Z_2$ topological insulator. We prove it by considering a process of cutting the three-dimensional inversion-symmetric HOTI along a plane, and study the spectral flow in the cutting process [1]. We show that the $Z_4$ indicators, which characterize three-dimensional inversion-symmetric HOTIs in classes A and AII, are directly related to the $Z_2$ indicators for the corresponding two-dimensional slabs with inversion symmetry, i.e. the Chern number parity and the $Z_2$ topological invariant, for classes A and AII respectively [2]. The existence of the gapless hinge states is understood from the conventional bulk-edge correspondence between the slab system and its edge states. Moreover, we also show that the spectral-flow analysis leads to another proof of the bulk-edge correspondence in one-dimensional inversion-symmetric insulators.


*This work was supported by JSPS KAKENHI Grant Numbers JP18J23289 and JP18H03678.

5:06PM J54.00014: Surface Topological Order for Higher-Order Topological Phases of Matter*  
APOORV TIWARI (Presenter), Paul Scherrer Institute, MINGHAO LI, Physics, ETH Zurich, ANDREI BERNEVIG, Princeton University, TITUS NEUPERT, Physics, University of Zurich, SIDDHARTH PARAMESWARAN, Physics, University of Oxford — We show that the chiral Dirac and Majorana hinge modes in three-dimensional higher-order topological insulators (HOTIs) and superconductors (HOTSCs) can be gapped while preserving the protecting $C_{2n}T$ symmetry upon the introduction of non-Abelian surface topological order. In both cases, the topological order on a single side surface breaks time reversal symmetry, but appears with its time-reversal conjugate on alternating sides in a $C_{2n}T$ preserving pattern. In the absence of the HOTI/HOTSC bulk, such a pattern necessarily involves gapless chiral modes on hinges between $C_{2n}T$-conjugate domains. However, using a combination of K-matrix and anyon condensation arguments, we show that on the boundary of a 3D HOTI/HOTSC these topological orders are fully gapped and hence `anomalous'. Our results suggest that new patterns of surface and hinge states can be engineered by selectively introducing topological order only on specific surfaces.

*This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Marie SklodowskaCurie grant agreement No 701647).

Tuesday, March 3, 2020 2:30 PM - 5:06 PM

Session J55 DCMP: Photoemission Studies of Topological Materials Mile
High Ballroom 2B - Michael Osofsky, United States Naval Research Laboratory
2:30PM J55.00001: Evolution of the band structure of α-Sn(001) thin film on InSb(001)  KO-HSUAN CHEN (Presenter), Department of Physics, National Tsing Hua University, KENG-YUNG LIN, Department of Physics, National Taiwan University, SHENG-WEN HUANG, Department of Physics, National Tsing Hua University, CHAO-KAI CHENG, Department of Physics, National Taiwan University, HSIAO-YU LIN, Department of Physics, National Tsing Hua University, SHANG-WEI LIEN, TAY-RONG CHANG, Department of Physics, National Cheng Kung University, CHENG-MAW CHENG, National Synchrotron Radiation Research Center, MINGHWEI HONG, Department of Physics, National Taiwan University, JUEINAI KWO, Department of Physics, National Tsing Hua University — Determining the topological phase of a material is a popular research route in condensed matter physics. For elemental material of α-Sn, its topological phase has been under debate. α-Sn(001) with in-plane compressive strain is expect to be a topological Dirac semimetal in theory, but experimental evidence of 3D Dirac state is still lacking. In contrast, a spin-momentum locked topological surface state (TSS) was found for α-Sn(001) on InSb(001), suggesting a topological insulator (TI). In this work, molecular beam epitaxy grown α-Sn(001) on InSb(001) and the thickness dependent angle-resolved photoemission spectroscopy (ARPES) study from 3 bilayers (BLs) to 370 BLs are reported. Streaky (2×1) reflection high energy electron diffraction patterns and narrow θ-rocking curve (FWHM of 0.0163°) in x-ray diffraction indicated an excellent crystallinity. Sharp TSSs were attained by ARPES in films thicker than 6 BLs without resorting to extra doping or surface treatments. No TSSs were observed for film thinner than 5 BLs, indicating a crossover from 3D TI to trivial insulator. In an extremely thick α-Sn film of 370 BLs, no evident k_z dependence on the Dirac state was found in photon energy range of 10-40 eV, suggesting α-Sn(001) on InSb(001) more likely to be in TI phase.


2:42PM J55.00002: Band structure study of elemental topological material α-Sn on InSb(111)B  KENG-YUNG LIN (Presenter), Natl Taiwan Univ, KO-HSUAN CHEN, SHENG-WEN HUANG, Natl Tsing Hua Univ, CHAO-KAI CHENG, Natl Taiwan Univ, CHENG-MAW CHENG, Natl Synchrotron Rad Res Ctr, MINGHWEI HONG, Natl Taiwan Univ, JUEINAI KWO, Natl Tsing Hua Univ — Research efforts on studying the band structure of elemental topological α-Sn have increased substantially in recent years. Bulk α-Sn is a zero-gap material with an inherent band inversion due to spin-orbit coupling. Interestingly, theoretical calculation proposed strained-induced topological phase transitions from topological Dirac semimetal (TDS) to topological insulator (TI) in α-Sn thin films. Among them, compressively strained α-Sn thin films on InSb(111)B were experimentally claimed to be a 3D TDS for 30-bilayer (BL) film by angle-resolved photoemission spectroscopy (ARPES). In this work, α-Sn thin films were grown on InSb(111)B by molecular beam epitaxy (MBE) with epi-InSb as the starting surfaces prepared in the same MBE chamber. Single-crystal α-Sn thin films with excellent crystallinity and smooth surface morphology were characterized by X-ray diffraction and atomic force microscopy; their band structures were studied by ARPES. Much clearer band dispersions were observed for our 30-BL film compared to those in the literature, with virtually no k_z dependence over a wide photon energy range from 18 eV to 52 eV for the claimed 3D Dirac state. Our results, therefore, do not support the 3D TDS phase observed in the previous work.

Clarifying superconducting proximity effects in topological insulating \((\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3\) films on niobium

JOSEPH HLEVYACK (Presenter), University of Illinois at Urbana-Champaign, SAHAND NAJAFZADEH, Institute for Solid State Physics, University of Tokyo, MENG-KAI LIN, University of Illinois at Urbana-Champaign, TAKAHIRO HASHIMOTO, AKIHIRO TSUZUKI, TSUBAKI NAGASHIMA, Institute for Solid State Physics, University of Tokyo, WEILU ZHANG, Shangzhi University, AKIKO FUKUSHIMA, Institute for Solid State Physics, University of Tokyo, YOJI NAKAZAKI, SHUK SHIN, Institute for Solid State Physics, University of Tokyo, DAVID FLOETOTTO, Center for Soft Nanoscience, University of Muenster, JOSE AVILA, Synchrotron SOLEIL, JAMES N ECKSTEIN, University of Illinois at Urbana-Champaign, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign — Coupling a topological insulator (TI) with an s-wave superconductor (SC) can initiate p-wave-like pairing in the nontrivial surface states. However, this proximity-induced pairing is still not well understood and challenging to realize, possibly due to a short superconducting coherence length and/or Fermi surface/lattice mismatch at the TI/SC interface. Using a novel cleavage-based “flip-chip” method, we have successfully prepared single-crystalline \((\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3\) thin films with a predetermined thickness (2-5 quintuple layers) on bulk Nb substrate. By carefully tuning the composition \(x\), we confirm using angle-resolved photoemission spectroscopy (ARPES) that the Fermi level lies in the band gap for all \((\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3\) films, thus yielding a lightly n-doped TI on a SC even in the thin-film limit. Proximity-induced superconducting gaps in these samples are measured by ultrahigh-resolution laser ARPES. The results will be compared with those from prior studies of heavily n-doped TI films on Nb. Our study helps to reveal the mechanisms of proximity-induced pairing in TIs and also underscores the limitations of using the proximity effect to realize topological superconductivity.

Topological chiral crystals

TYLER COCHRAN (Presenter), GUOQING CHANG, ILYA BELOPOLSKI, Princeton University, KAUSTUV MANNA, Max-Planck-Institute for Chemical Physics of Solids, DANIEL S SANCHEZ, ZIJIA CHENG, XIAN YANG, DANIEL MULTER, SONGTIAN ZHANG, NANA SHUMIYA, MAKSYM LITSKEVICH, JIAJIN YIN, Princeton University, SUYANG XU, Havard University, CLAUDIA FELSER, Max-Planck-Institute for Chemical Physics of Solids, HSIN LIN, Academia Sinica, ZAHID HASAN, Princeton University — Topological chiral crystals host guaranteed topological crossings in the bulk band structure and can possess Fermi arc surface states that span the entire surface Brillouin zone [1]. These materials can give rise to novel optical and magneto-transport response. In this presentation, we discuss recent photoemission experiments exploring the topology of chiral fermions [2]. By combining measurements with ultraviolet and soft x-ray incident photons, we determine the topological invariant directly. Our results shed new light on the relationship between structural chirality and topology.


*Work at Princeton was supported by the US DOE under Basic Energy Sciences programme (grant number DOE/BES DE-FG-02-05ER46200) and the Gordon and Betty Moore Foundation (GBMF4547/ Hasan). T.C. was supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. (#DGE-1656466).
3:18PM J55.00005: Observation of topological surface state in a superconducting material*  
GYANENDRA DHAKAL (Presenter), MD MOFAZZEL HOSEN, Univ of Central Florida, AYANA GHOSH, University of Connecticut, CHRISTOPHER LANE, Los Alamos National Laboratory, KAROLINA GÓRNICKA, MICHAL J. WINIARSKI, Gdansk University of Technology, KLAUSS DIMITRI, FIROZA KABIR, CHRISTOPHER SIMS, SABIN REGMI, WILLIAM NEFF, Univ of Central Florida, DARIUSZ KACZOROWSKI, Polish Academy of Sciences, JIAN-XIN ZHU, Los Alamos National Laboratory, TOMASZ KLIMCZUK, Gdansk University of Technology, MADHAB NEUPANE, Univ of Central Florida — The discovery of the topological insulator phase has ignited massive research interests in novel quantum materials. Topological materials with superconductivity further invigorate the importance of materials providing the platform to study the interplay between these two unique states. However, the candidates of such materials are rare. Here, we report a systematic angle-resolved photoemission spectroscopy (ARPES) study of superconducting material CaBi$_2$ [ $T_c$ = 2 K], corroborated by the first-principles calculations. Our study reveals the presence of topological Dirac state at the corner-point of the Brillouin zone with topological protection. Furthermore, our transport measurements show the presence of large magnetoresistance in this compound. Our results provide a platform to study the superconductivity and topology in CaBi$_2$.

*This project is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415.

3:30PM J55.00006: Electronic structure of PtPb$_4$ studied by Angle-Resolved Photoemission Spectroscopy*  
KYUNGCHAN LEE (Presenter), DAIXIANG MOU, LIN-LIN WANG, NA HYUN JO, YUN WU, BENJAMIN SCHRUNK, JOHN WILDE, MANH CUONG NGUYEN, AMELIA ESTRY, CAI-ZHUANG WANG, ANDREAS KREYSSIG, SERGEY L. BUD’KO, KAI-MING HO, PAUL C CANFIELD, ADAM KAMINSKI, Department of Physics and Astronomy, Iowa State University/Ames Laboratory — We investigate the electronic structure of PtPb$_4$ by using ultrahigh resolution, laser based Angle Resolved Photoemission Spectroscopy(ARPES) and Density functional theory(DFT) calculations. This material is a compound related to PtSn$_4$, which exhibits exotic topological properties such as Dirac node arcs. The Fermi surface(FS) of PtPb$_4$ has at least two electron pockets at the center of the Brillouin zone(BZ) and several hole pockets around the zone boundaries. Although the crystal structure has 4-fold symmetry, the ARPES data reveals a FS with only 2-fold symmetry, showing a rectangular FS sheet around X points and two intersected circular FS sheet around Y points. X-ray scattering data points to the stacking order as a key factor for the breaking of the 4-fold symmetry observed in ARPES data. The experimental results are in a reasonable agreement with the DFT calculations.

* Research at Ames Laboratory was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358.
3:42PM J55.00007: Gating monolayer WTe$_2$ devices in nano-ARPES  PAUL NGUYEN (Presenter), Physics, University of Washington, CHENG CHEN, ROLAND KOCH, AARON BOSTWICK, Advanced Light Source, Lawrence Berkeley National Laboratory, NATAILIE TEUTSCH, Physics, University of Warwick, VIKTOR KANDYBA, ALEX VICTOROVICH BARINOV, Elettra - Sincrotrone Trieste S.C.p.A, NEIL R WILSON, Physics, University of Warwick, YULIN CHEN, Physics, University of Oxford, ELI ROTENBERG, Advanced Light Source, Lawrence Berkeley National Laboratory, XIAODONG XU, DAVID COBDEN, Physics, University of Washington — We investigate the effects of electrostatic doping on a 2D topological semimetal, monolayer WTe$_2$, employing nanometer-resolution angle-resolved photoemission spectroscopy (nano-ARPES). The exfoliated WTe$_2$ monolayer flake rests on an hBN flake and is capped by a monolayer of hBN to prevent oxidation and allow cleaning. During the photoemission measurements a gate voltage can be applied between a thin graphite electrode beneath the hBN and a graphene contact that overlaps the WTe$_2$ on top. The gate is observed to shift the Fermi energy by more than 100 meV, from valence to conduction band of monolayer WTe$_2$. The temperature and doping dependence of the spectrum yield insights into the nature of the bulk conductivity.

3:54PM J55.00008: Electronic Structure of Topological Material CaMnSb$_2$  HONGTAO RONG (Presenter), JUNBAO HE, YONGQING CAI, GUODONG LIU, LIN ZHAO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, ZUYAN XU, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, XINGJIANG ZHOU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences — AMnPn$_2$ (A = Ca, Sr, Ba, Eu, Yb; Pn = Sb, Bi) compounds are new kind of topological materials. Theoretical studies indicate that AMnPn$_2$ host an anisotropic Dirac cone near the Fermi surface. Here we report our high-resolution laser-based angle-resolved photoemission measurements on the electronic structure of CaMnSb$_2$. The Fermi surface of CaMnSb$_2$ mainly consists of one hole pocket around the Brillouin zone center and two tiny hole pockets at the Brillouin zone boundary which are consistent with the first principle calculations. In addition, we observe four additional points located at the hole pocket around the Brillouin zone center along the high symmetry directions which is hard to be accounted for by band structure calculations.
4:06PM J55.00009: Coexistence of topological nontrivial phase and Rashba-type surface state in HoSb*  

MD MOFAZZEL HOSEN (Presenter), GYANENDRA DHAKAL, Univ of Central Florida, BAOKAI WANG, Northeastern University, NARAYAN POUDEL, Idaho National Laboratory, BAHADUR SINGH, Northeastern University, KLAUSS DIMITRI, FIROZA KABIR, CHRISTOPHER SIMS, SABIN REGMI, WILLIAM NEFF, Univ of Central Florida, DANIEL MURRAY, Idaho National Laboratory, FRANZISKA WEICKERT, National High Magnetic Field Laboratory, KRZYSZTOF GOFRYK, Idaho National Laboratory, OREST PAVLOSIUK, PIOTR WISNIEWSKI, DARIUSZ KACZOROWSKI, Polish Academy of Sciences, ARUN BANSIL, Northeastern University, MADHAB NEUPANE, Univ of Central Florida — Using the high resolution angle-resolved photoemission spectroscopy (ARPES), magnetotransport, and parallel first-principles modeling, we report the discovery of a topologically nontrivial state coexisting with a Rashba-type surface state in a rare earth monopnictide semimetal. Our theoretical analysis reveals the presence of bulk band inversions at the Γ and X points of the Brillouin zone (BZ). Interestingly, the upper part of the observed Rashba-type surface state coincides with the nontrivial surface state at the X point. Magnetotransport study indicates that HoSb can be characterized as a correlated nearly-complete electron-hole-compensated semimetal. Therefore, our findings provide HoSb as a new materials platform for exploring the interplay between coexisting topological and Rashba-type surface state and the non-saturating XMR effect in the rare earth monopnictide family.

*This project is supported by the Air Force Office of Scientific Research under Award No. FA9550-17-1-0415 and the Center for Thermal Energy Transport under Irradiation, an Energy Frontier Research Center funded by the U.S. DOE, Office of Basic Energy Sciences.

4:18PM J55.00010: Observation of spin polarized surface states in polar Weyl semimetal MoTe2  

YUMA TANAKA (Presenter), MOHAMMAD SAEED BAHRAMY, Department of Applied Physics, University of Tokyo, HIDEFUMI TAKAHASHI, Graduate School of Engineering Science, Osaka University, KENTA KURODA, KOICHIRO YAJI, AYUMI HARASAWA, TAKESHI KONDO, SHIK SHIN, Institute for Solid State Physics, University of Tokyo, SHINTARO ISHIWATA, Graduate School of Engineering Science, Osaka University, KYOKO ISHIZAKA, Department of Applied Physics, University of Tokyo — Since the theoretical prediction of the low temperature phase as a type-II Weyl semimetal, the electronic structure of β-MoTe2 has been actively studied by angle-resolved photoelectron spectroscopy. Until now, some segment-like band features resembling Fermi arcs are experimentally observed, which are indicative of the topological surface states connecting the bulk Weyl nodes. However, the band dispersions near the Fermi level is complicated, and clear interpretation is not easy. Here we investigate the spin polarizations of the Fermi arc features for both polar terminations by utilizing the high-resolution spin and angle-resolved photoelectron spectroscopy (SARPES). For respective surface terminations, the different patterns and spin polarizations of Fermi arcs are clearly observed. In the presentation, we will compare the result with the first-principles calculation and discuss the details of the spin polarized surface states.
Symmetry plays a major role in all disciplines of physics. Within the field of topological materials, there is a great interest in understanding how the mechanics of crystalline and internal symmetries protect nodal line type features in respect to spin orbit coupling. Additionally, the surface environment of a material can severely impact the surface states that are probed by angle resolved photoemission spectroscopy (ARPES). For the first time, we report the experimental observation of topological surface states in the nodal loop semimetal HfP2 using ARPES which is supported by our first principles calculations. Our study shows termination dependent surface states in this compound which are linked to three unique nodal loops that are confirmed to be topologically non-trivial. This work demonstrates that transition metal dipnictides provide a good platform to study non-trivial topological states protected by nonsymmorphic symmetry.

*This project is supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0415 and the National Science Foundation (NSF) CAREER award DMR-1847962.
Due to a higher order bulk boundary correspondence, a higher-order topological insulator hosts one-dimensional helical edge states around the hinges of the crystal. However, spectroscopic evidence for topological hinge states has been so far limited to semimetallic materials [1], where the measured edge conductivity is blurred by bulk carries. In this contribution, we show evidence for topological hinge states in a semiconducting quasi-one-dimensional material. Importantly, the crystal has naturally cleavable top and side surfaces which are stacked via van-der-Waals forces, and therefore the electronic structure around the hinge can be investigated in a cleaved surface or in an exfoliated thin flake. Our experiments by high-resolution angle-resolved photoemission spectroscopy reveal quasi-1D states inside the bulk band gap. Moreover, the corresponding signals with high conductivity are detected at the edges of the crystal by microwave impedance microscopy. These observations, therefore, indicate the existence of topological hinge states in a 1D stacking material.


Topological insulators are bulk semiconductors that manifest in-gap surface states with massless Dirac-like dispersion due to the topological bulk-boundary correspondence principle. These surface states can be manipulated by the interface environment to display various emergent phenomena. Here, we use angle-resolved photoemission spectroscopy (ARPES) and scanning tunnelling microscopy (STM) to investigate the interplay of crystallographic inhomogeneity with the topologically ordered band structure in a model topological insulator. We develop quantitative analysis methods to obtain spectroscopic information in spite of a limited dwell time on each measured point. We find that the band energies vary on the scale of 50 meV across the sample surface, and this enables single-sample measurements that are analogous to a multi-sample doping series. By focusing separately on the bulk and surface electrons we reveal a hybridisation-like interplay between fluctuations in the surface and bulk state energetics.
Topological Lifshitz transitions and Fermi arc manipulation in Weyl semimetal NbAs  
HAIFENG YANG (Presenter), ShanghaiTech University, LEXIAN YANG, Tsinghua University, ZHONGKAI LIU, ShanghaiTech University, YAN SUN, Max Planck Institute for Chemical Physics of Solids, ANDREI BERNEVIG, Princeton University, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, BINGHAI YAN, Weizmann Institute of Science, YULIN CHEN, University of Oxford — Surface Fermi arcs (SFAs), the unique open Fermi-surfaces (FSs) discovered recently in topological Weyl semimetals (TWSs), are unlike closed FSs in conventional materials and can give rise to many exotic phenomena, such as anomalous SFA-mediated quantum oscillations, chiral magnetic effects, three-dimensional quantum Hall effect, non-local voltage generation and anomalous electromagnetic wave transmission. Here, by using in-situ surface decoration, we demonstrate successful manipulation of the shape, size and even the connections of SFAs in a model TWS, NbAs, and observe their evolution that leads to an unusual topological Lifshitz transition not caused by the change of the carrier concentration. The phase transition teleports the SFAs between different parts of the surface Brillouin zone. Despite the dramatic surface evolution, the existence of SFAs is robust and each SFA remains tied to a pair of Weyl points of opposite chirality, as dictated by the bulk topology.

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Observation of unconventional chiral fermions with long Fermi arcs in CoSi  
ZHICHENG RAO (Presenter), Institute of Physics — In condensed system, Chiral fermions exist at nodes (that is, robust band-crossing points protected from being gapped by nontrivial band topology) that carry a nonzero Chern number. Recently, we reported two types of unconventional chiral fermions in CoSi, which are threefold-degenerate node at point and fourfold-degenerate node at R point. These nodes at point and R point carry nonzero Chern number and we observed two surface Fermi arcs on surface to connect their projection on (001) surface, which are related by a π rotation about Γ. Further, we show the two helical surface states encircle the projection of Γ point and R point, which can reveal the topological nature of bulk nodes in CoSi.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM  
Session J56 DCMP: Mott Physics Theory and Calculations  
Mile High Ballroom 2C - Congjun Wu, University of California, San Diego
Resistive switching, a phenomenon in which the resistance of a device can be modified by applying an electric field, is the basis for emerging technologies such as neuromorphic computing. Volatile switching is specially promising, as it may allow for the implementation of artificial spiking neurons. This type of switching is observed in Mott insulators featuring an insulator-to-metal transition which can be triggered by applying an external voltage: the material becomes conducting if a threshold is exceeded. Such switching takes place in a filamentary fashion. Despite intense research, it is not yet known how these filaments nucleate, grow and relax. We combine reflectivity and transport measurements to image the switching process with spatial and temporal resolution. Three Mott insulators are analyzed: VO$_2$, V$_2$O$_3$ and V$_3$O$_5$, finding remarkable differences in the filament expansion process. We will show how these differences provide a unique insight to identify which mechanism drives the Mott transition: Joule heating or electric field.

*Supported by the Quantum Materials for Energy Efficient Neuromorphic Computing (Q-MEEN-C) Energy Frontier Research Center (EFRC), funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award # DE-SC0019273.

The Mott transition as a topological phase transition

We show that the Mott metal-insulator transition in the standard one-band Hubbard model can be understood as a topological phase transition. The approach is inspired by the observation that the Mott pole in the self-energy is pinned throughout the insulating phase, similar to the zero-energy spectral pole corresponding to a localized surface state in topological systems. We use NRG-DMFT to solve the infinite-dimensional Hubbard model, and represent the resulting local self-energy in terms of the boundary Green's function of an auxiliary tight-binding chain without interactions. We find a rich structure in the parameters of the auxiliary chain, which we show are of generalized SSH model type. The Mott transition corresponds to a topological phase transition in this auxiliary system, characterized by its analytic properties. We devise simple toy models for the auxiliary chains that capture the basic physics of the metallic and insulating Hubbard model phases, as well as in the scaling limit near the transition.
Parting the Fermi Sea at the Mott Point: Dynamics of Correlated Electrons Reveals the Mechanism Underpinning Mottness

YUTING TAN (Presenter), NHMFL, Florida State University, ANDREJ PUSTOGOW, University of California, Los Angeles, ROLAND RÖSSLHUBER, ECE UYKUR, ANNETTE BÖHME, ANJA LÖHLE, RALPH HÜBNER, Physikalisches Institut, Universität Stuttgart, JOHN A SCHLUETER, Division of Materials Research, National Science Foundation, VLADIMIR DOBROSavljevic, NHMFL, Florida State University, MARTIN DRESSEL, Physikalisches Institut, Universität Stuttgart — By increasing the interaction among conduction electrons, a Fermi-liquid-type metal turns into a Mott insulator. This first-order phase transition should exhibit a regime where the adjacent ground states coexist, leading to electronic phase separation, but the range near T=0 remained unexplored because it is commonly concealed by antiferromagnetism. Here we map the genuine low-temperature Mott transition by applying dielectric spectroscopy under pressure to quantum-spin-liquid compounds. The dielectric permittivity uniquely distinguishes all conduction regimes around the Mott point, allowing us to reliably detect insulator-metal phase coexistence below the critical endpoint. Via state-of-the-art theoretical modeling we establish the coupling between segregated metallic puddles as the driving source of a colossal peak in the permittivity reaching $\varepsilon_1 \approx 10^5$ within the coexistence region. Our results indicate that the observed inhomogeneities are the consequence of phase separation emerging from strong correlation effects inherent to Mottness, suggesting a similar 'dielectric catastrophe' in other correlated materials.

This work is partially supported by the Center for Materials Theory as a part of the Computational Materials Science (CMS) program, funded by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Kinetics of thermal Mott metal-insulator transition in the Hubbard model

GIA-WEI CHERN (Presenter), Physics, University of Virginia — We present the first-ever microscopic dynamical simulation of the temperature-controlled Mott metal-insulator transition in the Hubbard model. By combining the efficient Gutzwiller method with molecular dynamics simulations, we demonstrate that the transformation from the correlated metal to the Mott insulator proceeds via the nucleation and growth of the Mott droplets. We show that after an initial incubation period, the early stage of the phase transformation is characterized by a constant nucleation rate and an interface-controlled cluster growth mechanism, consistent with the classical theory developed by Kolmogorov, Johnson, Mehl, and Avrami. This is followed by a novel intermediate stage of accelerated phase transformation that is characterized by avalanche behavior similar to the Barkhausen noise in magnetization dynamics. The implications of our findings for the recent nano-imaging experiments on metal-insulator transition of correlated materials are also discussed.

This work is partially supported by the Center for Materials Theory as a part of the Computational Materials Science (CMS) program, funded by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
3:18PM J56.00005: Nature of Mott transition in a hydrogen lattice  ZIJIAN LANG, Tsung-Dao Lee Institute & Shanghai JiaoTong University, SUDESHNA SEN, University College Dublin, VLADIMIR DOBROSAVLJEVIC (Presenter), Florida state University, WEI KU, Tsung-Dao Lee Institute & Shanghai JiaoTong University — Mott transition, an electron correlation induced metal-insulator transition, has long been realized in many materials. Yet, the microscopic nature of the transition proposed by Mott has not been carefully examined in these materials, even by modern theories. This is because Mott's original proposal makes use of non-linear change of screening of long-range Coulomb interaction that are almost always ignored in simple models used in previous study of Mott transition. Here we study the Mott transition of an artificial hydrogen lattice including both the long-range Coulomb interaction and the strong on-site correlation, via a dynamical mean-field extension of density functional calculation. We found that in the relevant range of lattice spacing, the system is in the charge-transfer regime, namely the charge fluctuation involves mostly higher energy orbitals beyond 1s one, rendering a single-band Hubbard model inadequate. Our study challenges Mott's original microscopic picture and reveal some key physics of metal-insulator transition in realistic materials.

3:30PM J56.00006: Mott Insulating States of Anisotropic SU(4) Dirac Fermions*  YU WANG (Presenter), HAN XU, School of Physics and Technology, Wuhan University, CONGJUN WU, Department of Physics, University of California, San Diego — We employ large-scale projector quantum Monte Carlo simulations to study the ground-state properties of the SU(4) Hubbard model on a square lattice with a staggered flux configuration. By varying the on-site repulsion and the flux, our simulations demonstrate phase transitions between the Dirac semimetal, antiferromagnetic (AFM) and valence-bond-solid (VBS) phases. We find a continuous AFM-VBS phase transition. The direct second-order transition between different symmetry-breaking phases suggests deconfined critical points which form the boundary between the AFM and VBS phases. Near the deconfined critical points, we show that the AFM and VBS Binder ratios have the same critical exponents. As Hubbard U increases, the VBS order drops to zero, while the AFM moment has a finite value in the Heisenberg limit. It infers that the system with any flux eventually enters the AFM phases with increasing Hubbard U. By analysis of the gap opening mechanism, it is shown that both the columnar VBS ordering and the plaquette VBS ordering emerge in the VBS phase, and thus the phase diagram features two tricritical points where the semimetal, AFM and VBS phases meet.

*This work is supported by the National Natural Science Foundation of China under Grants No. 11874292, No. 11729402, and No. 11574238.
**3:42PM J56.00007: Pseudogap, van Hove Singularity, Maximum in Entropy and Specific Heat for Hole-Doped Mott Insulators**

ALEXIS REYMBAUT, SIMON BERGERON, R. GARIOUD, M. THÉNAULT, MAXIME CHARLEBOIS, Institut quantique, Université de Sherbrooke, P. SÉMON, Brookhaven National Laboratory, ANDRE-MARIE TREMBLAY (Presenter), Institut quantique, Université de Sherbrooke — The first indication of a pseudogap in cuprates came from a sudden decrease of NMR Knight shift at a doping-dependent temperature $T^*$. Since then, experiments have found phase transitions at a lower $T^*_{\text{phase}}(\delta)$. Using plaquette cellular dynamical mean-field for the square-lattice Hubbard model at high temperature, where the results are reliable, we show that $T^*(\delta)$ shares many features of $T^*_{\text{phase}}(\delta)$. The remarkable agreement with several experiments, including quantum critical behavior of the electronic specific heat, supports the view that the pseudogap is controlled by a finite-doping extension of the Mott transition. We propose further experimental tests.


*Supported by NSERC under grant RGPIN-2014-04584, and by the Research Chair in the Theory of Quantum Materials. Computers provided by CFI, the Ministère de l’Éducation des Loisirs et du Sport (Québec), Calcul Québec, and Compute Canada. The work of P.S. was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences as a part of the Computational Materials Science Program. This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund.

**3:54PM J56.00008: Superconducting instability in an exactly solvable model of a doped Mott insulator**

PHILIP PHILLIPS, LUKE YEO (Presenter), EDWIN HUANG, University of Illinois at Urbana-Champaign — Regarding the cuprate superconductors as doped Mott insulators, we solve a toy model that exhibits both Mottness and superconductivity. We show that the Hatsugai-Kohmoto model, an exactly solvable model exhibiting a non-trivial Mott insulator-to-non-Fermi liquid metal transition, exhibits a superconducting instability. The instability is present in the non-Fermi liquid metal phase at half-filling, persists for a wide range of dopings away from half-filling, and terminates once the Mott parameter exceeds a critical strength.

*NSF DMR-1919143
4:06PM J56.00009: Intertwined Mott insulating behavior, magnetic quantum criticality, and superconductivity in a two-band Hubbard-like model: A Quantum Monte Carlo study
MORTEN HOLM CHRISTENSEN (Presenter), University of Minnesota, XIAOYU WANG, National High Magnetic Field Laboratory, Florida State University, YONI SCHATTNER, Department of Physics, Stanford University, EREZ BERG, Department of Physics, Weizmann Institute of Science, RAFAEL FERNANDES, University of Minnesota — The interplay between superconductivity and magnetism in correlated systems is an outstanding question in condensed matter physics. It has been recently shown that the two-band spin-fermion model, in which electrons interact with pre-existing magnetic fluctuations, can be simulated by Quantum Monte Carlo (QMC) without the fermionic sign-problem. Here we go beyond this approach and present sign-problem-free QMC results of a two-band microscopic model in which both superconductivity and magnetism arise from the very same inter-band repulsion, without pre-existing bosons mediating the electronic interactions. Our simulations reveal the interplay between a host of different phenomena as the interaction strength is increased. A wide magnetic dome appears at moderate values of the interaction, whereas a narrow superconducting dome emerges around the magnetic quantum critical point located on the less strongly correlated side of the phase diagram. Interestingly, a Mott transition is nearly coincident with this magnetic phase boundary, and is manifested by a change in the magnetic dynamics from overdamped to propagating. The emergence of superconductivity only in the former region provides important clues about the nature of the pairing glue in unconventional superconductors.

4:18PM J56.00010: Excitons in Mott insulator* TSUNG-SHENG HUANG (Presenter), CHRISTOPHER BALDWIN, MOHAMMAD HAFEZI, VICTOR GALITSKI, University of Maryland, College Park — We study the behaviors of excitons formed by spinless charges in the antiferromagnetically ordered phase of Mott insulators. We start from the slave fermion Hubbard model with linear spin wave approximation on the bosonic spinons and obtain the dispersion of dressed doublons and holons using self-consistent Born approximation. We derive the Bethe-Salpeter equation for the two particle Green's function of dressed doublon and holon to find the bound states between a doublon and a holon and identify them as excitons. We investigate several properties of Mott excitons.

*T-S. H. would like to thank Physics Frontier Center at the Joint Quantum Institute for supporting this project.
4:30PM J56.00011: Block-spiral magnetism of the low-dimensional orbital-selective Mott phase

JACEK HERBRYCH (Presenter), Wroclaw University of Science and Technology, JONAS HEVERHAGEN, University of Stuttgart, GONZALO ALVAREZ, Oak Ridge National Laboratory, MARIA DAGHOFER, University of Stuttgart, ADRIANA MOREO, ELBIO DAGOTTO, University of Tennessee — Competing interactions can lead to novel states of matter including frustrated magnetism, an extensive field of research both from the theoretical and experimental perspectives. Here, we show that competing energy scales present in the low-dimensional orbital-selective Mott phase (OSMP) induce an exotic magnetic order, never reported before. Neutron scattering experiments on iron-based 123 ladder materials (where OSMP is relevant) already confirmed theoretical prediction of block-magnetism (magnetic order of the form $\uparrow\uparrow\downarrow\downarrow$). Now we argue that another novel phase can be stabilized in multiorbital Hubbard models, i.e., `block-spiral state'. In the latter, the magnetic islands form a spiral propagating through the chain but with the blocks maintaining their identity, namely rigidly rotating. This complex spiral state is stabilized without any apparent frustration. Phenomenological simpler models that accurately capture both electronic and spin degrees of freedom are also discussed.

*(1) US Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division
(2) Polish National Agency of Academic Exchange (NAWA) PPN/PPO/2018/1/00035
(3) Deutsche Forschungsgemeinschaft, Emmy-Noether program (DA 1235/1-1) and FOR1807 (DA 1235/5-1)

4:42PM J56.00012: Local structural study of novel mott-insulating cousins of the iron pnictides

BHUPENDRA KARKI (Presenter), ALAA ALFAILAKAWI, Department of Physics and Astronomy, University of Louisville, BENJAMIN FRANDSEN, Department of Physics and Astronomy, Brigham Young University, MINGHU FANG, Department of Physics, Zhejiang University, M. S. EVERETT, JOERG C. NEUEFEIND, Neutron Scattering Division, Oak Ridge National Laboratory, BYRON FREEOLON, Department of Physics and Astronomy, University of Louisville — Iron oxy-chalcogenides, La$_2$O$_2$Fe$_2$OM$_2$ ($M = S, Se$), is the layered materials formed from stacking layered units of La$_2$O$_2$ and Fe$_2$OM$_2$ ($M = S, Se$). We describe the structural properties of the La$_2$O$_2$Fe$_2$OM$_2$ ($M = S, Se$), by using pair distribution function (PDF) analysis and Rietveld refinement methods applied to neutron diffraction data. Our results show that $M = S$ and Se possess similar nuclear structure at low and room temperatures. Local crystal structure was studied by investigating deviations in atomic positions and orthorhombicity. By tracking the orthorhombicity parameter, we observe the local scale distortions between the tetragonal and orthorhombic structure in a typical range of 1-2 nm. These spatially limited distortions represent fluctuating nematic order which suggests the ubiquity of nematic fluctuations in iron-based superconductors and related materials. In addition, we found the discontinuity in c-lattice which may arise due to the buckling of Fe$_2$O plane. We anticipate that this buckling might be due to the change in octahedral height or tilting of the octahedral structure. Overall, these results suggest that the structural distortion may play a role in absence of superconductivity in these materials.

*Department of Physics, University of Louisville, Louisville, KY 40208
4:54PM J56.00013: Pseudogap transition within the superconducting phase in the three-band Hubbard model*  
SIDHARTHA SHANKAR DASH (Presenter), DAVID SENECHAL, Université de Sherbrooke — We use cluster dynamical mean field theory on a three-band Hubbard model for high-$T_c$ superconductors to study the superconducting phase at zero temperature, obtained when doping the charge transfer insulator, for several values of $U$. We observe a first-order transition within the superconducting phase, which separates the so-called underdoped and overdoped solutions. The transition to the underdoped solution is marked by a jump in the spectral gap, and on further underdoping the spectral gap increases while the superconducting order parameter decreases. This, we conclude, is caused by the onset of the pseudogap in the underdoped region, which contributes to the increasing spectral gap; this is consistent with the change in the source of condensation energy from potential energy, in the overdoped region, to kinetic energy in the underdoped region. We also observe that the $d$-wave node disappears within the superconducting phase at low values of hole doping, within the underdoped region. We see this as a manifestation of Mott physics operating at very low doping.

*NSERC (Canada) and Compute Canada/Calcul Québec

5:06PM J56.00014: Extending the Gutzwiller approximation to intersite interactions*  
GARRY GOLDSTEIN (Presenter), GABRIEL KOTLIAR, Rutgers University, New Brunswick, NICOLA LANATA, Physics, Aarhus University — We develop an extension of the Gutzwiller Approximation (GA) formalism which includes the effects of Coulomb interactions of arbitrary range (including density density, exchange, pair hopping and Coulomb assisted hopping terms). This formalism reduces to the ordinary GA formalism for the multi-band Hubbard models in the presence of only local interactions. This is accomplished by combining the $1/z$ expansion - where $z$ is the coordination number and only the leading order terms contribute in the limit of infinite dimensions- with a $P^2-I$ expansion, where $P$ is the Gutzwiller projector on a site $R$. The method is conveniently formulated in terms of a Gutzwiller Lagrange function. We apply our theory to the single band $t$-$J$ model and the extended single band Hubbard model. We find a Mott transition but for the extended Hubbard model. An enhanced valence fluctuations transition is also discovered.

*This work was supported by the Computational Materials Sciences Program funded by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. N. L. was supported by the VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744).
5:18PM J56.00015: Dynamical t/U Expansion of the Doped Hubbard Model  WENXIN DING (Presenter), Anhui Univeristy, RONG YU, Renmin University — We construct a new U(1) slave spin representation for the single-band Hubbard model in the large-U limit. The mean-field theory in this representation is more amenable to describe both the spin-charge-separation physics of the Mott insulator at half-filling and the strange metal behavior at finite doping. By employing a dynamical Green's function theory for slave spins, we calculate the single-particle spectral function of electrons, and the result is comparable to that in dynamical mean-field theories. We then formulate a dynamical t/U expansion for the doped Hubbard model that reproduces the mean-field results at the lowest order of expansion. To the next order of expansion, it naturally yields an effective low-energy theory of a t – J model for spinons self-consistently coupled to an XXZ model for the slave spins. We show that the superexchange J is renormalized by doping, in agreement with the Gutzwiller approximation. Surprisingly, we find a new ferromagnetic channel of exchange interactions which survives in the infinite U limit, as a manifestation of the Nagaoka ferromagnetism.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J57 DMP DCOMP: 2D Semiconductors: opto-magnetic properties  Mile High Ballroom 3A - Jing Li, Los Alamos National Laboratory - Tag(s): Focus

2:30PM J57.00001: Landau quantized excitonic absorption and photoluminescence in a monolayer valley semiconductor  JEREMIAH VAN BAREN (Presenter), ERFU LIU, University of California, Riverside, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, YIA-CHUNG CHANG, Research Center for Applied Sciences, Academia Sinica, CHUN HUNG LUI, University of California, Riverside — We observe charge-density-dependent quantum oscillations in the excitonic absorption and luminescence of monolayer WSe$_2$ under magnetic fields up to B = 17.5 T. Valley-selective quantum oscillations occur for both the exciton and trions (or exciton-polarons) and reveal distinct intravalley and intervalley coupling between excitons and Landau levels (LLs). We observe spin- and valley-polarized LLs with filling factors $n = +0, +1$ in the lower conduction band and $n = -0$ to $-6$ in the valence band, including the Berry-curvature-induced $n = \pm 0$ LLs of massive Dirac fermions. The LL filling produces periodic plateaus in the exciton energy shift accompanied with sharp oscillations in the exciton absorption width and magnitude. This peculiar exciton behavior can be simulated by semi-empirical calculations. In addition, the experimentally deduced g-factors of the conduction band (g ~ 2.5) and valence band (g ~ 15) are much larger than the g-factors predicted in a single-particle model. Such g-factor enhancement implies strong many-body interactions at high charge density in monolayer WSe$_2$. The complex interplay between Landau quantization, excitonic effects, and many-body interactions, as demonstrated in our research, provides a new platform to explore novel correlated quantum phenomena.
Spin relaxation in InSe probed by time-resolved Kerr rotation

JOVAN NELSON (Presenter), Applied Physics Program, Northwestern University, TEODOR STANEV, Department of Physics and Astronomy, Northwestern University, TREVOR LAMOUNTAIN, Applied Physics Program, Northwestern University, HAOLIN CHEN, Department of Physics, Carnegie and Mellon, NATHANIEL PATRICK STERN, Department of Physics and Astronomy, Northwestern University — Two dimensional materials have shown much promise as a platform for novel optical and spin based devices. Recently, van der Waals layers of group-III monochalcogenide Indium Selenide (InSe) have attracted much attention because of their high electron mobility, strong second harmonic generation, and layered-dependent direct band gap. While these optical and electrical properties have been experimentally demonstrated, spin properties of InSe are still poorly understood despite intriguing predictions of layer-dependent optical spin selection rules. Here, we present measurements of spin relaxation in InSe using time-resolved Kerr rotation in the near infrared spectrum. These results will contribute to evaluating spin properties of the high-mobility carriers in InSe.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. 1324585, the National Science Foundation by award DMR-1905986 and the MRSEC program (DMR-1720319) at the Materials Research Center of Northwestern University.

Observation of strong valley magnetic response in monolayer transition metal dichalcogenide alloys of Mo$_{0.5}$W$_{0.5}$Se$_2$ and Mo$_{0.5}$W$_{0.5}$Se$_2$/WS$_2$ heterostructure

TING YU (Presenter), Nanyang Tech Univ — Monolayer (1L) transition metal dichalcogenide (TMD) alloys have emerged as a new material system towards future applications for electronic, optoelectronic and spintronic devices. Particularly, the unique valley physics associated with valley polarization and Zeeman effect opens new opportunities for valleytronic applications. However, valley magnetic response in 1L TMD alloys largely remains unexplored. Here, we report strong valley magnetic response of trions in Mo$_{0.5}$W$_{0.5}$Se$_2$ and Mo$_{0.5}$W$_{0.5}$Se$_2$/WS$_2$ heterostructures investigated by cryogenic magneto-photoluminescence microspectroscopy. The large $g$-factors have been extracted for Mo$_{0.5}$W$_{0.5}$Se$_2$ and Mo$_{0.5}$W$_{0.5}$Se$_2$/WS$_2$, respectively, which are attributed to the significant impact of strong Coulomb interactions on the trion emission under a perpendicular magnetic field. The reduction of the valley Zeeman splitting in the heterostructure of Mo$_{0.5}$W$_{0.5}$Se$_2$/WS$_2$ is explained in terms of the doping variation caused by the interlayer charge transfer between Mo$_{0.5}$W$_{0.5}$Se$_2$ and WS$_2$, which agrees well with our density functional theory calculations of the band alignment in the Mo$_{0.5}$W$_{0.5}$Se$_2$/WS$_2$ heterostructure. Our findings give new insights into the optical properties of 1L TMD alloys and the interlayer coupling and shed light on the valleytronics.
Revealing the exciton masses and dielectric properties of monolayer semiconductors with high magnetic fields

SCOTT CROOKER (Presenter), MATEUSZ GORYCA, JING LI, ANDREAS V. STIER, NHMFL - Los Alamos, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS-Tsukuba, EMMANUEL COURTADE, SHIVANGI SHREE, CEDRIC ROBERT, BERNHARD URBASZEK, XAVIER MARIE, INSA-Toulouse — In semiconductor physics, many essential optoelectronic material parameters can be experimentally revealed via optical spectroscopy in sufficiently large magnetic fields. For monolayer transition-metal dichalcogenide semiconductors, this field scale is substantial -- of order 100 tesla! -- due to heavy carrier masses and huge exciton binding energies. Here we report absorption spectroscopy of monolayer MoS$_2$, MoSe$_2$, MoTe$_2$, and WS$_2$ in very high magnetic fields to 91 T. We follow the diamagnetic shifts and valley Zeeman splittings of not only the exciton's 1s ground state but also its excited 2s, 3s, ... ns Rydberg states. This provides a direct experimental measure of the effective (reduced) exciton masses and dielectric properties. Exciton binding energies, exciton radii, and free-particle bandgaps are also determined. Unexpectedly, the measured exciton masses are significantly heavier than theoretically predicted, especially for the Mo-based monolayers. These results provide essential and quantitative parameters for the rational design of optoelectronic van der Waals heterostructures incorporating 2D semiconductors. [1] Goryca et al., Nature Comm. 10, 4172 (2019).

Spectroscopic signatures of few- and single layer MPS$_3$ ($M$= Mn, Ni, Fe) complexes

SABINE NEAL (Presenter), Department of Chemistry, University of Tennessee, Knoxville, HEUNG SIK KIM, Department of Physics, Kangwon University, KENNETH R O'NEAL, Department of Chemistry, University of Tennessee, Knoxville, AMANDA HAGLUND, Department of Materials Science and Engineering, University of Tennessee, KEVIN ARTHUR SMITH, Department of Chemistry, University of Tennessee, Knoxville, DAVID MANDRUS, Department of Materials Science and Engineering, University of Tennessee, HANS BECHTEL, Lawrence Berkeley National Lab, G CARR, Brookhaven National Lab, KRISTJAN HAULE, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, JANICE LYNN MUSFELDT, Department of Chemistry, University of Tennessee, Knoxville — Layered magnetic chalcogenides have become increasingly important over the last decade because they offer a unique platform for combining the complexity of bulk materials with the tunability of few- and single layer systems. These van der Waals complexes have been well studied by Raman spectroscopy, however, infrared spectroscopy is vastly underexplored due to the inability to overcome the diffraction limit. It is these ungerade infrared active modes that are vital in understanding material functionality. Synchrotron infrared nanospectroscopy, a fusion of near-field optical microscopy with high brightness infrared synchrotron radiation, has overcome this fight for photons and enabled a better understanding of size-induced effects, including symmetry breaking, that are quite different from the single crystal. This approach will be illustrated with members of the MPS$_3$ ($M$= Mn, Ni, Fe) family of complex chalcogenides.
3:30PM J57.00006: Imaging Spin-Split Impurity States in Monolayer Semiconductors

CALEB ZERGER (Presenter), ALEXANDER CONTRYMAN, HONG LI, TYLER LAYDEN, XIAOLIN ZHENG, HARI C. MANOHARAN, Stanford Univ — A two dimensional dilute magnetic semiconductor (2D-DMS) is a state sought after for its important implications for spintronics. It is predicted that this state could be achieved by doping monolayer transition metal dichalcogenides with magnetic dopants. Using scanning tunneling microscopy, we investigate the origins of a 2D-DMS state by probing the local density of states in magnetically doped monolayer dichalcogenide semiconductors. We find sharp features in the spectral maps due to an alignment of impurity states with the Fermi level due to tip-induced band bending (TIBB). By modeling the TIBB and comparing to density functional theory, we find evidence for strongly spin-split states in individual dopants, a necessary precursor to the 2D-DMS state. We also use these signatures to characterize impurity types in these samples, finding evidence for both transition metal substitutional dopants and dichalcogenide substitutions, which collectively alter the magnetic landscape.

3:42PM J57.00007: Spin-orbit coupling, exchange, and magnetism in exciton physics of 2D semiconductors

MENG WU (Presenter), ZHENGLU LI, TING CAO, STEVEN LOUIE, Department of Physics, University of California at Berkeley and Lawrence Berkeley National Laboratory — Interactions (e.g., spin-orbit coupling (SOC), electron-hole (e-h), magnetic ordering, etc.) often give rise to dramatic new features in the photophysics of 2D materials. With newly developed full-spinor \textit{ab initio} GW & Bethe-Salpeter equation (GW-BSE) methods, we investigate the interplay among these interactions in 2D semiconductors. We discover that e-h exchange interaction in monolayer transition metal dichalcogenides mixes the well-known A and B excitons that heretofore were believed to be completely independent of each other, since A and B excitons had been viewed as derived from inter-band transitions between different pairs of spin-polarized bands [1]. In another study, we elucidate the physical origin of giant excitonic and magneto-optical responses in monolayer CrI$_3$, a prototypical 2D ferromagnetic semiconductor [2]. Our calculations demonstrate that the optical properties of ferromagnetic monolayer CrI$_3$ are dominated by exciton states that extend over several unit cells. By simulating a realistic experimental setup, we further predict a strong dependence of magneto-optical Kerr effect signals on excitation frequency and substrate configuration.


*This work was supported by the Theory of Materials Program and the C2SEPEM at LBNL funded by the U.S. DOE under Contract No. DE-AC02-05CH11231, and by the National Science Foundation. Computational resources have been provided by NERSC and XSEDE.
Discovery of tunable excitons, giant valley orbital magnetic moment, and unconventional optical selection rules in bilayer graphene* [Invited]  LONG JU (Presenter), Massachusetts Institute of Technology MIT — Multilayer graphene in the rhombohedral stacking order is a unique semiconductor where the bandgap can be continuously controlled by an external electric field. It provides an exciting platform to study conventional exciton physics in the context of valley pseudospin and quantum geometry in an in situ tunable semiconductor bandgap. We employed the photocurrent spectroscopy technique to study AB-stacked bilayer graphene, and observed tunable exciton states with unusual optical selection rules, strong optical resonances and extremely narrow line width. Upon the application of a perpendicular magnetic field, a large valley-dependent magnetic moment was observed which can be traced back to the fundamental Berry curvature effect. We also observed inter Landau level transitions with unconventional optical selection rules, and established the continuous evolution from Coulomb-interaction-dominated to Landau-quantization-dominated optical response. We further used photoluminescence and Raman spectroscopy to study the exciton evolution with tunable carrier density. I will also discuss exciton physics in rhombohedral stacked graphene with more than 3 layers and the effect of Moire superlattice from hBN substrate.

*NSF

Investigation of the magnetic interactions in WSe$_2$/WS$_2$ moiré superlattice  YANHAO TANG (Presenter), LIZHONG LI, TINGXIN LI, YANG XU, Cornell University, SONG LIU, KATAYUN BARMAK, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National institute for materials science, ALLAN MACDONALD, University of Texas at Austin, JIE SHAN, KIN FAI MAK, Cornell University — Moiré superlattices formed in two-dimensional (2D) atomic crystals present a powerful platform to study interacting quantum particles in a lattice. Here, we present optical reflection spectroscopy studies on angle-aligned WSe$_2$/WS$_2$ bilayers, which form moiré superlattices because of the difference in lattice constant between the two materials. We measure the dependence of the lowest-energy moiré exciton on magnetic field and doping density. At half filling of the first hole moiré band, we observe a Mott insulating state with antiferromagnetic Curie-Weiss behavior. Past half filling, our experiment suggests an antiferromagnetic to weak ferromagnetic quantum phase transition near 0.6 filling. These results can be understood based on a triangular lattice Hubbard model in the strong interaction regime.
5:06PM J57.00010: Probing Electronic Structure and Carrier Dynamics in the Ferromagnetic Semiconductor CrSiTe3

GIRIRAJ JNAWALI (Presenter), HOWARD E JACKSON, LEIGH M SMITH, Department of Physics, University of Cincinnati, STEPHEN WILSON, Materials Engineering, University of California, Santa Barbara — The layered ferromagnetic semiconductor CrSiTe3 (CST) has attracted great scientific attention due to its potential as a 2-dimensional ferromagnet with higher $T_c$ than in its bulk form. In order to understand the nature of magnetic correlations and possible magneto-optoelectronic applications, it is crucial to understand the electronic structure and photoinduced response near the band-edge in nanoscale samples. Here we present transient optical spectroscopy on exfoliated CST nanosheet samples at 300 K as well as at 10 K over an extended photon energy: 0.3 – 1.2 eV. We find clear signatures of optical transitions around 0.5 and 1.15 eV, which agree well with theoretical calculations of the indirect and direct conduction band edges. Photoexcited carriers are thermalized within a ps to the lattice through strong coupling to optical phonons and the subsequent decay persists over a nanosecond before undergoing recombination. Our work not only demonstrates direct measurements of the band structure but also sheds light on scattering behavior of photoexcited carriers in CST, which are critical for its future applications.

*We acknowledge the financial support of the NSF through grants DMR 1507844, DMR 1531373, and ECCS 1509706. S.D.W. acknowledges the support of NSF DMR 1505549.

5:18PM J57.00011: First principles studies of valley splitting in monolayer transition metal dichalcogenides on BiFeO3

ELIZABETH A PETERSON (Presenter), JEFFREY B NEATON, Lawrence Berkeley National Laboratory — Control of the spin and valley degrees of freedom of monolayer transition metal dichalcogenides (TMDs) via time reversal symmetry breaking at K and K' has been successfully demonstrated via magnetic substrates [1], which can generate significantly larger valley splitting than applied magnetic fields. Multiferroic substrates offer an avenue to develop valleytronics devices with switchable in-situ polarization. Using first principles density functional theory calculations, we predict that the ferromagnetically-ordered surface of Fe-terminated (111)-BiFeO3 substrates can produce valley splittings in WSe2 an order of magnitude larger than previously proposed magnetic substrates. We discuss the details of the orbital exchange interactions driving the splitting; and we also develop design principles for tuning the valley splitting through lattice alignment of the TMD monolayer with the substrate, as well as the identity and spin state of the magnetic substrate ions.


*This work is supported by supported by the Air Force Office of Scientific Research Hybrid Materials MURI under award number FA9550-18-1-0480. Computational resources provided by the Department of Energy via NERSC.

Tuesday, March 3, 2020 2:30 PM - 5:06 PM
Steady-State Density Functional Theory for quantum transport and spectral functions

GIANLUCA STEFANUCCI (Presenter), Physics, University of Rome Tor Vergata, STEFAN KURTH, DAVID JACOB, NAHUAL SOBRINO, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU — Steady-State Density Functional Theory (i-DFT) is a formalism to describe open quantum systems in nonequilibrium steady states. i-DFT is based on the one-to-one correspondence between the pair density and steady current and the pair local potential and applied voltage. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the voltage. After revisiting the fundamentals of i-DFT we apply the formalism to strongly correlated quantum dots at finite current and temperature. We show that the well-known discontinuity of the DFT xc potential at integer particle number bifurcates as the current starts flowing. We also show that the i-DFT formalism can be used to calculate the quantum system spectral function, a relevant quantity in photoemission spectroscopy.

1) MIUR PRIN Grant No. 20173B72NB
2) “Grupos Consolidados UPV/EHU del Gobierno Vasco” (IT1249-19)
3) “Ministerio de Economia y Competividad (MINECO)” (FIS2016-79464-P)
3:06PM J58.00002: Linearized GW density matrix for molecules*  
FABIEN BRUNEVAL  
(Presenter), Service de Recherches de Métallurgie Physique, CEA-Saclay — The GW approximation is well known for the calculation of high-quality ionization potentials and electron affinities in solids and molecules. However, the Green's function contains much more information than the mere quasiparticle energies.

Most interestingly, an approximate density matrix can be obtained from the contraction of the GW Green's function. Here we test and assess the quality of this so-called linearized GW density matrix for several molecular properties. We show it is reliable to evaluate the total energy out of a non-self-consistent GW calculation, being an alternative to the famous RPA total energy expression.

Based on a comprehensive benchmark of 34 molecules, we compare the quality of the ionization potential [1] electronic density, Hartree energy, exchange energy, and the Fock operator expectation values [2] against other well-established quantum chemistry techniques. In particular, we show that the obtained linearized GW densities markedly differ from those calculated within the wide-spread quasiparticle self-consistent GW approximation.


*F.B. acknowledges HPC resources from GENCI-TGCC and GENCI-CINES (project gen6018).

3:18PM J58.00003: Dynamical excitations of charge states in diamond color centers*  
TATIANE PEREIRA DOS SANTOS (Presenter), ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — We perform a time-dependent computational study of nitrogen-vacancy centers in diamond under ion irradiation. The negatively charged nitrogen-vacancy (NV−) centers in diamond are potential candidates for solid-state qubits due to the possibility to manipulate single center's electronic spin states. However, the dynamics of charge transitions between NV centers of different charges, such as the neutral (NV0) and the positively charged (NV+) centers, are not fully understood. Using time-dependent ab initio calculations, we perform accurate dynamical simulations of ion projectiles propagating near NV centers in diamond and calculate the properties of the defect-related excited states under the projectile impact. We compare our results with a pristine diamond and calculate the dynamical properties of projectile-vacancy coupling for a set of ion projectiles at different velocities. We discuss the quantitative properties of the charge states of nitrogen-vacancy centers at a sufficiently short time-scale that are challenging to approach experimentally.

*We acknowledge ONR N00014-18-1-2605 for the financial support.
**3:30PM J58.00004: Recent progress in the first-principles quantum Monte Carlo: New algorithms in the all-electron calculations**  
KOSUKE NAKANO (Presenter), SISSA (International School for Advanced Studies), RYO MAEZONO, JAIST (Japan Advanced Institute of Science and Technology), SANDRO SORELLA, SISSA (International School for Advanced Studies) — First-principles quantum Monte Carlo (QMC) techniques, such as variational quantum Monte Carlo (VMC) and diffusion quantum Monte Carlo (DMC), are among the state-of-the-art numerical methods used to obtain highly accurate many-body wave functions. I will present recent improvements in a QMC code, TurboRVB: All-electron calculations in QMC are not as widely used as in DFT because the computational cost scales with $Z^{5.5-6.5}$, where $Z$ is the atomic number. We have recently developed new algorithms to drastically decrease computational costs of all-electron DFT (suitable for QMC)[1], and all-electron lattice regularized diffusion monte Carlo (LRDMC)[2,3]. I will present basic ideas of the new algorithms and show several applications such as a binding energy calculation of the sodium dimer[1].


*K. Nakano is grateful for a financial support from Simons Foundation. R. Maezono is grateful for financial supports from MEXT-KAKENHI (19H04692 and 16KK0097), from FLAGSHIP2020 (project nos. hp190169 and hp190167 at K-computer), and from the Air Force Office of Scientific Research(AFOSR-AOARD/FA2386-17-1-4049;FA2386-19-1-4015).

**3:42PM J58.00005: Thermo-Optical Properties of Organic Verdazyl Biradicals via UV-VIS Spectroscopy**  
OZGE GUNAYDIN-SEN (Presenter), CAITLYN CLARK, EMILY INGRAM, Lamar University, DAVID BROOK, San Jose State University — Recently, biradicals have attracted attention due to their magnetic properties which could be used in different fields such as electronics, computer technologies, and renewable energy. Unlike most of the other radicals, organic verdazyl biradicals are stable at room temperature which makes them easy to work with. We investigated the photo-physical properties (i.e. singlet-triplet spin gap) of verdazyl biradicals utilizing thermo-optical spectroscopy (UV-VIS) between room temperature and 400 K. The spectra were then analyzed using Beer's law and Curie population analysis to extract the singlet-triplet spin gap at several wavelengths by evaluating the excitations. The analysis suggests, stronger excitations are representative of $\pi \rightarrow \pi^*$ transitions while the weaker excitations are representative of forbidden $\pi \rightarrow \pi^*$ transitions. Switching between singlet ground and triplete excited states can lead to an improved understanding of the manipulation via change in temperature and possibly with the magnetic field.

*Welch foundation (V-0004) and SURF grant - Lamar University*
Semilocal exchange-correlation (xc) energy of a many-electron system is not exact for all one-electron densities. In 1981, Perdew and Zunger (PZ) subtracted the fully nonlocal self-interaction error orbital-by-orbital, making the corrected functional exact for all one-electron densities. Although the PZ self-interaction correction (SIC) eliminates many errors of semilocal functionals, it is often worse for equilibrium properties of molecules and solids. Nonempirical semilocal functionals are usually designed to be exact for uniform electron gases, but PZ SIC is not so designed. We have extrapolated from the Ne, Ar, Kr, and Xe atoms to estimate the relative errors of the PZ SIC xc energies (with localized SIC orbitals) in the limit of large atomic number: about +5.5% for the LSDA-SIC and about -3.5% for nonempirical generalized gradient (PBE)-SIC and meta-generalized gradient strongly constrained and appropriately normed (SCAN)-SIC approximations [1]. The SIC errors found here are considerably larger than the error previously estimated on the uniform gas using LSDA-SIC localized orbitals. These errors may explain the shortcomings of PZ SIC for equilibrium properties, opening the path to a generalized SIC.


*DE-SC0018331

The Fermi-Löwdin orbital self-interaction correction (FLO-SIC) method removes the spurious self-interaction from common density functional theory (DFT) approximations. Within FLO-SIC, Fermi orbitals are used as localized orbitals. Each of these orbitals is constructed using a point in real space, called Fermi-orbital descriptor (FOD). To obtain the minimum total energy, the set of FODs needs to be optimized. This optimization is challenging and time-consuming. Accordingly, ways to reduce the computational burden are desired. In this work, we present a way to constrain the FODs. We exploit the tendency of the FODs to arrange in symmetrical patterns considering different atomic shells and bonding situations [1]. We will show how such a constrained approach improves the efficiency of the FOD optimization by comparing to an unconstrained approach. Finally, we will discuss applications and future directions.


*This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, as part of the Computational Chemical Sciences Program under Award Number #DE-SC0018331.
4:18PM J58.00008: New Algorithms for the Fermi-Löwdin Orbital Self-Interaction Correction Calculations.* KAMAL SHARKAS (Presenter), JUAN E PERALTA, KOBLAR JACKSON, Central Michigan Univ — Self-interaction error (SIE) is in most approximate exchange-correlation functionals, and removing SIE is important for improving the performance of the Kohn-Sham density-functional theory (KS-DFT) when applied to systems of chemical and physical interest. The Fermi-Löwdin Orbital Self-Interaction Correction (FLO-SIC) methodology was recently introduced as a unitarily invariant reformulation of the Perdew-Zunger SIC scheme to remove unphysical SIE from DFT. We propose new algorithms that aim to speed up and extend the applicability of this methodology. The "two-step" algorithm was designed to reduce the number of times that orbital-dependent potentials need to be calculated in the self-consistency cycle, addressing one computational bottleneck of SIC calculations. We also introduced unified Hamiltonian formalism in FLOSIC as a way to solve the system of Schrödinger-like equations. An advantage of the unified Hamiltonian approach is that it can replace a cumbersome "Jacobi sweep" method with a well-optimized diagonalization routine. It also is a convenient formalism for allowing unoccupied states to "see" an SIC potential. We present atomic and molecular applications that show the performance of FLOSIC with these new algorithms.

*DE-SC0018331

4:30PM J58.00009: Perdew-Zunger Self-Interaction Correction in Neutral, Protonated, and Deprotonated Water Clusters* KAMAL WAGLE (Presenter), BISWAJIT SANTRA, Temple Univ, KAMAL SHARKAS, Central Michigan University, SHARMIN AKTER, RAJENDRA R ZOPE, TUNNA BARUAH, University of Texas, El Paso, KOBLAR JACKSON, JUAN E PERALTA, Central Michigan University, JOHN P. PERDEW, Temple Univ — We have assessed the importance of self-interaction correction (SIC) to density functional approximations (DFA) for the description of water-ion interactions. We have used LSDA, PBE, SCAN, and the Fermi-Löwdin orbital self-interaction correction (FLOSIC) in conjunction with these DFAs to calculate the binding energies of neutral, protonated [H$_3$O$^+$ (H$_2$O)$_n$], and deprotonated [OH$^-$(H$_2$O)$_n$] water clusters, where $n$ denotes the number of water molecules. Including SIC is important to obtain accurate binding energies for these clusters. We find that FLOSIC-SCAN not only improves the mean absolute error in the binding energy of all clusters but also preserves the energetic ordering of the low-lying water hexamers (prism, cage, book, and cyclic) that was difficult to achieve with many non-empirical DFAs. Moreover, many-body decomposition of the total binding energy reveals that FLOSIC-SCAN significantly reduces the two-body errors in SCAN calculations. The three-body and higher-order many-body errors are also small with FLOSIC-SCAN. This shows that FLOSIC-SCAN has the potential to overcome the limitations of SCAN in describing water and aqueous ions in condensed phases.


*DMR-1607868, DE-SC0018331
4:42PM J58.00010: Study of water cluster anions using the self-interaction corrected density functional approximations*  JORGE VARGAS (Presenter), PETER UFONDU, TUNNA BARUAH, University of Texas at El Paso, KOBLAR ALAN JACKSON, Central Michigan University, RAJENDRA ZOPE, University of Texas at El Paso — Accurate description of the excess charge in water cluster anions is challenging for standard semi-local and (global) hybrid density functional approximations (DFAs). Using the recent unitary invariant implementation of the Perdew-Zunger self-interaction correction (SIC) method by means of Fermi-Lowdin orbitals, we assess the effect of self-interaction error on the vertical detachment energies (vDEs) of water cluster anions with the local spin density approximation (LSDA), PBE-GGA, and the SCAN meta-GGA functionals. Removal of self interaction error corrects the electron overbinding tendency of the LSDA, PBE, and SCAN. The vDEs of water cluster anions, obtained from the total energy difference of anion and neutral, are significantly improved upon removal of self-interaction errors and are better than the hybrid B3LYP functional but fall short of MP2 accuracy. Removal of SIE results in substantial improvement to the eigenvalue of the extra electron. The negative of the highest occupied eigenvalue after SIC provides an excellent approximation to the vertical detachment energy especially for the SIC-PBE wherein the MAE of vDEs with respect to CCSD(T) is only 17 meV, the best amongst all approximations compared in this work.

*U.S. DOE under grants DE-SC0018331 and DE-SC0006818.

4:54PM J58.00011: Fermi-Lowdin orbital self-interaction corrections applied to water clusters: Polarizabilities, dipole moments, and ionization energies*  SHARMIN AKTER (Presenter), Computational Science Program, University of Texas at El Paso, YOH YAMAMOTO, RAJENDRA ZOPE, TUNNA BARUAH, Physics, University of Texas, El Paso — The self-interaction (SI) error in density functional approximations (DFA) often leads to excessive delocalization of electron density. We examine the effect of self-interaction correction on the static dipole polarizabilities of small water clusters (H2O)n for n=1-6 using the Fermi-Lowdin self-interaction correction (FLOSIC) method. The static polarizability of a molecule determines its response to an applied static electric field. Density functional approximations generally overestimate the polarizabilities of molecules and atoms which is found to be improved by incorporation of SI correction. The polarizabilities of the water clusters are calculated with DFAs at the local, generalized gradient and meta-GGA levels. Previously optimized geometries at the CCSD(T) level are used for this calculation. Results show that the lower level approximations, LDA and GGA, overestimate the polarizability values whereas FLOSIC corrects the polarizabilities leading to better agreement with reference CCSD(T) values. We also investigate the effect of removing the self-interaction error on the dipole moments and ionization potentials of these clusters with different functionals. The results will be presented and discussed.

*Support from DOE through Award # DE-SC0018331 is gratefully acknowledged.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J59 DMP: Magnetic Weyl semimetals  Mile High Ballroom 3C
2:30PM J59.00001: Single-crystal neutron diffraction study of Dirac material EuMnSb₂

JOHN WILDE (Presenter), Physics and Astronomy, Iowa State University/Ames Laboratory, BENJAMIN UELAND, SIMON XAVIER RIBEROLLES, Ames Laboratory, DOMINIC H RYAN, McGill University, ANDREAS KREYSSIG, Physics and Astronomy, Iowa State University/Ames Laboratory, DAVID VAKNIN, Ames Laboratory, THOMAS HEITMANN, University of Missouri, YONG LIU, SERGEY L. BUD'KO, Ames Laboratory, ROBERT MCQUEENEY, Physics and Astronomy, Iowa State University/Ames Laboratory — EuMnSb₂ is a potential Dirac semimetal with Dirac fermions located in the Sb layers. These Dirac fermions have the potential to be controlled by a magnetic field if the magnetic order of the Eu or Mn sublattices couples to them. A large anisotropic magnetoresistance suggests that this coupling is strong in EuMnSb₂. Here we present results from single-crystal neutron diffraction experiments on EuMnSb₂. We find that the Eu and Mn magnetic sublattices order antiferromagnetically (AF) at 24(1) K and 324(1) K, respectively, with an additional magnetic phase transition at 9(1) K related to the coupling between both magnetic sublattices. Neutron diffraction shows that each AF phase is characterized by a magnetic unit cell equal to the chemical unit cell in contrast to Mossbauer measurements which suggest incommensurability. Our analysis indicates that the ordered Eu moments chiefly point perpendicular to the Sb planes and that the Mn moments align within the planes.

*This work was supported by the CATS, an EFRC, and the DMSE, both funded by the U.S. DOE, Office of BES through the Ames Laboratory under its Contract No. DE-AC02-07CH11358.

2:42PM J59.00002: Visualization of Antiferromagnetic Domain Walls in the Topological Semimetal EuMnBi₂

WENBO GE (Presenter), PAUL SASS, WEIDA WU, Rutgers University, New Brunswick, DIMUTHU OBEYSEKERA, JUNJIE YANG, Central Michigan University — The layered compound EuMnBi₂ is one such system where magnetic order coexists with Dirac fermions. The interplay between the uniaxial A-type antiferromagnetic (AFM) Eu magnetic order and quasi-2D Dirac fermions was recently observed to give rise to a multilayer quantum Hall state at high magnetic field above the spin-flop transition (> 5 T)¹. In this talk we will present magnetic imaging of AFM domain walls (DW) and their evolution across the spin-flop transition in the topological semimetal EuMnBi₂ using our cryogenic magnetic force microscope². Our results reveal that curvilinear AFM DWs naturally form when the sample is cooled below Tₐ (~ 22 K). Magnetic field dependence of the DW signal suggests enhanced susceptibility inside the DWs in the A-type AFM state. The DWs disappear above the spin-flop transition, and re-nucleate at different locations after reentry into the A-type AFM state. The direct visualization of AFM DWs in topological semimetals will help in the understanding of topological phenomena in correlated magnetic systems.


*This work is supported by DOE BES under award DE-SC0018153.
2:54PM J59.00003: Signature of spin-fermion coupling in the magnetic excitations of Dirac semimetal YbMnBi₂.* AASHISH SAPKOTA (Presenter), IGOR ZALIZNYAK, JOHN TRANQUADA, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, LAURA CLASSEN, Brookhaven National Laboratory; University of Minnesota, CEDOMIR PETROVIC, AIFENG WANG, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, MATTHW STONE, ANDREI T SAVICI, VASILE O GARLEA, Oak Ridge National Laboratory — In Dirac semimetals, coupling of Dirac charge carriers with magnetism can lead to novel phenomena with potential for technological applications [1, 2]. From this perspective, 112 ternary pnictogens (A,R)MnX₂ (A=Ca,Sr; R=Yb,Eu; X=Bi,Sb) represent an interesting family of Dirac materials where both the magnetism and Dirac electrons coexist, thereby providing an opportunity to study the spin-fermion coupling between Mn spins and Dirac electrons in Bi layer [2]. Previous studies of spin excitations in (Sr,Ca)MnBi₂ using inelastic neutron scattering (INS) have found no indication of such coupling because anomalous broadening found in itinerant magnets was absent [2]. However, our recent INS measurements of spin waves on YbMnBi₂ found a small and q-independent broadening in the spin waves, which is consistent with a significant spin-Dirac fermion coupling. Theoretical calculations show that the effect of coupling on the spin excitations is suppressed by a vanishing carrier density of states at the Dirac point. [1] A. Sapkota et al, arxiv 1908.08114 (2019), [2] M. C. Rahn et al, Phys. Rev. B 95, 134405 (2017).

*Work at BNL was supported by Office of BES, U.S. DOE under Contract No. DE-SC0012704. Research conducted at ORNL’s SNS was sponsored by SUFD, Office of BES, U.S. DOE.

3:06PM J59.00004: A Charge Density Wave Transition in NaₓMnBiᵧ magnetic semimetal

DESPINA LOUCA (Presenter), AARON WEGNER, Univ of Virginia — The I-Mn-V antiferromagnet, NaMnBi, was recently reported to develop a very large magneto-resistance (MR) up to 10,000 % at 2 K under a magnetic field of 9 T. A strong positive MR is present in crystals showing a semiconductor-to-metal transition (SMT) while, in the absence of an SMT, a modest (20 %) MR is achieved. Here, we show that upon cooling below the magnetic transition, a spatial modulation appears due to charge and defect ordering in a checkerboard pattern, with two kinds of displacement vectors q₁=(2/3, 0, 1) and q₂=(2/3, 1/3, 1/2). This couples to a superlattice transition (Tₛ) that lowers the symmetry from centrosymmetric P4/nmm to non-centrosymmetric P-4m2. In crystals with a large MR a close to room temperature Tₛ is observed with both q₁ and q₂ present. In crystals with low MR however, Tₛ is lower and only q₁ is observed. Tₛ breaks spatial inversion symmetry and marks the onset of a charge density wave instability.
ILYA BELOPOLSKI (Presenter), GUOQING CHANG, TYLER COCHRAN, JIAXIN YIN, SONGTIAN SONIA ZHANG, ZIJIA CHENG, XIAN YANG, NANA SHUMIYA, DANIEL MULTER, MAKSIM LITSKEVICH, ZAHID HASAN, Princeton University — Topological electronic phases in intrinsic magnets are of current interest. One common magnetic topological object is the Weyl line, a two-fold band degeneracy along a closed curve in bulk momentum space. Weyl lines arise naturally in the absence of time-reversal symmetry (absent in magnets) and in the presence of mirror symmetry (common in many space groups). I will present the observation of Weyl lines by ARPES in the room temperature magnet Co$_2$MnGa [1]. On the surface of the magnet, I observe drumhead surface states, pinpointing the bulk-boundary correspondence and suggesting a Berry phase topological invariant associated with the Weyl line. Next, the intrinsic Berry curvature contribution to the anomalous Hall response, determined from quantum transport, agrees with a prediction of the Weyl line Berry curvature based on ARPES and first-principles calculations [1]. I will comment on composite topological structures arising from pinning and linking of different Weyl lines. Lastly, I will discuss future directions in Co$_2$MnGa and other topological Weyl line magnets.


*Work at Princeton was supported by the US DOE under the Basic Energy Sciences programme (Grant #: DOE/BES DE-FG-02-05ER46200).

YU LIU (Presenter), CHRISTIAN MATT, HARRIS PIRIE, Department of Physics, Harvard University, NATHAN DRUCKER, Department of Applied Physics, Harvard University, ROBERT-JAN SLAGER, Department of Physics, Harvard University, NA HYUN JO, BRINDA KUTHANAZHI, SERGEY L. BUD'KO, PAUL C CANFIELD, Department of Physics & Astronomy, Iowa State University/Ames Laboratory, JENNIFER E. HOFFMAN, Department of Physics, Harvard University — Weyl semimetals are characterized by topologically protected Weyl nodes in the bulk and Fermi-arcs states with momentum-locked spin or chirality on the surface. Among various Weyl semimetals, magnetic Weyl semimetals are particularly attractive because they have fewer, more widely separated Weyl nodes. Additionally, their Weyl nodes can potentially be manipulated by external magnetic field or changes in the local moment ordering. Here we present a scanning tunneling microscopy and quasiparticle interference (QPI) study of the magnetic Weyl semimetal candidate CeBi. In particular, we resolve splitting of the Bi $p$ and Ce $d$ bands of CeBi with 9T external magnetic field, which is the necessary precondition for Weyl nodes. We also observe signatures of Fermi-arcs in the QPI pattern. The QPI-derived band structure of CeBi in different magnetic phases is also studied.

*This work was supported by DOE EFRC, CATS
Swiss National Science foundation Grant P400P2_183890
Gordon and Betty Moore Foundation Grant GBMF4536 and Grant GBMF4411
U.S. DOE, BES, DMSE under Contract No. DE-AC02-07CH11358
3:42PM J59.00007: Magnetic semimetals and quantized anomalous Hall effect in EuB$_6$*  
MIN NIE (Presenter), Stanford Univ — Exploration of the novel relationship between magnetic order and topological semimetals has received enormous interest in a wide range of both fundamental and applied research. Here we predict that "soft" ferromagnetic (FM) material EuB$_6$ can achieve multiple topological semimetal phases by simply tuning the direction of the magnetic moment. Explicitly, EuB$_6$ is a topological nodal-line semimetal when the moment is aligned along the [001] direction, and it evolves into a Weyl semimetal with three pairs of Weyl nodes by rotating the moment to the [111] direction. Interestingly, we identify a novel semimetal phase featuring the coexistence of a nodal line and Weyl nodes with the moment in the [110] direction. Topological surface states and anomalous Hall conductivity, which is sensitive to the magnetic order, have been computed and are expected to be experimentally observable. Large-Chern-number quantum anomalous Hall effect can be realized in its [111]-oriented quantum-well structure.

*S. N. and F. P. are supported by Volkswagen of America and the Affiliates Program of the Nanoscale Protoyping Laboratory. Z. W. is supported by the National Thousand-Young-Talents Program. X.D. and H.M.W. are supported by the Ministry of Science and Technology of China.

3:54PM J59.00008: Real-space imaging of surface-magnetism in magnetic Weyl semimetal candidate CeBi*  
CHRISTIAN MATT (Presenter), YU LIU, NATHAN C DRUCKER, HARRIS PIRIE, ROBERT-JAN SLAGER, Harvard University, NA HYUN JO, Ames Laboratory, BRINDA KUTHANAZHI, SERGEY L. BUD’KO, PAUL C CANFIELD, Iowa State University, JENNIFER E. HOFFMAN, Harvard University — Magnetic Weyl semimetals host chiral Weyl nodes in their bulk which are formed by broken time-reversal symmetry, caused, for example, by intrinsic ferromagnetic order. While the bulk-surface correspondence dictates the formation of Fermi arcs connecting Weyl nodes with opposite chirality, their momentum-space contour and their connectivity (i.e. which Weyl points they are connecting to), depends on surface properties. Here we use spin-polarized scanning tunneling microscopy to map the magnetic structure on the surface of CeBi at various bulk-magnetic phases. We find unexpected surface-magnetic order with strongly bias-dependent magnetic contrast and phase. We discuss our observation in terms of Fermi arc connectivity and magnetic interactions in CeBi.

*This work was supported by DOE EFRC, Center for the Advancement of Topological Semimetals, Swiss National Science foundation under Grant P400P2_183890, U.S. DOE, BES, DMSE under Contract No. DEAC0207CH11358, and Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4536 and GBMF4411.
4:06PM J59.00009: Effect of chemical substitution on the anomalous Hall effect of chiral-lattice antiferromagnet CoNb$_3$S$_6$

DINA MICHEL (Presenter), NISHCHAL THAPA MAGAR, NICHOLAS BISHOP, Department of Physics and Astronomy, George Mason University, LEKHNATH POUDEL, Department of Materials Science and Engineering, University of Maryland, College Park, JEFFREY LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology, JOHN MITCHELL, Materials Science Division, Argonne National Lab, NIRMAL GHIMIRE, Department of Physics and Astronomy, George Mason University — An ordinary Hall effect in a conductor arises due to the Lorentz force acting on the charge carriers. In ferromagnets, an additional contribution to the Hall effect, the anomalous Hall effect (AHE), appears proportional to the magnetization. It is also known that the AHE can arise in non-collinear and non-coplanar antiferromagnets due to scalar spin chirality. However, recently a large AHE was observed in a collinear antiferromagnet CoNb$_3$S$_6$ [1]. More recent theories have indicated that the AHE in CoNb$_3$S$_6$ may be inherently related to the chirality associated with the crystal structure [2,3]. The presence of a small ferromagnetic component plays an important role in revealing the AHE in CoNb$_3$S$_6$ which was limited to a narrow temperature range just below the Néel temperature. Here we will show that partial substitution of Co by Fe widens the temperature range and that the AHE in Co$_{1-x}$Fe$_x$Nb$_3$S$_6$ saturates at lower temperatures. We will discuss the importance of this observation in the context of recent theories of the AHE in collinear antiferromagnets.


4:18PM J59.00010: In-plane antiferromagnetic moments in axion topological insulator candidate EuIn$_2$As$_2$

YANG ZHANG, the school of Physics, Sun Yat-Sen University, KE DENG, the school of Physics, Southern University of Science and Technology, XIAO ZHANG, MENG WANG, the school of Physics, Sun Yat-Sen University, CAI LIU, the school of Physics, Southern University of Science and Technology, EIKE F. SCHWIER, SHIV KUMAR, Hiroshima Synchrotron Radiation Center, Hiroshima University, CHAOYU CHEN, the school of Physics, Southern University of Science and Technology, BING SHEN (Presenter), the school of Physics, Sun Yat-Sen University — Topological insulator with antiferromagnetic order can serve as an ideal platform for the realization of axion electrodynamics. In this paper, we report a systematic study of the axion topological insulator candidate EuIn$_2$As$_2$. A linear energy dispersion across the Fermi level confirms the existence of the proposed hole-type Fermi pocket. Spin-flop transitions occur with magnetic fields applied within the $ab$-plane while are absent for fields parallel to the $c$-axis. Anisotropic magnetic phase diagrams are observed and the orientation of the ground magnetic moment is found to be within the $ab$-plane. The magneto-resistivity for EuIn$_2$As$_2$ behaves non-monotonic as a function of field strength. It exhibits angular dependent evolving due to field-driven and temperature-driven magnetic states. These results indicate that the magnetic states of EuIn$_2$As$_2$ strongly affect the transport properties as well as the topological nature.
Determination of the magnetic order in the EuIn$_2$As$_2$, an axion insulator candidate

SIMON RIBEROLLES (Presenter), Division of Materials Science & Engineering, Ames Laboratory, BRINDA KUTHANAZHI, NA HYUN JO, ADAM KAMINSKI, PAUL C CANFIELD, Ames Laboratory, Iowa State University, THOMAS HEITMANN, Missouri Research Reactor, University of Missouri, DOMINIC H RYAN, Physics, McGill University, BENJAMIN UELAND, Division of Materials Science & Engineering, Ames Laboratory, ROBERT MCQUEENEY, Ames Laboratory, Iowa State University — EuIn$_2$As$_2$ is a Zintl compound recently reported as a possible first example of axion insulator with antiferromagnetic (AF) long-range order and characteristic colossal negative magnetoresistance. It thus represents a unique platform to investigate the physics of axion insulators and, in particular, to focus on the interplay between the AF order and the topologically protected features of the electronic band structure. Here, we present results from single-crystal magnetic diffraction experiments. Surprisingly, our results reveal the successive stabilization of two different sets of magnetic Bragg reflections indexed with the propagation vectors $k_1=(0,0,0.31)$ and $k_2=(0,0,0)$ below $T_{N1}=17$ and $T_{N2}=15$ K, respectively, despite the chemical unit cell containing only a single Eu site. The two magnetic structures are believed to coexist at $T\leq T_{N2}$, and were individually determined from refinement analyses. We will describe both magnetic structures and discuss the influence of our results upon the current understanding of the material's topological features.

*Work supported by the Center for the Advancement of Topological Semimetals, an Energy Frontier Research Center funded by the U.S. DOE Office of Science, Office of BES, through Ames Laboratory under its Contract No. DE-AC02-07CH11358.

Anomalous Hall effect with colossal magnetic saturation and coercivity in (111)-oriented pyrochlore Eu$_2$Ir$_2$O$_7$ thin films

XIAORAN LIU (Presenter), WENBO GE, MIKHAIL KAREEV, FANGDI WEN, Rutgers University, New Brunswick, EUN SANG CHOI, National High Magnetic Field Laboratory, WEIDA WU, JAK CHAKHALIAN, Rutgers University, New Brunswick — The pyrochlore iridates are a class of candidate materials for the topological Weyl semimetal, which can host hidden topological and magnetic phases in the thin film form. To investigate the intrinsic properties relevant to the Ir sublattices, we fabricated high-quality epitaxial (111)-oriented pyrochlore Eu$_2$Ir$_2$O$_7$ thin films on YSZ substrates, in which the Eu$^{3+}$ ions are magnetically silent. Temperature-dependent transport reveals an onset of the metal-insulator transition at $T_C$ around 110 K, similar to the bulk value. However, magneto-transport measurements reveal that below $T_C$ in the insulating phase with the non-colicinear all-in-all-out antiferromagnetic order, a distinct anomalous Hall effect (AHE) emerges combined with a butterfly-shape hysteretic magnetoresistance. The AHE gets strongly pronounced at lower temperatures, with colossal enhancement of both the saturation field $H_S$ and the coercivity $H_C$. These findings are signatures of the emergent interacting topological phases in thin films of [111]-oriented pyrochlore iridates.
4:54PM J59.00013: Domain Wall-Dependent Electrical Transport in a Magnetic Weyl Semimetal*  NICHOLAS QUIRK (Presenter), GUANGMING CHEN, NAN YAO, N. PHUAN ONG, Princeton University — Magnetic force microscopy reveals that microscale lamellae fabricated by focused ion beam microscopy of Co$_2$MnGa—a ferromagnetic Weyl semimetal—contain just a few magnetic domains which form a pattern that is different on the top surface than on the bottom. Transport measurements of electrical devices made from these lamellae with contacts on both faces show large resistance anisotropies that depend on in-plane and out-of-plane magnetic fields in different ways. These data taken together describe a very non-homogeneous current distribution which may result from the interaction of the Weyl fermions in this material with the magnetic domain walls.

*Gordon and Betty Moore Foundation

5:06PM J59.00014: Imaging the Electronic Structures in Antiferromagnetic Dirac Semimetal GdSbTe*  BALAJI VENKATESAN, CHIH-CHUAN SU, Institute of Physics, Academia Sinica, RAMESH BABU, Department of Physics, National Taiwan University, RAMAN SANKAR, Institute of Physics, Academia Sinica, FANGCHANG CHOU, Center for Condensed Matter Sciences, National Taiwan University, GUANG-YU GUO, Department of Physics, National Taiwan University, TIEN-MING CHUANG (Presenter), Institute of Physics, Academia Sinica — Dirac semimetals (DSMs) are characterized by topology- or symmetry-protected band crossings near the Fermi level that can form Dirac points, nodal lines, nodal surface or nodal chains in the electronic band structures. These unique band crossings can give rise to interesting properties such as large anisotropic magnetoresistance, chiral anomaly and flat optical conductivity. Moreover, magnetic DSMs can break the time reversal symmetry, where the interplay of symmetry, relativistic effects and the magnetic order can lead to novel quantum phases and offer the tunability of these quantum states with magnetic field. GdSbTe is a non-symmorphic semimetal with an antiferromagnetic phase below T=13K. By using spectroscopic imaging - scanning tunneling microscopy and first principle calculation, we investigated the surface and bulk electronic structures in GdSbTe across the magnetic transition and under magnetic field. Our quasiparticle scattering interference imaging and calculation showed the linear dispersion from Dirac bands over a wide energy range and are robust against different magnetic orders, suggesting the rigidity of the non-symmorphic crystalline symmetry protection in GdSbTe.

*This work is supported by Academia Sinica and Ministry of Science and Technology in Taiwan.
5:18PM J59.00015: Interplay between topology and magnetic excitations in topological nodal semimetal CeAlGe* THANH NGUYEN (Presenter), MINGDA LI, FEI HAN, NINA ANDREJEVIC, RICARDO PABLO PEDRO, Massachusetts Institute of Technology MIT, MATTHEW STONE, SONGXUE CHI, JAIME FERNANDEZ-BACA, MASAAKI MATSUDA, DAVID TENNANT, Oak Ridge National Laboratory — Weyl semimetals (WSMs) comprise of a novel condensed matter phase that carries emergent quasiparticles of topologically nontrivial chiral Weyl fermions and represent a key recent advance in the realm of strongly spin-orbit-coupled materials. Magnetic WSMs, in which the nontrivial Weyl fermions break time-reversal symmetry, enable the possibility of further discovering unexplored spin-electronic phenomena enabling feasible spintronic applications. In this talk, I will present results obtained from neutron scattering experiments performed on predicted type-II WSM, CeAlGe. Our measurements of low-energy spin waves as well as crystal-field excitations using time-of-flight and triple-axis inelastic neutron scattering highlight phenomena intertwining its nontrivial topology with its unusually intricate magnetic structure. Through the investigation of these excitations, this study elucidates the substantial coupling between the exotic magnetic configuration and the topological semimetallic electronic structure within this material, which may see a valuable role in future practical applications.

*We acknowledge funding from U.S. Department of Energy (DOE), Office of Science (SC), Basic Energy Sciences (BES), award No. DE-SC0020148.

Tuesday, March 3, 2020 2:30 PM - 4:42 PM

Session J60 DMP: Josephson Junctions with Topological Insulator Weak Links Mile High Ballroom 4A - David Cobden, University of Washington - Tag(s): Focus

2:30PM J60.00001: Josephson Junctions Using Weak-Links of Topological Crystalline Insulators* [Invited] JAMES WILLIAMS (Presenter), University of Maryland, College Park — Topological Crystalline Insulators (TCI) produce topological states of matter that rely on crystalline symmetry, opening new avenues to create and control the novel properties of the surface state. In this talk I will elucidate the properties of Josephson junctions that use SnTe -- a candidate TCI material -- as the weak link. Deviations from conventional junction properties are observed, including signatures of broken time reversal symmetry. The genesis of these effects, which arise from a confluence of multiple electronic bands, ferroelectric distortions and topology, will be detailed.

*Synthesis of narrow SnTe nanowires was supported by NSF 1743896. Doping of indium and transport characterizations of SnTe nanowires were supported by DOE DE-SC0014476. Measurements in this work was sponsored by the grants National Science Foundation A “Quantum Leap” Demonstration of Topological Quantum Computing (DMR-1743913) and Physics Frontier Center at the Joint Quantum Institute (PHY-1430094).
3:06PM J60.00002: Fusion and parity readout of Majorana bound states in lateral S-TI-S Josephson junctions*  JESSICA MONTONE (Presenter), GUANG YUE, GILBERT ARIAS, University of Illinois at Urbana-Champaign, XIONG YAO, DEEPTI JAIN, JISOO MOON, SEONGSHIK OH, Rutgers University, New Brunswick, DALE J VAN HARLINGEN, University of Illinois at Urbana-Champaign — We propose experiments designed to demonstrate the fusion of Majorana bound states (MBS) and to measure their parity in S-TI-S (Superconductor-Topological Insulator-Superconductor) lateral Josephson junctions. These junctions are expected to host MBS at Josephson vortex cores where the phase difference across the junction is an odd multiple of $\pi$. Our approach is to integrate Al-AlO$_x$-Al single-electron transistors, which are sensitive to the parity of the MBS pairs, with Nb-Bi$_2$Se$_3$-Nb Josephson junctions, in which the MBS can be created and manipulated to carry out fusion and braiding operations. We report progress toward implementing these schemes and incorporating them into circuits for quantum information processing.

*This work is supported by the National Science Foundation grants DMR-1610114 and DMR-1745304.

3:18PM J60.00003: Interfacial effects of proximitizing superconductivity in topological insulators*  ILAN ROSEN (Presenter), MOLLY P ANDERSEN, LINSEY RODENBACH, Stanford Univ, PENG ZHANG, LIXUAN TAI, GEN YIN, UCLA, MARC A. KASTNER, Stanford Univ, KANG L. WANG, UCLA, DAVID GOLDHABER-GORDON, Stanford Univ — The proximitization of superconductivity into time-reversal invariant topological insulators, as well as their magnetic counterparts, has produced exciting observations including anomalous Fraunhofer patterns[1, 2], finite momentum pairing[3], and fractional quantized conductances[4]. Yet even as the quality of topological materials rapidly improves, variations in behavior across different experiments and groups are not well understood. We postulate that the properties of the interface between superconducting metals and topological insulators play a key role, and we discuss our attempts to characterize and manipulate such interfaces, focusing on the (BiSb)$_2$Te$_3$ family of topological insulators.


*Research supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.
3:30PM J60.00004: Interface and scattering potentials in topological insulator-superconductor heterostructures*  

EKLAVYA THAREJA (Presenter), ILYA VEKHTER, Louisiana State University, Baton Rouge — Many proposed applications of topological insulators rely on coupling them to superconductors in Josephson-type geometry. However, interface potentials at the boundary between a superconductor and a topological insulator can alter the dispersion and the spin texture of the topological states, thereby changing the nature of the proximity-induced superconducting order. Using effective low-energy models we study how these potentials, combined with the scattering at lateral junctions between superconducting and non-superconducting regions, change the spectra of the Andreev bound states and the Josephson current-phase relationship. We discuss the relevance of our findings to proposals for functional heterostructures.

*NSF via Grant No. DMR-1410741

3:42PM J60.00005: Superconductivity in \( \text{Sn}_{1-x}\text{In}_x\text{Te} \) thin films grown by molecular beam epitaxy*  

ANDREA BLIESENER (Presenter), JUNYA FENG, ALEXEY A TASKIN, YOICHI ANDO, Institute of Physics II, University of Cologne — \( \text{Sn}_{1-x}\text{In}_x\text{Te} \) is derived from the topological crystalline insulator \( \text{SnTe} \) which becomes superconducting when doped with Indium and it is one of the top candidates for topological superconductivity [1].

\( \text{Sn}_{1-x}\text{In}_x\text{Te} \) films have been grown by molecular beam epitaxy on a \( \text{Bi}_2\text{Te}_3 \) buffer layer, which has a good lattice matching for the growth in the (111) direction [2]. Using \textit{in situ} post-annealing procedures, we achieve robust superconductivity. To look for possible signatures of topological superconductivity, we fabricated tunnel junctions on the surface of the \( \text{Sn}_{1-x}\text{In}_x\text{Te} \) films. The tunnelling spectroscopy data shows a two-gap structure in the conductance spectra which points to the coexistence of bulk and surface superconductivity in the studied films.


*This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program (Grant Agreement No. 741121), the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under CRC 1238-277146847 (Subprojects A04, B01) as well as Germany’s Excellence Strategy—Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1-390534769.
3:54PM J60.00006: Superconductivity of Topological Surface States and Strong Proximity Effect in Sn$_{1-x}$Pb$_x$Te-Pb Heterostructures  JINFENG JIA (Presenter), HAO YANG, YAO-YI LI, TENG-TENG LIU, DANDAN GUAN, SHI-YONG WANG, HAO ZHENG, CANHUA LIU, Shanghai Jiao Tong Univ, LIANG FU, Physics, MIT — Superconducting topological crystalline insulators are expected to form a new type of topological superconductors to host Majorana zero modes under the protection of lattice symmetries. The bulk superconductivity of topological crystalline insulators has been induced through chemical doping and proximity effect. However, only conventional full gaps are observed, so the existence of topological superconductivity in topological crystalline insulators is still controversial. Here, we report the successful fabrication of atomically flat lateral and vertical Sn$_{1-x}$Pb$_x$Te-Pb heterostructures by molecular beam epitaxy. The superconductivity of the Sn$_{1-x}$Pb$_x$Te-Pb heterostructures can be directly investigated by scanning tunneling spectroscopy. Unconventional peak-dip-hump gap features and fourfold symmetric quasiparticle interference patterns taken at the zero energy support the presence of the topological superconductivity in superconducting Sn$_{1-x}$Pb$_x$Te. Strong superconducting proximity effect and easy preparation of various constructions between Sn$_{1-x}$Pb$_x$Te and Pb make the heterostructures to be a promising candidate for topological superconducting devices to detect and manipulate Majorana zero modes in the future.

4:06PM J60.00007: Probing the location of Josephson vortices and the Majorana states bound to them in S-TI-S lateral Josephson junctions via Scanning SQUID Microscopy*  GILBERT ARIAS (Presenter), JESSICA MONTONE, ERIK D HUEMILLER, GUANG YUE, DALE J VAN HARLINGEN, Physics, University of Illinois Urbana-Champaign — Superconducting-Topological Insulator-Superconducting (S-TI-S) Josephson junctions are a promising platform for creating and manipulating Majorana bound states (MBS). The MBS are localized at the cores of Josephson vortices where the phase difference across the junction is an odd-multiple of π. They can be manipulated by applying fields and currents to carry out braiding operations for quantum information processing. To optimize braiding protocols, it is useful to track the motion of the vortices via local magnetic imaging. We are developing a Scanning SQUID Microscope in which the probe is a superconducting pickup loop with submicron dimensions. It is inductively-coupled to a commercial dc SQUID, providing the required field sensitivity and spatial resolution. In this talk, we report our progress towards imaging the Josephson vortices and the currents carried by the Majorana states.

*This work was supported by the Department of Energy Basic Energy Sciences grant DE-SC0017888.
4:18PM J60.00008: Excess Vortex-Vortex Supercurrent as Method for Readout of Majorana Parity in Fe(Se,Te)*  
BENJAMIN NOVEMBER (Presenter), Physics, Harvard University, JAY SAU, Physics, University of Maryland, College Park, JAMES WILLIAMS, Joint Quantum Institue, JENNIFER E. HOFFMAN, Physics, Harvard University — Topological superconductors are one of the most exciting new platforms for the development of topological quantum computing. Specifically, the Fe(Se,Te) family has been shown to host Majorana zero-energy modes (MZMs) in vortex cores [1], pairs of which can potentially be used as topologically protected qubits. However, there has been no previous calculations to suggest that the two distinct parity states can be distinguished experimentally. Through the use of an effective two-dimensional Fu-Kane model on the surface of $\text{FeTe}_x\text{Se}_{1-x}$, we approximate the $(p_x + ip_y)$ superconductor as an internal s-wave proximity effect on the topological surface states. We then numerically calculate the wavefunction solution to the resulting Bogoliubov-de Gennes equation for both spatially separated single vortices and the double vortex limit of complete overlap of the single vortex pair. Using these wavefunction solutions, we compute supercurrent generated by zero-energy mode splitting and the resulting magnetic field gradient above the surface. We conclude it is possible to measure the presence of this excess supercurrent, and thus the quantum state of the MZM pair, using magnetic force microscopy.


*This work supported by NSF Grant No. ONA-1936246.

4:30PM J60.00009: Proximity effect at the superconducting-topological insulator interface from first principles*  
KYUNGWHA PARK (Presenter), Physics, Virginia Tech, BALAZS UJFALUSSY, Wigner Research Centre for Physics, Hungary — A topological insulator (TI) film in contact with an s-wave superconducting (SC) substrate has been extensively studied due to the possibility of hosting zero-energy Majorana states using the proximity effect. So far, theoretical studies have been carried out based on effective models. Experimental studies of TI-SC heterostructures showed inconsistent results on a dependence of the induced SC gap size on TI film thickness as well as on the proximity effect for the TI bulk states. The Fermi level is likely to cross both TI bulk and Dirac surface states. Here we investigate the proximity-induced SC gap at the interface TI and top TI surface states and bulk TI states, considering a Bi2Se3 film on a PdTe SC substrate within first-principles calculations. In this study, we solve the fully relativistic Kohn-Sham-Dirac-Bogoliubov-de Gennes equations for the heterostructure by introducing Cooper pairs within the screened Korringa-Kohn-Rostoker (SKKR) method. We present our results on the induced SC gap arising from TI bulk and surface states and its dependence on TI film thickness at several chemical potential values.

*The computational support was provided by SDSC under DMR060009N and VT ARC.
J60.00010: Multiple Pairs of Propagating Majorana Modes in the Vortex Line of Superconducting Quadratic Dirac Semimetals  
LUN HU, department of physics, University of California, San Diego, SHENSHAN QIN (Presenter), Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, CHEN FANG, JIANGPING HU, Beijing National Research Center for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, FU-CHUN ZHANG, Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences — We study the vortex bound states in a class of three dimensional (3D) time reversal invariant quadratic Dirac semimetals. Assuming intrinsic s-wave superconductivity, we find that multiple Majorana modes can be bound to the vortex line for certain range of doping level. Specifically, due to the quadratic Dirac points in the band structures, quasi-1D Majorana modes carrying angular momentum ±1 and ±2 can propagate along the vortex line; for quadratic Dirac semimetals with nontrival Z2 topological character, additional 0D Majorana zero modes carrying angular momentum 0 can be bound at the end of the vortex line. Together with our work in linear Dirac semimetals (Phys. Rev. Lett. 123, 027003), we establish a complete correspondence between the topological properties of the normal state band structures and the vortex bound states in the s-wave superconducting state.

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J61 DMP DCMP DCOMP: Fe-Based Superconductors - Nematicity III / ARPES  Mile High Ballroom 4B - Vitalii Vlasko-Vlasov, Argonne Natl Lab - Tag(s): Focus
2:30PM J61.00001: A local structure perspective on iron pnictides and chalcogenides: Insights gained from pair distribution function analysis* [Invited] BENJAMIN FRANDSEN (Presenter), Physics and Astronomy, Brigham Young University — The field of iron-based superconductivity, now well into its second decade of existence, continues to challenge and stimulate condensed matter physicists. One perennial issue of debate is the origin and implications of the electronic nematic phase. This state is characterized by a spontaneous breaking of four-fold rotational symmetry, which manifests as unequal occupations of the $d_{xz}$ and $d_{yz}$ orbitals, a tetragonal-to-orthorhombic structural phase transition, and (in many cases) stripe-type magnetic order. In addition to the statically ordered nematic phase observed widely in various families of iron-based superconductors, strong nematic fluctuations have also been found in broad regions of parameter space outside the ordered nematic state. Pair distribution function (PDF) analysis of x-ray and neutron total scattering data is a proven method of studying local, short-range structural correlations that deviate from the average structure, such as the orthorhombic distortions associated with nematic fluctuations in iron-based superconductors. Here, I will present recent PDF investigations of several representative families of iron-based superconductors. The results reveal the presence of local orthorhombic distortions across large regions of temperature-composition space and provide a detailed look at the temperature dependence and characteristic length scale of these distortions. The deeper understanding of the local structure of iron-based superconductors enabled by these PDF experiments will help clarify some of the outstanding questions relating to these fascinating materials.

*This work was supported in part by the U.S. Department of Energy under Contract No. DEAC02-05-CH11231 and by the College of Physical and Mathematical Sciences at Brigham Young University.
3:06PM J61.00002: Time Reversal Symmetry Breaking in the FeTe$_{1-x}$Se$_x$ family of high Tc superconductors.* [Invited] PETER JOHNSON (Presenter), Brookhaven National Laboratory — Laser-based ARPES with variable light polarization offers a powerful probe of the electronic structure near the center of the Brillouin zone. Here the technique is used to examine the Fe-based superconductor family, FeTe$_{1-x}$Se$_x$. At the zone center we observe the presence of Dirac cones with helical spin structure as expected for topological surface states and as previously reported in the related FeTe$_{0.55}$Se$_{0.45}$.[1] These studies are compared with theoretical studies that take account of the disordered local magnetic moments related to the paramagnetism observed in this system. Indeed including the magnetic contributions in the theoretical description is necessary to bring the chemical potential of the calculated electronic band structure into alignment with experimental observation. In the bulk superconducting state for FeTe$_{0.7}$Se$_{0.3}$ the topological state appears to acquire mass below T$_c$. With a single state at the center of the zone, mass acquisition is indicative of time reversal symmetry breaking which in turn suggests the potential formation of ferromagnetism in the surface layer.


*The work carried out at Brookhaven was supported in part by the U.S. DOE under Contract No. DE-AC02-98CH10886 and in part by the Center for Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy. C. W. at UCSD was supported by AFOSR FA9550-14-1-0168.

3:42PM J61.00003: Orbital transmutation in the nematic state of FeSe: the consequences for Raman and ARPES experiments* ANDREY CHUBUKOV (Presenter), University of Minnesota, MATTIA UDINA, MARCO GRILLI, LARA BENFATTO, Physics, "Sapienza" University of Rome, MORTEN HOLM CHRISTENSEN, RAFAEL FERNANDES, University of Minnesota — In this talk I will discuss nematicity induced change of the orbital composition of low-energy excitations in FeSe, and how it affects Raman and ARPES probes. I will argue that deep in the nematic state, hole and electron pockets become nearly mono-orbital, consistent with polarized ARPES measurements. I show that this leads to strong reduction of Raman intensity in B$_{1g}$ channel (in 1Fe zone), as observed in the measurements. The reduction comes about because for nearly mono-orbital pockets, B$_{1g}$ Raman response gets reduced by vertex corrections, which enforce charge conservation. I further discuss ARPES experiments at the M point ($\pi,\pi$). Deep in the nematic state, the two excitations, best visible in ARPES, have been identified as having xz and yz orbital character. However, they remain split above the nematic transition, in apparent contradiction to the fact that in the tetragonal phase the xz and yz orbitals are degenerate. We show that these experimental data are naturally explained by orbital transmutation of the excitations at M between tetragonal and nematic phases.

*The work was supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0014402.
3:54PM J61.00004: Time-reversal symmetry-breaking superconductivity in FeSe$_{1-x}$S$_x$*

MINGWEI QIU (Presenter), KOHEI MATSUURA, TAKAAKI TAKENAKA, YUICHI SUGIMURA, TAKASADA SHIBAUCHI, Univ of Tokyo, QI SHENG, KOHTARO YAMAKAWA, YASUTOMO J UEMURA, Department of Physics, Columbia University, YIPENG CAI, ANDREA DAMASCELLI, RYAN P DAY, KENJI KOJIMA, Stewart Blusson Quantum Matter Institute, University of British Columbia, JAMES W BEARE, GREGORIE LUKE, Department of Physics & Astronomy, McMaster University, ZHAO GUO QIANG, CHANGQING JIN, Institute of Physics, Chinese Academy of Sciences, YILUN GU, LICHENG FU, FANLONG NING, Department of Physics, Zhejiang University, MIKIHIKO SAITO, Univ of Tokyo — The FeSe$_{1-x}$S$_x$ superconductors involving non-magnetic nematic phase and its quantum criticality provide a unique platform to investigate the relationship between nematicity and superconductivity. The lifting of superconducting gap nodes due to twin boundaries has been observed experimentally, which suggests indirect evidence for time-reversal symmetry breaking (TRSB). It is consistent with the theoretical prediction that the superconducting order parameter breaks the time-reversal symmetry near the nematic twin boundaries. We have performed the muon spin rotation (μSR) measurements on FeSe and observed the spontaneous internal field below the superconducting transition temperature $T_c$, providing evidence for TRSB state in FeSe. Here we extend zero-field μSR studies to tetragonal FeSe$_{1-x}$S$_x$ (x=0.18, 0.2) without nematicity. We find that the μSR relaxation rate starts to grow below $T_c$ in these crystals. This indicates that weak but finite internal magnetic field is induced in the superconducting state, providing strong evidence for TRSB state not only near twin boundaries but also inside the bulk of FeSe$_{1-x}$S$_x$.

*Supported by a Grant-in-Aid for Scientific Research on Innovative Areas “Quantum Liquid Crystals” (KAKENHI Grant No. JP19H05824) from Japan Society for the Promotion of Science.

4:06PM J61.00005: An ARPES and STM/S investigation of the interplay between nematicity, orbital order, and superconductivity in FeSe*

MORGAN WALKER (Presenter), TIMOTHY BOYLE, ZITONG ZHAO, EDUARDO H DA SILVA NETO, JOURNEY BYLAND, JACKSON R BADGER, VALENTIN TAUFOUR, University of California, Davis, RYAN P DAY, SERGEY ZHDANOVICh, ANDREA DAMASCELLI, University of British Columbia, TOR PEDERSEN, SERGEY GOROVIKOV, Canadian Light Source — Nematic order coexists with a myriad of iron-based superconductors, suggesting it is an important actor in the mechanism behind the superconductivity in these compounds. Many of these materials also exhibit magnetism near the nematic and superconducting phases, complicating the quest to understand their relationship. Fortunately, FeSe has no magnetic ground state and is therefore a great candidate for disentangling the interplay between nematicity and superconductivity. We performed detailed scanning tunneling microscopy and spectroscopy (STM/S) and angle-resolved photoemission spectroscopy (ARPES) studies on single crystals of FeSe to investigate the interplay between nematicity, orbital order and superconductivity.

*This work was supported by the National Science Foundation (NSF) under grant DMR-1845994.
**4:18PM J61.00006: Nematicity studied with strain-dependent ARPES**

HEIKE PFAU (Presenter), Advanced Light Source, Lawrence Berkeley National Laboratory, SU-DI CHEN, Geballe Laboratory for Advanced Materials, Department of Applied Physics, Stanford University, MING YI, Department of Physics and Astronomy, Rice University, MAKOTO HASHIMOTO, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, COSTEL R. ROTUNDU, Stanford Institute of Materials and Energy Science, SLAC National Accelerator Laboratory, JOHANNA PALMSTROM, Geballe Laboratory for Advanced Materials, Department of Applied Physics, Stanford University, TONG CHEN, PENG-CHENG DAI, Department of Physics and Astronomy, Rice University, JOSHUA A STRAQUADINE, ALEXANDER T HRISTOV, Geballe Laboratory for Advanced Materials, Department of Applied Physics, Stanford University, ROBERT J BIRGENEAU, Department of Physics, University of California, Berkeley, DONGHUI LU, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, IAN FISHER, ZHIXUN SHEN, Geballe Laboratory for Advanced Materials, Department of Applied Physics, Stanford University —

Nematicity is a phenomenon found in an increasing number of strongly correlated materials in close proximity to other quantum phases such as unconventional superconductivity. It is therefore important to understand its microscopic origin. The phase diagram of most iron-based superconductors contains a nematic phase. It breaks rotational symmetry and involves an in-plane anisotropy of lattice, spin and charge degrees of freedom. It is currently debated whether spin or orbital degrees of freedom are the driving force and whether there is a common microscopic mechanism in iron-based superconductors with and without magnetic order. We were able to combine angel-resolved photoemission spectroscopy (ARPES) with in-situ tuneable uniaxial strain and determine the momentum dependence of the nematic order parameter in FeSe and BaFe$_2$As$_2$. The order parameter has the same non-trivial symmetry in both compounds suggesting a universal behavior and a common microscopic mechanism.

*Supported by the U.S. Department of Energy, Office of Basic Energy Sciences; Humboldt Foundation; German Science Foundation*

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**4:30PM J61.00007: Unprecedented Optical Anisotropy in Optimally Doped Iron-Based Superconductor**

LEONARDO DEGIORGI, ANIRBAN PAL (Presenter), MANUEL CHINOTTI, ETH Zurich —

The divergent nematic susceptibility, obeying a simple Curie-Weiss power law over a large temperature interval, is empirically found to be a ubiquitous signature in several iron-based materials across their doping-temperature phase diagram. The composition at which the associated Weiss temperature extrapolates to zero is found to be close to optimal doping, boosting the debate to what extent nematic fluctuations contribute to the pairing-mechanism and generally affect the electronic structure of iron-based superconductors. Here, we offer a comprehensive optical investigation [1] of the optimally hole-doped Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$ over a broad spectral range, as a function of temperature and of tunable applied stress, which acts as an external symmetry breaking field. We show that the stress-induced optical anisotropy in the infrared spectral range is reversible upon sweeping the applied stress and occurs only below the superconducting transition temperature. These findings demonstrate that there is a large electronic nematicity at optimal doping which extends right under the superconducting dome.

4:42PM J61.00008: Strain effects in Fe-based superconductors: Nematicity, exotic magnetism and superelasticity*  
ROSER VALENTI (Presenter), VLADISLAV BORISOV, KARIM ZANTOUT, SANANDA BISWAS, STEPHEN WINTER, Goethe University Frankfurt — In this talk we will analyze the role of strain in some families of Fe-based superconductors. 
Via a combination of first principles-based calculations and many-body approaches we investigate nematicity, possible exotic magnetism and superelasticity in 122 and 1144 systems [1,2] and discuss possible origins of the discrepancy between ARPES measurements and electronic structure calculations in the nematic phase of FeSe [3] with the help of strain. This work is a collaboration with Paul Canfield, Seok-Woo Lee, Rafael Fernandes, Peter Hirschfeld and Brian Andersen.

[3] Zantout et al. (in preparation)

*We thank the Deutsche Forschungsgemeinschaft for financial support

4:54PM J61.00009: Bilayer Spliting and Unusual Superconducting Gap in KCa$_2$Fe$_4$As$_4$F$_2$ Superconductor with Double Fe$_2$As$_2$ Layers  
DINGSONG WU (Presenter), WENSHAN HONG, CHENGXIAO DONG, JIANGPING HU, SHILIANG LI, HUIQIAN LUO, LIN ZHAO, XINGJIANG ZHOU, Institute of Physics, Chinese Academy of Science, Beijing 100190, China — We report the first high resolution laser Angle-Resolved Photoemission Spectroscopy (ARPES) measurements on a newly discovered iron based superconductor, KCa$_2$Fe$_4$As$_4$F$_2$ (K12442) which has the K+-cations connecting double Fe$_2$As$_2$ layers separated by the insulating Ca$_2$F$_2$ block with a high TC of 34 K at stoichiometric composition. Total five hole like Fermi surfaces are clearly identified around Brillouin zone center Γ(0,0) point and four of them are possible from the bilayer splitting of two Fermi surfaces. A tiny electron like pocket is shown around M(±π,±π) points surrounded by four strong spots with their top just below Fermi level. All the hole like pockets around Γ(0,0) point exhibit nearly isotropic nodeless superconducting gap symmetry but with different gap sizes. Their gap sizes can neither be understood in the simple $|\cos(k_x)+\cos(k_y)|$ functional form due to the biggest gap size from one middle Fermi surface, nor be consistent with the so-called quasi-nesting between the Fermi pockets around Γ and M points because of mismatch of Fermi pocket size. Our observations provide new information and require new insight to understand the superconductivity mechanism in iron based superconductor.
5:06PM J61.00010: Pairing symmetry and capping layer influence of the superconductivity at FeSe/SrTiO$_3$ interface  YANAN LI (Presenter), TIMOTHY PILLSBURY, Pennsylvania State University, GRANT SMITH, ERZSEBET VINCENT, University of Chicago, ANTHONY R. RICHARDELLA, Pennsylvania State University, DAVID AWSCHALOM, University of Chicago, NITIN SAMARTH, Pennsylvania State University — Single unit cell FeSe films on SrTiO$_3$ have attracted growing attention due to the enhancement of the superconducting critical temperature ($T_c$) over its bulk value and the possibility of topological superconductivity. The pairing symmetry and mechanisms underlying the superconducting gap have been studied via angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling spectroscopy (STS). Here, we report the synthesis and characterization of ultrathin FeSe films grown on SrTiO$_3$ by molecular beam epitaxy. We gain insight into the symmetry of the gap by measuring the angular dependence of the in-plane critical magnetic field. Additionally, to understand the discrepancy between $T_c$ measured by in-situ techniques (such as STS and ARPES) and ex-situ transport, we investigate how $T_c$ is influenced by varying the capping layer and Fermi energy. Supported by the University of Chicago, the Vannevar Bush Fellowship, and 2DCC-MIP/NSF DMR-1539916.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J62 DMP: Excitons and Exciton Transport in Nanostructures

2:30PM J62.0001: Novel exciton transport in double-layer graphene structures*  JIA LI (Presenter), Brown University, YIHANG ZENG, Columbia University, XIAOXUE LIU, Brown University, QIANHUI SHI, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, JAMES C HONE, CORY DEAN, Columbia University — A spatially indirect exciton is created when an electron and a hole, confined to separate layers of a double quantum well system, bind to form a composite boson. A system of such excitons is demonstrated to host a Bose–Einstein condensate phase at low temperature, featuring dissipationless exciton flow and perfect Coulomb drag. In this talk, I will discuss novel exciton phases in various double-layer structures characterized by exotic transport properties. In double monolayer graphene, an insulating exciton phase is stabilized in the presence of large density imbalance. With increasing temperature, the insulating phase “melts” into an exciton superfluid exhibiting perfect Coulomb drag. In double bilayer graphene, Coulomb drag measurement reveals strong anisotropy in exciton flow when $n = 0$ and $n = 1$ orbitals states are degenerate in one of the layers. Along the easy direction, drag measurement is consistent with an exciton condensate, whereas an anomalous drag response is observed in the orthogonal direction. These exotic exciton phases are studied in a multidimensional phase space defined by a variety of experimental parameters available to double-layer structures, which provides insight into the nature of electron correlation and the resulting physical structures.

*A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490 and the State of Florida.
Tunable polarons in a carbon nanotube electromechanical resonator

SERGIO DE BONIS (Presenter), CHANDAN SAMANTA, WEI YANG, CARLES URGELL, ICFO-The Institute of Photonic Sciences, BILJANA STAMENIC, BRIAN THIBEAULT, ECE Department, UCSB, FABIO PISTOLESI, CNRS, LOMA, Universite Bordeaux, ADRIAN BACHTOLD, ICFO-The Institute of Photonic Sciences — We demonstrate the formation of polarons in a nanotube electromechanical resonator by increasing the effect of the electron-phonon interaction to an unprecedented level. The polaronic nature of charge carriers results in the reduction of the electrical conductance by up to about half its value. The electron-phonon interaction suppresses the resonance frequency of the fundamental phonon mode by up to 25%. Our device is in the so-called ultra-strong coupling regime, where the electromechanical coupling per phonon is one order of magnitude larger than the resonance frequency. Our work establishes nanotube resonator as a possible platform for the demonstration of mechanical quantum bits and the study of quantum interference effects in the movement of an object consisting of 10^5–10^6 atoms.

Optical transition dipoles in quasi-two dimensional semiconductor nanomaterials

XUEDAN MA (Presenter), Argonne Natl Lab — Optical transition dipole moment is the key parameter in determining the interactions between an optical emitter and external electromagnetic fields. Understanding and having control over the transition dipole moments could lead to optoelectronic and photonic devices with unprecedented performance.[1,2] Transition dipole moments of materials can vary significantly depending on the materials’ band structures and compositions. In this work, we investigate the intrinsic optical transition dipole moments in quasi-two dimensional semiconductor nanomaterials, namely semiconductor nanoplatelets and quantum rings, to understand the influence of geometry and electronic structures on the transition dipole moments. Combining advanced quantum optical microscopy techniques with empirical tight-binding theory, we reveal strikingly different optical transition dipole properties in the two types of structures,[3,4] indicating the importance of material geometry and electronic structures in determining the transition dipole moments.

References:
3. X. Ma et al. Nano Lett. 2018, 18, 4647-4652
**3:30PM J62.00004: True Bilayer Exciton Condensate of One-Dimensional Electrons**

ADRIAN KANTIAN (Presenter), Uppsala Univ — We theoretically predict that a true bilayer exciton condensate, characterized by off-diagonal long-range order and global phase coherence, can be created in one-dimensional solid state electron systems. The mechanism by which this happens is to introduce a single particle hybridization of electron and hole populations, which locks the phase of the relevant mode and hence invalidates the Mermin-Wagner theorem. Electron-hole interactions then amplify this tendency towards off-diagonal long-range order, enhancing the condensate properties by more than an order of magnitude over the noninteracting limit. We show that the temperatures below which a substantial condensate fraction would form could reach hundreds of Kelvin, a benefit of the weak screening in one-dimensional systems.


*We thank Nordita for support. D. S. L. A. thanks ERC Project No. DM-321031 for financial support.*

**3:42PM J62.00005: Can trions crystallize in TMDC monolayers?**

ROMAN KEZERASHVILI (Presenter), Physics Department, New York City College of Technology, CUNY — Positively and negatively charged trions in monolayers of transition metal dichalcogenides (TMD) are bound with binding energies of 20-30 meV [1]. Based on the existence of the trions in TMD monolayers, one can propose that a dilute gas of trions, as composite fermions, forms a 2D Wigner crystal. This is similar to the 2D Wigner crystal formed by a dilute system of electrons. The formation of 2D Wigner crystal of the dilute system of trions in TMD monolayers is studied. We show how the reduction of dimensionality affects the binding energy of trions and their crystallization in TMD monolayers. The 2D trion gas in TMD is described using a Charge-Charge, Charge-Exciton, Exciton-Exciton interactions based on the screened Coulomb interaction - Keldysh potential [2]. The formation of the 2D Wigner crystal in the dilute system of trions in TMD monolayers, when the average distance between the trions is much larger than the radius of each trion is predicted. It is shown that the critical density of the formation of the trion Wigner crystal is greater than the critical density of the electron Wigner crystal in the same material.


*The work is supported by the U.S. DOD Grant No. W911NF1810433*
Direct Visualization of Exciton Transport in Semiconductor Quantum Dot Nanostructures Using Time-Resolved Superresolution Microscopy*  

ALAN VAN ORDEN  
(Presenter), MEGAN DUNLAP, Department of Chemistry, Colorado State University, DUNCAN P. RYAN, PETER GOODWIN, JAMES WERNER, JENNIFER A HOLLINGSWORTH, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, MARTIN PAUL GELFAND, Department of Physics, Colorado State University — A time-resolved superresolution microscope to localize single emitters with nanometer precision and image their lifetimes with sub-nanosecond time resolution is described. This technique has been used to image semiconductor quantum dot (QD) nanostructures composed of single QD emitters that interact via resonance energy transfer. Photoemission from the nanostructures is imaged onto a 2x2 optical fiber array, and the fiber outputs are monitored using time-correlated single photon counting. The relative intensities reveal changes in the emission center as the QDs blink on and off. Emission centers separated by 10-nm or less can be distinguished based on changes in intensity and lifetime that occur when energy is transferred from donor to acceptor QDs. The distribution of centroid positions provide a direct visualization of the energy transport pathway through the nanostructure.

*This work was funded by the Los Alamos Laboratory-Directed Research and Development Exploratory Research Program (20180189ER) and performed, in part, at the Center for Integrated Nanotechnologies, a User Facility operated for the U.S. Department of Energy (DOE) Office of Science. AVO acknowledges the Los Alamos Institute for Materials Science for a Rapid Response grant. LA-UR-19-30557, unlimited release.

Electron-hole superfluidity controlled by a periodic potential in double layers of two-dimensional material*  

OLEG BERMAN  
(Presenter), ROMAN KEZERASHVILI, New York City College of Technology, YURI LOZOVIK, Institute of Spectroscopy, KLAUS ZIEGLER, University of Augsburg — We propose to control of electron-hole superfluidity in semiconductor coupled quantum wells and double layers of 2D material by an external periodic potential [1]. The latter can either be created by periodic gates attached to quantum wells or the double layers of 2D material or by the Moiré pattern of two twisted layers. Treating the electron-hole pairing within the mean-field approach, we apply the tight-binding approximation of the single electron spectrum and study the effect of the additional periodic potential on the electron-hole plasma-superfluid transition. The electron-hole pairing order parameter as a function of the temperature, the charge carrier density, and the gate parameters are obtained by minimization of the mean-field free energy. The second order phase transition between superfluid and electron-hole plasma, controlled by the external periodic potential, is studied for various parameters.


Exciton- and phonon-mediated electron ultrafast dynamics in semiconducting carbon nanotubes

STEFANO DAL FORNO (Presenter), MARCO BATTIATO, School of Physical and Mathematical Sciences, Nanyang Technological University — Semiconducting single-wall carbon nanotubes (SWCNTs) are ideal one-dimensional materials that have attracted much attention in the construction of novel optoelectronic devices. Their exceptional properties arise from the tunability of quantities such as chirality, twist angle and diameter. The understanding of scattering processes in CNTs is complex due to the non trivial interplay of different quasiparticles such as electrons, holes, phonons and excitons. In particular, due to the low dimensionality and the relatively high dielectric constant, excitons in SWCNTs possess very high binding energy and large spatial extent. It is therefore critical to model this theoretically hard problem to allow for the exploitation of CNTs properties in applications like low dimensional electronics or THz emission.

In this work we study the role of electron, hole, phonon and exciton coupling in (6,5) SWCNTs by theoretically modelling the experimental time-resolved absorption spectrum. We solve the full Boltzmann transport equation explicitly for high order scatterings and strongly out of equilibrium regimes. Our results show excellent agreement with experiments and show the capabilities of our newly developed numerical approach.

Electroluminescence from multi-particle exciton complexes in transition metal dichalcogenide semiconductors

MATTHIAS PAUR (Presenter), ADAY J. MOLINA-MENDOZA, Photonics Institute, TU Wien, RUDOLF BRATSCHITSCH, Institute of Physics and Center for Nanotechnology, University of Münster, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, THOMAS MUELLER, Photonics Institute, TU Wien — Light emission from higher-order correlated excitonic states has been recently reported in hBN-encapsulated monolayer WSe2 and WS2 upon optical excitation. These exciton complexes are found to be bound states of excitons residing in opposite valleys in momentum space, a promising feature that could be employed in valleytronics or other novel optoelectronic devices. However, electrically-driven light emission from such exciton species is still lacking. Here we report electroluminescence from bright and dark excitons, negatively charged trions and neutral and negatively charged biexcitons, generated by a pulsed gate voltage, in hexagonal boron nitride encapsulated monolayer WSe2 and WS2 with graphene as electrode. By tailoring the pulse parameters we are able to tune the emission intensity of the different exciton species in both materials. We find the electroluminescence from charged biexcitons and dark excitons to be as narrow as 2.8 meV.

*Nanyang Technological University, NAP-SUG grant.
4:42PM J62.00010: Strong plasmon coupling to high-energy band-nested excitons in 2D TMDCs

AARON ROSE (Presenter), JEREMY R. DUNKLIN, HANYU ZHANG, SANJINI U NANAYAKKARA, ELISA M MILLER, JAO VAN DE LAGEMAAT, National Renewable Energy Laboratory —

We show Rabi splitting of 244 meV at the C-exciton in the two-dimensional (2D) transition metal dichalcogenide (TMDC) MoS$_2$. The splitting is 9.5% of the transition energy (2.57 eV) in $k$-space (607 meV or 23.6% in $\theta$-space), which is ~2.5× the ratio observed in similar experiments at the A- and B-excitons and approaches the ultrastrong coupling limit. The large enhancement in the coupling strength is likely due to the nested conduction and valence bands found in the 2D TMDCs which leads to strong absorption. We measured the $k$-space dispersion of few-layer MoS$_2$ in a tunable plasmonic cavity at room temperature to observe the Rabi splitting. The band-nesting region of 2D TMDCs is under study for spontaneous charge-separation and slowed hot carrier cooling. Our observation suggests that strong coupling of the C-exciton in the 2D TMDCs may improve carrier lifetimes as well as enhance other quantum coherent phenomena such as polariton condensation or molecular hybridization for chemical reactions.

*Funding was provided by DOE Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, Solar Photochemistry Program.

4:54PM J62.00011: Study of exciton diffusion in carbon-nanotube thin-films

YICHEN LI (Presenter), SAMUEL W BELLING, AMIRHOSSEIN DAVOODY, IRENA KNEZEVIC, Electrical and Computer Engineering, University of Wisconsin-Madison —

Carbon nanotubes have attracted considerable attention for their potential use in organic thin-film photovoltaic devices. Given the fact that the exciton-transfer properties are directly related to improving the efficiency of these devices, it is crucial to develop a model of exciton diffusion in various carbon nanotube composites and study the diffusion mechanism. Here, we focus on the role of different properties of carbon nanotubes, including chirality and spacing, on exciton diffusion. We generate realistic nanotube meshes with different properties through which the motion of excitons is tracked using a Monte Carlo simulation. Finally, we compare the calculated exciton diffusion rate and diffusion length to experiment and develop an understanding of how different conditions of carbon nanotube aggregation affect diffusion properties.

*This work was supported by DOE BES, award DE-SC0008712.
5:06PM J62.00012: Electric Field Effect of $T_C$ in Thin Flakes of the Excitonic Insulator Ta$_2$NiSe$_5$$^*$

MICHAEL MASTALISH (Presenter), ARASH FEREIDOUNI, KRISHNA PANDEY, RABINDRA BASNET, JIN HU, HUGH CHURCHILL, Physics, Univ of Arkansas-Fayetteville — The layered, small-gap semiconductor Ta$_2$NiSe$_5$ is a prominent excitonic insulator candidate with a $T_C$ of 326 K. We investigated the electric field effect of the excitonic insulator transition temperature in a device fabricated with thin (15 nm) Ta$_2$NiSe$_5$. Flakes of Ta$_2$NiSe$_5$ were obtained by mechanical exfoliation and transferred onto narrow bottom gates insulated with Al$_2$O$_3$, and the Ta$_2$NiSe$_5$ was then contacted with Cr/Au. Measurements of source-drain current as a function of temperature revealed a small yet sharp drop in current near $T_C$. A modest, reproducible shift of $T_C$ by approximately 1 K was observed under a transverse electric field of +/- 0.5 V/nm. Future experiments with this and similar devices will probe the origin of this field effect on $T_C$, as well as the unexpected sign of the change in current at $T_C$.

*We acknowledge support from DOE award DE-SC0019467 and NSF award DMR-1851919.

5:18PM J62.00013: Potential gradient control of room-temperature triangular-whispering gallery polariton condensate$$^*$

HYUN GYU SONG (Presenter), SUNGHAN CHOI, CHUNG HYUN PARK, SU-HYUN GONG, CHULWON LEE, MIN SIK KWON, DAE GWANG CHOI, KIE YOUNG WOO, YONG-HOON CHO, KAIST — Exciton polaritons offer hybrid nature of excitons and photons, which are interactive quasi-particles providing the potential energy manipulation. Although wide bandgap semiconductors form room-temperature polaritons, the fabrication of homogeneous planar microcavities is challenging due to low refractive index contrast and large lattice misfit in III-nitride systems. Consequently, lateral localization of planar cavities by disorder (potential fluctuation and dephasing) hinder the establishment of ballistic extensions of polariton condensates, an essential factor for any quantum controls. We introduce a room-temperature polariton system with low disorder capable of one-dimensional (1D) ballistic extension. Selectively grown GaN wires reduce disorder in both excitons by dislocation bending and photons by crystallographically defined hexagonal facet. This high-quality wire allows us to form room-temperature triangular-whispering gallery polariton condensates with ballistic extension controlled by the optical potential gradient. The correlation between transport characteristics from momentum and real space offers a strong indication of ballistic transport in this 1D system.

1. H. G. Song et al, Optica 6, 1313 (2019)

*National Research Foundation of Korea (NRF2019R1A2B5B03070642).

Tuesday, March 3, 2020 2:30 PM - 5:18 PM

Session J63 DMP DCMP FIAP: Optical Probes and Imaging of Defects

High Ballroom 4D - Leora Dresselhaus-Cooper, Lawrence Livermore Natl Lab - Tag(s): Focus
Multi-modal microscopy and spectroscopy of wide band gap semiconductors

RACHEL OLIVER (Presenter), Materials Science and Metallurgy, University of Cambridge — The heart of materials science is the link between materials structure and properties. Traditionally, the small-scale structure of materials is often assessed using microscopy techniques, which may provide access to topography, crystallography, composition etc. The physical properties of material are more commonly assessed at a macroscopic level, often using spectroscopy techniques. Increasingly, however, advanced microscopes allow spectroscopy or other physical property measurements with nanoscale resolution.

One established technique that allows direct correlation of microscopy and spectroscopy is cathodoluminescence (CL) in the scanning electron microscope (SEM), in which the recombination of electron-hole pairs excited by the electron beam leads to emission of light that is collected and analysed spectroscopically. CL can be collected alongside structural/compositional data recorded in the SEM. This approach is often simply used for the collection of panchromatic CL images, mapping the total intensity of light emitted at each pixel. However, sophisticated CL systems allow not only the collection of time-integrated spectra, but also time-resolved measurements on the tens of picosecond timescale and data collection across a range of temperatures.

I will discuss the application of temperature- and time-dependent CL to a range of problems in wide-bandgap semiconductors, particularly defects and quantum wells in gallium nitride, addressing both the standard hexagonal form of this material and metastable cubic GaN. However, SEM only provides a limited subset of the structural information a materials scientist desires. Thus, I will introduce methods that allow different microscopy techniques to be brought to bear on exactly the same nanoscale structure, revealing more about its characteristics than any individual technique could achieve alone. In particular, I will discuss methods for combining SEM-CL with transmission electron microscopy, and scanning probe microscopy.

Far-infrared spectroscopy of shallow thermal donors and dilute impurities in high-purity silicon

VLADIMIR MARTINEZ (Presenter), DAVID BURNHAM TANNER, Department of Physics, University of Florida, Gainesville, FL, 32611, USA, RANA ADHIKARI, KOJI ARAI, AIDAN F BROOKS, CHRISTOPHER WIPF, LIGO, California Institute of Technology, Pasadena, CA 91125, USA — Silicon has uses as test-mass material for future gravitational-wave detectors and in high-resolution infrared spectroscopy in astronomy. The transparency of Si in the infrared region is critical to the effectiveness of these new devices. The temperature-dependent infrared transmission has been measured for high-purity silicon samples with impurity concentrations of \(\sim 10^{15}\) per cc. Measurements were made in a frequency range from 10–2000 cm\(^{-1}\) and temperatures from 10–300K. At 10 K, silicon is transparent in the far infrared (10–600 cm\(^{-1}\)) apart from narrow absorption lines caused by residual impurities. These absorption lines are mostly due to hydrogen-like transitions in donor and acceptor atoms as well as interstitial oxygen and will have a significant effect on the optimal operation of the Si device. At higher temperatures the electrons are ionized by the thermal energy in the crystal and become free elections, causing a Drude-like response in the far-infrared. Using the results of our transmission spectra, we can determine the type of impurities in the sample and their concentration.

*Supported by the NSF PHY-1707835 and PHY-0757058.
**3:18PM J63.00003: Multidimensional Coherent Spectroscopy of Erbium Doped GaAs Quantum Wells**  
ROBERT BOUTELLE (Presenter), TRAVIS AUTRY, RICHARD MIRIN, KEVIN SILVERMAN, National Institute of Standards and Technology Boulder — Rare-earth ions are appealing for a broad array of applications. When embedded in crystalline matrices, they combine well protected spin and optically active transitions which are useful to store and process quantum information. When doped in semiconductors, they have been intensely investigated as a new class of electrically active infrared-emitting materials. To better understand the interaction of rare-earth doping, we investigate the effect of dilute erbium doping in GaAs quantum wells. When doped into GaAs, the Er$^{3+}$ ion substitutes Ga$^{3+}$ forming ErAs, which is known to have “coupled” magnetic and electronic properties. As a magnetic material, there is a strong exchange coupling between the relatively large local moments of the 4f and valence and conduction electrons near the Fermi level. Using multidimensional coherent spectroscopy, we attempt to elucidate excited-state structure and interactions of the Er$^{3+}$ doping in GaAs at different doping concentrations. This spectroscopy can characterize excited state dynamics and interactions.

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**3:30PM J63.00004: Deep UV Photoluminescence and Chemical composition Analysis of Residual Impurities in Hexagonal boron nitride**  
NIKESH MAHARJAN (Presenter), Physics, Brooklyn College and the Graduate Center of CUNY, NEELAM KHAN, School of Science and Technology, George Gwinnett College, JAMES H. EDGAR, ELI JANZEN, Tim Taylor Department of Chemical Engineering, Kansas State University, MIM L NAKARMI, Physics, Brooklyn College and the Graduate Center of CUNY — Single crystal hexagonal boron nitride (h-BN) is an ultrawide (~6.0 eV) semiconductor under development for electronic, optoelectronic and nanophotonic devices. A key issue in these applications is the effect of impurities, especially oxygen, on its properties. Here the properties and compositions of h-BN and oxidized h-BN were compared. The deep UV photoluminescence spectra from h-BN samples were oxidized at 900 °C in dry and ambient air, had strong phonon-assisted band edge emissions along with a sharp atomic-like emission line at 4.09 eV, and its phonon replicas at 3.89 and 3.69 eV. The sharp emission line and phonon replicas were not observed in unoxidized sample. Comparative chemical composition analysis of the residual impurities was carried out using X-ray photoelectron spectroscopy (XPS) and time-of-flight secondary ion mass spectroscopy (TOF-SIMS) in order to identify the impurities related to the sharp transition. Our results of atomic like features could have potential applications in the solid-state single photon source for quantum information technologies.
3:42PM J63.00005: Independent determination of carrier densities and analysis of different recombination channels in GaAs PL and EL through Raman scattering of LO phonon – plasmon coupled mode*  
FAN ZHANG (Presenter), YONG ZHANG, Univ of North Carolina - Charlotte  
— Determining the carrier (electron) density $n$ is critical in many material and device characterization. An ABC model is widely used to describe the carrier recombination, where the contributions of non-radiative, radiative, and Auger recombination are partitioned, respectively, into the three terms in $R = A_n + B_n^2 + C_n^3$. In general, not only the partition is questionable, e.g., nonradiative contribution could be non-linear in $n$, but also a number of approximations are needed in order to determine $n$. It has been demonstrated recently that by combining photoluminescence (PL) and Raman imaging one can simultaneously obtain the spatial distribution of electron and hole density in a semiconductor material or device by first determining the electron density through Raman scattering of LO phonon – plasmon coupled (LOPP) mode [1]. This approach is extended to analyze carrier recombination processes in both PL and electro-luminescence (EL) with varying laser excitation and current injection level. The results indicate that nonradiative recombination typically exhibits non-linear dependence on $n$, as suggested by a recent analysis of EL in an InGaN LED [2].  
*ARO/Electronics (W911NF-16-1-0263)

3:54PM J63.00006: Understanding the Fluorescence Mechanism of Carbon Dots through Single-Molecule Excited-State Imaging*  
HUY NGUYEN (Presenter), University of Illinois at Urbana-Champaign, INDRAJIT SRIVASTAVA, Carle Illinois College of Medicine, JOSEPH W LYDING, University of Illinois at Urbana-Champaign, DIPANJAN PAN, Carle Illinois College of Medicine, MARTIN GRUEBELE, University of Illinois at Urbana-Champaign — We employed scanning tunneling microscopy (STM) and single molecule absorption STM (SMA-STM) to study the fluorescence mechanism in carbon dots (Cdots). The red- and blue-fluorescing Cdot samples were previously purified and characterized in bulk with standard spectroscopic techniques. Carbon dots were deposited on a thin hybrid PtAu film over a sapphire substrate via solvent-based aerosol deposition. We first performed current imaging tunneling spectroscopy (CITS) to resolve the spatial electronic structure of the adsorbed Cdots, estimating the quantity of defects, whether they were active or inactive as optical absorbers, and measuring energy levels of dopants. Then we applied SMA-STM to spatially resolve electronically excited defects, and used scanning tunneling spectroscopy (STS) in situ to look at the density of states at these locations during laser excitation and otherwise. We observed significant spatial variations in the band structure and detected increased defect quantity as fluorescence red-shifts. We further identified the energy levels involved in fluorescence and ultimately discuss the most plausible fluorescence mechanism, which does not depend on the size of the Cdot.  
*James R. Eiszner Chair in Chemistry.  
Ullyot and Sloan fellowships support Huy Nguyen.
Charge sensing in CMOS devices using reflectometry

JOFFREY RIVARD (Presenter), CLÉMENT GODFRIN, Institut quantique, Universite de Sherbrooke, Canada, ALEXEI ORLOV, Departement of Electrical Engineering, University of Notre-Dame, USA, EVA DUPONT-FERRIER, Institut quantique, Universite de Sherbrooke, Canada —

Spin qubits in silicon are great candidates for scalable quantum information processors due to their long coherence time and compatibility with industrial CMOS fabrication lines.[1] Usual spin-readout techniques imply spin-to-charge conversion and charge readout by transport measurement. This requires multiple leads and limits the scalability of the system. A solution is to do charge sensing using RF-reflectometry measurement[2] for which only one lead is necessary to control and read the qubit.[3] The critical part is to obtain an impedance matching, at low temperature, between the resonant circuit and the RF-line. Finding this matching condition can be challenging considering the temperature dependence of each of the tank circuit component and the sample-to-sample capacitance variability. A solution is to use a varactor[4] to adjust in situ the circuit impedance. In this talk, we report on optimization of reflectometry setups at low temperature and discuss the use of tunable capacitors for in situ tuning targeting high sensitivity RF-measurement for spin qubit readout.


Infrared Transmission of Ge:Mn Thick Films Prepared by Ion Implantation and Post-Annealing*

LAILA HASSAN OBIED, Brock University, SJOERD ROORDA, Physics, University of Montreal, SHENQIANG ZHOU, SLAWOMIR PRUCNAL, Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum, Dresden-Rossendorf, DAVID CRANDLES (Presenter), Brock University —

Approximately 3 micrometer thick Ge:Mn films were prepared by low temperature ion-implantation followed by post-annealing. XRD, SIMS, magnetometry and infrared transmission (100-6500 cm\(^{-1}\)) were used to characterize the films. The average Mn concentration in the amorphous implanted films is less than 0.3%. Annealing causes approximately 40-70% of Mn atoms to migrate to Mn-rich clusters or form Mn\(_5\)Ge\(_3\) while the remainder enters the Ge lattice and creates free holes. If annealed at high enough temperature the amorphous films become polycrystalline. Solid phase epitaxy does not occur. A Drude peak and structure in the mid-infrared absorption observed by infrared transmission provide evidence for free holes. The data suggest that the maximum solubility of Mn in Ge is less than 0.08 %.

*Work supported by NSERC and the Helmholtz-Gemeinschaft Deutscher Forschungszentren (HGF-VH-NG-713)
**4:30PM J63.00009: Photon Statistics as an Analytical Tool in Solid-State Defect Systems**

REBECCA FISHMAN (Presenter), RAJ PATEL, DAVID HOPPER, TZU-YUNG HUANG, LEE BASSETT, University of Pennsylvania — Photon correlation spectroscopy is a versatile and widely used analysis technique with a broad history of applications ranging from molecular spectroscopy to exploration of fundamental quantum mechanical concepts. More recently, this method has been used to study quantum emission from defect complexes in solid-state systems for a variety of quantum technological applications. The predominant use of photon statistics in solid-state systems is as an indicator of single-photon emission, a desirable property for applications such as quantum key distribution and quantum repeaters. However, a more thorough analysis of photon statistics offers the potential to reveal characteristics of the system such as electronic structure, multi-level optical dynamics, and responses to external fields. We briefly discuss the history and development of photon correlation spectroscopy as a measurement tool and outline methods for proper acquisition and analysis of photon statistics. In addition, we use this analysis framework to study quantum emitters in hexagonal boron nitride and discuss how these methods can allow the determination of their electronic structure and optical dynamics.

*This work was supported by the National Science Foundation under award DMR-1922278.

**4:42PM J63.00010: Spatiotemporal Microwave Imaging of Photo-carrier Dynamics in Monolayer Semiconductors**

ZHAODONG CHU (Presenter), CHUN YUAN WANG, JIAMIN QUAN, University of Texas at Austin, CHENHUI ZHANG, King Abdullah University of Science and Technology, CHAO LEI, University of Texas at Austin, ALI HAN, King Abdullah University of Science and Technology, XUEJIAN MA, University of Texas at Austin, HAO-LING TANG, King Abdullah University of Science and Technology, DISHAN ABEYSINGHE, MATTHEW STAAB, University of Texas at Austin, XIXIANG ZHANG, King Abdullah University of Science and Technology, ALLAN MACDONALD, University of Texas at Austin, VINCENT TUNG, King Abdullah University of Science and Technology, CHIH-KANG SHIH, XIAOQIN (ELAINE) LI, KEJI LAI, University of Texas at Austin — The spatiotemporal evolution of photo-generated charge carriers in two-dimensional transition-metal dichalcogenides (TMDs) plays a crucial role for their optoelectronic applications. A comprehensive understanding of such dynamics, however, remains a challenging task. Here, we report the simultaneous spatial and temporal photoconductivity imaging in WS$_2$ monolayers by laser-illuminated microwave impedance microscopy. The diffusion length and carrier lifetime were directly measured. Time-resolved experiments indicate that the critical process for photo-carriers is the escape of holes from defect-induced trap states, which prolong the apparent lifetime of mobile electrons in the conduction band. This work provides fundamental knowledge on the defect-mediated spatiotemporal dynamics of charge carriers in 2D TMDs, paving the way for their applications in novel optoelectronic devices.
4:54PM J63.00011: Photodegradation of Si-doped GaAs Nanowire*  ANA CLARA SAMPAIO PIMENTA (Presenter), Univ Fed de Minas Gerais, HENRIQUE LIMBORÇO, Microscopy Centre of UFMG, JUAN CARLOS GONZÁLEZ PÉREZ, NESTOR CIFUENTES TABORDA, Univ Fed de Minas Gerais, SÉRGIO LUÍS LIMA DE MORAES RAMOS, Centre for Nanomaterial technology and Graphene, FRANKLIN MASSAMI MATINAGA, Univ Fed de Minas Gerais — Researching optical effects in nanowires (NWs) may requires high pump intensity that under ambient conditions can degrade NWs due to thermal oxidation. In this work we investigated the photodegradation of a single Si-doped GaAs NW by laser heating in air. To understand the changes occurred on the NW we carried out scanning electron microscopy (SEM), and energy dispersive X-ray (EDS), micro-Raman (μ-RS), micro-photoluminescence (μ-PL) spectroscopies in laser damaged regions as well as in non-affected ones. From Stokes and anti-Stokes peaks we estimated that the oxidation process starts at 661 K, resulting in two new modes at 200 and 259 cm\(^{-1}\). SEM and EDS showed a significant loss of As in the oxidized regions, but no erosion of the NW. μ-PL showed the near-band-edge emission of GaAs along the NW, as well as a new emission band at 755 nm corresponding to polycrystalline β-Ga\(_2\)O\(_3\) formation. Our results also indicate that neither amorphous As, nor crystalline As, were deposited at the surface of the NW. Combining different experimental techniques, this study showed the formation of polycrystalline β-Ga\(_2\)O\(_3\) by oxidation of the NW surface and the limits to perform spectroscopic investigations on individual GaAs NWs under ambient conditions.

*This work was funded by CNPq, FAPEMIG and CAPES.

5:06PM J63.00012: Defect induced photoluminescence in SnO\(_2\) nanostructures: Evaluation and Utilization for optical sensing and waveguide application  BINAYA SAHU (Presenter), RABINDRANATH JUINE, ARINDAM DAS, Indira Gandhi Centre for Atomic Research — Despite having an excellent reputation in resistive sensing and profound optical properties, SnO\(_2\) is less explored for optical sensing and waveguide application. In the current project SnO\(_2\) quantum dots [QDs~2.4 nm] and 1D NSs [d~500nm], are utilized for photoluminescence (PL) based NH\(_3\) sensing and waveguide application respectively. PL spectra collected from SnO\(_2\) QDs using 325 nm excitation show the rise of peaks at 2.77 and 2.96 eV in the presence of NH\(_3\). Sensor response (R) is calculated in different concentrations of NH\(_3\), (10-500 ppm) using the formula \(R = (I_{\text{gas}}-I_0)/I_0\) [I\(_{\text{gas}}\) and I\(_0\), PL intensity in the presence and absence of NH\(_3\)]. Defects on the surface of QDs, supported by pre-edge SnM\(_5\) resonance peak in XAS spectrum collected from QDs, form energy band just above the valance band and causes diminished PL peak at 2.77 and 2.96 eV. During the interaction, NH\(_3\) provides electron to SnO\(_2\) and enhance 2.77 and 2.96 eV related transition. Room temperature NH\(_3\) detection with excellent selectivity and high recovery rate ensures the technical importance of this work. Further waveguide application using SnO\(_2\) 1D NSs is realized by exciting single 1-D NSs with 325 nm LASER. Optical images and PL spectra were captured to confirm the defect induced PL is guided through 1D NSs.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM
2:30PM J64.00001: Tuning the electronic and thermoelectric response of oxide superlattices by confinement, strain and interface polarity* [Invited] ROSSITZA PENTCHEVA (Presenter), Department of Physics, University of Duisburg-Essen — Transition metal oxides are prospective candidates for energy conversion applications e.g. as thermoelectrics owing to their chemical and thermal stability and in particular to their complex correlated nature. Nanostructuring and reduced dimensionality can lead to further performance enhancement. By combining DFT+U calculations and Boltzmann transport theory we explore the implications of interface polarity, confinement and strain on the thermoelectric properties of perovskite superlattices. Taking as an example LaNiO$_3$/SrTiO$_3$(001), we demonstrate that compatible n- and p-type materials can be realized by selective choice of the layer stacking at polar interfaces [1]. On the other hand, a strongly enhanced thermoelectric response is obtained in nonpolar LaNiO$_3$/LaAlO$_3$(001) superlattices due to the confinement-driven metal-to-insulator transition [2]. This concept is further extended to (SrXO$_3$)$_1$/(SrTiO$_3$)$_n$(001) SL with $X = V$, Cr, and Mn [3]. Last but not least, the thermoelectric response of topologically nontrivial phases is discussed.


*German Science Foundation CRC/TRR80, projects G3,G8.
A new method for heat to electricity conversion which takes advantage of the first order phase transformation of ferroelectric materials will be presented. Low temperature waste heat can be utilized with the proposed device in which a transfer of energy was successfully shown using a BaTiO$_3$ single crystal heated and cooled repeatedly through its phase transformation. [1] We use these results as a motivation for our discussion on the growth of ferroelectric thin films using the hybrid molecular beam epitaxy approach. High quality, epitaxial single crystal BaTiO$_3$ thin films were grown using this technique and showed a bulk-like phase transformation with thickness of 350 nm, an encouraging behavior for our device. By alloying with BaSnO$_3$, we also explore the BaTiO$_3$-BaSnO$_3$ system for its potential advantages for energy conversion including control over dielectric constant and Curie temperature. We will analyze structure and composition through high resolution x-ray diffraction and x-ray photoelectron spectroscopy as well discuss their effect on dielectric and ferroelectric properties.

3:18PM J64.00003: Artificial two-dimensional ferroelectric metal at room temperature*

MIKHAIL KAREEV (Presenter), Rutgers University, New Brunswick, YANWEI CAO, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, ZHEN WANG, Louisiana State University, SE YOUNG PARK, University of California Berkeley, Berkeley, YAKUN YUAN, Pennsylvania State University, XIAORAN LIU, Rutgers University, New Brunswick, SERGEY M NIKITIN, HIROFUMI AKAMATSU, Pennsylvania State University, DEREK MEYERS, Brookhaven National Laboratory, SRIMANTA MIDDEY, Indian Institute of Science, PAUL THOMPSON, European Synchrotron Radiation Facility, PHILIP RYAN, Argonne National Laboratory, PADRIAC SHAFER, ALPHA T. N’DIAYE, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, VENKATRAMAN GOPALAN, Pennsylvania State University, YIMEI ZHU, Brookhaven National Laboratory, KARIN M RABE, JAK CHAKHALIAN, Rutgers University, New Brunswick — Polar metals, commonly defined by the coexistence of polar crystal structure and metallicity, are thought to be scarce because the long-range electrostatic fields are expected to be fully screened by the conduction electrons of a metal. Moreover, reducing from three to two dimensions, it remains an open question whether a polar metal can exist. Here we report on the realization of a room temperature two-dimensional ferroelectric metal in a tri-color superlattice BaTiO3/SrTiO3/LaTiO3. A combination of advanced probes and DFT calculations have revealed the microscopic mechanisms of unusual periodic electric polarization, charge distribution, and orbital symmetry. Our results provide a route to create all-oxide artificial non-centrosymmetric quasi-two-dimensional metals with exotic quantum and topological states including potentially coexisting ferroelectric, ferromagnetic, and superconducting phases.

*This work was supported by the Gordon and Betty Moore Foundation EPiQS Initiative (GBMF4534).

3:30PM J64.00004: Tuning the correlation strength via cation order in double perovskites*

TURAN BIROL (Presenter), ARPITA PAUL, University of Minnesota — \( \text{A}_2\text{BB'O}_6 \) double perovskites often behave very differently than their parent compounds. This can lead to phenomena such as frustrated magnetism or half metallicity, which are often driven by inter-cationic charge transfer. In this talk, we study the V-Nb double perovskites, where V and Nb ions attain different valences despite coming from the same column in the periodic table. By performing first principles Density Functional Theory + Dynamical Mean Field Theory (DFT+DMFT) calculations, we show that the interplay of cation order and this charge transfer affect the electronic structure of \( \text{Sr}_2\text{VNB'O}_6 \) in a very interesting way, and gives rise to a phase diagram that includes correlated Hund's metallic, as well as Mott insulating phases.

*This work was supported by the National Science Foundation through the UMN MRSEC under DMR-1420013.
Ferroelectric Polarization Induced Magnetic Order and Topological Hall Effect at the PbZr$_{0.2}$Ti$_{0.8}$O$_3$/SrIrO$_3$ Heterointerface* LE ZHANG (Presenter), Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln, MYUNG-GEUN HAN, YIMEI ZHU, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln — The 5$d$ Iridate SrIrO$_3$ (SIO) is a paramagnetic semimetal with strong spin-orbit coupling (SOC) when prepared in the orthorhombic phase. In this study, we explore the possibility of inducing magnetic order and nontrivial chiral spin structures in ultrathin SIO films using the polarization field of a neighboring ferroelectric layer. We have fabricated high quality epitaxial PbZr$_{0.2}$Ti$_{0.8}$O$_3$ (PZT)/SIO (1.6-2 nm) heterostructures and demonstrated nonvolatile ferroelectric field-effect modulation of channel resistance. For the 1.6 nm SIO channel, we can reversibly control SIO between the metallic and insulating phases by switching the polarization field of PZT. More interestingly, in the insulating phase, the Hall effect measurements reveal features of hysteresis and topological Hall effect, suggesting a polarization-induced antiferromagnetic order. We ascribe it to the emerging interfacial Dzyaloshinskii–Moriya interaction due to strong SOC and polarization-enhanced inversion symmetry breaking. Our results demonstrate a feasible way to achieve electrically controlled magnetic order and design topological electronics at the heterointerface of complex oxides.

*This work was primarily supported by NSF under Award No. DMR-1710461.

Charge Engineering in Nickelate-based Mott Transistors Gated by Ferroelectrics* YIFEI HAO (Presenter), XUEGANG CHEN, LE ZHANG, XIA HONG, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska - Lincoln — We present a comprehensive study of ferroelectric-gated Mott transistors based on high quality epitaxial heterostructures composed of a ferroelectric Pb(Zr,Ti)O$_3$ (PZT) gate and a correlated oxide RNiO$_3$ ($R = \text{La, Nd, Sm}$) channel. For single layer nickelate channels, including Sm$_{0.5}$Nd$_{0.5}$NiO$_3$, NdNiO$_3$ (NNO), and LaNiO$_3$ (LNO), the resistance switching ratio $\Delta R/R_{\text{on}}$ increases exponentially with decreasing channel thickness until it approaches the electrical dead layer thickness, with the maximum $\Delta R/R_{\text{on}}$~194% observed in 1 nm LNO channel. Inserting a La$_{1-x}$Sr$_x$MnO$_3$ (LSMO) buffer layer results in up to two orders of magnitude increase in $\Delta R/R_{\text{on}}$ for devices with the same total channel thickness, with the maximum $\Delta R/R_{\text{on}}$ reaching 1,225% in the NNO/LSMO channel. The giant enhancement is attributed to the interfacial charge transfer effect between RNiO$_3$ and LSMO, which effectively reduces the carrier density in the active channel. Our studies address the key materials challenges that limit the application potential of epitaxial complex oxide-based field effect transistors.

*This work was supported by NSF Grant No. DMR-1710461 and SRC under GRC Task Number 2831.001.
Spin-dependent charge transport in crystalline BaTiO$_3$-germanium tunnel junctions* YICHEN JIA (Presenter), CHARLES H AHN, FREDERICK J WALKER, Yale University — The epitaxial integration of functional oxides on conventional semiconductors using advanced molecular beam epitaxy opens new opportunities for coupling their unique properties with semiconductors for post-CMOS computing paradigms. Here we measure spin-dependent transport in Permalloy-BaTiO$_3$-Ge tunnel junctions using the three-terminal Hanle technique. We show that the aligned conduction bands at the epitaxial BaTiO$_3$-Ge interface allow controllable charge transport between quantum tunneling and trap-assisted conduction through an external bias. In the quantum tunneling region, we observe a negative magnetoresistance with a full width at half maximum of ~100 mT when an external magnetic field is applied perpendicular to the BaTiO$_3$-Ge interface. The negative magnetoresistance evolves into a superposition of two peaks with opposite polarity and distinct linewidth when the trap-assisted conduction becomes dominant. Possible mechanisms include a spin-dependent transport model involving defect states in the heterostructure. The correlation between charge transport and magneto-resistive response is the basis of a sensitive technique to measure defects in oxide semiconductor heterostructures.

*Y.J. acknowledges partial support from the James Kouvel Fellowship Fund.

In plane strained Barium Titanate thin films directly integrable on Silicon* MARC REYNAUD (Presenter), Department of Physics, University of Texas at Austin, PEI-YU CHEN, Department of Chemical Engineering, University of Texas at Austin, SUNAH KWON, Department of Materials Science and Engineering, University of Texas at Dallas, BRYCE EDMONSON, Department of Chemical Engineering, University of Texas at Austin, MOON KIM, Department of Materials Science and Engineering, University of Texas at Dallas, JOHN G. EKERDT, Department of Chemical Engineering, University of Texas at Austin, AGHAM POSADAS, ALEXANDER DEMKOV, Department of Physics, University of Texas at Austin — Integrating ferroelectric materials onto Si is a critical part of the design new photonic devices such as optical modulators and switches. However, a difficult question to answer thus far has been how to optimize the crystalline orientation in these materials. One interesting material is Barium Titanate (BTO), because it exhibits the largest known Pockels effect which is the modulation of the refractive index by an electric field. However, many applications and device geometries require BTO with the polarization pointing in plane with the substrate, but so far it has proven difficult to optimize BTO to maximize in plane domains. Here, we present a method for the growth of single crystal BTO films that are entirely in plane and strain tunable. In this study, we use extensive X-ray characterization, TEM imaging and direct measurement of the Pockels coefficient in these films to show that the films are entirely in plane oriented BTO. This provides a method for high quality in plane oriented BTO to be directly integrated on Silicon.

*This work was funded by the Air Force Office of Scientific Research under Grant FA9550-18-1-0053.
Switching Rashba spin texture via interface with a ferroelectric compound*  XIAOLI ZHANG (Presenter), CARLOS MERA, ALEX ZUNGER, University of Colorado, Boulder — We study the microscopic factors controlling the switching of a Rashba(R) spin texture by switching the ferroelectric (FE) polarization of an underlying FE substrate. The spin polarization (SP) in R band depends on the direction of the intrinsic R electric dipole. Thus, an electric field changing the ferroelectric polarization should be able to reverse the Rashba SP. We study a heterojunction between FE PbTiO$_3$ (with TiO2 layers termination), and a R film of Pt, Pb, Rh, Ir, Au and Ag. We determine the role of FE slab thickness, passivation and atom relaxation on both the creation of R bands and SP switching. The FE polarization up (down) corresponds to the structural configuration with Ti above (below) O. Therefore, the R material, mainly interacts with Ti (O) for polarization up (Down). The R material then receives (donate) electrons for polarization up (down). Since Ti and O atoms mainly form the conduction and valence bands, respectively, we find that for up (down) polarization, R bands appear at the conduction (valence) bands. We find these R bands exhibit opposite helical spin texture for opposite ferroelectric polarization directions, allowing the possibility of control the SP direction with electric fields with an external electric field.

*Supported by NSF-DMR-CMMT.

Reversal of Tunneling Electroresistance in Ferroelectric Tunnel Junctions by Interface Engineering  MING LI (Presenter), LINGLING TAO, EVGENY Y TSYMBAL, University of Nebraska - Lincoln — A ferroelectric tunnel junction (FTJ) consists of two metal electrodes separated by a nm-thick ferroelectric barrier which allows quantum-mechanical tunneling through it. A tunneling electroresistance (TER) effect is a sizable change in resistance of a FTJ with reversal of ferroelectric polarization. Depending on the energy alignment between electrodes and barrier, the tunneling conductance can be dominated by either electrons or holes. For electron (hole) tunneling, the Fermi energy lies closer to the conduction band minimum (valence band maximum) of the barrier. Low (high) resistance is achieved when polarization is pointing to the electrode with longer screening length for electron (hole) tunneling, referred to as positive (negative) TER. In this work, using density functional theory calculations, we demonstrate the crossover between the electron-like and hole-like tunneling in a practical FTJ La$_{1-x}$Sr$_x$MnO$_3$/BaTiO$_3$/Pt with positive (La$_{1-x}$Sr$_x$O)$_{1-x}$/TiO$_2$ and negative (MnO$_2$)$_{x-1}$/BaO interface terminations. The positively (negatively) charged interface pulls down (up) the electrostatic potential energy at the interface and thus shifts Fermi energy of La$_{1-x}$Sr$_x$MnO$_3$ closer to the conduction band minimum (valence band maximum) of BaTiO$_3$, leading to positive (negative) TER.
**4:54PM J64.00011: Effect of Strain and Doping on the Magnetoelectric Coupling at LSMO/PZT Multiferroic Interfaces: An Ab Initio Study**  
KRISHNA ACHARYA (Presenter), IGOR VASILIEV, New Mexico State Univ — The magnetic properties of multiferroic materials can be controlled by the applied electric field. We apply *ab initio* methods based on density functional theory (DFT) to study the influence of strain on the magnetoelectric coupling at the (0,0,1) interface between PZT (PbZr$_{0.2}$Ti$_{0.8}$O$_3$) and LSMO at two different doping levels (La$_{0.5}$Sr$_{0.5}$MnO$_3$ and La$_{0.8}$Sr$_{0.2}$MnO$_3$). The effects of strain are modeled by applying a ±1%, uniaxial strain in the direction orthogonal to the LSMO/PZT interface. Our calculations show that the magnetic properties of the LSMO layer are strongly influenced by both the doping concentration and the applied uniaxial strain. The results of our study are consistent with the available experimental data.

**5:06PM J64.00012: Effect of confinement and octahedral rotations on the electronic, magnetic, and thermoelectric properties of Sr$X$O$_3$/SrTiO$_3$(001) superlattices, ($X$ = V, Cr, and Mn)*  
MANISH VERMA (Presenter), BENJAMIN GEISLER, ROSSITZA PENTCHEVA, Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — Transition metal oxides are an attractive class of materials for thermoelectric applications due to their chemical and thermal stability and environmental friendliness. Here we explore the effect of confinement and octahedral rotations on the electronic and thermoelectric properties of (Sr$X$O$_3$)$_1$/SrTiO$_3$$_n$(001) ($X$ = V, Cr, and Mn; n = 1, 3) superlattices by combining *ab-initio* simulations including an on-site Coulomb repulsion term and Boltzmann theory. We find that in the ground state, the superlattices always display finite octahedral rotations, which drive an orbital reconstruction and metal-to-insulator transition in SrVO$_3$ and SrCrO$_3$ single layers with ferro- and antiferromagnetic spin order, respectively. On the other hand, SrMnO$_3$ based superlattices exhibit antiferromagnetic spin order along with bulk-like properties. We show that tuning the quantum confinement plays an important role in improving the thermoelectric performance in these superlattices and the estimated electronic power factors compare favorably with some of the best performing transition metal oxide thermoelectrics.


*Funding by the DFG within CRC/TRR80 (G3 and G8) and computational time on LRZ supercomputer (pr87ro) are acknowledged.*
5:18PM J64.00013: Depth-resolved electronic structure of a BiFeO$_3$/La$_{0.7}$Sr$_{0.3}$MnO$_3$ superlattice investigated by standing-wave hard X-ray photoemission spectroscopy (SW-HXPS)  
HENRIQUE MARTINS (Presenter), University of California, Davis, ALEXANDER GRAY, Temple University, GIUSEPPINA CONTI, Materials Sciences Division, LBNL, INNA VISHIK, University of California, Davis, SLAVOMIR NEMSAK, Advanced Light Source, LBNL — Studies of artificially designed interfaces of transition metal oxide heterostructures enable opportunities to engineer new stable phases of matter, leading to novel complex devices. However, it is a challenge to identify the features in the electronic structure that induce these emergent interfacial phenomena. Here we have studied a prototypical ferroelectric/ferromagnetic interface between two perovskite oxides, BiFeO$_3$ and La$_{0.7}$Sr$_{0.3}$MnO$_3$, by Bragg-reflection standing-wave hard X-ray photoemission spectroscopy (SW-HXPS). The superior depth precision of the SW-HXPS provides information on interfacial and “bulk” signals, and it allows us to identify the character of the interfacial features in the electronic structure in correlation with the detailed depth information on chemical states.

* This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0014697.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J65 DMP: Semiconductors, Superconductors, and Molecular Qubits Mile High Ballroom 4F - Han Htoon, Los Alamos Natl Lab - Tag(s): Focus

2:30PM J65.00001: Magnetoelectric behavior in metal-organic complexes including spin crossovers compounds [Invited] VIVIEN ZAPF (Presenter), National High Magnetic Field Lab, Los Alamos National Lab — We explore metal-organic complexes that show unconventional routes to magnetoelectric behavior. Traditionally, magnetoelectric behavior has been most commonly studied in inorganic oxides, where ferro or antiferromagnetism couples to dielectric or ferroelectric properties. Such coupling allows an electric field to control and switch e.g. a quantum magnetic state or vice versa. This field contains a wealth of intriguing fundamental science, as well as applications being targeted in ultra-low power sensing, qubits, memories, tunable antennas, and other devices. In this talk I will review several of our recent efforts to extend this field of magnetoelectrics to metal-organic complexes, which contain transition metal ions and organic ligands. These compounds tend to have soft lattices that mediate magnetoelastic coupling, and a broad array of intriguing forms of magnetism going beyond (anti) ferromagnetism. I will begin with spin crossovers where the spin state of a transition metal ion changes with applied magnetic fields, thereby modifying the electric polarization. I will show results on Mn-based spin crossovers where magnetic fields toggle the spin state and thereby induce structural phase transitions or Jahn Teller effects. These structural changes result in very strong magnetoelastic coupling as well as complex phase diagrams. I will also discuss metal-organic frameworks that are effectively intrinsic heterostructures where magnetic and electric properties can be combined with flexible architectures. I will review the state of this nascent field and potential new directions.
On-chip Integrable Highly Spectrally Uniform Ordered Semiconductor Quantum Dot Single Photon Source Arrays for Scalable Quantum Optical Networks

JIEFEI ZHANG (Presenter), SWARNABHA CHATTARAJ, Univ of Southern California, SIYUAN LU, IBM Thomas J. Watson Research Center, ANUPAM MADHUKAR, Univ of Southern California — Scalable optical networks demand ordered and spectrally uniform single photon source (SPS) array integrable on-chip with photon manipulating units. Recently we demonstrated such SPSs based on a new class of spatially ordered and spectrally uniform InGaAs/GaAs mesa top single quantum dots (MTSQDs) [1,2] that are readily integrable, on-chip, with dielectric light manipulating units (LMUs) [1,3] based on 2D photonic crystal platform or collective Mie-like resonance of dielectric building block based metastructures. These MTSQDs have single photon emission purity > 99% ($g^{(2)}(0)<0.02$) at 9.4K [2]. The spectral uniformity of the nominally In$_{0.5}$Ga$_{0.5}$As MTSQD array is ~8nm limited by alloy fluctuation, but importantly reveal pairs of MTSQDs emitting within 300μeV [1,3]. In this talk we report studies on binary InAs/GaAs MTSQD in 5X8 arrays demonstrating striking spectral uniformity of 1.8nm (<2meV) over 1000um$^2$ area. The results highlight the potential of the spatially-ordered MTSQDs-LMU integrated system for realizing quantum optical circuits [3].


Funded by AFOSR (FA9550-17-01-0353) and ARO (W911NF-19-1-0025)

Fused LiNbO$_3$-(Al)GaAs hybrids for quantum dots optomechanics

EMELINE NYSTEN (Presenter), Lehrstuhl für Experimentalphysik I, Augsburg University, YONG-HENG HUO, Division of Quantum Physics and Quantum Information, University of Science and Technology of China, HAILONG YU, GUO-FENG SONG, Nano-Optoelectronics Laboratory, Chinese Academy of Sciences, ARMANDO RASTELLI, Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, HUBERT KRENNER, Lehrstuhl für Experimentalphysik I, Augsburg University — Surface acoustic waves (SAW) are a useful tool to control the emission of quantum dots (QDs). In particular, SAWs enable the injection of charge carriers into the dot or the modulation of their energy levels [1,2,3]. Here, we explore the possibility to enhance the interaction between the SAW and the QDs by transferring them on a strong piezoelectric LiNbO$_3$ substrate by epitaxial lift-off [4]. By employing multiharmonic transducers, we generate SAWs on LiNbO$_3$ over a wide range of radiofrequencies. We monitor their coupling to and propagation across the semiconductor membrane, both in the electrical and optical domain. We demonstrate the enhanced optomechanical tuning of the embedded QDs with increasing frequencies. This effect is verified by finite element modelling of our device geometry and attributed to an increased localization of the acoustic field within the semiconductor membrane [5]. The results of our study clearly show the large potential of our hybrid platform to integrate complex phononic and optomechanical circuitry with integrated QDs to study sound-matter coupling.

**3:30PM J65.00004: Optomechanical single photon frequency division multiplexing**

MATTHIAS WEISS (Presenter), Augsburg University, DANIEL WIGGER, Münster University, MAXIMILIAN NÄGELE, Augsburg University, KAI MÜLLER, JONATHAN J. FINLEY, Walter Schottky Institute, TU Munich, T. KUHN, Münster University, PAWEL MACHNIKOWSKI, Wroclaw University of Science and Technology, HUBERT KRENNER, Augsburg University — Here we report on the implementation of a hybrid nonlinear optomechanical scheme to generate frequency multiplexed of single photons from a single quantum dot. To this end, the excitonic optical transition of a single semiconductor quantum dot (QD) is coherently driven by a laser with a frequency of approximately 330THz and simultaneously dynamically strained by a surface acoustic wave (SAW) in the low GHz regime. The coherent optomechanical interaction caused by the QD mixes optical and acoustic frequencies, resulting in the generation of a frequency comb. Thus the collected resonance fluorescence signal, consisting of single photons, is emitted into these frequency bins, precisely split by the frequency $\omega_{\text{SAW}}$ of the SAW.

Furthermore the nonlinear interaction between two mutually coherent SAWs with frequencies $\omega_{\text{SAW}}$ and $2\omega_{\text{SAW}}$ allow for the intensity modulation of certain teeth of the comb. The probability of a single photon being emitted in a given frequency bin can be programmed, by the relative phase between the two SAWs. Introducing a frequency detuning of 50μHz between the two SAWs an intensity modulation of the teeth of the frequency comb with a period of approximately 5½ hours can directly be observed, verifying the extraordinary stability of our scheme.

**3:42PM J65.00005: Tailoring Nanoscale Crystal Polytype Selection for Quantum Confinement Engineering**

HONGLING LU (Presenter), SAMAN MONIRI, CALEB REESE, SUNYEOL JEON, ADAM KATCHER, TYLER HILL, HUI DENG, RACHEL GOLDMAN, Univ of Michigan - Ann Arbor — Electrically-controlled and integrable single photon sources are essential components of quantum information systems. Although semiconductor quantum dots (QDs), including InGaN/GaN QDs-in-nanowires, are promising for room temperature applications, their scalability is limited by alloy composition fluctuations. Here, we aim to create alloy-fluctuation-free QD arrays, namely poly-type QDs-in-NWs, using self-catalyzed NW growth at vapor-liquid-solid (VLS) triple-junctions. We demonstrate, for the first time, epitaxy of GaN NW ensembles and films with a significant ZB content on Si(001). In addition to presenting our novel two-step molecular-beam epitaxy (TS-MBE) approach to control Si$_x$N$_y$ layer formation and subsequent GaN phase selection, we reveal new insight into the relative roles of surface and step-edge diffusion on film to nanowire transitions. The NWs exhibit remarkable photoluminescence (PL) characteristics consisting of distinct emission from donor-acceptor pairs (DAP) and excitonic transitions related to both ZB and WZ GaN. This first demonstration of epitaxial growth and PL emission from ZB GaN NWs on Si(001) provides a crucial step toward the realization of GaN QDs-in-NWs for single photon emitters.

*National Science Foundation grant No. DMR-1120923.
3:54PM J65.00006: Multiferroic triangular molecular qubits*  MARK PEDERSON (Presenter), Physics, University of Texas, El Paso, CARLO M CANALI, FHOKRUL ISLAM, Department of Physics and Electrical Engineering, Linneaus University, ALEXANDER I JOHNSON, Physics, Central Michigan University — The frustrated triangular single molecule magnets with half integer spins from an important class of molecular magnets that have potential application as qubits in quantum computing. The lack of inversion symmetry allows these molecular qubits to be manipulated by an external electric field. Among several candidate triangular molecules, Fe$_3$O(NC$_5$H$_5$)$_3$(O$_2$CC$_6$H$_5$)$_6$ molecular cation is particularly exciting since to date this is the only molecule in which the spin-electric coupling effect is observed experimentally. In this work, using standard density-functional methods, we demonstrate that the spin-electric behavior of this molecule could be even more interesting as there are energetically competitive reference states associated with both high and low local spins (S=5/2 vs. S=1/2) on the Fe$^{3+}$ ions. Each of these spin structures allow spin-electric coupling in their respective chiral ground states. The presence of nearly degenerate reference states, composed of high-spin and low-spin centers, is of potential interest for quantum sensing applications. In this talk we will also discuss the possibility of inducing spin-crossover between the low and high spin configurations by an external electric field.

*Supported by UTEP, Texas STARS, Swedish Research Council & Carl Tryggers Stiftelse.

4:06PM J65.00007: Supercurrent in All-Van-der-Waals Josephson Tunnel Junction*  QING LI (Presenter), Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, JOEL WANG, Research Laboratory of Electronics, Massachusetts Institute of Technology, MEGAN YAMOAH, DENIS BANDURIN, Department of Physics, Massachusetts Institute of Technology, DAVID K KIM, ALEXANDER MELVILLE, JONILYN YODER, Massachusetts Institute of Technology (MIT) Lincoln Laboratory, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, WILLIAM OLIVER, Research Laboratory of Electronics, Massachusetts Institute of Technology — Superconducting quantum circuits have demonstrated tremendous progress over the past decade. However, current state-of-art of superconducting qubits still suffer strongly from dielectric two-level-systems (TLS), a major cause of qubit decoherence. Further advancement of qubit lifetime ultimately requires material and fabrication improvements that reduce TLS loss. In this work, we construct superconducting quantum devices with van der Waals (vdW) materials and their heterostructures, which feature crystalline layers with atomically precise interface. We fabricate high-quality, all-vdW parallel-plate capacitors and Josephson junctions – two key components in superconducting qubits. We then characterize the dielectric loss of the vdW capacitors and measure the Josephson response of the vdW tunnel junctions. We expect the advent of vdW qubits will enable both high coherence and small form factors.

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Shadow lithography for in-situ growth of generic semiconductor/superconductor devices  DAMON CARRAD (Presenter), MARTIN BJERGFELT, THOMAS KANNE NORDQVIST, Center for Quantum Devices, University of Copenhagen, MARTIN AAGESEN, Danish Defense Research Center, FILIP KRIZEK, Center for Quantum Devices, University of Copenhagen, ELISABETTA FIORDALISO, DTU Nanolab, Technical University of Denmark, ERIK JOHNSON, Department of Mechanical Engineering, Technical University of Denmark, JESPER NYGÅRD, THOMAS SAND JESPERSEN, Center for Quantum Devices, University of Copenhagen — Current progress in Majorana and Andreev qubits and devices using semiconductor/superconductor nanowires is built on the hard proximity-induced superconducting gap obtained from epitaxial indium arsenide/aluminium interfaces. Devices are conventionally obtained by selectively etching superconductor segments from the semiconductor. However, this is currently only possible for InAs/Al hybrids, excluding the use of potentially more desirable materials (e.g. Nb, InSb) in functional devices. Here, we present a crystal growth platform based on three-dimensional structuring of growth substrates for synthesising semiconductor nanowires with in-situ patterned superconductor shells. The shadow lithography platform enables independent choice of material since etching is no longer required, and is highly flexible with regard to device geometry. We grow and characterise tunnel probe devices, Josephson junctions and Majorana islands using aluminium, niobium, tantalum and vanadium. The devices exhibit increased yield and electrostatic stability compared to etched devices, which we attribute to the obviation of damaging etch processes. The shadow lithography platform promises high yield, stable, reproducible Majorana devices using the best possible materials.

Engineered Chirality of One-Dimensional Nanowires* MEGAN BRIGGEMAN (Presenter), JIANAN LI, Physics and Astronomy, University of Pittsburgh, MENGCHEN HUANG, Physics, University of California-Santa Barbara, HYUNGWOO LEE, JUNG-WOO LEE, CHANG-BEOM EOM, Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Physics and Astronomy, University of Pittsburgh — Quantum transport in 1D geometries is fascinating in its own right, but it can also be regarded as a building-block for creating and exploring a variety of quantum systems. We have developed a flexible platform for creating 1D nanostructures at the LaAlO$_3$/SrTiO$_3$ interface using a conductive atomic force microscope lithography technique. Straight nanowire segments behave as electron waveguides with subband occupation that can be tuned with a gate and an external magnetic field. We can periodically perturb this waveguide, with 10 nm periodicity, to yield a chiral nanowire which exhibits striking oscillatory transmission as a function of both magnetic field and chemical potential. We discuss these results in terms of an engineered axial in-plane spin-orbit interaction within the spiral electron waveguide. These findings represent an important advance in the ability to design new families of quantum materials with emergent properties, and mark a milestone in the development of a solid-state 1D quantum simulation platform.

**4:42PM J65.00010: InSb Nanostructures for Advanced Quantum Devices**  GHADA BADAWY (Presenter), SASA GAZIBEGOVIC, PHILIPP LEUBNER, Eindhoven University of Technology, FRANCESCO BORSOI, TU Delft, SEBASTIAN HEEDT, Microsoft Corp Delft, JIE SHEN, TU Delft, FOLKERT DE VRIES, ETH Zurich, SEBASTIAN KOELLING, Eindhoven University of Technology, MARCEL VERHEIJEN, Eurofins, LEO P KOUWENHOVEN, Microsoft Corp Delft, ERIK BAKKERS, Eindhoven University of Technology — Indium-antimonide (InSb) nanowires (NWs) constitute a suitable platform for hosting Majorana zero modes, a key requirement for fault-tolerant topological quantum computing, due to their high electron mobility and strong spin-orbit coupling. Building devices based on InSb nanostructures, while maintaining their pristine quality has proven to be rather challenging. Firstly, brought forth by the difficulties to obtain high quality nanostructures and secondly due to the fabrication steps required to transform a single nanostructure into a working device.

Here, we show the growth of pure zinc blende InSb NWs and nanosheets. The high chemical purity of these nanostructures is reflected in the higher electron mobility values as compared to so far reported values for InSb nanostructures. Further, we use the high degree of control over growing both 1-dimensional (1D) and 2-dimensional (2D) nanostructures on the same substrate, to design *in-situ* quantum device structures. In particular, by relying on both InSb NWs and nanosheets to shadow deposit superconductors and normal metals we design a variety of devices ranging from Josephson Junctions to hybrid superconductor/semiconductor devices, while circumventing the harsh processing steps which degrade the device quality.

**4:54PM J65.00011: InSbAs two-dimensional electron gases as a platform for topological superconductivity**  CHRISTIAN MOEHLE (Presenter), CHUNG-TING KE, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, CANDICE THOMAS, Department of Physics and Astronomy and Station Q Purdue, Purdue University, MARIO LODARI, GIORDANO SCAPPUCCI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, SAURABH KARWAL, QuTech and Netherlands Organization for Applied Scientific Research (TNO), SARA METTI, CHARLES R. GUINN, Department of Physics and Astronomy and Station Q Purdue, Purdue University, RAY KALLAHER, GEOFFREY C. GARDNER, Microsoft Quantum at Station Q Purdue, Purdue University, MICHAEL MANFRA, Department of Physics and Astronomy and Station Q Purdue, Purdue University, SRIJIT GOSWAMI, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Majorana zero modes, the fundamental building blocks of topologically protected qubits, can be realized in semiconductor-superconductor hybrid systems. Two-dimensional electron gases (2DEGs) with strong spin-orbit coupling offer a scalable platform for Majorana devices. Here, we investigate a new 2D hybrid system consisting of ternary InSbAs 2DEGs with epitaxially grown aluminum. Studying Josephson junctions in these systems allows us to estimate a large induced gap (200 μeV) and high interface transparencies (≈0.9). Furthermore, through weak anti-localization and quantum Hall measurements, we show that InSbAs has exceptionally strong spin-orbit interaction and a g-factor comparable to pure InSb. This unique combination of properties make InSbAs/Al 2DEGs a promising platform to study topological superconductivity.
5:06PM J65.00012: Stable quantum dots in an InSb two-dimensional electron gas  IVAN KULESH (Presenter), CHUNG-TING KE, Delft University of Technology, CANDICE THOMAS, Purdue University, SAURABH KARWAL, Netherlands Organization for Applied Scientific Research (TNO), CHRISTIAN MOEHLE, Delft University of Technology, SARA METTI, RAY KALLAHER, GEOFFREY C. GARDNER, MICHAEL MANFRA, Purdue University, SRIJIT GOSWAMI, Delft University of Technology — Indium antimonide (InSb) two-dimensional electron gases (2DEGs) have a unique combination of material properties: high electron mobility, strong spin-orbit interaction, large Landé g-factor, and small effective mass. This makes them an attractive platform to explore a variety of mesoscopic phenomena ranging from spintronics to topological superconductivity. However, there exist limited studies of quantum confined systems in these 2DEGs, often attributed to charge instabilities and gate drifts. We overcome this by removing the δ-doping layer from the heterostructure, and induce carriers electrostatically. This allows us to perform the first detailed study of stable gate-defined quantum dots in InSb 2DEGs. We demonstrate two distinct strategies for carrier confinement and study the charge stability of the dots. The small effective mass results in a relatively large single particle spacing, allowing for the observation of an even-odd variation in the addition energy. By tracking the Coulomb oscillations in a parallel magnetic field we determine the ground state spin configuration and show that the large g-factor (∼30) results in a singlet-triplet transition at magnetic fields as low as 0.3 T.

5:18PM J65.00013: Electron-phonon coupling in nitride superconductors from first principles: The effect of epitaxial strain and nitrogen concentration on superconducting properties*  BETUL PAMUK (Presenter), GURU KHALSA, Cornell University — The recent all-epitaxial integration of NbN superconductors with the III-Nitride family of semiconductors by molecular beam epitaxy has created an opportunity for scalable, integrated semiconductor/superconductor devices with access to industrial fabrication processes [Nature 555, 183–189 (2018)]. NbN has a large superconducting critical temperature ($T_c$) that makes it a useful superconducting component at liquid helium temperature, but its structural, metallic, and superconducting properties are extremely sensitive to growth conditions and nitrogen concentration. Group IV-B Nitrides (Ti, Zr, Hf) are chemically more stable than NbN, but their $T_c$’s are markedly smaller. Can the recent demonstration of epitaxial integration of transition metal nitrides with III-Nitrides be used as a strategy for tailoring their superconducting properties?

Using first-principles approaches we explore the effect of epitaxial strain and nitrogen concentration on Group IV-B Nitride superconducting properties. We find that both epitaxial strain and nitrogen concentration can drastically alter the electron-phonon coupling and potentially increase $T_c$ to temperature ranges sensible for superconducting devices.

*NSF PARADIM: DMR-1539918
ONR (monitored by Dr. Paul Maki)
Session J66 DCMP: The Superconductor-Insulator Transition: Beyond Universal Scaling

2:30PM J66.00001: Collapse of the Cooper pair phase coherence length at a superconductor-to-insulator transition* [Invited] SHAWNA HOLLEN (Presenter), Univ of New Hampshire — The superconductor-to-insulator transition (SIT) in quasi-2D thin films now serves as a canonical quantum phase transition (QPT). However, variation in its features between different material systems continues to raise perplexing questions about universality and universality classes in QPTs. A key to understanding the different manifestations of SITs has been through experimental probes of microscopic transport mechanisms. In this talk, I will present transport experiments on two morphologies of amorphous Bi quench-condensed films patterned with a nanohoneycomb array of holes, where the holes provide an embedded probe of local phase coherence. Films with smooth, nano-scale undulations in thickness exhibit a bosonic insulating phase that includes a giant magnetoresistance peak. In contrast, films of uniform thickness exhibit a fermionic insulating phase. The distinct phases are supported by the presence or absence of magneto-resistance oscillations that occur when Cooper pairs are phase coherent over a scale similar to the spacing of the nanohoneycomb array. These data provide a microscopic view of locally phase coherent Cooper pairs, confirm the existence of the bose insulator, and distinguish two classes of disorder-tuned SITs.

*This work was supported by the AAUW, the NSF through Grant No. DMR-0605797 and No. DMR-0907357, by the AFRL, and by the ONR.

3:06PM J66.00002: Experimentally observed magnetic-field driven quantum phase transition in superconducting nanowires and its striking agreement with critical theory.* [Invited] ANDREY ROGACHEV (Presenter), University of Utah — We have discovered that a magnetic-field driven quantum phase transition (QPT) in MoGe superconducting nanowires can be fully explained by the pair-breaking critical theory with exponents $\nu=1$ and $z\approx 2$. We find that in the quantum critical regime, the electrical conductivity is in agreement with a theoretically predicted scaling function and, moreover, that the theory quantitatively describes the nonuniversal dependence of conductivity on the critical temperature, field magnitude and orientation, nanowire cross-sectional area, and microscopic parameters of the nanowire material. Our data analysis is very different from what was used in the past for QPT in superconducting films: (i) we have subtracted contribution of normal electrons, both Drude and quantum corrections, and found that QPT occurs only in the superconducting part of the system, (ii) we also have kept the critical exponents fixed to their theoretical values and not varied them in the scaling procedure. In the second part of the talk, we will briefly comment on reliability of the finite-size scaling analysis and present our work-in-progress on QPT in MoGe films. In these films we have not observed the bosonic “strange metal” phase. However, we have found some evidences of a pair-breaking QPT that occurs at about 0.1 of quantum conductance of Cooper pairs.

*This research was supported in part by the National Science Foundation under award numbers DMR-1611421 and DMR-1553991 and by the ERC Grant QUEST number 637815.
Theory of the pair-breaking quantum phase transition in superconducting nanowires* [Invited]  ADRIAN DEL MAESTRO (Presenter), Physics, University of Vermont, FRÉDÉRIC GAY, BENJAMIN SACÉPÉ, Univ. Grenoble Alpes, Institut Néel, ANDREY ROGACHEV, Physics, University of Utah — We present a theoretical description of a zero temperature phase transition between superconducting and diffusive metallic states in ultra thin wires induced by Cooper pair-breaking perturbations. Fluctuation corrections to BCS theory motivate a dissipative field theory that can be used to compute the universal scaling of the electrical and thermal conductivity in the quantum critical regime. In the large-N limit, we obtain predictions for transport in striking agreement with recent experimental measurements of the fluctuation conductivity of metallic nanowires in parallel and transverse magnetic fields. The ability to quantitatively describe the experiment goes beyond the usual scaling approach and validates the underlying pair-breaking mechanisms near the quantum phase transition. Extensions of the theory including the effects of disorder and higher dimensions are considered, with implications for the interpretation of transport measurements in superconducting films.

*This research was supported in part by the National Science Foundation under award numbers DMR-1611421 (A.R.) and DMR-1553991 (A.D.) and by the ERC Grant QUEST number 637815 (B.S.).

Low-temperature anomaly in disordered superconductors near $B_{c2}$ [Invited]  BENJAMIN SACEPE (Presenter), Institut Neel, CNRS Grenoble — Strongly disordered superconductors in a magnetic field display many characteristic properties of type-II superconductivity --except at low temperatures where an anomalous linear T-dependence of the resistive critical field $B_{c2}$ is routinely observed. This behavior violates the conventional theory of superconductivity, and its origin remains a long-standing puzzle. In this talk I will present systematic measurements of the critical magnetic field and current on disordered superconducting films of various levels of disorder. Surprisingly, our measurements show that the $B_{c2}$ anomaly near zero-temperature is accompanied by a clear mean-field like scaling behavior of the critical current. Our experimental findings together with theoretical considerations on the inherent vortex-glass state and its thermal fluctuations enable to explain the linear-T anomaly to occur in films as well as bulk superconductors with a slope that depends on the normal-state sheet resistance, in full agreement with the data.
4:54PM J66.00005: Quasiparticle screening near a bosonic superconductor-insulator transition revealed by magnetic impurity doping* [Invited] JAMES VALLES (Presenter), Brown University — While bosonic superconductor-insulator transitions (SIT) have been clearly observed in a number of thin film systems, the mechanisms driving the Cooper pair localization remain to be established. These SITs feature thermally activated Cooper pair transport in the insulating phase with an activation energy $T_0$ that grows continuously from zero at the critical point. Some models attribute this behavior to disorder effects that give rise to Anderson localization of Cooper pairs while others invoke Coulomb interaction effects that drive a Mott transition. I will describe experiments on ultrathin, nanoporous $\alpha$-Bi films that focus on how $T_0$ depends on the pairbreaking effects induced by magnetic impurity doping. I will discuss how the data provide strong evidence that the bosonic SIT in thin films is a Mott transition driven by Coulomb interactions that are screened by virtual quasi-particle excitations[1]. The dependence of these SITs on on underlying fermionic degrees of freedom distinguishes them from those occuring in micro-fabricated Josephson Junction Arrays, cold atom systems, and likely in high temperature superconductors with nodes in their quasiparticle density of states.

Work done in collaboration with: Xue Zhang, James Joy, Wu Chunshu, and Jimmy Xu

*We are grateful for the support of NSF Grant No. DMR-1307290

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J67 DCMP: Correlations and Topology in Moiré Superlattices
Four Seasons 2-3 - Pablo Jarillo-Herrero, Massachusetts Institute of Technology MIT - Tag(s): Invited

2:30PM J67.00001: Correlated electronic states and Fermi surface topology in flat-band graphene layers* [Invited] EVA ANDREI (Presenter), Rutgers University, New Brunswick — Stacking two-dimensional atomic crystals, or applying a spatially periodic potential can radically change their electronic properties. In particular, it is possible to engineer conditions leading to the creation of extremely narrow energy, flat bands, where the quenched kinetic energy facilitates the emergence of correlated electronic states. This talk will highlight two examples where the electronic ground state and Fermi surface topology depend sensitively on the filling of the flat bands: stacked graphene layers$^{1,2}$ with a relative twist angle close to a magic value of $\sim 1^\circ$, and buckled graphene layers in which a periodically modulated pseudo-magnetic field creates flat electronic bands.


*Support through NSF-DMR 1708158 and DOE-FG02-99ER45742 is gratefully acknowledged.
Until recently, flat bands were achieved as Landau levels at high magnetic field. Recently, Pablo Jarillo-Herrero of MIT and coworkers demonstrated flat minibands in graphene-based superlattices, discovering correlated insulators and superconductors at different fillings. We have now discovered dramatic magnetic states in such systems. Specifically, in magic-angle twisted bilayer graphene also aligned with a hexagonal boron nitride (hBN) cladding layer, we observe a giant anomalous Hall effect and signs of chiral edge states. This all occurs at zero magnetic field, near 3 electrons per moire cell in the conduction miniband [1]. Remarkably, the magnetization of the sample can be reversed by applying a small DC current. Although the anomalous Hall resistance is not quantized, and dissipation is significant, we suggest that the system is an incipient Chern insulator, similar to an integer quantum Hall state. In a different superlattice system, ABC-trilayer graphene aligned with hBN, again near 3 electrons per moire cell a Chern insulator emerges [2]. A magnetic field of order 100 mT is needed to quantize the anomalous hall signal. This trilayer system can be tuned in-situ to display superconductivity instead of magnetism [3]. We will discuss possible magnetic states, and complementary probes to examine which state actually emerges as the ground state in each system.


*This research was primarily supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under contract DE-AC02-76SF00515.
In moire narrow band systems, periodic interlayer interactions can be used to engineer isolated superlattice bands in which the Coulomb interaction is comparable to the bandwidth. As in a Landau level, this leads to electron interaction dominated physics despite the low density of electrons, enabling full density control using electrostatic gates. Unlike Landau levels, however, moire flat bands occur under time reversal symmetric conditions. I will discuss experiments that observe the spontaneous breaking of time reversal symmetry in twisted bilayer graphene, observed as magnetic hysteresis. Remarkably, hysteresis is accompanied by a quantized anomalous Hall effect, persisting to zero magnetic field and elevated temperatures. I will discuss the origins of this effect in the spontaneous orbital polarization of the electron system into a single, topological nontrivial superlattice band, and show magnetic imaging data acquired using nanoSQUID on tip microscopy that confirms the orbital character of the magnetism and reveals mesoscopic domain dynamics.
Mapping the twist-angle disorder and unconventional Landau levels in magic angle graphene

The emergence of flat electronic bands and of the strongly correlated and superconducting phases in twisted bilayer graphene crucially depends on the interlayer twist angle upon approaching the magic angle $1.1^\circ$. Although advanced fabrication methods allow alignment of graphene layers with global twist angle control of about $0.1^\circ$, little information is currently available on the distribution of the local twist angles in actual magic angle graphene (MAG) transport devices. Here we map the local variations in hBN encapsulated devices with relative precision better than $0.002^\circ$ and spatial resolution of a few moiré periods. Utilizing a scanning nanoSQUID-on-tip, we attain tomographic imaging of the Landau levels in the quantum Hall state in MAG, which provides a highly sensitive probe of the charge disorder and of the local band structure determined by the local twist angle [1]. We find a correlation between the degree of twist angle disorder and the quality of the MAG transport characteristics. However, even state-of-the-art transport devices, exhibiting pronounced global MAG features, such as multiple correlated insulator states, high-quality Landau fan diagrams, and superconductivity, display significant variations in the local with a span that can be close to $0.1^\circ$. Devices may even have substantial areas where no local MAG behavior is detected, yet still display global MAG characteristics in transport. The derived maps reveal substantial gradients and a network of jumps. We show that the twist angle gradients generate large unscreened electric fields that drastically change the quantum Hall state by forming edge states in the bulk of the sample, and may also significantly affect the phase diagram of correlated and superconducting states. The findings call for exploration of band structure engineering utilizing twist-angle gradients and gate-tunable built-in planar electric fields for novel correlated phenomena and applications.

4:54PM J67.00005: Theory of flat bands, correlated insulators and superconductivity in graphene Moire heterostructures [Invited]  ESLAM KHALAF (Presenter), Harvard University — The remarkable discovery of correlated insulating behavior and superconductivity in twisted bilayer graphene (TBG) inspired a vast theoretical and experiment effort to (i) understand the origin of this behavior including the nature of symmetry breaking and the mechanism of the superconductivity and (ii) find similar systems which share some of its interesting properties while differing in some details leading to a wider range of possible phases. The purpose of this talk is to present some recent works contributing to the progress on these two fronts. In regards to (i), we will present an exhaustive discussion of possible mean field symmetry broken states in TBG [1]. By highlighting the existence of a hidden approximate symmetry in the model, we will identify a manifold of low-energy states whose competition is settled by small symmetry breaking terms and present numerical results supporting this argument. Furthermore, we will discuss their possible experimental signatures and comment on their compatibility with different experiments. Regarding (ii), we will discuss a related Moire system, twisted double bilayer graphene (TDB), which was recently synthesized experimentally [2] and shown to exhibit correlated insulating behavior and spin-triplet superconductivity. We will show the results of a thorough analysis of its band structure, correlated insulating state and superconducting phase which compare favorably with experimental findings [3].


Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J68 DBIO: Theory Meets High-Precision Biology: Emergent Simplicity in Stochastic Organismal Dynamics  Four Seasons 4 - Srividya Iyer-Biswas, Purdue Univ - Tag(s): Invited

2:30PM J68.00001: Johan Paulsson Invited Talk [Invited] —
3:06PM J68.00002: Self-driven phase transitions in living matter [Invited]  JOSHUA SHAEVITZ  
(Presenter), Princeton University — The soil dwelling bacterium *Myxococcus xanthus* is an amazing organism that uses collective motility to hunt in giant packs when near prey and to form beautiful and protective macroscopic structures comprising millions of cells when food is scarce. I will present an overview of how these cells move and how they regulate that motion to produce different phases of collective behavior. Inspired by recent work on active matter and the physics of liquid crystals, I will discuss experiments that reveal how these cells generate nematic order, how defect structure can dictate global behavior, and how Myxo actively tune the Péclet number of the population to drive a phase transition from a gas-like flocking state to an aggregated liquid-droplet state during starvation.

3:42PM J68.00003: Stochastic intergenerational cell size homeostasis: Precision measurements, exact kinematics and emergent simplicities [Invited]  SRVIDYA IYER-BISWAS  
(Presenter), Purdue Univ — In this talk I will first establish that intergenerational bacterial cell size homeostasis is maintained under appropriate growth conditions, using our high-precision data on growth and division of individual *C. Crescentus* cells. Next, the emergent simplicities revealed by these data. To conclude, a theoretical framework consistent with observed scaling laws, sans fitting parameters, which captures the exact kinematics of stochastic intergenerational cell size homeostasis.

4:18PM J68.00004: Jamming and dynamic arrest in sheltered microbial communities* [Invited]  
OSKAR HALLATSCHEK (Presenter), University of California, Berkeley — Microbes often colonize spatially-constrained habitats, such as pores in the skin or crypts in the colon. The resulting micro-communities are often stable and contribute to the genetic diversity and function of our microbiomes. It is, however, unclear how spatial constraints influence microbial community assembly. By monitoring and modeling microbial populations under controlled microfluidic confinement, we find a rich spectrum of dynamical patterns that are controlled by the competition between density-dependent outflow and population growth. Our results show that density-dependent passive diffusion can drive a reproducing population to a jamming threshold. The resulting loss of mixing and intra-species competition controls the resilience and evolution of these sheltered communities.

*Simons Investigator award from the Simons Foundation (#327934)  
National Institute Of General Medical Sciences of the National Institutes of Health (#R01GM115851)
How cell growth triggers cell division

JAN SKOTHEIM (Presenter), EVGENY ZATULOVSKIY, SHICONG XIE, SHUYUAN ZHANG, MARDO KOIVOMAGI, BENJAMIN REYES TOPACIO, DANIEL BERENSON, Stanford University — Cell size is fundamental to function in different cell types across the human body because it sets the scale of organelle structures, biosynthesis, and surface transport. Tiny lymphocytes squeeze through tight spaces to reach sites of infection, while the four orders of magnitude larger oocyte divides without growth to form the ~100 cell pre-implantation embryo. Despite the vast size range across cell types, cells of a given type are typically uniform in size because cells accurately couple cell growth to division. While some genes affecting cell size have been identified, the molecular mechanisms through which cell growth drives cell division had remained elusive. While it was expected that growth would act to increase the activities of the cyclin-dependent kinases (Cdk) known to promote cell division, this is not the case. Rather, we found that cell growth acts in the opposite manner. Cell growth triggers division by diluting proteins that inhibit cell division, Whi5 in yeast, and the retinoblastoma tumor suppressor Rb in human cells. Thus, inhibitor dilution provides one long sought mechanism coupling cell growth to cell division.

Tuesday, March 3, 2020 2:30 PM - 5:30 PM

Session J70 DPOLY DSOFT GSNP DFD: 3D Printing of Polymers and Soft Materials II

208 - Jinhye Bae, University of California, San Diego - Tag(s): Focus

2:30PM J70.00001: BREAK —

3:06PM J70.00002: Printing direction dependent microstructures in direct ink writing
LEANNE FRIEDRICH (Presenter), MATTHEW BEGLEY, University of California, Santa Barbara — Direct ink writing (DIW) can be combined with external fields to enable deposition of composite filaments with designed microstructures. Using acoustophoresis, we establish a narrow distribution of microparticles at the center of a direct write nozzle. In low-viscosity shear thinning inks, the particle distribution shifts and widens after deposition depending on the printing direction. We use particle image velocimetry and digital image analysis to characterize the flow field and particle distributions in the printed filament as a function of printing direction. We propose an analytical model for diagnosing sources of printing direction-dependent flows and particle distributions. Sources include anisotropy of the particle distribution in the nozzle, an asymmetric inertial disturbed zone near the nozzle, reshaping of a fluid-like square filament, rotation of a solid-like square filament, and printer calibration. Using the model, we propose strategies for mitigating or amplifying direction-dependent microstructures obtained via direct ink writing. The analytical model can also be adapted to similar direct-write applications to diagnose sources of direction dependence of printed microstructures.
3:18PM J70.00003: Polymer Network Formation in Epoxy-Acrylate Dual-Cure Thermoset Resins for Direct Ink Write Additive Manufacturing* LEAH APPELHANS (Presenter), JESSICA KOPATZ, JACLYNN UNANGST, Organic Materials, Sandia National Laboratory, ADAM COOK, DEREK REINHOLTZ, Advanced Materials Laboratory, Sandia National Laboratory — Dual-cure thermoset resins have been studied for many years for applications in adhesives and coatings. More recently dual-cure approaches have elicited interest for application to additive manufacturing methods such as stereolithography (SLA) and direct-ink-write (DIW). Development of methods to additively manufacture thermoset resins will enable additive approaches for a broad scope of materials including structural materials and advanced composites. The development of a dual-cure epoxy-acrylate thermoset resin for direct-ink-write AM will be described and the effect of resin composition and cure profiles on polymer network formation and final mechanical properties explored. Initial studies on the use of functionalized fillers as network crosslinkers will also be described.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

3:30PM J70.00004: Understanding the structure-property relationships of nanostructured epoxy inks for direct ink writing DEBORAH LIU, GAVIN DONELY, SIMON A ROGERS, DANIEL KROGSTAD (Presenter), University of Illinois at Urbana-Champaign — Direct ink writing (DIW) figures to be an important additive manufacturing technique in the future due to the wide variety of the materials that can be printed including polymers, hydrogels, nanocomposites and ceramic/metal slurries. Rather than material limitations, the main limitations are imposed by the rheological requirements of the inks – they need to behave as solids with no shear applied, yet readily flow when pressure is applied during the printing process. Over the last few years, we have been studying the structure-property relationships of nanostructured, 3D printable epoxy inks. Nanostructure has been imparted to the inks through the use of block copolymer micelles and/or inorganic nanoparticles. In this presentation, we will discuss how these nanostructures affects the rheology and the printability of the inks as well as the epoxy crosslinking kinetics.

3:42PM J70.00005: Chemical Approaches to Diversifying the 3D Printing Ecosystem [Invited] ANDREW BOYDSTON (Presenter), University of Wisconsin - Madison — Our research team focuses on discovering and developing new chemistry for additive manufacturing that can be integrated with cutting-edge engineering technologies. We place emphasis on: 1) incorporation of functional materials, particularly those that respond via conversion of mechanical force into chemical reactivity; 2) expansion of the materials space available for AM; and 3) selective multi-material printing from “all-in-one” mixed-resin vats. As a representative example, we will discuss progress toward simultaneous photo-radical/photo-cationic printing mechanisms for production of multimaterial parts.
**4:18PM J70.00006: 3D Control of Properties in Single-Material Digital Stereolithography for the Treatment of Growth Plate Injury**  
ASAIS CAMILA UZCATEGUI (Presenter), Materials Science and Engineering, University of Colorado, Boulder, CALLIE I. HIGGINS, National Institute of Standards and Technology, JOHN HERGERT, ARCHISH MURALIDHARAN, Materials Science and Engineering, University of Colorado, Boulder, JASON KILGORE, National Institute of Standards and Technology, STEPHANIE J. BRYANT, ROBERT R. MCLEOD, Materials Science and Engineering, University of Colorado, Boulder — A predominant challenge in tissue engineering is the need of a technique for producing structures with precise three-dimensional control of mechanical properties. We use pediatric physeal tissue engineering as a model application because damaged cartilage within the physis (growth plate) can lead to bone formation and asymmetric growth arrest. The growth plate has three distinct zones where cells evolve differently depending on the chemical and mechanical environment. Here, we present the first demonstration of micron scale 3D control of mechanical properties using a single cytocompatible material. Our findings indicate that the mechanical and chemical properties of materials patterned using stereolithography can be programmed by a model that accounts for the non-reciprocal relationship between intensity, time and conversion. In this work we use a poly(ethylene glycol) diacrylate based hydrogel to implement a step function and a gradual change in mechanical properties in 3D scaffolds. The model is validated by a novel application of atomic force microscopy. As a proof of concept, pillar structures were implanted into a rabbit model of physeal injury and there was an apparent reduction in bony bar reformation after 8 weeks of implantation.

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**GAANN,NSFGRFP, NIH1R01AR069060,R21HD090696**

**4:30PM J70.00007: Cure Depth Effects on Photopolymer Reactivity in Stereolithography 3D Printing**  
ANNA SMALLWOOD (Presenter), RYKELLE B. ADLEY, CAIUS J. JACOTT, CHANG RYU, Chemistry and Chemical Biology, Rensselaer Polytechnic Institute — The quality of 3D printed polymers produced by stereolithography (SLA) 3D printing depends heavily on the characteristics of the liquid photopolymer resin. Layer delamination may occur if a resin reacts too quickly upon UV irradiation, resulting in a failed print. Monomer conversion upon UV irradiation will be minimal if a resin reacts too slowly, which leads to the same result. Several characteristics of SLA resins show an ideal range within which print conditions are optimal. Resin characteristics may be tuned within this zone to achieve consistent 3D printing and desirable mechanical properties. These characteristics include monomer conversion, rate of polymerization, and photopolymerization onset time as a function of curing depth. This study seeks to investigate the effect of photoinitiator concentration on these characteristics. Resin reactivity will be monitored via real-time Fourier infrared spectroscopy by attenuated total reflectance (RT-FTIR ATR). Two photoinitiators will be employed as an additive to a commercial SLA resin and the reactive species in an original resin. A monochromatic UV LED will be employed at varying intensity as the UV source. Prints will be attempted with varying photoinitiator content and mechanical properties will be studied by tensile testing.
4:42PM J70.00008: Design and Fabrication of 3D Printed Polymer Composites using Grayscale Stereolithography  JOHN HERGERT (Presenter), ASAIS CAMILA UZCATEGUI, ARCHISH MURALIDHARAN, ROBERT R. MCLEOD, University of Colorado, Boulder — Polymer composites are fabricated using stereolithography by spatially modulating the intensity of light used to fabricate a part with regions of varying crosslinking density. A second polymer is preferentially in-swollen into the printed part where crosslinking density is low, thus forming a 3D printed composite with regions of varying stiffness. The initial part is printed using rubbery poly(ethylene glycol) diacrylate which is later swollen with acrylamide. The acrylamide monomer is polymerized to form an interpenetrating network that is glassy in regions where the acrylamide volume fraction is sufficiently high. A deterministic model for polymer conversion in the printing process is utilized to inform printing conditions such that final composite properties can be predicted. This model is validated using confocal Raman microscopy to independently resolve the local concentration of the two polymers throughout the composite.

4:54PM J70.00009: WITHDRAWN ABSTRACT —

5:06PM J70.00010: Theory and Implementation of Volumetric 3D Printing*  CHARLES RACKSON (Presenter), University of Colorado, Boulder, MAXIM SHUSTEFF, Center for Engineered Materials and Manufacturing, Lawrence Livermore, ROBERT R. MCLEOD, University of Colorado, Boulder — We discuss Volumetric 3D Printing, a type of additive manufacturing in which 2D patterns of light are projected into a rotating volume of photosensitive polymer material. The temporally-separated, spatially-overlapping patterns crosslink the material, resulting in an arbitrary (to within voxel resolution) 3D distribution of conversion within the material. We describe theoretical limitations to the method, experimental implementation, and how the coupling of optics and materials informs system design. Polymer design requirements such as viscosity and absorptivity are reviewed, as well as optical requirements including wavelength choice, brightness, and speckle mitigation.

*Funding provided by Lawrence Livermore National Laboratory
Stiffness can mediate the balance between hydrodynamic forces and avidity to impact the targeting of flexible polymeric nanoparticles in flow*  

SAMANEH FAROKHIRAD (Presenter), Department of Mechanical and Industrial Engineering, New Jersey Institute of Technology, ABHAY RANGANATHAN, Department of Anesthesiology and Critical Care, University of Pennsylvania, JACOB MYERSON, Department of Pharmacology, University of Pennsylvania, VLADIMIR R. MUZYKANTOV, Department of Pharmacology, University of Pennsylvania, PORTONOVO AYYASWAMY, Department of Mechanical and Aerospace Engineering, University of California, Los Angeles, DAVID M. ECKMANN, Department of Anesthesiology, Ohio State University, RAVI RADHAKRISHNAN, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — We report computational investigations of deformable polymeric nanoparticles (NPs) under colloidal suspension flow and adhesive environment. We employ a coarse-grained model for the polymeric NP and perform Brownian dynamics simulations with hydrodynamic interactions and in presence of wall-confinement, particulate margination, and wall-adhesion for obtaining NP microstructure, shape, and anisotropic and inhomogeneous transport properties for different NP stiffness. Comparing our computational results for the amount of NP margination to the near-wall adhesion regime with those of our binding experiments in cell culture under shear, as well as those of tissue targeting measurements in vivo in mice, we found quantitative agreement on shear-enhanced binding, effects of particulate volume fraction, and effects of NP stiffness. The reported combined computational approach and results are expected to enable fine-tuning of design and optimization of flexible NP in targeted drug delivery applications.

*We acknowledge support from the National Institutes of Health through grants 1R01EB006818, U01EB016027, and 1U54CA193417. Computational resources were provided in part by the Penn Bioengineering, MRSEC and by the Extreme Science and Engineering Discovery Environment (XSEDE) grant MCB060006.

Tuesday, March 3, 2020 2:30 PM - 4:00 PM

Session J71 APS: Graduate School Fair Reception (2:30pm - 4:00pm)
Exhibit Hall C/D - Tag(s): Careers, Education, Undergrad Friendly

2:30PM J71.00001: Graduate School Fair Reception (2:30pm - 4:00pm) —

Tuesday, March 3, 2020 4:30 PM - 6:30 PM

Session K02 APS: Meet the Physical Review Journal Editors Reception (4:30pm - 6:30pm) Lobby D - Tag(s): Undergrad Friendly

4:30PM K02.00001: Meet the Physical Review Journal Editors Reception (4:30pm-6:30pm) —
The Editors of the Physical Review journals invite you to join them for conversation on Tuesday, March 3, 4:30-6:30PM. The Editors will be available to answer questions, hear your ideas, and discuss any comments about the journals. All are welcome. Light refreshments will be served.
Session K03 APS: Student Reception (5:30pm - 8:30pm)
Careers, Undergrad Friendly

Tuesday, March 3, 2020 5:30 PM - 6:30 PM

Session K08 APS: Town Hall: Guide to Effective Practices for Physics Departments: Implications for Program Review and Accreditation
Program review is a reality for all colleges and universities. Whether this is regional accreditation, periodic external program review, or the department seeking certification or accreditation, there is a substantial amount of work required. The joint APS / AAPT guide: Effective Practices for Physics Programs (EP3), is a community-based effort to help physics programs conduct meaningful self-assessments, and respond to regional accreditation in ways that will maximize the value from the time spent by the department in developing and conducting these assessments. The guide will provide an opportunity for the department to transform the chore of self-assessment into a culture of continuous improvement, informed by evidence-based practices. It will include strategies for chairs to implement reforms, information on assessment practices, and a set of resources informing all aspects of a physics program. EP3 will train departmental reviewers to use these strategies and design principles in external program reviews.

Tuesday, March 3, 2020 5:45 PM - 6:45 PM

Session K21 GERA: GERA Business Meeting (5:45pm-6:45pm)

Tuesday, March 3, 2020 5:45 PM - 6:45 PM

Session K25 GSNP: GSNP Business Meeting (5:45pm-6:45pm)
Tuesday, March 3, 2020 5:45 PM - 6:45 PM

Session K34 DPOLY: DPOLY Business Meeting (5:45pm-6:45pm) 506
5:45PM K34.00001: DPOLY Business Meeting (5:45pm-6:45pm) —

Tuesday, March 3, 2020 5:45 PM - 6:45 PM

Session K36 DQI: DQI Business Meeting (5:45pm-6:45pm) 601
5:45PM K36.00001: DQI Business Meeting (5:45pm-6:45pm) —

Tuesday, March 3, 2020 5:45 PM - 6:45 PM

Session K46 GMAG: GMAG Business Meeting (5:45pm-6:45pm) 708
5:45PM K46.00001: GMAG Business Meeting (5:45pm-6:45pm) —

Tuesday, March 3, 2020 5:45 PM - 6:45 PM

Session K58 DCP: DCP Business Meeting (5:45pm-6:45pm) Mile High Ballroom 3B
5:45PM K58.00001: DCP Business Meeting (5:45pm-6:45pm) —

Tuesday, March 3, 2020 5:45 PM - 6:45 PM

Session K60 GMED: GMED Business Meeting (5:45pm-6:45pm) 110
5:45PM K60.00001: GMED Business Meeting (5:45pm-6:45pm) —

Tuesday, March 3, 2020 6:00 PM - 9:00 PM

Session K04 APS: Google Cloud Hero Workshop Mile High Ballroom 2A
6:00PM K04.00001: Google Cloud Hero Workshop —
Tuesday, March 3, 2020 6:45 PM - 7:45 PM

Session K59 DPOLY: NSF Question & Answer Session on Polymers and Soft Matter 506 - Andrew Lovinger, National Science Foundation

6:45PM K59.00001: NSF Question & Answer Session on Polymers and Soft Matter  —

Tuesday, March 3, 2020 7:00 PM - 8:00 PM

Session K01 DCMP: DCMP Business Meeting (7:00pm-8:00pm) 103

7:00PM K01.00001: DCMP Business Meeting (7:00pm-8:00pm)  —

Tuesday, March 3, 2020 7:00 PM - 8:30 PM

Session K06 DBIO: DBIO Town Hall for National Academies Physics of Biology Decadal Survey 401

7:00PM K06.00001: DBIO Town Hall for National Academies Physics of Biology Decadal Survey  —

Tuesday, March 3, 2020 7:30 PM - 8:30 PM

Session K07 DMP: DMP Business Meeting (7:30pm-8:30pm) 102

7:30PM K07.00001: DMP Business Meeting (7:30pm-8:30pm)  —

Tuesday, March 3, 2020 7:30 PM - 8:30 PM

Session K68 APS: Physics of NASCAR Four Seasons 4 - Tag(s): Outreach, Undergrad Friendly

7:30PM K68.00001: Physics of NASCAR  —

Tuesday, March 3, 2020 7:30 PM - 9:00 PM

Session K09 APS: Screening of the film: LIGO 506-507 - Tag(s): Outreach
**7:30PM K09.00001: Screening of the Film: LIGO** — “LIGO” is director Les Guthman’s inside story of the LIGO collaboration and its historic discovery of gravitational waves. He began filming a few weeks before the detection of GW150914, and, through great good fortune, was on location at the LIGO Livingston Observatory in Louisiana on the day the binary black hole signal came in. He filmed during the four months LIGO kept the detection secret and continued through 2016 and the summer of 2017, when LIGO and Virgo made a second seminal detection — of two colliding neutron stars — and launched a new era in multi-messenger astronomy. Guthman’s final shoot was in Stockholm in December 2017 with Rai Weiss, Kip Thorne and Barry Barish. “LIGO” was produced by his Advanced LIGO Documentary Project, under a grant from the National Science Foundation and funding from MathWorks, Caltech and MIT.

**Wednesday, March 4, 2020 8:00 AM - 11:00 AM**

**Session L01 DAMOP: Long-Ranged Interactions and Nonequilibrium Systems** 103 - Mikael Rechtsman, Pennsylvania State University

**8:00AM L01.00001: George E. Valley Jr. Prize Talk: Prethermal phases of matter in long-range interacting and classical many-body systems** [Invited] NORMAN YAO (Presenter), University of California, Berkeley — Recent advances suggest that physical systems, which are taken out of equilibrium, can exhibit phenomena fundamentally richer than their static counterparts. For example, certain phases of matter that are provably forbidden in equilibrium, such as discrete time crystals, have found new life in periodically driven, non-equilibrium systems. In this talk, I will define the essential features of time crystalline order and describe two new venues where such order can be observed: 1) in a 1D disorder-free, long-range interacting system and 2) in a classical spin system. In both cases, the underlying workhorse is Floquet prethermalization - a phenomena which occurs in the high frequency limit of periodically driven many-body systems; in particular, when the drive frequency is large compared with the local energy scales of the system, there can exist a long-lived quasi-steady state - a so-called "prethermal" state - in which ordered phases of matter can remain stable for exponentially long time scales.

**8:36AM L01.00002: Spin squeezing in the XXZ model with power-law interactions** CHUNLEI QU (Presenter), ANA M. REY, JILA, University of Colorado, Boulder — Spin squeezed states are known to be a useful resource for quantum metrology. Although there have been many proposals on how to generate spin squeezing, most of the dynamical generations involve collective Ising interactions via the so-called one axis twisting (OAT) model. In this talk, we will present our recent results on spin squeezing generation in the XXZ model with power-law interactions. Despite the inhomogeneous character of the spin couplings, we find this system can exhibit a level of spin-squeezing similar to that generated by the OAT model. We will report on our systematic investigation of this model and explain the mechanism responsible for the large spin squeezing generation. Our results are useful for state-of-the-art ultracold polar molecular experiments where pinned molecules in an optical lattice can interact with each other by long-range dipolar interactions and for trapped ion crystals featuring long-range interactions mediated by the phonon modes of the crystal.
8:48AM L01.00003: Persistence of power-law correlations in nonequilibrium steady states of gapped quantum spin chains  
JARRETT LANCASTER (Presenter), Physics, High Point University,  
JOSEPH P GODOY, Physics, Appalachian State University — The existence of quasi-long range order is demonstrated in nonequilibrium steady states in isotropic XY spin chains including of two types of additional terms that generate a gap in the energy spectrum. The system is driven out of equilibrium by initializing a domain-wall magnetization profile through application of external magnetic field and switching off the magnetic field at the same time the energy gap is activated. An energy gap is produced by either applying a staggered magnetic field in the transverse direction or introducing a modulation to the XY coupling. The magnetization, spin current and spin-spin correlation functions are computed in the thermodynamic limit at long times after the quench. For both types of systems, we find the persistence of power-law correlations despite the ground state correlation functions exhibiting exponential decay. It is discussed how these power-law correlations appear related to the periodic nature of the perturbation which generates the energy gap.

9:00AM L01.00004: Locality and Heating in Periodically Driven, Power-law Interacting Systems  
MINH CONG TRAN, JQI/QuICS, NIST/University of Maryland, College Park and KITP, UCSB,  
ADAM EHRENBERG, ANDREW GUO (Presenter), JQI/QuICS, NIST/University of Maryland, College Park,  
PARAJ TITUM, JQI/QuICS, NIST/University of Maryland, College Park and Applied Physics Laboratory, JHU,  
Dmitry Abanin, University of Geneva, ALEXEY V GORSHKOV, JQI/QuICS, NIST/University of Maryland, College Park and KITP, UCSB — Periodically driven quantum systems with local interactions take exponentially long to heat up. We study the heating time in periodically driven $D$-dimensional systems with interaction strengths that decay with the distance $r$ as a power-law $1/r^\alpha$. Using a theory based on linear response, we show that the heating time is exponentially long as a function of the drive frequency for $\alpha > D$. For systems that may not obey linear response theory, we use a more general Magnus-like expansion to show the existence of quasi-conserved observables, which implies exponentially long heating time for $\alpha > 2D$. We also generalize recent state-of-the-art Lieb-Robinson bounds for power-law systems from two-body to $k$-body interactions and thereby obtain a longer heating time than previously established in the literature. Additionally, we conjecture that the gap between the bounds from the linear response theory and the Magnus-like expansion does not stem from physical differences in the theories, but rather from the lack of tight Lieb-Robinson bounds for power-law interactions. We show that the gap vanishes in the presence of a hypothetical, tight bound, and report on recent steps toward achieving this ideal bound for one-dimensional systems.
9:12AM L01.00005: Origin of the slow growth of entanglement entropy in long-range interacting spin systems  SILVIA PAPPALARDI (Presenter), ALESSIO LEROSE, Interational School of Advanced Studies, SISSA — Long-range interactions allow far-distance quantum correlations to build up very fast. Nevertheless, numerical simulations demonstrated a dramatic slowdown of entanglement entropy growth after a sudden quench. In this work, we unveil the general mechanism underlying this counterintuitive phenomenon for generic d-dimensional quantum spin systems with slowly-decaying interactions. We demonstrate that the semiclassical rate of collective spin squeezing governs the dynamics of entanglement, leading to a universal logarithmic growth in the absence of semiclassical chaos. In fact, the standard quasiparticle contribution is shown to get suppressed as the interaction range is sufficiently increased. All our analytical results agree with numerical computations for quantum Ising chains with long-range couplings. Our findings thus identify a qualitative change in the entanglement production induced by long-range interactions and are experimentally relevant for accessing entanglement in highly-controllable platforms, including trapped ions, atomic condensates, and cavity-QED systems.

9:24AM L01.00006: Orthogonality catastrophe with long-range interactions  WEI XIA (Presenter), XIAOPENG LI, Department of Physics, Fudan University — Anderson orthogonality catastrophe is a fundamental property of fermions with a fermi surface subjected to a scattering potential. The case of finite-range potential has been well-understood. Recently, long-range interaction has been achieved in numerous quantum systems such as trapped ions, Rydberg atoms, and polar atoms/molecules. In this talk, I will present our recent study on Anderson orthogonality catastrophe with long-range interaction in one, two, and three dimensions. With a power-law type long-range interaction 1/r^α, we find in one dimension that there is critical α below which the conventional AOC scenario does not hold. In both two and three dimensions, we establish that the AOC holds generically for any value of α. This can be attributed to the energy barrier produced by angular motion in two and three dimensions, which is absent in one dimension. We show our theoretical results can be readily tested in trapped ions and tweezer-array confined Rydberg atoms.
Measurement-Induced Phase Transitions in Long-range Quantum Circuits

MAXWELL BLOCK (Presenter), YIMU BAO, SOONWON CHOI, EHUD ALTMAN, NORMAN YAO, Physics, University of California, Berkeley — Hybrid quantum circuits, in which random unitary gates are interspersed with projective measurements, can exhibit a phase transition between volume- and area-law scaling of steady-state entanglement entropy, owing to the competition between information scrambling and measurements. Long-range interactions can scramble information parametrically faster than short-range interactions, suggesting they may qualitatively modify the transition. In this talk, we study 1D long-range hybrid quantum circuits where each unitary is a random two-qubit Clifford gate with range sampled from a $1/r^\alpha$ power law distribution. We find that the presence of long-range interactions changes the universality of the transition: for $\alpha>3$, the critical exponents agree with studies of nearest-neighbor hybrid circuits, while for $\alpha<3$ the critical exponents change continuously with $\alpha$. In particular, we find the dynamical exponent $z<1$ for $\alpha<3$, indicating the transition cannot be described by conformal field theory. Moreover, for $\alpha<2$ the area-law scaling crosses over to a sub-volume law scaling in which entanglement entropy grows with system size, even under high measurement rates. Our work is especially relevant for hybrid quantum circuits realized in experimental systems with inherently long-range interactions.

Quantum Simulation and Computation with Programmable Rydberg Atom Arrays

ALEXANDER KEESLING (Presenter), HARRY LEVINE, AHMED OMRAN, GIULIA SEMEGHINI, SEPEHR EBADI, DOLEV BLUVSTEIN, HANNES PICHLER, MARKUS GREINER, Harvard University, VLADAN VULETIC, MIT, MIKHAIL LUKIN, Harvard University — Arrays of neutral atoms in reconfigurable geometries has arisen as a powerful platform for quantum science in the past few years. Strong and controllable interactions introduced through the Rydberg blockade mechanism lead to a rich set of both equilibrium and non-equilibrium many-body phenomena. Recently we have used a one-dimensional version of this platform to study the critical properties of various quantum phase transitions, generate large N-partite entangled states, and develop new techniques to implement two- and three-qubit quantum logic gates with high fidelity.

I will present recent progress towards extending our experimental platform to control hundreds of atoms in arbitrary two-dimensional geometries, and the new prospects for quantum simulation and computation in these large-scale atom arrays.

*We acknowledge financial support from the Center for Ultracold Atoms, the National Science Foundation, Vannevar Bush Faculty Fellowship, the U.S. Department of Energy, and the Office of Naval Research.
10:00AM L01.00009: Observation of nanoscale hydrodynamics in a strongly interacting dipolar spin ensemble in diamond --- Theory  FRANCISCO MACHADO (Presenter), CHONG ZU, BINGTIAN YE, BRYCE H KOBRIN, THOMAS MITTIGA, SATCHER HSIEH, PRABUDHYA BHATTACHARYYA, TIM O HOEHN, SOONWON CHOI, University of California, Berkeley, CHRISTOPHER LAUMANN, Boston University, DMITRY BUDKER, NORMAN YAO, University of California, Berkeley — Establishing a quantitative connection between the microscopic description of a quantum many-body system and its emergent macroscopic phenomena remains an important open problem. In this talk, we introduce a novel method that combines analytical, numerical, and experimental approaches to address this challenge. Strongly motivated by recent experiments that utilize strongly interacting dipolar spin ensembles in diamond, we present a framework to efficiently describe the spin dynamics. More specifically, starting from a microscopic Hamiltonian description of the spin ensemble, we construct an effective classical description of the spin polarization dynamics that accurately captures the experimental observations. Our method highlights a hybrid approach to study emergent hydrodynamics in strongly interacting quantum systems.

10:12AM L01.00010: Observation of nanoscale hydrodynamics in a strongly interacting dipolar spin ensemble in diamond --- Experiment*  CHONG ZU (Presenter), FRANCISCO MACHADO, BINGTIAN YE, BRYCE H KOBRIN, THOMAS MITTIGA, SATCHER HSIEH, PRABUDHYA BHATTACHARYYA, TIM O HOEHN, SOONWON CHOI, University of California, Berkeley, CHRISTOPHER LAUMANN, Boston University, DMITRY BUDKER, NORMAN YAO, University of California, Berkeley — Bridging the gap between microscopic quantum dynamics and macroscopic emergent phenomena is an important open problem in quantum many-body physics. In this talk, we introduce a novel platform, based upon nitrogen-vacancy (NV) color centers surrounded by a dense ensemble of substitutional nitrogen (P1) centers in diamond, to experimentally probe nanoscale spin diffusion. In this platform, the NV centers serve as both entropy sinks for initializing the P1 ensemble and time-resolved probes of local spin dynamics. Using a combination of static and driven fields, we are able to independently control different parameters such as the strength of interaction and disorder, allowing us to probe the quench dynamics of the strongly interacting spin ensemble under various conditions. We find that the late time dynamics of the P1 ensemble agrees with an effective description based on emergent hydrodynamics, from which we estimate diffusion coefficients.

*This work was supported as part of the Center for Novel Pathways to Quantum Coherence in Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-AC02-05CH11231.
A reconfigurable blue-detuned lattice for neutral atom quantum computing*  BRANDON GRINKEMEYER (Presenter), Harvard University, TRENT GRAHAM, MINHO KWON, ZACHARY A MARRA, XIAOYU JIANG, University of Wisconsin - Madison, MARTIN LICHTMAN, University of Maryland, College Park, MATTHEW F EBERT, MARK SAFFMAN, University of Wisconsin - Madison — We present a novel approach to forming a blue-detuned optical lattice for single Cesium atoms. This approach makes use of Acousto-Optic Deflectors (AOD) in conjunction with diffractive elements to form a lattice of crossed lines. Due to the frequency shifts introduced by the AOD we eliminate Talbot planes that have posed problems for previous blue-detuned trapping schemes. By using AODs we also gain control over the size and spacing of the traps. The tunability of the size of the trap offers a parameter that can be used to find a magic trapping condition for the ground and Rydberg states of the atom. Additionally, the ability to reconfigure spacing allows us to tune Rydberg interaction strengths. The combination of these degrees of freedom makes this trap ideal for studying quantum computation and simulation with neutral Rydberg atoms.

*We acknowledge support from NSF PHY-1720220, the ARL-CDQI, DOE award de-sc0019465, and ColdQuanta, Inc.

The Measurement-Driven Entanglement Phase Transition: Relation to Cluster Fragmentation*  SAGAR VIJAY (Presenter), Harvard University — We study the dynamics of a collection of spins evolving under unitary gates and random projective measurements, and in the absence of spatial locality. For a certain choice of Clifford unitary gates, we map the wavefunction of the spins to the state of an evolving cluster, which undergoes a dynamical "fragmentation" transition as a function of the measurement rate. This classical dynamical transition corresponds to a phase transition in the asymptotic state of the spins; above a critical rate of applied measurements, the system exists in a product state over extensively many subsystems, while below this threshold, the wavefunction is no longer separable, and all subsystems develop volume-law entanglement. We show that the scaling of the entanglement entropy, which is related to the connectivity of the evolving cluster, distinguishes between the two phases, and identify a protocol to measure a local order parameter for this transition. The dynamics of the cluster may be studied analytically to determine other properties of the state of the spins, such as the distribution of stabilizer lengths. We discuss the relevance of our results to the measurement-driven entanglement transition that has been observed in higher dimensions.

*S.V. is supported by the Harvard Society of Fellows.
10:48AM L01.00013: Measurement-Induced Phase Transitions in Many-Body Localized and Integrable Systems  
YIMU BAO (Presenter), SOONWON CHOI, EHUD ALTMAN, University of California, Berkeley — Recent works have shown the competition between scrambling unitary dynamics and local projective measurements can lead to a phase transition in the dynamics of entanglement entropy. In integrable systems, the extensive number of conserved quantities strongly constrains the information scrambling. Here, we show that such systems can still exhibit an entanglement phase transition given an appropriate choice of measurement basis. We analyze a toy model of many-body localized systems as a paradigmatic example. If the observables being measured are not scrambled in unitary evolution, the growth of entanglement is prohibited by any finite rate of measurements. In contrast, if measured observables are scrambled, the unitary evolution can hide and protect quantum correlations from measurements, leading to a phase transition at a nonvanishing measurement rate. The phase transition in other integrable systems, such as free fermionic and Bethe-ansatz solvable systems are also explored. Our results further corroborate the understanding of the phase transition in terms of quantum error correcting properties of the scrambling dynamics.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM

Session L02 DAMOP: Interacting Ultracold Gases, Light-Matter Coupling, and Cavities

8:00AM L02.00001: Three-color fermions under local and next-neighbor interactions*  
ARTURO PÉREZ, ROBERTO FRANCO PEÑAVALOZA, JERESON SILVA VALENCIA (Presenter), Universidad Nacional de Colombia, Bogota — Graphene, Bechgaard salts, polymers and systems of adatoms on semiconductor surfaces can be described by an extended SU(2) Fermi-Hubbard model, which has a rich phase diagram that has been studied for decades. Ultracold atom setups have allowed testing and extending many ideas and concepts of condensed matter. Confining alkaline-earth-metal atoms, which have several hyperfine states allow to obtain SU(N>2) Fermi-Hubbard systems experimentally.

We study three-color (N=3) fermions confined in a one-dimensional optical lattice and consider local and next-neighbor interactions, obtaining an extended SU(3) Fermi-Hubbard model. Using DMRG, we build a phase diagram that contains two different charge density wave phases, a phase separation and spin-density wave phases for a global density of one-third.

*J.S.-V. is thankful for the support of DIEB-Universidad Nacional de Colombia (Grant No. 41402)
In conventional solid-state electron systems with localized states the ac absorption is linear since the inelastic widths of the energy levels exceeds the drive amplitude. The situation is different in the systems of cold atoms in which phonons are absent. Then even a weak drive leads to saturation of the ac absorption within resonant pairs, so that the population of levels oscillates with the Rabi frequency. We demonstrate that, in the presence of weak dipole-dipole interactions, the response of the system acquires a long-time component which oscillates with frequency much smaller than the Rabi frequency. The underlying mechanism of this long-time behavior is that the fields created in the course of the Rabi oscillations serve as resonant drive for the second-generation Rabi oscillations in pairs with level spacings close to the Rabi frequency. The frequency of the second-generation oscillations is of the order of interaction strength. As these oscillations develop, they can initiate the next-generation Rabi oscillations, and so on. Formation of the second-generation oscillations is facilitated by the non-diagonal component of the dipole-dipole interaction tensor.

*The work was supported by the Department of Energy, Office of Basic Energy Sciences, Grant No. DE- FG02- 06ER46313.

Unidirectional flow of solitons with nonlinearity management MAJED ALOTAIBI (Presenter), Kuwait Univ, S. M. AL-MARZOUQ, H. BAHLOULI, Physics, King Fahd University of Petroleum and Minerals, U. AL KHAWAJA, United Arab Emirates University — Unidirectional flow of solitons is obtained with a localized modulation of the nonlinearity strength. The modulation takes the shape of an asymmetric double well with a slight difference between the potential depths. The results were established using numerical computations and then verified qualitatively using a variational approach. Our results suggest that the most important physics at the origin of the unidirectional flow is the excitation of the breathing modes in the scattering region. Simplified variational equations of motion suggested that the phenomenon can be observed if the soliton is scattered by a generic asymmetric effective double potential well.
**8:36AM L02.00004: Cooperative Light Emission in the Presence of Strong Inhomogeneous Broadening**

CHEN SUN (Presenter), Brown University, VLADIMIR Y CHERNYAK, Wayne State University, ANDREI PIRYATINSKI, NIKOLAI SINITSYN, Los Alamos National Laboratory — We study photon emission by an ensemble of two-level systems, with strong inhomogeneous broadening and coupled to a cavity mode whose frequency has linear time-dependence. The analysis shows that, regardless the distribution of energy level splittings, a sharp phase transition occurs between the weak and strong cooperative emission phases near a critical photonic frequency sweeping rate. The associated scaling exponent is determined. We suggest that this phase transition can be observed in an ensemble of negatively charged NV centers in diamond interacting with a microwave half-wavelength cavity mode even in the regime of weak coupling and at strong disorder of two-level splittings.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, Condensed Matter Theory Program (V.Y. C. and N.A.S.), and by the J. Michael Kosterlitz Postdoctoral Fellowship at Brown University (C.S.). N.A.S. and A.P. also thank the support from the LDRD program at LANL.

**8:48AM L02.00005: "Signal Energy" of an Excited Dipolar Bose Gas driven by an Oscillating Dimple**

ASAAD R SAKHEL (Presenter), Physics, Al-Balqa Applied University, Salt 19117, Jordan, ROGER RAJI SAKHEL, Physics, Isra University, Amman 11622, Jordan — It is known that dipolar Bose-Einstein condensates (DBECs) display rich and fascinating features that are not observable in nonpolar BECs (Lahaye et al., Rep. Prog. Phys. 72, 126401 (2009)). As such, the present examination studies the dynamics of a DBEC, being motivated by the work of Sabari and Kumar (Eur. Phys. J. D 72, 48 (2018)) who examined the effect of an oscillating obstacle in a DBEC. We thus examine the "signal energy" of a trapped DBEC that is driven by an oscillating dimple potential. For this purpose we numerically solve the time-dependent Gross-Pitaevskii equation. The signal energy is related to the energy spectral density. It is demonstrated that the signal energy displays parametric resonances (PRs) at specific values of the dipole-dipole interaction parameter that can be controlled via the trapping geometry. The spacings between these values have been found to reveal information about the energy level structure of the external trap. The dynamics of the harmonic-oscillator (HO)-states occupancy obtainable from the modal coefficients $C_n(t)$ arising in the decomposition of the wave function $\Psi(x;t) = \sum_{n=0} C_n(t) \varphi_n(x)$, where $\varphi_n(x)$ is the usual HO function, as well as the phase-mismatch between $C_0(t)$ and $C_1(t)$ have been found to display challenging features at PR.
9:00AM L02.00006: Contour-time approach to the 2D disordered Bose-Hubbard model in the strong coupling regime.* MATTHEW FITZPATRICK (Presenter), ALI MOKHTARI-JAZI, MALCOLM P KENNEDY, Simon Fraser Univ — We develop a strong-coupling approach for calculating spatio-temporal correlations in the disordered Bose-Hubbard model. We consider systems that are prepared in highly-excited out-of-equilibrium density patterns and derive equations of motion for the disorder-averaged single-particle Green's function, allowing us to study the relaxation dynamics. We discuss how our formalism can be applied to the study of Bose glass and possibly many-body localized states in the context of recent cold experiments.

*Supported by NSERC

9:12AM L02.00007: Study of Low Energy Excitations of Cold Atomic Fermi Systems using Quantum Monte Carlo Methods KAELEYN DAUER (Presenter), ETTORE VITALI, ANNETTE LOPEZ, PATRICK KELLY, California State University, Fresno — The calculation of dynamical properties of quantum many-body theories is a big challenge from both the theoretical and computational point of view. Quantum Monte Carlo methods are considered to be some of the most accurate approaches for unravelling physical mechanisms in systems where correlations are so strong that simple approaches are doomed to fail. Most of the success of Quantum Monte Carlo techniques involve static properties of physical systems, like phase diagrams and density correlations. The extension to dynamical quantities, like the spectrum of density fluctuations or the spectral function is still a major challenge, despite some important recent successes. Cold atomic Fermi systems are unique due to the unprecedented experimental control that can be achieved and due to the flexibility of hamiltonians that can be engineered. This makes them a unique test ground for correlated methodologies like Quantum Monte Carlo. In this presentation we will review important recent advances in the calculations, and we will present new results about the spectrum of density fluctuations and spectral functions of Fermi gases.
**9:24AM L02.00008: Broadband sensitivity improvement via coherent quantum feedback with PT symmetry***

Xiang Li (Presenter), Rana Adhikari, California Institute of Technology, Vaishali Adya, Australian National University, Yanbei Chen, California Institute of Technology, Yifan Chen, Chinese Academy of Sciences, Maxim Goryachev, University of Western Australia, Yiqiu Ma, Huazhong University of Science and Technology, Jing Shu, Chinese Academy of Sciences, Michael Tobar, University of Western Australia, Robert L Ward, Australian National University, Chunnong Zhao, University of Western Australia — A conventional resonant detector is subject to a trade-off between bandwidth and peak sensitivity. This limitation can be traced back to the Quantum Cramer Rao Bound and the coherent state of the conventional resonator. The trade-off can be broken by injecting non-classical states (e.g., squeezed vacuum), but it often has stringent requirements on optical losses. Anomalous dispersion due to an unstable quantum system has been shown to be able to improve the bandwidth-sensitivity product by signal amplification and thus suffer less from losses. But stabilizing the system may cause technical complications and conceptual issues. Here we propose a simple stable quantum amplifier enabled by two-mode non-degenerate parametric amplification. We demonstrate that coherent broadband signal amplification can be achieved without incurring instability. As the amplifier operates at the threshold, one mode of the amplifier forms a PT-symmetric system of the original detector mode, while the other mode collects the signal and transfer it to the readout. We will discuss how to apply this strategy to gravitational-wave detectors.

*The work of X.L, Y.C and Y.M are supported by NSF Grants PHY 1612816, 1708212 and 1708213, the Brinson Foundation, and the Simons Foundation (Award Number 568762).

**9:36AM L02.00009: Interacting Bose-Bose mixtures at finite temperature***

Arko Roy (Presenter), Miki Ota, Alessio Recati, Franco Dalfovo, University of Trento, INO-BEC Center and Dept. of Physics — We examine the role of thermal fluctuations in 2D uniform binary condensate mixtures of dilute atomic gases. In particular, we use the Stochastic Projected Gross-Pitaevskii formalism to probe the impact of non-condensate atoms to the phenomenon of phase-separation in two-component Bose-Einstein condensates. We demonstrate that, in comparison to zero temperature, there is a suppression in the phase-separation of the binary condensates at non-zero temperature. We also show that a mixed phase gives rise to a fully separated one at finite temperature. Finally, these phases are characterized by measuring the speed of sound at finite temperature.

*Provincia Autonoma di Trento*
9:48AM L02.00010: Superradiant Peierls transition in a multi-mode optical cavity  COLIN RYLANDS (Presenter), University of Maryland, College Park, BENJAMIN L LEV, Stanford University, JONATHAN KEELING, University of St. Andrews, VICTOR GALITSKI, University of Maryland, College Park — The strong matter-light coupling attainable in optical cavities has been employed with remarkable success to study quantum systems. It has facilitated the realization of many exciting phenomena from superradiance and self organization of matter to exciton-polaritons condensates. We consider such a system in which a one dimensional interacting Bose gas is loaded into a multi-mode optical cavity and subject to a pump field. Focusing on the steady state properties of the system we find that for sufficiently strong repulsive interactions a superradiant transition takes place which is accompanied by a metal insulator transition in the atomic system. In the limit of infinite repulsion this is attributable to the Peierls instability. Away from this special point we show that this still occurs however the nature of the transition changes and upon further reducing the interaction strength the system undergoes a transition to a gapless normal state.

10:00AM L02.00011: Microscopic Origins of the Hess-Fairbank Effect and its Consistency with the Second Law of Thermodynamics  ANTHONY J LEGGETT, DOUGLAS PACKARD (Presenter), University of Illinois at Urbana-Champaign — The history of applying kinetic theory to help us understand superfluid and BEC phenomena is a long and storied one, going back to the work of Landau and Khalatnikov [1]. Further developments were made using quantum field theoretic [2] and quantum optical methods [3]. We use these methods to study the nonequilibrium physics of Bose condensation and superfluid formation in a rotating quantum fluid. In particular, we examine the quantization of angular velocity observed at low rotational speeds, i.e. the Hess-Fairbank effect. We present results relating the transfer of atoms into a condensate or superfluid mode (at rest in the lab frame) to the overall generation of entropy, taking the rotating container of the fluid itself into account. Finally, we attempt to relate these results to the phenomenon of flux expulsion from a bulk superconductor, in light of recent critical papers on this topic [4].

Structure of chaotic eigenstates and their entanglement entropy

CHAITANYA MURTHY (Presenter), MARK SREDNICKI, University of California, Santa Barbara — We consider a chaotic many-body system (i.e., one that satisfies the eigenstate thermalization hypothesis) that is split into two subsystems, with an interaction along their mutual boundary, and study the entanglement properties of an energy eigenstate with nonzero energy density. When the two subsystems have nearly equal volumes, we find a universal correction to the entanglement entropy that is proportional to the square root of the system's heat capacity (or a sum of capacities, if there are conserved quantities in addition to energy). This phenomenon was first noted by Vidmar and Rigol in a specific system; our analysis shows that it is generic, and expresses it in terms of thermodynamic properties of the system. Our conclusions are based on a refined version of a model of a chaotic eigenstate originally due to Deutsch, and analyzed more recently by Lu and Grover.


This work was supported in part by the Microsoft Corporation.

Mixed spectra and partially extended states in a two-dimensional quasiperiodic model

ATTILA SZABO (Presenter), ULRICH SCHNEIDER, Univ of Cambridge — We introduce a two-dimensional generalisation of the quasiperiodic Aubry-André model. Even though this model exhibits the same duality relation as the one-dimensional version, its localisation properties are found to be substantially more complex. In particular, partially extended single-particle states appear for arbitrarily strong quasiperiodic modulation. They are concentrated on a network of low-disorder lattice lines, while the rest of the lattice hosts localised states. This spatial separation protects the localised states from delocalisation, so no mobility edge emerges in the spectrum; instead, localised and partially extended states are interspersed, giving rise to an unusual type of mixed spectrum. In the absence of interactions, this mixed spectrum also gives rise to complex dynamics, such as ballistic transport across the low-disorder lines, while the rest of the system remains localised. This behaviour is robust against disorder and other weak perturbations. Our model is thus directly amenable to experimental studies and promises fascinating many-body localisation properties.

This work was partly funded by the European Commision ERC Starting Grant QUASICRYSTAL and the EPSRC Grant (EP/R044627/1) and Programme Grant DesOEQ (EP/P009565/1).
Efimov physics in the presence of a Fermi sea  

MINGYUAN SUN  
(Presenter), Beijing University of Posts and Telecommunications — I will introduce the Efimov correlation in atomic system of two heavy bosons ($^{133}$Cs) immersed in a bath of light fermions ($^6$Li). Using the Born-Oppenheimer approximation, we identify two different regimes, depending on the Fermi momentum of light fermions ($k_F$) and the boson-fermion scattering length $a_s(< 0)$, where the presence of underlying Fermi sea plays distinct roles in the Efimov-type binding of bosons. Namely, in the regime $k_F |a_s| < 1$ ($k_F |a_s| > 1$), the Fermi sea induces an attractive (repulsive) effective interaction between bosons and thus favors (disfavors) the formation of bound state, which can be seen as the Efimov trimer dressed by the fermion cloud. Interestingly, this implies a non-monotonic behavior of these bound states as increasing the fermion density (or $k_F$). Moreover, we establish a generalized universal scaling law for the emergence/variation of such dressed Efimov bound states when incorporating a new scale ($k_F$) brought by the Fermi sea.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L03 GSCCM: Materials in Extremes: Phase Transitions  
Heather Whitley, Lawrence Livermore Natl Lab - Tag(s): Focus
8:00AM L03.00001: Probing liquid-liquid phase transitions under dynamic compression: an X-ray diffraction and ab initio MD study of selenium* [Invited] RICHARD BRIGGS (Presenter), AMY L COLEMAN, SHUAI ZHANG, Lawrence Livermore Natl Lab, DAVID R MCGONEGLE, Oxford University, FEDERICA COPPARI, AMALIA FERNANDEZ, MARTIN G GORMAN, MICHELLE C MARSHALL, RAYMOND SMITH, Lawrence Livermore Natl Lab, ORIANNA BALL, RYAN S MCWILLIAMS, University of Edinburgh, VITALI PRANKAPENKA, GSECARS, University of Chicago, CONOR KRILL, VINAY RASTOGI, JUNE WICKS, John Hopkins University, CYNTHIA BOLME, Los Alamos National Laboratory, PHILIP HEIMANN, ERIC CUNNINGHAM, HAEJA LEE, SLAC national accelerator laboratory, MALCOLM I MCMANON, University of Edinburgh, JON HENRY EGGERT, DAYNE FRATANDUONO, Lawrence Livermore Natl Lab — One of the most interesting phenomena of non-crystalline materials is polyamorphism, or the ability of an amorphous material, with medium range order, to exist in several distinct modifications. In liquids, the transition between these states has been termed the liquid-liquid phase transition (LLPT) and has been observed experimentally under static compression experiments in several materials. In selenium, ab initio calculations have shown significant changes in the liquid structure with increasing pressure, yet experimental data at high-pressure is limited. Even less is known regarding the evolution of the liquid structure under rapid shock compression and whether a LLPT between complex liquid structures can occur on nanosecond timescales. Here we report on femtosecond X-ray diffraction measurements of the LLPT in selenium following shock compression and release and find that the liquid structure transformations are dramatic and we show that they can occur on nanosecond timescales. The results are supported by molecular dynamic simulations of the liquid state at a range of pressure, temperature, density states covering the LLPT. Experiments were performed at the Matter at Extreme Conditions end-station of the Linac Coherent Light Source (LCLS). This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344.

*This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344. Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515.

8:36AM L03.00002: Ab-initio calculations of the phase diagram of Gold JOHANN BOUCHET (Presenter), FRANCOIS BOTTIN, VANINA RECOULES, GUNNAR WECK, CEA de Bruyeres-le-Chatel — We will present first principles calculations on the phase diagram of Gold up to 1TPa. To calculate the Gibbs free energies of the different structures (fcc, hcp, bcc...) we have performed calculations on the unit cells to obtain the cold curves and ab-initio molecular dynamics coupled with the temperature dependent energy potential (TDEP) method to calculate the vibational contribution to the free energy and capture the anharmonicity at high temperature. We compare our results to previous calculations and experimental data. We will also show results on thermodynamic data: thermal dilatation, Gruneisen parameter... and our calculations of the melting curve.
8:48AM L03.00003: A new metastable phase for shock compressed Copper  NILANJAN MITRA (Presenter), Indian Institute of Technology Kharagpur — Copper is utilized in many different applications within the shock compression community (such as pistons in NIF) primarily because it is believed that it does not undergo any solid-solid phase transition prior to melting. However, studies have demonstrated coordination number loss behind shock front. A recent MD study by the authors group demonstrated that solid-solid phase transition occurs in Cu under shock compression to that of the BCT phase [1]. However, any MD calculations are dependent on the interatomic force potentials used, which for the previous study was taken as EAM-Mishin potential for Cu having valence shell containing “s” orbitals. To rule out any forcefield issues, DFT studies were carried out. DFT studies are for 0K temperature, whereas under shock compression there is a significant rise in temperature for Cu samples. Thereby, Gibbs free energy calculation within the quasiharmonic approximation is carried out to demonstrate the feasibility of existence of BCT phase for Cu shock compressed along 001 direction [2], supporting previous postulation by Friedel.

Ref.

9:00AM L03.00004: Measurement of high pressure crystal structure and the pressure-temperature melt conditions in shock-compressed silicon carbide  RAYMOND SMITH (Presenter), Lawrence Livermore Natl Lab, ZIXUAN YE, JUNE WICKS, Johns Hopkins University, MARIUS MILLOT, DAYNE FRATANDUONO, DAVID J ERSKINE, JON HENRY EGGERT, Lawrence Livermore Natl Lab — Silicon Carbide (SiC) has many attractive properties including low density, high strength, high melting point, low wear coefficient and high chemical stability that lead to its extensive use in a wide range of industrial applications including as abrasives, shielding material on space craft; personal armor and as a potential ablator material for fusion capsules. Silicon carbide is also important in geology and planetary science. SiC grains - found in meteorites and impact sites – have an unusual isotopic signature which indicate that they are pre-solar in origin and provide constraints on stellar nucleosynthesis and on the stellar sources for the origin of the solar system. Several studies have also explored possible interior structure of carbon-rich planets in which SiC is a likely main constituent, but experimental data for the high-pressure properties of SiC is currently unavailable to test these models. Here we report on laser-driven nanosecond x-ray diffraction and shock-decay experiments on the Omega-EP laser facility located at the Laboratory for Laser Energetics (NY, USA). We present new data on the high pressure crystal structure, and pressure-temperature conditions for melt in single-crystal SiC samples.
Hurry up or take your time: kinetics of shock-driven phase transitions and dynamic x-ray diffraction.* [Invited] PATRICIA KALITA (Presenter), Sandia National Laboratories

— One of the unanswered questions in physics is how much time does a shock-driven phase transition need - i.e. its kinetics? And how does this time influence the end-result of the shock process?

Traditionally, phase transitions in dynamic compression are inferred from continuum data and compared to results from static compression experiments, shock-recovery, or calculations. With the development of time-resolved synchrotron dynamic x-ray diffraction (DXRD) combined with shock compression a new dawn is rising for the field of shock physics, as one can now probe atomic-scale changes in situ, with nanosecond resolution.

We will illustrate the atomic- and nanosecond-scale quantification of kinetics of shock-driven phase transitions in example materials. We will also show how we leverage two user facilities of the Advanced Photon Source: DCS and HPCAT, in synergistic dynamic/static compression experiments.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

This work describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the work do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Portions of this work were performed at DCS (Sector 35), APS, ANL. DCS is operated by WSU under the U.S. DOE/NNSA award no. DE-NA0002442. Portions of this work were performed at HPCAT (Sector 16), APS, ANL. HPCAT operations are supported by DOE-NNSA's Office of Experimental Sciences.
The APS is a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by ANL under Contract No. DE-AC02-06CH11357.
Experimental data analysis methods for the physics-based description of phase transition kinetics

JONATHAN BELOF (Presenter), PHILIP C MYINT, Lawrence Livermore Natl Lab, DANE M STERBENTZ, University of California, Davis — Experimental data analysis techniques for the determination of phase transformation kinetics under ramp compression are presented. The new techniques, which do not require any simulations, are described in three parts: (I) estimation of nucleation and growth rates via analysis of the velocimetry wave profile “loop”, (II) bounding of the metastability limit or “maximum over-pressurization” and (III) application of a universal scaling relation that sheds light on the time-dependence of the phase transition. The relatively simple analysis techniques presented are made available in an open source code for the community.

Funding support of this work was partially provided from the LLNL LDRD program under 16-ERD-037. This work is performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Experiments and Simulations of Shocked and Ramp-Compressed Metals to 5 Mbars

JEFFREY NGUYEN (Presenter), MINTA C AKIN, Lawrence Livermore Natl Lab, PAUL D ASIMOW, California Institute of Technology — In this report, we present a series of shocked and ramp compressed data on various metals including tantalum, iron and tin. These samples were shocked and ramp-compressed to pressures as high as 5 Mbars with graded density impactors (GDI). To analyze these data, we utilize both backward (characteristics) and forward analyses. The former method does not require a priori knowledge of a pressure drive, and often fails in the presence of strength or phase transition. By employing simulations in analysis of these experiments, we can improve experimental uncertainty as well as gain better understanding of phase transition and strength during ramp compression. In particular, we will examine the alpha-epsilon and solid-liquid transitions in iron. We will also report on recent efforts to characterize GDI in situ impedance profile.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
Experimental measures of the orientation dependence of the B1-B2 transformation in shock-compressed MgO

June Wicks (Presenter), Johns Hopkins University, Raymond Smith, Lawrence Livermore, Zixuan Ye, Johns Hopkins University, Marius Millot, Lawrence Livermore

Of the over 6,000 confirmed and candidate extrasolar planets discovered to date, those 1-4 times the radius of the Earth are found to be most abundant. MgO is expected to be a major component of the deep mantles of terrestrial planets and exoplanets. Its high-pressure transformation from a rocksalt (B1) structure to the B2 (CsCl) structure is expected to occur in rocky exoplanets greater than about 5 Earth masses in size. In this work, the structure and temperature of MgO upon shock compression over the 200-700 GPa pressure range was examined at the Omega-EP Laser facility. Laser drives of up to 2 kJ over 10 ns were used to shock compress single-crystal MgO. At peak compression, the sample was probed with He-α X-rays from a laser-plasma source. Diffracted X-rays were recorded on image plates lining the inner walls of a box attached to the target package. For each shot we measure pressure (velocity interferometry), density (x-ray diffraction) and shock temperature (pyrometry). We also probe orientation-dependence of the shock Hugoniot by conducting laser-driven decaying shock measurements of single crystal MgO [100], [111] and [110], and will discuss the importance of single crystal experiments to better improve phase diagram models of materials at extreme conditions.

Metastable conducting solid hydrogen at high pressures.

Ilnur Saitov (Presenter), Genry Norman, National Research University Higher School of Economics

The possibility of formation of metastable metallic hydrogen at normal pressure was predicted in [1]. In the present work, the density functional theory is applied for the calculation of the equation of state, the pair correlation function and density of states of solid hydrogen in the region of the possible formation of the conducting phase. A hysteresis of the dependence of pressure on density is observed in the pressure range from 350 GPa to 625 GPa. During compression, the transition of molecular hydrogen with the C2/c symmetry to a conducting atomic state with the C222_1 symmetry through an intermediate conducting molecular phase with Cmca-4 symmetry is observed. The results of calculation of the band structure of the molecular state Cmca-4 point to the semimetallic mechanism of conductivity. The possibility of the existence of conductive atomic solid hydrogen with P2_1/c symmetry under expansion up to a pressure of 350 GPa is shown.


*The study was prepared within the framework of the HSE University Basic Research Program and funded by the Russian Academic Excellence Project '5-100'
10:36AM L03.00010: Ionization of H in iron oxy-hydroxide QINGYANG HU (Presenter), HPSTAR (Beijing) — The symmetrization of O-H bonds in hydroxide often induces a slightly first order phase transition. However, the phase transition causes dramatic reconfiguring of electronic properties. In this work, we pressurized a piece of iron oxy-hydroxide (FeO\textsubscript{2}H) up to 60 GPa. Upon the asymmetric O-H bonds symmetrize to O-H-O, the measured electric conductivity surged a few orders of magnitude higher. Combining with first-principle simulation, the symmetrization separates H\textsuperscript{+} ion from the hydroxyl OH\textsuperscript{-1} group by forming ionic-type double O-H bonds. Although the pressure range of symmetrization coincides with the high-low spin transition of Fe, the sudden boost of electric conductivity is against conventional spin-transition effect, which reduces conductivity. Therefore, the ionic phase transition of H is likely to be responsible for the change of conductivity. The ionization of H is among the many intriguing behaviors of H under extreme pressure conditions and may have profound influences for the fundamental processes in Earth’s deep interiors.

10:48AM L03.00011: High-Pressure-Induced Phase Transition in 1,3-Diphenylurea: the Approaching of N−H⋯O Hydrogen-Bonded Chains YUXIANG DAI (Presenter), YANG QI, Northeastern University — Under extreme pressure conditions, supramolecular materials can undergo many novel phenomena such as phase transition, polymerization, piezochromism, and negative compression. In our research plan, we selected a series of low-dimensional supramolecular materials to study the evolution of crystal structure and intermolecular interactions under high pressure. In this study, the crystal structure and hydrogen-bonded chains of 1,3-diphenylurea were found to appear abrupt changes when the pressure increased to 1.8 GPa. The intermolecular interactions, the vibrations of chemical groups and the molecular conformation were clearly distinguished from the initial state. The anisotropic compression of the original crystal structure and the occurrence of structural phase transition were derived from the remarkable shrink of distance between hydrogen-bonded chains. This study demonstrates that excessively reducing the space between of hydrogen-bonded chains will rearrange the self-assembly of supramolecular materials.

Reference:
8:00AM L04.00001: Semiconductor Junctions for Photon Up and Downconversion: From Nanocrystals to Bulk Solids* [Invited] EMILY K RAULERSON, INKI LEE, BRITTANY R POLLOK, JON A BENDER, DANIEL E COTTON, SEAN ROBERTS (Presenter), University of Texas at Austin — Materials that repackage the energy of incoherent light, by either summing its photons together or dividing them into lower energy pairs, offer potential for new technologies for solar energy conversion, photon detection, catalysis, and quantum information science. Organic dimers, polymers, and extended solids that undergo singlet fission offer a potential means for achieving this goal as this process converts high-energy single spin-triplet excitons into pairs of low-energy spin-triplet exciton pairs. Likewise, singlet fission’s inverse, triplet fusion, can be used to combine low-energy exciton pairs into high-energy states. However, designing applications based on these materials necessitates design of both highly stable singlet fission/triplet fusion materials as well as hybrid organic:inorganic junctions that allow triplet excitons to interface with commercial semiconductor technologies. In this presentation, I will review our group’s efforts to produce covalently tethered structures for this purpose. The presentation’s first half will focus on the design of photostable single fission-capable solids based on perylenediimide dyes while its second half will focus on model semiconductor junctions that interface these and related materials with semiconductor quantum dots. Lessons learned from these studies will be used as a basis for designing silicon:organic structures that allow for spin-triplet exciton transfer across their junction.

*This work is supported in part by the National Science Foundation (CHE-1610412, CHE-1654404), W. M. Keck Foundation, Research Corporation for Science Advancement (Grant 24489), and the Welch Foundation (F-1885).

8:36AM L04.00002: Efficient Triplet Harvesting in an Air-stable Diketopyrrolopyrrole Singlet Fission Solar Cell ANDREW LEVINE, JOSEPH HAMMER, SAUL BLAIN, MAJHARUL HOQUE, VISHAL NARANG, ADAM BRAUNSCHWEIG, MILAN BEGLIARBEKOV (Presenter), NanoScience, CUNY Advanced Science Research Center — Diketopyrrolopyrrole (DPP) is an air-stable molecule which has recently been shown through spectroscopic investigation to host excitonic singlet fission (SF). Here we synthesize DPP-based solar cells using dicyano naphthalene diimide (dCN NDI) acceptor molecules and quantify SF generated carrier extraction efficiency. The characteristic dependence of the photocurrent as a function of magnetic field, which is the unambiguous signature of SF, is observed. Furthermore, we show that DPP-based photovoltaic devices are remarkably air-stable, unencapsulated devices do not exhibit a degradation of electrical or photovoltaic properties as a result of aging. Therefore, DPP is promising material for organic SF photovoltaic devices.
A Kinetic Description of Ultrafast Excitation, Relaxation, and Charge Transfer in Ru Dye-Semiconductor Systems

THOMAS CHESHIRE (Presenter), Chemical Science Division, Lawrence Berkeley National Laboratory, JEB BOODRY, Department of Chemical and Biochemical Engineering, University of California, Berkeley, M KYLE BRENNAMAN, Department of Chemistry, University Of North Carolina Chapel Hill, PAUL G. GIOKAS, Coherent Inc., DAVID F. ZIGLER, Chemistry & Biochemistry Department, California Polytechnic State University, ANDREW MORAN, JOHN MICHAEL PAPANIKOLAS, GERALD J. MEYER, THOMAS MEYER, Department of Chemistry, University Of North Carolina Chapel Hill, FRANCES HOULE, Chemical Science Division, Lawrence Berkeley National Laboratory — We describe a predictive kinetic framework for ultrafast photophysics of ruthenium polypyridyl dyes in solution and on solid surfaces to probe how kinetic processes such as absorption, relaxation, and intersystem crossing affect excited state lifetimes. Employing a form of kinetic Monte Carlo that produces an absolute time base, we compute transient absorption (TA) signals and find excellent agreement with experimental spectroscopic data. We compare dye photophysics in solution to that of sensitized metal oxide films, where charge injection from the excited states may occur. Dye molecules have similar excitation and decay kinetics in solution and on ZrO$_2$ films where there is no charge transfer. In contrast, charge transfer to the semiconductor competes with intramolecular transitions for dyes bound to TiO$_2$. Comparison of simulated TA spectra to experiment allow rate coefficients for charge injection to be estimated. The kinetic framework is readily integrated into multiscale models for dye-sensitized light harvesting systems.

*Supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Solar Photochemistry Program (No. DE-AC02-05CH11231) and the UNC EFRC Center for Solar Fuels, an Energy Frontier Research Center by (No. DE-SC0001011).

Fast algorithm for simulating nonlinear ultrafast spectroscopies

PETER ROSE (Presenter), JACOB KRICH, Univ of Ottawa — We present Ultrafast Ultrafast (UF$^2$) spectroscopy, a fast algorithm for calculating perturbative n-wave mixing signals in nonlinear optical spectroscopies including arbitrary optical pulse shapes and overlaps. It was demonstrated for closed systems, and we present here the extension to open systems, including vibronic systems with Lindblad or Redfield evolution. UF$^2$ is more computationally efficient than any method of which we are aware when the dimension of the relevant system Hilbert space is sufficiently small, as in energy-transfer systems. The speed of UF$^2$ comes from working in the eigenbasis of the time evolution operator, which enables costless time evolution between pulses, and performing the time evolution due to the pulses using the FFT and convolution theorem. We characterize the computational cost for a range of system sizes, showing when UF$^2$ gives significant speed improvements over other methods.

UF$^2$ automatically generates all Feynman diagrams for a specified phase-matching condition. It is well-suited to calculating higher-order signals (6-wave mixing and above). UF$^2$ allows easy and quick prediction of nonlinear optical spectra for a wide range of system parameters and optical pulse shapes.
9:12AM L04.00005: Enhancing vibrationally assisted energy transfer via vibrational cooperation and interference*  
ZENGZHAO LI (Presenter), LIWEN KO, ZHIBO YANG, Department of Chemistry, University of California, Berkeley, MOHAN SAROVAR, Sandia National Laboratories, BIRGITTA K WHALEY, Department of Chemistry, University of California, Berkeley — Vibrationally assisted energy transfer has recently been engineered in a trapped-ion quantum simulator [Gorman et al., Phys. Rev. X 8, 011038 (2018)]. Motivated by this demonstration, we investigate how cooperativity and interference of multiple vibrations enhance energy transfer. This is a step in the quest to reveal the extent of vibrational or vibronic mechanisms behind the phenomenon of long-time coherences in photosynthetic light harvesting systems. By analyzing a donor-bridge-acceptor trimeric chromophore system coupled to two vibrations, we identify features of one-, two-, and even four-phonon transfer processes and signatures of cooperativity and interference that provide maximum enhancement of energy transfer. Our findings of vibrational cooperativity and interference in excited state energy transfer are verifiable in trapped-ion quantum simulators.

*Sandia National Laboratories is a multimission laboratory managed and operated by NTESS, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's NNSA under contract DE-NA-0003525. This work is supported by the U.S. DOE, Office of Science, Office of Basic Energy Sciences in the Materials and Chemical Sciences Research for Quantum Information Research program under contract DE- FOA-0001909.

9:24AM L04.00006: Electrochemical tuning Localized Surface Plasmon Resonance of Au-Ag core-shell nanoparticle for Surface-Enhanced Raman Scattering*  
JING GUO (Presenter), Physics, Florida International University, EUGENE LI, Herbert A. Ammons Middle, JIN HE, Physics, Florida International University — Active control of the localized surface plasmon in metallic nanoparticles is of fundamental importance for surface-enhanced Raman spectroscopy (SERS) application. By oxidation-reduction chemistry of Ag-AgCl shells or clusters on the surfaces of AuNP, we induced dielectric-conductive shell or clusters between AuNP and GME. Self-assembled monolayer modified on GME experienced different electromagnetic field produced by surface plasmon of Ag/AuNP or AgCl/AuNP, thus, induced extreme but reversible changes in SERS intensity. Meanwhile, the redox process of Ag-AgCl is confirmed by time-resolved electrochemical current (i-t). Simultaneously SERS and i-t measurement on Ag/AuNP-on-GME show our ability to manipulate the morphology of narrow inter AuNP-GME gaps. With the assistant of Ag shell or cluster on AuNP-on-GME, Raman enhancements can be tuned much more dramatically by electrochemical bias.

*This work is supported by the Engineering Research Centers Program of the National Science Foundation under NSF Cooperative Agreement No. EEC-1647837 and NSF (CBET1454544). We want to thank FIU AMERI for the use of SEM.
9:36AM L04.00007: Phonon-induced Spin State Relaxation in spin crossover molecule*
HAECHAN PARK (Presenter), HAI-PING CHENG, JIA CHEN, University of Florida — Spin crossover (SCO) materials have drawn intense attention lately due to its unique property to switch from low-spin to high-spin state by external stimuli. The relaxation time of the spin state is a critical quantity in all application areas. Whether SCO molecules are in solution or in crystal form, it is crucial to understand the spin dynamics of a single molecule. This study describes a method development that goes beyond our previous work on phonon-assisted electron relaxation processes where the total spin of the system remains unchanged. We discuss using spin-orbit coupling instead of kinetic energy of nuclei as a perturbation between states of different total spins. This method considers different nuclear positions in the configuration space generated by ab-initio molecular dynamics, which provides a suitable description for coupling between the vibrational modes of nuclei and the electron spins. We will demonstrate the dynamics of spin-dependent relaxation using our simulations


*This work is supported as part of M²QM, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0019330.

9:48AM L04.00008: Reveal the interplay between high frequency and low frequency intramolecular vibrational mode in ultrafast electron transfer reaction*
SHAHNAWAZ RATHER, BO FU (Presenter), GREG SCHOLES, Princeton University — We are presenting a theoretical study of an ultrafast electron transfer reaction by employing the Redfield theory of quantum dissipation dynamics and a model Hamiltonian involving three electronic states and two vibrational modes. Accompanying a pump-probe spectroscopy experiment of N, N'-Bis(2,6-methylphenyl)-3,4,9,10-pyrenetetracarboxylic Diimide (PDI) emerging in an electron-donating solvent, we are able to identify the role of vibronic coherence and the timescale separation due to the interplay between the high-frequency mode and the low-frequency mode. We found that vibronic coherences provide a complete blueprint of a three-stage process: an ultrafast ET event, an impulsive response of nuclear coherences (truest manifestation of Born-Oppenheimer approximation), and the relaxation of coherently prepared hot vibrational states. The outcome of this work also provides a potential design principle for preventing detrimental charge recombination in organic photovoltaics.

*S.R., B.F. and G.D.S. acknowledge support from the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences, of the U.S. Department of Energy through Grant No. DE-SC0015429.
The complex dynamics of ultrafast photoinduced reactions such as singlet fission are governed by their evolution along vibronically coupled potential energy surfaces. Here, I will describe our recent work on both understanding this coupling and manipulating it using ultrafast optical spectroscopy. Combining excited-state time-domain Raman spectroscopy and tree-tensor network state simulations, we construct the full 108-atom molecular movie of ultrafast singlet fission in a pentacene dimer, explicitly treating 252 vibrational modes on 5 electronic states. Our combined experimental and theoretical approach reveals the atomic-scale singlet fission mechanism and can be generalized to other ultrafast photoinduced reactions in complex systems. In other singlet fission systems, polydiacetylene and carotenoids, we experimentally demonstrate that S1 state (21Ag-) is a superposition state with strong contributions from spin-entangled pairs of triplet excitons (1(TT)). We further show that optical manipulation of the S1 (21Ag-) wavefunction using triplet absorption transitions allows selective projection of the 1(TT) component into a manifold of spatially separated triplet-pairs with lifetimes enhanced by up to one order of magnitude and whose yield is strongly dependent on the level of inter-chromophore coupling.

*This work was supported by the Engineering and Physical Sciences Research Council, UK (Grant Numbers EP/M025330/1, EP/M01083X/1, EP/L015552/1 and EP/M006360/1) and the Winton Programme for the Physics of Sustainability. J.W. acknowledges financial support from Singapore MOE Tier 3 Programme (MOE2014-T3-1-004). T.W. acknowledges the Marie Curie Intra European Fellowship (PIEF-GA-2013-623652) within the 7th European Community Framework Programme. C.S. acknowledges financial support by the Royal Commission for the Exhibition of 1851.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM
8:00AM L05.00001: Manipulating nonadiabatic conical intersection dynamics by optical cavities [invited]  SHAUL MUKAMEL (Presenter), BING GU, Chemistry, University of California Irvine — Optical cavities hold great promise to manipulate and control the photochemistry of molecules. We demonstrate how molecular photochemical processes can be manipulated by strong light-matter coupling. For a molecule with an inherent conical intersection, optical cavities can induce significant changes in the nonadiabatic dynamics by either splitting the pristine conical intersections into two novel polaritonic conical intersections or by creating light-induced avoided crossings in the polaritonic surfaces. This is demonstrated by exact real-time quantum dynamics simulations of a three-state two-mode model of pyrazine strongly coupled to a single cavity photon mode. We further explore the effects of external environments through dissipative polaritonic dynamics computed using the hierarchical equation of motion method. We find that cavity-controlled photochemistry can be immune to external environments. We demonstrate that the polariton-induced changes in the dynamics can be monitored by transient absorption spectroscopy.

References


8:36AM L05.00002: Effect of Stokes shift on molecular polariton dynamics*  JUSSI TOPPARI (Presenter), Department of Physics and Nanoscience Center, University of Jyväskylä, GERRIT GROENHOF, Department of Chemistry and Nanoscience Center, University of Jyväskylä, TERO T HEIKKILÄ, Department of Physics and Nanoscience Center, University of Jyväskylä — Strong coupling between molecules and confined light, like surface plasmon polaritons (SPP) or cavity photons (CP), leads to a formation of polariton states manifested by a Rabi split in the absorption spectrum. This changes the energy landscape of the molecules and can alter their chemical behavior. However, the Stokes shift of the molecule can play an essential role here.

We have studied molecular polaritons involving SPPs or optical cavities and different molecules. While the emission of SPP is purely transverse magnetic (TM), that of a SPP-molecule polariton has also a transverse electric (TE) component with the TE/TM ratio following the molecular contribution. Interestingly, we observe that the larger the Stokes shift of the molecule is, the lower is the TE emission. For cavities, the angle dependent emission of the lower CP-molecule polariton while exciting the upper polariton, reveals different pathways depending again on the Stokes shift. While molecules with high Stokes shift seem to induce regular molecule relaxation and excitation of the lower polariton via the fluorescing state, the molecules with no Stokes shift relax to the lower polariton via coupling to vibrational states. In both cases the effect of the molecular relaxation is eminent.

*Funding by Academy of Finland
OLEKSIY ROSLYAK (Presenter), Department of Physics and Engineering Physics, Fordham University, ERIC BITTNER, Department of Chemistry, University of Houston, ANDREI PIRYATINSKI, Theoretical Division, Los Alamos National Laboratory — Using our generalization of the Dicke model for quantum emitters coupled to surface plasmon modes, we have predicted a reach phase diagram of plasmon-exciton-polaritons states depending on the interaction strengths between the surface plasmon modes and quantum emitters.¹ For the purpose of practical implications, we study R6G rhodamine dye quantum emitters placed in a plasmonic cavity. The cavity is constituted from metal nanoparticles forming a rectangular 2D lattice. CDA analysis reveals intricate combinations of a bright local surface plasmon resonance (LSPR) on each nanoparticle and dark diffractive orders present in periodic structures resulting in a sharp Fano shaped surface lattice resonance (SLR). Concentration dependent coupling to R6G simulated via effective dielectric medium approach at CDA and RCWA levels. Extracted coupling rates between the SLR and the rhodamine dyes allow us to map the problem on the Dicke Hamiltonian. The polariton branches of the Hamiltonian are evaluated and subsequent analysis of the associated state photon emission properties is performed.

Bose-Einstein condensation has been realized for various particles or quasi-particles, such as atoms, molecules, photons, magnons and semiconductor exciton polaritons. We have experimentally realized a new type of condensate: a BEC of hybrids of surface plasmons and light in a nanoparticle array [1]. The condensate forms at room temperature and shows ultrafast dynamics. We utilized a special measurement technique, based on formation of the condensate under propagation of the plasmonic excitations, to monitor the sub-picosecond thermalization dynamics of the system. Recently, we have achieved such Bose-Einstein condensation also at the strong coupling regime, and shown by varying the lattice size that the thermalization in these systems is a simulated process that occurs in 100 femtosecond scale [2]. This new platform is ideal for studies of differences and connections between BEC and lasing [3,4,5]. While usually lasing in nanoparticle arrays occurs at the centre of the Brillouin zone, we have now demonstrated lasing also at the K-point [6]. The lasing mode can be identified with the help of group theory. Clear lasing is observed despite a narrow band gap at the K-point, which is promising considering future studies of topological photonics.

References
Tailoring weak-to-strong coupling of a plasmonic-photonic cavity*

FENG PAN (Presenter), RANDALL H. GOLDSMITH, University of Wisconsin - Madison — Control of light-matter interactions is important to a number of advances in quantum communication, information and sensing. Tailoring coupling strength relative to loss rates is central to exert control over the interactions. Recently we have demonstrated we could pin down a high dynamic range of system parameters in a coupled plasmonic-photonic cavity. Embedding the coupled cavity with an index-matching polymer matrix allows plasmonic and photonic modes to be largely overlapped and thus lifts up $g$ to the same order of magnitude as dominant nonradiative loss rate, potentially leading to a strongly coupled cavity. After the coupled cavity is embedded by polydimethylsiloxane (PDMS). Plasmonic resonance of a gold nanorod (AuNR) is red-shifted due to change of local dielectric environment around the AuNR. Decreasing the aspect ratio blue-shifts its plasmon resonance back to our spectral window and then we observe a splitting spectral feature that signifies strong coupling. This demonstration provides an avenue for tailoring weak-to-strong coupling, which foreshadows the potential of entangling multiple plasmonic systems through photonic mode for protection against decoherence in quantum communication.

*CHE-1836482; DMR-1610345

Strong coupling beyond the light-line*

KISHAN MENGHRAJANI (Presenter), WILLIAM L BARNES, University of Exeter — Many experiments on strong coupling of molecules make use of metal-clad microcavities. Coupling is usually investigated between the excitonic or vibronic molecular resonance (as appropriate) and the lowest order cavity mode. However, metal-clad microcavities also support a coupled surface plasmon mode, something that appears to have been ignored in previous work, probably because it exists beyond the light-line. Here we show that this coupled plasmon mode also interacts with molecular resonances to produce hybrid polariton modes.

We use a vibrational resonance in the polymer PMMA, incorporated into a microcavity with gold mirrors. Although the asymmetrically coupled surface plasmon (TM$_{1}$) mode has no cut-off, it lies outside the air light-line, we bring that mode inside the air light line by incorporating a grating structure into the lower gold mirror. The grating-scattered coupled plasmon mode is observed to strongly couple with the vibrational resonance. Our results indicate that this coupled plasmon mode should be taken into account when looking at how strong coupling may be used to alter/create molecular properties via strong coupling.

*Engineering and Physical Sciences Research Council (EPSRC, EP/L015331/1). European Research Council (ERC-2016-AdG-742222).
10:00AM L05.00007: Modified excited states dynamics in the nanoparticle plasmon – molecular exciton hybrids under strong coupling regime [Invited] TIMUR SHEGAI (Presenter), Physics, Chalmers University of Technology — Strong light-matter interactions in microcavities have been long known to provide means to alter optical and nonlinear properties of the coupled system. As a result of this interaction, one typically observes the emergence of new polaritonic eigenstates. These states are of hybrid nature and possess both light and matter characteristics, which is reflected in vacuum Rabi splitting, observed in the absorption or transmission spectra. Because of the hybrid nature of these states, the excited state temporal dynamics can be significantly altered in comparison to the uncoupled system dynamics. This, in turn, can have profound effects on the emission and photochemical processes.

Here, we show that individual plasmonic nanoantennas can strongly couple to molecular J-aggregates, resulting in splitting up to 400 meV, i.e. ~20% of the resonance energy. Moreover, we observe mode splitting not only in elastic scattering response but also in photoluminescence of individual hybrid nanosystems, which manifests a direct proof of strong coupling in plasmon-exciton nanoparticles. This situation is drastically different from the photoluminescence of uncoupled molecules, which signals the involvement of polaritonic states into the relaxation pathways of the hybrid system. We also discuss how the involvement of these pathways can modify excited state dynamics, including such important photochemical processes as photobleaching.

10:36AM L05.00008: Cavity Induced Non-adiabatic Effects and Modifications of the Spin-orbit Coupling* DOMINIK SIDLER (Presenter), MICHAEL RUGGENTHALER, HEIKO APPEL, ANGEL RUBIO, Max Planck Inst Structure & Dynamics of Matter — A numerically exact diagonalisation of the non-relativistic Pauli-Fierz Hamiltonian is performed for quantized three-body problems coupled to one cavity mode in 3D. The resulting 10-dimensional setup can be transformed into an effectively five dimensional problem, which is fully diagonalisable with state-of-the-art computers. This allows to investigate polaritonic effects for real systems (e.g. He or HD+) with high accuracy, potentially giving access to cavity induced non-adiabatic effects. Modifications of the fine-structure arising from the coupling to a quantized cavity mode can be treated perturbatively.

*Project RouTe (13N14839) is sponsored by the Federal Ministry of Education and Research

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L07 DQI: Autonomous QEC and Bosonic Codes 102 - Theodore Yoder, IBM

TJ Watson Research Center - Tag(s): Focus
Protecting a bosonic qubit with autonomous quantum error correction I – Theory

CHEN WANG (Presenter), JEFFREY GERTLER, Univ of Mass - Amherst — Existing demonstrations of quantum error correction are based on an active schedule of measurement and recovery operations which is hardware intensive and incurs additional error overhead. It is theoretically possible to correct quantum errors with dissipation in a continuous and autonomous fashion, without a classical controller. While dissipative confinement of a quantum system to a two-state manifold had been demonstrated, so far it has remained challenging to achieve a dissipation operator that counters the dominant natural errors in order to extend the lifetime of an encoded qubit. Here we present an autonomous error correction scheme for a bosonic qubit in a superconducting cavity, which directly corrects the dominant error channel of the system: single photon loss. In this Part I of the talk, we discuss this dissipative error correction protocol, its design considerations, as well as its expected performance and limitations.

*This research was supported by the U.S. Air Force for Scientific Research (AFOSR) and Army Research Office (ARO).

Protecting a bosonic qubit with autonomous quantum error correction II – Experiment

JEFFREY GERTLER (Presenter), Univ of Mass - Amherst, BRIAN BAKER, Physics and Astronomy, Northwestern University, JULIANG LI, Univ of Mass - Amherst, JENS KOCH, Physics and Astronomy, Northwestern University, CHEN WANG, Univ of Mass - Amherst — Existing demonstrations of quantum error correction are based on an active schedule of measurement and recovery operations which is hardware intensive and incurs additional error overhead. It is theoretically possible to correct quantum errors using dissipation in a continuous and autonomous fashion, without a classical controller. While dissipative confinement of a quantum system to a two-state manifold had been demonstrated, so far it has remained challenging to achieve a dissipation operator that counters the dominant natural errors in order to extend the lifetime of an encoded qubit. Here we present an autonomous error correction scheme for a bosonic qubit in a superconducting cavity, which directly corrects the dominant error channel of the system: single photon loss. In this Part II of the talk, we present our circuit QED setup and experimental results.

*This research was supported by the U.S. Air Force for Scientific Research (AFOSR) and Army Research Office (ARO).
8:24AM L07.00003: All-Gaussian universality and fault tolerance with the Gottesman-Kitaev-Preskill code*  
BEN Q BARAGIOLA, GIACOMO PANTALEONI, Center for Quantum Computation and Communication Technology, School of Science, RMIT, RAFAEL ALEXANDER (Presenter), Center for Quantum Information and Control, University of New Mexico, ANGELA KARANJAI, Centre for Engineered Quantum Systems, School of Physics, The University of Sydney, NICOLAS C MENICUCCI, Center for Quantum Computation and Communication Technology, School of Science, RMIT — The Gottesman-Kitaev-Preskill (GKP) encoding of a qubit within an oscillator is particularly appealing for fault-tolerant quantum computing with bosons because Gaussian operations on encoded Pauli eigenstates enable Clifford quantum computing with error correction. We show that applying GKP error correction to Gaussian input states, such as vacuum, produces distillable magic states, achieving universality without additional non-Gaussian elements. Fault tolerance is possible with sufficient squeezing and low enough external noise. Thus, Gaussian operations are sufficient for fault-tolerant, universal quantum computing given a supply of GKP-encoded Pauli eigenstates.  
*R.N.A. is supported by National Science Foundation Grant No. PHY-1630114. A.K. is supported by the Australian Research Council Centre of Excellence for Engineered Quantum Systems (Project No. CE170100009). This work is supported by the Australian Research Council Centre of Excellence for Quantum Computation and Communication Technology (Project No. CE170100012).

8:36AM L07.00004: Stabilization of finite-energy Gottesman-Kitaev-Preskill bosonic codes*  
BAPTISTE ROYER (Presenter), SHRADDHA SINGH, STEVEN GIRVIN, Department of Physics, Yale University — Due to their large Hilbert space and their high quality factors, microwave cavities are an attractive candidate for the encoding of logical quantum information. One promising choice of encoding in these cavities is the Gottesman-Kitaev-Preskill (GKP) code which allows to protect against small displacements in phase space. However, in their ideal form, GKP codewords contain an infinite amount of energy and, consequently, their experimental implementation cannot be exact. Nevertheless, recent experiments [Flühmann et al., Nature (2019), Campagne-Ibarcq et al., arXiv:1907.12487] have demonstrated that it is possible to obtain long coherence times for GKP logical qubits. In this talk, we investigate improved stabilization strategies tailored specifically for finite-energy GKP codes and study how these protocols perform in a superconducting implementation with realistic parameters.  
*This work was undertaken thanks in part to funding from the Army Research Office, grant No. W911NF-18-1-0212.
Path-independent gates for error-corrected quantum computing: Theory

WEN-LONG MA (Presenter), Pritzker School of Molecular Engineering, University of Chicago, PHILIP REINHOLD, SERGE ROSENBLUM, ROBERT SCHOELKOPF, Departments of Applied Physics and Physics, Yale University, LIANG JIANG, Pritzker School of Molecular Engineering, University of Chicago — Universal control of a quantum system can usually not be achieved by direct control of the system. To realize the missing unitary gates for universal control, we can couple an ancilla system with more complete functionality to the logical system and jointly control both systems. However, the ancilla often suffers much stronger noise than the logical system. Here, we propose a general class of quantum gates on the logical system that is path independent (PI) of Markovian ancilla error trajectories, including both ancilla relaxation and dephasing errors. By fixing the initial and final ancilla states, the designed gates can be PI of infinite-order ancilla dephasing errors, finite-order ancilla relaxation errors, and the combination of both. The PI gates can also be made error-transparent to the first-order logical system errors. As an example, we show that the photon-number selective arbitrary phase (SNAP) gates in circuit QED belong to such a class of PI gates. This proposal provides a hardware-efficient approach toward fault-tolerant quantum computation with system-specific error models.

Path-independent gates for error-corrected quantum computing: Experiment

SERGE ROSENBLUM (Presenter), PHILIP REINHOLD, Departments of Applied Physics and Physics, Yale University, WEN-LONG MA, Pritzker School of Molecular Engineering, University of Chicago, LUIGI FRUNZIO, Departments of Applied Physics and Physics, Yale University, LIANG JIANG, Pritzker School of Molecular Engineering, University of Chicago, ROBERT SCHOELKOPF, Departments of Applied Physics and Physics, Yale University — In future fault-tolerant quantum computers, errors resulting from noise and decoherence must be detected and corrected in real-time. This is particularly important while applying logical gates, which can cause errors to quickly spread throughout the system. Here, we present an error-corrected construction for a logical gate set [1] enacted by a multilevel transmon ancilla on a cavity-encoded logical qubit. We show that the logical information is maintained by detecting ancilla errors and applying the appropriate corrections to the logical qubit. The error-corrected operation is path-independent of dominant ancilla errors, leading to a sixfold suppression of the gate error with increased energy relaxation, and a fourfold suppression with increased dephasing noise. The results support the viability of hardware-efficient bosonic quantum computation by showing that bosonic qubits can be controlled by error-prone ancillas without inheriting their inferior performance.


*This research was supported by the Army Research Office (W911NF-18-1-0212), and the Air Force Office of Scientific Research (FA9550-14-1-0052 and FA9550-15-1-0015).
9:12AM L07.00007: Error-transparent operations on a logical qubit protected by quantum error correction
YUWEI MA (Presenter), YUAN XU, XIANGHAO MU, WEIZHOU CAI, LING HU, WEITING WANG, XIAOXUAN PAN, HAIYAN WANG, YIPU SONG, Tsinghua University, CHANGLING ZOU, USTC, LUYAN SUN, Tsinghua University — Universal quantum computation is striking for its unprecedented capability in processing information, but its scalability is challenging in practice because of the inevitable environment noise. Although quantum error correction (QEC) techniques have been developed to protect stored quantum information from leading orders of errors, the noise-resilient processing of the QEC-protected quantum information is highly demanded but remains elusive. Here, we demonstrate phase gate operations on a logical qubit encoded in a bosonic oscillator in an error-transparent (ET) manner. The ET gates are extended to the bosonic code and are able to tolerate errors during the gate operations, regardless of the random occurrence time of the error. With precisely designed gate Hamiltonians through photon-number-resolved AC-Stark shifts, the ET condition is fulfilled experimentally. We verify that the ET gates outperform the non-ET gates with a substantial improvement of the gate fidelity after an occurrence of the single-photon-loss error. Our ET gates in the superconducting quantum circuits are readily for extending to multiple encoded qubits and a universal gate set is within reach, paving the way towards fault-tolerant quantum computation.

9:24AM L07.00008: High-impedance circuits for parity measurements of cat qubits
CLARKE SMITH (Presenter), MARIUS VILLIERS, RAPHAËL LESCANNE, ANTOINE MARQUET, Ecole Normale Supérieure, CAMILLE BERDOU, MINES ParisTech, TAKIS KONTOS, Ecole Normale Supérieure, MAZYAR MIRRAHIMI, INRIA, ZAKI LEGHTAS, MINES ParisTech — Encoding a qubit in the two degenerate steady states of an oscillator—which only exchanges pairs of photons with its environment—can exponentially suppress the bit-flip rate for large phase-space separations. The unsuppressed phase flips of these so-called "cat qubits" correspond to a change in the photon number parity of the oscillator, and they could be corrected using redundant encoding. In such a scheme, errors are detected via measurements of the joint parity between cat qubits, which could be implemented at the Hamiltonian level using effective parity-type couplings. We show that a parity-type Hamiltonian emerges from the conventional Josephson potential in the limit of high oscillator impedance. Here, the high impedance guarantees large fluctuations of the superconducting phase, which translates into large displacements in oscillator phase space. We present the design of a superconducting circuit that effectively realizes the parity-type Hamiltonian, as well as the status of its experimental implementation.

*Funding provided by ANR, Ville de Paris
9:36AM L07.00009: Experimental implementation of fault-tolerant error syndrome measurement for pair-cat code (1/2)*  AKSHAY KOOTTANDAVIDA (Presenter), IOANNIS TSIOUTSIOS, SHANTANU O MUNDHADA, LUIGI FRUNZIO, MICHEL H. DEVORET, Yale University — Stabilized quantum manifolds of a bosonic system can encode error-protected qubits. In particular, a single-mode manifold spanned by cat states can exponentially suppress against phase-flip errors. However, errors due to photon loss cannot be corrected without stopping the stabilization process, using existing microwave superconducting circuit technology. Phase-flip suppression can also be achieved by stabilizing a manifold spanned by pair-cat states, which are superpositions of the two-mode states called Barut-Girardello/pair-coherent states. Moreover, it is now possible to detect, in a fault-tolerant manner, photon-loss errors in either mode, simultaneously with the manifold stabilization, by monitoring the photon-number difference between them. In this talk, we will present an experimental implementation of cavities and superconducting devices that is compatible with such encoding. We will also report on techniques of continuous monitoring of the photon number difference between the modes. Part-one of this two-part presentation will introduce the basic theoretical concepts of pair-cat codes and the design parameters of our experimental implementation.

*ARO, ONR, NSF, AFOSR, and YINQE

9:48AM L07.00010: Experimental implementation of fault-tolerant error syndrome measurement for pair-cat code (2/2)*  IOANNIS TSIOUTSIOS (Presenter), AKSHAY KOOTTANDAVIDA, SHANTANU O MUNDHADA, LUIGI FRUNZIO, MICHEL H. DEVORET, Department of Applied Physics, Yale University — Stabilized quantum manifolds of a bosonic system can encode error-protected qubits. In particular, a single-mode manifold spanned by cat states can exponentially suppress against phase-flip errors. However, errors due to photon loss cannot be corrected without stopping the stabilization process, using existing microwave superconducting circuit technology. Phase-flip suppression can also be achieved by stabilizing a manifold spanned by pair-cat states, which are superpositions of the two-mode states called Barut-Girardello/pair-coherent states. Moreover, it is now possible to detect, in a fault-tolerant manner, photon-loss errors in either mode, simultaneously with the manifold stabilization, by monitoring the photon-number difference between them. In this talk, we will present an experimental implementation of cavities and superconducting devices that is compatible with such encoding. We will also report on techniques of continuous monitoring of the photon number difference between the modes. Part-two of this two-part presentation will present our most recent experimental progress.

*Work supported by: ARO, ONR, NSF, AFOSR, and YINQE
10:00AM L07.00011: Progress on fault-tolerant quantum computing with concatenated bosonic-qubit codes* ARNE GRIMSMO (Presenter), STEFANUS EDGAR TANUARTA, JULIETTE SOULE, Univ of Sydney, BEN Q BARAGIOLA, RMIT University, JOSHUA L. A. COMBES, University of Queensland — In this talk I will discuss ongoing work to quantify the performance of bosonic error correcting codes concatenated with conventional qubit codes. There are two questions we are trying to answer: 1. When does using a bosonic code at the ground level of a concatenated scheme outperform using two-level systems? 2. How do different bosonic codes compare to each other. We would like to answer both of these questions in a fault-tolerant setting that includes state preparation and measurement noise, as well as noise during the error correction circuit.

*This work was supported by the Australian Research Council (ARC) via a Discovery Early Career Research Award (DE190100380).

10:12AM L07.00012: Fault-Tolerant Bosonic Quantum Error Correction with the Surface-GKP Code KYUNGJOO NOH (Presenter), Yale University, CHRISTOPHER CHAMBERLAND, IBM Thomas J. Watson Research Center — Bosonic quantum error correction is a viable option for realizing error-corrected quantum information processing in continuous-variable bosonic systems. Here, we consider the concatenation of the bosonic Gottesman-Kitaev-Preskill (GKP) code with the surface code, namely, the surface-GKP code. In particular, we thoroughly investigate the performance of the surface-GKP code by assuming realistic GKP states with a finite squeezing and noisy circuit elements due to photon losses. By using a minimum-weight perfect matching decoding algorithm on a 3D space-time graph, we show that fault-tolerant bosonic quantum error correction is possible with the surface-GKP code if the squeezing of the GKP states is higher than 11.2dB in the case where the GKP states are the only noisy elements. We also show that the squeezing threshold changes to 18.6dB when both the GKP states and circuit elements are comparably noisy. At this threshold, each circuit component fails with probability 0.69%. Finally, if the GKP states are noiseless, fault-tolerant quantum error correction with the surface-GKP code is possible if each circuit element fails with probability less than 0.81%.
10:24AM L07.00013: Majorana dimer models of holographic quantum error correction

ALEXANDER JAHN (Presenter), MAREK GLUZA, FERNANDO PASTAWSKI, JENS EISERT, Dahlem Center for Complex Quantum Systems, Free University of Berlin — Holographic quantum error-correcting codes have been proposed as toy models describing key aspects of the AdS/CFT correspondence. In this talk, we introduce a versatile framework of Majorana dimers capturing the intersection of stabilizer and Gaussian Majorana states. This picture allows for an efficient contraction with a simple diagrammatic interpretation and is amenable to analytical study of holographic quantum error-correcting codes. Equipped with this framework, we revisit the recently proposed hyperbolic pentagon code (HyPeC) and demonstrate efficient computation of boundary state properties for generic logical bulk input. We show that the dimers characterizing boundary states of the HyPeC follow discrete bulk geodesics. From this geometric picture, properties of entanglement, quantum error correction, and bulk/boundary operator mapping immediately follow, offering a fresh perspective on holography. We also elaborate upon the emergence of the Ryu-Takayanagi formula from our model, which shares many properties of the recent bit thread proposal.

Our work thus elucidates the connection between bulk geometry, entanglement, and quantum error correction in AdS/CFT, and lays the foundation for new models of holography. We close with an outlook on the boundary symmetries of holographic Majorana dimer models and discuss the connection to the strong disorder renormalization group.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM

Session L08 DQI: Superconducting Qubits: Materials, Fabrication and Coherence II 104 - Martin Weides, Univ of Glasgow

8:00AM L08.00001: PAMBE grown NbTiN-AlN-NbTiN Josephson junction heterostructures for superconducting quantum circuits

CHRISTOPHER RICHARDSON (Presenter), AUSTIN THOMAS, ASHISH ALEXANDER, CHRISTOPHER WEDDLE, ALAN KRAMER, Laboratory for Physical Sciences, MATTHEW OLSZTA, BRUCE AREY, Pacific Northwest National Laboratory — Plasma assisted molecular beam epitaxy (PAMBE) is used to grow niobium titanium nitride alloys (Nb$_x$Ti$_{1-x}$N) superconductors and wide bandgap nitride (AlN) trilayers directly on c-plane sapphire wafer. This combination of nitride materials provides sufficient degrees of freedom that synthesis of an epitaxial Josephson junction may be possible. Using a structure first approach to design optimization, the structural, surface topology, bonding, and interface characteristics will be described. Superconducting characteristics including microwave loss and work towards IV transport through Josephson junction devices will be discussed.
As the lifetime of superconducting qubits has increased, large temporal fluctuations in the relaxation time $T_1$ of the excited state have been observed by different groups. We have measured such fluctuations in several Al/AlOx/Al transmons mounted in 3-D aluminum cavities. Our longest lived device showed $T_1$ that varied from 100 to 300 μs at 20 mK. Comparing with shorter lived transmons, we find that the size of the fluctuations in $T_1$ appears to scale with $T_1$. Measurements of $T_1$ versus temperature from 20 to 300 mK reveal that the fluctuations depend on temperature and support the idea that non-equilibrium quasiparticles are the dominant source of dissipation in these devices.

*This work was supported by the Maryland Quantum Materials Center, the Joint Quantum Institute, and the Laboratory for Physical Sciences.

Protecting superconducting qubits from low-frequency noise is important for advancing superconducting quantum computation. We present a protocol for engineering dynamical sweet spots protecting against 1/f noise, using a periodic drive. The position and strength of dynamical sweet spots can be obtained analytically in the framework of Floquet theory. For the example of fluxonium biased slightly away from half a flux quantum, we predict an improvement in pure-dephasing time from less than 1 μs to over 1 ms. Using the Floquet eigenstates as the computational basis, we show that high-fidelity single-qubit gates can be implemented at dynamical sweet spots. We further confirm that qubit readout can be performed by adiabatically mapping the qubit's Floquet states to the static qubit states, and subsequently employing standard measurement techniques.

*Army Research Office Grant No. W911NF1910016
8:36AM L08.00004: Investigating the mechanisms of charge-parity switching in offset-charge-sensitive transmons* SPENCER DIAMOND (Presenter), Department of Applied Physics, Yale University, KYLE SERNIAK, MIT Lincoln Lab, MAX HAYS, VALLA FATEMI, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Department of Applied Physics, Yale University, GIANLUIGI CATELANI, Forschungszentrum Julich, MANUEL HOUZET, CEA Grenoble, LEONID GLAZMAN, MICHEL H. DEVORET, Department of Applied Physics, Yale University — Charge-parity switches in superconducting qubits contribute to decoherence and limit qubit performance. In the past, such decoherence was exclusively attributed to pre-existing non-equilibrium quasiparticles tunneling across Josephson junctions and exchanging energy with the qubit. However, it was recently predicted that high-frequency photons can be efficiently absorbed at transmon Josephson junctions and cause charge-parity switches. This process requires no pre-existing quasiparticles, but in fact generates two quasiparticles and can likewise change the qubit state. These two types of charge-parity switches are distinguishable by their relative rates of qubit excitation and relaxation, which have been measured in single-junction offset-charge-sensitive transmons. The transition rates were found to be inconsistent with a thermal distribution of quasiparticles in the superconductor tunneling across the junction, but may be explained by photon-assisted tunneling events. Here, we will present experimental results demonstrating that adding flux-tunability to our device can further distinguish between these charge-parity switch-induced decoherence mechanisms.

*Work supported by: ARO, ONR, AFOSR, NSF and YINQE

8:48AM L08.00005: Effect of external high-energy radiation on coherence of superconducting qubits ANTTI VEPSALAINEN (Presenter), AMIR KARAMLOU, Massachusetts Institute of Technology MIT, JOHN LAURENCE ORRELL, Pacific Northwest National Laboratory, AKSHUNNA S DOGRA, FRANISICA VASCONCELOS, Massachusetts Institute of Technology MIT, BEN LOER, Pacific Northwest National Laboratory, BETHANY NIEDZIELSKI, ALEXANDER MELVILLE, DAVID KIM, MOLLIE SCHWARTZ, JONILYN YODER, MIT Lincoln Laboratory, BRENT A VANDEVENDER, Pacific Northwest National Laboratory, SIMON GUSTAVSSON, WILLIAM OLIVER, Massachusetts Institute of Technology MIT — There is an anomalously high density of broken Cooper pairs in superconductors, which has been universally seen in experiments. It has been shown that external radiation can break Cooper pairs in superconducting circuits, causing elevated quasiparticle densities. The origin of the radiation has been a source of extensive research over several decades, but no conclusive answer has been found. It is known that thermal effects cause a finite quasi-particle density, but the observed densities are several orders of magnitudes higher than predicted by thermal equilibrium model. In superconducting devices infrared photons have shown to contribute to non-equilibrium quasi-particle densities through connected microwave lines. We propose that in addition to this effect, gamma-rays from radioactive decays in the environment are also a significant source of quasi-particle breaking radiation. We have measured the strength of the external radiation in our laboratory and demonstrated the effect of the high-energy radiation on qubit coherence using a Cu64 source with time-varying intensity. We show that proper shielding from gamma-rays is required for reaching high coherence times in transmon qubits.
9:00AM L08.00006: Synchrotron X-ray studies of superconducting qubit materials*  IGNACE JARRIGE (Presenter), National Synchrotron Light Source II, Brookhaven National Laboratory, ANJALI PREMKUMAR, Department of Electrical Engineering, Princeton University, CONAN R WEILAND, Materials Measurement Science Division, National Institute of Standards and Technology, JACK BERTHOLD, ALEXANDER PLACE, Department of Electrical Engineering, Princeton University, IRA WALUYO, ADRIAN HUNT, ANDREW M. KISS, YONG CHU, VALENTINA BISOGNI, JONATHAN PELLICIARI, ABDUL K RUMAIZ, National Synchrotron Light Source II, Brookhaven National Laboratory, MIKE MILLER, PAULA RUSSO, Angstrom Engineering Inc., DAVID I SCHUSTER, Department of Physics and the James Franck Institute, University of Chicago, ANDREW HOUCK, Department of Electrical Engineering, Princeton University — Despite dramatic improvements in the coherence times of superconducting qubits over the past decade, further progress is still needed to push quantum computers towards reality. Recent breakthroughs highlighted the paramount role played by the defect-prone native surface oxide layers in limiting the coherence of qubits. However, very little is known about the defects and their mechanism of coupling to the qubit degree of freedom, in part due to the lack of suitable probes for defects in thin amorphous layers. Here, we report on the combined use of synchrotron X-ray scattering and spectroscopic tools to probe the surface electronic and bulk structural properties of Nb thin films deposited on sapphire, which emulate qubit capacitor pads. The thin films were deposited using four different techniques yielding varying film qualities and densities. Material properties, including crystalline grain sizes and surface oxide layer thicknesses and compositions, will be discussed in light of the coherence times obtained for transmon qubits using Nb capacitor pads deposited with the same four techniques. We will discuss possible scenarios for the correlations between the material properties and the qubit performance.

*AP, BJ, & AP thank ARO, NSF GRF, Humboldt Foundation, & NDSEG.

9:12AM L08.00007: Highly uniform submicron junction arrays and applications to next generation photodetectors*  JOHN MARK KREIKEBAUM (Presenter), University of California, Berkeley, KEVIN O'BRIEN, Massachusetts Institute of Technology, BAPTISTE ROYER, Universite de Sherbrooke, ARNE GRIMSMO, University of Sydney, ALEXANDREblaís, Universite de Sherbrooke, IRFAN SIDDIQI, University of California, Berkeley — Josephson junctions are an ubiquitous circuit element in cQED experiments. In complex devices with many such junctions, such as state-of-the-art microwave photon detectors, precise control over each junction's critical current is often required, and thus variations of the junction area and tunnel barrier thickness must be sufficiently minimized. Analyzing junction array resistance distributions from many wafers, we have identified several key processing variables to improve uniformity. Using this optimized recipe, we have fabricated and benchmarked a single microwave photon detector utilizing four identical transmons to mediate cross-Kerr coupling between a photon input waveguide and a readout resonator. Plans to increase detector performance by distributing the coupling over 1000's of junctions will be discussed; a very challenging device to build without the uniformity improvements presented.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05-CH11231.
9:24AM L08.00008: Loss Characterization in Superconducting Resonators  
ALEXANDER MELVILLE (Presenter), GREG CALUSINE, WAYNE WOODS, KYLE SERNIAK, EVAN GOLDEN, ARJAN SEVI, JONILYN YODER, WILLIAM OLIVER, MIT Lincoln Laboratory — Uniquely characterizing loss from two-level systems (TLS) in dielectric materials in coplanar waveguide resonators is challenging due to the nearly proportional scaling of the electric field participation in response to changes in geometry and anisotropic trench depth [1]. We tailor our resonator design and fabrication process to focus the participation into specific dielectric regions such that we can characterize the specific loss tangent of each dielectric [2]. In this talk, we characterize the change in overall quality factor and dielectric-specific loss tangent arising from specific changes to the fabrication process.


*This material is based upon work supported by the Department of Defense under Air Force Contract No. FA8721-05-C-0002. Any opinions, findings, conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the Department of Defense.

9:36AM L08.00009: Modeling geometric dependence of dielectric losses in superconducting coplanar-waveguide resonators  
VALTTERI LAHTINEN (Presenter), MIKKO MOTTONEN, Aalto University — Superconducting coplanar-waveguide (CPW) resonators are essential devices in circuit quantum electrodynamics (cQED). Their performance is limited by dielectric losses in the substrate and in the thin lossy oxide layers on the material interfaces. Reliable modeling is required to aid in the design of low-loss CPW structures for cQED. We analyze the geometric dependence of the dielectric losses in CPW structures using finite-element modeling of the participation ratios of the lossy regions. Material and device specific parameters of these regions are generally not known accurately enough, introducing uncertainty in the simulations. To this end, we carry out simulations on a range of CPW geometries and parameters. Combining the simulations with measured two-level-system-limited Q factors of CPW resonators, we solve an inverse problem to find optimal model parameters producing these values. Utilizing this model and our geometric-dependence analysis, we predict high Q factors obtainable by optimizing the cross-sectional geometries of the measured CPW structures. Our results guide the fabrication of low-loss CPW resonators for cQED.

*Support from Jane and Aatos Erkko Foundation, Vilho, Yrjö and Kalle Väisälä Foundation and the Technology Industries of Finland Centennial Foundation.
Reducing dephasing for flux control of superconducting qubits

NICOLAS DIDIER (Presenter), Rigetti Quantum Computing — Scaling up superconducting quantum processors with optimized performance requires sufficient flexibility in the choice of operating points for single and two qubit gates to maximize their fidelity and cope with imperfections. Flux control is an efficient technique to manipulate the parameters of tunable qubits, in particular to activate entangling gates. It however suffers from enhanced dephasing, induced by the ubiquitous 1/f flux noise at flux sensitive points of operation. We consider how flux pulses can protect a tunable qubit from slow flux noise for a range of frequencies in the tunability band. Preserving long coherence times during qubit interactions could furthermore alleviate the constraints on coupling strength and unlocks high fidelities for both single and two qubit gates in a scalable architecture based on static couplings.

Characterizing noise for capacitively-shunted flux qubits

VINAY TRIPATHI (Presenter), MOSTAFA KHEZRI, HUO CHEN, DANIEL A LIDAR, Univ of Southern California — Capacitively-shunted flux qubits (CSFQs), due to their high anharmonicity together with reduced persistent currents allow for relatively fast control pulses and long coherence times. This makes them a suitable candidate for both gate model quantum computing and quantum annealing. We report a joint theoretical-experimental study of 1/f noise in CSFQs using Macroscopic Resonance Tunneling (MRT). MRT has been used for flux qubits to characterize low-frequency flux noise using well established theoretical models. A detailed theoretical explanation of higher order MRT with correction of junction asymmetry is important for our understanding of noise in CSFQs. We carry out analyses of different theoretical models that account for relaxation and dephasing to explain experimental $T_1$ and $T_2$ results obtained from studies of CSFQs.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.
Hexagonal boron nitride (hBN), an insulating 2-D(van der Waals) material that features an essentially defect-free bulk and atomically flat surfaces through mechanical exfoliation, may be used to build high-quality Josephson elements and qubit capacitors. We study hBN in the microwave regime via lateral capacitive coupling and parallel plate capacitors. In the single-photon limit, the extracted quality factor of hBN is bounded below at ~ 200,000. Beyond hBN, this measurement technique can also be used to explore new material platforms for superconducting technologies.

*This research was funded in part by the ARO grant No. W911NF-18-1-0116; and by the Department of Defense via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.
10:24AM L08.00013: Loss Mechanisms in Superconducting Quantum Transmission Line Metamaterials* TAMIN TAI (Presenter), JINGNAN CAI, STEVEN ANLAGE, Physics Department, University of Maryland, College Park — Superconducting quantum bits (qubits) coupled with resonators are widely utilized for applications in quantum computing. Efforts are under way to scale up the numbers of qubits, but there are many recurring issues of dielectric loss of substrate materials, two level systems, and quasi-particles loss, all leading to decoherence of superconducting qubits. In order to understand different loss mechanisms, our group is fabricating many high-quality aluminum half wavelength transmission line resonators by e-beam deposition and photo-lithography methods. Through the investigation of power dependence and temperature dependence of these transmission line resonators, and comparison with different theoretical models, the dominant loss mechanism in our half wavelength transmission line can be identified. This transmission line will later host many flux qubits to study the collective behavior of a quantum metamaterial system.

*This work is funded by US Department of Energy through Grant # DESC0018788 and CNAM.

10:36AM L08.00014: Over-100µs tunable planar transmons: epitaxial Josephson Junctions and design optimization* ANASTASIYA PISHCHIMOVA, DMITRIY MOSKALEV, ALEKSEI MATANIN (Presenter), FMN Laboratory, Bauman Moscow State Technical University, ALINA DOBRONOSOVA, Dukhov Automatics Research Institute, (VNIIA), DARIA EZENKOVA, FMN Laboratory, Bauman Moscow State Technical University, ELIZAVETA IL'INICHNA MALEVANNAYA, Dukhov Automatics Research Institute, (VNIIA), ILYA BESEDIN, National University of Science and Technology, OLGA SOROKINA, LUCIA ALMIROVNA GANIEVA, Dukhov Automatics Research Institute, (VNIIA), ANDRONIC MICHAEL, VLADIMIR VLADIMIROVICH ECHEISTOV, FMN Laboratory, Bauman Moscow State Technical University, ALEXANDER VYACHESLAHOVICH ZVEREV, Dukhov Automatics Research Institute, (VNIIA), DMITRIY SERGEEVICH YAKOVLEV, Institute of Solid State Physics, Russian Academy of Sciences, ILYA RODIONOV, FMN Laboratory, Bauman Moscow State Technical University — Since superconducting qubits discovery over twenty years ago energy relaxation times has been improved by several orders. Josephson junctions, a crucial nonlinear component of superconducting qubits, are still fabricated from two aluminum polycrystalline electrodes with lossy amorphous aluminum oxide in between. Here we demonstrate our results in reducing two-level states (TLS) in amorphous oxides by means of Josephson Junctions optimization, thus reducing the participation of the lossy materials and interfaces. We carry out a comparative analysis of tunable X-mon qubit lifetimes based on various Josephson Junctions design types, demonstrating several times coherence improvement. From the other hand, we propose novel superconducting qubits fabrication technique based on Josephson junction epitaxial growth with inorganic masks. To experimentally test the proposed approaches we demonstrate tunable X-mon qubits with coherence over 100 microseconds.

*Devices were fabricated at the BMSTU Nanofabrication Facility (Functional Micro/Nanosystems, FMNS REC, ID 74300).
8:00AM L09.00001: Breakdown of phenomenological Lindblad master equations in the strong coupling regime*  
BRUNO TAKETANI (Presenter), Univ Federal de Santa Catarina, J. MAURICIO TORRES, Instituto de Física, Benemérita Universidad Autónoma de Puebla, RALF BETZHOLZ, School of Physics and International Joint Laboratory on Quantum Sensing and Quantum Metrology, Huazhong University of Science and Technology — The Lindblad form of the master equation has proven to be one of the most convenient ways to describe the impact of an environment interacting with the quantum systems of interest. For single quantum systems, the jump operators that characterize this interaction usually take simple forms, with clear experimental/physical interpretation. However, for coupled quantum systems the jump operators can take significantly different forms and in general the total Lindbladian for the system cannot be described by separate Lindbladians acting on the individual quantum systems. In this talk we investigate the effects of such separate, phenomenological description in optomechanical and spin-boson systems, which are particularly pronounced in the strong coupling regime and compare the results with a more realistic microscopic derivation of the master equation. We show that these approaches, phenomenological and microscopic, lead to different solutions to the model and we explore the parameter regime and conditions where these differences manifest themselves in an experiment. We propose an experiment with superconducting systems to investigate these issues and the breakdown of the phenomenological approach with increasing coupling strength.

*Supported by CAPES PROCAD, CNPq INCT-IQ 465469/2014-0.
Entanglement classifier in chemical reactions*  
JUNXU LI (Presenter), SABRE KAIS, Department of Chemistry and Physics, Purdue Univ — The Einstein, Podolsky, and Rosen (EPR) entanglement, which features the essential difference between classical and quantum physics, has received wide theoretical and experimental attentions. Recently, the desire to understand and create quantum entanglement between particles such as spins, photons, atoms, and molecules is fueled by the development of quantum teleportation, quantum communication, quantum cryptography, and quantum computation. Although most of the work has focused on showing that entanglement violates the famous Bell's inequality and its generalization for discrete measurements, few recent attempts focus on continuous measurement results. Here, we have developed a general practical inequality to test entanglement for continuous measurement results, particularly scattering of chemical reactions. After we explain how to implement this inequality to classify entanglement in scattering experiments, we propose a specific chemical reaction to test the violation of this inequality. The method is general and could be used to classify entanglement for continuous measurement results.

*This study is based on work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under award number DE-SC0019215.

Concurrence and Discord measurements in a Kitaev type 1D Spin chain  
VIMALESH VIMAL (Presenter), IIT Kanpur — We present the study of concurrence and quantum discord in the ground state of 1D spins. The spins have the nearest neighbor Kitaev type interaction with the external transverse magnetic field. The system with periodic boundary condition gives the translation symmetry which simplifies the study to pairwise concurrence and discord at the odd and the even pair of sites separately. The correlation measures do not depend on the direction of the external field. They show dependence on spin length in the smaller chain but saturate quickly. The concurrence and the discord show the peak structure in the critical region but their derivatives do not show pronounced singularity to trace the phase transition of the system. The discord quantifies the correlation better as it gives finite correlation in the region where concurrence goes to zero.

Reference:  
8:36AM L09.00004: Triangle Nonlocality: genuine quantum nonlocality and quantum Finner inequality* [Invited] Marc-Olivier Renou (Presenter), ICFO Barcelona, Salman Beigi, IPM Theran, Nicolas Brunner, Nicolas Gisin, Sadra Boreiri, University of Geneva, Yuyi Wang, Computer Science, ETH Zurich, Elisa Bäumer, ETH Zurich — Network nonlocality extends standard Bell nonlocality to networks, where several independent sources are distributed to several parties according to the network structure. Contrary to standard Bell Nonlocality, this problem is non convex: no efficient systematic way to tackle it is known, either for local or quantum correlations. It is only partially understood for the simplest scenarios of bilocality (extended to star-locality and nonlocality on a line). However, for scenarios with loops, e.g. the triangle network, nothing is known except examples directly deduced from the usual form of quantum nonlocality (via the violation of a standard Bell inequality). This can even be done without using inputs. The question of finding a genuine quantum violation of triangle network locality was open the last years.

In this talk, we first present a novel example of quantum nonlocality without inputs in the triangle network, which we believe represent a new form of quantum nonlocality, genuine to the triangle network. It involves both entangled qubit states and joint entangled measurements. We generalize it to qutrits shared states and any odd-cycle networks.

Then, we move to the question of the characterization of local and quantum correlations. We derive a bound, the quantum Finner inequality (already known to hold for local resources), which we also demonstrate to hold when the sources are arbitrary no-signaling boxes which can be wired together. We generalize this bound to all networks involving bipartite sources. We discuss it as an application for the device-independent characterization of the topology of a quantum network.

We conclude with some open questions related to quantum network nonlocality.

This talk is based on the two letters arXiv:1905.04902 and arXiv:1901.08287.

*Swiss national science foundation (Starting grant DIAQ, NCCR-QSIT and NCCR-Swissmap).

9:12AM L09.00005: Evolution of entanglement in collective excitations in linear atomic chains Emily Townsend (Presenter), Garnett Bryant, National Institute of Standards and Technology, Abhikbrata Sarkar, Indian Institute of Technology, Kharagpur, India. — Quantum simulation of small physically realizable systems (e.g. chains of precision placed dopant atoms in silicon) provides an opportunity to learn about many-body physics at larger scale. Electrons in 1-D atomic chains with a long range coulomb interaction support plasmonic excitations of various modes and occupations of these modes, as linear superpositions of single particle excitations. We examine the time evolution of entanglement following plasmonic excitation due to coupling between the atomic chain and dipole emitters. We compare the results for a wide range of interaction strength between the electrons, from non interacting to strongly coupled and for pumping various plasmonic modes.
9:24AM L09.00006: Entanglement and impropriety*  BRIAN LA COUR (Presenter), THOMAS YUDICHAK, University of Texas at Austin — We describe a classical model of quantum entanglement corresponding to spontaneous parametric downconversion. Specifically, we consider the interaction of classical stochastic vacuum modes from the zero-point field and a high intensity pump with a nonlinear optical medium. The vacuum modes are treated as proper complex Gaussian random variables and are the sole source of randomness in the model. Phase matching conditions mimic the quantum mechanical energy and momentum conservation laws and result in outgoing classical fields of maximum intensity. The resulting transformation resembles the Bogoliubov transformation for multi-mode squeezed light, albeit with operators replaced by random variables, and yields a vector of improper complex Gaussian random variables. Using an amplitude threshold detection and post-selection measurement scheme, the degree of impropriety is found to correspond to the degree of entanglement in the corresponding quantum description.

*This work was supported by the Office of Naval Research under Grant No. N00014-14-1-2107.

9:36AM L09.00007: Tripartite information, scrambling, and the role of Hilbert space partitioning in quantum lattice models*  OSKAR SCHNAACK, NIKLAS BÖLTER, SEBASTIAN PAECKEL, SALVATORE MANMANA (Presenter), STEFAN KEHREIN, University of Gottingen, MARKUS SCHMITT, University of California, Berkeley — For the characterization of the dynamics in quantum many-body systems the question how information spreads and becomes distributed over the constituent degrees of freedom is of fundamental interest. The delocalization of information under many-body dynamics has been dubbed scrambling and out-of-time-order correlators were proposed to probe this behavior. In this work we investigate the time evolution of tripartite information as a natural operator-independent measure of scrambling, which quantifies to which extent the initially localized information can only be recovered by global measurements. Studying the dynamics of quantum lattice models with tunable integrability breaking we demonstrate that in contrast to quadratic models generic interacting systems scramble information irrespective of the chosen partitioning of the Hilbert space, which justifies the characterization as scrambler. Without interactions the dynamics of tripartite information in momentum space reveals unambiguously the absence of scrambling.

*We acknowledge financial support by SFB/CRC 1073 (project B03) and by Research Unit FOR 1807 (project P7) of the DFG, the Studienstiftung des Deutschen Volkes, the Leopoldina Fellowship Programme of the German Nat. Acad. of Sciences Leopoldina, and by the Simons Foundation.
9:48AM L09.00008: Tsirelson Polytopes and Randomness Generation* PETER BIERHORST (Presenter), Mathematics, University of New Orleans, YANBAO ZHANG, NTT Corporation, EMANUEL H KNILL, National Institute of Standards and Technology — We classify the extreme points of polytopes of probability distributions in the (2,2,2) Bell-CHSH setting that are induced by a single Tsirelson bound. We also do the same for a parametrized family of polytopes obtained from two Tsirelson bounds that interact non-trivially. Such constructions can be applied to device-independent random number generation using the method of probability estimation factors (PRA 98:040304(R) (2018), arXiv:1812.07786, arXiv:1806.04553). We demonstrate a meaningful improvement in certified randomness applying the new polytopes characterized here.

*This work was partially supported by NSF grant number 1839223 and Louisiana Board of Regents contract number LEQSF(2019-22)-RD-A-27.

10:00AM L09.00009: Experimental Certification of a Minimal Informationally Complete Positive Operator-Valued Measure in a Device-Independent Protocol* MASSIMILIANO SMANIA (Presenter), Stockholm University, PIOTR MIRONOWICZ, Gdansk University of Technology, MOHAMED NAWAREG, Stockholm University, MARCIN PAWLOWSKI, University of Gdansk, ADAN CABELLO, Universidad de Sevilla, MOHAMED BOURENNANE, Stockholm University — Minimal informationally complete positive operator-valued measures (MIC-POVMs) are a special kind of measurements in quantum theory that have the property that the statistics of their $d^2$-outcomes are enough to reconstruct any $d$-dimensional quantum state. For this reason, MIC-POVMs are referred to as "standard" measurements for quantum information, and are of the utmost interest in quantum information theory and applications, where they have been shown to be the ultimate tools for quantum state tomography [1], quantum key distribution [2] and randomness certification [3], among other fields.

We report on an experiment with entangled photon pairs that certifies for the first time a MIC-POVM for qubits following a device-independent protocol. That is, modeling the state preparation and the measurement devices as black boxes and using only the statistics of the inputs and outputs.

1. J. Reháček et al., PRA 70, 052321 (2004)
3. A. Acín et al., PRA 93, 040102(R) (2016)

*VR (Sweden); Knut and Alice Wallenberg Foundation (Sweden); MINECO-MICINN (Spain); Conserjería de Conocimiento, Investigación y Universidad, Junta de Andalucía (Spain); National Science Centre (Poland); DS Programs, Gdansk University of Technology (Poland);
Many-particle interference and entanglement controlled by undetected particles  MAYUKH LAHIRI (Presenter), Department of Physics, Oklahoma State University — Creating and manipulating entangled states are essential for performing various tasks in quantum information science. We present a unique interferometric scheme that allows us to generate many-particle entangled states. The unique feature of the scheme is that the entangled states can be manipulated without interacting with the entangled particles [1]. We illustrate the scheme by two special cases in which Bell states and GHZ-class states are produced. The scheme also emphasizes the connection between interference and entanglement, a connection that has been of interest in fundamental physics [2-4].


Quantum State Reduction: Generalized Bipartitions from Algebras of Observables*  OLEG KABERNIK, JASON POLLACK, Department of Physics and Astronomy, University of British Columbia, ASHMEET SINGH (Presenter), Walter Burke Institute for Theoretical Physics, California Institute of Technology — Reduced density matrices are a powerful tool in the analysis of entanglement structure, coarse-grained dynamics, decoherence, and the emergence of classicality. While one often uses the partial trace map to produce a reduced density matrix, in many natural situations (such as limited resolution experiments) this reduction may not be achievable. We investigate the general problem of identifying how the quantum state reduces given a restriction on the observables where the appropriate state-reduction map can be defined via a generalized bipartition, which is associated with the structure of irreducible representations of the algebra generated by the restricted set of observables. One of our main technical results is a general algorithm for finding irreducible representations of matrix algebras. We demonstrate the viability of this approach with two examples of limited-resolution observables. The definition of quantum state reductions can also be extended beyond algebras of observables by a more flexible notion of bipartition, the partial bipartition, which describes coarse-grainings preserving information about a limited set (not necessarily algebra) of observables.

*NSERC, Canada;
Simons Foundation;
Burke Institute at Caltech by DOE grant DE-SC0011632;
FQXi
L09.00012: Optimality in Quantum Data Compression using Dynamical Entropy
GEORGE ANDROULAKIS (Presenter), Univ of South Carolina — In this joint work with Duncan Wright we study lossless compression of strings of pure quantum states of indeterminate-length quantum codes which were introduced by Schumacher and Westmoreland. Past work has assumed that the strings of quantum data are prepared to be encoded in an independent and identically distributed way. We introduce the notion of quantum stochastic ensembles, allowing us to consider strings of quantum states prepared in a more general way. For any identically distributed quantum stochastic ensemble we define an associated quantum Markov chain and prove that the optimal average codeword length via lossless coding is equal to the quantum dynamical entropy of the associated quantum Markov chain.

L09.00013: Experimental Test of Leggett's Inequalities with Solid-State Spins
XIANZHI HUANG (Presenter), XIAOLONG OUYANG, WENGANG ZHANG, XIN WANG, HUILI ZHANG, YEFEI YU, DONGLING DENG, LUMING DUAN, Center for Quantum Information, IIIS, Tsinghua University, Beijing 100084, P. R. China — Bell's theorem states that no local hidden variable model is compatible with quantum mechanics. Surprisingly, even if we release the locality constraint, certain nonlocal hidden variable models, such as the one proposed by Leggett, may still be at variance with the predictions of quantum physics. Here, we report an experimental test of Leggett's nonlocal model with solid-state spins in a diamond nitrogen-vacancy center. We entangle an electron spin with a surrounding weakly coupled $^{13}$C nuclear spin and observe that the entangled states violate Leggett-type inequalities by more than 6.4 and 10.1 standard deviations for six and eight measurement settings, respectively. Our experiment results are in full agreement with quantum predictions and render Leggett's nonlocal hidden variable model disputable with a high level of confidence.

Wednesday, March 4, 2020 8:00 AM - 9:36 AM

Session L10 GIMS: Fundamental Measurement Science
National Institute of Standards and Technology
8:00AM L10.00001: Propellant Quantity Gauging in Microgravity Using Radio Frequency Tank Modes*  
GREGORY ZIMMERLI (Presenter), NASA Glenn Research Center, MARIUS ASIPAUSKAS, Universities Space Research Association, CAMERON DONG, NASA Glenn Research Center — The Radio Frequency Mass Gauge (RFMG) is a novel propellant quantity gauging technique developed at NASA for the purpose of gauging cryogenic propellant tanks in low-gravity. The RFMG operates by sensing several resonant electromagnetic modes of a tank and comparing the measured tank mode frequencies to a lookup table of results from several thousand numerical simulations. The numerical simulations are performed in advance in order to predict the electromagnetic eigenmode frequencies at different propellant fill levels, liquid configurations, and temperatures. A best match between measured and simulated eigenmode frequencies is used to gauge the fluid mass inside the tank. An RFMG instrument flew on the International Space Station (ISS) and was used to gauge the mass of liquid methane in a 50 L tank as part of the Robotic Refueling Mission 3 (RRM3) payload operations. Shifts to the measured tank RF spectra during the mission indicated significant changes to the fluid configuration as a result of various ISS maneuvers and payload tests. During the four months of RRM3 cryogenic payload operations the RFMG produced a mean gauged mass of 19.0 kg, in agreement with the expected value, with a one-sigma error distribution of ±2% of the full-scale mass.

*This work was funded by NASA.

8:12AM L10.00002: Stretching the bandwidth of physical measurements by compressed sensing  
SHUNSUKE FUJISAWA (Presenter), SUSUMU FUKATSU, Graduate School of Arts and Sciences, University of Tokyo — The bandwidth limit is an issue in any class of physical measurements. To restore the original full-band spectrum from the available data sets that have been severely bandwidth-limited due to measurement is a challenge. Compressed sensing (CS), which is essentially an estimation based on L1 norm minimization, is a powerful technique to retrieve signals using a small number of clues on the assumption of sparsity. Here we attempt the CS in frequency domain to restore the otherwise lost part of the spectrum with good fidelity. The proof-of-concept experiment was done on a model system with bandwidth-limiting properties by first acquiring the prior knowledge of its step response in the form of discretized impulse response function. The original input waveform was mixed with random signal to spread the spectrum over the entire frequency range, i.e., omni-frequency heterodyne. Then the CS was implemented by using repetitive interleaved random sampling over the captured signals that are linearly coupled with the random mixing signals through the step response. Successful recovery of the original full-band spectrum with well over 70%-fidelity holds promise for high-Z and the many strongly bandwidth-limiting measurements. Single-shot and real-timeliness issues will also be discussed.
The Role of Noise in \textit{PT}-Symmetric Systems*  

BAHAR JAFARI ZADEH (Presenter), FRED M ELLIS, Wesleyan Univ — \textit{PT}-symmetric systems have provided a remarkable variety of phenomena related to signal manipulation ranging from unconventional state management to enhanced sensitivity at exceptional points. Although ideal models have been proposed for many different systems, the role of noise has typically not been the focus of previous papers. In this study, we compare the consequences of noise, both internally generated and externally received, between a non-\textit{PT} regenerative resonator and a \textit{PT} resonator pair. We show that, in general, there is no advantage of the \textit{PT} system from a signal-to-noise perspective.

*We acknowledge partial support from the National Science Foundation through awards DMR-1420451 and CMMI-1925543, and from Wesleyan University

Characterization of Acoustic Standing Waves Surrounding A Cylindrical Inertia Block in an Ultra-Low Vibration Facility*  

JULIET NWAGWU UME-EZEOKE (Presenter), YU LIU, JENNIFER E. HOFFMAN, Harvard University — In facilities working with scanning tunneling microscopes (STM), it has been found that the vibrations of the surface on which the STM is placed can significantly alter results. To mitigate this issue, more research is being done into low-vibration laboratories. The low-vibration facility at Harvard University employs a massive cylindrical inertia block mounted on pneumatic isolators. The block has been made cylindrical to avoid coupling of acoustic standing waves between the walls of the room and the inertial block. We have used COMSOL Multiphysics to perform finite element analysis to simulate coupling of the acoustic standing waves in the room to the resonant modes of the inertial block. To check the results of the simulation, a speaker is used to generate a range of frequencies in order to excite the block. We then measure the acoustic standing waves using a microphone.

*This work was funded by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4536, the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319, and NSF MRI Grant No. DMR-1828569.

Optimizing mechanical resonator sensitivity for thin film internal friction and shear modulus measurements*  

THOMAS METCALF (Presenter), XIAO LIU, BATTOGTOKH JUGDERSUREN, United States Naval Research Laboratory — The double-paddle oscillator is a mechanical resonator with an extremely high quality factor at liquid helium temperatures, enabling sensitiv measurements of the internal friction and shear modulus of thin film materials. Since its development more than twenty years ago, several energy loss mechanisms that establish its background quality factor have been identified and quantitatively modeled, including thermoelastic dissipation and attachment loss. Building on work that led to the successful design of a companion resonator (one that measures Young’s modulus), here we use Finite Element Modeling (FEM) of variations on resonator geometry to seek lower thermoelastic and attachment losses as well as to increase the frequency-space separation of resonant modes. Four candidate resonator geometries were identified and fabricated. We compare measurements of these designs to that of the standard resonator geometry.

*Work supported by the Office of Naval Research
9:00AM L10.00006: Progress on the Detection of Single Free Helium Atoms through Field Ionization for a Dark Matter Detector* DAVID OSTERMAN (Presenter), HUMPHREY J MARIS, GEORGE M SEIDEL, DEREK STEIN, Physics, Brown University —
We describe recent progress on the detection of free helium atoms by field ionization, which is a key element of a new liquid helium-based method of dark matter detection proposed by Maris, Seidel and Stein [1]. When a dark matter particle collides with a liquid He atom it produces phonons and rotons which propagate through the superfluid, eventually arriving at the surface. These excitations can then evaporate a He atom, which can then be detected through field ionization, the process of ionizing them in a strong electric field using sharp, metal nanotips. The ability of field ionization to detect even a single helium atom, combined with the < 1 meV binding energy of a He atom to the superfluid surface, could potentially allow for the detection of dark matter particles with masses down to 1 MeV/c².

*NASA EPScOR RID: NNX15AK52A
NASA RI Space Grant: NNX15AI06H

9:12AM L10.00007: Digitizer nonlinearity correction with an AC Josephson Voltage Standard JASON M UNDERWOOD (Presenter), BRYAN C WALTRIP, Physical Measurement Laboratory, National Institute of Standards and Technology — High-fidelity conversion of physical measurement data to the digital domain is desirable in many fields of science. Numerous techniques are available for the correction of nonlinearities in analog-to-digital converters (ADCs). However, implicit in these methods is the availability of a source with a higher resolution and/or lower nonlinearity than that of the ADC under test, which is challenging to realize for ADCs with resolutions exceeding 20 bits. An AC Josephson Voltage Standard (ACJVS) is capable of generating pure tones with distortion below 1 part per billion and amplitude accuracies in the single parts per million. These characteristics make it an ideal source for evaluating nonlinearities in high-resolution digitizers commonly used in audio and dynamic force measurements. In this talk I will describe the framework for performing such nonlinearity corrections with the ACJVS, share results and limitations, and discuss possible ways that this technique can be used to account for phase distortion.
9:24AM L10.00008: Effect of chiral dopant and nanoparticles on liquid crystal based microlenses  
KELUM PERERA (Presenter), AHLAM NEMATI, TORSTEN HEGMANN, ANTAL ISTVAN JAKLI, Kent State Univ - Kent — Microlenses apply to optical devices such as biomimetic optical systems, optical fiber switches, light deflection devices, solar concentrators, etc. [1,2]. Piotr et al. [1] demonstrated and characterized chiral nematic liquid crystal (LC) films suspended in the transmission electron microscope (TEM) grids that form converging spherical microlenses when immersed in water. Here we report on the tunability of the focal length of the TEM grids suspended 4-cyano-4-pentylbiphenyl (5CB) microlenses by adding different concentrations chiral dopant CD1 (ZLI 811) and mixing chiral nanoparticles with 5CB to detect various sources of chirality and make various shapes of microlenses with tunable focal lengths. Additionally, the effects of chiral dopants on the hybrid alignment of LC microlenses is also presented.

Reference

Wednesday, March 4, 2020 8:00 AM - 9:00 AM

Session L15 DFD GSNP: Fluid Structure Interactions 210/212 - Claudio Falcon, Univ de Chile

8:00AM L15.00001: Observation of broad-band water wave guiding in shallow water*  
CLAUDIO FALCON (Presenter), FABIÁN SEPULVEDA, DIEGO GUZMÁN, RODRIGO VICENCIO, Univ de Chile — We report on the observation and characterization of broad-band wave guiding of surface gravity waves in an open channel in the shallow water limit. The wave guide is constructed by changing locally the depth of the fluid layer, which creates conditions for surfaces waves to propagate along the guide. We present experimental and numerical results of this shallow water wave guiding, which can be straightforwardly matched to the one-dimensional wave equation of shallow water waves. Furthermore, we also probe the possibility of wave guiding in curve guides and measure how this changes wave propagation.

*ICM Millennium Nucleus of Soft Smart Mechanical Metamaterials
ICM Millenium Institute for Research in Optics (MIRO)
8:12AM L15.00002: Designing an All-Carbon Membrane for Water Desalination* DAVID TOMANEK (Presenter), Michigan State University, ANDRII KYRYLCHUK, National Academy of Sciences of Ukraine — We design an all-carbon membrane for the filtration and desalination of water. A unique layered assembly of carbon nanostructures including graphite oxide (GO), buckypaper consisting of carbon nanotubes, and a strong carbon fabric provides high mechanical strength and thermal stability, resilience to harsh chemical cleaning agents and electrical conductivity, thus addressing major shortcomings of commercial reverse osmosis membranes. We use ab initio density functional theory calculations to obtain atomic-level insight into the permeation of water molecules in-between GO layers and across in-layer vacancy defects. Our calculations elucidate the reason for selective rejection of solvated Na\(^+\) ions in an optimized GO membrane that is structurally stabilized in a sandwich arrangement in-between layers of buckypaper, which are protected on both sides by strong carbon fabric layers.


*NSF/AFOSR EFRI 2-DARE grant number EFMA-1433459

8:24AM L15.00003: Separation and collision dynamics in biomimetic wind-driven fog harvesting AIDA SHAHROKHIAN (Presenter), Polymer Science, University of Akron, FAN KIAT CHAN, University of Illinois at Urbana-Champaign, JIANSHE FENG, Polymer Science, University of Akron, MATTIA GAZZOLA, University of Illinois at Urbana-Champaign, HUNTER KING, Polymer Science, University of Akron — In regions where foggy days are recurrent and other water sources scarce, harvesting fog is a practical solution. Physical and behavioral techniques developed over eons by plants and animals in these regions can provide useful insight to do it better. O.unguicularis, a Namib desert beetle, goes to the top of the sand dunes on foggy days and uses its forewings to intercept the inertial microdroplets carried by the wind. Adaptation of this beetle has been extensively studied through the lens of surface wettability and its role in transporting accumulated water. Yet, how the interaction between flow dynamics and surface topography of beetle elytra can induce collision of droplets and increase accumulation of water has not been considered. Here, we show in careful experiments accompanied by numerical flow simulations that surface morphology, independent of wettability, plays a dominant role in deposition efficiency of beetle-like geometries. Furthermore, we investigate the potential role of hydrodynamic forces in near collision dynamics where surface mechanics and texture can limit the possibility of collision. The results suggest that manipulation of the collision mechanism via geometry and mechanics can be an alternative driver of the physical adaptation of the fog basking beetles.
8:36AM L15.00004: Pair interaction between sedimenting polar objects in the Stokes regime*

ALYSSA CONWAY (Presenter), NARAYANAN MENON, RAHUL CHAJWA, SRIRAM RAMASWAMY, Univ of Mass - Amherst — We study triangles placed in a quasi-two-dimensional container and sedimented at low Reynolds number as a model of the stokesian sedimentation of polar objects. Individual polar objects, unlike non-polar axisymmetric objects, rotate as they sediment due to coupling between the orientational and translational degrees of freedom and ultimately reorient into stable orientations [Jayaweera, Mason, J. Fluid Mech. 22 (1965)]. In order to study the pair interaction between polar objects, we sediment pairs of triangles with initial conditions that include both stable and unstable orientations of the individual triangles. Surprisingly, none of the periodic motions observed [Chajwa, Menon, Phys. Rev. Lett. 122 (2019)] with non-polar object pairs are seen with pairs of triangles. Instead, we observe that triangles reorient and translate away from each other until both objects achieve a stable orientation. As a special case, we also observe that equilateral triangle pairs (which have three-fold, rather than polar, symmetry) continuously rotate in their steady state.

*We acknowledge funding from NSF DMR 1905698.

8:48AM L15.00005: Sedimenting disk arrays: waves and transient growth*

RAHUL CHAJWA (Presenter), RAMA GOVINDARAJAN, International Centre for Theoretical Sciences TIFR, Survey no. 151 Shivakote, Bengaluru 560089, NARAYANAN MENON, Physics Department, University of Massachusetts Amherst MA 01003, SRIRAM RAMASWAMY, Department of Physics, Indian Institute of Science, Bengaluru 560 012 — We study experimentally the Stokesian sedimentation (Re \(\sim 10^{-4}\)) of one-dimensional lattice of disks in a quasi two-dimensional geometry with trajectories of disk centres lying in a plane. We induce initial positional perturbations over a uniformly spaced configuration of disks with their separation vectors and normals aligned, and perpendicular to gravity. For various perturbation wavenumbers \(q\) and interparticle separations \(d\), we find two classes of behaviour: (i) wavelike propagation of orientations coupled with number-density fluctuations and (ii) clumping instability resembling that of spheres, decorated with orientations. We construct equations of motion using pairwise addition of forces and torques in an array of spheroids. Linear stability analysis of the dispersion relation predicts non-modal transient growth, which we observe experimentally; and a phase boundary in the \(q-d\) plane separating neutrally stable and unstable regimes, consistent with our experimental observations. We predict a critical density of the lattice of spheroids below which all wavenumbers are asymptotically linearly stable, showing that orientable particles need not be subject to the inevitable clumping instability of spheres.

*NSF DMR 1905698; SERB (India); Tata Education and Development Trust; and TIFR

Wednesday, March 4, 2020 8:00 AM - 10:36 AM

Session L16 DQI: Quantum Annealing and Optimization II 201 - Yudong Cao, Zapata - Tag(s): Focus
Adaptive measurement approach towards controlling non-adiabatic transitions in quantum annealing

SALIL BEDKIHAL (Presenter), MEHMET CANTURK, YONGCHAO TANG, ANTONIO MARTINEZ, ADRIAN LUPASCU, University of Waterloo, SONG ZHANG, JUAN ATALAYA, BIRGITTA K WHALEY, University of California, Berkeley — Non-adiabatic transitions arising from extremely small energy gaps present a challenge to quantum annealing and adiabatic quantum computing. In realistic quantum annealing scenarios, one does not have a priori knowledge of the energy-spectrum and hence the location of minimum energy gaps; thereby making it difficult to design strategies that will slow down close to the points of enhanced transition probability out of the ground state. In this work, we present an adaptive annealing protocol based on measurement of the energy-level curvature. Numerical results are presented for a random transverse field Ising model. We also discuss the relationship between the measurement operator and the fidelity-susceptibility, a measure allowing analysis of quantum phase transitions in many-body systems.

This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).

Elucidating the interplay between non-stoquasticity and the sign problem

LALIT GUPTA (Presenter), ITAY HEN, Univ of Southern California — The sign problem is a key challenge in computational physics, encapsulating our inability to properly understand many important quantum many-body phenomena in physics, chemistry and the material sciences. Despite its centrality, the circumstances under which the problem arises or can be resolved as well as its interplay with the related notion of ‘non-stoquasticity’ are often not very well understood. In this study, we make an attempt to elucidate the circumstances under which the sign problem emerges and to clear up some of the confusion surrounding this intricate computational phenomenon. To that aim, we make use of the recently introduced off-diagonal series expansion quantum Monte Carlo scheme with which we analyze in detail a number of examples that capture the essence of our results.

*The research is based upon work (partially) supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.
8:24AM L16.00003: All-optical Ising machine by spatial light modulation  
DAVIDE PIERANGELI (Presenter), GIULIA MARCUCCI, CLAUDIO CONTI, Univ of Rome La Sapienza — A broad class of computationally intractable problems maps to the search of the ground state of a spin system. Quantum and classical setups that evolve according to an Ising Hamiltonian are thus emerging as novel computing architectures for solving combinatorial optimizations that cannot be tackled on large scales by conventional hardware. Among these, photonic platforms can process data at light speed and in parallel, through multiple spatial or frequency channels. However, the realized photonic Ising machines either involve a limited number of spins or electronic spin couplings or lack of scalability.

Here, we make use of optical spins that are encoded and controlled by spatial light modulation to realize a large-scale all-optical Ising machine [1]. We implement photonic spin configurations with an unprecedented number of interacting nodes that settle in the corresponding Ising ground state. The setup, which is based on the sole spatial coherence of light, suggests a scalable and efficient approach for optical computing. Our results open the route to Ising machines that exploit spatial degrees of freedom of light for parallel spin processing.


8:36AM L16.00004: Is Fault Welcoming Quantum Computing Realistic?*  
ELIOT KAPIT (Presenter), Physics, Colorado School of Mines, VADIM OGANESYAN, Physics, City University of New York — An error-corrected, fault tolerant quantum computer is one of the most important long term goals of quantum computing research. In these systems random noise is an obstacle that must be overcome through error correction. Here we explore a new possibility, fault-welcoming quantum computing, where a system can not only maintain a quantum speedup for a given (likely non-universal) class of quantum algorithms against realistic noise, but actually performs better than an idealized copy with no noise. We modify flux qubit quantum annealing by including random, coherent low-frequency oscillations in the directions of the transverse field terms during evolution. Through analytical and numerical calculations, we show that this produces a quantum speedup for finding ground states in the Grover problem and quantum random energy model, and thus should be widely applicable to other hard spin glass problems. Further, we show that this speedup should be resilient to two realistic noise channels, and that another channel, bath-assisted phase transitions, accelerates optimization and may outweigh the others, thus potentially making the system fault welcoming. The modifications we consider could be explored with current technology.

*NSF grant # PHY-1653820
8:48AM L16.00005: Schrieffer-Wolff Methods for Annealing Qubits* RUDOLPH MAGYAR (Presenter), DAVID GEORGE FERGUSON, Northrop Grumman - Mission Systems — A robust method for characterizing the low-energy Pauli decomposition of coupled superconducting qubits is based on a generalization of Bravyi et al's Schrieffer-Wolff transformation but applied in infinitesimal steps [1]. This method has several desirable properties. The effective Hamiltonian remains block diagonal so that the computational subspace is completely decoupled from the non-computational one. The adiabatic connection terms generated by the time-dependence of the computational subspace are block off-diagonal and thus do not generate any terms within the computational subspace. This work is a continuation of work described last year focused on the readout of single flux qubits. Subsequent numerical advances now permit the extension of the method to interacting tunable flux qubits including novel flux qubits capable of implementing strong non-stoquastic interactions.


*This material is supported by the Intelligence Advanced Research Projects Activity (IARPA) through the Army Research Office (ARO) Contract No. W911NF-17-C-0050.

9:00AM L16.00006: Beyond Standard Quantum Annealing* [Invited] TAMEEM ALBASH (Presenter), University of New Mexico — Quantum annealing is typically studied (and experimentally realized) in terms of an interpolation between a driver and a problem Hamiltonian, often taken to be a uniform transverse field and an Ising Hamiltonian respectively. Nothing restricts the time-dependent Hamiltonian to take such a simple form, and greater control of experimental systems has revived the study of more exotic interpolations. We review recent work exploring new quantum annealing protocols, including adiabatic reverse annealing and the introduction of catalyst Hamiltonians. While providing an exponential improvement in performance for solving certain highly symmetric toy models, no recipe is known for how to use these new proposals to give performance enhancements more generally. This highlights the need for dramatically new insights and methods but also more experimental capabilities to further explore the performance of non-standard quantum annealing.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.
9:12AM L16.00007: A real-time path integral representation of driven quantum algorithms*

FRANK WILHELM, Univ des Saarlandes, DAVID K HEADLEY (Presenter), Group Research, Future Technologies, Daimler AG, Stuttgart, Germany, PETER SCHUHMACHER, Univ des Saarlandes — Both adiabatic quantum computing / quantum annealing and the quantum approximate optimization algorithm combine a problem Hamiltonian with a non-commuting driver Hamiltonian in order to efficiently explore the complete state space of an optimization problem. We develop a representation of such algorithms as a real-time path integral that directly and rigorously implements the otherwise colloquial idea that quantum algorithms follow all possible computations at the same time. We apply path integral techniques such as eikonals and semiclassics in order to provide a way to better understanding under which conditions we can expect these algorithms to reliably converge.

*Funded in parts by IARPA under the QEO program

9:24AM L16.00008: Updates to Hybrid Quantum-Classical Annealing*

PETER SCHUHMACHER (Presenter), ADITI MISRA, Univ des Saarlandes, SALIL BEDKIHAL, XI DAI, ADRIAN LUPASCU, University of Waterloo, FRANK WILHELM, Univ des Saarlandes — Last year. we proposed an efficient gap-independent cooling scheme for a quantum annealer that benefits from finite temperatures. We chose a system based on superconducting flux qubits as a prominent example of current quantum annealing platforms and proposed coupling the qubit systemtransversely to a coplanar waveguide to counter noise and heating that arise from always-present longitudinal thermal noise. We provide a schematic circuit layout for the system and showed we achieve global performance enhancements. However, the work covered only single-qubit annealing. In this work, we discuss different strategies to generalize HQCA to larger qubit numbers.

*The research is based upon work (partially) supported by the Office of the Director of National Intelligence(ODNI), Intelligence Advanced Research Projects Activ-ity (IARPA), via the U.S. Army Research Office con-tract W911NF-17-C-0050. The views and conclusionscontained herein are those of the authors and shouldnot be interpreted as necessarily representing the officialpolicies or endorsements, either expressed or implied, ofthe ODNI, IARPA, or the U.S. Government. The U.S.Government is authorized to reproduce and distributereprints for Governmental purposes notwithstanding anycopyright annotation thereon.
9:36 AM L16.00009: Non-stoquastic interactions of superconducting circuits in the low frequency regime* MARIUS SCHÖNDORF (Presenter), FRANK WILHELM, Univ des Saarlandes — Non-stoquastic interactions are hard to realize in experimental setups using superconducting qubits. On the other hand they are important or even necessary for the construction of adiabatic quantum computers which show a real quantum speedup. In ArXiv:1903.06139, Ozfidan et al. show that they can realize non-stoquastic qubit-qubit interactions in a superconducting circuit architecture. The non-stoquastic nature only appears when the system is restricted to the low energy qubit subspace, since the full circuit Hamiltonian itself is stoquastic. Here we study the origin of these non-stoquastic interactions arising when projecting stoquastic Hamiltonians to the low energy spectrum. For this we use different theoretical tools, e.g. renormalization group techniques.

*This work was funded by IARPA in connection with the quantum enhanced optimization (QEO) program.

9:48 AM L16.00010: Oscillatory quantum optimization methods applied to problems with large ground state bands* ZHIJIE TANG (Presenter), ELIOT KAPIT, Colorado Sch of Mines — RFQA is a promising new quantum method for solving optimization problems, where by adding local oscillations to transverse fields, it can provide a polynomial quantum speedup over traditional quantum annealing methods. Inspired both by the performance of RFQA in trial problems with few ground states, and by the phenomenology of NP-complete problems, we consider RFQA applied to problems with exponentially many ground states, but where these states are an exponentially small fraction of the total configuration space. We explore how accelerated thermalization in low energy bands can provide a potentially noise tolerant quantum speedup for optimization and machine learning.

*NSF grant (PHY-1653820)

10:00 AM L16.00011: How Quantum is the Speedup in Adiabatic Unstructured Search?* ITAY HEN (Presenter), Univ of Southern California — In classical computing, analog approaches have sometimes appeared to be more powerful than they really are. This occurs when resources, particularly precision, are not appropriately taken into account. While the same should also hold for analog quantum computing, precision issues are often neglected from the analysis. I will discuss in the above context the sensitivity of the quantum adiabatic unstructured search algorithm [Roland and Cerf, Phys. Rev. A 65, 042308 (2002)] against various types of imperfections and show that the speedup associated with the algorithm is generally not robust against the presence of finite precision. In addition, I will present a classical analog algorithm for unstructured search that can be viewed as analogous to the quantum adiabatic unstructured search algorithm and which provides a quadratic speedup over standard digital unstructured search.

*The research is based upon work (partially) supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.
Recent advances in adiabatic quantum computing and quantum annealers has centered around using more advance and novel Hamiltonians to solve optimization problems. One of these advances has centered around the development of driver Hamiltonians that commute with the constraints of an optimization problem. This approach has been shown to be able to use sparser connectivity to embed several practical problems on quantum devices in comparison to other methods. Designing the driver Hamiltonians that successfully commute with several constraints has largely been based on strong intuition for specific problems and with no general algorithm for arbitrary constraints. In this work, we develop an algebraic framework for reasoning about the commutation of Hamiltonians with linear constraints - one that allows us to classify the complexity of finding a driver Hamiltonian for a set of constraints as NP-Hard through a reduction to the Subset Equal Sums problem as well as design a simple algorithm to solve the problem for Hamiltonians with bounded number of higher body interaction terms.

*This work was supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.

8:00AM L17.00001: Strong photon coupling to the quadrupole moment of an electron in a triple quantum dot* [Invited] JONNE KOSKI, ANDREAS LANDIG, ETH Zurich, MAXIMILIAN RUSS, Department of Physics, University of Konstanz, JOSE CARLOS ABADILLO-URIEL, Department of Physics, University of Wisconsin-Madison, PASQUALE SCARLINO, BENEDIKT KRATOCHWIL, CHRISTIAN REICHL, WERNER WEGSCHEIDER, ETH Zurich, GUIDO BURKARD, Department of Physics, University of Konstanz, SUSAN NAN COPPERSMITH, Department of Physics, University of Wisconsin-Madison, ANDREAS WALLRAFF, KLAUS ENSSLIN, THOMAS IHN (Presenter), ETH Zurich — We experimentally couple the photonic excitations of a superconducting microwave resonator to a single electron hosted in a quantum dot charge qubit. The two qubit states with a 4.3 GHz separation arise in a four-electron triple quantum dot formed by locally gating a two-dimensional electron gas in GaAs. We demonstrate strong electron-photon coupling via the quadrupole moment in a parameter regime with negligible dipole coupling. The quadrupolar qubit-photon coupling strength is estimated from the vacuum Rabi mode splitting to be $g_0/2\pi = 150$ MHz. The qubit can also be tuned into a regime where it operates as a conventional double quantum dot charge qubit dipole coupled to the resonator. The experiment is motivated by a recent proposal [1,2] which aims at avoiding decoherence by distant charge fluctuations. Using spectroscopy measurements we determine the decoherence rate of the quadrupolar qubit to be $\gamma_2/2\pi = 32$ MHz. Comparing the coupling of charge noise to the conventional dipolar qubit and the quadrupolar qubit, we find that the coherence of the system is limited by short-range charge noise originating from noise sources residing near the triple quantum dot.


*Work supported by the Swiss National Science Foundation through the National Center of Competence in Research (NCCR) Quantum Science and Technology. SNC and MF acknowledge support by the Vannevar Bush Faculty Fellowship program sponsored by the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering and funded by the Office of Naval Research through Grant No. N00014-15-1-0029. MR and GB acknowledge funding from ARO through Grant No. W911NF-15-1-0149 and the DFG through SFB 767. MF and JCAU acknowledge support by ARO (W911NF-17-1-0274).
8:36AM L17.00002: Efficient orthogonal control of tunnel couplings in a quantum dot array

TZU-KAN HSIAO (Presenter), CORNELIS VAN DIEPEN, UDITENDU MUKHOPADHYAY, Delft University of Technology, CHRISTIAN REICHL, WERNER WEGSCHEIDER, ETH Zurich, LIEVEN M VANDERSYPEN, Delft University of Technology — Electrostatically defined semiconductor quantum dot arrays offer a promising platform for quantum computation and quantum simulation. However, crosstalk of gate voltages to dot potentials and inter-dot tunnel couplings complicates the tuning of the device parameters. To date, cross-talk to the dot potentials is routinely and efficiently compensated using virtual gates, but cross-talk to the tunnel barriers is currently compensated through a slow iterative process, due to exponential dependence of tunnel couplings on gate voltages. Here we show that the crosstalk on tunnel barriers can be compensated using a linear combination of gate voltages, since the exponential dependence applies to all gates. We demonstrate efficient calibration of crosstalk in a quadruple dot and define a set of virtual barrier gates as linear combinations of physical gate voltages. We then demonstrate orthogonal control of tunnel couplings in the quadruple dot using these virtual barrier gates. Our method marks a key step forward in the scalability of the tuning process of large-scale quantum dot arrays.

*This work was supported by NWO Vici, ERC Synergy and the Swiss National Science Foundation.

8:48AM L17.00003: Barrier-Controlled Multi-Qubit Exchange

HAIFENG QIAO (Presenter), YADAV KANDEL, University of Rochester, SAEED FALLAHI, GEOFF C GARDNER, MICHAEL MANFRA, Purdue University, JOHN NICHOL, University of Rochester — Heisenberg exchange coupling between neighboring electron spins in semiconductor quantum dots provides a powerful tool for coherent qubit manipulation in spin-based quantum computing and quantum information processing. Various other phenomena such as many body localization and time crystals in semiconductor quantum dots also require tunable exchange couplings. However, controlling multiple exchange couplings in large quantum dot arrays proves to be challenging, due to non-linear and non-local dependence of the exchange couplings on the confinement gate voltages. In this work we demonstrate simultaneous control of multiple barrier-induced exchange couplings in a four-qubit processor. We model the dependence of the exchange couplings on all barrier gate voltages, which provides a means of precisely and simultaneously controlling multiple exchange couplings. We demonstrate two-, three-, and four-qubit exchange oscillations, and compare the experimental data to the simulated predictions.

*This research was sponsored the Defense Advanced Research Projects Agency under Grant No. D18AC00025; the Army Research Office under Grant Nos. W911NF16-1-0260, and W911NF-19-1-0167.
9:00AM L17.00004: Coherent Spin-State Transfer via Heisenberg Exchange*  YADAV KANDEL  
(Presenter), HAIFENG QIAO, University of Rochester, SAEED FALLAHI, GEOFFREY C. GARDNER, MICHAEL MANFRA, Purdue University, JOHN NICHOL, University of Rochester — Spin qubits in semiconductors are a promising scalable architecture for quantum computing. Long chains of spin qubits have already been realized in different semiconductor platforms but transferring quantum information throughout such chains is still a challenge. Here we present the first experimental demonstration of the coherent transfer of electron spin states back and forth across a chain of four quantum-dot spin qubits using Heisenberg exchange coupling between neighboring electrons, which arises from the overlap of their wavefunctions. We swap the spin states of a pair of electrons via precisely-controlled exchange pulses. Successive SWAP operations between different pairs can transfer a quantum spin state to a distant qubit, without moving any electrons. Because this method is scalable to long chains of spin qubits, coherent spin-state transfer using Heisenberg exchange will be useful in multi qubit operations, measurement-based entanglement swapping and gate teleportation, and error correction in spin-based quantum computers.

*This research was funded by the University of Rochester, ARO/LPS through Grant No. W911NF-17-1- 0260, and the DARPA DRINQS program through Grant No. D18AC00025.

9:12AM L17.00005: Noise-resilient driven exchange gate for quantum dot spin qubits*  
STEPHAN PHILIPS (Presenter), MAXIMILIAN RUSS, LIEVEN M VANDERSYPEN, Delft University of Technology — Spin qubits in silicon quantum dots are a promising candidate for high-fidelity quantum computation due to long decoherence times and fast operations. Demonstrations of single qubit gates with fidelities up to 99.9% have been shown [1,2]. Recent demonstrations of two-qubit gates show fidelities of 92-98% [2,3]. These two-qubit gate implementations are not robust against low-frequency charge noise, which couples in via the exchange interaction, causing a limited fidelity. We propose a simple yet effective scheme that is resilient against low-frequency charge noise. We use a combination of analytic calculations and numerical simulations under realistic conditions to obtain estimated gate fidelities greater than 99%, which allow for fault-tolerant two qubit gates. We directly compare these realizations with existing proposals and will present our experimental efforts towards achieving this goal.


*We acknowledge financial support from the Marie Sklodowska-Curie actions—Nanoscale solidstate spin systems in emerging quantum technologies—Spin-NANO, grant agreement number 676108 and from the European Research Council (ERC-Synergy).
**9:24AM L17.00006: Interplay of exchange and superexchange in triple quantum dots**

KUANGYIN DENG (Presenter), EDWIN BARNES, Virginia Tech — Recent experiments on semiconductor quantum dots have demonstrated the ability to utilize a large quantum dot to mediate superexchange interactions and generate entanglement between distant spins. This opens up a possible mechanism for selectively coupling pairs of remote spins in a larger network of quantum dots. We will describe our theoretical efforts to understand the controllability of superexchange interactions in these systems. We focus on a triple-dot system arranged in a triangular configuration and use configuration interaction calculations to investigate the interplay of superexchange and nearest-neighbor exchange interactions as the geometry and detuning of the mediating dot are varied. We also study how the strength and sign of the superexchange coupling depends on the number of electrons in the mediator. Our results can be used as a guide to assist further experimental efforts towards scaling up to larger, two-dimensional quantum dot arrays.

*This work is supported by the Army Research Office (W911NF-17-0287).

**9:36AM L17.00007: Coherent manipulation of three-spin states in a Si/SiGe triple quantum dot**

KENTA TAKEDA (Presenter), AKITO NOIRI, TAKASHI NAKAJIMA, JUN YONEDA, TAKASHI KOBAYASHI, SEIGO TARUCHA, RIKEN — Quantum dot arrays provide a promising platform for quantum information processing. In Si-based devices, recent technological advances make it possible to implement single- and two-qubit operations with high fidelities. A three-qubit system is a next step toward scaling up and it is particularly important for realizing a quantum error-correcting code. In this work, we demonstrate coherent manipulation of three individual spins in a Si/SiGe triple quantum dot by site-selective electric dipole spin resonance. Spins in the left and right dots are read out by a spin-selective tunneling technique while the center spin is measured by reading out the left spin subsequently to a controlled-rotation operation. We also report our recent progress on controlled-controlled-rotation where the resonance frequency of the center spin depends on both left and right spin states.


*This work was supported financially by Core Research for Evolutional Science and Technology (CREST), Japan Science and Technology Agency (JST) (JPMJCR15N2 and JPMJCR1675) and MEXT Quantum Leap Flagship Program (MEXT Q-LEAP) grant No. JPMXS0118069228.
9:48AM L17.00008: Full Permutation Dynamical Decoupling in an Encoded Triple-Dot Qubit
BO SUN (Presenter), HRL Laboratories, LLC — Dynamical decoupling (DD) sequences can mitigate decoherence induced by slowly varying interactions between a qubit and a bath by using appropriately timed qubit rotations. For an exchange only qubit encoded in the spins of three electrons, dynamical decoupling can be achieved by applying a series of full-SWAP operations on the constituent spins which fully permute their locations across the three dots [1]. Using gate-defined quantum dots in an enriched Si/SiGe device, we demonstrate that repeated applications of the full permutation sequence can echo low frequency charge and magnetic noise, resulting a dynamically decoupled coherence time of 100s of microseconds. We find that the first order DD sequence is susceptible to rotations about the Y-axis of the Bloch sphere, driven by either real magnetic field gradients or spin-orbit pseudo-gradients. Initializing the qubit along the Y axis renders the experiment insensitive to these errors, as implied by measurements of qubit leakage in this configuration. The resulting experiment is only sensitive to high-frequency noise sources and is similar to noise spectroscopy. We compare our results to simulations which include various types of high-frequency charge noise.

10:00AM L17.00009: Highly tunable exchange-only singlet-only qubit in a GaAs triple quantum dot
ARNAU SALA (Presenter), JØRGEN HOLME QVIST, JEROEN DANON, NTNU — Quantum-dot based exchange-only spin qubits offer fast manipulation and full electric control but decohere rapidly in the presence of Zeeman field gradients, such as those resulting from the hyperfine interaction with randomly polarized nuclear-spin ensembles in the dots. A solution is to encode the qubit in the decoherence-free subspace spanned by two four-particle singlet states in a quadruple-dot setup [1].

Here we propose an implementation of this singlet-only qubit in a triple quantum dot with a (1,4,1) charge occupation. In the central multi-electron dot, the interplay between Coulomb interaction and an out-of-plane magnetic field creates an energy spectrum with a tunable singlet-triplet splitting and this feature can be exploited to create a six-particle singlet-only qubit with a qubit splitting that can straightforwardly be tuned over several μeV by adjusting the external magnetic field. We confirm the full exchange-based electric control of the qubit and demonstrate its superior coherence properties due to its singlet-only nature.

10:12AM L17.00010: Correcting Distortion of Base-band Exchange Pulses in Quantum Dot Qubits  DAVID BARNES (Presenter), HRL Laboratories, LLC — Repeatedly identical control waveforms are necessary for high fidelity qubit control. In triple-dot exchange-only spin qubits, full Bloch-sphere control is achieved via baseband voltage pulses alone. This makes them sensitive to the effects of pulse distortion extending from kHz to GHz frequencies. Here we present a technique to correct the known distortion of our arbitrary waveform generators. The application of this correction lead to a reduction of single qubit infidelity from 0.5% to 0.2% as measured by the “blind randomized benchmarking” protocol [1]. Additionally, we will cover an extension to this routine where we are able to estimate and potentially correct residual pulse distortion using coherent qubit control experiments.


10:24AM L17.00011: Long-Distance Charge Transport in a Single Electron Conveyor Device in (Al,Ga)As  MATTHIAS KUENNE (Presenter), JARA-FIT Institute for Quantum Information, Forschungszentrum Juelich GmbH and RWTH Aachen University, D-52074 Aachen, Germany, STEFAN TRELLenkAMP, Helmholtz Nano Facility, Forschungszentrum Juelich GmbH, D-52425 Juelich, Germany, JULIAN RITZMANN, ARNE LUDWIG, ANDREAS WIECK, Lehrstuhl für angewandte Festkoerperphysik, Ruhr-Universität Bochum, D-44801 Bochum, Germany, HENDRIK BLUHM, JARA-FIT Institute for Quantum Information, Forschungszentrum Juelich GmbH and RWTH Aachen University, D-52074 Aachen, Germany — For the realization of scalable quantum computing architectures enabling topological error correction, a transfer of the qubit information over distances of at least a few microns is required for making space for signal vias and allowing for tiling of qubit registers with classical control-circuits. Instead of coupling qubits by employing surface acoustic waves, we chose a one-dimensional, gate-defined conveyor belt-like device layout where electrons are moved between qubit sites by translating the potential minima in which the electrons are trapped. Here, the direction and the velocity of the electron transport are not limited by the crystal’s properties.

In this talk, I will present a device designed to allow the shuttling of electrons over 7 µm with only four voltage signals, whereby in principle arbitrary distances are feasible. We employed high-yield, multi-layer electron beam lithography in order to fabricate the required 100 metallic gates. I will show results on pumping charges from one reservoir to the other by filling each potential minimum in the conveyor with up to five electrons. We observed charge transport which is independent of a bias voltage and linear in frequency.
10:36AM L17.00012: Computer-automated tuning procedures for semiconductor quantum dot arrays* ADAM MILLS (Presenter), MAYER M FELDMAN, Princeton University, CARA MONICAL, PHILLIP J LEWIS, KURT W LARSON, ANDREW M MOUNCE, Sandia National Laboratories, JASON PETTA, Princeton University — As with any quantum computing platform, semiconductor quantum dot devices require sophisticated hardware and controls for operation. The increasing complexity of quantum dot devices necessitates the advancement of automated data collection and control software. By automating the analysis of charge stability diagrams, we can easily create tools to tune charge occupancy and interdot tunnel couplings in our quantum dot arrays. We use an image analysis toolbox developed in Python to automate the calibration of virtual gates, a process that previously involved a large amount of user intervention. Moreover, we show that straightforward feedback protocols can be used to simultaneously tune multiple tunnel couplings in a triple quantum dot1.


10:48AM L17.00013: Designing CPHASE Gates with Arbitrary Phase by Structural Modification of the Fong-Wandzura Sequence DANIEL ZEUCH (Presenter), Peter Grünberg Institut, Forschungszentrum Jülich, NICHOLAS EVANS BONESTEEL, Department of Physics, Florida State University and NHMFL — We design efficient arbitrary CPHASE gates for exchange-only spin-based quantum computation in which quantum gates are carried out by sequences of exchange pulses acting on qubits encoded using three or more spins. The construction we present is motivated by our analytic derivation [1] of the Fong-Wandzura sequence [2], the shortest known pulse sequence for an exact CNOT gate (for a linear array of spins). This earlier derivation is based on a type of elevation of a simple five-pulse sequence consisting only of SWAP or trivial pulses, which captures the essential structure of the Fong-Wandzura sequence. In the present construction, we introduce and evaluate a modified simple five-pulse sequence consisting of four SWAP pulses and one pulse of arbitrary duration. We then show how this sequence can be elevated in a fashion similar to that of our Fong-Wandzura derivation, to yield a leakage-free entangling two-qubit sequence that carries out a gate operation locally equivalent to arbitrary CPHASE.


Wednesday, March 4, 2020 8:00 AM - 11:00 AM
8:00AM L18.00001: New experimental approaches for exploring condensed matter physics
[Invited] AMIR YACOBY (Presenter), Harvard University — The magnetic fields generated by spins and currents provide a unique window into the physics of correlated-electron materials and devices. Proposed only a decade ago, magnetometry based on the electron spin of nitrogen-vacancy (NV) defects in diamond is emerging as a platform that is exceptionally suited for probing condensed matter systems: it can be operated from cryogenic temperatures to above room temperature, has a dynamic range spanning from DC to GHz, and allows sensor-sample distances as small as a few nanometers. As such, NV magnetometry provides access to static and dynamic magnetic and electronic phenomena with nanoscale spatial resolution.

While pioneering work focused on proof-of-principle demonstrations of its nanoscale imaging resolution and magnetic field sensitivity, now experiments are starting to probe the correlated-electron physics of magnets and superconductors and to explore the current distributions in low-dimensional materials. In this talk, I will review some of our recent work that uses NV center magnetometry to image skyrmions in thin magnetic films, measure the spin chemical potential in magnetic insulators, and image hydrodynamic electron flow in graphene.

8:36AM L18.00002: Virginia O Lorenz Invited Talk
[Invited] —

9:12AM L18.00003: Hybrid sensing approaches for quantum spin sensors* [Invited] MICHAEL FLATTÉ (Presenter), Univ of Iowa — Quantum sensing, for example using diamond NV spin centers, has been effectively demonstrated for magnetic and electric fields as well as to measure the local temperature. Novel methods using hybrid sensing modalities, in which auxiliary entities are exploited to interact with the quantum sensor, are now under intense investigation. These include using a nearby ferromagnetic particle with a freely orientable magnetization, which amplifies the magnetic field of a sensed object to the point where it can be detected by a quantum spin sensor. Here I will describe two recent proposals for hybrid sensing modalities. In the first proposal the magnetic field of the NV spin itself is used to generate a magnetic response from a nearby material, and the resulting magnetic field is detected by the spin center. This extends quantum sensing to diamagnetic materials, for which the magnetic susceptibility is the desired metric. In the second proposal single-photon detection by a photoreceptive molecule, which changes its conformation in response to the absorption of a photon, can be measured using quantum sensing of the resulting electric dipole change due to the new shape of the molecule. These results suggest many new hybrid modalities are possible based on current quantum spin sensors. This work done in collaboration with J. van Bree and N. J. Harmon.

*This work was supported by an AFOSR MURI and DARPA/DETECT.
9:48AM L18.00004: Defect spins in two-dimensional materials for quantum sensing and nanophotonics* [Invited]  LEE BASSETT (Presenter), University of Pennsylvania — Optically addressable spin defects like the diamond nitrogen-vacancy center enable versatile applications in precision sensing and nanoscale imaging. Related defects in other materials, especially two-dimensional materials such as hexagonal boron nitride (hBN), offer potential advantages and novel sensing capabilities. Van der Waals materials like hBN can host defects in a precise two-dimensional layer, at a surface that is potentially cleaner than that three-dimensional semiconductors. This talk will introduce the properties of optically active defects in hBN, focusing in particular on their room-temperature optical and spin properties [1,2]. We will also discuss the role of new materials and defects more broadly for use in quantum sensing and other applications in quantum science [3].


*This work was supported by the Army Research Office (W911NF-15-1-0589) and the National Science Foundation (DMR-1922278).

10:24AM L18.00005: What would you do with a quantum-limited torque magnetometer?* [Invited]  JOHN DAVIS (Presenter), Physics, University of Alberta — In the past decade, cavity optomechanics has demonstrated its awesome potential to bring quantum mechanics into the study of mechanical systems. Yet little work has been done to use cavity optomechanics for sensing applications, such as the study of condensed matter systems. At the University of Alberta, we have focused on harnessing cavity optomechanical detection to measure ever smaller moment of inertia resonators, thereby improving torque sensing. Combining this with low temperature operation, we have reached torque sensitivities on the order of $10^{-24}$ N m/√Hz, just ten times the device’s standard quantum limit. To date, we have used such cavity optomechanical torque sensors to explore nanomagnetic vortices, collective spin dynamics, and phase-shift keying applications, but potential quantum sensing applications are numerous. Looking forward, it will also be possible to use the toolbox of quantum optics such as single photon detectors and squeezed states, along with cavity optomechanics, to enable new frontiers of quantum sensing and to push beyond the standard quantum limit.

*The University of Alberta; the Natural Sciences and Engineering Research Council, Canada (Grants No. RGPIN-04523-16, No. DAS-492947-16, No. STPGP 494024-16, and No. CREATE-495446-17); and the Canada Foundation for Innovation.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM
Light induced phase transitions in charge density waves

GEDIK (Presenter), Massachusetts Institute of Technology MIT — Upon excitation with an intense laser pulse, materials can undergo a non-equilibrium phase transition through pathways different from those in thermal equilibrium. The mechanism underlying these photoinduced phase transitions has long been researched, but many details in this ultrafast, non-adiabatic regime still remain to be clarified. To this end, we studied light induced phase transitions in two different charge density wave (CDW) systems. First, we investigated the photo-induced melting of a unidirectional CDW in LaTe$_3$. Using a suite of time-resolved probes, we independently track the amplitude and phase dynamics of the CDW. We find that a fast (approximately 1 picosecond) recovery of the CDW amplitude is followed by a slower re-establishment of phase coherence dictated by the presence of topological defects in CDW. Furthermore, after the suppression of the original CDW by photoexcitation, a different, competing CDW along the perpendicular direction emerges. The timescales characterizing the relaxation of this new transient CDW and the reestablishment of the original CDW are nearly identical, which points towards a strong competition between the two orders. Secondly, I will also report the realization of optical chiral induction and the observation of a gyrotropically ordered CDW phase in 1T-TiSe$_2$. Our results provide a framework for understanding other photoinduced phase transitions and for unleashing novel states of matter that are “trapped” under equilibrium conditions.

Quantum Beats by Lightwave Acceleration of Broken-Symmetry Supercurrents

JIGANG WANG (Presenter), Department of Physics and Astronomy, Iowa State University & Ames Laboratory — Light-induced supercurrents chart a path forward for the electromagnetic design of emergent materials phases and collective modes for quantum engineering applications. In this talk, I will discuss our recent progress towards applying this new tuning knob, enabled by using single- and few-cycle THz pulses, to reveal some distinguishing features of quantum systems: Anderson pseudo-spin precessions and higher harmonics forbidden by equilibrium symmetry, hidden emergent phases that are difficult to be accessed by other tuning methods, Higgs modes in unconventional superconductors. We will also discuss how to extend THz light-driven coherence and subcycle symmetry breaking for quantum control of other complex systems including topological matter, with implications on quantum gate and sensing applications.

*The author is grateful for collaborations with Ilias E. Perakis and Chang-Beom Eom. Work at Iowa State University was supported by the National Science Foundation.
Local Symmetry Breaking and Spin Momentum Locking in Cuprates Superconductors [Invited] ALESSANDRA LANZARA (Presenter), University of California, Berkeley — The 20th century has been dominated by the realization that symmetry and symmetry breaking are keys to much of the novel phenomena observed in physics today. Superconductivity for example requires both time-reversal and inversion symmetry, and the removal of one of these (e.g. time reversal through a magnetic field) leads to the suppression of the superconducting order. Recently however it has been realized that, even if the global symmetry of the system is retained, a local symmetry breaking can still induce a variety of novel fascinating behaviors. In this talk I will present the effect of local breaking of inversion symmetry in cuprates superconductors and show that this leads to unusual phenomena and the appearance of a non-zero spin polarization with a well-defined spin momentum locking, that is strictly linked to the Fermi surface topology.

These results were enabled by the combination of UV laser with a state-of-the-art time of flight spectrometer combined with exchange scattering, allowing to perform spin and angle resolved photoemission spectroscopy experiments with unprecedented spin, time, energy and momentum resolution.

Femtosecond Covariance Spectroscopy to Control Multimode Quantum Correlations* [Invited] DANIELE FAUSTI (Presenter), Università di Trieste e Elettra Sincrotrone Trieste — The vast majority of nonlinear optical spectroscopies work in an integrated mode, namely they use the mean-value signal, properly averaged over several stroboscopic repetitions. While ensuring an adequate signal-to-noise ratio, this approach relies strongly on pulse-to-pulse consistency and has thus motivated significant efforts in pursuit of perfect experimental stability. By contrast, we have developed a fundamentally different approach, named Femtosecond Covariance Spectroscopy (FCS), which identifies noise as a powerful and unique asset to access information that standard mean-value experiments miss. FCS is based on covariance rather than mean-value observables and relies on the study of multimode quantum correlations imprinted on stochastic ultrashort pulses by light-matter interactions. As a proof of principle, we have successfully applied such approach to the study of Raman-active vibrational modes excited through Impulsive Stimulated Raman Scattering (ISRS) in crystalline quartz. Nevertheless, the impact of FCS is not only limited to the field of condensed matter physics. Indeed, given the formal analogy between the quantum description of ISRS and optomechanical experiments, FCS could pave the way to a new generation of experiments in which the coupling between the electromagnetic field and the mechanical oscillator, could be reproduced by the interaction between light pulses and phonon modes.

*Funding Agencies: ERC_StG2015, Project INCEPT

Mariano Trigo Invited Talk [Invited] —

Wednesday, March 4, 2020 8:00 AM - 10:48 AM
8:00AM L20.00001: Tubulin shape controls the kinetics and mechanism of microtubule depolymerization*  
JONATHAN BOLLINGER (Presenter), ZACHARY IMAM, MARK STEVENS, GEORGE BACHAND, Sandia National Laboratories — Microtubules exhibit alternating phases of growth and shrinkage thought to be controlled by the conformation of tubulin dimers. Specifically, compression of tubulin due to the hydrolysis of GTP has been suggested to generate stress and drive catastrophic depolymerization. We use molecular dynamics simulations and ex vivo experiments to investigate how depolymerization is affected by the presence of uncompressed (unhydrolysed) dimers in the microtubule lattice. Both methods reveal exponential decay in the kinetics of depolymerization corresponding to the relative number of uncompressed dimers. This slowdown is accompanied by a morphological change from ram's horns to blunt-ended dissociation. Collectively these data show that uncompressed dimers can alter depolymerization consistent with promoting rescue events.

*This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA0003525.
8:12AM L20.00002: Stutter: a Transient Microtubule Dynamic Instability Phase that is Strongly Associated with Catastrophe* [invited] SHANT MAHSEREJIAN, Pacific Northwest National Lab, JARED SCRIPTURE, AVA MAURO, University of Notre Dame, ELIZABETH LAWRENCE, MARIJA ZANIC, Vanderbilt, MARK ALBER, University of California, Riverside, HOLLY GOODSON (Presenter), University of Notre Dame — Microtubules (MTs) are dynamic polymers with critical roles in processes ranging from membrane transport to chromosome separation. Central to MT function is dynamic instability (DI), a behavior typically assumed to consist of growth and shortening, with sharp transitions in between. However, this two-state assumption disregards details in MT behavior that are evident in high-resolution data. For example, MTs exhibit growth rate variability, and pinpointing where transitions begin can be difficult when viewed at high spatiotemporal resolution. These observations suggest that MT behavior is more complicated than implied by standard quantification methods. To address these problems, we developed STADIA (Statistical Tool for Automated Dynamic Instability Analysis). STADIA’s methods are rooted in machine learning to objectively analyze and quantify macro-level DI behaviors exhibited by MTs. Applying STADIA to MT length-history data revealed a transient, intermediate phase that we term ‘stutter’, during which the rate of MT length change is smaller in magnitude than growth or shortening phases. Significantly, most catastrophe events in both simulations and experiments are preceded by stutters, suggesting that this newly recognized phase is mechanistically involved in catastrophes. Consistent with this idea, a MT anti-catastrophe factor (CLASP2γ) increases the likelihood of growth following a stutter phase in experiments. We conclude that STADIA enables unbiased identification of DI phases including stutters, producing more complete and accurate DI measurements than possible with classical analysis methods. Identifying stutters as a distinct and quantifiable phase provides a new target for mechanistic studies regarding DI phase transitions and their regulation by MT binding proteins.

*NSF MCB 1817966

8:48AM L20.00003: Molecular dynamics study of Katanin oligomers: A MT-severing enzyme* MANGESH DAMRE (Presenter), ROHITH ANAND VARIKOTI, RUXANDRA I DIMA, Univ of Cincinnati — Microtubule (MT) severing enzymes, such as katanin, belong to the AAA ATPases family and play an important role in meiosis and mitosis through their cutting action on MTs. The severing action is driven by ATP hydrolysis, which induces transitions between distinct conformations of the oligomeric state of the severing enzyme. Two of these oligomeric structures, one in a spiral and the other in a closed ring arrangement, have recently been solved using cryo-EM. ATP is present in all the chains from the spiral conformation, while there is only partial occupancy of ATP in the ring conformation. At the same time, reports from the literature suggest that such high-order oligomeric states of severing enzymes are stable only in the presence of nucleotides and the substrate. We will describe our all-atom molecular dynamics simulations performed on the apo, the ATP bound, and minimal substrate-bound states of katanin. Our results help identify the factors that account for the stability of the oligomeric states and characterize the allosteric transitions that underlie the action of severing enzymes.

*The National Science Foundation (NSF)
9:00AM L20.00004: Role of substrate cooperativity and motor concentration in microtubule severing*  ROHITH ANAND VARIKOTI (Presenter), Univ of Cincinnati, JENNIFER L ROSS, Department of Physics, Syracuse University, RUXANDRA I DIMA, Univ of Cincinnati — Microtubules (MTs) associated proteins (MAPs) regulate the dynamic behavior of MTs during cellular processes. Severing enzymes are MAPs which destabilize MTs by removing subunits from the filament. Because severing enzymes belong to the AAA+ unfoldases family, we probed the severing mechanism characterized by the enzymes applying pulling forces on the C-terminal regions of MT subunits. Due to the large size of the system, we employed coarse grained molecular simulations of different MT lattices and at varying concentration of severing enzymes. Comparison of results from our simulations with data from in-vitro severing assays shows that the cooperative removal of protofilament fragments, at increased concentration of severing enzymes, is a likely MT destabilization scenario. Moreover, we found that optimization of energetics is not a strong requirement if severing proceeds entirely by an unfoldase mechanism.

*National Science Foundation

9:12AM L20.00005: Dynamic stability of actin cytoskeletal networks with mixed geometries  PASHA TABATABAI (Presenter), LAURA LANIER, MICHAEL MURRELL, Yale University — Cells dynamically remodel their cytoskeleton while simultaneously utilizing it to carry out vital tasks such as migration and division. In cells, multiple distinct actin structures coexist, and it is unclear how this coexistence of multiple dynamic networks affects the stability of each network. To this end, we re-engineer a dynamic cytoskeletal system using a minimal set of purified proteins to simultaneously nucleate filamentous actin networks containing mixtures of both branched Arp2/3 and linear formin networks. With this system, we investigate the effect of coexistence of networks with different geometries and growth rates on steady-state structure. Additionally, we explore the influence of both filament severing activity and molecular motor activity on network stability.

9:24AM L20.00006: Actin crosslinking controls mobility, microtubule crosslinkers control co-localization in a composite cytoskeletal network*  LEILA FARHADI (Presenter), Physics, University of Massachusetts Amherst, MICHAEL RUST, Department of Molecular Genetics and Cell Biology, University of Chicago, MOUMITA DAS, School of Physics and Astronomy, Rochester Institute of Technology, RAE M ROBERTSON-ANDERSON, Department of Physics and Biophysics, University of San Diego, JENNIFER L ROSS, Physics, Syracuse University — Actin and microtubule filaments are cytoskeletal biopolymers with various vital roles in the cell. Despite decades of studying them separately, they have recently been shown to interact in networks mechanically and chemically. Here, we are interested in the composite network mechanics and mobility as the actin and microtubules are increasingly crosslinked. We use biotin-NeutrAvidin crosslinkers to irreversibly crosslink actin and MAP65, an antiparallel microtubule crosslinker to bundle microtubules. Cytoskeleton networks are imaged over time using fluorescent microscopy and the mobility characteristics are measured. We find that actin crosslinkers tune the mobility of this composite network, while microtubule crosslinkers can control the co-localization of actin and microtubules.

*Funding: W.M. Keck Foundation Research Grant.
**Avalanches in simulations of branched actomyosin networks with the Arp2/3 complex**

JAMES LIMAN (Presenter), Department of Bioengineering, Rice University, CARLOS BUENO, Systems, Synthetic, and Physical Biology, Rice University, YOSSI ELIAZ, Department of Physics, University of Houston, NICHOLAS SCHAFTER, Center for Theoretical Biological Physics, Rice University, NEAL WAXHAM, Department of Neurobiology and Anatomy, McGovern Medical School at The University of Texas Health Science Center at Houston, PETER G WOLYNES, Center for Theoretical Biological Physics, Rice University, HERBERT LEVINE, Department of Physics, Northeastern University, MARGARET CHEUNG, Department of Physics, University of Houston — Actomyosin networks are ubiquitous in biology. They provide structure to cells and are involved in cell movement, growth, and division. The dynamics of actomyosin networks are active processes and are greatly influenced by actin binding-proteins (ABPs). These ABPs include both motor proteins (non-muscle myosin IIA heavy chain (NMIIA)) and cross-linker proteins (α-actinin). Another important ABP, the Arp2/3 complex, nucleates branched filaments thereby influencing the topology of the network. In this work, we simulate the spatiotemporal configurations of actomyosin networks with and without the Arp2/3 complex. The simulations show that the branched actomyosin networks that include the Arp2/3 complex exhibit sporadic convulsive movements, which we call avalanches, that release built-up stress in the network. We then identify and characterize these avalanches. The characteristics of these avalanches observed in the simulations are consistent with the recent experimental observation of “cytoquakes.”

*This work is supported by the National Science Foundation CHE 1743392 and the Center for Theoretical Biological Physics PHY 1427654.

**A dynamic contractile F-actin network reconstituted in Xenopus egg extract**

JIANGUO ZHAO (Presenter), CHRISTOPH F. SCHMIDT, Department of Physics and Soft Matter Center, Duke University — The actin cytoskeleton in most animal cells is a highly dynamic multi-component network that rapidly turns over, adapts, generates forces and moves. The continuous remodelling of the cytoskeleton and spontaneous flows have been extensively visualized in a variety of cellular processes, including intracellular transport, cell migration and division. It remains unclear how the spatiotemporal interactions of the various components self-organize to give rise to global F-actin flows. We reconstituted a fully active model cytoskeleton in water-in-oil emulsion droplets containing xenopus egg extract. We observed steady state directed flows and non-equilibrium phase separation. We analysed the flow and examined the contractile stress generated by actin-myosin interactions.
10:00AM L20.00009: Controlling ‘cell’ size and shape to elucidate the mechanics of microtubule aster positioning* [Invited]  
JAY GATLIN (Presenter), TAYLOR SULERUD, ABDULLAH SAMI, ZACH GEISTERFER, Molecular Biology, University of Wyoming, JOHN OKEY, Chemical Engineering, University of Wyoming — The microtubule (MT) cytoskeleton plays critically important roles in numerous eukaryotic cellular functions, and it does so across a functionally diverse and morphologically disparate range of cell types. In these roles, MT assemblies must adopt distinct cell cycle-dependent morphologies and physical dimensions to perform specific functions. During interphase, the MT network takes the form of a radial astral array (aster) that functions to center the nucleus, a by proxy the mitotic spindle, which ultimately dictates the position of the cell division plane. The mechanical underpinnings of this positioning phenomenon remain elusive despite its fundamental importance to both symmetric and asymmetric vision and intensive study. To address this gap in our collective understanding, we have combined photo-labile hydrogels with cell-free extracts in a new experimental platform that affords exquisite control of “cell” shape and volume. By observing the behavior/dynamics of MT asters confined in hydrogel micro-containers of different geometries, we have elucidated the relative contribution of MT-based pushing forces to aster positioning and have begun to characterize the length scales over which they operate.

*This research was supported by the National Institute Of General Medical Sciences of the National Institutes of Health under Award Numbers P20GM103432 and R01GM113028. The authors would also like to thank the Pew Biomedical Scholars Program for its support as well.

10:36AM L20.00010: Active Composites of Actin and Kinesin-driven Microtubules*  
JOHN BEREZNEY (Presenter), SETH FRADEN, Brandeis Univ, ZVONIMIR DOGIC, Physics, University of California, Santa Barbara — Two major structural proteins, actin and microtubules, form multiple co-existing and interpenetrating filamentous protein networks within the cell cytoplasm. The out-of-equilibrium active reorganization of these structures by molecular motors is necessary for basic physiological processes such as cell division, cell motility, and environmental sensing. While the passive structure and mechanics of such materials have been well documented, the effects of their steady-state out-of-equilibrium reorganization is a site of current research. To demonstrate some of the mechanics governing the active reorganization of these materials, we have built a polymer blend of kinesin-driven microtubule networks which reorganize a passive entangled actin network. We find both the mechanics of the actin network as well as its initial structure can have dramatic effects on the steady-state behavior of the system. To capture the range of behaviors, we build a state diagram which captures the non-equilibrium phenomena we observe.

*We acknowledge financial support from the NSF MRSEC DMR-1420382

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

8:00AM L21.00001: Development of a Machine-Learned Density Functional Tight Binding for TiH₂ Bulk and Surface Chemistry* NIR GOLDMAN (Presenter), Lawrence Livermore Natl Lab — Knowledge of chemical defect energies and kinetics is essential for assessing potential hydrogen storage materials like TiH₂, where hydrogen point defects need to be assessed accurately and efficiently. The Density Functional Tight Binding (DFTB) method is a highly efficient semi-empirical quantum approach that can accurately probe these properties, but can be challenging to parameterize for each system of interest due to the different bonding types that can occur. Here, we have created a machine learning-based approach for determining the DFTB models which is both rapidly optimized, systematically improvable, and highly transferable. Our method leverages the Chebyshev Interaction Model for Efficient Simulation (ChIMES), a reactive many-body molecular dynamics force field where interactions are represented by linear combinations of Chebyshev polynomials. In this work, we discuss our ChIMES/DFTB models for TiH₂, and show its accuracy for both bulk and surface properties. Our approach is easy to implement and can yield accurate DFTB models for a number of challenging materials and conditions where chemical events can be difficult to model with standard quantum approaches alone.

*Prepared by LLNL under Contract DE-AC52-07NA27344.

8:12AM L21.00002: Molecular Dynamics Modeling of Plasma Material Interactions using Machine Learned Interatomic Potentials* MARY ALICE CUSENTINO (Presenter), MITCHELL WOOD, AIDAN THOMPSON, Sandia National Laboratories — Multiple materials, namely tungsten and beryllium, will be present in future fusion reactors as plasma facing components. Experiments of beryllium implantation in tungsten indicate the formation of W-Be intermetallics on the surface, which can affect the performance of the tungsten divertor. Molecular dynamics (MD) can provide insight into physical processes related to experimental observations. However, MD is limited by the accuracy of the interatomic potential used. Recently, machine learning methods are being used to develop more accurate, quantum-informed potentials. In this work, we have developed a machine learned Spectral Neighbor Analysis Potential (SNAP) for W-Be and used this potential to study beryllium implantation in tungsten. An amorphous W-Be layer forms within the first 50 ns that is limited to the near surface region and an exchange mechanism that allows tungsten to migrate from the substrate into the amorphous layer was observed. Ordered structures similar to expected intermetallic configurations were seen within the amorphous layer. These results show the early stages of a surface W-Be layer that can provide further insight into the formation of the intermetallics observed in experiments.

*SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525
8:24AM L21.00003: Machine learning modeling of the Curie temperature for ferromagnetic intermetallics*

HONGBIN ZHANG (Presenter), TENG LONG, NUNO FORTUNATO, YIXUAN ZHANG, OLIVER GUTFLEISCH, Technische Universität Darmstadt — Magnetic materials play an essential role in green energy and informatics applications, such as efficient energy harvesting and conversion and low energy cost spintronic devices. Currently the key challenge is how to optimize the performance of existing systems and to design novel materials for broader applications. In this talk, a random forest model is trained to classify ferromagnetic and antiferromagnetic orderings and to predict the transition temperature ($T_C$) of the ferromagnets, using 2805 known intermetallic compounds. The resulting accuracy is 86% for classification and 92% for regression (with a mean absolute error of 58K), comparing favourably with first-principles methods. We apply these models to 5183 intermetallic compounds found in the Materials Project database, predicting their magnetic ordering and $T_C$. This enables us to make reliable predictions, particularly by combing high throughput and machine learning methods, paving the way to accelerate the discovery of novel magnetic compounds for technological applications.

*We thank the financial support from European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (Grant No. 743116-project Cool Innov) and the Chinese Scholarship Council.

8:36AM L21.00004: Comparison of Classical Molecular Dynamics and Ab initio Molecular Dynamics with Different Equilibration Methods for Modeling Solvent - Lithium Salt Systems in Lithium Air Batteries*

EMILY CRABB (Presenter), ARTHUR FRANCE-LANORD, GRAHAM MICHAEL LEVERICK, Massachusetts Institute of Technology MIT, RYAN STEPHENS, Shell International Exploration & Production Inc., YANG SHAO-HORN, JEFFREY C GROSSMAN, Massachusetts Institute of Technology MIT — Lithium-air batteries are an active area of research because of their potential to have a much higher energy density than traditional lithium-ion batteries. However, they are not yet commercially viable due to poor efficiency, high charging voltages, and low cycle lifetimes. In Li-air batteries, $O_2$ reduction starts when superoxide forms in solvent and reacts with $Li^+$ to form lithium superoxide ($LiO_2$). Solid $Li_2O_2$ then forms as the final discharge product on the cathode. Recent experimental work suggests that the choice of solvent and the presence of lithium salts in the system may have a large impact on how the discharge product forms at the cathode. We therefore modeled the clustering of lithium salt molecules in solvent without $LiO_2$ present with explicit solvent calculations using both classical and ab initio molecular dynamics simulations. For each ab initio simulation, we also used one of two equilibration procedures: (1) performing a classical molecular dynamics simulation or (2) performing shorter ab initio simulations at higher temperatures. A comparison of these computational approaches for properties such as coordination numbers will be presented.

*This work is supported by a grant from Shell, as well as partial support from a DOE fellowship.
8:48AM L21.00005: Benchmarking SCAN functional for two-dimensional crystal structures*
GRACIE CHANEY (Presenter), DANIEL WINES, JARON KROPP, FATIH ERSAN, CAN ATACA, Univ of Maryland-Baltimore County — It has recently been reported that the strongly constrained and appropriately normed (SCAN) meta-GGA functional has performed exceptionally well for density functional theory (DFT) calculations involving molecular and crystalline systems. In addition, the computational cost of SCAN is argued to be much less than that of the highly demanding hybrid functional methods with comparable accuracy. SCAN has been applied to several three-dimensional systems, but has not been widely used for two-dimensional materials such as transition metal (M) monochalcogenides (MX), M dichalcogenides (MX₂), and M trichalcogenides (MX₃). In this study, we provide a comprehensive set of data obtained by SCAN, hybrid functionals (HSE), and PBE. Specifically, we compare lattice constants, band gaps, electronic/thermal transport and magnetic properties, and computational cost. We also study optical properties with GW approximation, using DFT orbitals obtained from SCAN and PBE. Our goal is to benchmark results from SCAN, PBE, HSE, PBE+GW, and SCAN+GW and to create a detailed picture of how SCAN performs compared to other well established DFT functionals. This work is the terminal paper for benchmarking different DFT functionals and will guide further theoretical studies involving 2D materials.

*NDF DMR-1726213

9:00AM L21.00006: Theoretical study on the electric-double layer formed at interlayer of transition-metal-carbide MXene by quantum-classical hybrid interface simulation
YASUNOBU ANDO (Presenter), CD-FMat, AIST, MASASHI OKUBO, The University of Tokyo, MINORU OTANI, CD-FMat, AIST, ATSUO YAMADA, The University of Tokyo — Two-dimensional transition-metal carbide MXene has been known as a promising material of high-performance electrode for energy storage applications with both non-aqueous and aqueous electrolytes because it has electronic conductivity, ion capability in interlayer nanospace, and the redox activity of Ti. Here, we performed a microscopic theoretical analysis of the electric-double layer capacitance in the interlayer nanospace of the MXene electrode by combining first-principles calculations and implicit solvation theory named 3D-RISM method[1]. As a result, we found that hydration shell of Li⁺ and Na⁺ overscreens the electric field, or shows “negative dielectric constant”, and enhances its electronic-double layer capacity[2, 3].

First-principles analysis of band offsets, phase stability, and alkali incorporation in (Ag,Cu)(In,Ga)Se$_2$ solar cells*  KOSTIANTYN SOPIHA (Presenter), JES LARSEN, JAN KELLER, MARIKA EDOFF, CHARLOTTE PLATZER-BJÖRKMAN, Ångström Solar Center, Division of Solid State Electronics, Uppsala University, CLAS PERSSON, Department of Physics/Centre for Materials Science and Nanotechnology, University of Oslo, JONATHAN SCRAGG, Ångström Solar Center, Division of Solid State Electronics, Uppsala University — Over the years, thin-film photovoltaics based on Cu(In,Ga)Se$_2$ (CIGS) have undergone continuous improvements, with recent efficiency records indicating that CIGS is yet to unleash its full potential. Ag-alloying (forming ACIGS) is emerging as an exciting focus area, since ACIGS demonstrates better crystallinity and lower $V_{OC}$ losses than CIGS alone. In this work, we investigate the fundamental origin of these improvements by performing detailed first-principles analysis of ACIGS alloys. Based on the computed electronic properties, we establish a correlation between the composition and conduction band minimum, which allows rational tuning of band offsets at ACIGS/buffer (CdS or Cd-free) interface with a desired band gap of the absorber. From a thermodynamic analysis, we reveal the existence of a miscibility gap that can induce phase separation and Ag grading during thin film growth. Furthermore, from a defect analysis, we show that Ag promotes solubility of alkalis during post-deposition treatment. The obtained results are verified by measuring device and material characteristics for different ACIGS films, which showed a good agreement with the theoretical predictions.

*We thank Swedish Foundation for Strategic Research and Research Council of Norway for their financial support.

Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods  FRANCESCA TAVAZZA (Presenter), KAMAL CHOU DHARY, Materials Measurement Lab, National Institute of Standards and Technology — Solar energy plays an important role in solving serious environmental problems and meeting the high energy demand. However, the lack of suitable materials hinders further progress of this technology. Here, we present the largest inorganic solar cell material search till date using density functional theory (DFT) and machine-learning approaches. We calculated the spectroscopic limited maximum efficiency (SLME) using the Tran–Blaha-modified Becke–Johnson potential for 5097 nonmetallic materials and identified 1997 candidates with an SLME higher than 10%, including 934 candidates with a suitable convex-hull stability and an effective carrier mass. Screening for two-dimensional-layered cases, we found 58 potential materials and performed $G_0W_0$ calculations on a subset to estimate the prediction uncertainty. As the above DFT methods are still computationally expensive, we developed a high accuracy machine-learning model to prescreen efficient materials and applied it to over a million materials. The data and tools are publicly distributed at: https://www.ctcms.nist.gov/~knc6/JVASP.html, https://www.ctcms.nist.gov/jarvisml/, https://jarvis.nist.gov/, and https://github.com/usnistgov/jarvis.
9:36AM L21.00009: Electrical property dominated promising half-Heusler thermoelectrics through high-throughput material computations*  SHUPING GUO (Presenter), TIANTIAN JIA, Institute of Solid State Physics, Chinese Academy of Sciences, SHASHWAT ANAND, Department of Materials Science and Engineering, Northwestern University, YONGSHENG ZHANG, Institute of Solid State Physics, Chinese Academy of Sciences, JEFF SNYDER, Department of Materials Science and Engineering, Northwestern University — Half-Heusler (HH) compounds are one of the state-of-the-art thermoelectric materials with high electrical properties. Here, we carry out high-throughput computations on 95 HH compounds. Using the thermoelectric properties of NbFeSb and ZrNiSn as the screening criterion, we filter out nine p-type and six n-type promising candidates with environmentally friendly elements. Scrutinizing their electronic structures, we find that the cooperative effects of high band degeneracy, small deformation potential, light band, and large phonon velocity contribute to the large power factor. It is interesting to notice that the electrical properties dominate the thermoelectric performance in HH compounds. Balancing the excellent electrical properties and relatively low thermal conductivities, three HH compounds are predicted to be promising thermoelectric candidates. Our work not only provides novel promising materials for future experimental investigation but also offers insights into understanding the underlying physical nature of high thermoelectric performance.

*We acknowledge supports from the National NSF of China (grant no. 11774347), the “Designing Materials to Revolutionize and Engineer our Future” program of the NSF under Award No. 1729487 and the U.S. DOE, Office of EERE.

9:48AM L21.00010: Computational Discovery of an Enormous Class of Stable Quaternary Chalcogenides with Very Low Lattice Thermal Conductivity  KOUSHIK PAL (Presenter), CHRISTOPHER MARK WOLVERTON, Northwestern University — The development of efficient thermal energy management devices such as thermoelectrics, barrier coatings, and thermal data storage disks relies on compounds which possess low lattice thermal conductivity ($\kappa_l$). Here, we present an enormous class of thermodynamically stable quaternary chalcogenides $\text{AMM'}\text{Q}_3$ (A=Alkali, alkaline earth, post transition metals; M,M'=transition metals, lanthanides; Q= chalcogens) that possess intrinsically low $\kappa_l$ using high-throughput DFT calculations. Leveraging the computed energetics of hundreds of thousands of multinary compounds in the Open Quantum Materials Database (OQMD), we discovered a large number (nearly 1000) of thermodynamically stable chalcogenides through successive screening based on the calculations on multiple crystallographic prototypes of the experimentally known $\text{AMM'}\text{Q}_3$ compounds. We validate the low-$\kappa_l$ in this family of compounds by calculating the lattice thermal conductivity taking several representative compounds using the highly accurate anharmonic lattice dynamics methods. Our predictions suggest new experimental research opportunities in the synthesis and characterization of these stable, low-$\kappa_l$ compounds.
10:00AM L21.00011: Electron-phonon scattering effects on the transport properties of ZrS$_2$

HITOSHI MORI (Presenter), MASAYUKI OCHI, KAZUHIKO KUROKI, Osaka Univ — Multi-valley structure is known as one of the favorable band structures for enhancing thermoelectric efficiency. N-type TiS$_2$ has electronic structure with multi-valley character, and its power factor is relatively high: ~40 μW/cmK$^2$ at room temperature. In previous experimental studies, the electrical resistivity of TiS$_2$ has been found to exhibit strong temperature dependence of ~T$^2$. One of the previous studies indicated that inter-valley scattering among conduction band valleys may be related to the peculiar temperature dependence of the electrical resistivity [1].

Since understanding the inter-valley scattering effect on the transport properties may provide a clue toward designing materials with higher thermoelectric efficiency, in the present study, we perform DFT calculations and calculate the electronic transport properties by considering the electron-phonon scattering effect using the EPW code [2]. As a target material in this study, we consider not TiS$_2$, but instead its analogous compound ZrS$_2$. We will discuss the role of the inter-valley scattering played in the electronic transport properties of ZrS$_2$.


10:12AM L21.00012: Li and Na migration in Guest-free, type I clathrates evaluated via ab initio methods*

XIHONG PENG (Presenter), ANDREW DOPILKA, CANDACE CHAN, Arizona State Univ — Open, cage-like clathrates Tt$_{46}$ (Tt = Si, Ge, Sn) has a potential as anodes in Li/Na-ion batteries. Density-functional theory calculations were performed to explore ionic mobility of Li/Na through clathrate crystals. Local energy minima of Li/Na locations inside the clathrates were determined, the Li/Na migration paths/barriers were calculated using nudged elastic band method. It was found that it is favorable for Li to occupy the Tt$_{20}$ cage center while preferring the off-center positions in larger Tt$_{24}$ cages. The lowest Li migration barriers were found to be 0.35, 0.13 and 0.37 eV for Si$_{46}$, Ge$_{46}$, and Sn$_{46}$, respectively. In contrast, Na shows preference for the cage centers and higher migration barriers than Li. In general, the Tt$_{24}$ channels in the guest-free, type I clathrates are ideal for fast Li diffusion, while Na is too large to migrate effectively between cages. The energy landscape for Li inside the clathrates is uniquely different than that in diamond allotropes, leading to significantly lower energy barriers for Li migration. These results suggest that open frameworks of intermetallic clathrates may enable facile Li migration and have potential as anodes in Li-ion batteries.


*NSF DMR-1710017
**10:24AM L21.00013: Effect of Bulk Diffusivities of Co-solvents on the Microscopic Dynamics of an Ionic Liquid**  
NARESH C OSTI (Presenter), Neutron Scattering Division, Oak Ridge National Laboratory, RAY MATSUMOTO, MATTHEW THOMPSON, PETER THOMAS CUMMINGS, Chemical and Biomolecular Engineering, Vanderbilt University, MADHUSUDAN TYAGI, NIST Center for Neutron Research, National Institute of Standards and Technology, EUGENE MAMONTOV, Neutron Scattering Division, Oak Ridge National Laboratory — Room temperature ionic liquids (RTILs) are considered superior over organic electrolytes in terms of their thermal stability, volatility, voltage window, and device life expectancy, making them promising electrolyte materials for electrical double layer capacitors. However, pure RTILs often exhibit high viscosity, low conductivity, and poor diffusivity, which can affect the charging and discharging rates, impacting device performances. The addition of co-solvents is found to change the viscosity of RTILs, leading to improved physico-chemical characteristics that affect their bulk and interfacial properties. Even though a direct correlation of co-solvent polarity with cation diffusivity has been established, an impact of co-solvent bulk diffusivity on the cation dynamics of RTILs has never been explored. Here, using different neutron scattering spectrometers and molecular dynamics simulation, we showed a presence of a phase separation into an ionic liquid-rich and a solvent-rich phase of 1-butyl-3-methyl-imidazolium bis(trifluoromethylsulfonyl)imide, [Bmim$^+$][TFSI$^-$], mixed with four different co-solvents of nearly the same dipole moment, where we observed a scaling of long-range translational mobility of the [Bmim$^+$] cation with the bulk diffusivities of the organic solvents.

**10:36AM L21.00014: Properties of V$_2$O$_5$ polymorphs from first principles**  
SAKTHI KASTHURIRENGAN (Presenter), HARTWIN PEELAERS, Univ of Kansas — V$_2$O$_5$ is a very promising battery electrode material that can intercalate not only Li, but also more abundant alkaline metals such as Na and K, and even multivalent ions such as Mg, Ca, Zn, and Al. V$_2$O$_5$ can occur in several polymorphs, with at least 5 different polymorphs observed. During intercalation phase transitions can take place, and such phase transitions can be detrimental to battery performance. Understanding these transitions requires knowledge of the energetics and structural properties of the various V$_2$O$_5$ polymorphs.

We provide such understanding by employing density functional theory (DFT) calculations based on hybrid functionals. Since several of the polymorphs are layered, van der Waals interactions are important. However, this interaction is not included in standard DFT calculations. We therefore tested several approaches to include these interactions in combination with hybrid functionals. Based on our results we discuss the structural and electronic properties of the various polymorphs, and show the role polarons play in electronic transport. The obtained insights can be used to optimize future V$_2$O$_5$-based battery electrodes.
Computational Design and Study of Small D-A Type Organic Molecule with Ambipolar Characteristics and Rich Linear and Non-Linear Optical Properties

DWAIPAYAN CHAKRABORTY (Presenter), PRIYA JOHARI, Shiv Nadar Univ — Push-pull type small organic molecule has recently gained a huge scientific research owing to their remarkable charge transfer properties, high non-linear optical response, reduced HOMO-LUMO gap and hence broad range of absorption spectrum, air stability etc. which collectively promotes this class of molecules as potential candidate for non-linear optical devices, OFETs and organic solar cells. In this effort, we therefore rationally designed a promising Donor(D)-π-Acceptor(A) (i.e, push-pull) type molecule NNDM-NH$_2$, a trans-stilbene derivative. We predicted its crystal structure starting from the experimental crystal structure of another stilbene derivative and calculated the charge transport properties, electronic band structure, gas-phase linear and non-linear optical properties. We also did the Hirshfeld surface analysis and plotted the molecular electrostatic potential to get insight into the structure-property correlation. We found that this new organic semiconductor owns a high charge carrier mobility for hole and electron, together with desirable electronic and linear and non-linear optical properties revealing NNDM-NH$_2$ as a potential candidate for the opto-electronic devices.

*Shiv Nadar University

**Wednesday, March 4, 2020 8:00 AM - 10:36 AM**

**Session L22 DBIO DCP DMP DPOLY: Biomaterials III: Tissue-Scale Physics** 303 - Esther Amstad - Tag(s): Focus
8:00AM L22.00001: Filament Nucleation Tunes Mechanical Memory in Active Polymer Networks* [Invited] VIKRANT YADAV, Yale University, DEB BANERJEE, Physics, University College London, ALAN TABATABAI, Yale University, DAVID KOVAR, Division of Biological Sciences, University of Chicago, TAEGYOON KIM, Biomedical Engineering, Purdue University, SHILADITYA BANERJEE, Physics, University College London, MICHAEL MURRELL (Presenter), Yale University — Incorporating growth into contemporary material functionality presents a grand challenge in materials design. The F-actin cytoskeleton is an active polymer network which serves as the mechanical scaffolding for eukaryotic cells, growing and remodeling in order to determine changes in cell shape. Nucleated from the membrane, filaments polymerize and grow into a dense network whose dynamics of assembly and disassembly, or ‘turnover’, coordinates both fluidity and rigidity. Here, we vary the extent of F-actin nucleation from a membrane surface in a biomimetic model of the cytoskeleton constructed from purified protein. We find that nucleation of F-actin mediates the accumulation and dissipation of polymerization-induced F-actin bending energy. At high and low nucleation, bending energies are low and easily relaxed yielding an isotropic material. However, at an intermediate critical nucleation, stresses are not relaxed by turnover and the internal energy accumulates 100-fold. In this case, high filament curvatures template further assembly of F-actin, driving the formation and stabilization of vortex-like topological defects. Thus, nucleation coordinates mechanical and chemical timescales to encode shape memory into active materials.

*ARO MURI W911NF-14-1-0403, CMMI-1525316, NIH RO1 GM126256, U54 CA209992, HFSP RGY0073/2018

8:36AM L22.00002: Bioinspired materials with self-adaptable mechanical behaviors* SANTIAGO ORREGO, Temple University, ZHEZHI CHEN, URSZULA KREKORA, DECHENG HOU, SEUNG-YEOL JEON, MATTHEW PITTMAN, Johns Hopkins University, CAROLINA MONTOYA, Temple University, YUN CHEN, SUNG KANG (Presenter), Johns Hopkins University — Nature produces outstanding biomaterials for structural applications such as bones and woods that can adapt to their surrounding environment. However, it is a challenge for synthetic materials to change and adapt their structures and properties to address the changes in loading conditions. To overcome the issue, we have investigated synthetic materials inspired by bone that trigger mineral syntheses from ionic solutions on scaffolds upon mechanical loadings so that they can self-adapt to mechanical loadings. For example, we observed a 30-180% increase in the modulus of the material upon different magnitudes of periodic loadings. Moreover, the mechanism allows a one-step route for making graded materials by controlling stress distribution along the scaffold. The findings can contribute to addressing the current challenges of synthetic materials for load-bearing applications from self-adaptive capabilities.

*This work is supported by the Air Force Office of Scientific Research Young Investigator Program Award (Award number: FA9550-18-1-0073, Program manager: Dr. Byung-Lip (Les) Lee), Johns Hopkins University Whiting School of Engineering start-up fund, and Temple University Maurice Kornberg School of Dentistry start-up fund (PI: Orrego).
8:48AM L22.00003: The continuum of allosteric behavior in mechanical networks  JASON ROCKS (Presenter), Physics, Boston University, ANDREA JO-WEI LIU, ELENI KATIFORI, Physics and Astronomy, University of Pennsylvania — Allosteric regulation in proteins is often accompanied by conformational transitions, facilitating the transmission of mechanical signals between distant ligand binding sites. Analyses of allosteric proteins have revealed a variety of archetypal motions ranging from hinge-like or shear mechanisms to allosteric strain pathways connecting different binding sites. Here we investigate the range of possible motions that can be achieved in mechanical networks tuned to perform allostery. Using an analysis based on persistent homology, we develop a description of allosteric motion which quantifies and unifies all mechanisms into a single framework. We show that while some networks fall into distinct classes of archetypal designs, most fall along a continuum consisting of combinations of hinges, strain pathways and isostatic architectures. We apply this analysis to a collection of proteins, allowing us to identify potential sets of residues that are important for facilitating allosteric communication between different binding sites.

9:00AM L22.00004: A microfluidic model of periarterial spaces in the glymphatic system* KEELIN QUIRK (Presenter), KERSTIN N. NORDSTROM, Mt Holyoke Coll, DOUGLAS H KELLEY, University of Rochester — In the glymphatic system, cerebrospinal fluid enters through periarterial spaces and removes metabolic waste from the brain's interstitial spaces. Previous experiments in live mice have found that a wave along artery walls produced by the heartbeat induces flow in the surrounding perivascular space. However, the mechanisms driving the flow are still not well understood, as many mechanisms may be acting simultaneously. We have designed microfluidic devices to serve as two-dimensional models of periarterial spaces. Using particle tracking velocimetry, we analyze induced flow driven by a peristaltic wave at the frequency range representative of human heartbeats. We find the overall bulk flow induced by the membrane wave travels in the same direction as the wave and increases with frequency. However, during an individual pump cycle, we observe both forward and backwards flow. We also measure the phase shift of the induced flow.

*This work was supported by the Clare Boothe Luce Program at Mount Holyoke College, a grant from the NIH/National Institute of Aging (RF1 AG057575-01) and a grant from the Army Research Office (MURI W911NF1910280)
9:12AM L22.00005: Ultrafast Finger Snap is Mediated by a Frictional Skin Latch  RAGHAV
ACHARYA (Presenter), ELIO CHALLITA, SAAD BHAMLA, Chemical and Biomolecular Engineering, Georgia
Institute of Technology — The snap of a finger is a ubiquitous motion that has been seen across
cultures and times. Using high-speed imaging, we analyze finger snap dynamics for the first time.
We find that the mechanics of the snap are strongly mediated by human skin friction, which acts
as a latch to generate rapid motion. The skin frictional latch is optimally tuned to enable
maximum kinematic performance as the angular accelerations observed during a snap are one
of the fastest human motions known. A simple scaling relationship is found that links the latch
geometry to the performance of snapping motion across multiple organisms from termites to
humans. Ultimately, our work reveals how friction between surfaces can be harnessed as tunable
and scalable latching mechanism, with applications ranging from increasing grip in biomedical
prosthetic surfaces to generating high force and accelerations in tiny robots.

9:24AM L22.00006: Unveiling Interfacial Properties of Surfactant Assemblies Mimicking
Healthy and Diseased States in Lung Membranes*  MARILYN PORRAS-GOMEZ (Presenter),
CECILIA LEAL, University of Illinois at Urbana-Champaign — Lipid-protein complexes conform the
basis of pulmonary surfactants covering the respiratory surface and mediating gas exchange in
lungs, yet how they contribute to alveoli membrane functions in healthy and diseased conditions
is not sufficiently understood. Alveolar stability appears to be controlled by the passive elastic
properties of the pulmonary tissue as well as the mechanical performance of the surfactant
membranes and an unbalance of these is associated with different respiratory dysfunctions and
pathologies. Cardiolipin is a mitochondrial lipid overexpressed in mammalian lungs infected by
bacterial pneumonia, likely to play a role in alveolar stability. We performed structural and
mechanical characterization by GISAXS, AFM and Fast Force Mapping on lipid-based mimicking
pulmonary membranes in healthy and diseased states. Our preliminary results unveiled that
pulmonary membranes suffer structural transformations induced by cardiolipin and calcium
ions. Membrane contacts, or stalks, might induce a significant increase in oxygen gas permeation
that can lead to imbalance in alveoli gas exchange.

*National Institutes of Health under grant No. 1DP2EB024377
US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, under Contract
No. DE-AC02-06CH11357
9:36AM L22.00007: Hybrid active matter: particles and cellular aggregates*  FRANCOISE BROCHARD-WYART (Presenter), PhysicochimieCurie, Institut Curie — We investigate the collective migration of cell on adhesive substrates, using 3D cellular aggregates as a model system. Aggregates spread by expanding outwards a cell monolayer, which may dewet, causing the aggregates to move as “Giant Keratocytes”. We interpret this motion by a symmetry-breaking of cell polarity in analogy to active droplets.

We then describe mixture of dead and living matter and how microparticles play with cells. The size of the particles is varied from nanometers to few microns. Nanoparticles (size 20nm) can be used as a glue “nanostickers” to stick cells together and have important applications for cellular therapy and cancer treatment. Micro-particles MiPs (size ≈ micron) are used to study the spreading of cell aggregates on substrates decorated with MiPs. A cell monolayer expands around the aggregate. Cells at the periphery uptake the microparticles “gluttonous cells” by phagocytosis, forming an aureole of cells full of particles. Macro-particles MaPs (size ≈10 microns) are too big to be eaten and they are put into active motion “dancing”. We study also phase separations in hybrid particles -cells aggregate versus beads volume fraction.

*CelTisPhyBio and PIC3D of the Institut Curie and the WPI-Program, Japan,

9:48AM L22.00008: The role of heterogeneous environments and docetaxel gradients in the emergence of polyploid, mesenchymal and resistant prostate cancer cells.*  ROBERT AUSTIN (Presenter), Princeton University — The ability of a population of PC3 prostate epithelial cancer cells to become resistant to docetaxel therapy and progress to a mesenchymal state remains a fundamental problem. The progression towards resistance is difficult to directly study in heterogeneous ecological environments such as tumors. In this work, we use a micro-fabricated “evolution accelerator” environment to create a complex heterogeneous yet controllable in-vitro environment with a spatially-varying drug concentration. With such a structure we observe the rapid emergence of a surprisingly large number of polyploid giant cancer cells (PGCCs) in regions of very high drug concentration, which does not occur in conventional cell culture of uniform concentration. This emergence of PGCCs in a high drug environment is due to migration of diploid epithelial cells from regions of low drug concentration, where they proliferate, to regions of high drug concentration, where they rapidly convert to PGCCs. Such a mechanism can only occur in spatially-varying rather than homogeneous environments.

*This work was supported by NSF PHY-1659940
10:00AM L22.00009: Predicting Pericellular Matrix Structure from Simple Models of Hyaluronan Secretion* JAN SCRIMGEOUR (Presenter), Clarkson Univ — The synthesis and release of hyaluronan (HA) from the surface of living cells is essential to the maintenance of living tissues and fluids. HA synthesis is controlled by the hyaluronan synthase enzyme, which assembles the polymer chain, and extrudes it through the cell membrane before it is released into the extracellular space. This enzymatic process forms a critical link between the state of the cellular system (protein expression, metabolism, etc) and the properties of cellular interfaces, the extracellular matrix and many biofluids. I present a simple kinetic model that allows an examination of the secretion process. This model enables simulation of the synthesis and release process, enabling prediction of the molecular weight distributions of HA that are tethered to, and released from the cell surface. In so doing this model offers direct insight into the structure of the pericellular matrix, a cell tethered, hyaluronan-rich interface that mediates many cell processes such as adhesion and cell surface access. In addition, the simulations suggest that time-resolved analysis of the hyaluronan molecular weight distributions produced by living cells after PCM digestion can reveal critical details of hyaluronan synthase function.

*National Science Foundation (CAREER), DMR 1847786

10:12AM L22.00010: Electrical detection of Hachimoji nucleobases via a nanopore device incorporated in a graphene/h-BN heterostructure* GANESH SIVARAMAN, Argonne Leadership Computing Facility, Argonne National Laboratory, FABIO ARTHUR LEAO DE SOUZA, Instituto Federal do Espírito Santo, MARIA FYTA, Institute for Computational Physics, University of Stuttgart, RALPH HENDRIK SCHEICHER, Department of Physics and Astronomy, Uppsala University, WANDERLA L. SCOPEL, Department of Physics, Universidade Federal do Espírito Santo, RODRIGO G. AMORIM (Presenter), Department of Physics, ICEx, Universidade Federal Fluminense - UFF — Solid-state nanopores based on 2D materials have been proposed as a candidate for next generation sequencing (NGS) to achieve high throughput, label-free DNA and protein sequencing at low costs. A recent endeavor in synthetic biology resulted in the creation of stable DNA/RNA systems based on 8 (`hachi`) letter (`moji`) building blocks (i.e. 4 synthetic and 4 natural nucleobases) [1]. Although mutations and methylations of the natural nucleobases have been extensively investigated, synthetic nucleobases reported in the hachimoji system remain unexplored with such NGS methods. Hence in this talk, we propose a computational study based on density functional theory and non-equilibrium Green’s function formalism, to unravel the electrical read-out of synthetic and natural nucleobases. To this end, we propose a hybrid 2D nanopore formed in a graphene nanorod embedded within hexagonal boron nitride to perform the electrical read. We will go on to show that the proposed hybrid 2D nanopore can qualitatively discriminate natural and synthetic nucleobases.


*US DOE Office of Science (DE-AC02-06CH11357).
10:24AM L22.00011: Modeling the rheology of dense biological tissues JUNXIANG HUANG
(Presenter), DAPENG BI, Northeastern University — Shear forces in tissues are prevalent in many important biological processes including embryonic development, organogenesis and tumor invasion. However, the intercellular transmission of shear forces and the rheological response of a tissue remains poorly understood. In this work, we use a minimal vertex-based model to investigate the rheology of confluent epithelial tissues. We systematically probe the effects single-cell stiffness, polarized cell motility and the strain rate on the monolayer stress. We also elucidate how the interplay of these parameters affect the cellular rearrangements such as T1 transitions and the statistics of cell shapes in the tissue.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM

Session L23 DBIO GSNP: Physics of the Brain: Structure and Dynamics

8:00AM L23.00001: A structured representation of odors in the fly mushroom body* [Invited] JIE-YOON YANG, ELIZABETH J HONG (Presenter), Division of Biology & Biological Engineering, California Institute of Technology — The mushroom body (MB) is a third-order olfactory area in the insect brain required for adaptive olfactory behaviors, such as learning odor associations, and is loosely analogous to olfactory cortex in mammals. In the vinegar fly Drosophila melanogaster, the chemical selectivity of each of the ~2200 principal neurons of the MB, called Kenyon cells (KCs), is determined by the pooling of odor information from a small random subset of the ~50 channels of olfactory input. The random integration of olfactory inputs in KCs contrasts with connectivity rules in other third-order olfactory areas, such as the lateral horn, where feature selectivity is determined by the invariant integration of specific combinations of olfactory inputs. The distinct connectivity statistics in different third-order olfactory areas has led to the idea that odor representations in the MB are “unstructured” and individualized in every brain, and must acquire meaning through learning, whereas invariant, chemotopic representations in the lateral horn support innate behaviors. We present a method using genetically enabled, in vivo two-photon functional imaging to measure near complete population representations of odors in KCs. We find that the relationship among neural representations of odors in the MB is invariant across individual brains. Furthermore, we apply a simple computational model of MB odor responses to illustrate that sparse, random connectivity can result in invariant relationships among odor representations, the structure of which is at least partially dictated by the correlational structure of the peripheral olfactory code. However, the experimentally observed structure of MB representational space deviates significantly from the predictions of the model for some regions of odor space. We discuss possible reasons for this discrepancy and future experimental directions to distinguish among these possibilities.

*This work was funded by NIMH, the Curci Foundation, and the NSF Ideas Lab.
8:36AM L23.00002: Inferring causality in highly-synchronized dynamics*  JOSUAN CALDERON (Presenter), GORDON BERMAN, Emory University — The brain is a complex system with intricate neural dynamics, exhibiting interactions that are thought to be crucial for emergent cognitive functions. Causality methods provide a powerful tool for the characterization of these functional circuits by identifying directed functional interactions from time-series data. A frequently-stated hypothesis is that synchronization of oscillatory activity plays a key role for the communication of information between distant sites of the brain. However, quantitatively assessing the strength and the direction of these interactions has proven difficult, especially in the highly-synchronized states that are often observed. Here we explore how synchronization affects the capability to mathematically measure causal interactions in both artificial systems and data. Performing a comparative analysis of often-used causality metrics, we show how synchronization introduces biases. These results suggest a new framework that could be used to assess causality across a wide range of synchronization states in the brain and elsewhere.

*HFSP (RGY0076/2018)

8:48AM L23.00003: Modularity allows classification of human brain networks during music and speech perception*  MELIA BONOMO (Presenter), Department of Physics and Astronomy, Rice University, CHRISTOF KARMONIK, Magnetic Resonance Imaging Core, Center for Performing Arts Medicine, Houston Methodist Research Institute, ANTHONY K BRANDT, Shepherd School of Music, Rice University, J TODD FRAZIER, Center for Performing Arts Medicine, Houston Methodist Hospital — Therapeutic music engagement is effective for improving cognitive health in patients suffering from neurological disease or trauma, however, little is known about the mechanism of action. Here, we investigated a means to quantify individual differences in functional brain activity while subjects listened to a variety of auditory pieces. Modularity was used to measure the degree to which functional activity within a group of brain regions was more highly correlated than activity between groups. We found consistent modules of the brain regions responsible for auditory processing among subjects, but differing whole-brain connection patterns and co-activation of regions responsible for autobiographical memory, prospection, and processing emotion ultimately led to differing modular structure. Significant trends were seen for individuals with higher or lower modularity during their self-selected musical piece. The use of modularity as a classifier of functional brain activity during auditory processing paves the way for creating personalized music therapy interventions and understanding how music benefits the brain.

*This work was supported by the Center for Theoretical Biological Physics at Rice University and the Ting Tsung & Wei Fong Chao Foundation.
Synchronization, waves and stochasticity in spatially structured neuronal networks

JONAS RANFT, IBEIN, Ecole Normale Superieure, ANIRUDH KULKARNI, Institut de la Vision, Inserm, VINCENT HAKIM (Presenter), Ecole Normale Superieure — Synchronization between distant brain regions, in the 20-30 Hz frequency range, has been observed in areas such as V1 or in the motor cortex during movement preparation. In order to shed light on these data, we have revisited the synchronization properties of distinct oscillating local Excitatory-Inhibitory (E-I) modules induced by distance-dependent long-range excitation. First, focusing on the sparsely synchronized oscillation regime which prevails in vivo, we have developed a rate model that accurately describes the stochastic oscillations of a single spiking E-I module. Second, we have considered the case of a chain of E-I modules with long-range excitation that decreases with distance. For modules of large sizes, complex dynamical regimes are observed in a sufficiently long chain, when long-range excitation mainly targets excitatory neurons. Synchronization of the module oscillations is otherwise observed. For modules with a moderate and biologically realistic size, stochasticity plays an important role in the observed dynamics. We show that its effect can be quantitatively described by modifications of the well-known Edwards-Wilkinson or KPZ equations. We analyse the resulting stochastic dynamics and discuss their relations to observed experimental observations.

Searching for emergent long time scales without fine tuning

XIAOWEN CHEN (Presenter), WILLIAM S BIALEK, Princeton University — Most of animal and human behavior occurs on time scales much longer than the response times of individual neurons. In many cases it is plausible that these long time scales emerge from the recurrent dynamics of electrical activity in networks of neurons. In linear models, time scales are set by the eigenvalues of a dynamical matrix whose elements measure the strengths of connections between neurons. It is not clear to what extent connection strengths need to be tuned in order to generate sufficiently long time scales; in some cases, one needs not just a single long time scale but a whole range. For a system with random symmetric connections, random matrix theory allows us to show that imposing a global stability constraint is sufficient to generate a diverging density of arbitrarily slow modes. But as soon as the detection mechanism for stability is set to be biologically plausible, these modes disappear for all system sizes. We will give a progress report on the more realistic, and challenging, case of asymmetric interactions.

*This work was supported in part by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030).
Neurons in the brain receive inputs from thousands of afferents. The high dimensionality of neural input spaces is tightly linked to the ability of neurons to realize difficult classification tasks through simple decision surfaces. However, this advantage of high dimensional neural representations comes at a price: Learning is difficult in high dimensional spaces. In particular, a neuron's ability to generalize from a limited number of training examples can be impaired by overfitting when the number of free parameters, i.e. synaptic efficacies, is large.

Constituting a major breakthrough in machine learning, learning in high-dimensional spaces has been greatly improved by margin techniques that maximize the minimal distance between available training examples and the learned decision boundary. Maximal margin techniques have been applied successfully in artificial neural networks with graded responses where standard metrics apply. By contrast, the use of margin learning has been much less straightforward in networks of spiking neurons that consist of neuron models that (like nerve cells in the brain) respond to inputs by eliciting trains of discrete all-or-nothing events (action potentials).

Recently, we have introduced the spike-threshold-surface to define a continuous distance between the responses of spiking neurons. Here we extend this notion to capture the margins between responses of spiking neurons. We show that a family of gradient-based learning rules that operate on these margins strongly improves the learning capabilities of spiking neurons. We discuss their biologically plausible implementation through empirically observed synaptic learning rules. This work transfers powerful margin-based learning concepts from machine to neurobiological learning.

In collaboration with Timo Wunderlich

*Charite Medical School Berlin, Berlin Institute of Health, ERC Synergy Grant BrainPlay
Randomly connected networks generate emergent selectivity and predict decoding properties of large populations of neurons* AUDREY SEDERBERG (Presenter), ILYA M NEMENMAN, Emory University — Modern recording methods enable sampling of thousands of neurons during the performance of behavioral tasks, raising the question of how recorded activity relates to theoretical models. In the context of decision making, functional connectivity between choice-selective cortical neurons was recently reported[1]. The straightforward interpretation of these data suggests the existence of selective pools of inhibitory and excitatory neurons. Computationally investigating an alternative mechanism for these experimental observations, we find that a randomly connected network of excitatory and inhibitory neurons generates single-cell selectivity, patterns of pairwise correlations, and indistinguishable excitatory and inhibitory readout weight distributions, as in experimental observations. We predict that, for this task, there are no anatomically defined subpopulations of neurons representing choice, and that choice preference of a particular neuron changes with the details of the task. We suggest distributed stimulus selectivity and functional organization in population codes are emergent properties of randomly connected networks.


Impact of correlated connections in large recurrent networks with mesoscopic structure ALEXANDER KUCZALA (Presenter), TATYANA OLEGIVNA SHARPEE, Salk Inst — Random recurrent networks serve as a useful tool for the tractable analysis of large neural networks. The spectrum of the connectivity matrix determines the network's linear dynamics as well as the stability of the nonlinear dynamics. Knowledge of the onset of chaos helps determine the networks computational capabilities and memory capacity. However, fully homogeneous random networks lack the non-trivial structures found in real world networks, such as cell types and plasticity induced correlations in neural networks. We address this deficiency by investigating the impact of correlations between forward and reverse connections, which may depend on the neuronal type. Using random matrix theory, we derive a set of self consistent equations that efficiently compute the eigenvalue spectrum of large random matrices with block-structured correlations. The inclusion of structured correlations distorts the eigenvalue distribution in a nontrivial way; the distribution is neither a circle nor an ellipse. We find that layered networks with strong interlayer correlations have gapped spectra. For antisymmetric layered networks, oscillatory modes dominate the linear dynamics. In simple cases we find analytic expressions for the support of the eigenvalue distribution.
10:24AM L23.00009: Relationships Between Lognormal Distributions of Neural Properties and Connectivities

PETER ROBINSON (Presenter), XIAO GAO, YINUO HAN, Physics, Univ of Sydney — Relationships between convergence of inputs onto neurons, divergence of outputs from them, synaptic strengths, nonlinear firing properties, and randomness of axonal ranges are systematically explored by interrelating means and variances of synaptic strengths, firing rates, and soma voltages. Imposition of self-consistency yields broad distributions of synaptic strength as a necessary concomitant of the massive convergence of inputs to individual neurons, and widths of lognormal distributions of synaptic strength and firing rate are explained. The strongest individual synapses are shown to have an effect on soma voltage comparable to the standard deviation of all others combined. Remarkably, inclusion of moderate randomness in axonal ranges accounts for the observed ~10^3-fold variability in two-point connectivity at a given separation, and ~10^5-fold overall when the known mean exponential fall-off is included, consistent with observed near-lognormal distributions.

*The Australian Research Council supported this work under Laureate Fellowship grant FL1401000225 and Center of Excellence Grant CE140100007.

10:36AM L23.00010: Directed effective connectivity of in vitro neuronal networks revealed from electrophysiological recordings

CHUMIN SUN, K.C. LIN, Department of Physics, Chinese Univ of Hong Kong, YU-TING, HUANG, Institute of Physics, Academia Sinica, EMILY S.C. CHING (Presenter), Department of Physics, Chinese Univ of Hong Kong, PIK-YIN LAI, Dept. of Physics and Center for Complex Systems, National Central University, C.K. CHAN, Institute of Physics, Academia Sinica — Studying connectivity of in vitro neuronal network revealed from electrophysiological recordings can provide insights for understanding the brain network. Existing methods focus on estimating functional connectivity defined by statistical dependencies between neuronal activities but it is effective connectivity that captures the relevant direct casual interactions. We present a method that makes explicit use of a theoretical result that effective connectivity is contained in the relation between time-lagged cross-covariance and equal-time cross-covariance. Applying this method to data recorded by multi-electrode arrays of over 4000 electrodes, we estimate the directed effective connectivity and synaptic weights of neuronal cultures at different days in vitro. Our analyses show that the neuronal networks are highly nonrandom with a fraction of inhibitory nodes close to the values measured in monkey cerebral cortex, have small-world topology and feeder hubs of large outgoing degree and the distributions of the average incoming and outgoing synaptic strength are non-Gaussian with long tails.

*The work of CS, KCL, and ESCC has been supported by the Hong Kong Research Grants Council under grants no. CUHK 14300914 and 14304017 and that by YTH, PYL and CKC is supported by MoST of Taiwan.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM

Session L24 GSNP DSOFT: Jamming, Criticality, and the Gardner Transition 401 - Corey O'Hern, Yale University - Tag(s): Focus
Pressure-dependent shear response of jammed packings of frictionless, spherical particles* [Invited] KYLE VANDERWERF (Presenter), ARMAN BOROMAND, Yale University, MARK SHATTUCK, The City College of New York, COREY SHANE O’HERN, Yale University — The mechanical response of packings of purely repulsive, spherical particles to athermal, quasistatic simple shear near jamming onset is highly nonlinear. Previous studies have shown that, at small pressure $p$, the ensemble-averaged static shear modulus $<G>G_0$ scales with $p^\alpha$, where $\alpha \approx 1$, but above a characteristic pressure $p^{**}$, $<G>G_0$ scales with $p^\beta$, where $\beta \approx 0.5$. However, we find that the shear modulus $G_i$ for an individual packing typically decreases linearly with $p$ along a geometrical family where the contact network does not change. We resolve this discrepancy by showing that, while the shear modulus does decrease linearly within geometrical families, $<G>$ also depends on a contribution from discontinuous jumps in $G_i$ that occur at the transitions between geometrical families. For $p > p^{**}$, geometrical-family and rearrangement contributions to $<G>$ are of opposite signs and remain comparable for all system sizes. $<G>$ can be described by a scaling function that smoothly transitions between two power-law exponents $\alpha$ and $\beta$. We also demonstrate the phenomenon of compression unjamming, where a jammed packing unjams via isotropic compression.

*We acknowledge support from NSF Grants Nos. CBET-1605178 (K. V. and C. O.), CMMI-1463455 (M. S.), and PHY-1522467 (A. B.).

Gardner physics in three-dimensional structural glasses* CAMILLE SCALLIET (Presenter), DAMTP, Univ of Cambridge, LUDOVIC BERTHIER, L2C, University of Montpellier, FRANCESCO ZAMPONI, Laboratoire de Physique, ENS Paris — The discovery of Gardner phases in structural glasses has profound consequences for their physical behavior, e.g. elasticity, rheology, low-temperature transport. It is therefore crucial to understand which type of materials, and under which physical conditions, are in the Gardner phase. Based on mean-field results [1], we present a comprehensive numerical study of 3d glasses. By changing external parameters, we explore regimes relevant to granular, colloidal, and molecular glasses. We delimit two separate regimes. We find that glasses close enough to jamming present a hierarchical landscape [2], and rejuvenation and memory effects expected in a Gardner phase [3]. In the regime far from jamming, relevant to atomic glasses, no Gardner physics is observed. Our study reveals instead the presence of localised excitations, whose role in low-temperature transport is analyzed. Our results suggest that Gardner physics should be observed in colloidal and non-Brownian particles near jamming.


*The authors thank the Fondation l’Oréal (CS) and the Simons Foundation (LB, FZ).
8:48AM L24.00003: Dimensional Dependence of Scaling Prefactors in Overjammed Systems
JAMES SARTOR (Presenter), ERIC CORWIN, Univ of Oregon — Granular materials express universal properties regardless of the material properties of the individual grains. This universality of granular packings is a direct consequence of the statistics of contact forces between grains. When packing fraction changes, material properties are governed by the creation and destruction of new contacts. The number of excess contacts, packing fraction, and pressure all characterize distance to the jamming transition and are related by scaling theory made possible by the universality of granular materials. While the scalings between these parameters follow simple power laws, the prefactors to these scalings are not universal. We present measurements of these prefactors in dimensions 2-10. These prefactors depend nontrivially on dimension and differ from the asymptotic high dimensional values predicted by mean field theory.

9:00AM L24.00004: Vibrational Properties of Hard and Soft Spheres are Unified at Jamming
FRANCESCO ARCERI (Presenter), ERIC CORWIN, Physics, University of Oregon — Glasses and granular materials are characterized by the appearance of amorphous rigidity at the jamming point. While grains described as soft spheres jam in the limit of zero pressure, in a thermal hard sphere glass jamming is only achieved at infinite pressure when all the available space is filled and particles are in enduring contact with one another. The criticality near jamming has been largely explored from the soft side of the transition both in theory and numerics. The study of the vibrational properties in hard spheres has proven to be challenging to measure numerically because no analytic interaction is defined. Recently, an effective interaction between hard spheres at zero temperature has been proposed, of which minimization is able to produce typical configurations of low temperature colloidal glasses. This protocol ensures a proper definition of the vibrational spectrum near and at jamming. We observe a variety of low frequency modes which, for a certain range of density, agree with those found in jammed soft spheres. Therefore, the vibrational properties of hard and soft spheres near jamming are fully governed by the geometry of the system and the critical point represents a smooth joining between the two descriptions.
Effect of annealing on the nature of the yielding transition of amorphous solids

SRIKANTH SASTRY (Presenter), HIMANGSU BHAUMIK, Jawaharlal Nehru Ctr Adv Sci, GIUSEPPE FOFFI, LPS, Université Paris-Sud, France — Recently it has been demonstrated employing athermal quasi-static cyclic shear that an atomistic model glass former exhibits a sharp yielding transition across a sharply defined critical amplitude [1], which is further characterized by strain localization at the post yield regime [2], and the attainment of low energy structures approaching the yielding point. Here, we study the applicability of these results to a model of silica, and further, study the effect of annealing on the nature of yielding in both the model systems. We analyse the manner in which the discontinuous nature of the transition changes with annealing and compare our results with recent results analysing the effect of annealing in glasses [4].

References:


Universal non-mean-field scaling in the density of states of amorphous solids

HARUKUNI IKEDA (Presenter), Ecole normale supérieure — Amorphous solids have excess soft modes in addition to the phonon modes described by the Debye theory. Recent numerical results show that if the phonon modes are carefully removed, the density of state of the excess soft modes exhibit universal quartic scaling, independent of the interaction potential, preparation protocol, and spatial dimensions. We hereby provide a theoretical framework to describe this universal scaling behavior. For this purpose, we extend the mean-field theory to include the effects of finite-dimensional fluctuation. Based on a semiphenomenological argument, we show that mean-field quadratic scaling is replaced by the quartic scaling in finite dimensions. Furthermore, we apply our formalism to explain the pressure and protocol dependence of the excess soft modes.

*This project received funding from the European Research Coineduncil (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant Agreement No. 723955-GlassUniversality).
A jamming plane of sphere packings*  
YULIANG JIN (Presenter), Institute of Theoretical Physics, Chinese Academy of Sciences, HAJIME YOSHINO, Cybermedia Center, Osaka University — The concept of jamming has attracted great research interest due to its broad relevance in soft matter such as liquids, glasses, colloids, foams, and granular materials, and its deep connection to the sphere packing problem and phase transitions. Here we show numerically that the phase space of frictionlessly jammed states can be extended from the well-known jamming-point along the density axis to a jamming plane spanned by the density and shear-strain axes. We discuss how this jamming plane can be explored by standard athermal and thermal jamming protocols, and relate the protocol-dependence of the explored phase space to the reversibility of the routes to the jammed states. While all jammed states are isostatic and in the same universality class, their anisotropies and amorphous orders depend on the density and the shear strain. Among all points on the jamming plane, the jamming-point is special: it sets a sharp lower bound in the thermodynamic limit for the jamming density of all frictionless random packings, and the configurations there have the minimum amorphous order.

*This work was supported by KAKENHI (No. 25103005 “Fluctuation & Structure” and No. 50335337) from MEXT, Japan, by the Chinese Academy of Sciences Pioneer Hundred-Talent Program (Yuliang Jin).

Out-of-equilibrium jamming of liquids and glasses: memory and criticality*  
PETER MORSE (Presenter), PATRICK CHARBONNEAU, Duke University — The emergence of memory in glass-forming liquids has recently been described by mean-field theory. Liquids equilibrated below the onset packing fraction (or above the onset temperature) share the same set of inherent states, while on the other side of that onset the set of inherent states depends on the equilibrated liquid properties. The resulting jammed states then have memory of the original liquid. In this talk, we present a new method to jam hard sphere liquids efficiently, which enables us to reliably detect this onset and relate its value with the mean-field prediction. This jamming algorithm also exhibits a signature of an out-of-equilibrium Gardner transition, corresponding to the point at which the roughness of the optimization landscape becomes algorithmically notable. Taken together these results will help inform a theory of out-of-equilibrium liquids and glasses.

*This research is supported by a grant from the Simons Foundation (#454937, Patrick Charbonneau).
10:00AM L24.00009: Creating ultra-stable jammed packings by training on pressure  VARDA FAGHIR HAGH (Presenter), Physics, University of Chicago, ERIC CORWIN, Physics, University of Oregon, M. LISA MANNING, Physics, Syracuse University, ANDREA JO-WEI LIU, Physics, University of Pennsylvania, SIDNEY ROBERT NAGEL, Physics, University of Chicago — Disordered materials are highly trainable because of their rugged energy landscapes. The idea of training is to evolve the physical properties of the microscopic constituents in a given system until a macroscopic state with desired emergent properties is achieved. Here, we train packings of soft harmonic spheres based on their per-particle pressures. First, the pressure on each particle is measured and then the radius of each particle is changed proportional to the inverse of its pressure, (i.e. particles with larger pressure get slightly smaller and particles with smaller pressure grow slightly larger). This process is repeated iteratively until pressure fluctuations disappear from the system. The final trained packings have a much lower energy and are mechanically ultra-stable regardless of original (untrained) packings' distance from the instability. This training process moves the critical packing fraction to a higher value and engraves a memory of training in the system that does not disappear under decompression.

10:12AM L24.00010: Intruder dynamics in granular flow  SCOTT NEWLON (Presenter), Southern Illinois University Carbondale, LEO SILBERT, Department of Physics, Central New Mexico Community College — The dynamics and kinematics of a single intruder particle in two dimensional, disordered packings of frictionless bidisperse discs interacting through linear and non-linear contact forces are investigated using computer simulations. To initiate motion of the intruder requires a threshold force to be exceeded which depends on the pressure of the packing. Beyond this critical force, for a given driving force, the average intruder velocity scales with the excess driving force. The velocity curves for different pressures are found to obey an universal scaling relation that depends on the initial packing pressure. We also find that the critical, threshold force is related to the shear modulus, thereby connecting the microrheological properties of the intruder at the grain scale to the bulk, macroscopic mechanical properties of the packing.

10:24AM L24.00011: One-step replica-symmetry-breaking phase in low-dimensional spin glasses*  JUDITH HOELLER (Presenter), NICHOLAS READ, Yale University — It is long known that mean-field theory of an Ising spin glass predicts a second-order phase boundary in the temperature–magnetic field plane between a paramagnet and a replica-symmetry-breaking phase. Here, we show that at nonzero magnetic fields and just above six dimensions, this phase diagram is modified by the appearance of a one-step replica symmetry-breaking phase below the transition, and a tricritical point beyond which the transition becomes quasi-first-order. These results may explain the reported absence of a diverging correlation length in the presence of a magnetic field in less-than-six-dimensional spin glasses in simulations and high-temperature series expansions.

*NSF grant no. DMR-1724923
10:36AM L24.00012: Origin of Two-Step Glass Transition in 2D Colloidal Suspension of Rods*

XINZHUO LIU, HUAGUANG WANG, ZEXIN ZHANG, Institute for Advanced Study, Soochow University, XINSHEING LING (Presenter), Brown University — We report an experimental study of monolayers of colloidal rods which exhibits a two-step glass transition with no appearance of nematic domains. Instead, it was found that rods tend to align with each other randomly in two preferred configurations, parallel, or perpendicular. We argue that the bi-modal distribution of the relative angles of the rods in the glassy phase is due to the existence of an activation barrier separating two local free energy minima in the configurational space. This barrier increases significantly when the first transition is approached, thereby freezing out the rotational motion while the translational motion remains diffusive. The results suggest that the activation barrier for rods rotating relative to each other is the key to the two-step glass transition.

*This work was financially supported by National Natural Science Foundation of China (Grant Nos. 11574222, 11704269, and 21522404), Natural Science Foundation of the Jiangsu Higher Education Institutions of China (Grant No. 17KJB140020), and the PAPD program of Jiangsu Higher Education Institutions.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L25 GSNP DSOFT DCP: Physics of Liquids III 402 - Fausto Martelli, IBM TJ
Watson Research Center - Tag(s): Focus

8:00AM L25.00001: Energy landscapes: from molecules and nanodevices to glasses and machine learning [Invited] DAVID WALES (Presenter), University of Cambridge — The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science. This talk will highlight connections between glassy systems and emergent phenomena in clusters, biomolecules and soft matter. Applications will be presented to illustrate new approaches for global optimisation, quantum dynamics, enhanced sampling of systems exhibiting broken ergodicity, and rare event dynamics. The key aim is to explain how the energy landscape perspective can unify our understanding of apparently disparate systems. A range of applications will be presented, from spectroscopy, biomolecules, and structural glass-formers, along with coarse-grained models and some recent results for machine learning landscapes.

Effects of random pinning on the potential energy landscape of a supercooled liquid, JCP, 149, 114503, 2018.
Defining and quantifying frustration in the energy landscape, JCP, 146, 124103, 2017.
8:36AM L25.00002: Nanoscale dynamics of liquids: $S(Q,\omega)$ with 0.8 meV resolution using x-rays    ALFRED Q. R. BARON (Presenter), DAISUKE ISHIKAWA, Materials Dynamics Laboratory, RIKEN SPring-8 Center — We describe a new instrument for measuring the dynamic structure factor of liquids, $S(Q,\omega)$, at the RIKEN SPring-8 Center in Japan using inelastic x-ray scattering (IXS) (see https://arxiv.org/abs/1504.01098). A long, 15m, insertion device provides unprecedented x-ray intensity, making practical experiments possible with sub-meV resolution at sub nm$^{-1}$ momentum transfers. This allows new insight into the mesoscale crossover regions between hydrodynamic and atomistic behavior of liquids. The performance will be illustrated with examples, including new results from liquid water [Ishikawa & Baron, submitted] and liquid iron [Baron, Inui, Ishikawa, et al, work in progress], demonstrating the range of the instrument and its applicability to even rather difficult experiments.

8:48AM L25.00003: The formation of nanoripples by ultra-low energy ion irradiation reveals the liquidus nature of metallic glass surface    PENG LUO (Presenter), CAMILO JARAMILLO CORREA, JESSICA CRYSTAL SPEAR, University of Illinois at Urbana-Champaign, JEAN PAUL ALLAIN, The Pennsylvania State University, YANG ZHANG, University of Illinois at Urbana-Champaign — We report an experimental investigation of ion irradiation on metallic glasses (MGs), with extremely low ion energy of 50–225 eV, orders of magnitude lower than that often used in previous studies. Highly periodic ripples with a wavelength of 20 nm and an amplitude of 0.5 nm were developed on MG surfaces under irradiation. With increasing irradiation time, we can identify three regimes: appearance of initial random islands, coarsening of the pattern through annihilation reactions of mobile defects, and finally saturation of the ripples. No change is observed for the devitrified counterparts with the same treatment. These findings reveal the liquidus nature of glass surface even far below the glass transition temperature and provide new clues for surface modification of amorphous materials.

9:00AM L25.00004: Study of Mesoscale Structure and Dynamics of Associated Liquid 2-propanol by Neutron Scattering and Molecular Dynamics Simulations    YANQIN ZHAI (Presenter), Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, ANTONIO FARAOINE, NIST Center for Neutron Research, National Institute of Standards and Technology, YANG ZHANG, Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign — Monohydroxy alcohols are good model systems for studying the impact of hydrogen bonding on the structure and dynamics of liquids and on the macroscopic transport properties such as viscosity. We investigated 2-propanol by static and quasielastic neutron scattering experiments on a series of partially and fully deuterated samples at temperatures ranging from the liquid, the deeply supercooled, to the glassy state. Corresponding Molecular Dynamics (MD) simulations are performed to further understand the collective dynamics of the system. We focus on the mesoscale structures associated to the structure factor pre-peak at wavevector $Q \sim 0.8$ Å$^{-1}$. The dynamics of these molecular associates is at least one order of magnitude slower than the dynamics at the structure factor peak, at $Q \sim 1.4$ Å$^{-1}$. MD simulations show that 2-propanol molecules prefer to form chain-like structures with approximately 10% of the rings although the hydroxyl group is located in a non-terminal position. The emergence of multiple relaxation processes as the system is cooled towards the melting temperature and below is observed, which could be related to the non-Arrhenius increase of the viscosity.
TIMOTHY PRISK (Presenter), National Institute of Standards and Technology, SCOTT HANNA, Winston Churchill High School, RICHARD AZUAH, National Institute of Standards and Technology — Quantum zero-point motion plays an important role in determining the properties and behavior of liquid hydrogen. For example, by comparing the predictions of classical molecular dynamics with centroid molecular dynamics, several theoretical studies have suggested that the self-diffusion constant of liquid para-hydrogen is dominated by zero-point motion. In this presentation, we report quasi-elastic neutron scattering measurements of liquid normal hydrogen under saturated vapor pressure. Our empirical estimates of the self-diffusion constant and Arrhenius activation energy are in good agreement with accepted values obtained by nuclear magnetic resonance. As previous theoretical work has generally focused upon temperatures near the triple point, we will argue that further development in this area would be useful.

*We acknowledge the support of the National Institute of Standards and Technology, U.S. Department of Commerce, in providing the neutron facilities used in this work. Support for Scott hanna was provided by the Center for High Resolution Neutron SCattering, a partnership between the National Institute of Standards and Technology and the National Science Foundation under Agreement No. DMR-1508249.

YADU KRISHNAN SARATHCHANDRAN (Presenter), University of Tennessee, Knoxville, YUYA SHINOHARA, EUGENE MAMONTOV, Oak Ridge National Laboratory, WOJCIECH DMOWSKI, TAKESHI EGAMI, University of Tennessee, Knoxville — Water exhibits an anomalously high dielectric constant, $\varepsilon=78$, at ambient temperature. This is caused by a Debye peak in the dielectric spectrum with a maximum at ~20 GHz. It is reported that this Debye peak reflects some hydrogen bond mediated, collective dipolar dynamics in water. However, a clear microscopic description of this phenomenon is lacking. We report our study on the microscopic picture of water's dielectric relaxation using the time-dependent pair-distribution function, the Van Hove function. The dynamic structure factor of water, $S(Q, E)$, is measured using quasi-elastic neutron scattering over a wide momentum transfer range by making use of recent advances in analyzer crystal options at BASIS, SNS. $S(Q, E)$ is double Fourier transformed to obtain the Van Hove function, $g(r, t)$, to investigate the temporal evolution of molecular correlations in real-space up to 10 picoseconds. Our findings align with previous studies on the time-scale of the Debye process and the higher frequency excess Debye process, although significantly differ in the microscopic description.

*"This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials and Science and Engineering Division.”
9:36AM L25.00007: Atomic dynamics of liquid Hg studied by high-resolution inelastic x-ray scattering

DAISUKE ISHIKAWA (Presenter), Japan Synchrotron Radiation Research Institute, ALFRED Q. R. BARON, RIKEN SPring-8 Center — High-resolution Inelastic X-ray Scattering (IXS) is a powerful tool for measuring the dynamic structure factor, S(Q,ω), in liquids. Very recently, we began to operate a new instrument that allows practical measurements on liquids of the most interesting low Q region at BL43LXU of the RIKEN SPring-8 Center in Japan. Liquid dynamics in this region is important since this region corresponds to transition from hydrodynamic to solid-like elastic regimes. Liquid metals are particularly interesting since they behave quite differently from molecular liquids due to strong atomic interactions. We use the new setup to investigate liquid Hg with energy resolution >0.8 meV at temperature near the melting point T_m = 234.3 K. We will discuss details of transition of the speed of sound in liquid Hg, the quasi-elastic line-width, and a new approach to fitting dynamical spectra.

9:48AM L25.00008: Isotope effect in liquid water explored by X-ray absorption spectroscopy

CHUNYI ZHANG (Presenter), Temple University, LINFENG ZHANG, Princeton University, JIANHANG XU, FUJIE TANG, XIFAN WU, Temple University — The X-ray absorption spectra (XAS) of both liquid H_2O and D_2O are computed using our recently developed approximate computational approach in solving Bethe-Salpeter equation. In the above, the molecular structures are obtained from the well-equilibrated trajectories generated by path-integral deep potential molecular dynamics (DPMD). In particular, the DPMD force field is constructed from ab initio path-integral molecular dynamics based on the strongly constrained and appropriately normed (SCAN) density functional. Our preliminary results indicate that the experimentally observed isotope effects in the XAS spectra are qualitatively reproduced by our theoretical prediction. The H-bond network in heavy water is slightly more structured than that in light water, which is consistent with the less prominent pre-edge and main-edge of theoretical XAS spectrum of D_2O than that of H_2O.

*This work was primarily supported by National Science Foundation through Awards No. DMR-1552287.
10:00AM L25.00009: The Long-range Ordering of Ions in Aqueous Salt Solutions  EVGENII FETISOV (Presenter), JOHN L FULTON, SHAWN MICHAEL KATHMANN, CHRISTOPHER J MUNDY, GREGORY K SCHENTER, Pacific Northwest National Laboratory — The importance of understanding the long-range structure in aqueous salt solutions has recently come to the forefront when it was suggested that the ordering of water in the presence of ions possibly reaches length scales up to 10 nm. A much more important question regards the long-range ordering of the ions themselves since their arrangement critically affects processes such as nucleation/crystallization and the solution energetics related to activity coefficients and osmotic pressure. We use a combination of molecular dynamics and X-ray diffraction to correlate experimentally measured long-range structure to the precise spatial distribution of species in aqueous solutions of alkali and alkali earth halides. For the first time, we quantitatively differentiate and explain a separate region in the fluid structure factor containing diffraction-like features at low Q values (“pre-peaks”) that lead to the oscillatory behavior in the ion-ion and ion-water pair distribution functions. These features are shown to be due to a combination of correlated (e.g., cation-cation and cation-water) and anti-correlated (cation-anion and anion-water) atomic positions. In addition, we also explore the influence of salt concentration on the position and magnitude of the pre-peaks.

10:12AM L25.00010: Influence of ionic species on water broadband electrodynamics  VASILY G. ARTEMOV (Presenter), HENNI OUERDANE, Skolkovo Institute of Science and Technology — Proton exchange plays a central role in modern electrochemical systems. While it is well described for times larger than milliseconds [1], it is an important process not fully understood on nanoscale distances and subpicosecond timescales. Here, we discuss the dynamical structure of water from femtoseconds to seconds time intervals using a combination of broadband dielectric spectroscopy and infrared spectroscopy methods. Accounting for dielectric properties [2], isotopic effects [3] and confinement effects [4], we present a model of water based on the time-dependence of the ionic species concentration, over the whole time interval between the intermolecular direct current (below microseconds) and intramolecular infrared vibrations (sub-picoseconds), which so far was hardly achievable. Our approach provides a new vision on the hydrogen bonding in water taking into account the role of ionic species on the intermolecular interactions; and we discuss how this paves the way to innovative design of electrochemical energy storage devices.

HOSSAM FARAG (Presenter), Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, ILYA A SHKROB, LU ZHANG, LEI CHENG, Chemical Sciences and Engineering Division, Argonne National Laboratory, YANG ZHANG, Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign — Non-aqueous electrolytes enable batteries to operate at higher cell potentials compared to its aqueous counterpart due to the wider electrochemical stability window of the former. Super-concentrated electrolytic solutions are emerging as a new class of liquid electrolytes with various unusual functionalities beneficial for advanced Li battery applications. However, a desired high ionic conductivity is missing in the high-concentrated regime due to a reduction in ionic mobility. Reduced ionic motility is ascribed to an increase in solution viscosity whose mechanism is still not fully understood. We hypothesize that we could tune the solution viscosity via modulating the supramolecular interactions enabling a groundbreaking solution for fast recharging rate of these batteries. We carried out MD simulations to investigate the mechanism by which the ionic conductivity decreases. We first observed a reduction in the number free-ion carriers via formation of contact ion pair in this high concentration regime. Further investigation of the mechanism by which viscosity increases is still undergoing. Herein, we present the simulation results and relative analysis.

10:36AM L25.00012: Local Dynamics in Metallic Liquids Studied by Inelastic Neutron Scattering*  
ZENGQUAN WANG (Presenter), HUI WANG, WOJCIECH DMOWSKI, University of Tennessee, Knoxville, KENNETH F KELTON, Washington University, St. Louis, TAKESHI EGAMI, University of Tennessee, Knoxville — Local dynamics in liquid metals has been poorly understood when compared to their crystalline counterparts. For instance, the atomistic origin of the viscous behavior is not well elucidated, even though viscosity is one of the most basic properties for liquids. In this research, inelastic neutron scattering (INS) experiments were carried out on various metallic liquid droplets (including single, binary, and complex BMG forming liquids), using an electro-static levitator, at different temperatures at SNS. The dynamic structure function $S(Q, E)$ and the Van Hove correlation function $G(r,t)$ were then obtained. Compared with Molecular Dynamics (MD) simulation results, the local configuration change was analyzed based on distinct $G(r,t)$ and proved as the elementary excitation in high temperature metallic liquids, thus controlling their shear viscosity. Also, self diffusion behaviors were analyzed based on self $G(r,t)$. A comprehensive understanding of the local dynamics was made in various metallic liquids.

*This work is supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division.
High-resolution neutron imaging study of kinetics of H$_2$O water vapor uptake from air into sessile heavy water droplets

JAE KWAN IM (Presenter), LEEKYO JUNG, Physics, Ulsan Natl Inst of Sci & Tech, JAN CRHA, PAVEL TRTIK, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, JOONWOO JEONG, Physics, Ulsan Natl Inst of Sci & Tech — At the surface of a liquid, the liquid molecules escape and enter the encompassing air as a gas, and the gas molecules join the liquid concurrently. Here we report the neutron imaging of a sessile heavy water (D$_2$O) droplet that absorbs light water (H$_2$O) vapor from the ambient air. A quantitative image analysis utilizing the Beer-Lambert law enables us to measure the attenuation coefficient of the specimen and estimate H$_2$O content within the droplet. We double-check this result with a quantitative Fourier-transform infrared spectroscopy and conclude that small D$_2$O droplets with a large surface-to-volume ratio can be very hygroscopic, e.g., the 15 percent of a D$_2$O droplet of 10 microliters can be replaced with H$_2$O in 10 minutes.

The neutron imaging was performed at the ICON beamline of SINQ at Paul Scherrer Institut, Switzerland, under the proposal-number 20180136. The authors acknowledge support from the 2018 Research Fund (1.180069.01) of UNIST (Ulsan National Institute of Science and Technology) and IBS-R020-D1 funded by the Korean Government.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM

Session L26 DBIO DSOFT GSNP DPOLY: Mechanics of Cells and Tissues Across Scales V

How does extracellular matrix rigidity affect the fluidity of an embedded spheroid?

AMANDA PARKER (Presenter), Physics, Syracuse University, M CRISTINA MARCHETTI, Physics, UC Santa Barbara, M. LISA MANNING, J M SCHWARZ, Physics, Syracuse University — The extracellular matrix (ECM) that surrounds a tissue, such as a cancer spheroid, is known to regulate spheroid behavior, with stiffer ECM promoting invasion. Using a computational model, we explore how a simple mechanical interaction between a spheroid and its ECM promotes changes in the spheroid's rigidity, morphology and the shapes of its constituent cells, as well as the ECM's rigidity and structure. We model the spheroid using a vertex model and the ECM using a spring network model, with an additional term describing the interfacial tension between the spheroid and ECM. Both vertex and spring network models transition between rigid and floppy phases, depending on their respective tuning parameters (cell shape and spring rest length) and imposed strain. Therefore, we expect, and find, that by mechanically coupling the two systems, changes to the phase of one system can drive changes to the phase of the other. We identify two regimes of interest—one in which compression of the spheroid dominates and one in which stretching dominate. We find that isotropic compression promotes fluidity of tissue and preserves the relationship between cell shape and tissue phase, while stretching by the ECM results in rather different behavior.

This work is supported by NSF-POLS 1607416
8:12AM L26.00002: Self-organized vasculogenesis in 3D printed mixed cell populations
SARAH ELLISON (Presenter), THOMAS ANGELINI, University of Florida — In the process of vasculogenesis during embryotic development, endothelial cells create blood vessel networks necessary for the survival and function of tissues. In tissue engineering, creating functional vasculature remains among the largest impediments to achieving healthy tissues. Deeper understanding of cell self-organization during vasculogenesis could therefore have impacts in developmental biology and tissue engineering. To fabricate 3D multicellular systems of designed consistency, we 3D print structures made from mixtures of hepatocytes, endothelial cells, and extracellular matrix. These structures are fabricated directly in a 3D growth medium made from jammed microgels. By observing cellular spatial organization and testing biological markers, we investigate how endothelial cells and hepatocytes self-organize into co-continuous interpenetrating networks, resulting in vasculature and improved overall cellular function. Preliminary data and analysis will be presented.

8:24AM L26.00003: Interrogating collagen mechanics at the single-molecule level* NANCY R. FORDE (Presenter), Department of Physics, Simon Fraser University — Collagen is the fundamental structural protein in vertebrates, forming a variety of hierarchical material structures. In spite of its prevalence and mechanical importance in biology, its mechanics at the molecular level – where it possesses a unique triple-helical structure – are surprisingly controversial: its flexibility is unresolved, as is its response to stress. My research group has been investigating these properties through single-molecule experiments. To do so, we have developed imaging algorithms to use in atomic-force microscopy (AFM), developed a model for polymers with inherent curvature (the curved worm-like chain model - cWLC), and built an instrument for high-throughput single-molecule force spectroscopy, the mini-radio centrifuge force microscope (MR.CFM). I'll describe what we have learned about collagen's flexibility and stress response, how local sequence context matters, and how our work resolves some of the many contentious findings regarding collagen's mechanics.

*This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC).

8:36AM L26.00004: Mechanical response of the vitreous gel in our eyes: Results from an inhomogeneous two-fluid model* PANCY LWIN (Presenter), SCOTT V FRANKLIN, GEORGE THURSTON, DAVID ROSS, MOUMITA DAS, Rochester Institute of Technology — The vitreous gel is a viscoelastic gel present between the eye lens and the retina. It is made up of a composite network of stiff collagen fibers and softer hyaluronic acid (HA) polymers, and water. Its mechanical properties are critical to proper functioning of the eye, and undergo changes with aging and disease. We study rheological properties of this gel by simulating it as a two-fluid model made of an inhomogeneous polymer network interacting with a fluid. Our results relate the time-varying mechanical response of the gel to the composition of the network, the material properties of the network and the fluid, and the strength of the coupling of between the network and the fluid. These results may provide insights into changes in mechanical-structure function properties of the vitreous gel in vitreous disorders.

*The research was funded by the National Science Foundation via the award NSF/CBET-1604712.
8:48AM L26.00005: Kinetics of Cell Adhesion Through Biomimetic Glycocalyx*  
YU JING, SHLOMI COHEN, JESSICA FAUBEL, JENNIFER CURTIS (Presenter), School of Physics, Georgia Institute of Technology — Giant polysaccharides grafted to the external cell surface interfere with receptor-ligand binding and can strain molecular bonds. This is relevant in cell-matrix interactions during cell migration as well as in cell-cell interactions, such as T-cell immune response. We introduce a biomimetic glycocalyx platform to investigate the kinetics of cell adhesion in the presence of sugar-rich interfaces. With this approach, we study the mechanisms by which cells penetrate the thick polymer brush-like interface and how this process depends on initial brush thickness.

*The authors gratefully acknowledge funding from NSF DMR #1709897.

9:00AM L26.00006: Length regulation of epithelial cell junctions  
MICHAEL STADDON (Presenter), University College London, KATE E CAVANAUGH, EDWIN M MUNRO, MARGARET GARDEL, University of Chicago, SHILADITYA BANERJEE, University College London — Morphogenesis of epithelial tissues involve precise spatiotemporal coordination of cell shape changes. In vivo, many morphogenetic events are driven by pulsatile contractions of intercellular junctions, producing irreversible deformations at tissue scales. The biophysical functions of these oscillatory contractions and the significance of their temporal structure remain unknown. Here, we combine theory and experiments to demonstrate that pulsatory contractions serve as a mechanical ratchet to guide directed morphogenesis. We propose a new theory for epithelial tissue mechanics that highlights two essential properties of intercellular junctions. First, epithelial junctions must overcome a critical strain threshold to trigger irreversible tension remodelling and junction length changes. Second, continuous relaxation of junctional strain promotes gradual loss of mechanical memory from the system, which makes the system refractory to continuous input, enabling frequency-dependent modulation of cell shape changes via junctional ratcheting. Taken together, the combination of mechanosensitive tension remodelling and strain relaxation provides a robust mechanism for directed tissue morphogenesis and the maintenance of tissue homeostasis in response to small amplitude contractions.
The physics of lipid bilayer in cell membranes is one of the most exciting topics in modern science. We have investigated the molecular dynamics of complex phospholipid membranes in their fluid phases by neutron spin echo spectroscopy. Our study reveals the origin of anomalous motions in different phospholipids that leaves a generalized fingerprint in their mean square displacement (MSD). It shows a $t^{0.26}$ dependence in the pico- to nanosecond region that indicates a new localized motion that is related to the tail group of the lipid. At longer times, $t > 3$ ns, the MSD shows a $t^{0.66}$ dependence describing membrane undulation, followed by a translational diffusion ($t^1$), that is visible at the edge of instrumental resolution. The analysis reveals the range in which we can analyze the membrane fluctuations to determine the membrane rigidity. Our study reveals the existence of the complex dynamic organization of the lipid bilayer in terms of localized anomalous motions. In biological cell membranes, these anomalous motions would imply a substantial difference in cellular signaling and regulatory processes.


*DOE-EPSCoR GRANT DE-SC0012432

In vitro characterization and numerical simulations of red blood cell transmigration through splenic inter-endothelial slits

During their circulation through the spleen, red blood cells (RBCs) are forced to squeeze through gaps between endothelial cells that are ~8 times narrower than its diameter. The ensuing squeezing motion causes large RBC deformations that remove old and diseased cells from the circulation. There is limited data about the deformation and stress experienced by RBCs. To study the mechanics of RBC splenic filtration, we designed and characterized a family of microfluidic devices where a suspension of human RBCs flows through an array of channels of controlled length (L), width (W) and height (H). We varied these geometrical parameters ($0.75 < W < 3$, $4.5 < H < 10$ and $1 < L < 5$ um) and imaged the time-evolving RBC shape while crossing each channel, as well as the flow field through the channel by μ-PIV. We also investigated this process computationally by coupling a multiscale model of the RBC membrane with a boundary integral formulation of the fluids. The computationally flow field and cell deformation are consistent with experiments. In wider channels RBCs reorient into the direction of less constrain, whereas in narrower channels, cells fold (U shape) experimenting large deformations. We examined computationally the mechanics of folded cell shapes under different flow rates and slit geometries.
Nucleation and Formation of a Primary Clot in Insect Blood Probed by Magnetic Rotational Spectroscopy

KONSTANTIN KORNEV (Presenter), PAVEL APRELEV, PETER ADLER, ARTIS BRASOVS, Clemson University — Blood clotting at wound sites is critical for preventing blood loss and invasion by microorganisms in multicellular animals, especially small insects vulnerable to dehydration. The mechanistic reaction of the clot is the first step in providing scaffolding for the formation of new epithelial and cuticular tissue. The clot, therefore, requires special materials properties. We have developed and used nano-rheological magnetic rotational spectroscopy with nanorods to quantitatively study nucleation of cell aggregates that occurs within fractions of a second. Using larvae of Manduca sexta, we discovered that clot nucleation is a two-step process whereby cell aggregation is the time-limiting step followed by rigidification of the aggregate. Clot nucleation and transformation of viscous blood into a visco-elastic aggregate happens in a few minutes, which is hundreds of times faster than wound plugging and scab formation. This discovery sets a time scale for insect clotting phenomena, establishing a materials metric for the kinetics of biochemical reaction cascades.

Microfluidic platform for label-free viability cell sorting

FATIMA EZAHRA CHRIT (Presenter), ABHISHEK RAJ, NICK STONE, TODD SULCHEK, ALEXANDER ALEXEEV, Georgia Inst of Tech — Cell biomechanical properties often change in predictable ways with important cell phenotypes changes, such as cell loss of viability. We propose a biophysical approach for cell viability sensing, enumeration, and purification that is label-free and continuous. Using microfluidics, we show that we can separate viable cells from nonviable cells based on the difference in their stiffness with an enrichment factor of >5 and an overall recovery of 95%. The technology consists of a microchannel with diagonal ridges that direct cells along different paths in a manner dependent on cell biomechanical properties. As a result, the sorted viable and nonviable cells are collected at different microchannel outlets. To investigate the sorting process, we use a tracking algorithm that tracks cells moving through the microchannel. Sorting outcomes are correlated with the tracking metrics such as the cell deflection per ridge and the interaction time with ridges in the channel. The approach can be used for cell characterization and purification either in-line with cell bioreactors or after cell manufacture and prior to administration to improve outcomes.

The work is supported by NSF Engineering Research Center for Cell Manufacturing Technologies and NSF CBET 1928262.
**10:00AM L26.00011: Simultaneous Measurement of Electrical and Mechanical Properties of Biological Cells Using a Tuning Fork-Coupled Conductive Probe**  
MARK SCHILLER (Presenter), 
Physics, Boston College, ALEXANDRA M IVANOV, MEGI MACI, Biology, Boston College, EVA K PONTRELLI, Physics, Boston College, JUAN MERLO, Physics and Astronomy, Vassar College, TIMOTHY CONNOLLY, Biology, Boston College, MICHAEL NAUGHTON, Physics, Boston College — AFM-style probes have commonly been used to measure mechanical properties of materials such as their Young's Modulus. This technique has also been implemented to further explore biological cells\(^1\). Differentiation, pluripotency, and other attributes have been linked to certain mechanical properties of cells as well their membrane potential\(^2,3,4\). Simultaneous measurements of these quantities can help determine their inter-relation and inform on their relationship(s) with other properties. We have devised a conductive tip tuning fork probe, which is intended to simultaneously measure mechanical properties and membrane potential of a cell. We discuss fabrication and preliminary experimental results using conductive tip tuning forks to probe HeLa cells.

\(^1\)S. Vahabi et al., Iran J. Med. Sci. 38(2) 76-83, 2013  
\(^4\)K Hammerick et al., Tissue Eng. 17, 495-502 (2011)

**10:12AM L26.00012: Brain Mechanics Drive Cavitation and Fracture Response**  
CAREY DOUGAN (Presenter), SUALYNETH GALARZA, Chemical Engineering, University of Massachusetts, CHRISTOPHER BARNEY, Polymer Science and Engineering, University of Massachusetts, YUE ZHENG, SHENGQIANG CAI, Department of Mechanical and Aerospace Engineering, University of California San Diego, ALFRED J CROSBY, Polymer Science and Engineering, University of Massachusetts, SHELLY PEYTON, Chemical Engineering, University of Massachusetts — Roughly 1.7 million cases of Traumatic Brain Injury occur in the U.S. every year. It has been suggested that impact injuries and non-impact injuries due to explosive blasts result in “cavitation-related damage.” This cavitation event is the formation of bubbles in the brain that can lead to fracture upon collapse. Therefore, it is essential to understand how brain mechanics contributes to the propagation of cavitation and fracture related damage \textit{in vivo}. Needle-induced cavitation (NIC) is a useful technique to study localized deformation within brain tissue and how modulus and strain rate contribute to fracture. Utilizing the techniques of NIC and indentation we observe a significant correlation between modulus and strain rate. This strain rate dependency for NIC can result in visible fracture of specific brain regions of varying moduli at large strains. With the help of modeling, we use the NIC measurements to understand the fracture properties of brain tissue. By understanding the strain rate deformation of specific areas of the brain, we aim to gain further insight into how cavitation-related events lead to irreversible damage.

*This research was supported by the Office of Naval Research under N00014-17-1-2056.*
Rheological properties of cellular aggregates formed by pilus mediated interactions

HUI-SHUN KUAN (Presenter), Friedrich-Alexander Uni Erlangen-Nürnberg & Max-Planck-Zentrum für Physik und Medizin, FRANK JULICHER, Max Planck Institute for the Physics of Complex Systems, VASILY ZABURDAEV, Friedrich-Alexander Uni Erlangen-Nürnberg & Max-Planck-Zentrum für Physik und Medizin — Aggregates of living cells are an example of active materials with unconventional material properties. The rheological properties of cellular aggregates can, therefore, be markedly different from those exhibited by passive soft systems. Motivated by colonies of *Neisseria gonorrhoeae* bacteria, we develop a continuum theory to study cellular aggregates formed by attractive pili mediated intercellular interactions. We find that the formation of cellular aggregates is an active phase separation process and we discuss the activity-induced viscoelastic properties of such aggregates. By studying the behaviour of aggregates under oscillatory shear, we can link the loss and storage moduli of the aggregates to the dynamics of the active intercellular forces. Due to the turnover of pili, the aggregates show a liquid-like behaviour at large times and strong shear-thinning effect under the large amplitude oscillatory shear. Our theory provides an important insight on how pilus mediated intercellular forces in cellular aggregates govern their material properties which in the future could be tested experimentally.

Optical tweezer application with Autofocusing Airy-Bessel beams

YI LIANG (Presenter), Guangxi Key Lab for Relativistic Astrophysics, Center on Nanoenergy Research, School of Physical Science and Technology, Guangxi University, YINXIAO XIANG, West Virginia Univ, FAN SHI, Tianjin University of Technology — We proposed a new autofocusing beams named autofocusing Airy-Bessel beams (AABB). Compared with traditional circular autofocusing beams (CAB), autofocusing Airy-Bessel beams exhibited a shorter autofocusing propagation distance and two times stronger peak intensity at the focusing point. We adopted this new kind of autofocusing beams as an optical tweezer to trap particles and red blood cells. This kind of optical tweezer presented a larger trapping stiffness, which corresponded a stronger trapping force as compared with conventional autofocusing beams. In other words, it could reduce the photodamage on sample especially some biological sample such as different kind of cells at realizing a same trapping. Generally, the trapping ability of this kind of optical tweezer was found to be proportion to the laser power. This new type of tweezer may find new applications in optical manipulation and biomedical research.

*This work was supported by the National Natural Science Foundation of China (11604058), the Guangxi Natural Science Foundation (No. 2016GXNSFBA380244).
**8:00AM L27.00001: Highly Efficient Vertical SnS₂ Nanoflake Photodetector Decorated with PbS Colloidal Quantum Dots**  
BINOD GIRI (Presenter), PRATAP RAO, Worcester Polytech Inst — Tin disulfide (SnS₂) is a 2D material with excellent optoelectronic properties suitable for various solar conversion and sensing applications. SnS₂ has been used in photodetectors due to its high carrier mobility and bandgap of 2.2eV. In applications where the detection of longer wavelengths of light is desired, other materials such as lead sulfide quantum dots (PbS QDs) with tunable band gaps are used together with SnS₂ to maximize light absorption and charge collection. Although several reports have demonstrated high sensitivity and responsivity of few-layer-SnS₂/PbS QDs photodetectors, their large scale production has not been addressed. These devices are often made by mechanically exfoliating bulk SnS₂ and depositing narrow metal contacts using e-beam lithography, which are both not scalable. In this work, we have fabricated photodetectors from vertical SnS₂ nanoflakes grown by a scalable close space sublimation and decorated by colloidal PbS QDs. The SnS₂/PbS QD device is fabricated on SiO₂/Si substrates with gold contacts patterned using standard photolithography. These devices exhibit excellent responsivity, on-off ratios and transient response critical for a photodetector. Our work presents a scalable method of fabricating photodetectors from SnS₂ nanoflakes and PbS QDs.

**8:12AM L27.00002: Fundamental limits on the performance of electromagnetic devices**  
RAHUL TRIVEDI (Presenter), GUILLERMO ANGERIS, Electrical Engineering, Stanford University, LOGAN SU, Applied Physics, Stanford University, SHANHUI FAN, JELENA VUCKOVIC, Electrical Engineering, Stanford University — Formulating the design of electromagnetic devices as an optimization problem has opened up the possibility of achieving performance metrics that have eluded common design techniques. However, since these optimization problems can only be approximately solved, it is not clear what performance metrics (e.g. transmission and cross-talk) are achievable for an optical device, subject to constraints on device footprint, refractive index contrast, and feature size. In this work, we show how to efficiently calculate provable bounds on performance metrics that are expressible as a quadratic form in the electric field for a general class of linear-optical devices using Lagrangian duality and convex relaxations. We illustrate these techniques by calculating bounds on some representative 1D and 2D electromagnetic design problems: the reflectivity of a 1D mirror and the focusing efficiency of a 2D lens.

*Rahul Trivedi acknowledges funding from Kailath Graduate Fellowship.*
8:24AM L27.00003: Optical sensor development for toxic elements detection in liquids*  
C BHATT (Presenter), DANIEL HARTZLER, DUSTIN MCINTYRE, National Energy Technology Lab — Laser induced breakdown spectroscopy (LIBS) based sensor methodology was developed for the detection of three toxic elements; As, S, and Se in liquid. This concept will be used to develop a sensor for the in-situ analysis of coal power plant wastewater. Real time probe for the monitoring of the EPA regulated species is needed to control effluent streams in the power plants. Single and double pulse LIBS systems with 1064 nm Nd:YAG lasers were utilized to generate micro plasma from the surface of liquid jet containing these elements in ppm levels. Plasma emission was collected at 45 degree with the laser beam for As and Se emission lines detection in UV range while that was collected in collinear mode with laser beam for S line detection in near IR. Atomic emission lines at wavelengths 274.4 nm, 278.0 nm for As, 921 nm for S, and 196.09 nm, 203.9 nm, and 206.32 nm for Se were detected in LIBS spectra.

*This work was performed in support of the US Department of Energy’s Fossil Energy Crosscutting Research Program. The Research was executed through the NETL Research and Innovation Center’s Water Management for Power Systems Field Work Proposal. Research performed by Leidos Research Support Team staff was conducted under the RSS contract 89243318CFE000003.

8:36AM L27.00004: Cryogenic Operation of Silicon Photonic Electro-Optic Modulators based on DC Kerr Effect*  
UTTARA CHAKRABORTY (Presenter), JACQUES CAROLAN, Research Laboratory of Electronics, Massachusetts Institute of Technology, GENEVIEVE CLARK, MITRE Corporation, DARIUS BUNANDAR, JELENA NOTAROS, MICHAEL R. WATTS, DIRK R. ENGLUND, Research Laboratory of Electronics, Massachusetts Institute of Technology — Scalable photonic integrated circuits operating at cryogenic temperatures are essential for quantum information processing and supercomputing. The silicon-on-insulator platform is highly promising for its compactness and CMOS compatibility. However, efficient electro-optic modulation in silicon at cryogenic temperatures remains an outstanding challenge, owing to carrier freeze-out at cryogenic temperatures in conventional plasma-dispersion-based modulators [1]. The generation of an induced second-order nonlinearity in silicon with an applied DC electric field has been demonstrated at room temperature [2]. In this work, we demonstrate DC Kerr-based modulation in silicon at a temperature of 5K at GHz speeds, showing the potential of DC Kerr modulators for use in large-scale silicon photonic integrated circuits for cryogenic computing.


*U.C. is supported by a National Defense Science and Engineering Graduate (NDSEG) Fellowship. J.C. is supported by EU H2020 Marie Sklodowska-Curie Grant Number 751016. Devices were fabricated under the Defense Advanced Research Projects Agency (DARPA) DODOS program (Grant No. HR0011-15-C-0056). This work is supported in part by PsiQuantum.
Pump-probe experiment in a non-linear chaotic photonic cavity: modulation of a Physically Unclonable Function*  
SAMUEL METAIS, AMY C. FOSTER (Presenter), MARK A FOSTER, Johns Hopkins University — How to design a PUF, physically unclonable function[1], is a recurrent problem in information theory and cryptography. In our group, we use a non-linear truncated disk of silicon in a silicon dioxide background as a semi-chaotic cavity[2]. Silicon waveguides show non-linear effect during the propagation of high-amplitude pulses, which further complexifies the underlying physics of our device. From known results and performances of actual devices[3], we will first show here how one can enhance the photon lifetime in such a cavity to increase the information content in our operating bandwidth, and in a second part use a co-propagating laser pump in order to locally modulate the refractive index, allowing us to control the cavity’s response.


*The author recognizes funding from the IARPA under the contract number # 2018-18041100006.

Large emission enhancement and emergence of strong coupling with plasmons in nanoassemblies: Role of quantum interactions and finite emitter size.*  
RIYA DUTTA (Presenter), Indian Institute of Science - Dept of Physics, KRITIKA JAIN, MURUGESAN VENKATAPATHI, Computational and Statistical Physics Laboratory, INDIAN INSTITUTE OF SCIENCE, JAYDEEP BASU, Indian Institute of Science - Dept of Physics — Next-generation photonic devices, optical quantum communication, and information processing will rely on generating Quantum Emitter assemblies with high photonic efficiencies, that can be coupled to sources of localized radiation typically enabled by plasmons in ultrasmall metal nanoparticles. The Purcell effect has been the basis for several decades in understanding enhancement of photonic efficiency and decay rates of emitters through their coupling to cavity modes and metal nanostructures. However, it is not clear whether this regime of radiative enhancements can be extended to ultrasmall nanoparticle sizes or interparticle distances. Here we report large radiative enhancements of quantum dot assemblies with extremely small metal nanoparticles and emitter-particle separations R of a few nanometers, where Purcell effect would lead to either no enhancements or quenching. We invoke a new regime of radiative enhancements to explain the experimental data and also correctly predict the emergence of strong coupling below certain R, as observed in experiments. In addition, we show that the widely used point emitter approximations diverge from actual observations in the case of finite size emitters at such small separations. REF- PHYSICAL REVIEW B 100, 155413 (2019)

*DST, SERB India.
9:12AM L27.00007: Multiscale electrothermal simulation of quantum cascade lasers

MICHELLE KING (Presenter), Materials Science and Engineering, University of Wisconsin-Madison, SINA SOLEIMANIKAHNOJ, IRENA KNEZEVIC, Electrical and Computer Engineering, University of Wisconsin-Madison — Quantum cascade lasers (QCLs) are high-power, coherent light sources that emit at midinfrared and terahertz frequencies. The active core of these devices is a periodic multiple-quantum-well heterostructure where the electronic and lattice systems exist far from equilibrium and are strongly coupled. Heat generated in the active core (the part responsible for light emission) diffuses throughout the rest of the device. Coupled charge and heat transport in QCLs present a multiscale and multiphysics problem that governs device properties observed in experiment, such as the current-voltage characteristics, gain, and internal quantum efficiency. We present a strategy for simulating coupled heat and charge transport in QCLs, which occur on drastically different spatial scales, that employs a coupled ensemble Monte Carlo for electrons and phonons in a stage-level simulation of the active core and couples to a device-level heat diffusion simulation.

*DOE BES DE-SC0008712; AFOSR FA9550-18-1-0340

9:24AM L27.00008: Selectively launching propagating surface plasmon from designed symmetric plasmonic structures

YU GONG (Presenter), College of Charleston, ALAN G. JOLY, PATRICK Z. EL-KHOURY, WAYNE P. HESS, Pacific Northwest National Laboratory — The next generation signal processing technology demands high speed and energy efficient information carriers. Surface plasmon polaritons (SPPs) can be one of the most promising candidates since they propagate at almost the speed of light, and can be confined to sub-wavelength dimensions using designed nanostructures. In our studies, we show the intensity of propagating SPPs launched from opposing edges of a symmetric trench structure can be controlled by the linear polarization of the optical field. Through the FDTD simulations, we reveal that the coupling efficiency of the propagating SPPs is inversely proportional to that of the localized surface plasmon excited at the trench edges. We also explored the generation of propagating SPPs from a protruded silver cap structure with s-polarized femtosecond laser excitation. Surprisingly, our results show the SPPs propagate with a bifurcated spatial structure with an antisymmetric mirror plane and may be regarded as two spatially distinct, temporally phase-locked wave packets. Our findings can facilitate the design of plasmonic devices/components in nanophotonic circuits.

*The authors acknowledge support from the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences.
9:36AM L27.00009: Fundamental thermal noise limits for high-Q/V optical microcavities
CHRISTOPHER PANUSKI (Presenter), RYAN HAMERLY, DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — Thermo-refractive noise — refractive index perturbations driven by fundamental thermal fluctuations — have recently been identified as a limiting noise source in various optical microcavities. Here, we present a theoretical and experimental characterization of this thermal noise in high quality factor \((Q)\), small mode volume \((V)\) photonic crystal cavities. The theory reveals a mode volume-dependent maximum “effective” \(Q\)-factor due to thermal dephasing. We quantify the implications for quantum optical devices operating in the qubit limit of cavity nonlinear optics and compare these results to calibrated frequency stability measurements of common 2D silicon photonic crystal cavities. The results highlight the importance of considering thermal noise in state-of-the-art high-Q/V optical resonators, but also inform design choices which minimize its impact on device performance.

9:48AM L27.00010: Cryogenic electro-optic interconnect for superconducting circuits
ITAY SHOMRONI (Presenter), AMIR YOUSSEFI, NATHAN R BERNIER, YASH JOSHI, Ecole Polytechnique Federale de Lausanne, PHILIPP JOHANN UHRICH, University of Heidelberg, TOBIAS J. KIPPENBERG, Ecole Polytechnique Federale de Lausanne — Encoding information onto optical fields is the backbone of modern telecommunication networks. Optical fibers offer low loss transport and vast bandwidth compared to electrical cables, and are currently also replacing copper cables for short-range communications. Optical fibers also exhibit significantly lower thermal conductivity, making optical interconnects attractive for interfacing with superconducting circuits and devices. Yet little is known about modulation at cryogenic temperatures. Here we demonstrate a proof-of-principle experiment, showing that currently employed Ti-doped LiNbO modulators maintain the Pockels coefficient at 3K—a base temperature for classical microwave amplifier circuitry. We realize electro-optical read-out of a superconducting electromechanical circuit to perform both coherent spectroscopy, measuring optomechanically-induced transparency, and incoherent thermometry, encoding the thermomechanical sidebands in an optical signal. Although the achieved noise figures are high, approaches that match the lower-bandwidth microwave signals, use integrated devices or materials with higher EO coefficient, should achieve added noise similar to current HEMT amplifiers, providing a route to parallel readout for emerging quantum or classical computing platforms.
10:00AM L27.00011: Photon Mediation of Electron Transitions in Quantum Cascade Lasers

SINA SOLEIMANIKAHNOJ (Presenter), MICHELLE KING, IRENA KNEZEVIC, University of Wisconsin - Madison — Quantum cascade lasers (QCLs) are unipolar coherent light sources emitting in the terahertz and midinfrared portion of the electromagnetic spectrum. The active region of a QCL consist of periodic stacks of alternating semiconductor materials forming quantum wells which confine electrons in space and ensure they have desired discrete energy levels. Lasing is achieved by electron transition between these energy levels. In QCLs with the so-called diagonal design, this transition involves quantum tunneling between states with a small spatial overlap, separated by a potential barrier. This electron tunneling is mediated by photons present in the active region of the QCL and is referred to as photon-assisted (PA) tunneling. So far, theoretical studies dedicated to PA tunneling in QCLs have been limited to simple rate equations accompanied by empirical or phenomenological scattering rates. In this work, we present a quantum-transport study of PA tunneling in QCLs based on a Markovian master equation for the density matrix and investigate the effect of PA tunneling on electron dynamics and state lifetime.

*Funding: DOE BES DE-SC0008712; AFOSR FA9550-18-1-0340

10:12AM L27.00012: Extreme laser background suppression for resonance fluorescence in semiconductor nanostructures

MERYEM BENELAJLA (Presenter), attocube systems AG, MERYEM BENELAJLA, CNRS/INSA Toulouse, ELENA KAMMANN, KHALED KARRAI, attocube systems AG — Semiconductor nanostructures are promising candidates for developing single photon technologies. Relevant demonstrations in this field has been carried out by resonantly coupling a laser beam to a quantum emitter. Such challenging measurements require the suppression of laser background by several order of magnitudes. One way to do that is to use cross polarization confocal microscopy. Normally, high quality commercial crossed polarizers allows a laser suppression down to 5 to 6 orders of magnitudes. Surprisingly, when used in combination with a confocal microscope, the extinction ratio is boosted up to 9 order of magnitudes. This unexpected but very welcome enhancement finds its origin in the Imbert-Fedorov effect, now commonly referred to as Spin Hall effect of light, which manifests itself in the reflectivity of a Gaussian laser beam off a mirror. In this presentation, we will discuss in details the physics and optics of such a remarkable effect, which we mapped in details for the first time.
Quantized Microwave Faraday Rotation

VISHNUNARAYANAN SURESH (Presenter), EDOUARD PINSOLLE, CHRISTIAN LUPIEN, Universite de Sherbrooke, TALIA MARTZ-OBERLANDER, Department of Physics, McGill University, MICHAEL P LILLY, JOHN RENO, Center for Integrated Nanotechnologies, Sandia National Laboratories, GUILLAUME GERVAIS, Department of Physics, McGill University, THOMAS SZKOPEK, Electrical and Computer Engineering, McGill University, BERTRAND M REULET, Universite de Sherbrooke — The phenomenon of rotation of polarization in the presence of static magnetic field known as Faraday rotation [1] is very well known. Here we present the quantitative observation of microwave Faraday rotation conducted with GaAs/AlGaAs semiconductor heterostructure. The microwave Faraday rotation observed in high mobility two-dimensional electron gas arises as a result of cyclotron motion of charge carriers. The Faraday rotation induced can be understood by Fresnel analysis for the transmission of right and left handed circularly polarized microwaves. As with the Hall effect, a continuous classical as well as quantized Faraday rotation is observed. In the quantum Hall regime, the Faraday rotation is quantized in units of fine structure constant. The dielectric response of the semiconductor host, and the modification of the wave impedance and field distribution by a wave guide [2] will lead to a modification of the quantized Faraday rotation away from the vacuum fine structure constant, $\alpha \approx 1/137$. The effect of frequency dependent electromagnetic confinement can be accounted with an effective fine structure constant $\alpha^*$. 


In-chip laser nano-structuring inside silicon with spatially modulated beams

ONUR TOKEL (Presenter), AQIQ ISHRAQ, RANA ASGARI SABET, Bilkent Univ — Recently, we demonstrated a laser-writing method that exploits nonlinear interactions to form subsurface (in-chip) modifications, created deep inside silicon [1]. This single-step, maskless method introduced a new capability, i.e., controlled 3D microfabrication capability at 1-µm resolution inside Si [1]. Here, we expand the technique for demonstrating, to the best of our knowledge, the first nanofabrication capability in Si, realized without damaging the wafer surface. In order to achieve this, we exploit the ‘non-diffracting’ nature of Bessel beams, which offer better spatial control in comparison to Gaussian beams. The laser pulses of ~5 ns, 1.55 µm and a few-microjoules energy are modulated with a spatial light modulator, before directed with a lens system, forming Bessel pattern inside the sample. The crystal structure is disrupted in the form of rod-like structures that have high aspect-ratios > 500, with structure-widths that are on the order of 250 nm, and of roughness ~30 nm. These in-chip nano-structures can potentially lead to novel infrared photonic elements for phase and polarization control at the nanoscale.

L27.00015: Visible quantum dot light-emitting diodes with simultaneous high brightness and efficiency*  

HUAI BIN SHEN, Hua University, Kaifeng, China, QIANG GAO, University of Science and Technology of China, Hefei, China, YANBIN ZHANG, Henan University, Kaifeng, China, YUE LIN, University of Science and Technology of China, Hefei, China, QINGLI LIN, ZHAOHAN LI, LING CHEN, ZAIPING ZENG, Henan University, Kaifeng, China, XIAOGUANG LI, Shenzhen University, Shenzhen, China, YU JIA, SHUJIE WANG, ZULIANG DU, LIN SONG LI, Henan University, Kaifeng, China, ZHENYU ZHANG (Presenter), University of Science and Technology of China, Hefei, China — Quantum dot light-emitting diodes are promising light sources for applications in displays. However, to date, there have been no reports of devices that simultaneously offer both high brightness and high external quantum efficiency. Here, we report red, green and blue quantum dot light-emitting diodes based on CdSe/ZnSe core/shell structures that have these attributes. We demonstrate devices with maximum external quantum efficiencies of 21.6%, 22.9% and 8.05% for red, green and blue colours with corresponding brightness of 13,300 cd m^{-2}, 52,500 cd m^{-2} and 10,100 cd m^{-2}. The devices also offer peak luminance of 356,000 cd m^{-2}, 614,000 cd m^{-2} and 62,600 cd m^{-2}, respectively. We postulate that this high performance is due to the use of Se throughout the core/shell regions and the existence of alloyed bridging layers at the core/shell interfaces. This study suggests that in the future visible quantum dot light-emitting diodes will also be suitable for lighting applications.


*Supported by NNSF of China and MOST.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L28 FIAP GERA: Seeing the Energy Future 405-407 - Carlos Gutierrez, Sandia National Laboratories - Tag(s): Industry, Invited, Undergrad Friendly

8:00AM L28.00001: Robert Andosca Invited Talk [Invited] —
ANDREW SPECK (Presenter), Schlumberger — Over the last few years, the Oil & Gas Industry has increasingly been driven to provide the most cost-effective and reliable supply of energy possible in order to continue providing over half of the world’s energy mix sustainably. This has required service providers for the industry to relentlessly optimize their technology performance and service delivery to improve asset economics both in existing fields as well as in new developments. A key location for optimization is in the multi-billion-dollar investments in subsea fields which require continual operational expenditures for services such as Inspection, Maintenance, and Repair (IMR) to ensure asset integrity.

IMR service providers currently utilize remotely operated vehicles (ROV) tethered to a surface vessel and piloted in real-time. Recent progress in underwater perception, maritime autonomy, and artificial intelligence can disrupt this old method and allow developing a leaner service model that significantly reduces the costly vessel and personnel support while improving data quality. uROV (untethered ROV) is unique in its approach to this problem. Around producing subsea fields, a higher level of supervision than “launch and forget” is needed. Thus, the uROV platform is based around supervised autonomy wherein a “person in the loop” has real-time feedback from onboard sensors and is then able to update the operation.

This talk will present the novel sensor architecture embedded on the uROV platform to enable this vision. Results include a first demonstration of remote acoustic visualization and control of subsea LiDAR during a high-resolution scan of a P-38 wreck. Extensions under development will enable remote mapping of infrastructure surface temperatures as well as detection and localization of potential hydrocarbon leaks. I will lastly present progress towards utilizing the data generated by these sensors for localization and cluttered environment navigation to safely approach high value assets.

ROSS KONINGSTEIN (Presenter), Research, Climate and Energy, Google — Tentative notional abstract. Work in progress.

Opening up the future of energy requires making bold advances in stationary and mobile power production.

In energy, more so than in most industries, most of the resources go into incremental advances. History teaches us that the marked differences between the past and today are due to fundamental changes.

So let’s look at what some fundamental changes could look like, and why this field could be the most exciting one to place revolutionary bets in.
In an increasingly electrified technology driven world, power electronics is central to the entire manufacturing economy. Silicon (Si) power devices have dominated power electronics due to their low cost volume production, excellent starting material quality, ease of processing, and proven reliability. Although Si power devices continue to make progress, they are approaching their operational limits primarily due to their relatively low bandgap and critical electric field that result in high conduction and switching losses, and poor high temperature performance.

In this presentation, the favorable material properties of Silicon Carbide (SiC) devices, which allow for highly efficient power electronic systems with reduced form factor and reduced cooling requirements, will be highlighted. Emphasis will be placed on high impact application opportunities where SiC devices are expected to displace their incumbent Si counterparts. These include “more electric aerospace” with weight, volume, and cooling system reductions contributing to energy savings and low emissions; automotive power electronics with reduced losses and relaxed cooling requirements; more efficient, flexible, and reliable grid applications with reduced system footprint; variable frequency drives for efficient high power electric motors at reduced overall system cost; and novel data center topologies with reduced cooling loads and higher efficiencies. Cost reduction strategies will be outlined elucidating the path to the projected $1.9 billion SiC device market by 2024.

*PowerAmerica is an Innovation Manufacturing Institute funded by the U.S. Department of Energy.
8:00AM L29.00001: Coarse-grained theory for motion of solitons and skyrmions* CHENG LONG (Presenter), JONATHAN SELINGER, Kent State Univ - Kent — Recent experiments have found that applied electric fields can induce motion of skyrmions in chiral nematic liquid crystals [1]. To understand the magnitude and direction of the induced motion, we develop a coarse-grained approach to describe dynamics of skyrmions, similar to our group’s previous work on the dynamics of disclinations [2]. In this approach, we represent a localized excitation in terms of a few macroscopic degrees of freedom, including the position of the excitation and the orientation of the background director. We then derive the Rayleigh dissipation function, and hence the equations of motion, in terms of these macroscopic variables. We demonstrate this theoretical approach for 1D motion of a sine-Gordon soliton, and then extend it to 2D motion of a skyrmion. Our results show that skyrmions move in a direction perpendicular to the induced tilt of the background director. When the applied field is removed, skyrmions move in the opposite direction but not with equal magnitude, and hence the overall motion may be rectified.


*This work was supported by NSF Grant No. DMR-1409658.

8:12AM L29.00002: Energy dependence of resonant x-ray scattering for the twist bend nematic phase, a helix of liquid crystals* YU CAO, State Key Laboratory for Mechanical Behavior of Materials, Shaanxi International Research Center for Soft Matter, School of Materials Science and Engineering, Xi’an Jiaotong, JUN FENG, Advanced Light Source, Lawrence Berkeley National Laboratory, ASRITHA NALLAPANENI, Department of Polymer Engineering, University of Akron, YUKI ARAKAWA, Department of Applied Chemistry and Life Science, Toyohashi University of Technology, KEQING ZHAO, College of Chemistry, Sichuan Normal University, FENG LIU, State Key Laboratory for Mechanical Behavior of Materials, Shaanxi International Research Center for Soft Matter, School of Materials Science and Engineering, Xi’an Jiaotong, CHENHUI ZHU (Presenter), Advanced Light Source, Lawrence Berkeley National Laboratory — We examined the manifestation of resonance effects in twist bend nematic (NTB), smectic A (SmA) and crystalline phases via tender resonant X-ray scattering (TReXS) at sulfur K-edge. While SmA layering peak is partially resonant, scattering peak of NTB is purely resonant visible only near S K-edge. The difference is attributed to the periodic molecular orientation variation with weak electron density modulation. We further demonstrate that the energy-dependence of such scattering peak arising from pure orientation variation scales with the sum of $f_1(E)^2$ and $f_2(E)^2$, corresponding to the real and imaginary parts of dispersion correction respectively, while the resonant contribution in sulfur-containing SmA scales with $f_1(E)$, and is a first order perturbation to the relatively strong non-resonant peak from electron density modulation.

*Director of the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under contract no. DE-AC02-05CH11231. The work was also supported by National Natural Science Foundation of China (No. 21774099, 21761132033 and 51603166), Science and Technology Agency of Shaanxi Province (2016KW-050 and 2018KWZ-03). Y.C. also thanks China Scholarship Council (CSC) for providing financial support (201706280170).
8:24AM L29.00003: Behavior of Superparamagnetic Microbeads in Smectic Films*
EMMANUEL BAMIDELE (Presenter), Material Science and Engineering Program and Soft Materials Research Center, University of Colorado, XI CHEN, JACKSON DURM, CHEOL PARK, JOSEPH E MACLENNAN, NOEL ANTHONY CLARK, Physics and Soft Materials Research Center, University of Colorado — We investigate the behaviour and magnetic response of superparamagnetic, silica-coated iron oxide microbeads embedded in freely suspended films of the smectic A liquid crystal 8CB. The microbeads, which are 5 mm in diameter, are mixed into the liquid crystal material at the edge of the film holder before the films of a few smectic layers are spread. Small aggregates and short chains of beads are observed in the film a few minutes after spreading, with longer chains forming along layer steps and at the heavily dislocated meniscus. The microbeads appear to affect the line tension of the layer steps, resulting in an increased tendency for thicker material to sweep in from the meniscus onto the initially thin film and causing islands to shrink much more rapidly than in films of neat 8CB. Moderate applied magnetic fields can be used to translate the beads on the film and to change the rate of island shrinkage.

*This work was supported by NASA Grant No. NNX-13AQ81G and NAG No. NNX17AC74G and by the Soft Materials Research Center under NSF MRSEC Grant No. DMR-1420736.

8:36AM L29.00004: Dynamics of magnetically induced defect walls in Nematic Lenses
ZOLTAN KARASZI (Presenter), HAUMED RAHMANI, Kent State Univ - Kent, VIKTOR KENDERESI, PETER SALAMON, AGNES BUKA, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, ANTAL ISTVAN JAKLI, Kent State Univ - Kent — We studied nematic liquid crystal (NLC) droplets with lens-shaped free surface placed on solid substrates under magnetic field applied parallel to the solid substrate. Both the solid substrate and the air pose homeotropic anchoring of the NLC director. At low magnetic-fields, the director field with a small radial in-plane component becomes distorted toward the field. At moderate fields it transforms into two regions with opposite tilt direction, separated by a wall. Polarizing optical microscopy (POM) with monochromatic light illumination reveals two sources of magnetic field driven fringe generation. At high fields, a Helfrich-type inversion defect wall arises normal to the magnetic field and moves outward. In addition to the experimental POM results, we present a simple theory and computer simulations that explain the magnetic field dependence of the director field and the time dependence of the outward motion of the inversion wall at constant magnetic fields.
8:48AM L29.00005: Dynamic pattern generation of topological defect arrays in nematic liquid crystals*  MINSU KIM (Presenter), FRANCESCA SERRA, Johns Hopkins University — Some photonic devices use the periodic nature of repeating lattices to modulate light.[1] Here we create tunable patterns of topological defect arrays in nematic liquid crystals (LCs) that can be simply controlled by electrical waveforms.[2,3] The refractive index of LCs is spatially modulated owing to the presence of the topological defect arrays. The symmetry and regularity of patterns is controllable thanks to micro-pillars created by photolithography. Adjusting the frequency and amplitude of electrical waveforms changes the defect spacing. Where the defect spacing is reduced, the number density of defects increases, compatibly with the presence of the pillars. The patterns are in two dimensions and this opens up more possibilities for the arrangement of the defects. When a laser beam propagates through the spatially modulated refractive index LC layer, the direction of the wave front changes and the beam can be split and steered. We utilize these complex patterns as a diffraction grating, which can change both diffraction (polar) angle and azimuthal angles.


*ACS PRF 59931-DN110

9:00AM L29.00006: Elongation of Tactoids in the presence of an electric field*

MOHAMMADAMIN SAFDARI (Presenter), University of California, Riverside, PAUL VAN DER SCHOOT, Physics, Eindhoven University of Technology, ROYA ZANDI, University of California, Riverside — Tactoids are spindle-shaped droplets of a nematic phase suspended in the co-existing isotropic phase. They are found in dispersions of a wide variety of elongated colloidal particles, including actin, fd virus, carbon nanotubes, vanadium peroxide, and chitin nanocrystals. Recent experiments on tactoids of chitin nanocrystals dispersed in water show that electrical fields can strongly elongate tactoids, but only if the tactoids have a sufficiently large volume. We explain this by extending the Oseen-Frank elastic model of Kaznacheev et al. [1] and Prinsen et al. [2] to partially bipolar tactoids and evaluate the level of elongation of the tactoids as a function of the surface tension, elastic constants, volume, and electric field strength. By invoking a free-energy-based relaxational dynamics, we also describe the time evolution after switching on the electric field, confirming that, counterintuitively, large tactoids take more time to elongate to their equilibrium value in an electric field than small ones do.

[2] Peter Prinsen et al, 2003, Shape and director-field transformation of tactoids

*National Science Foundation, DMR-171955
9:12AM L29.00007: Observation of Ferroelectricity in a Thermotropic Nematic Liquid Crystal Using its Spectacular Electro-Optics* XI CHEN (Presenter), Department of Physics, University of Colorado, Boulder, EVA KORBLOVA, Department of Chemistry, University of Colorado, Boulder, RENFAN SHAO, LEO RADZIHOVSKY, MATTHEW GLASER, JOSEPH E MACLENNAN, Department of Physics, University of Colorado, Boulder, DAVID M. WALBA, Department of Chemistry, University of Colorado, Boulder, NOEL ANTHONY CLARK, Department of Physics, University of Colorado, Boulder — We have synthesized and studied the literature compound RM734 [1], a polar rod shaped molecule exhibiting a typical nematic phase and a second nematic phase assigned to be a "splay nematic" state [2]. We find that the second phase is rather a thermotropic ferroelectric nematic, an identification based on the first observation in a nematic of the defining characteristics of ferroelectricity: (1) the formation, in absence of applied electric field, of spontaneously polar domains of opposite sign of polarization separated by distinct domain boundaries; and (2) field-induced polarization reversal mediated by movement of these domain boundaries. A truly remarkable feature of this phase is the magnitude of its spontaneous polarization, saturating at 6 μC/cm², the largest ever reported for an organic material or for any fluid, and larger than that of all but a few crystalline ferroelectrics.

Works Cited

*Acknowledgements: Work supported by NSF Grants 1420736 (MRSEC) and 1710711.

9:24AM L29.00008: Ferromagnetic Fréedericksz transition in ferromagnetic nematic filaments* MIN SHUAI (Presenter), XI CHEN, NATHAN COBASKO, JOSEPH E MACLENNAN, MATTHEW A. GLASER, NOEL ANTHONY CLARK, University of Colorado, Boulder — Barium hexaferrite nanoplates at sufficiently high concentrations in 1-butanol spontaneously form a ferromagnetic nematic phase due to the interplay between Onsager excluded volume effects and magnetic dipole-dipole interactions [Nat Comm, 7: 10394, 2016]. We have discovered a rich variety of ferromagnetic structures, such as droplets, toroids, and filaments, which form in the isotropic background when the concentration of the nanoplates is within the isotropic-nematic phase coexistence region. Here, we demonstrate a Fréedericksz transition in such ferromagnetic filaments. In the absence of applied magnetic field, the local magnetization direction of the filaments is parallel to their long axes. When a magnetic field is applied parallel to the magnetization direction, the existing alignment of the nanoplates is reinforced and the shape of the filaments remain unchanged. However, when a sufficiently strong magnetic field is applied antiparallel to the magnetization direction, an undulation instability sets in and the filaments form wavy structures. A simple model was developed to describe the deformation of the filaments close to the transition points.

*This work is supported by NSF MRSEC Grant DMR-1420736 and NASA Grant No. NNX17AC74G.
**9:36AM L29.00009: Electrostatically controlled surface boundary conditions in hybrid molecular-colloidal liquid crystals**

HARIDAS MUNDOOR (Presenter), BOHDAN SENYUK, MAHMOUD ALMANSOURI, SUNGOH PARK, BLAISE FLEURY, University of Colorado, Boulder, HENRICUS WENSINK, Laboratoire de Physique des Solides, Université Paris-Sud, IVAN I SMALYUKH, University of Colorado, Boulder — In fundamental studies of liquid crystal (LC) colloids, surface interactions define the boundary conditions for molecules on particle surfaces and ultimately determine the induced defects and interactions. We study the influence of surface charge and ions on surface anchoring properties, with a focus on defining the behavior of anisotropic colloids dispersed in a nematic LC. We demonstrate a systematic variation of boundary conditions through controlling the competing aligning effects of surface functionalization and electric field arising from surface charging and bulk counterions. The control of ionic content in the bulk and at surfaces allows for tuning the equilibrium orientations of charged colloidal particles with respect to the far-field director \( \mathbf{n} \). When dispersed in high concentration, the charged colloids form biaxial nematic, columnar, and crystalline assemblies with tunable symmetries and ordering enabled by the anisotropic elastic and electrostatic interactions.

**9:48AM L29.00010: Cellulose Nanocrystal well alignment with addition magnetic nanoplates in weak gradient magnetic field**

MINGFENG CHEN (Presenter), ZHENGDONG CHENG, DALI HUANG, Texas A&M University — Rod like Cellulose nanocrystal (CNCs) are emerging nanomaterials that form chiral nematic liquid crystals and the controlling of orientation of formed liquid crystal phased has attracted broad attention. To enhance the response of CNC rods in the magnetic field, barium hexaferrite (BF) nanoplates, with positive magnetic susceptibility and mean nanoplatelet magnetization is \( m_0 = 2 \times 10^{-18} \) A m\(^2\), were introduced. Here, we investigated the effect of addition BF nanoplatelets on the phase transition and orientation of CNCs suspension in a weak external gradient magnetic field (Several hundred Gauss) . We observed the nematic phase prefer to move to the lower magnetic field region and a floating nematic phase is formed when the direction of magnetic field is contrast with the gravity field. We also demonstrate the gradient magnetic field can accelerate the phase separation. Based on these, we establish a method to control the phase separation speed and the position of nematic phase, since the movement of nematic phase depends on the competition of magnetic and gravity field. Moreover, the nematic phase were nearly perfect alignment along the magnetic field, which indicate with the BF magnetic nanoplates, the CNCs can be aligned by very weak magnetic field.
10:00AM L29.00011: Application of monolayer WSe\textsubscript{2} as the planar-alignment agent in an electro-optic liquid crystal device*  
RAJRATAN BASU, LUKAS J ATWOOD (Presenter), US Naval Academy — Two-dimensional (2D) tungsten diselenide (WSe\textsubscript{2}) nanosheets were transferred onto indium tin oxide (ITO) coated glass slides. Two such 2D WSe\textsubscript{2}-covered ITO glass slides were placed together to fabricate a liquid crystal (LC) cell. A nematic LC inside this WSe\textsubscript{2}-based cell exhibits uniform planar-alignment. This planar-alignment at the molecular scale is achieved due to the coherent overlay of the LC molecules along the selenium (Se) array on the WSe\textsubscript{2} lattice. This WSe\textsubscript{2}-based LC device shows the typical electro-optical effect when an electric field is applied via ITO electrodes. This electro-optical effect also reveals a standard Fréedericksz transition of the LC, confirming that the 2D WSe\textsubscript{2}, as the planar-alignment agent, supplies adequate planar anchoring energy—which can be overcome by the Fréedericksz threshold voltage.

*This work was supported by the Office of Naval Research (N0001419WX01126; N0001419WX01219; N0001419WX00566) and the USNA 2019 Kinnear Fellowship Award.

10:12AM L29.00012: Topographical variations in thin liquid crystal films*  
TIM ATHERTON (Presenter), Physics and Astronomy, Tufts University, ANDREW FERRIS, CHARLES ROSENBLATT, Physics, Case Western Reserve University — A thin film of isotropic fluid with a free interface is always perfectly flat far away from boundaries and inclusions. In contrast, liquid crystals can, in principle, sustain a surface topography because elastic distortions in the bulk can be relaxed by deformation(s) of the surface. In practice, surface tension tends to dominate over elastic forces and so boundary deformations are usually neglected. (However, these have been observed in smectics and in nematics, as De Gennes famously predicted, where defects are confined to the boundary.) Here we present a different scenario: Topography at the free interface is induced by surface patterning of the substrate in a thin, hybrid-aligned nematic liquid crystal. The proposed mechanism requires finite anchoring at the free interface leading to modulation of the nematic orientation; deformation of the surface then allows the nematic to better satisfy the anchoring condition. We present analytical and numerical theory for several surface patterns, which are compared with our experimental actualizations.

*This material is based upon work supported by the National Science Foundation under Grant Nos. DMR-1654283 and DMR-1901797 and by NASA under Grant No. NNX17AC76G.
10:24AM L29.00013: Microscopic look at mesogen interactions with two-dimensional nanosheets*  
PAUL BROWN (Presenter), ASEE Fellow for Naval Research Laboratory, SEAN A FISCHER, JAKUB KOLACZ, CHRISTOPHER SPILLMANN, DANIEL GUNLYCKE, United States Naval Research Laboratory — Recent interest surrounding the combination of liquid crystals (LC) and two-dimensional (2D) nanosheets has shown when 2D nanosheets are utilized liquid crystal-optical refractors obtain faster response times, smaller device dimensions, and the replacement of mechanical components that suffer from deterioration. Additionally, 2D materials can operate as an electrode and alignment agent simultaneously. In this talk, we use density functional theory to focus on the microscopic origins of recent observations where liquid crystals are combined with two-dimensional nanosheets. We highlight the origins of critical interactions between 5CB and graphene, boron nitride, and phosphorene. We demonstrate qualitatively different band structures among the substrates, and, in particular, boron nitride shows an alignment dependence for 5CB. The effect associated with the 5CB orientations on boron nitride will be discussed in more detail, where the possibility of edge modes form. Finally, we discuss the influence of point defects in the crystal lattice of each substrate.

*This work has been supported by the Office of Naval Research, directly and through the U.S. Naval Research Laboratory.

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XIAO LI (Presenter), Univ of North Texas, KANGHO PARK, Korea Advanced Institute of Science and Technology, JOSE MARTÍNEZ-GONZÁLEZ, Universidad Autónoma de San Luis Potosí, ORLANDO GUZMAN, Universidad Autonóma Metropolitana, JUAN DE PABLO, PAUL F NEALEY, University of Chicago — In condensed matter, the correlation length is an essential parameter for describing the distance over which a material maintains its structural properties. In liquid crystals, such a characteristic length is of the order of 10 µm while in solid crystals it can be extent up to macroscopic dimensions. Here, we report how to measure the correlation length of blue-phases (BPs), which are chiral liquid crystals with long-range 3D-crystalline structures and submicron-sized lattice-parameters. We design patterned substrates made of a binary array of regions with different anchoring, which facilitate a uniform nucleation and growth of BP-crystals with (100)-lattice orientation and a simple cubic symmetry. Our results indicate that this simple cubic blue-phase (BPII), forms first on the patterned surface, thereby setting the growth of domains in directions that can be parallel or perpendicular to the patterned regions. These results are used to understand the emergence of a surface anchoring assisted BPII-coherence length in terms of time and pattern characteristics. We found that BPII single crystals can be achieved on patterned regions whose lateral dimensions are equal or larger than 10 µm, which is consistent with our measurements of the BPII-coherence length.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM
8:00AM L30.00001: Conformal elasticity of two-dimensional dilational maximally auxetic materials [Invited]  

ZEB ROCKLIN (Presenter), Georgia Tech — The elastic response of a structure depends not only on its material, but on its geometry, as when the thinness of a sheet gives rise to out-of-plane bending fundamentally distinct from the response of a thick slab. Such thinness is similarly exploited in mechanical metamaterials which permit counter-rotations of stiff adjoining elements, ranging from corner-sharing square or triangular pieces to disordered networks. Such behavior can be described via a micromorphic theory which includes these abrupt local rearrangements, giving rise to a long-wavelength elastic theory which resembles conventional Cauchy elasticity with a dramatically reduced bulk modulus. The low-energy deformations consist predominantly of local rotations, translations and dilations without shears and are hence exactly the conformal maps of complex analysis, which admit a simple analytical theory extending even into the nonlinear regime. Despite finite-size effects, bending resistance and disorder, this theory accurately captures response in both finite-element simulations and experimental systems, opening new avenues for shape-changing, programmability and nonlinear response.

8:36AM L30.00002: Control and design of response in disordered networks: Geometry and self-stresses.*  

ANWESA BOSE, STEVEN A. VAN DUIJNHOVEN, MATTHIJS F.J. VERMEULEN, WOUTER G ELLENBROEK, CORNELIS STORM (Presenter), Applied Physics, Eindhoven University of Technology — The mechanical response of elastic networks is not only controlled by the elastic properties of its constituents, but also by their architecture. This is evident for crystalline structures, but equally true for random networks. I share two recent examples where we use geometry to elicit nonstandard mechanical response from disordered networks. In the first, we design freestanding frames that are mechanically overconstrained, and demonstrate that by engaging their states of self stress (i.e., applying internal loads that produce no strain) we can tune the overall mechanical response and induce softness, bi- and instabilities of purely geometric origin [1]. In the second example, we design random periodic lattices and structurally optimize them to exhibit specific responsiveness manifested, f.i., by extreme auxeticity (deeply negative Poisson's ratios). Together, these examples illustrate that the power of geometry may be harnessed to coax tailored, highly non-generic response even out of fully disordered materials.


*Funding from the Netherlands Organisation for Scientific Research (NWO) under the Marginal Soft Matter programme (FOM12CSM01) and the Computational Sciences for Energy Research programme (14CSER005) is gratefully acknowledged
8:48AM L30.00003: Coulomb Floppy Networks: from soft to hard matter.* ALEXEI TKACHENKO (Presenter), IGOR ZALIZNYAK, Brookhaven National Laboratory — Floppy Networks (FNs) play a prominent role in soft condensed matter physics, from polymeric gels and rubber to biomolecules, glasses, and granular materials. We demonstrate how the very same concept emerges in the context of a family of open-framework ionic solids, e.g. ScF$_3$, which can be conceptualized as Coulomb FNs. They exhibit unusual properties, including quantum structural phase transition near ambient pressure and negative thermal expansion (NTE). We connect these phenomena to FN-like crystalline architecture, stabilized by the net electrostatic repulsion, playing a role similar to the osmotic pressure in a polymeric gel. Our theory provides an accurate quantitative description of NTE and structural transition. Entropic stabilization of criticality explains the observed phase behavior. In addition, a significant entropic contribution to elasticity accounts for the marked discrepancy between numerical and experimentally observed compressibilities.

*The work was performed at Brookhaven National Laboratory under DOE contract DE-SC0012704. It used resources of the Center for Functional Nanomaterials (CFN), a user facility of the Office of Basic Energy Sciences (BES), and was partially supported Division of Materials Sciences and Engineering of BES.

9:00AM L30.00004: Emergence of rigidity, microscopic rearrangements and viscoelastic response in soft particle gels EMANUELA DEL GADO (Presenter), Georgetown University, BAVAND KESHAVARZ, Mechanical Engineering, MIT, MINASPI BANTAWA, Georgetown University, MICHELA GERI, Mechanical Engineering, MIT, MEHDI BOUZID, LPTMS, Universite Paris Sud, THIBAUT DIVOUX, CNRS, MIT, GARETH H MCKINLEY, Mechanical Engineering, MIT — We have investigated the connection between the structural and mechanical heterogeneities of soft particulate gels and their viscoelastic spectrum in a 3-D microscopic numerical model, using large scale simulations with Optimally Windowed Chirp (OWCh) signals. In the model, particles spontaneously self-assemble into disordered, stable porous networks (even at low volume fractions) that feature extended relaxation spectra, microscopic dynamics, and mechanics consistent with several observations in colloidal and protein gels. To recapitulate the basic features of the particle contacts in those systems, the main ingredients of the model are short-range attractive interactions and bending stiffness for the inter-particle bonds. We have analyzed the emergence of rigidity, the shape of the frequency-dependent dynamic modulus G*(ω) and its dependence on the gel connectivity, and the distribution of microscopic non-affine rearrangements the network experiences under small-amplitude oscillatory deformation. We show how the viscoelastic response of different gels can be captured in a unique master curve through a fractional constitutive model and discuss how the underlying microscopic dynamical processes determine the rheological response.

9:12AM L30.00005: Pseudomomentum balance in thin structures JAMES HANNA (Presenter), University of Nevada, Reno, HARMMEET SINGH, École Polytechnique Fédérale de Lausanne — The balance of pseudomomentum is associated with material symmetry in continua. We will employ it in the context of thin, flexible structures, to explain conserved quantities in rotating conical membranes and propulsive forces on confined elastic rods.
9:24AM L30.00006: Asymptotic isometry and wrinkle-to-fold transition in a simplified Lamé problem*  ANSHUMAN PAL (Presenter), THOMAS WITTEN, University of Chicago — Azimuthal wrinkling in the annular (Lamé) geometry serves as an archetype for understanding geometry-influenced elastic response in thin sheets. In most experiments, the annulus is subjected to radial tension at both the inner and outer boundaries, generating compression and wrinkling in the azimuthal direction ([1]). In our work, we study an even simpler version of this problem, using theory and simulations, where the annulus is subjected to only a radial pull at the inner boundary. This creates azimuthal wrinkling with a simpler, one-dimensional phase space spanned by the dimensionless 'bendability' parameter, $\varepsilon^{-1}$. We focus on the large $\varepsilon^{-1}$ (small thickness and/or large load) limit — here, in contrast to previous experiments, the sheet becomes asymptotically isometric, and the wavenumber coarsens and hits a lower limit set by the geometry of the sheet and the boundary conditions. If we now loosen the boundary condition, the wrinkles transition to a single fold that consumes all the excess length. Although purely numerical, to the best of our knowledge, this is the first realisation of a wrinkle-to-fold transition ([2]) on an unsupported membrane.

References -
1. Davidovitch et al, PNAS 2011

*This work is partly supported by NSF-MRSEC DMR-1420709

9:36AM L30.00007: Geometry, mechanics, and dynamics of leaves, flowers, and sea slugs KENNETH YAMAMOTO (Presenter), SHANKAR VENKATARAMANI, Univ of Arizona — Why are there intricate, self-similar wrinkles along the edges of growing leaves, blooming flowers, torn plastic sheets, and frilly sea slugs? We argue that the mechanics and dynamics of these non-Euclidean elastic sheets are governed by interacting non-smooth geometric defects in the material. I will describe novel ideas stemming from characterizing and analyzing these defects using discrete differential geometry in order to uncover fundamental insights into the elastic behavior and properties of thin hyperbolic bodies. New theories based on the mechanics of non-smooth defects may (i) explain biological phenomena, from the morphogenesis of leaves, flowers, etc. to the biomechanics of sea slugs, as well as (ii) introduce new paradigms for materials design and actuation in a variety of new technologies, e.g., soft robotics.
9:48AM L30.00008: Mechanics and geometry of soft beams and shells
DANIELE BATTISTA (Presenter), MICHELE CURATOLO, PAOLA NARDINOCCHI, Univ of Rome La Sapienza — We investigate swelling-induced morphing in thin soft polymer based plates and shells. Starting from flat geometries, sphere-like and nearly developable shapes are realized and the ability to control a specific shaping, shifting from one shape to another, under anisotropic swelling is investigated. Starting from nearly developable shapes, the effects on the geometry of swelling and shrinking is also studied. The mathematical model accounts for both diffusion and nonlinear mechanics (stress-diffusion model). It is implemented in a finite element code and a campaign of numerical experiments is planned. Reduced analytical or semi-analytical approaches will be used to catch the experimental results above.

The Authors thank PRIN 2017 "Mathematics of active materials: From mechanobiology to smart devices", project n. 2017KL4EF3, for financial support.

10:00AM L30.00009: Capture of particles by a flexible granular envelope
KATHARINE BANCROFT (Presenter), THEODORE ANTHONY BRZINSKI, Haverford College — The capture of small particles by a flexible envelope can model many common phenomena. For example, in the rotating environment of a commercial dryer, large, flexible, non-convex objects like fitted sheets and duvet covers often capture smaller items like socks that fail to dry as a result. Amoeba exploit a similar process for prey capture by extruding pseudopodia in which smaller organisms become trapped. We have developed a quasi-2D granular system with qualitatively similar dynamics: a granular chain envelope composed of custom ball chain in a background dispersion of spherical grains inside a rotating drum. The particle-scale geometry of the granular chain determines the available conformations of the envelope, leading to a biased convexity. We share the results of our investigation of the kinetics of particle capture for this novel model system.

10:12AM L30.00010: Predicting the onset of disclination defects on curved open surfaces
SIDDHANSH AGARWAL (Presenter), SASCHA HILGENFELDT, University of Illinois at Urbana-Champaign — Ordered structures on surfaces with Gaussian curvature are topologically constrained to contain a finite defect charge, while the positioning of these defects is determined by optimization of the surface’s elastic energy. Open surfaces of sufficiently small curvature minimize energy without defects in the bulk, while stronger curvature favors the appearance of a disclination in the ground state; the presence of a boundary adds subtlety to the local screening of Gaussian curvature by defects. We find that, in contrast to previous heuristic arguments, the onset of transition is governed neither by local values of Gaussian curvature nor by its global integral. Starting from stringent energy minimization, we instead propose a weighted integral Gaussian curvature as an improved predictor for the transition - one that is universally valid for a large class of bounded rotationally symmetric surfaces. Our formalism also allows for analysis of the first or second order character of the transition, and how it is modified by boundary stresses and/or breaking symmetries of shape or material properties. These findings are of practical and fundamental importance in both engineering and biological cellular systems, such as the pattern of visual processing in invertebrate eyes.
10:24AM L30.00011: Facets and Folds: A model for fragmentation kinetics of crumpled thin sheets

JOVANA ANDREJEVIC (Presenter), LISA M LEE, SHMUEL RUBINSTEIN, CHRISTOPHER RYCRFT, Harvard University — As a confined thin sheet crumples, a unique arrangement of sharp ridges emerges, delineating approximately flat facets. Viewed collectively, this mosaic of ridges and facets exhibits striking statistical reproducibility - the total length traced out by ridges, for instance, has been shown to grow logarithmically with the number of crumpling and unfolding repetitions. Here, we explore the correspondence between crumpling and a general fragmentation process. We identify a physical model for the evolution of facet area distribution in crumpled sheets that captures a wide range of data samples with a single variable parameter. We then demonstrate the capacity of this model to reproduce experimental observations such as the characteristic logarithmic scaling of total ridge length, thereby supplying a missing physical basis for the observed phenomenon.

*We acknowledge support from the National Science Foundation under Grants No. DMR-1420570 and DGE-1745303.

10:36AM L30.00012: Stress Relaxation of Drying Colloids

ZHIYU JIANG (Presenter), CHONG SHEN, LANFANG LI, Physics, Lehigh University, MEGAN VALENTINE, Mechanical Engineering, University of California, Santa Barbara, YE XU, Mechanical Engineering, Beihang University, H DANIEL OU-YANG, Physics, Lehigh University — Stress relaxation during the drying of coatings is of interest due to its importance in the thin film-formation process that dictates the final properties of coatings. Using drying colloidal suspensions as a model system, this study examines how stresses in the colloidal matrix relax when particles are compacted during uniaxial drying in a microfluidics. Microscopic oil droplets co-suspended in the colloids are used as probes for local stresses and strains as these droplets are deformed by the changing matrix of particles. Balance of the interfacial stress of the oil in the colloids and the stress produced by the compacting colloids dictates the shape evolution of the droplets. The evolution of the deformations of multiple droplets is recorded by confocal fluorescence microscopy. Images of the time evolutions of the droplet shapes and the positions of fluorescent tracer particles nearby the droplets are analyzed by digital image correlation. The talk will address questions on the roles of the viscous damping, interfacial tension between the oil and colloidal matrix, the anisotropy of the strain and stress distributions and the mechanical properties of compacting colloidal particles before the coating is fully dried.
Physics Behind the Snapping of a Twisted Balloon

YU-CHUAN CHENG (Presenter), HUNG-CHIEH FAN CHIANG, HSIN-HUEI LI, WEI-CHIH LI, TZAY-MING HONG, Physics, National Tsing Hua University — It is childhood experience to twist balloons and turn them into dogs and flower. In this talk we investigate the process that leads up to the snap of a cylindrical balloon. For a twisted short balloon (1<\(L/D\)<7 where \(L\), \(D\) : length and diameter), its phase transits from (1) being sheared and wrinkle-free while torque (\(t\)) is linear to \(\theta\), (2) appearance of a neck without wrinkles, while radius and shear angle are found to obey \(r^3\!d\theta/dx=\text{const}\), (3) development of parallel wrinkles whose number \(\sim 12\) is insensitive to \(L\), \(D\), and thickness. \(\tau\) increases concavely with \(\theta\), to (4) wrinkles cross one another eventually and are followed by a sudden snap into two segments, as for a bended drinking straw. For a medium-size balloon (7<\(L/D\)<15), (a) similar to (1), (b) skip (2, 3) to become curled with a low-amplitude oscillation in \(\theta\), (c) similar to (4). When the balloon is long (15<\(L/D\)), (i) similar to (1) (ii) similar to (b), but develop a supercoil while accompanied by a suddenly drop in \(\tau\), (iii) repeat (i, ii). Heuristic models are proposed to understand the physics behind different phases. MD simulation is also performed to reveal energetics. Furthermore, to verify whether the above properties are unique to a quasi-1D object (balloons), a thread (real 1D) and ribbon (2D) are also studied.

*MoST

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L31 DSOFT: DSOFT Early Career Award and Directed Assembly
8:00AM L31.00001: Early Career Award for Soft Matter Research talk* [Invited] STEFANO SACANNA (Presenter), New York Univ NYU — Colloidal self-assembly today is increasingly focused on the development of particles that mimic atomic properties. Atoms serve as inspiration for what simple but ideal building blocks are capable of, and through the mastery of relatively few design principles, such as directionality, valence, and well-defined bonds, many target architectures become rationally accessible. A colloidal diamond lattice, for example, theoretically operates as an exotic semiconductor for light, and is just now becoming available through molecular mimetic routes. Myriad syntheses have been developed to accomplish this by targeting specific geometries and surface patterns, which serve to direct assembly. In this talk, I will break down and categorize the wide selection of colloidal reactions available by using an analogy to synthetic chemistry, helping to index and navigate the ever-expanding colloidal toolbox. Beginning with elementary colloidal particles, I will define the set of directions synthetic routes can take, firstly, through inter-particle reactions, which combine disparate particles into new well-defined units and secondly through intra-particle reactions, which occur through a particle’s internal transformation. I will also discuss the most prominent colloidal interactions available for assembly, and which are most useful for a given synthetic route. Today, long-sought-after target structures are just coming to fruition, so it is an ideal time in the colloidal community to examine the most efficient ways to generate particles and how to make them assemble. Drawing from many fields including colloid and surface chemistry, supramolecular chemistry, biochemistry, and photonics, molecular mimetic colloids represent a point of interest for any materials scientist.

*This work was supported by the NSF CAREER award DMR-1653465

8:36AM L31.00002: Colloidal Diamond Crystals MINGXIN HE (Presenter), Department of Chemical and Biomolecular Engineering, New York University, JOHNATHON GALES, ETIENNE DUCROT, Department of Physics, New York University, ZHE GONG, Department of Chemistry, New York University, GI-RA YI, School of Chemical Engineering, Sungkyunkwan University, STEFANO SACANNA, Department of Chemistry, New York University, DAVID J PINE, Department of Chemical and Biomolecular Engineering, New York University — Self-assembling colloidal diamond has been a longstanding goal because of the structure’s potential for photonic applications. Because particles in a diamond lattice are tetrahedrally coordinated, one approach has been to self-assemble spherical particles with tetrahedral sticky patches. Difficulties persist, however, because the patchy particles possess no mechanism to select the proper staggered orientation of tetrahedral bonds on nearest-neighbor particles, a necessary requirement for cubic diamond. Here, we show that by using partially compressed clusters with retracted sticky patches, colloidal cubic diamond can be self-assembled using patch-patch adhesion together with a steric interlock mechanism that selects the proper staggered bond orientation. Colloidal particles in the self-assembled diamond structure are highly constrained and mechanically stable, which makes it possible to dry the suspension and retain the diamond structure. The inverse lattice exhibits promising photonic properties, including a complete photonic bandgap.
8:48AM L31.00003: Colloidal Diamond Photonic Bands  JOHNATHON GALES (Presenter), MINGXIN HE, DAVID J PINE, New York Univ NYU — We have designed a new set of patchy tetrahedral colloidal clusters that can self-assemble into a diamond lattice. Like the conventional colloidal diamond of spheres, we find that the diamond lattice of clusters we have assembled exhibits a strong photonic band gap for appropriate parameters. Inverting the lattice leads to a particularly strong band gap after optimizing a few geometric parameters. We also provide a method for achieving the inverse lattice.

9:00AM L31.00004: Photonic band gaps in self-assembled colloidal structures  DUANDUAN WAN (Presenter), Wuhan Univ, SHARON C GLOTZER, University of Michigan — An intriguing feature of colloids is their ability of self-assembly, i.e., colloidal particles arrange themselves into an ordered structure. Using computer simulations, we explore the effect of thermal disorder on the photonic band gap in a self-assembled photonic crystal. We find that photonic band gaps can exist over a large range of intermediate packing fractions and that the widest gap does not necessarily appear at the densest packing fraction. Further, we show that with judicious choices of particle shape, packing fraction, and particle internal structure, self-assembly can be a promising method to make photonic crystals with large band gaps despite the presence of disorder.

9:12AM L31.00005: Rational Design of Patchy Colloids Capable of Self-Assembling into Open Crystal Lattices with Complete Photonic Bandgaps*  YUTAO MA (Presenter), ANDREW L FERGUSON, University of Chicago — Patchy colloids equipped with anisotropic interactions are promising building blocks whose self-assembly provides a powerful tool for forming many complex functional materials. A main challenge in the self-assembly of patchy colloids is the design of colloidal geometry and chemistry that favor the formation of target structure thermodynamically and kinetically. We have previously developed a rational design protocol, called landscape engineering, in which we recover the free energy surface governing colloidal self-assembly process by combining molecular simulation with nonlinear dimensionality reduction technique and sculpt the free energy surface by modifying the colloidal design using genetic algorithm to make target structure thermodynamically favorable. We have applied this protocol to successfully design patchy colloids capable of self-assembling into pyrochlore lattice and cubic diamond lattice consisting of tetrahedral clusters via two-stage temperature control. Both structures are defect-free and possess complete photonic bandgaps. Our method may be extended to the rational design of self-assembling colloidal molecules and other systems such as peptides.

*NSF Grant No.DMR-1841800
9:24AM L31.00006: Nanoparticle Superlattices with Polymer Ligands*  ALEX TRAVESSET  
(Presenter), Physics and Astronomy, Iowa State University and Ames Lab, NATHAN R HORST, Ames Lab, JIANSHE XIA, HONGXIA GUO, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China — We provide a study of the assembly of single component nanocrystals (nanoparticles) NCs capped with polystyrene by solvent evaporation. We investigate regimes from the colloidal $R_G/R_C<<1$ with $R_C$ (core radius) and $R_G$ (ligand gyration radius) to the polymer limit $R_G/R_C>>1$. We show that for increasing chain length, there is the emergence of a ```cascade effect```, i.e. an abrupt drop in internal energy with the resulting potential of mean force dominated by configurations wherein the chains bend over the core in order to maximize contacts with the other NC, which accounts for the large magnitude of the many body effects in the superlattice free energy. Interestingly, the Orbifold Topolgical Model (OTM) that successfully characterizes the nanocrystal interaction in the colloidal limit, quantitatively describes the polymer limit as well. Our results establish that bcc is the equilibrium phase. Implications for recent and future experiments are discussed.

*NSF, DMR-CMMT 1606336  
XSEDE grant TG-MCB140071.  
NSF of China (21574142, 21790343)

9:36AM L31.00007: Binary colloidal compounds with depletants*  ALI EHLEN (Presenter), HECTOR MANUEL LOPEZ RIOS, MONICA OLVERA DE LA CRUZ, Northwestern University — We study the effects of depletants on binary size-asymmetric colloidal crystals. Specifically, we discuss the mechanism that leads to two types of systems: 1) stable compound crystals of large repulsive particles with smaller particles; and 2) crystals of large repulsive particles stabilized by a mobile sublattice of small particles. This talk will address the impact of the presence of depletants in both the compounds and in the sublattice-melted crystals, as well as the relative significance of the attractive interaction between the particles and the depletion forces.

*We acknowledge the support of the Sherman Fairchild Foundation for this work.
9:48AM L31.00008: Phase Diagram and Structure Map of Binary Nanoparticle Superlattices from a Lennard-Jones Model*  SHANG REN (Presenter), Department of Physics and Astronomy, Rutgers University, YANG SUN, FENG ZHANG, Ames Laboratory, ALEX TRAVESSET, CAI-ZHUANG WANG, KAI-MING HO, Department of Physics and Astronomy, Iowa State University — In this work, we show that a binary system interacting through Lennard-Jones (LJ) potential predicts all phases reported in experiments in which nanoparticles are effectively described as quasi hard spheres. Furthermore, we show that binary lattices may be described as combinations of a small number of particle clusters, motifs, which generalize the four Z-N that describe Frank Kasper phases. We report a phase diagram consisting of 53 equilibrium phases, whose stability is quite insensitive to the microscopic details of the potentials, thus giving raise to some universality. Our results show that meta-stable phases share the same motifs as equilibrium phases. Connections with packing models, phase diagrams with repulsive potentials and the prediction of new superlattices in experiments are thoroughly discussed.

*Work at Ames Laboratory was supported by the US Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division, under Contract No. DE-AC02-07CH11358, including a grant of computer time at the National Energy Research Supercomputing Center (NERSC) in Berkeley, CA. The Laboratory Directed Research and Development (LDRD) program of Ames Laboratory supported the use of GPU-accelerated computing.

10:00AM L31.00009: Novel mesophase behavior in two-dimensional binary solid solutions*  PRAJWAL BANGALORE PRAKASH (Presenter), FERNANDO A ESCOBEDO, Cornell University — Towards the goal of designing new complex materials, Monte Carlo simulations were used to study the entropic-driven assembly of binary mixtures of hard polygons and disks. Two distinct types of mixtures were studied, such that individual components either form distinct crystal lattices, like squares and disks, or similar crystal lattices, like hexagons and disks. Our focus was the 2D phase behavior of mixtures where the components have size ratios that optimize their co-assembly into solid solutions, and over the full range of compositions and concentrations to further detect any partially ordered phases (mesophases). Besides the enhanced regions with solid miscibility, a novel mosaic/polycrystalline phase was found for the disk+square mixtures and a rotator-plastic solid phase for the disk+hexagon mixtures. The mosaic phase has interspersed clusters of locally ordered 4-fold squares and 6-fold disks, distributed throughout the domain with random orientations. The plastic-solid rotator mesophase of hexagons and disks exhibits long-range translational and short-range orientational order. Changes in phase behavior for different component size ratios were also investigated to assess the importance of the optimal size ratio in promoting mesophase behavior.

*NSF award CBET-1907369
10:12AM L31.00010: Diffusion of DNA-coated colloids on DNA coated surface* JEANA(AOJIE) ZHENG (Presenter), New York Univ NYU, SOPHIE MARBACH, MIRANDA HOLMES-CERFON, Courant Institute of Mathematical Sciences, New York University, DAVID J PINE, New York Univ NYU — DNA-coated colloids can self-assemble and crystalize into a wide variety of structures. In order for DNA-coated colloids to anneal and form crystals, they must roll and diffuse while attached to each other. Here we report on the diffusion of DNA-coated colloidal spheres on a flat DNA-coated substrate. Near the DNA-melting temperature, the mean square displacement is linear in time as expected for normal diffusion, but the diffusion coefficient is much smaller than for free diffusion. As the temperature is lowered, the motion becomes sub-diffusive, which suggests the presence of random free energy barriers in the DNA-mediated interactions. We have found that DNA induced interactions are highly sensitive to the density and homogeneity of the DNA distribution. As we reduce the DNA density, the DNA coated colloids diffuse slower. Here we also report the modeling of melting curve for particle - substrate binding, allowing to understand and predict how binding properties depend on parameters of the DNA-coated colloids (salt concentrations, DNA sequence, etc.) This study is important for designing and optimizing self-assembly structure of DNA coated colloids.

*MRSEC Program of the National Science Foundation under Award Number DMR-1420073

10:24AM L31.00011: 3D self-replication of DNA nanostructures* FENG ZHOU (Presenter), HENG NI, RUOJIE SHA, NADRIAN C SEEMAN, PAUL M CHAIKIN, New York Univ NYU — Self-replication is a natural process that can generate materials and pass along information. We have seen several examples of artificial self-replication in which the template assembles, organizes and directs formation of the target nanostructure. However, the self-assembly procedure increases the template's dimensionality, which makes it challenging to template and replicate a 3D object. Here, we report the direct self-replication of a 3D object. First, we fabricate a three face cube corner as our template. The replication proceeds by self-assembling three daughter origami tiles to three edges of the cube corner. DNA single strands on each cube face and daughter tile hybridize to fold the tiles inward and complete the cubic box. The daughter tiles are then cross-linked into a new cube corner. Heating releases the two complementary cube corners. This method provides a general approach for conducting high-order self-replication by organizing the materials via folding. Considering that the 3D DNA nanostructure is a functional platform, this type of 3D self-replication can produce new materials, such as chiral plasmonic nanomaterials, by passing the steric information through successive generations.

*This research has been primarily supported by DOE DE-SC0007991 and DE-SC0000989.
10:36AM L31.00012: Self-assembled helical structures of ABCD star tetrablock copolymer within cylindrical confinement  PARESH CHOKSHI (Presenter), SUPRIYA GUPTA, Department of Chemical Engineering, Indian Institute of Technology Delhi — Physical confinement of block copolymers plays an important role in generating a rich variety of novel ordered phases not seen in bulk systems. These novel ordered microstructures, arising mainly out of structural frustration and confinement-induced entropy loss, provide ideal templates to self-assemble nanoparticles. In order to generate novel multicomponent helical structures, we investigate the four-armed ABCD star tetrablock copolymers for their equilibrium states under cylindrical nanopore confinement with the help of self-consistent field theory. The ABCD star tetrablock copolymer exhibits rich self-assembly behaviour with myriads of three-dimensional ordered phases ranging from one-component, two-components and three-components helices to honeycomb-like structures depending upon the individual block fractions and the size of cylindrical nanopore. Such chiral structural motifs generated from achiral polymeric molecules are fascinating due to superior performance in sophisticated optical functions. The comprehensive understanding of the self-assembly behaviour enables one to design novel nanostructured materials with desired material properties.

10:48AM L31.00013: Toward generating colloidal cubic phases: Shape sensitivity of the Ia(-3)d gyroid phase in hard pear-shaped particle systems  PHILIPP SCHÖNHÖFER (Presenter), University of Michigan, GERD SCHROEDER-TURK, Murdoch University — The ambition to mimic highly complex and functional nanostructures found in living organisms marks one of the pillars of today's research in bio- and soft matter physics. Here, self-assembly has evolved into a prominent strategy in nanostructure formation. However, it is still a challenge to design and realise particle properties such that they self-organise into the desired target configuration. One key design parameter is the (effective) shape of the constituent particles.

We address the entropically driven colloidal self-assembly of tapered ellipsoids, reminiscent of "pear-shaped" particles, including the formation of structures based on triply periodic minimal surfaces (TPMS) such as the gyroid. Using computational simulations, we investigate the influence of variations in shape on the stability of the gyroid phase. We show that the formation of the gyroid reported earlier in the so-called pear hard Gaussian overlap (PHGO) approximation, is due to small non-additive properties of that potential. This phase does not form in pears with a "true" hard pear-shaped potential. In particular, the slight differences in shape favour the formation of interdigitated bilayers in the PHGO particle ensemble, which indicates a two-step hierarchical mechanism to generate TPMS phases.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM

Session L32 DPOLY DSOFT DCP: Dynamics of Glassy Polymers Under Nanoscale Confinement II  504 - Biao Zuo, Zhejiang Sci-Tech University - Tag(s): Focus
8:00AM L32.00001: Measuring dynamic mechanical properties of thin polymer films [Invited]
YUNLONG GUO (Presenter), PEI BAI, Shanghai Jiao Tong Univ — Polymer dynamics under confinement on nanoscale exhibits substantial deviation from the bulk and has received a great deal of research interests in the past two decades. To date, some representative physical properties of confined polymers such as glass transition temperature and structural relaxation, have been studied extensively. Despite milestone progress in measuring Young's modulus, creep, and stress-strain curves of thin polymers, mechanical properties of confined polymers are still far from well understood, and remain to be elucidated in many other aspects. Here we demonstrate an experimental apparatus for direct measurement of dynamic mechanical response of thin polymer films. We utilize a sinusoidal pressure wave on a polymer film to induce vibration, and the response of the material is record by a high-speed digital camera. By analyzing the data on stress, strain, and the phase difference in between, we obtained dynamic mechanical properties of polymer films with various thickness.

8:36AM L32.00002: An explanation of how nanoconfinement affects the control of local dynamic relaxation*  
JANE E LIPSON (Presenter), RONALD WHITE, Dartmouth Coll — The dynamics of local segmental relaxation in glass forming systems is linked to fundamental material properties and control variables that reflect the influence of thermodynamics on the relaxation time, tau. In the Cooperative Free Volume (CFV) model the key variables are temperature (T) and free volume (V_{free}), which is related to density. The general CFV result is that \( \log \tau \sim (1/V_{\text{free}}) \times f(T) \). We find that our result for \( f(T) \) works equally well for the bulk under highly varying pressure conditions, and for all types of confinement. The presence of \( V_{\text{free}} \) in the CFV expression for \( \log \tau \) results in a sensitivity to density changes that becomes strong at low T, and also reflective of the presence of interfaces, whether in film or nanocomposite. In this talk these CFV features will be illustrated through extensive connection with experimental data on a variety of systems.

*NSF DMR-1708542
8:48AM L32.00003: Is there a general compensation rule governing the relaxation dynamics of polymeric surface patterns?  SONAL BHADAURIYA, Department of Polymer Engineering, University of Akron, CHRISTOPHER M STAFFORD, JACK DOUGLAS, Materials Science and Engineering Division, National Institute of Standards and Technology, ALAMGIR KARIM (Presenter), Department of Chemical and Biomolecular Engineering, University of Houston — Understanding the mechanism and decay kinetics of patterned polymeric surfaces is a pertinent issue in nanotechnology. Herein, we present the relaxation behaviour of nanoparticle-brush filled imprinted and wrinkled polymer films showing similar compensation effect. Entropy-enthalpy compensation (EEC) effect signifies a linear correlation between the activation parameters of a relaxation process and is routinely observed in the relaxation dynamics of many condensed materials such as molecular additives and glass-forming materials. For the first time, we experimentally observed a full mapped out transition of pattern decay kinetics as a function of temperature (below and above the glass transition of the matrix) and additive concentration by utilizing decay of polymeric surface wrinkles. We observe EEC effect for an athermal and a favorable interacting composite system, thereby ensuring the robustness of the observed phenomenon. As a consequence of this compensation effect, relaxation kinetics for composite wrinkled films is faster than the neat polymer film below the characteristic compensation temperature, $T_{comp}$ and faster above the $T_{comp}$. EEC proves itself to be the underlying mechanism for patterned polymer decay, governing the kinetics of any polymeric surface with patterns.

9:00AM L32.00004: A simulation study on nonlinear mechanical responses of glassy polymer nanofibers*  TAEJIN KWON (Presenter), BONG JUNE SUNG, Sogang Univ — The confined polymer glasses, such as glassy polymer fibers, exhibit unique glassy behaviors that differ from bulk polymer glasses. We perform molecular dynamics simulations and study nonlinear mechanical responses of glassy polymer nanofibers under uniaxial deformation. We investigate not only nonlinear mechanical responses but also the dependence of mechanical properties on the strain rates of typical polymer glasses, which were also observed in previous experiments. We find from our simulations that the local stress in the surface regions of fibers is greater than that in the core region of fibers, for which the stress of glassy polymer fibers is greater than that of bulk polymer glasses in our simulations. The distance between monomers in glassy polymer fibers are more stretched than that in bulk polymer glasses. Also, the non-affine displacements in the surface regions of glassy polymer fibers are greater than those in bulk polymer glasses. These results indicate that the microscopic events during deformation relate closely to the mechanical responses of polymer glasses.

*This work was supported by the Samsung Science and Technology Foundation under Project Number SSTF-BA1502-07.
9:12AM L32.00005: Gradient overlap effects in the thin films

ASIEH GHANEKARADE (Presenter), DAVID SIMMONS, Univ of South Florida — The dynamics of polymer and other glass-forming liquids can exhibit massive gradients in the nanoscale vicinity of interfaces – an effect that is not locally correlated with microscopic changes in structure. A major outstanding question is how these gradients behave in extremely thin films, where gradients emanating from distinct interfaces can interact. Here we report on the results of ultra-thin film simulations probing dynamics and glass formation locally and globally in this gradient-overlap regime. Results point to three general regimes of thin film behavior: one when the film thickness is greater than twice the gradient range; one in which the gradients overlap but do not individually span the film; and an ultra-thin-film limit in which each gradient span fully to the other interface. We report on distinct behaviors in these regimes in terms of the form of the gradients, the presence or absence of a bulk-like domain, and the breadth of the overall film glass transition. These findings have implications for the interpretation of dynamical data in ultra-thin films and for the underlying origin of alterations in dynamics in the nanoscale vicinity of interfaces.

*This material is based upon work supported by the National Science Foundation under Grant No. CBET1705738.

9:24AM L32.00006: Dynamical gradients, barrier factorization and interface coupling in thick and thin films of glass-forming liquids

KENNETH SCHWEIZER (Presenter), University of Illinois at Urbana-Champaign, ANH D. PHAN, Phenikaa University, Hanoi, Vietnam — We have developed a microscopic theory for the spatially heterogeneous dynamics of glassy polymer liquids near a vapor interface. The key activated event involves cage scale hopping facilitated by a collective elastic distortion of the surrounding medium. Three coupled physical effects enter for thick films: reduction of neighbors and weakened caging constraints nucleated very near the surface, dynamical transfer of weakened constraints in a layer-by-layer manner into the bulk, and modification of the collective elastic barrier both near and far from the interface. Predictions include an exponential spatial variation of caging constraints and the local glass transition temperature, the near factorization of the temperature and spatial location dependences of the total activation barrier, a double exponential form of the alpha time gradient characterized by a nearly constant correlation length, and position-dependent power law decoupling of the relaxation time from its bulk analog. Generalization of the ideas to thin films predicts nonadditive dynamical gradient interference effects resulting in a further enhancement of relaxation and reduction of the film averaged effective barrier with decreasing film thickness. Comparisons to simulation and experiment will be presented.
The surface glass transition temperature \(T_{g_{\text{surf}}}\) of polystyrene (PS) films supported by silica was studied for film thickness, \(h\), from 7 nm to 100 nm by time-of-flight secondary ion mass spectrometry (ToF-SIMS). The width of the surface glass transition, \(\Delta T_{g_{\text{surf}}}=(T_{g_{\text{surf}+}}-T_{g_{\text{surf}-}})\) and \(T_{g_{\text{surf}}}=(T_{g_{\text{surf}+}}+T_{g_{\text{surf}-}})/2\) were extracted from the end group intensity as a function of temperature. We found that \(T_{g_{\text{surf}}}\) decreases with decreases \(h\) and is \(~20\) K lower than the glass transition temperature \((T_g)\) of the film for any given \(h\). We attribute this observation to effects of the free surface. On the other hand, \(\Delta T_{g_{\text{surf}}}\) increases with decreasing \(h\) starting from large \(h\ (>\sim60\text{nm})\). We explore possible origins for the noted broadening in surface glass transition of thin films.

*We acknowledge supports of the Research Grant Council of Hong Kong through the Projects 16303418 and 16302917.

Despite more than two decades of study, there remain many fundamental unanswered questions about the dynamics of glass-forming materials confined to thin films. In particularly, several experiments show evidence of a qualitative change in behavior upon confinement to sufficiently thin films. For example, the viscosity of amorphous thin films has been shown to exhibit a sharp transition from glassy to liquid-like behavior when film thickness is reduced below 30 nm [Y. Zhang et al., J. Chem. Phys. 145, 114502 (2016)]. Here, we provide evidence that this transition is due to the films inability to support an inactive, low-mobility, dynamic phase near a free surface. Active to inactive dynamical phase transitions have been found for a number of bulk glassy systems by biasing trajectories to low-mobility states using a field \(s\). For a model polymer system, we find that thin films require a dramatically larger field strength than the bulk to reach the inactive phase suggesting that it may be inaccessible for thin enough films. This sheds light on why the dynamics on the surface of amorphous materials is so different from bulk behavior.

*Funded by NSF grants MRSEC/DMR-1720530.
10:00AM L32.00009: Modeling the Glass Transition in Polymers using a Mean-Field “TS2” Model: Bulk and Thin Films* VALERIY GINZBURG (Presenter), Dow Chemical Co — A phenomenological model is proposed to describe the equilibrium dynamic behavior of amorphous, glass-forming polymers. We postulate that a material can be represented by a lattice of cooperatively re-arranging regions (CRR), with each CRR having two states, the low-temperature “Solid” and the high-temperature “Liquid”. At low temperatures, the material exhibits two characteristic relaxation times, corresponding to the slow large-scale motion involving multiple “solid” CRRs (α-relaxation) and the faster local motion within individual CRRs (β-relaxation). At high temperatures, the α- and β-relaxation times merge, as observed experimentally and suggested by the “Coupling Model” framework. This approach is labeled “Two-state, two (time)scale model” or TS2. We show that the TS2 treatment can successfully describe the low-temperature Arrhenius a-relaxation time behavior described in several recent experiments. We also apply TS2 to describe the molecular-weight dependence of the glass transition temperature in bulk polymers, as well as its dependence on film thickness in thin films.

*This work was supported by Dow.

10:12AM L32.00010: Tuning the Effective Viscosity of Random Copolymer films of Styrene and 4-Methoxystyrene by Varying the Copolymer Composition* JIANQUAN XU (Presenter), Hong Kong University of Science and Technology, CHAO LV, BINYANG DU, Zhejiang University, OPHELIA TSUI, Hong Kong University of Science and Technology — We show that thickness dependence of effective viscosity, $\eta_{\text{eff}}(h_0)$, of random copolymer films of styrene (St) and 4-methoxystyrene (MeOS) supported by silica (SiOx) can be easily tuned by using different MeOS concentrations, $X_{\text{MeOS}}$. When $X_{\text{MeOS}}$ is increased from 0% to 100%, $\eta_{\text{eff}}$ of nanometer films changes steadily from suppressed to enhanced. At $X_{\text{MeOS}} = 10\%$, $\eta_{\text{eff}}(h_0)$ displays a non-monotonic variation. We explain our results by suggesting that MeOS interacts more strongly with SiOx than St does and the behavior of $\eta_{\text{eff}}(h_0)$ is due to competitions between substrate effect and free surface effect. If substrate effect is stronger, $\eta_{\text{eff}}$ of nanometer films is enhanced. If free surface effect is stronger, $\eta_{\text{eff}}$ reduction occurs. When the two effects are comparable, our $X_{\text{MeOS}} = 10\%$ data suggests that substrate effect dominates in nanometer films but free surface effect dominates in thicker films, resulting in a non-monotonic $\eta_{\text{eff}}(h_0)$ dependence.

*We acknowledge supports of the Research Grant Council of Hong Kong through the Projects 16302917 and 16303418. B.D. acknowledges support of the National Science Foundation of China through the Projects 21674097 and 21875214.
10:24AM L32.00011: The Glass Transition Behavior and Structural Recovery of 2D Stacked Polystyrene Nanorods  MADHUSUDHAN REDDY PALLAKA, SINDEE L SIMON (Presenter), Texas Tech Univ —

The behavior of glass-forming materials confined at the nanoscale has been of considerable interest over the past two decades with conflicting results sparking debate. Here the focus is on the glass transition and associated structural relaxation kinetics of 20 and 350 nm stacked polystyrene nanorods using the Mettler Toledo Flash differential scanning calorimeter (DSC). The $T_g$ of 20 nm stacked polystyrene nanorods is depressed by 20 K and 10 K at cooling rates of 0.1 and 1000 K/s, respectively, whereas bulk-like behavior is observed for 350 nm stacked polystyrene nanorods. Structural recovery is also performed on 20 and 350 nm stacked polystyrene rods as a function of aging time and temperature, and the evolution of the enthalpy is followed. The structural recovery rate is found to be enhanced in the case of 20 nm stacked polystyrene rods when compared to the 350 nm stacked rods. The effect of spatial dimensionality on $T_g$ and structural recovery is also evaluated; in addition, a relaxation time map is constructed to better understand the glass transition and structural recovery kinetics. The results will also be discussed in the context of current controversies in the field.

10:36AM L32.00012: The Importance of Density in Segmental Dynamics: Applications of the Cooperative Free Volume Rate Model and Connections with the Density Scaling Approach*
RONALD WHITE (Presenter), JANE E LIPSON, Dartmouth College — A focus in our work is to make predictive connections with real experimental systems. For example, while segmental relaxation data is sometimes collected only at atmospheric pressure, deeper insight is only possible by accounting for pressure-dependent dynamics. This enables the analysis of the contributions due to independent changes in temperature ($T$) and volume ($V$), which gives a much deeper representation of the experimental system. It also leads to natural connections with that system’s dynamics under confinement. In this talk we discuss our recent work in modeling and predicting alpha relaxation times, $\tau(T,V)$, using the cooperative free volume rate model (CFV), in which the system's (well-defined and thermodynamically quantified) free volume controls the molecular cooperativity, and thus the activation energy. In addition to presenting our analysis of experimental systems, we will also feature connections and comparisons with the widely applied density scaling approach. We will show how the key parameters of the two approaches are connected and contrast their predictive power. A strength of the CFV model is its more efficient use of the same thermodynamic information to characterize the form of the corresponding dynamics.

*This work is supported by NSF, DMR-1708542.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L33 DPOLY DSOFT: Hierarchical Structural Emergence in Elastomer Nanocomposites: Dispersion, Dynamics, Structure, Modeling, and Simulation I  505 - Anne-Caroline Genix, Université de Montpellier - Tag(s): Focus
8:00AM L33.00001: Rheological and Electrical Percolation Behavior of Carbon Black Suspended in Propylene Carbonate  JEFFREY RICHARDS (Presenter), Northwestern University, JULIE HIPP, NORMAN J. WAGNER, Chemical and Biological Engineering, University of Delaware — In this work, the microstructural origin of the rheo-electric behavior of carbon black gels and suspensions is studied. These materials find widespread use as conductive fillers in composites and slurry-based electrochemical energy storage technologies. In these applications, both the viscosity and electrical conductivity are key design parameters. We use microstructural, rheological and electrical measurements to understand the origin of percolation in these suspensions and rationalize the results using a fluid-cluster-gel transition. The results of these studies explain many emerging observations of the macroscopic behavior of filled carbon black suspensions and guide the way toward improving their rheological and electrical performance.

8:12AM L33.00002: Dielectric & Dynamic response of emergent hierarchical filler networks in polymer nanocomposites*  KABIR RISHI (Presenter), Univ of Cincinnati, ASHISH GOGIA, University of Dayton, GREG BEAUCAGE, Univ of Cincinnati, VIKRAM KUPPA, University of Dayton, ANH TANG, Univ of Cincinnati — Commercial nanocomposites such as tire compounds are composed of dispersions of carbon black/silica mass fractal aggregates in an elastomer/oil blend, the performance of which is related to the nano-aggregate network structure, the interfacial chemical affinity and extent of dispersion based on accumulated strain. These composites display a complex hierarchical structure intimately tied to their inherent incompatibility and processing history. On the nanoscale carbon black displays primary particles aggregated into mass fractal aggregates that percolate locally above about 5wt.% into a network cluster. In the linear viscoelastic regime, this network dictates the high-frequency response.\textsuperscript{1} At higher concentrations near 20wt.% the local aggregated clusters agglomerate into a micron-scale mass fractal network associated with electrical conductivity that influence the gel-like dynamic response at low frequencies.\textsuperscript{2} The impact of the inherent particle structure, the attributes of the nano-scale and meso-scale networks on the dynamic and electrical moduli of these systems was explored using different industrial grade carbon blacks.

\textsuperscript{1}K. Rishi et al., Macromolecules 51, 7893 (2018)
\textsuperscript{2}H. H. Winter et al., Colloid Polym. Sci. 266, 494 (1988)

*NSF CMMI- 1635865, 1636036; DOE APS DE-AC02-06CH11357
8:24AM L33.00003: Rheology and Shear-Induced Structural Evolution in Model Conductive Carbon Black Suspensions  JULIE HIPP (Presenter), Chemical and Biomolecular Engineering, University of Delaware, JEFFREY RICHARDS, Chemical & Biological Engineering, Northwestern University, NORMAN J. WAGNER, Chemical and Biomolecular Engineering, University of Delaware — Carbon black is commonly used in many technological applications ranging from tire rubbers and inks to electrochemical energy storage devices. In these applications, shear plays an important role in determining end performance due to the shear-induced structural changes and resulting change in properties that occur during mixing, processing, and application steps. To understand this shear-dependent behavior, the microstructure of carbon black suspensions is directly measured by performing Rheo-USANS (Ultra-Small Angle Neutron Scattering) experiments at a range of applied shear rates for suspensions with varying interaction strength, particle loading, and building block characteristics. These experiments show that a dramatic structural transformation from large, dense agglomerates to small, open agglomerates is predictable using the inverse Bingham number, which compares the measured stress to the yield stress of the suspension. Additionally, at high shear rates, the self-similar breakdown of agglomerates is shown to be dependent on the Mason number, which compares shear forces to interparticle attractions. This structural evolution explains many behaviors that are not well understood such as apparent shear-thickening and tunability of yield stress and elasticity.

8:36AM L33.00004: Polyisoprene silica nanocomposites and its structure property relationship*  DEBOLEENA DHARA (Presenter), ANDREW JIMENEZ, Columbia Univ, ZAID M ABBAS, Department of Chemistry and Biochemistry, University of South Carolina, MORTON M DENN, The City College of New York, BRIAN C BENICEWICZ, Department of Chemistry and Biochemistry, University of South Carolina, SANAT KUMAR, Columbia Univ — Recently, tire companies have sought to improve their fuel economy to meet the demand for a higher fuel efficiency and environmental sustainability. To achieve this goal, tire technologies have looked to improving the tire rolling resistance. In this talk, we investigate the structure-property relationship of polymer grafted nanoparticles, where the grafted polymer provides a better control over the dispersion of the particles in a polymer matrix. The dispersion and resulting morphologies of various systems were studied and followed by rheology and dynamic mechanical testing to probe the impact of the various structures on the mechanical properties, in the melt and the crosslinked forms. Using small amplitude oscillatory shear, we found that increasing nanoparticle loading significantly contributed to mechanical reinforcement. Reduction in tan delta that accompanies this reinforcement indicates an improvement in rolling resistance. In addition, creep measurements help us to expand the frequency window of our study, allowing access to the lower frequencies that are relevant to the operating frequencies of a tire.

*National Science Foundation-1709061
8:48AM L33.00005: Microscopic Origins of Dynamic Mechanical Properties of Filled Rubber Investigated with X-ray Photon Correlation Spectroscopy*  
DILLON PRESTO (Presenter), Polymer Science, University of Akron, SURESH NARAYANAN, Advanced Photon Source, Argonne National Laboratory, BRYCE MEYER, Mathematics, University of Akron, JOHN MEYERHOFER, Polymer Science, University of Akron, SERGIO MOCTEZUMA, Dynasol Elastómeros, MARK SUTTON, Physics, McGill University, MARK FOSTER, Polymer Science, University of Akron — The mechanical properties of nanoparticle filled rubber are largely determined by the structure of the filler network and filler/polymer interactions. These reinforced rubbers have broad commercial utility, such as use in tire tread technology. The dynamic mechanical properties of these systems have a major impact on tire safety and fuel economy. Despite their importance, the connections between microscale filler behavior and macroscale performance are not well understood. Recent developments in X-ray photon correlation spectroscopy (XPCS) allow us to probe the microscale dynamics of filler particle networks and determine how this influences macroscale properties. We have used in-situ XPCS on styrene-butadiene rubber (SBR) filled with silicas of different surface chemistries under dynamic strain to probe the rearrangement of the filler network. We draw connections between the filler/polymer interaction and the resulting network structure, filler dynamics, and macroscopic properties.

*We thank Dynasol Group for funding and sample preparation. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

9:00AM L33.00006: Probing dynamics and crosslink morphology of thermosets during cure via XPCS*  
EDWARD TRIGG (Presenter), HILMAR KOERNER, Air Force Research Lab - WPAFB — Epoxy-based systems have been widely used for decades, from aircraft parts to consumer goods. However, there are still gaps in the fundamental understanding of their crosslinking (curing) behavior, specifically heterogeneities in crosslink topology depending on cure cycle rates. Optimization of cure cycles is key to agile polymer matrix processing in industry and government. Here, we use X-ray photon correlation spectroscopy (XPCS) to study the crosslinking of epoxies in real time, with dilute nanoparticles as tracers to study the effect of the progressing crosslink topology as it confines the dynamics of the tracer. A series of six epoxy systems are presented, wherein the ratio of two curing agents is systematically varied. The fully cured systems range from linear polymers to densely crosslinked resins, enabling a deeper understanding of their cure mechanisms and crosslink topologies. XPCS shows diffusive motion at low degrees of cure, and a sharp transition to ballistic motion at higher cure, which depends on composition. DSC, in situ near-FTIR, and MC simulations complement the XPCS data. XPCS can be used as a tool to interpret crosslinking mechanisms without dynamically perturbing the system as is done in rheology.

*NRC Fellowship (NAS)  
AFOSR  
CHX Beamline, NSLS-II (DOE)
9:12AM L33.00007: Influence of Graft Density on Dynamically Coupled Polymer Grafted Nanocomposites* ANDREW EHLERS (Presenter), Materials Science and Engineering, Rensselaer Polytechnic Institute, PINAR AKCORA, Chemical Engineering and Materials Science, Stevens Institute of Technology, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — The viscoelastic behavior of polymer grafted nanocomposites (PGNs) with significantly different glass transition temperatures ($T_g$s) between the graft and matrix polymers is investigated with molecular dynamics simulations. These types of PGNs have been shown to have reversible and repeatable stiffening behavior upon heating (Senses, E.; Isherwood, A.; Akcora, P. ACS Appl. Mater. Interfaces 2015, 7, 14682). This unique thermal stiffening behavior was attributed to the dynamic coupling of the high-$T_g$ adsorbed chains and the low-$T_g$ matrix chains. The PGN studied in the current work consists of a nanoparticle with grafted high-$T_g$ polymer chains in a low $T_g$ polymer matrix. The effect of the dynamic coupling of the grafted and matrix polymer chains is studied by molecular dynamics (MD) simulations. Results of MD simulations indicate that grafted chains drastically slow down matrix chain dynamics and also form a percolated network at high nanoparticle concentrations. The influence of the graft density on viscoelastic properties is investigated to identify the mechanism of the observed stiffening in these types of PGNs.

*This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1825254.

9:24AM L33.00008: The emergence of quasi-sinusoidal nonlinearity in particle-filled polymer solutions WENTAO XIONG (Presenter), XIAORONG WANG, School of Chemical Science and Engineering, Tongji University — Systematic rheometric measurements are carried out to explore the nonlinear responses of carbon black-filled polyisoprene/squalene solutions with the polymer concentrations $f$ in the matrix ranging from the coil overlapping state ($\Phi = \Phi^*$) to the melt state ($\Phi = 1$). At the coil overlapping state when $\Phi \ll 1$, the system shows the classic nonlinearity, where the storage modulus $G'$ decreases as strain amplitude increases and the resulting stress responses are deviated from sinusoidal waves. At the melting state when $\Phi = 1$, the system displays a new nonlinearity, where the stress responses are surprisingly sinusoidal regardless the reduction of $G'$. Between the two states when $\Phi^* < \Phi < 1$, the system exhibits a complex nonlinear behavior throughout a wide range of $\Phi$. The ratio of the third to the first harmonics $I_3/I_1$ in the stress responses first decreases rapidly reaching a minimum when $\Phi \approx 0.1$, then increases to a maximum when $\Phi \approx 0.3$, after which it decreases again as $\Phi$ approaches 1. Remarkably, the filler flocculation in the system also displays the corresponding minimum and maximum values. The quasi-sinusoidal response in a system is apparently due to the restoration of broken filler network requiring longer than the time scale of a typical dynamic perturbation.
9:36AM L33.00009: Single Particle Tracking of Sticky and Non-Sticky Nanoparticles in Polymer Melts  JINSEOK PARK (Presenter), ERIC BAILEY, RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — While nanoparticle (NP) diffusion in polymer melts is important to the fabrication and applications of polymer nanocomposites, the influence of the NP/polymer interaction is poorly understood. Investigation of the weak NP/polymer interactions is experimentally challenging tendency for nanoparticle aggregation. Here, the diffusion coefficients of weakly attracting (methyl capped, CH$_3$ QDs) and strongly attracting (carboxylic acid capped, COOH QDs) nanoparticles (radius ~ 6.5 nm) in poly(propylene glycol) (PPG) melts were measured by single particle tracking (SPT). The mean-squared displacements and van Hove distribution of nanoparticle motion show Brownian motion of non-aggregated nanoparticle, in the long-time diffusion regime (~1s). For weakly interacting CH$_3$ QDs, the effective nanoparticle radius is independent of PPG $M_W$ due to the absence of a bound layer. For strongly interacting COOH QDs, the effective radius of the nanoparticle increases with the PPG molecular weight as $M_W^{0.5}$, indicating a long-lived bound layer. By obtaining spatial and temporal diffusion behavior of single nanoparticles, SPT provides previously inaccessible information on the nanoparticle diffusion in polymer melts.

9:48AM L33.00010: A Coarse Grained Model for the Simulation of dynamic Properties of Filled Elastomers  MARIIA VIKTOROVA, REINHARD HENTSCHKE (Presenter), School of Mathematics and Natural Sciences, Bergische Universitaet, Wuppertal, Germany, HOSSEIN ALI KARIMI-VARZANEH, Continental Reifen Deutschland GmbH, D-30419 Hannover, Germany — The properties of rubber are strongly influenced by the distribution of filler within the polymer matrix. We describe a modelling approach to the calculation of dynamic moduli of filled elastomers based on filler morphologies derived from the experimental interface tensions of the material's components. A Monte Carlo-based morphology generator, developed previously [1], is used to build model compounds on the µm-scale. Subsequently the Monte Carlo morphologies are mapped onto on a coarse grained model, allowing to obtain the amplitude and frequency dependence of the dynamic moduli during cyclic deformations. This combination of models ties the experimental surface tensions, characterizing the individual components, to the dynamic behavior of the macroscopic material. We consider selected examples of binary polymer blends containing a single type of filler at variable concentration. In addition to the dynamic moduli we also compute attendant transmission micrographs, wetting envelopes and work of adhesion plots.

10:00AM L33.00011: The influence of shear rate and adsorbed polymer chain flexibility on thermally stiffening nanocomposites*  
CHEN GONG (Presenter), Materials Science and Engineering, Rensselaer Polytechnic Institute, PINAR AKCORA, Chemical and Materials Engineering, Stevens Institute of Technology, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — The novelty of the nanocomposite used in the current work is that it thermally stiffens with increasing temperature. It consists of a low glass transition temperature ($T_g$) polymer matrix incorporating silica nanoparticles that contain an adsorbed high-$T_g$ polymer. Although the unique thermal-stiffening property has great application potential, the weak interactions between the adsorbed polymer and nanoparticles make it vulnerable to severe shear stresses that are prevalent in standard processing operations. In the current study, a laboratory mixing extruder was used to process nanocomposites that were initially solution blended, as a function of shear rate and adsorbed polymer chemistry. The extrudates were characterized via multiple methods such as electron microscopy, small angle X-ray scattering, and rheometry. Results indicated that the extrusion process altered the dispersion and distribution of nanoparticles, thereby, leading to changes in the mechanical properties depending on the adsorbed polymer chain flexibility – systems with flexible adsorbed chains recovered most of their mechanical performance. The effect of adsorbed chain flexibility provides an insight into designing thermally stiffening nanocomposites with better processability.

*Supported by NSF Grant 1825254.

10:12AM L33.00012: Understanding the Dispersion and Aggregation of fillers in Polymer Nanocomposites using Dissipative Particle Dynamics (DPD) Simulations of Polymer-Filler Blends*  
ASHISH GOGIA (Presenter), University of Dayton Research Institute, University of Dayton, 1700 Curran Place, Dayton, OH 45409-0170, KABIR RISHI, ALEX M MCGLASSON, GREG BEAUCAGE, Dept. Chem. and Mat. Eng., University of Cincinnati, VIKRAM KUPPA, University of Dayton Research Institute, University of Dayton, 1700 Curran Place, Dayton, OH 45409-0170 — Enhancing the properties of polymeric systems such as natural rubber by the addition of suitable additives provides for interesting applications, both mundane and novel. Such nanocomposites contain nanoscale fillers of varying miscibility, including carbon black, silica, metal oxides, pigments, and/or various combinations thereof. These complex systems exhibit rich phase behavior resulting from thermodynamic interactions and kinetic history. In this research, we perform Dissipative Particle Dynamics (DPD) simulation of polymer chains with aggregated and free filler particles, varying polymer-polymer, filler-filler, and polymer-filler interaction energy, to understand the hierarchical structure and dispersion over multiple length and time-scales. Our results demonstrate the role of concentration, temperature and interaction strength on the clustering of fillers, investigated via their fractal dimension, the radius of gyration, mesh size and population distributions, and are compared with small-angle x-ray scattering data.

*NSF CMMI - 1635865, 1636036.
FRANÇOIS BOUÉ (Presenter), Laboratory Léon Brillouin CNRS-CEA-UPSay — We review work from Laboratory Léon Brillouin and associated groups, on the structure of polymer-nanoparticles composites, under deformation, in relation with mechanical properties improvement of plastics. First, the nanoparticles: depending on preparation, but also on composition (non grafted or grafted particles), and on the matrix chains molecular weight, they can show individually dispersion, fractal aggregation, compact aggregation (1), or initially anisotropic aggregates. These conditions can be created by physicochemical ways, like solution casting, or combined with an external field, or by industrial protocols like in tyre industry... We will review how to obtain the different cases, and their response to deformation (2). For this we will use first different chemical synthesis, including chain grafting on the particles; second, physical characterization: Small Angle Scattering, mostly from X Rays (SAXS), complemented by Electronic Transmission Microscopy to help us for interpretation of the scattering.

Second, the polymer chains: we will observe them in the matrix (non-crystalline), as well as the grafted ones, combining now X Rays with neutron radiation (SANS), in nanocomposites at rest, and under deformation (3). This leads to striking comparison with measured stress-strain curves. We will compare and harmonise with results of other groups (4), for a more global view.

(2) N. Jouault, F. Dalmas, F. Boué, J. Jestin, Polymer, Polymer 2014, 55, 2523-2534.

* PhD fundings: CEA, Région Bretagne, Michelin.
Beamtime: LLB & SOLEIL, Paris-Saclay, ILL & ESRF, Grenoble.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L34 DPOLY DCOMP: Molecular Design of Polymers: Structure, Mechanics and Thermal Properties 506 - Joerg Rottler, University of British Columbia - Tag(s):
Focus
Tunable thermal transport and reversible thermal conductivity switching in topologically networked bio-inspired materials

John Tomko (Presenter), University of Virginia, ABDON PENA-FRANCESCH, HUIHUN JUNG, Pennsylvania State University, MADHUSUDAN TYAGI, Center for Neutron Research, NIST, BENJAMIN ALLEN, MELIK DEMIREL, Pennsylvania State University, PATRICK HOPKINS, University of Virginia

The dynamic control of thermal transport properties in solids must contend with the fact that phonons are inherently broadband. Thus, efforts to create reversible thermal conductivity switches have resulted in only modest on/off ratios, since only a relatively narrow portion of the phononic spectrum is impacted. Here, we report on the ability to modulate the thermal conductivity of topologically networked materials by nearly a factor of four following hydration, through manipulation of the displacement amplitude of atomic vibrations. By varying the network topology, or crosslinked structure, of squid ring teeth-based bio-polymers through tandem-repetition of DNA sequences, we show that this thermal switching ratio can be directly programmed. This on/off ratio in thermal conductivity switching is over a factor of three larger than the current state-of-the-art thermal switch, offering the possibility of engineering thermally conductive biological materials with dynamic responsivity to heat.


A Thermal Resistance Network Model for Heat Conduction of Amorphous Polymers

Jun Zhou, Qing Xi, Tongji University, Jixiong He, North Carolina State University, Nakayama Tsuneyoshi, Hokkaido University, Yuanyuan Wang, Shanghai Second Polytechnic University, Jun Liu (Presenter), North Carolina State University

Thermal conductivities (TCs) of the vast majority of amorphous polymers are in a very narrow range, 0.1 ~ 0.5 W m⁻¹ K⁻¹, although single polymer chains possess TC of orders-of-magnitude higher. Entanglement of polymer chains plays an important role in determining the TC of bulk polymers. We propose a thermal resistance network (TRN) model for TC in amorphous polymers taking into account the entanglement of molecular chains. Our model explains well the physical origin of universally low TC observed in amorphous polymers. The empirical formulae of pressure and temperature dependence of TC can be successfully reproduced from our model not only in solid polymers but also in polymer melts. We further quantitatively explain the anisotropic TC in oriented polymers.

We acknowledge funding from NC State University Faculty Research and Professional Development Fund, National Key R&D Program of China (No. 2017YFB0406004), National Natural Science Foundation of China (No. 11890703), and Shanghai Key Laboratory of Special Artificial Microstructure Materials and Technology (2019 ~2022).
8:24AM L34.00003: Improving ductility of glassy semicrystalline polymers by pre-deformation*  TRAVIS SMITH, MASOUD RAZAVI, SHIQING WANG (Presenter), Univ of Akron — Having developed some elementary understanding of how glassy polymers gain ductility [1, 2], we have begun to explore molecular mechanics of semicrystalline polymers whose Tg > ambient, to which poly(L-lactic acid) (PLLA), poly(ethylene terephthalate) (PET), and syndiotactic polystyrene (sPS) belong. Our objective is to explain why crystallization can turn a ductile glassy polymer to a brittle material, as is the case for PLLA [3]. Based on PET and s-PS, the present study will show how the ductility of such polymers can be predicted to improve upon introducing predeformation effect that alters the morphology and network structure. In doing so, we are able to further advance our theoretical understanding of factors that influence polymer ductility.

[2] Masoud Razavi, Shiwang Cheng, Da Huang, Shufan Zhang and Shi-Qing Wang, “Crazing and yielding in glassy polymers of high molecular weight, manuscript in preparation for Polymer”.

*This work is supported by NSF (DMR-1905870).

8:36AM L34.00004: Low, high, and switchable thermal conductivity in soft materials [Invited] DAVID CAHILL (Presenter), University of Illinois at Urbana-Champaign — A century of experiment and theory have produced a thorough understanding of heat conduction by phonons in simple inorganic crystals. By contrast, basic understanding of heat conduction by molecular vibrations in soft materials (amorphous and crystalline polymers, small molecule solids, biological materials) is much less mature. Complex, non-periodic structures spanning multiple length scales are difficult to characterize and model. Low thermal conductivity, fiber morphologies, poor control of defects, and anisotropy created by molecular order create daunting challenges for experiment. I will discuss our past work on the thermal conductivity and elastic constants of a wide variety of polymeric materials in the form of thin films and fibers that span a factor of 300 in thermal conductivity, 0.06 to 20 W/m-K. Time-domain thermoreflectance (TDTR) provides a common experimental platform for these studies; varying the thickness and modulation frequency changes the relative sensitivities of the TDTR measurement to thermal conductivity and heat capacity. Our recent work has employed light-activated changes in the morphology azo-polymers to switch by a factor of 3 between a low conductivity amorphous form and higher thermal conductivity crystalline form. We are developing frequency-domain probe beam-deflection and optical-fiber-based TDTR measurements to provide new capabilities for measurements of the thermal conductivity, effusivity and diffusivity of small volumes of soft materials.
9:12AM L34.00005: Making transparent, super-ductile and heat-resistant semi-crystalline polymers*  MASOUD RAZAVI (Presenter), SHIQING WANG, Univ of Akron — Based on our recent molecular picture [1], chain networking is a key factor that affords ductility for polymer glasses during tensile deformation. Therefore, it is essential, when considering the mechanics of semicrystalline polymers, that crystallization does not disrupt the chain network, which is typically not the case for semicrystalline polymers that crystallize slowly. We explore a molecular strategy to avoid depletion by crystallization of the polymer entanglement associated with the interchain uncrossability. The present study will characterize the conditions for producing such a new crystalline state and examine its mechanical behavior using class B semicrystalline polymers such as PLA and PET whose Tg is above room temperature.


*This work is supported by NSF (DMR-1905870) and ACS PRF# 60897-ND7.

9:24AM L34.00006: Estimation of mechanical properties of interfaces in polymer nanocomposites using molecular dynamics*  ABHISHEK SHANDILYA (Presenter), Materials Science and Engineering, Rensselaer Polytechnic Institute, PRAJAKTA PRABHUNE, CATHERINE BRINSON, Mechanical Engineering and Materials Science, Duke University, RAVISHANKAR SUNDARARAMAN, Materials Science and Engineering, Rensselaer Polytechnic Institute — Polymer nanocomposites are candidates for the next-generation of cable insulation and capacitor dielectrics. Nanoscale fillers, due to their high surface area, drastically increase the interfacial region which improves the dielectric permittivity and breakdown strength of the nanocomposites. Understanding the role of these interfaces in mechanical response of nanocomposites is crucial for their robust design. Modelling them at the molecular scale can capture the nanoscale features of the filler surface, the amorphous nature of the polymer and the interaction between them, while keeping the computational cost low. Using molecular dynamics, we calculate mechanical response of an ensemble of composites where polymer chains are grafted on a filler surface. We study the role of graft density and filler surface curvature on the stress and displacement field near the interface. We use an iterative finite-element-based approach to extract elastic modulus variation near the interface from the molecular dynamics stress and displacement profiles, which provides a starting point for large-scale modeling of composite nanostructures from first principles.

*This work was supported by the National Science Foundation under Grant No. 1729452.
A grand challenge in designing polymeric materials is to tune their properties by macromolecular engineering. Here, applications of polymers are often hindered by their low thermal conductivity $k$. While low $k$ values are highly desirable for thermoelectric materials, they create severe problems when used under the high temperature conditions. Going from the polymers dictated by weak Van der Waals to hydrogen-bonded interactions, $k$ varies between 0.1-0.4 W/Km. Using molecular dynamics simulations, we study thermal transport and its links to the elastic response of polymers and polymer blends in their solid states. We find that there exists a maximum attainable stiffness, thus providing an upper bound of $k$ for solid polymers. The specific chemical structures and the glass transition temperature play no role in controlling $k$, especially when the microscopic interaction is hydrogen bonded. These results are consistent with the minimum thermal conductivity model and existing experiments.


Employing Boltzmann transport equation coupled with Density-Functional Theory and non-equilibrium molecular dynamics simulation, we developed a combined scheme of calculating the thermoelectric property for polymeric materials. In the case of PEDOT doped with PSS, theory can give optimal carrier density for the power factor. It is found that the ideal crystalline polymer leads to a tiny thermoelectric figure of merit because of the extremely high thermal conductivity. Thus, engineering of disordered structure at nanoscale is essential.

We find that the formation of polaron band upon doping is essential to understand the "abnormal Seebeck effect", namely, for the potassium doped nickel-coordinated polymer, the Seebeck coefficient first increases with temperature and then suddenly drops. We proposed a two-band transport model to explain such exotic behavior.

*This work is supported by the National Natural Science Foundation of China (Grant No. 21788102) and the Ministry of Science and Technology (Grant No. 2017YFA0204501)
10:36AM L34.00010: Effect of polymer architecture on the gas separation performance of PIM-1 membranes  VENKAT PADMANABHAN (Presenter), Tennessee Tech Univ — Molecular simulations are used to demonstrate the effects of chain architectures on the gas separation performance of PIM-1 membranes. Four different architectures (linear, H-shape, star, and dendritic) are considered to investigate the transport properties of four industrially relevant gases (CO₂, CH₄, O₂, and N₂). The simulations indicate that it is possible to tune the free volume morphology of PIM-1 membranes by choosing the appropriate architecture. An inverse relationship between the density and fractional free volume was observed as expected, with the highest density and lowest FFV obtained for the dendritic PIM-1. While the linear PIM-1 showed larger pores that enhanced the diffusivity of all small gases, the branched architectures (H-shape, star and dendritic) showed smaller interconnected pores with several bottle-neck morphologies. The observed modifications resulted in significant differences in the diffusivity of mid-range size gas molecules such as N₂, pushing the performance of CO₂/N₂ and O₂/N₂ separation performance beyond the Robeson’s 2008 upper bound.

10:48AM L34.00011: Surface Segregation of Branched Chain-ends in PDMS  MONICA MARKS (Presenter), School of Materials Science and Engineering, Georgia Institute of Technology, KYRIAKI KALAITZIDOU, George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, WILL GUTEKUNST, School of Chemistry and Biochemistry, Georgia Institute of Technology — It is well known that polymeric materials reorganize at their surfaces in order to minimize surface tension and free energy. This reorganization, driven by enthalpic and/or entropic forces, creates surface properties that can dramatically differ from the bulk. Enthalpically driven reorganization allows low energy groups to surface segregate and dominate the surface properties of the material. This is the case with polydimethylsiloxane (PDMS), where low surface energy pendant methyl groups accumulate at the surface. However, in some cases, higher energy groups can surface segregate when incorporated into branched or bulky polymer chain-ends. This process is entropically driven, in order to maximize polymer configurations in the bulk, despite increasing the enthalpy of the system. This research aims to study the surface segregation behavior of high energy, branched chain-ends within a PDMS network. Novel Silicone additives consisting of linear PDMS polymers, chain-end functionalized with branched polyester dendrimers containing quaternary ammonium cations (QACs) have been synthesized. The QACs provide the observable property of antimicrobial activity, which will be used to probe the surface segregation of the additive chain-ends.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L35 DPOLY: Sustainable Biopolymers for Enhanced Applications 507 - John Dutcher, Univ of Guelph - Tag(s): Focus
8:00AM L35.00001: Dendrimeric Morphology and Mechanical Modulus of Soft Phytoglycogen Nanoparticles Revealed by AFM Force Spectroscopy  BENJAMIN BAYLIS (Presenter), ERIN SHELTON, JOHN DUTCHER, Univ of Guelph — Phytoglycogen is a naturally occurring glucose polymer that is produced in the form of highly branched, compact nanoparticles by sweet corn. The deformability, unique hydration and inherent safety of the particles makes them desirable for applications in personal care, nutrition and biomedicine. We have used atomic force microscopy (AFM) force spectroscopy to measure the size, morphology, and stiffness of the phytoglycogen nanoparticles in both water and air. For measurements in water, we were successful in covalently bonding isolated phytoglycogen particles to gold using an intermediate layer of 4-mercaptophenylboronic acid. We used the Quantitative Imaging mode of our JPK AFM to collect high resolution force-distance maps of a large number of individual phytoglycogen particles, which revealed the inner dendrimeric morphology of the particles at the largest applied forces and allowed us to quantify the increase in the elastic modulus in going from the outer to the inner regions of the particles. We also observed large increases in the modulus for dry particles in air, quantifying the effect of hydration on the mechanical stiffness of the particles.

8:12AM L35.00002: Structure of Native and Hydrophobically Modified Phytoglycogen Nanoparticles Using Small Angle Neutron Scattering  JOHN H ATKINSON (Presenter), Univ of Guelph, JONATHAN NICKELS, Univ of Cincinnati, MICHELLE MICHALSKI, MICHAEL GROSSUTTI, ADRIAN SCHWAN, Univ of Guelph, JOHN KATSARAS, Oak Ridge National Laboratory, JOHN DUTCHER, Univ of Guelph — Phytoglycogen is a highly branched polymer of glucose produced as soft, compact nanoparticles by sweet corn. Properties such as softness, porosity and mechanical integrity, combined with nontoxicity and biodegradability, make phytoglycogen nanoparticles ideal for applications involving the human body. We describe small angle neutron scattering (SANS) measurements of native phytoglycogen and phytoglycogen that was hydrophobically modified using octenyl succinic anhydride (OSA) in both its hydrogenated (hOSA) and deuterated (dOSA) forms. The data for the native particles was well described by a core-coil model, in which the outer surfaces of the particles are covered by short chains. The data for highly modified hOSA-phytoglycogen was consistent with a “raspberry” model, in which the outermost chains decorated with hOSA collapsed to form “seeds” with a well-defined size and separation. For lower DS values for both hOSA and dOSA-phytoglycogen, the data was well described using a core-shell particle geometry in which the composition of the shell was consistent with measured DS values. The results of the present study offer new insights into the morphology of phytoglycogen nanoparticles and the physical nature of their modification with OSA.
8:24AM L35.00003: Hydration water structure, hydration forces, and mechanical properties of polysaccharide films  
MICHAEL GROSSUTTI (Presenter), JOHN DUTCHER, Univ of Guelph — We have used ellipsometry at controlled relative humidity (RH) to measure the equilibrium swelling of ultrathin films of polysaccharides, including native and modified phytoglycogen nanoparticles as well as dextran and hyaluronic acid. At high humidities (RH > 70%), the RH-driven swelling of hydrophilic polymers can be described by exponentially decaying interstitial hydration forces. We have used two complementary approaches to analyse this high RH swelling regime to measure the length scale $\lambda_0$ that characterizes exponentially decaying hydration forces and to quantify the associated bulk modulus $K_p$ of the films. We further probe this swelling regime using attenuated total reflection infrared (ATR-IR) spectroscopy to investigate the hydrogen bond structure of the hydration water in the polysaccharide films. By combining ellipsometry and ATR-IR spectroscopy we find that the structuring of the hydration water hydrogen bond network in this regime correlates with both the hydration force decay length and film mechanical stiffness. These measurements provide insight into the relationship between the hydration water structure, hydration forces, and mechanical properties of polysaccharides, and suggest that a more ordered water hydrogen bond network leads to a smaller $\lambda_0$ and larger $K_p$.

8:36AM L35.00004: Carbohydrate-Based Polymers and Nanomaterials for Advanced Technologies* [Invited]  
MAREN ROMAN (Presenter), KEVIN EDGAR, Department of Sustainable Biomaterials, Virginia Tech, ALAN ROGER ESKER, Department of Chemistry, Virginia Tech — Carbohydrate-based polymers, termed polysaccharides, are ubiquitous in Nature. They perform a wide range of functions, including providing structural support in plant cell walls, generating swelling pressure in mammalian tissues, protecting microbes from dehydration and toxins, storing solar energy, and regulating binding events on cell surfaces. Owing to their diverse structures and properties, polysaccharides have found numerous industrial and medical applications. For example, they are used to increase the viscosity of food products and drilling fluids, stabilize emulsions, suspensions, and foams, form gels, prevent ice crystal formation, and protect wounds during healing. This presentation will showcase recent efforts at Virginia Tech toward the development of polysaccharide-based advanced technologies with biomedical and drug delivery applications.

*This work was supported by the National Science Foundation under Grant Nos. CHE-0724126 and DMR-0907567, the United States Department of Agriculture under Grant Nos. 2005-35504-16088 and 2011-67009-20090, the Deutsche Forschungsgemeinschaft under Grant No. HE 2054/11-1, Omnova Solutions, Inc., Tembec, Inc., the Institute for Critical Technologies and Applied Science, the Macromolecules Innovation Institute, and the Department of Sustainable Biomaterials at Virginia Tech.
**9:12AM L35.00005: Structure-Property Mappings for Bio-Advantaged Polyhydroxyalkanoate (PHA)-based Polymers**

KARTEEK BEJAGAM (Presenter), CARL N. IVerson, BABETTA L. MARRONE, GHANSHYAM PILANIA, Los Alamos National Laboratory — A steady increase in the consumption and rapid disposal of plastic products is currently imposing a stringent burden on the environment—translating into a range of severe problems from destruction of ecosystems to climate change. As a potential solution, biosynthetic and biodegradable polymers, such as Polyhydroxyalkanoates (PHAs), have emerged as a possible alternative material that can help drive the transition of our society to a more sustainable future. The underlying large combinatorial chemical space, however, poses a significant bottleneck towards identification of application-specific promising PHA-based candidate polymers. While a direct experimental-based exploration is impractical in this vast space, data-enabled screening approaches rely on our ability to accumulate accurate databases of key polymer properties. Towards this end, we are currently involved in an effort that employs molecular dynamics simulations—in a close coupling with experiments—to understand and establish accurate structure-property relationships for this bio-advantaged polymer class. In addition to providing molecular-level insights into the mechanistic origins of polymer functionalities, the generated data is expected to serve as an input for further informatics-based analysis.

**9:24AM L35.00006: Enabling Circular Polymer Chemistry Through Computation**

ALEXANDER EPSTEIN (Presenter), Materials Science and Engineering, University of California, Berkeley, PETER CHRISTENSEN, The Molecular Foundry, Lawrence Berkeley National Laboratory, TREVOR SEGUIN, Energy Technologies Division, Lawrence Berkeley National Laboratory, BRETT HELMS, The Molecular Foundry, Lawrence Berkeley National Laboratory, KRISTIN PERSSON, Materials Science and Engineering, University of California, Berkeley — Monomer-to-monomer recycling is a promising solution to the global plastic pollution crisis. However, most conventional plastics are difficult to depolymerize due to the large energy input required to degrade a carbon-carbon backbone. Instead, one can design polymers to incorporate bonds that are reversible in specific processes. This work demonstrates how quantum chemistry tools can be used to develop design rules for bonds that enable monomer-to-monomer recycling. Specifically, design rules were discovered for an exciting new polymer platform, called poly(dikeotenamine)s, which has been shown to display chemical circularity with >90% monomer yield. Design rules were developed from analysis of the simulated reaction pathway for the acid-catalyzed hydrolysis of the polymer with several heteroatom substitutions of the basic platform. Considering the ubiquity of the addition-elimination reaction in depolymerization processes, this analysis can inform design of a wide variety of monomer-to-monomer recycling techniques.

*US Department of Energy Bioenergy Technology Office: BioEnergy Engineering for Products Synthesis*
9:36AM L35.00007: Compression of Acid Hydrolyzed Phytoglycogen Nanoparticles at High Packing Densities  HURMIZ SHAMANA (Presenter), JOHN DUTCHER, Univ of Guelph — Phytoglycogen is a natural polysaccharide produced in the form of compact, 44 nm diameter nanoparticles in the kernels of sweet corn. Its highly branched, dendrimeric structure leads to interesting and useful properties that make the particles ideal as unique additives in personal care, nutrition and biomedical formulations. The properties of phytoglycogen nanoparticles can be altered through chemical modifications such as acid hydrolysis, which not only reduces their diameter but also produces significant changes to the interactions between particles in highly concentrated dispersions. At sufficiently small concentrations ($C < 30\% \text{ w/w}$), the acid hydrolyzed particles exhibit typical soft sphere behaviour characterized by an increase in the zero-shear viscosity with concentration, reaching a value that exceeds that of water by a factor of $\sim 10^3$ at $C \sim 30\% \text{ w/w}$. As the concentration is increased beyond 30% w/w (the concentration at which the particles begin to be compressed against one another), the dependence of zero-shear viscosity versus concentration data shows a pronounced kink, with increases beyond 30% w/w significantly more gradual. This result is consistent with a reduction in stiffness for acid hydrolyzed phytoglycogen nanoparticles.

9:48AM L35.00008: Tunable Yield Stress of Aqueous Dispersions of Hydrophobically-Modified Phytoglycogen Nanoparticles  CARLEY MIKI (Presenter), HURMIZ SHAMANA, JOHN DUTCHER, Univ of Guelph — Phytoglycogen is a natural polysaccharide produced in the form of compact, 44 nm diameter nanoparticles in the kernels of sweet corn. Its highly branched, dendrimeric structure leads to interesting and useful properties that make the particles ideal as unique additives in personal care, nutrition and biomedical formulations. The properties of phytoglycogen can be readily altered through chemical modification. We consider a hydrophobic modification of phytoglycogen by covalently attaching charged, hydrophobic octenyl succinic anhydride (OSA) chains to the weakly charged, hydrophilic surface of phytoglycogen. When dispersed in water at moderate concentrations ($C \sim 20\% \text{ w/w}$), the OSA-modified particles form a shear-sensitive gel with a low shear viscosity that exceeds by a factor of $\sim 10^6$ that of native phytoglycogen dispersions of the same concentration. Furthermore, the dispersions exhibit a well-defined yield stress, as measured using different rheology techniques. The yield stress vanishes as the pH of the dispersions is reduced below the pKa of the acidic group of OSA, with the material transitioning from a shear-sensitive gel to a flowing liquid. This pH-sensitivity suggests new applications for OSA-modified phytoglycogen.
10:00AM L35.00009: Binding of Proteins to a Phytoglycogen-Functionalized Surface Plasmon Resonance Sensor Surface  
KATHLEEN CHARLESWORTH, NICHOLAS VAN HEIJST (Presenter), AIDAN MAXWELL, MICHAEL GROSSUTTI, JOHN DUTCHER, Univ of Guelph — Phytoglycogen is a highly branched polymer of glucose produced as soft, compact nanoparticles by sweet corn. Properties such as softness, porosity and mechanical integrity, combined with nontoxicity and biodegradability, make phytoglycogen nanoparticles ideal for applications involving the human body. Many of these applications rely on the binding of small molecules onto phytoglycogen nanoparticles. Surface Plasmon Resonance (SPR) is a sensitive experimental technique, based on the resonant absorption of light within an ultrathin gold film, that can be used to measure the binding kinetics and affinities of small molecules. We have successfully created a stable phytoglycogen-functionalized SPR sensor surface, using 4-mercaptophenylboronic acid as a linker between the gold layer and phytoglycogen. This has allowed us to use SPR to measure the association constant between phytoglycogen and Concanavalin A (ConA) to be $2.87 \pm 0.44 \times 10^5$ M$^{-1}$ by fitting the data to the Langmuir adsorption model. By measuring the amide bands of ConA bound to phytoglycogen using infrared spectroscopy, we find that ConA maintains a large amount of its native beta-sheet content, suggesting that phytoglycogen helps to preserve its bioactivity.

10:12AM L35.00010: Plastic Resins for the Circular Economy: from Wind Turbines to Gummy Bear Candy and Beyond.*  
JOHN DORGAN (Presenter), BIN TAN, HARSHAL BAMBHANIA, Michigan State Univ — Plastics and composites have concerning sustainability metrics including high embedded energy and associated greenhouse gas emissions, low recyclability rates, and generation of microplastics pollution. Composites are notoriously difficult to recycle but are critical for wind turbine, lightweight vehicle, and other sustainable technologies. An economically viable, fully recyclable, composite resin is demonstrated; physical properties of composites produced from the reclaimed resin show true “turbine-to-turbine” recycling is possible. Various end-of-use options are established; regrinding produces short fiber moldable materials. Base catalyzed digestion produces poly(methyl methacrylate) or the superabsorbent poly(methacrylic acid). Distillation of the digestate produces methanol, water, and food grade potassium lactate; the resulting lactate has been incorporated into gummy bear candies. Judicious formulation of polymer resins enables complete circularity in low-embedded energy materials; exploitation of triggerable degradation provides varied and intriguing end-of-use recycling options.

*Support through the David and Denise Endowment gift to the Michigan State University Foundation is gratefully acknowledged.
10:24AM L35.00011: Performance-advantaged bioproducts from biomass* [Invited]  GREGG BECKHAM (Presenter), NREL — Chemical intermediates accessible from selective processing of lignocellulose, namely carbohydrates from polysaccharides and aromatic oxygenated compounds from lignin, offer the potential for atom-efficient biological and catalytic transformations to new building blocks for biopolymers that are difficult to access from petroleum-derived, hydrocarbon intermediates. To that end, this talk will cover several new biopolymers via biological and catalytic transformations of carbohydrates and lignin-derived aromatic compounds that exhibit performance-advantaged properties relative to existing petroleum-based polymers. Performance-advantaged bioproducts, such as those described here, could potentially incentivize the development of a viable bioeconomy alongside biofuels production.

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Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L36 FED DCOMP: {$PICUP}: Integrating Computation in Introductory and Upper-Level Physics Courses 601/603 - Amy Liu, Georgetown University - Tag(s): Education, Invited, Undergrad Friendly

8:00AM L36.00001: Integrating computation using materials from the PICUP collection in Introductory Physics* [Invited] MARIE LOPEZ DEL PUERTO (Presenter), University of St. Thomas — The Partnership for Integrating Computation into Undergraduate Physics (PICUP, www.gopicup.org) runs workshops, hosts an online collection of curricular materials, and supports a growing community of interested faculty with the goal of making it easier for faculty to integrate computation into their courses. In this talk, I will share my experience integrating computation into the introductory physics sequence. I will highlight materials in the PICUP collection that I adapted, discuss how those materials fit into and enhance the course, and talk about how I integrate computation into a workshop-style course. I will then present different approaches used by faculty who integrate computation into introductory physics courses in a variety of institutional settings, so attendees can see how they might integrate computation in their own introductory courses.

*This work is supported in part by NSF grant DUE-1525062.
8:36AM L36.00002: Enhancement of Student Experience and Content Coverage in Physics Courses Through Integration of Computation* [Invited]  KELLY ROOS (Presenter), Bradley University — Integrating computational activities into undergraduate physics courses adds educational value to the physics curriculum through providing deeper conceptual understanding of physical principles, introducing marketable skills, enhancing problem-solving, and expanding topical coverage. In this presentation, I shall provide a few examples of these computational activities that add educational value to the undergraduate physics curriculum in introductory and upper level courses, and offer suggestions (based on more than 25 years of “trying things”) on how to effectively implement such activities into the traditional course format, i.e. the conventional lecture-lab mode of physics instruction.

*Support from the National Science Foundation, grants NSF-1525525, NSF-1524963, NSF-1525062, NSF-1524128, and NSF-1524493, is gratefully acknowledged.

9:12AM L36.00003: Title: Upper-Division Computational Physics at Syracuse and its Lasting Impact on Students [Invited]  WALTER FREEMAN (Presenter), Syracuse University — The value of incorporating computational physics into the undergraduate curriculum is now widely accepted, both because it facilitates student learning of core physical concepts and because computational skills are needed in graduate research and industry. However, computation doesn't just let us train the same sort of physicists more efficiently; students with computation as a core part of their training develop a richer, more insightful, more fundamentally grounded, and ultimately more fruitful perspective on physics as a discipline. In short, they become a different sort of physicist -- one with a clearer view of what physics shows us about the world and with more freedom to apply their knowledge to understand physical phenomena.

I will present case studies of students from Syracuse University who have studied computational physics as part of their upper-division and graduate training, and argue that their outlook on the physical world and approach to physics as a whole has benefited from this experience.

9:48AM L36.00004: Modern Computer Applications in the Advanced Laboratory [Invited]  DANIEL BORRERO-ECHEVERRY (Presenter), Willamette University — While computers have long played an important part in Physics laboratory instruction, the scope of their use is often limited to relatively simple data processing tasks like fitting experimental data to well-established analytical models. While these applications are obviously important, they are not representative of the full range of ways that computers are used in modern physics research laboratories. In this talk, I will discuss how the Physics department at Willamette University has created engaging laboratory experiences that tightly integrate experiment, theory, and computational modeling and incorporate modern computational tasks like data visualization, simulation of experimental systems, and computer-aided design of experimental apparatus. These activities have reduced the time that faculty spend training undergraduates to work in their labs allowing students to make more significant research contributions, while also helping them acquire crucial computation skills that they will need as they join the 21st century workforce.
10:24AM L36.00005: Normalizing computation through continuous student engagement in the undergraduate physics curriculum* [Invited]  YOGESH JOGLEKAR (Presenter), GAUTAM VEMURI, ANDREW D GAVRIN, Indiana University - Purdue University Indianapolis — Physics is, by definition, the most fundamental empirical science. Broadly construed, the laws of physics allow us to explain phenomena and predict outcomes on scales that range from astronomical to the microscopic. And yet, anecdotal surveys show that high-school and undergraduate students largely perceive physics as “theoretical” with little to no day-to-day consequences. This gap between the reality and the perception is fueled, in part, by undergraduate curriculum where majority of the courses mostly focus on examples that have the distinct advantage of being analytically solvable. In this talk, I will present a department-wide initiative to normalize computation across the physics curriculum – an intervention that is designed to bridge the gap by enabling students to explore realistic physics and engineering examples. It consists of a meta-course comprising computational modules developed by the departmental faculty for every course in the undergraduate curriculum, a redesigned “Introduction to Computational Physics” course, and a sustained engagement of students through assignments and exams that involve computational problems. I will present preliminary results of surveys from each semester under intervention.

*This work was supported IUPUI SEIRI seed grant.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L37 GIMS: Nanoscale Characterization of Correlated and Entangled Quantum Phenomena 605 - Stephen Jesse, Oak Ridge National Laboratory - Tag(s): Invited

8:00AM L37.00001: Markus B. Raschke Invited Talk [Invited]  MARKUS B. RASCHKE (Presenter), University of Colorado, Boulder — TBD
8:36AM L37.00002: Revealing topological quantum states with STM-based spectroscopy*

[Invited] AN-PING LI (Presenter), Oak Ridge National Lab — Topological insulators possess a massless Dirac dispersion with spin–momentum locking at the surface. The onset of a spontaneous magnetization or a broken time-reversal symmetry leads to the formation of an exchange gap in the Dirac band dispersion. In this work, we will present two examples to show how STM spectroscopy can be used to detect these signatures of topological quantum states. (1), Spin helical states on Bi2Te2Se. A multi-probe STM with spin-polarized tips allows us to perform in situ transport measurement to differentiate surface conductance from the bulk and spin-up chemical potential from the spin-down. As a result, a spin-momentum-locked current is revealed which shows ultra-high mobility and polarization. (2), Gapped surface states on MnBi2Te4. Quasiparticle interference patterns are used to probe local dispersions of both surface and bulk electronic structures. The theoretically predicted gapped surface states are evaluated with high spatial resolution. It is expected that tuning of the Fermi level in the exchange gap will result in the emergence of a quantum anomalous Hall effect.

*This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.
9:12AM L37.00003: Atomic precision advanced manufacturing for electronic devices* [Invited]  
DAN R. WARD, TZU-MING LU, LISA A TRACY, XUJIAO GAO, ANDREW D. BACZEWSKI, AARON KATZENMEYER, SCOTT W SCHMUCKER, EVAN ANDERSON, JEFFREY IVIE, DENIS MAMALUY, EZRA BUSSMANN, SHASHANK MISRA (Presenter), Sandia National Laboratories — Since the advent of atomic manipulation with the scanning tunneling microscope (STM), a significant challenge for atomic scale fabrication has been to build structures large enough to exhibit emergent system-level phenomena that can be understood at a macroscopic level. Using fabrication to build a bridge between atomistic details and macroscopic properties promises to deepen our understanding of physical phenomena that are otherwise understood only in a coarse-grained way. STM-based hydrogen lithography on silicon can be used to place individual donor atoms comprising a device, a process we refer to as atomic precision advanced manufacturing (APAM). Although this capability promises to bolster our semiclassical understanding of electron transport in electronic devices, application of this technique has been held back by two factors that are the focus of this talk. In this talk, I will detail our efforts to make more atomically perfect devices, attempting to control both the precision placement of dopants and also their surroundings, and more complex devices, incorporating metal-oxide-semiconductor (MOS) gates. In the future, advanced devices could open the door to understanding the limitations of some fundamental assumptions in device physics including semiclassical approximations and linear response.

*This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, for the U.S. Department of Energy's National Nuclear Security. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

9:48AM L37.00004: Interrogating Entangled Matter with Entangled Probes [Invited]  
PATRICK BLACKSTONE (Presenter), ABU ASHIK MD. IRFAN, GERARDO ORTIZ, Indiana University - Bloomington — We developed an Entangled Scattering theory that extends the scope of standard scattering approaches to study entangled matter, such as unconventional phases of strongly correlated systems. Our presentation will focus on a neutron beam probe that is entangled in spin and path, although similar ideas also apply to photon probes. Our theory generalizes the ubiquitous van Hove Theory whereby the differential cross-section is written as a particular linear combination of two-point correlation functions. Controlling the degree of entanglement of the neutron probe (e.g., the microscopic spin-echo length) allows us to identify the relevant entangled excitations of the investigated target material. This theory and future experiments that it informs may shed light on complex phases exhibited by novel materials such as multiferroics, unconventional superconductors, quantum spin liquids, and frustrated magnets.
Toward practical quantum-enhanced microscopies* [Invited]  

BENJAMIN J LAWRIE (Presenter), RAPHAEL POOSER, Oak Ridge National Laboratory — Quantum light sources are increasingly essential to the development of the next generation of sensors and microscopes. While squeezed light exhibiting quantum noise reduction has been leveraged to enable quantum-enhanced measurements of microcantilever beam displacement [1], substantial further improvements are required to enable realistic quantum-enhanced scanning probe microscopy. We will discuss an approach to scanning probe microscopy based on truncated nonlinear interferometry that enables minimum photon back-action noise while also operating below the photon shot noise limit [2]. Further, we will explore photon correlation measurements in cathodoluminescence microscopies as a path toward the sub-diffraction-limited characterization of single color centers and excitons in nanostructured and 2D materials.


*This research was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. The experimental concept was conceived and initial experiments were performed as part of the Laboratory-Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC for the U.S. Department of Energy.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L38 COM: TEAM-UP: The Time is Now for Systemic Changes to Increase the Number of African American Bachelor’s in Physics and Astronomy  

607 - Garfield Warren, Indiana University Bloomington - Tag(s): Diversity

8:00AM L38.00001: Philip W Hammer Invited Talk [Invited] —
8:15AM L38.00002: The TEAM-UP Report: Major Findings and Recommendations [Invited]
MARY B JAMES (Presenter), Reed College — The TEAM-UP task force collected quantitative and qualitative data from over 250 undergraduate physics students and 40 physics departments to examine and assess the reasons for the persistent under-representation of African American (AA) students in physics and astronomy at the bachelor's level. The task forces embraced social science research methods and perspectives to investigate four key questions:
1. How does physics culture enhance or diminish AA students’ success?
2. What are the key experiences that lead to AA student persistence or failure to persist in undergraduate physics and astronomy programs?
3. What programmatic factors lead to the persistence of AA students in obtaining B.S./B.A. degrees in Physics/Astronomy?
4. What impedes or promotes culture change in the physics and astronomy community necessary to increase the persistence of AA students in Physics and Astronomy?

In this talk we describe the major findings and evidence-based recommendations for AIP Member Societies, physics and astronomy departments, and other stakeholders to increase the number and percentage of African American students obtaining bachelor's degrees in physics and astronomy.

8:45AM L38.00003: TEAM-UP’s Recommendations on Systemic Change [Invited] EDMUND BERTSCHINGER (Presenter), Massachusetts Institute of Technology — The TEAM-UP report identifies the structural and systemic causes explaining why African Americans have not experienced the growth in bachelor's degrees in physics the way they have in other fields or as other minority groups have experienced in physics over the past two decades. Solving these problems requires changing not only the way physicists train students, but how they think about training students. Research on change in higher education suggests the need for physicists and astronomers to recognize and question the norms, values, and culture of their fields. The TEAM-UP report’s highest priority recommendations provide a guide to cultural transformation in the profession. The evidence and theories presented in this report call for a new way of thinking by physicists, much as the Davisson-Germer experiment did nearly a century ago.


9:45AM L38.00005: Maria Ong Invited Talk [Invited] —

10:15AM L38.00006: PANEL DISCUSSION [Invited] —

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L39 DCOMP GDS DMP: Machine Learning for Quantum Matter
I 703 - Miles Stoudenmire, Simons Foundation - Tag(s): Focus
ANNABELLE BOHRDT (Presenter), Tech Univ Muenchen, CHRISTIE S. CHIU, GEOFFREY JI, MUQING XU, DANIEL GREIF, MARKUS GREINER, EUGENE DEMLER, Physics Department, Harvard University, FABIAN GRUSDT, MICHAEL KNAP, Tech Univ Muenchen — Quantum gas microscopes for ultracold atoms provide real-space snapshots of complex many-body systems with single site resolution. We use machine learning techniques to analyse and classify such snapshots of ultracold atoms. Specifically, we study the two-dimensional Fermi-Hubbard model, which is believed to capture the rich physics of high-temperature superconductivity and other phases such as the strange metal, stripe, antiferromagnet, or pseudo-gap phase. While a large number of theories exist to describe this system, each with its own merits, a unifying analytic understanding is still lacking. We compare the data from an experimental realization of the two-dimensional Fermi–Hubbard model to two theoretical approaches: a doped quantum spin liquid state of resonating valence bond type, and the geometric string theory, describing a state with hidden spin order. This method considers all available information without a potential bias towards one particular theory by the choice of an observable and can therefore select the theory that is more predictive in general. Up to intermediate doping values, our algorithm tends to classify experimental snapshots as geometric-string-like, as compared to the doped spin liquid. Our results demonstrate the potential for machine learning in processing the wealth of data obtained through quantum gas microscopy for new physical insights.


ELMER GUARDADO-SANCHEZ, BENJAMIN M SPAR, Princeton University, JUAN CARRASQUILLA, Vector Institute for Artificial Intelligence, RICHARD THEODORE SCALETTAR, University of California, Davis, WASEEM S BAKR, Princeton University, EHSAN KHATAMI (Presenter), San Jose State University — Quantum gas microscopes for ultracold atoms in optical lattices have transformed quantum simulations of many-body Hamiltonians. Statistical analysis of atomic snapshots can produce expectation values for various charge and spin correlation functions and has led to new discoveries for the Fermi-Hubbard model in two dimensions. Here, we enlist the help of artificial intelligence to look for possible patterns in the snapshots not captured by conventional indicators. We try this unbiased approach on images taken in the non-Fermi liquid phase of the Hubbard model around optimal doping.

*E.K. acknowledges support from the NSF under Grant No. DMR-1609560.
8:48AM L39.00003: Unsupervised machine learning of topological phase transitions*
JOAQUIN RODRIGUEZ NIEVA, MATHIAS SCHEURER (Presenter), Department of Physics, Harvard University — In the traditional theory of phase transitions, pioneered by Landau, different phases are characterized by the symmetries they break. However, physical systems can also exhibit phase transitions between two states that share the same symmetries, but can be sharply distinguished by their “topological” properties. While symmetry-breaking phase transitions are readily captured with machine learning, topological phase transitions are significantly more difficult, which is related to their non-local nature. In this talk, I will discuss an unsupervised machine-learning approach that we propose [see Nature Physics 15, 790-795 (2019)], which is capable of “learning” topological invariants from raw, unlabeled data. The success of the approach is demonstrated on several different models and we also discuss a mapping of the output of the machine learning to the eigenvalues and wavefunctions of an auxiliary quantum problem. This will allow us to use physical intuition of quantum mechanics to understand how the machine-learning algorithm performs the topological classification.

*JRN: support from AFOSR-MURI: Photonic Quantum Matter (award FA95501610323); MSS: support from the German National Academy of Sciences Leopoldina, grant no. LPDS 2016-12, and from the NSF under grant no. DMR-1664842.

9:00AM L39.00004: Classification of optical quantum states using machine learning
SHAHNAWAZ AHMED (Presenter), MC2, Chalmers University of Technology, CARLOS SÁNCHEZ MUÑOZ, Physics, Oxford University, FRANCO NORI, Theoretical Quantum Physics, Riken, ANTON FRISK KOCKUM, MC2, Chalmers University of Technology — Machine-learning techniques for quantum state tomography can give significantly faster results, e.g., by using adaptive measurements to avoid redundant data acquisition, or by finding efficient parameterizations of a quantum state to escape the "curse of dimensionality". Here, we explore a similar idea for optical quantum states by using deep neural networks (DNNs). We train a DNN to classify different optical quantum states, e.g., cat or thermal states, with a high accuracy. Our DNN can also predict interesting physical properties, such as Wigner negativity, directly from measurement data without requiring a full reconstruction. We study the influence of various factors such as noise, Hilbert-space cutoff, and measurement settings on the predictions and show that the DNN approach is robust. We also apply standard methods for analyzing neural network predictions, such as Grad-CAM, to determine the features used by the network to make its predictions. To benchmark our method, we compare with a naive classifier using maximum likelihood estimation. Our results indicate that the DNN can be a fast and efficient real-time classifier to distinguish various optical quantum states in the lab.
9:12AM L39.00005: Unsupervised learning of quantum phase transitions using nonlinear
dimension reduction methods  ALEXANDER LIDIAK (Presenter), ZHEXUAN GONG, Physics,
Colorado School of Mines — Quantum simulators have reached a complexity that understanding
measurement data they generated has become a daunting task for traditional data analysis
methods. To make scientific discoveries based on experimental data where theoretical
understanding is lacking, unsupervised machine learning can be a powerful tool. However,
existing approaches to unsupervised learning of quantum many-body states are largely focused
linear dimension reduction methods such as principle component analysis (PCA), or
generalizations such as kernel PCA. These methods often fail when order parameters of the
states are nonlinear functions, i.e. states with valence-bond order, topological order, many-body
localization, etc. This motivates us to investigate nonlinear dimension reduction methods such as
diffusion maps and autoencoders. By studying a 1D chiral Z3 clock model (experimentally a chain
of Rydberg atoms), we find PCA detects only the Z3 phase while diffusion maps detects the full
phase map including a incommensurate phase. In addition, diffusion maps directly detect the Z3
symmetry of model and predict the number of clusters. We find these nonlinear dimension
reduction methods also useful in learning valence-bond order and Gaussian-type topological
phase transitions in quantum spin systems.

9:24AM L39.00006: Machine learning the Mattis glass transformation  DANIEL LOZANO-
GOMEZ (Presenter), DARREN PEREIRA, MICHEL J P GINGRAS, University of Waterloo — Machine
learning techniques are being actively explored to ascertain their usefulness in many areas of
physics. Within condensed matter physics, one of the goals these techniques are being
investigated for is per their ability to identify the different phases of a system. As such, the
identification of a system's symmetries and underlying gauges is taken as a crucial step to
accomplish this endeavor. In this context, we consider classical spin models in which we
introduce a so-called Mattis gauge transformation. This transformation turns the standard
ferromagnetic Ising model into a non-frustrated random bond Ising model, and the
ferromagnetic XY model into an XY model with random Dzyaloshinskii-Moriya interactions. We
show through a simple unsupervised method, the Principal Component Analysis (PCA), that PCA
is able to expose the introduced, albeit hidden, gauge transformation for both models. For the
Ising Mattis-model, the original Ising model structure is recovered by PCA, and a rough estimate
of the gauge distribution is extracted. For the XY gauge model, we show that while the gauge
transformation is `hidden'' in the clustering structure for the full data set, it is nevertheless
uncovered when studying a specific component of the spins.
9:36AM L39.00007: Augmenting machine learning algorithms with the addition of a physics based intelligence prior  CHRISTOPHER SINGH (Presenter), MATTHEW REDELL, Physics, Binghamton University, MOHANNAD ELHAMOD, JIE BU, ANUJ KARPATNE, Computer Science, Virginia Tech, WEI-CHENG LEE, Physics, Binghamton University — Improving the predictive power of machine learning models is one of the greatest challenges to the science of learning. Here we demonstrate with the simplest of neural networks that the addition of an intelligence prior can drastically improve the learning capabilities. We outline this simple mechanism to decrease the number of exposures, and enhance the predictive power with a number of examples relevant to the study of quantum phase transitions. We find that guided networks are uniquely capable to identify key features of quantum phases where unguided models fail, and that while the mean square error of topologically equivalent models may be commensurate, the structure of the predictions produced by the models is qualitatively very different. In many situations where knowledge of a physical system is available, but direct sampling of the entire phase space is computationally intractable, this approach offers a superior learning alternative.

9:48AM L39.00008: Adversarial machine learning for modeling the distribution of large-scale ultracold atom experiments*  CORNEEL CASERT (Presenter), Ghent University, KYLE MILLS, Ontario Tech University, TOM VIEIJRA, JAN RYCKEBUSCH, Ghent University, ISAAC TAMBLYN, National Research Council of Canada — Directly generating microstates with desired properties from the configuration space of many-body systems is infeasible due to its high-dimensional nature. Instead, traditional generation methods rely on computationally costly algorithms or carefully controlled experimental setups, which limits the number of particles that can be investigated. We present how artificial neural networks allow for the direct and targeted generation of large-scale microstates, while restricting the time-consuming simulations or measurements to a small number of particles. Their potential is illustrated on a data set of experimental snapshots of a doped Fermi-Hubbard model realized by ultracold atoms trapped in an optical lattice. The adversarial machine learning method we develop here is broadly applicable and can also be used for speeding up computer simulations of both equilibrium and nonequilibrium physical systems.

*This research is supported by an NVIDIA hardware grant.
10:00AM L39.00009: Using Convolutional Neural Networks to analyze phase transitions and calculate critical exponents  NISHAD MASKARA (Presenter), EVERT VAN NIEUWENBURG, MANUEL ENDRES, Physics, California Institute of Technology — Identifying phase transitions and their corresponding order parameters is a central problem in physics, but estimation of order parameters from experimental measurements is difficult. In this work, we present an alternative framework for analyzing phase transitions by using neural networks to learn order parameters directly from data. By introducing a type of convolutional architecture, we show how these methods can be made more robust by systematically increasing the convolutional window size. We investigate the extraction of correlation length critical exponents by performing finite-size scaling on the network, and use this to analyze the 1D TFIM phase transition from measurements in different bases. This work is a step towards a machine learning toolkit for characterizing phase transitions without prior knowledge.

10:12AM L39.00010: Unsupervised learning of topological indices  OLEKSANDR BALABANOV (Presenter), MATS GRANATH, University of Gothenburg — I will present an unsupervised protocol for learning topological indices of quantum systems [1]. The idea is to produce ensembles of topologically equivalent data and then train a specially designed neural-network-based regressor for classifying them. The datasets of topologically equivalent samples are derived by continuously deforming some selected parent systems and this procedure does not require any knowledge of the topological numbers or how they are constructed. I will explicitly illustrate the protocol with two examples: It will be employed for classifying 1d band insulators in symmetry class AIII, characterized by a winding number, and 2d band insulators in symmetry class A, characterized by a Chern number.


10:24AM L39.00011: Machine Learning based BCS superconductivity Predictor from Normal State Properties  FEI HAN (Presenter), NINA ANDREJEVIC, THANH NGUYEN, QUYNH NGUYEN, SHREYA PARJAN, Wellesley College, MINGDA LI, Massachusetts Institute of Technology MIT — BCS theory is the widely accepted microscopic mechanism for conventional superconductivity. However, despite decades’ research effort, it is still challenging to judge that whether a material is superconducting or not, not to mention a faithful estimation on the superconducting critical temperature $T_c$. In this study, we employed a few deep learning architectures to correlate the normal state properties to superconductivity. A few normal state properties are found to be closely related to the formation of superconductivity with further link to $T_c$. Our work might offer an alternative avenue to rapidly identify superconducting materials.
Unlocking quantum critical phenomena with physics guided artificial intelligence

CHRISTOPHER SINGH, MATTHEW REDELL (Presenter), Binghamton University, MOHANNAD ELHAMOD, JIE BU, Virginia Tech, WEI-CHENG LEE, Binghamton University, ANUJ KARPATNE, Virginia Tech — Breakthroughs in cold atom experiments, advances in quantum computing, developments in spin liquids, and the proliferating importance of quantum critical phenomena compel the application of machine learning techniques to difficult quantum problems. In an age where data can drive unparalleled discoveries, expensive-to-acquire data such as measurements of quantum computer states or cold atom chains can be used by the community to distill new information. Thus, more effective ways of prediction and distillation are required to efficiently identify the criticality. While many have done this using a classification algorithm, we have pioneered a method to predict quantum critical phenomena using machine learning in the absence of direct exposure to states on either side of the transition by directly predicting the ground state wavefunction. By analyzing the predictions for the total phase space, we can confidently identify the location of criticality from the evolution of the predicted wavefunctions. Through further development, this type of machine could help researchers quickly, and cheaply, identify regions of the phase space that are of the utmost interest.

Neural-Network Approach to Dissipative Quantum Many-Body Dynamics

MICHAEL HARTMANN (Presenter), Univ Erlangen Nuremberg, GIUSEPPE CARLEO, Flatiron Institute — In experimentally realistic situations, quantum systems are never perfectly isolated and the coupling to their environment needs to be taken into account. Often, the effect of the environment can be well approximated by a Markovian master equation. However, solving this master equation for quantum many-body systems becomes exceedingly hard due to the high dimension of the Hilbert space. Here we present an approach to the effective simulation of the dynamics of open quantum many-body systems based on machine-learning techniques. We represent the mixed many-body quantum states with neural networks in the form of restricted Boltzmann machines and derive a variational Monte Carlo algorithm for their time evolution and stationary states. We document the accuracy of the approach with numerical examples for a dissipative spin lattice system.

Wednesday, March 4, 2020 8:00 AM - 10:12 AM

Session L40 DCOMP DMP: Matter in Extreme Environments III: Warm Dense Matter
Warm and extremely dense matter, having densities ranging from tens to millions of grams per cubic centimeters and temperatures of 104 to 106 K, widely exist in the universe such as giant planet cores and white dwarfs. Thanks to advances in technology, such extreme conditions can now be created in laboratories by powerful lasers or pulsed-power machines. Experimental advances have certainly helped us to unravel how matter behaves under warm and superdense conditions. On the theory and computation side, first-principles tools such as thermal density-functional theory (DFT) are often used to reveal novel properties of warm and extremely dense matter. Many new phenomena, for example, unusual K-edge shifting,[1] dynamical Ka-line movement,[2] and interspecies radiative transition,[3] have been predicted by ab-initio DFT calculations. Some of them have recently been confirmed by experimental measurements. In this talk, we will cover the recent progress in understanding the physics of matter in such extreme environments through both computational and experimental studies. This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856.


8:36AM L40.00002: Ultrafast electron-ion coupled dynamics of iron nano-foil in warm dense matter (WDM) conditions studies by time resolved XANES and ab-initio simulations*

AMALIA FERNANDEZ (Presenter), ALFREDO A. CORREA, SEBASTIEN HAMEL, Lawrence Livermore Natl Lab, DAVID PRENDERGAST, Lawrence Berkeley Nationa Laboratory, SRI CHAITANYA DAS PEMMARAJU, PHILIP HEIMANN, SLAC, ROGER WIRTH FALCONE, University of California Berkeley, JON HENRY EGGERT, YUAN PING, TADASHI OGITSU, Lawrence Livermore Natl Lab — In recent years, significant progresses have been made in both ultrafast experimental measurements techniques as well as in computational modeling that allow us to access to fundamental properties such as electron-phonon coupling under electron-ion non-equilibrium conditions. In this presentation, we will discuss how a combination of time-resolved XANES experiment and ab-initio derived two-temperature model coupled with XANES simulation is used to study the spatiotemporal electron-ion relaxation behavior of nano-meter thin iron foil that is exposed to femto second laser pulse. We show that the current level of experimental time resolution is already sufficient to constraint thermophysical properties under non-equilibrium WDM conditions within a few tens of percent, however, for the optimal sensitivity, which depends strongly on the choices of geometrical design of target as well as corresponding laser fluence.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344 with support from DOE OFES Early Career program.

8:48AM L40.00003: First-principles Stopping Power in Warm Dense Matter*  

ATTILA CANGI (Presenter), ANDREW BACZEWSKI, STEPHANIE B HANSEN, Sandia National Laboratories — Recent experiments provide measurements of fusion-product stopping powers in warm dense targets [1, 2]. State-of-the-art numerical modeling complements these critical advances in our empirical knowledge and phenomenological understanding of transport properties in this thermodynamic regime. In anticipation of future experiments, we assess the ability of real-time time-dependent density functional theory (TDDFT) to reproduce these results and compare its predictions with linear response TDDFT and average-atom models.


*Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.
9:00AM L40.00004: Thermoelectric properties from time-dependent density functional theory*  ALICIA WELDEN (Presenter), XAVIER ANDRADE, ALFREDO A. CORREA, Lawrence Livermore Natl Lab — The goal of this work is to develop computational methods to predict electrical and thermal transport properties from ab-initio quantum simulations. We apply a microscopic theory of quantum transport to obtain conductivities from first principles. The new methods, based on simulating real time electron dynamics, are able to access larger systems than the standard Kubo-Greenwood approach and are also applicable in non-linear regimes. We investigate liquid metallic hydrogen at 1400 K and 400 GPa, in order to see if there is nonlinear behavior under conditions that are typically accessible by experiments.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344." LDRD: Quantum Non-Equilibrium Dynamics of Electronic Transport in Nonlinear Regimes [18-ERD-031 2018] RELEASE:LLNL-POST-773049

9:12AM L40.00005: Thermal gradient effect on the transport properties of helium and intrinsic defects in tungsten*  ENRIQUE MARTINEZ SAEZ (Presenter), Theoretical Division, Los Alamos National Laboratory, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, BRIAN WIRTH, Department of Nuclear Engineering, University of Tennessee — Plasma-facing materials (PFMs) in a fusion reactor are expected to withstand stringent conditions, with high heat and particle fluxes that modify the materials microstructure. These fluxes create strong gradients of temperature and concentration of diverse species. Besides the He ash, neutron particles will create intrinsic point defects, such as vacancies and self-interstitials atoms (SIAs), and their clusters. These species will then migrate in the presence of the afore-mentioned gradients. In this work, we use nonequilibrium molecular dynamics simulations to study the transport properties of He, vacancies, and SIAs in the presence of a thermal gradient in tungsten. In all cases, the defects and impurity atoms tend to migrate toward the hot regions of the material. The resulting concentration profiles are in agreement with irreversible thermodynamics. We compute a negative heat of transport for all species, which indicates that the respective driven species fluxes are directed opposite to the heat flux. We demonstrate that, when the mass-heat transport coupling is considered, the resulting steady-state profiles vary significantly from those when species transport is decoupled from heat transport.

*SciDAC project on Plasma Surface Interactions under award number DE-SC0008875.
Electronic structure approach to compute Dark Matter-Electron scattering cross-sections in Direct Detection experiments

CHENG ZHEN (Presenter), ROUVEN ESSIG, MARIVI FERNANDEZ SERRA, State Univ of NY - Stony Brook — The existence of dark matter in the Universe is nowadays overwhelming. Numerous direct detection experiments are currently on going or planned all around the world. As the mass of these dark matter particles is unknown, these experiments explore different mass ranges, with a large majority being sensitive to masses above the GeV range. In these experiments dark matter is assumed to scatter from the nuclei and background models are built upon a combined theoretical and experimental characterization of nuclear recoils in the detectors. Recently, however, dark matter in the sub-GeV mass range has received much attention, and several well-motivated theoretical models exist for candidates in this mass range. The traditional method of detecting the nuclear recoil does not apply for sub-GeV dark matter because the recoil energy falls below the detector threshold. However, the scattering of dark matter with atomic electrons can produce observable ionization signals. In this talk we present the theoretical model to estimate the dark matter-electron scattering event rate using first principle methods. We will show how this rate estimation depends on the underlying theoretical approximations. We also show results for different systems like liquid Xe, Si and Ge.

Accurate Calculations of a Solid State Test Set with Quantum Monte Carlo Methods

CODY MELTON (Presenter), Sandia National Laboratories, JARON KROGEL, Oak Ridge National Laboratory, FIONN MALONE, MIGUEL A MORALES, Lawrence Livermore National Laboratory, LUKE SHULENBURGER, Sandia National Laboratories — Quantum Monte Carlo (QMC) methods serve as some of the most promising techniques for studying correlated materials across large spans of system size. Here, we revisit a solid state test set for QMC ranging from ionic, metallic, covalent, and van der Waals materials.

Using the familiar fixed-node Diffusion Monte Carlo (DMC) and the more recent auxiliary field quantum Monte Carlo (AFQMC), we examine the bulk ground state properties from ambient conditions up to nearly 300 GPa. One of the key limitations to the accuracy of previous DMC calculations for this set was the quality of the effective core potentials utilized. In this work, we use the recently developed correlation consistent effective core potentials and compare to previous calculations to quantify the size of the pseudopotential errors in DMC on the calculated structural properties. Additionally, we directly compare AFQMC to DMC in order to understand the relative strengths and weaknesses of the two methods for these calculations.

This work was supported by the Center for Predictive Simulation of Functional Materials, a DOE-BES center. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525
Materials Informatics for Dark Matter Detection

RICHARD GEILHUFE (Presenter), BART OLSTHOORN, NORDITA, ALFREDO FERELLA, Stockholm University, TIMO KOSKI, KTH Royal Institute of Technology, FELIX KAHLHÖFER, RWTH Aachen, JAN CONRAD, Stockholm University, ALEXANDER V BALATSKY, NORDITA — Dark Matter particles are commonly assumed to be weakly interacting massive particles (WIMPs) with a mass in the GeV to TeV range. Recent interest has shifted toward lighter WIMPs, which are more difficult to probe experimentally. A detection of sub-GeV WIMPs requires the use of small gap materials in sensors. Using recent WIMP mass estimates, we identify the relevant target space toward small gap materials (100 to 10 meV). Dirac Materials, a class of small- or zero-gap materials, emerge as natural candidates Dark Matter sensors. We propose the use of informatics tools to rapidly assay materials band structures to search for small gap semiconductors and semimetals, rather than focusing on a few preselected compounds. As a specific example of the proposed strategy, we use the organic materials database (https://omdb.mathub.io) to identify organic candidate materials. We outline a novel and powerful approach to search for dark matter detection sensor materials by means of a rapid assay of materials using informatics tools.

We acknowledge support from VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744), the European Research Council under the European Unions Seventh Framework ERS-2018-SYG 810451 HERO, and the Knut and Alice Wallenberg Foundation.

Extreme Electric Fields in DFT

MICHAEL ASHTON (Presenter), CHRISTOPH FREYSOLDT, JOERG NEUGEBAUER, Max Planck Inst fuer Eisenforschung GmbH — Strong (10^10 V/m) electric fields can be used to trigger chemical processes with extreme precision by selectively stabilizing or weakening bonds to initiate reactions which are otherwise slow or do not proceed at all. The ability to manipulate electric fields to tailor and stimulate bond-breaking events is a powerful experimental control knob, but one whose effects are difficult to predict due to a lack of suitable tools to probe its associated atomic-scale mechanisms. Here we introduce a novel approach, which we term the Generalized Dipole Correction (GDC), that enables the direct study of ultra-high fields effecting bond-breaking and desorption at the level of single atoms using Density Functional Theory (DFT). As a prototype application, we consider field evaporation from a kinked W (110) surface. We reveal two qualitatively different competing mechanisms that can be switched by the applied field.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L41 GMAG: Magnetic dynamics and magnetic switching

Yabin Fan, Massachusetts Institute of Technology MIT - Tag(s): Focus
The coupling between electronic and magnetic phenomena was one of the riddles propelling the development of modern electromagnetism. Today, the fully controlled electric field evolution of ultrashort laser pulses permits the direct and ultrafast control of electronic properties of matter and is the cornerstone of light-wave electronics. In sharp contrast, because there is no first order interaction between light and spins, the magnetic properties of matter can only be affected indirectly on the much slower tens-of-femtosecond timescale in a sequence of optical excitation followed by the rearrangement of the spin structure.

I will discuss an experiment recording an orders of magnitude faster magnetic switching with sub-femtosecond response time by initiating optical excitations with near-single-cycle laser pulses in a ferromagnetic layer stack. The unfolding dynamics are tracked in real-time by a novel attosecond time-resolved magnetic circular dichroism (atto-MCD) detection scheme revealing optically induced spin and orbital momentum transfer (OISTR) in synchrony with light field driven charge relocation. In tandem with ab-initio quantum dynamical modelling, we show how this mechanism provides simultaneous control over electronic and magnetic properties that are at the heart of spintronic functionality. This first incarnation of attomagnetism observes light field coherent control of spin-dynamics in the initial non-dissipative temporal regime and paves the way towards coherent spintronic applications with Petahertz clock rates.
8:36AM L41.00002: Unification of ultrafast demagnetization and switching* GUOPING ZHANG (Presenter), M MURAKAMI, Y. H. BAI, Indiana State University, THOMAS F GEORGE, University of Missouri-St. Louis, XIAOSHAN WU, Nanjing University — All-optical spin switching and demagnetization are two sides of the same physics. We find a way to unify them through the same model that takes into account the Heisenberg exchange between spins and spin-orbit coupling. We include both the kinetic energy term and potential energy term, so that we can account for the realistic interaction between the laser and the system. To have efficient spin switching, the electron initial momentum direction must closely follow the spin's orientation, so that the orbital angular momentum is transverse to the spin, and consequently the spin-orbit torque lies in the same direction as the spin. Both left and right circularly polarized light have stronger but different effects in both uniform spin domains and The demagnetization can be understood from the spin-orbit coupling-mediated spin-wave excitation. The efficiency of laser-induced demagnetization is very high. We also observe the collapse of the spin-spin correlation length within 20 fs, consistent with the experimental findings.


*the U.S. Department of Energy under Contract No. DE-FG02-06ER46304.

8:48AM L41.00003: Ultrafast Magnetic Spectroscopy, Scattering and Full-Field Imaging Using Tabletop High Harmonic Sources* PETER JOHNSEN (Presenter), CHRISTIAN GENTRY, ROBERT M KARL, SINEAD RYAN, JEREMY THURSTON, HENRY KAPTEYN, MARGARET MURNANE, JILA — The observation and manipulation of spin dynamics on the nanoscale is a crucial ability in our quest to engineer quantum materials. We present spectroscopy, scattering, and full field imaging of magnetic nanostructures using EUV high harmonic sources. Our control of EUV polarization, spin and orbital angular momentum, along with high spatial and temporal coherence, allows us to uniquely control and probe spin dynamics on few-femtosecond timescales on up.

*STROBE NSF Science and Technology Center
NSF Graduate Research Fellowship Program
9:00AM L41.00004: Revealing angular momentum transfer channels and timescales in the ultrafast demagnetization process of ferromagnetic semiconductors  ZHANGHUI CHEN (Presenter), Lawrence Berkeley National Laboratory, JUN-WEI LUO, Chinese Academy of Sciences, LIN-WANG WANG, Lawrence Berkeley National Laboratory — Ultrafast control of magnetic order by light provides a promising realization for spintronic devices beyond Moore's Law. Here, we unravel the laser-induced demagnetization mechanism of ferromagnetic semiconductor GaMnAs, using an efficient time-dependent density functional theory approach that enables the direct real-time snapshot of the demagnetization process. Our results show a clear spin-transfer trajectory from the localized Mn-d electrons to itinerant carriers within 20 fs, illustrating the dominant role of \( sp-d \) interaction. We find that the total spin of localized electrons and itinerant carriers is not conserved in the presence of spin-orbit coupling (SOC). Immediately after laser excitation, a growing percentage of spin-angular momentum is quickly transferred to the electron orbital via SOC in about 1 ps, then slowly to the lattice via electron–phonon coupling in a few picoseconds. The spin-relaxation time via SOC is about 300 fs for itinerant carriers and about 700 fs for Mn-d electrons. These results provide a quantum-mechanical microscopic picture for the long-standing questions regarding the channels and timescales of spin transfer, as well as the roles of different interactions underlying the GaMnAs demagnetization process.

9:12AM L41.00005: Magnetic Entropy Dynamics in Ultrafast Demagnetization  SAHAR GOHARSHENASANESFAHANI (Presenter), SERBAN SMADICI, Univ of Louisville — Development of femtosecond laser sources and magneto-optical pump-probe techniques enabled measurements of ultrafast demagnetization in ferromagnets. It is necessary to measure two quantities to thermodynamically describe a magnetic state. In particular, measuring the magnetic entropy dynamics of a material in addition to its magnetization dynamics is crucial for fully understanding the transient magnetic state.

Time-resolved magneto-optical Kerr effect measurements of magnetization and magnetic entropy dynamics were made for ferromagnetic Co/Au/glass thin films. An intense 1030 nm pump pulse excited the film and a weak 515 nm time-delayed probe pulse was detected after reflecting off the sample. An external magnetic field was applied along the film surface. Different powers of the pump were used, increasing the film temperature to Curie temperature. Measurements revealed unexplored properties of the magnetic state at ultrafast timescales. Results will be compared to predictions of the Landau model and computer simulations.
9:24AM L41.00006: Analytic modeling of switching time dynamics of monodomain ferromagnets with biaxial energy landscape* ANKIT SHUKLA (Presenter), Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, ARUN PARTHASARATHY, Electrical and Computer Engineering, New York University, SHALOO RAKHEJA, Electrical and Computer Engineering, University of Illinois at Urbana-Champaign — Assuming the macrospin model, we develop analytic models to describe the magnetization dynamics of an in-plane-anisotropy ferromagnet driven by spin-transfer-torque with spin polarization collinear to the easy axis orientation. Thus far, the physics of in-plane magnets has been analyzed using numerical solution of the Landau Lifshitz Gilbert (LLG) equation, while analytic expressions of switching time probability, which are needed for memory design and optimization, are lacking. In the limit of small torque, low damping and zero temperature, we construct an average energy flow equation to describe the dynamics of the in-plane magnet. We approximate the elliptic integrals in the flow equation with rational functions and obtain the switching time of the magnetization as a function of energy landscape, material parameters, and input spin current. We also evaluate analytical expressions for switching time probability and cumulative distribution functions assuming a Boltzmann equilibrium distribution of magnetization in the initial energy basin. Good agreement between the model and numerically evaluated results based on Monte Carlo simulations of the LLG equation is demonstrated.

*This work is supported by the National Science Foundation Grant no. 1930620

9:36AM L41.00007: Elastic Properties of Encapsulation Epoxy for Vanadium Tetracyanoethylene Devices Measured Using Brillouin Light Scattering (BLS)* KATHERINE E. NYGREN (Presenter), Department of Physics, Colorado State University, ANDREW FRANSON, SETH KURFMAN, EZEKIEL JOHNSTON-HALPERIN, Department of Physics, The Ohio State University, KRISTEN S. BUCHANAN, Department of Physics, Colorado State University — The organic-based ferrimagnetic coordination compound vanadium tetracyanoethylene (VTCNE) shows promise for microwave applications because it has low damping, similar to that of yttrium iron garnet (YIG), it exhibits conformal deposition on a variety of substrates, and the deposition process does not require high temperatures, which allows for simple integration into large scale semiconductor fabrication processes. Like many organic materials, however, it is sensitive to oxygen. The use of organic-friendly epoxy for encapsulation is a common method for protecting the organic that can easily be integrated into device fabrication processes on a large scale, and epoxies that protect the VTCNE without compromising the damping have been identified. Recent measurements suggest, however, that the magnetic properties, particularly the anisotropy, of VTCNE may be sensitive to strain. Consequently, understanding the mechanical properties of the encapsulating epoxy under typical device conditions is important. Here, we have used Brillouin light scattering (BLS) spectroscopy to probe the elastic properties of the cured encapsulating epoxy via phonon spectra measurements as a function of the angle of incidence and light polarization.

*This work is supported by NSF-EFRI award #1741666.
Overcoming the spectroscopic limitations of inelastic light scattering by sub-diffraction light confinement

RYAN M FREEMAN (Presenter), Department of Physics, Emory University, VLADISLAV DEMIDOV, SERGEJ DEMOKRITOV, Institute for Applied Physics and Center for Nonlinear Science, University of Muenster, JINJUN DING, MINGZHONG WU, Department of Physics, Colorado State University, HAYK HARUTYUNYAN, SERGEI URAZHDIN, Department of Physics, Emory University — The small momentum of light strongly limits inelastic light scattering techniques. For instance, only long-wavelength spin waves are accessible to Brillouin light spectroscopy (BLS) widely utilized in studies of magnetic materials and nanostructures [1,2]. We overcome this limitation by utilizing a nanoscale metallic antenna on yttrium iron garnet (YIG) film. The antenna facilitates sub-diffraction confinement of light, generating momentum significantly larger than that of free-space light, and simultaneously enhances the local field due to a combination of geometric phase matching and optical reflection. We also present evidence for the plasmonic effects further enhancing the sensitivity and the spectral range. Our approach can be extended to other types of excitations and light scattering techniques. The demonstrated momentum enhancement can also facilitate light absorption in indirect-gap semiconductors, improving the efficiency of solar cells and optical detectors.


*R.F. and S.U. were supported by the NSF ECCS-1804198, J.D. and M.W – by NSF EFMA-1641989 and ECCS-1915849. The work by H.H. was supported by the US DOE Office of Science, BES Award DE-SC0020101.
10:00AM L41.00009: Terahertz emission from circular photogalvanic effect in bismuth thin films* YOSHUA HIRAI (Presenter), NAOTAKA YOSHIKAWA, HANA HIROSE, MASASHI KAWAGUCHI, MASAMITSU HAYASHI, Department of Physics, University of Tokyo, RYO SHIMANO, Cryogenic Research Center and Department of Physics, University of Tokyo — When circularly polarized light is shined onto a sample, optical selection rules lead to spin-dependent excitations. This can cause helicity-dependent spin-polarized photocurrents within the sample, referred to as the circular photogalvanic effect (CPGE). Bismuth is a highly expected material to host spin-dependent photocurrents, due to its large spin Hall angle and Rashba-like surface states. Recently, helicity dependent photocurrents have been demonstrated in bismuth/copper heterostructures by dc transport measurements [1]. Correspondingly, ultrafast transient photocurrents are expected to occur under the illumination of femtosecond laser pulses, resulting in the emission of terahertz (THz) pulse radiation. Here, we present the observation of THz emission from bismuth thin films under near-infrared (800 nm, 1.55 eV) pulse excitation. A polarization dependent THz emission is observed in both bismuth thin films and bismuth/metal heterostructures. The opposite polarities of the emitted THz pulse with the left/right-hand circular polarized excitation evidences the transient photocurrent with the opposite direction due to CPGE.


*This work was supported by JST CREST Grant Number JPMJCR19T3, Japan.

10:12AM L41.00010: Ultrafast Spin Seebeck Measurements on Rare-Earth Iron Garnets* VICTOR ORTIZ (Presenter), Physics and Astronomy, University of California, Riverside, MICHAEL J GOMEZ, Mechanical Engineering, University of California, Riverside, YAWEN LIU, MOHAMMED ALDOSARY, JING SHI, Physics and Astronomy, University of California, Riverside, RICHARD WILSON, Mechanical Engineering, University of California, Riverside — Understanding the thermal generation of spin currents in magnetic materials is an important goal for the field of spin caloritronics. Among magnetic materials, rare earth iron garnets (REIG) display intriguing magnetic transport properties as result of strong antiferromagnetic exchange interactions and low magnetic damping. We report on ultrafast longitudinal spin Seebeck effect (LSSE) experiments on thin film REIG / heavy metal (HM) heterostructures (RE: Y, Tm, Eu, Tb; HM: Au). We use time-resolved magneto optic Kerr effect measurements to directly observe the transfer of magnetization from the REIG into the HM on femto-second timescales, allowing us to selectively probe the interfacial SSE. We observe a factor of 4 difference in the magnitude of the LSSE among the different REIG samples. Our results provide insight regarding the different contributions to the spin current from the different REIGs and the relevance of the interface between the REIG and the HM layers.

*This work was supported by the U.S. Army Research Laboratory and the U.S. Army Research Office under contract/grant number W911NF-18-1-0364; and SHINES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award SC0012670.
10:24AM L41.00011: Controlled nonlinear magnetic damping in spin-Hall nano-devices*
BORIS DIVINSKIY (Presenter), Institute for Applied Physics and Center for Nonlinear Science, University of Muenster, SERGEI URAZHDIN, Department of Physics, Emory University, SERGEJ DEMOKRITOV, VLADISLAV DEMIDOV, Institute for Applied Physics and Center for Nonlinear Science, University of Muenster — One of the fundamental dynamical phenomena in magnetic systems is the nonlinear damping enhancement, which imposes strict limitations on the operation and efficiency of magnetic nanodevices. For instance, nonlinear damping prevents coherent magnetization auto-oscillations driven by the spin injection into spatially extended magnetic regions [1].
We utilize micro-focus Brillouin light spectroscopy (BLS) to demonstrate that nonlinear damping can be controlled by the ellipticity of magnetization precession. By balancing the demagnetizing field with the magnetic anisotropy in a Pt/Co/Ni heterostructure, we minimize ellipticity and achieve coherent magnetization oscillations in a microscopic CoNi disk, driven by spatially extended injection of spin current generated in Pt by the spin Hall effect. Micromagnetic simulations show that the mechanism responsible for the nonlinear damping is non-resonant parametric pumping enabled by the precession ellipticity. Our results provide a novel route for the implementation of efficient active spintronic and magnonic devices driven by spin current.


*Supported by the NSF award #ECCS-1804198

10:36AM L41.00012: Conductivity-Like Gilbert Damping due to Intraband Scattering in Epitaxial Iron*
BEHROUZ KHODADADI, Virginia Tech, ANISH RAI, ARJUN SAPKOTA, ABHISHEK SRIVASTAVA, BHUWAN NEPAL, University of Alabama, YOUNGMIN LIM, DAVID SMITH, Virginia Tech, CLAUDIA K.A. MEWES, SUJAN BUDHATHOKI, ADAM JOSEPH HAUSER, University of Alabama, MIN GAO, JIE-FANG LI, DWIGHT D VIEHLAND, ZIJIAN JIANG, JEAN J HEREMANS, Virginia Tech, PRASANNA V BALACHANDRAN, University of Virginia, TIM MEWES, University of Alabama, SATORU EMORI (Presenter), Virginia Tech — Confirming the origin of Gilbert damping by experiment has remained a challenge for many decades, even for some of the simplest ferromagnetic metals. Here, we experimentally identify Gilbert damping that increases with decreasing electronic scattering in thin films of BCC Fe. The observed conductivity-like damping, which cannot be accounted for by classical eddy current loss, is in excellent quantitative agreement with theoretical predictions of Gilbert damping due to intraband scattering. These results resolve the longstanding question since the 1970s about the role of intraband scattering in Gilbert damping. Our results also indicate that – somewhat counterintuitively – disorder can reduce intrinsic damping at low temperatures in ferromagnetic metals, such that optimally disordered films may be well suited for cryogenic spintronic and quantum applications.

*This research was funded in part by 4-VA, a collaborative partnership for advancing the Commonwealth of Virginia. A. Sapkota and C. Mewes would like to acknowledge support by NSF-CAREER Award No. 1452670, and A. Srivastava would like to acknowledge support by NASA Award No. CAN80NSSC18M0023.
Manipulation of terahertz spectrum using microfabricated magnetic heterostructures*  WEIPENG WU (Presenter), SERGI LENDINEZ, MOJTABA TAGHIPOUR KAFFASH, Department of Physics and Astronomy, University of Delaware, RICHARD D SCHALLER, Department of Chemistry, Northwestern University, HAIDAN WEN, Advanced Photon Source, Argonne National Laboratory, MATTHIAS BENJAMIN JUNGFLEISCH, Department of Physics and Astronomy, University of Delaware — Terahertz (THz) radiation with sub-micrometer wavelength falls in the gap between the optical and radio frequency range. Conventional THz emitters rely only on the electron's charge. However, recently it was found that spin-based effects occur on the ultrafast time scale. Upon excitation with a femtosecond laser pulse a diffusive spin current is created in a ferromagnet that leads to THz transients in an adjacent heavy metal layer due to a conversion by the inverse spin Hall effect. Here, we demonstrate generation and control of THz radiation from microstructured Fe/Pt bilayers. We compare the THz spectrum of different patterns and an extended film using time-domain THz spectroscopy. The microstructures are fabricated using optical lithography and sputtering deposition. The THz spectrum is experimentally observed and interpreted in terms of a simplified multi-slit diffraction model, which captures the main experimental features. Our results show an efficient control of the emitted THz light. This is a crucial step forward for the design and realization of directional spin-based THz sources.

*This work was supported by the National Science Foundation under Grant No. 1833000.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM

Session L42 GMAG DMP FIAP DCOMP: Spin Phenomena in Nonmagnetic 2D Materials 709/711 - Brian Zhou, Boston College - Tag(s): Focus

Extracting spin-orbit coupling strength using realistic device simulations  BAS NIJHOLT, Kavli Institute for Nanoscience, Delft University of Technology, P.O. Box 4056, 2600 GA Delft, The Netherlands, GEORG WINKLER (Presenter), JUKKA VAYRYNEN, Microsoft Quantum, Microsoft Station Q, University of California Santa Barbara, Santa Barbara, CA 93106, USA, GUANZHONG WANG, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands, GIJS DE LANGE, Microsoft Quantum Lab Delft, 2628 CJ, Delft, The Netherlands, LUCA BINCI, ALBERTO BORDIN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands, ROMAN LUTCHYN, Microsoft Quantum, Microsoft Station Q, University of California Santa Barbara, Santa Barbara, CA 93106, USA — We do realistic device simulations of semiconductor nanowires and calculate the weak antilocalization correction. We match our numerical simulation to magnetoconductance measurements and accurately extract the spin-orbit coupling strength from experiment. Unlike analytic approaches, our approach considers the electrostatic potential, works for arbitrary wire cross sections, and arbitrary finite mean free paths, including the complicated cross over regime where mean free path is comparable to wire width. After verifying our technique against known analytical results, we extract the spin-orbit coupling strength of semiconductor nanowires produced by selective area growth.
Far out-of-equilibrium spin populations trigger giant spin injection into atomically thin MoS$_2$  

EE MIN CHIA (Presenter), Nanyang Tech Univ — Injecting spins from ferromagnetic metals into semiconductors efficiently is a crucial step towards the seamless integration of charge- and spin-information processing in a single device. However, efficient spin injection into semiconductors has remained an elusive challenge due to the extremely low injection efficiencies originating from impedance mismatch, or technological challenges due to stability and cost issues. In Co/MoS$_2$, by making use of the strongly out-of-equilibrium character of the injected spins, we demonstrate a highly-efficient spin injection from a ferromagnet (Co) into a semiconductor (MoS$_2$), thus overcoming the crippling problem of impedance mismatch. Astonishingly, we measure a giant spin current that is orders of magnitude larger than typical injected spin current densities using currently available techniques. Our result demonstrates that technologically relevant spin currents can be driven by ultralow-intensity laser pulses, finally enabling ultrashort spin-current pulses to be a technologically viable information carrier for terahertz spintronics. *Nature Physics*, DOI:10.1038/s41567-018-0406-3 (2019).

*A*STAR PHAROS Programme on Topological Insulators (SERC Grant No. 152 74 00026) and 2D Materials (SERC Grant No. 152 70 00012 and 152 70 00016).

Introducing CVD WS$_2$ in Magnetic Tunnel Junctions  

VICTOR ZATKO (Presenter), MARTA GALBIATI, CNRS/THALES, SIMON MUTIEN-MARIE DUBOIS, Université Catholique de Louvain, Institute of Condensed Matter and Nanosciences, MAURO OCH, CECILIA MATTEVI, Department of Materials, Imperial College London, PIERRE BRUS, ODILE BEZENCENET, MARIE-BLANDINE MARTIN, BERNARD SERVET, Thales Research and Technology France, JEAN-CHRISTOPHE CHARLIER, Université Catholique de Louvain, Institute of Condensed Matter and Nanosciences, FLORIAN GODEL, FRÉDÉRIC PETROFF, ALBERT FERT, BRUNO DLUBAK, PIERRE SENEOR, CNRS/THALES — The use of the spin variable as the vector of information has been largely applied from hard drives read-heads to MRAMs, with novel propositions beyond spin-logics for neuromorphic, stochastic and quantum calculations. While very recent, the introduction of 2D materials such as graphene and the 2D insulator h-BN in Magnetic Tunnel Junctions (MTJs) vertical spin valves has already shown some promising properties[1]. The advent of the 2D semiconductors families opened new opportunities for further tailoring of spintronics properties[2]. Here, we will present results on the scarcely studied WS$_2$ 2D semiconductor for spintronics. We will detail a protocol to fabricate spin valves based on CVD grown WS$_2$, with step by step characterizations in support (Raman spectroscopy, photoluminescence, AFM). We will then present our spin transport measurements obtained in a CVD WS$_2$ based MTJ. Our measured MR signals, above state of the art for 2D semiconductor based MTJs, validates our fabrication approach. These results open the way to the integration of different members of the very large 2D semiconductor families, TMDC and beyond, in order to reveal their spin transport properties in MTJs.

Defect induced magnetism in monolayer semiconducting PtSe$_2$  

AHMET AVSAR (Presenter), CHEOL-YEON CHEON, MICHELE PIZZOCHERO, ALBERTO CIARROCCHI, OLEG V. YAZYEV, ANDRAS KIS, Ecole Polytechnique Federale de Lausanne — Intrinsic disorders such as metal vacancies and antisites in 2D TMDCs are generally accompanied by local magnetic moments which could induce long range magnetic ordering if disorder concentration is sufficient. Towards this, we have recently shown that platinum (Pt) vacancy defects located at the surfaces of multilayer metallic PtSe$_2$ act as magnetic centers [1]. For both fundamental studies and technological applications, it is critical to explore magnetism in ultra-thin PtSe$_2$ as this material shows a complete switching from a metal to a semiconductor as its thickness is reduced [2]. Here, we will present our magneto-transport measurements together with first-principles calculations which clearly demonstrate that Pt vacancy defect yields an antiferro- (ferro-)magnetic ordering in mono (bi-)layer PtSe$_2$. We will also demonstrate that these air-stable crystals can be employed as a magnetic substrate to induce novel proximity phenomena into adjacent nonmagnetic layers. Our findings broaden the horizon of 2D magnets to include normally nonmagnetic stable materials by defect engineering.


Weak anti-localization in undoped Ge/GeSn heterostructures*  

JIUN-YUN LI, CHIA-TSE TAI (Presenter), CHENG-YU LIN, CHIA-YOU LIU, TZU-MING WANG, Natl Taiwan Univ, CHARLES HARRIS, TZU-MING LU, Sandia National Laboratories — In this work, we demonstrate weak anti-localization (WAL) in undoped Ge/GeSn heterostructures. We used gated Hall-bar devices to induce two-dimensional hole gases (2DHGs) in strained GeSn quantum wells for magnetotransport experiment at 1.2 to 10 K. Transition from weak localization to WAL is observed as the density increases due to density dependent spin-orbit coupling. By fitting to the HLN formula, phase coherence and spin-orbit times of 2DHGs as well as the spin-orbit splitting energy in undoped Ge/GeSn heterostructures are extracted. Our data show that the scattering lifetime is shorter than the spin-orbit time at all densities, indicating that the system is in the spin-diffusive regime.

*This work at NTU was supported by MOST (107-2112-M-002-014- and 108-2112-M-002-011-) and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy (DOE), Office of Basic Energy Sciences user facility. Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. DOE’s National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.
**9:00AM L42.00006: Magnetic order and anisotropy at 3d ferromagnet/2D material heterojunctions**

DER-HSIN WEI (Presenter), Scientific Research Division, National Synchrotron Radiation Research Center, CHUN-I LU, Department of Physics, National Taiwan Normal University, CHIH-HENG HUANG, International PhD Program for Science, National Sun Yat-sen University, YANNWEN LAN, Department of Physics, National Taiwan Normal University, CHIEN-CHEN KUO, Department of Physics, National Sun Yat-sen University, TZU-HUNG CHUANG, Scientific Research Division, National Synchrotron Radiation Research Center — Layered (opto-)electronic devices integrated with two dimensional (2D) materials is an exciting research field that packs with new possibilities and challenges. For example, a high spin injection efficiency from ferromagnetic (FM) electrode to 2D-materials is thought possible, but it needs to work with the complex orbital hybridization and proximity effect at heterojunctions. Here we report the magnetic properties of two 3d ferromagnet/2D material heterojunctions; Co/MoS$_2$ and Fe/graphene. Both macroscopic magnetic orders and microscopic magnetic configurations of these two heterojunctions are examined. In addition, the interplay between FM materials and 2D materials are studied with the X-ray micro-spectroscopy. We find a heterojunction can exhibit the magnetic anisotropy, but it seems crystalline structure of FM layer is not responsible for it. I will present the experimental data followed by a brief discussion.

*Supported by MOST 107-2112-M-213-003-MY3, and National Synchrotron Radiation Research Center

**9:12AM L42.00007: Spin-to-charge interconversion in van der Waals heterostructures** [Invited]

CK SAFEER (Presenter), CIC NanoGUNE, San seanstan, Spain — Graphene has been known as an excellent material for long-distance spin transport due to its weak spin-orbit coupling (SOC). However, the same reason makes graphene an adverse candidate for different spintronics applications in which strong SOC is required, such as the Datta and Das proposal or spin-charge interconversions. It has recently been predicted theoretically that SOC can be induced in graphene so that exotic spin-orbit phenomena such as spin Hall effect (SHE) or Rashba-Edelstein effect can be obtained. In our work, by using van der Waals heterostructure-based lateral spin valves, we experimentally demonstrate spin-to-charge conversion (SCC) due to SHE in graphene via spin-orbit proximity with MoS$_2$, a transition metal dichalcogenide (TMD)$^1$. The combination of long-distance spin transport and large spin-to-charge conversion in a van der Waals heterostructure gives rise to a hitherto unreported efficiency for the spin-to-charge voltage output. Using a similar approach, we observed large multidirectional SCC in Weyl semimetal MoTe$_2$. Here, due to the low symmetry of MoTe$_2$ crystal, we detect, along with the conventional SCC, an unconventional SCC where the spin polarization and the charge current are parallel. Our finding enables the simultaneous conversion of spin currents with any in-plane spin polarization in one single experimental configuration. All in all, these exceptional effects obtained by the unique properties of 2D materials open exciting opportunities in a variety of future spintronic applications.

Two-dimensional spin-valley locking spin valve

LINGLING TAO (Presenter),
EVGENY Y TSYMBAL, Department of Physics and Astronomy, University of Nebraska-Lincoln —

Valleytronics is an emerging field of research which employs energy valleys in the band structure of two-dimensional (2D) electronic materials to encode information. A special interest has been triggered by the associated spin-valley coupling which reveals rich fundamental physics and enables new functionalities. Here, we propose exploiting the spin-valley locking in 2D materials with a large spin-orbit coupling and electric field reversible valley spin polarization, such as germanene, stanene, a 1T' transition metal dichalcogenide (TMDC) monolayer, and a 2H-TMDC bilayer, to realize a valley spin valve (VSV). The valley spin polarization in these materials can be switched by an external electric field, which enables functionalities of a valley spin polarizer or a valley spin analyzer. When placed in series, they constitute the proposed VSV—a device whose conductance state is ON or OFF depending on the relative valley spin polarization of the polarizer and the analyzer. Using quantum-transport calculations based on an adequate tight-binding model, we predict a giant VSV ratio of nearly 100% for both germanene- and stanene-based VSV devices. Our results demonstrate the implication of the spin-valley coupling in 2D materials for the novel device concept promising for valleytronics.

Group-IV tellurides as a route towards all-in-one spin transistors

JAGODA SLAWINSKA (Presenter), FRANK T CERASOLI, PRIYA GOPAL, Univ of North Texas, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, Univ of North Texas —

Simple displacive ferroelectrics GeTe and SnTe have been studied for decades but their intriguing physics based on spin-orbit coupling remained unexplored until few years ago. In particular, they are prototype examples of ferroelectric Rashba semiconductors, a class of materials in which the unique coupling between spin and polar degrees of freedom enables the electrical manipulation of spins. Such a property, combined with a sizable spin Hall effect recently predicted in these materials opens a perspective to integrate different functionalities and construct ferromagnets-free spin devices. Here, we reveal even more intriguing phenomena emerging at the limit of the monolayer. More specifically, we explore the persistent spin texture intrinsically present in the ferroelectric phase which protects the spin from decoherence and supports extraordinarily long spin lifetime. Our first-principles calculations followed by symmetry arguments revealed that such a spin wave mode can be externally detuned by perpendicular electric field, leading to spin randomization and decrease in spin lifetime. We propose this mechanism as an operation principle of an all-in-one spin transistor, in which spin injection/detection can be accomplished via spin Hall effects.
10:12AM L42.00010: Atomically-resolved theory of the magnitude of the bulk Rashba effect* CARLOS MERA (Presenter), University of Colorado, Boulder, ELTON OGOSHI, ABC university, Santo Andre, SP, Brazil, ADALBERTO FAZZIO, Brazilian Nanotechnology National Laboratory, Campinas, SP, Brazil, GUSTAVO M. DALPIAN, ABC university, Santo Andre, SP, Brazil, ALEX ZUNGER, University of Colorado, Boulder — Rashba effect based-mechanisms to control and generate spin-polarized states have been one of the cornerstones of spintronics. A strong Rashba effect -- as measured by the Rashba coefficient $\alpha_R$ -- is required for applications. However, the physical mechanism defining the $R$ scale, i.e., the magnitude of $\alpha_R$, is unknown. We find an intrinsic separation between strong Rashba effect associated with anti-crossing bands, and weak Rashba effect associated with no anti-crossing bands. As an application of the proposed theory, we use this design principle to guide the selection of strong Rashba compounds. First, we illustrate that since topological insulators (TIs) intrinsically have anti-crossing bands, strong Rashba compounds could then be identified almost effortlessly by isolating TIs that are non-centrosymmetric, thus establishing a case for cross-functionality of topological Rashba materials. Second, we predict 34 strong Rashba materials by performing DFT calculations for ~800 potential Rashba compounds and filtering those with anti-crossing bands. This reveals rationally designed cases including known GeTe and BiTeI, and compounds that were previously made but unnoticed as Rashba compounds BiTeCl ($P6_3mc$) and BaCdK2Sb2 ($Pmc2_1$).

*Supported by NSF-DMR-CMMT and FAPESP (Grant 19/03663-7).

10:24AM L42.00011: All-electrical creation and control of giant spin-galvanic effect in 1T’-MoTe$_2$/graphene heterostructures at room temperature MD ANAMUL HOQUE (Presenter), DMITRII KHOKHRIAKOV, BOGDAN KARPIAK, SAROJ DASH, Chalmers Univ of Tech — The ability to engineer new states of matter and to control their electronic and spintronic properties by electric fields is at the heart of the modern information technology and driving force behind recent advances in van der Waals (vdW) heterostructures of two-dimensional materials. Here, we exploit a proximity-induced Rashba-Edelstein (REE) effect in vdW heterostructures of Weyl semimetal candidate MoTe$_2$ and CVD graphene, where an unprecedented gate-controlled switching of spin-galvanic effect emerges due to an efficient spin-to-charge conversion at room temperature [1]. The magnitude of the measured spin-galvanic signal is found to be an order of magnitude larger than the other systems, giving rise to a giant REE. The magnitude and the sign of the spin-galvanic signal are shown to be strongly modulated by gate electric field near the charge neutrality point, which can be understood considering the spin textures of the Rashba spin-orbit coupling-induced spin-splitting in conduction and valence bands of the heterostructure. These findings open opportunities for utilization of gate-controlled switching of spin-galvanic effects in spintronic memory and logic technologies.

References:
10:36AM L42.00012: Highly tunable nonlinear Hall effects induced by spin-orbit couplings in strained polar transition-metal dichalcogenides* CHENG-PING ZHANG (Presenter), TONG ZHOU, KAM TUEN LAW, Hong Kong University of Science and Technology — Recently, signatures of nonlinear Hall effects induced by Berry curvature dipoles have been found in atomically thin 1T'/T_d-WTe_2. In this work, we show that in strained polar transition-metal dichalcogenides (TMDs) with 2H-structures, Berry curvature dipoles created by spin degrees of freedom lead to strong nonlinear Hall effects. Under easily accessible uniaxial strain of order ~ 0.2%, strong nonlinear Hall signals, characterized by Berry curvature dipole in the order of ~ 1Å, arise in electron-doped polar TMDs such as MoSSe, which is easily detectable experimentally. Moreover, the magnitude and sign of the nonlinear Hall current can be easily tuned by electric gating and strain. These properties can be used to distinguish nonlinear Hall effects from classical mechanisms such as ratchet effects. Importantly, our system provides a potential scheme for building electrically switchable energy harvesting rectifiers.

*KTL acknowledges the support of Croucher Foundation, Dr. Tai-chin Lo Foundation and HKRGC through C6026-16W, 16309718, 16307117 and 16324216.

L42.00013: Research on the valley-related properties based on multilayer transition metal dichalcogenides HONGMING GUAN (Presenter), NING TANG, XIAOYUE ZHANG, XINGCHEN LIU, WEIKUN GE, BO SHEN, State Key Laboratory of Artificial Microstructure and Mesoscopic Physics, School of Physics, Peking Univ — Monolayer transition metal dichalcogenides (TMDCs), owing to the unique valley-related phenomena, have aroused great attention. However, in multilayer TMDCs, for the presence of the spatial-inversion symmetry, the valley-related phenomena are absent, which limits the developments of valleytronics. In this report, by utilizing the ionic liquid (IL) covering on top of the multilayer TMDC samples, the spatial-inversion symmetry is broken by the out-of-plane electric field induced by IL. The valley-related properties are therefore induced. Firstly, we investigated the circular photogalvanic effect (CPGE) in multilayer MoS_2. Upon the electric field induced by IL, the valley-coupled CPGE signals emerge. Via the wavelength-dependent measurements, it is confirmed only with resonant excitation of K (K') valley can the CPGE signals be detected. Furtherly, we studied the circular photon assisted valley Hall effect in multilayer WSe_2. With the application of IL, a Hall-oriented photocurrent signal in proportional to the drain-source voltage is detected, illustrating the valley Hall effect is successfully observed. These results imply the valley degree of freedom could be reborn in multilayer TMDCs.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L43 DCOMP DMP DCP: First-principles modeling of excited-state phenomena in materials VII: Electronic excitations: DFT and Beyond 702 - Michiel van Setten, IMEC - Tag(s): Focus
Transition to metallization in warm dense helium-hydrogen mixtures using stochastic density functional theory* [Invited] YAEL CYTTER, The Hebrew University of Jerusalem, ERAN RABANI (Presenter), University of California, Berkeley, DANIEL NEUHAUSER, University of California, Los Angeles, MARTIN PREISING, RONALD A. REDMER, University of Rostock, ROI BAER, The Hebrew University of Jerusalem — The Kubo-Greenwood (KG) formula is often used in conjunction with Kohn-Sham (KS) density functional theory (DFT) to compute the optical conductivity, particularly for warm dense matter. For applying the KG formula, all KS eigenstates and eigenvalues up to an energy cutoff are required and thus the approach becomes computationally expensive, especially for high temperatures and large systems, scaling cubically with both system size and temperature.

In this talk, I will review our recent developments to calculate the KS conductivity within the stochastic DFT framework, which requires knowledge only of the KS Hamiltonian but not its eigenstates and values. The method allows for an accurate description of the entire spectrum, including the high-frequency range, unlike the deterministic method which is compelled to introduce a high-frequency cutoff due to memory and computational time constraints. The computational effort associated with the method scales linearly with system size and reduces in proportion to the temperature, unlike the cubic increase with traditional deterministic approaches.

We applied the method to helium-hydrogen mixtures in the warm dense matter regime at temperatures of \( \sim 60,000 \) K and find that the system displays two conductivity phases, where a transition from nonmetal to metal occurs when hydrogen atoms constitute \( \sim 0.3 \) of the total atoms in the system.

*Work supported in part by the Center for Computational Study of Excited State Phenomena in Energy Materials (C2SEPEM) at the Lawrence Berkeley National Laboratory, which is funded by the U.S. Department of Energy, Office of Science, Basic energy Sciences, Materials Sciences and Engineering Division under Contract No. DEAC02-05CH11231 as part of the Computational Materials Sciences Program.
Towards a systematic multi-scale method for excitations in molecular materials in the BigDFT code

MARTINA STELLA (Presenter), LAURA E RATCLIFF, Imperial College London, LUIGI GENOVESE, CEA Grenoble Center, France — Understanding excitations is critical in spectroscopy as well as in technological applications, e.g. identifying where excited states lay for molecules in crystals is crucial for guiding experimentalists in locating excitation sources. Another example is thermally activated delayed fluorescence (TADF), a mechanism for designing the next generation of OLEDs (Organic Light Emitting Diodes materials) that are less environmentally harmful than the previous generation. Excitations in TADF materials exhibit an intricate mixture of charge-transfer and local nature and can be strongly influenced by the host material.

Modelling TADF (e.g identifying the best performing material) or locating excited states, thus, requires an accurate methodology that explicitly includes environmental effects. We are developing a multi-scale approach in the BigDFT code where high accuracy is combined with the ability of treating big systems to eventually go beyond implicit models. BigDFT runs on parallel architectures and can treat large systems with high, controllable precision. As a first step towards a robust methodology, we assess the performance of a promising new constrained-DFT approach recently developed in our group for various classes of excitations in comparison to standard methods (TDDFT).

*EPSRC

MuST: An integrated ab initio framework for the study of disordered structures

YANG WANG (Presenter), Pittsburgh Supercomput Ctr, Carnegie Mellon University, MARKUS EISENBACH, XIANGLIN LIU, Oak Ridge National Laboratory, KHORGOLKUHU ODBADRAKH, University of Tennessee Knoxville, HANNA TERLETSKA, Department of Physics, Middle Tennessee State University, KA-MING TAM, Department of Physics, Louisiana State University, YI ZHANG, University of the Chinese Academy of Sciences, LIVIU CHIONCEL, Institute of Physics, University of Augsburg — The effect of disorder in materials is of great fundamental and technological interest. In this presentation, I will introduce a new public software package, called MuST, designed for enabling first principles investigation of disordered materials. MuST is developed based on full-potential multiple scattering theory with Green function approach, and is built upon decades of development of research codes that include Korringa-Kohn-Rostoker Coherent Potential Approximation (KKR-CPA), a highly efficient ab initio method for the study of random alloys, and Locally Self-consistent Multiple Scattering (LSMS) method, a linear scaling ab initio code capable of treating extremely large disordered systems from the first principles using the largest parallel supercomputers available. Strong disorder and localization effects can also be studied in real system within the LSMS formalism with cluster embedding in an effective medium with the Typical Medium Dynamical Cluster Approximation (TMDCA), which enables a scalable approach for first principles studies of quantum materials.

*This work is jointly supported by the NSF OCA and DMR under award number 1931525/1931367/1931445, and is supported in parts by the Office of Science of DOE and the LDRD Program of ORNL.
9:00AM L43.00004: Understanding the chemical enhancement mechanism of 2D substrate enhanced Raman Spectroscopy (2D-SERS). KANCHAN ULMAN (Presenter), SU YING QUEK, Natl Univ of Singapore — Surface-enhanced Raman spectroscopy (SERS) is a well established field which utilizes the enhancement of Raman signals for molecules on metal substrates, resulting in applications of this phenomena for detection and identification of trace concentrations of molecules. In recent years, two-dimensional (2D) materials like graphene, h-BN and MoS$_2$ are being used as substrates for SERS, giving rise to rapidly growing field of 2D-substrate enhanced Raman spectroscopy (2D-SERS). In conventional SERS, the enhancement factor is dominated by an electromagnetic enhancement mechanism, as compared to the smaller chemical enhancement effect. In 2D-SERS however, this chemical enhancement effect (which stems from electron-phonon coupling within the molecule and substrate) is thought to play a dominating role. Yet, the detailed understanding of the chemical enhancement effect in 2D-SERS is still lacking. Using first principles calculations, we study the chemical enhancement mechanism using typical probe molecules such as pyridine and pthalocyanine on 2D substrates, highlighting the role of electron-phonon coupling and charge-transfer excitons in the chemical enhancement mechanism of 2D-SERS.

9:12AM L43.00005: Local mixing in modified Becke-Johnson potential for low-dimensional systems TOMAS RAUCH (Presenter), IFTO, FSU Jena, Germany, MIGUEL MARQUES, Institute of Physics, MLU Halle-Wittenberg, Germany, SILVANA BOTTI, IFTO, FSU Jena, Germany — We propose an extension to the modified Becke-Johnson potential [1] that enables its use to study both heterogeneous and low-dimensional systems. This is achieved by using a coordinate-dependent expression for the $c$ parameter, in contrast to the original global formulation. Our functional builds on the excellent description of bulk band gaps of the modified Becke-Johnson potential and preserves its modest computational effort. Furthermore, it yields with one single calculation band-diagrams and band-offsets of heterostructures, interfaces, and surfaces. We exemplify the usefulness and efficiency of our local functional by testing it for a series of semiconductor interfaces, surfaces, two-dimensional systems, and molecules.

9:24AM L43.00006: Periodic Electronic Structure Calculations With Density Matrix Embedding Theory*  
HUNG Q PHAM, MATTHEW R HERMES, LAURA GAGLIARDI (Presenter), University of Minnesota — We developed a periodic version of density matrix embedding theory, DMET, with which it is possible to perform electronic structure calculations on periodic systems, and compute the band structure of solid-state materials. Electron correlation can be captured by means of a local impurity model using various wave function methods, like, for example, full configuration interaction, coupled cluster and multiconfigurational methods. The method is able to describe not only the ground-state energy but also the quasiparticle band picture via the real-momentum space implementation. We investigate the performance of periodic DMET in describing the ground-state energy as well as the electronic band structure for one-dimensional solids. Our results show that DMET is in good agreement with other many-body techniques at a cheaper computational cost. We anticipate that periodic DMET can be a promising first principle method for strongly correlated materials.

*This research is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences under Award DEFG02-17ER16362.

9:36AM L43.00007: Density Functional Theory-based study of charge transfer in doped silicon nanowire with gold leads: A toy model for the p-n junction photovoltaic device  
NATHAN WALKER (Presenter), DMITRI KILIN, ANDREI KRYJEVSKI, North Dakota State Univ — We analyze a toy model for p-n junction photovoltaic devices by simulating photoexcited state dynamics in silicon nanowires doped with aluminum and phosphorus atoms and capped with gold leads. We use Boltzmann transport equation (BE) that includes phonon emission, carrier multiplication (CM), and exciton transfer. BE rates are computed using non-equilibrium finite-temperature many-body perturbation theory (MBPT) based on Density Functional Theory simulations, including excitonic effects from Bethe-Salpeter Equation (see A. Kryjevski, D. Mihaylov, and D. Kilin, J. of Phys. Chem. Lett., 9(19) (2018), A. Kryjevski, D.Mihaylov, S. Kilina, and D. Kilin, J. of Chem. Phys., 147, 154106 (2017)). We compute total charge transfer amount generated from the initial photoexcitation and find an enhancement when CM is included.
**9:48AM L43.00008: Hj-Aggregate Theory Applied to Interacting SP³-Hybridization Defects in Carbon Nanotubes**  
BRADEN WEIGHT (Presenter), Department of Physics, North Dakota State University, ANDREW E SIFAIN, US Army Research Laboratory, BRENDAN J GIFFORD, Center for Nonlinear Studies, Los Alamos National Laboratory, SVETLANA KILINA, Department of Chemistry and Biochemistry, North Dakota State University, SERGEI TRETIAK, Center for Nonlinear Studies, Los Alamos National Laboratory — Single-walled carbon nanotubes (CNTs) have been recently studied in greater depth due to their promise of superior electronic properties for tunable emission of infrared energies. Optical features of functionalized CNTs (via SP³-hybridization defects) have been narrowed to only a few main parameters: (I) chirality, (II) defect configuration, and (III) defect electronegativity. Previous theoretical studies have been directed at single defects (comprised of a pair of functional groups) attached to the CNT surface, and, until recently, no literature has discussed the effects of defect concentration on CNTs in any depth [1,2]. In this work, we aim to model the interactions between nearby defects using density functional theory (DFT) and, extending to excited states, time-dependent DFT (TD-DFT) in order to fit these interactions to a well-known descriptor of analogous systems known as Hj-aggregate theory.


*Los Alamos National Laboratory LDRD Program*

**10:00AM L43.00009: Identifying sources of error in finite temperature calculations for molecules and solids using density matrix quantum Monte Carlo**  
HAYLEY PETRAS, SAI RAMADUGU, JAMES SHEPHERD (Presenter), Department of Chemistry, University of Iowa — Density matrix quantum Monte Carlo (DMQMC) calculates exact-on-average finite temperature electronic energies in a finite basis. This method has shown promise when applied to model systems like the electron gas (Phys. Rev. Lett. 117, 115701) but it is not well understood whether these findings are transferrable to real systems and to what extent strong correlation can affect our ability to run calculations on a system. Calculations on small molecules and solids (in a periodic basis set) will be presented including a resolution to previous convergence issues for the H10 chain. Finally, the computational cost scaling of DMQMC will be identified.

*We acknowledge the University of Iowa for funding.*
10:12AM L43.00010: Dynamical configuration interaction study of free base porphyrin*
MARC DVORAK (Presenter), PATRICK RINKE, Aalto University — We apply the recently developed dynamical configuration interaction (DCI) theory to study the low-lying excited states of free base porphyrin. In DCI [1,2], we diagonalize the exact many-body Hamiltonian in the strongly-correlated active space with the wave function technique of configuration interaction (CI). Additionally, the effects of the surrounding degrees of freedom are downfolded onto an energy-dependent correction added to the bare CI Hamiltonian. These corrections are approximated with many-body Green's function theory in the GW approximation. Free-base porphyrin is the largest system studied with DCI so far and serves as an important test of the numerical implementation, scalability, and size consistency of the theory. Our DCI results for excitation energies of porphyrin are in good agreement with past work.


*This work is supported by the Academy of Finland grant no. 316347.

10:24AM L43.00011: Light driven Non-Thermal Amorphization Mechanism of Phase Change Material*
SUBODH TIWARI (Presenter), AIICHIRO NAKANO, Univ of Southern California, FUYUKI SHIMOJO, Department of Physics, Kumamoto University, RAJIV KALIA, PAULO BRANICIO, PRIYA VASHISHTA, Univ of Southern California — Phase-change materials (PCM) are exploited in modern electronics due to the extreme electro-optical contrast between crystalline and amorphous states. However, atomistic mechanisms governing photoexcitation-induced athermal amorphization processes are still unknown. We perform excited-state dynamics within the framework of density functional theory to understand the mechanism behind such crystalline-to-amorphous transition for Germanium Telluride (GeTe). Amorphous phase induced due to excited-state dynamics was characterized by computing diffraction pattern. Further analysis of bond-overlap population shows charge transfer of electron from Ge-Te bonding orbitals to Ge-Ge antibonding orbitals. Such charge transfer process leads to the destabilization of GeTe crystals, eventually leading to amorphization. Rapid heat extraction during excited-state simulation does not lead to amorphous phase. Since structural transformation limits the lifetime of PCM-based devices, a complete understanding behind mechanism may allow us to a new avenue to design better devices.

*This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC0014607
First Principles Simulations of Hg$_x$Cd$_{1-x}$(S,Se) Optical Properties*  
ERICK HERNANDEZ ALVAREZ (Presenter), ANDREW MICHAEL SMITH, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Mercury cadmium chalcogenide alloy quantum dots (QDs) are a promising material to meet the rapidly growing need for materials with emission in the biological near-infrared (NIR) window (700-2,000 nm) where tissue transparency is high and autofluorescence noise is low. Cation exchange-mediated alloying is an effective way to tune the QD emission wavelength continuously across the entire visible and NIR spectra without altering the QD’s physical dimensions. Here we describe the optical properties of zinc blende Hg$_x$Cd$_{1-x}$S and Hg$_x$Cd$_{1-x}$Se alloys from first principles simulations across the compositional space. We use density functional theory to compute electronic band structures of the binary mercury and cadmium chalcogenide systems and their intermediate ternary alloys. We then compute the corresponding optical spectra and describe the extent of the effect of spin-orbit coupling on the calculated photophysical properties. Comparison to measured absorption spectra of mercury cadmium chalcogenide alloy QDs provides insights into how photophysical parameters can be achieved with specific compositions and nanocrystal sizes.

*Support by the National Science Foundation Graduate Research Fellowship Program

DFT: the lore of smoothing and tetrahedra is wrong*  
JEREMY JORGENSEN (Presenter), GUS HART, Brigham Young Univ - Provo — Smoothing and tetrahedron methods in density functional theory (DFT) codes were developed to improve the robustness and efficiency of DFT codes. Tests we have performed demonstrate that both methods fail to accomplish either assertion. We have run ~20,000 DFT calculations in VASP and Quantum Espresso with various types and amounts of smoothing on 12 metals. The rate of convergence of the total energy for calculations with smoothing is often worse than those without smoothing, and smoothing does not result in a reduction in the number of self-consistency cycles when compared to runs without smoothing. We obtained similar results in comparisons involving tetrahedron methods.

*Funding from ONR (MURI N00014-13-1-0635)
8:00AM L44.00001: Beyond Fourier's law: viscous heat equations [Invited] ANDREA CEPELLOTTI (Presenter), School of Engineering and Applied Sciences, Harvard University — Heat hydrodynamics is undergoing a renewed wave of interest, after it has been theoretically proposed to take place in 2D materials and recent experimental observations in graphite. In particular, heat hydrodynamics emerges when the momentum carried by phonons is weakly dissipated, making it possible, for example, to observe second-sound, a wave-like propagation of heat. The macroscopic description of this regime, however, is still object of investigations, as the commonly used Fourier’s law isn’t capable of describing hydrodynamic transport.

In this talk, we will first introduce a first-principles formalism to compute the thermal viscosity, the transport coefficient determining the diffusion of momentum (as opposed to thermal conductivity, which describes energy diffusion). Using an exact solution of the phonon Boltzmann transport equation (BTE) based on relaxons, the eigenvectors of the scattering matrix, we show how the thermal viscosity is fully determined by the even part of the relaxon spectrum, whereas the odd part describes thermal conductivity.

Next, we show that thermal conductivity and viscosity parametrize a set of viscous heat equations, the thermal counterpart of the Navier-Stokes equations in the linear and laminar regime, with heat transport being described in terms of temperature and drift-velocity fields. These equations reduce to Fourier’s law in the limit of strong momentum dissipation, yet, if momentum dissipation is weak, can also describe second sound. These equations can be parametrized with first-principles calculations, and then solved at a similar complexity of Fourier’s law. We test the formalism on silicon, diamond and graphite, replicating for graphite the experimental observations of a hydrodynamic window and suggesting the existence of hydrodynamic transport in diamond. These equations pave the way to the description of heat transport in devices at the mesoscale.

8:36AM L44.00002: Quantum thermal transport in glasses: the role of anharmonicity
MICHELE SIMONCELLI (Presenter), Ecole Polytechnique Federale de Lausanne, FRANCESCO MAURI, Physics, Sapienza University of Rome, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne — Thermal transport in glasses is often described by the harmonic theory introduced by Allen and Feldman [Phys. Rev. Lett., 62(6) (1989)], where heat is carried by couplings between vibrational modes and disorder limits the thermal conductivity. Hitherto, the effects of anharmonicity on heat conduction in glasses have been investigated using molecular simulations, combined with empirical quantum corrections to address discrepancies with experiments at low temperature. Recently, a unified theory of thermal transport in crystals and glasses has been formulated [Simoncelli, Marzari, and Mauri, Nat. Phys., 15 (2019)], allowing to account rigorously for quantum and anharmonic effects also in glassy or disordered systems. Here, we show that quantum effects and anharmonicity are crucial to explain the increasing non-saturating trend of the thermal conductivity with temperature observed in silica glass --- and not explained by the saturating Allen-Feldman harmonic theory. We analyze amorphous silica as a prototypical glass and provide recipes to perform first-principles quantum thermal conductivity calculations in glasses, which are accurate over a wide temperature range.

*Research supported by the NCCR MARVEL, funded by the Swiss National Science Foundation.
8:48AM L44.00003: Thermal transport modeling of nanoscale graphene devices using a Peierls-Boltzmann treatment  ALI KEFAYATI (Presenter), State Univ of NY - Buffalo, PHILIP ALLEN, Department of Physics and Astronomy, Stony Brook University, VASILI PEREBEINOS, State Univ of NY - Buffalo — In nonmagnetic insulators, phonons are the carriers of heat. If heat enters in a region and temperature is measured at a point within a phonon mean free paths of the heated region, ballistic propagation causes a nonlocal relation between local temperature and heat insertion. Our work focuses on the solution of the Peierls-Boltzmann equation (PBE) for nanoscale graphene devices. We use a realistic anharmonic scattering potential and examine different approximations such as the relaxation time approximation and the definition of local temperature. The results illustrate the expected local (diffusive) response for minimum phonon mean free path \(\lambda_{\text{min}} \ll L\), and a diffusive to ballistic crossover as \(\lambda_{\text{min}}\) increases toward the scale of the device size \(L\).

9:00AM L44.00004: Heat transport in resonant condensed systems: Thermal conductivity reduction by coherent mechanisms* [Invited]  MAHMOUD I. HUSSEIN (Presenter), CHIA-NIEN TSAI, HOSSEIN HONARVAR, University of Colorado, Boulder — The notion of a locally resonant metamaterial—widely applied to light and sound—has recently been introduced to heat, whereby the thermal conductivity is reduced primarily by intrinsic localized atomic vibrations (vibrons) rather than scattering mechanisms. The localized vibration modes manifest by the introduction of intrinsic nanoresonators within, or attached to, a host crystalline material, ideally a semiconductor. The phonon band structure under such conditions exhibit a myriad of horizontal bands representing each resonant degree of freedom. These bands hybridize with the underlying phonon modes carrying the heat in the host medium, which leads to significant reductions in the phonon group velocities and to mode localizations within the nanoresonators. Moderate reductions in the phonon lifetimes also occur. The nature of nanoscale thermal conduction under such conditions is fundamentally transformed due to these effects. A key requirement for the realization of phonon-vibron couplings and the subsequent effects mentioned above is the presence of a sufficient level of coherent wave behavior, which is only possible when there is a relatively wide distribution of the phonon mean free path. An example of a “nanophononic metamaterial” is a silicon membrane with nanopillars distributed on the surface. In this work, we provide predictions—by theory and simulations—of the thermal transport properties of this system.

*This research is partially supported by the Advanced Research Projects Agency-Energy (ARPA-E) grant number DE-AR0001056.
Minimizing Heat Transport by Ballistic Confinement in Phononic Metalattices

WEINAN CHEN (Presenter), DISHA TALREJA, DEVIN GOODLING, PRATIBHA MAHALE, NABILA NOVA, HIU CHENG, JENNIFER RUSSELL, SHIHYING YU, NICOLAS POILVERT, GERALD D MAHAN, SUZANNE MOHNEY, VINCENT CREPSI, THOMAS MALLOUK, JOHN BADDING, BRIAN FOLEY, VENKATRAMAN GOPALAN, ISMAILA DABO, Pennsylvania State University — We study the thermal conductivity of phononic metalattices, a class of newly synthesized nanostructures exhibiting long-range periodicity commensurate with the mean free paths of the phonons. In this work, we present a computational approach that is capable of computing the ballistic phonon mean free paths in periodic metamaterials by embedding an explicit model of phonon radiation into a continuum density of scatters, closing the gap between existing analytical models and numerical simulations. Our computational predictions supported by sensitive measurements indicate that the thermal conductivity minimum of metalattices can be as low as 0.15 W/m/K, which is among the smallest lattice conductivities reported for two- and three-dimensional silicon-based materials. This exceptional reduction in the heat conductivity establishes metalattices as a useful platform to achieve order-of-magnitude tunability in the thermal response of crystalline semiconductors.

Thermal boundary conductance of beyond graphene two-dimensional materials

CAMERON FOSS (Presenter), ZLATAN AKSAMIJA, Univ of Mass - Amherst — An ongoing concern for 2D materials is their ability to thermally couple with an underlying substrate which acts as the primary pathway for heat removal in 2D devices. The thermal pathway from the 2D layer to substrate has been studied rigorously in graphene and various transition metal dichalcogenides. However, the literature still lacks a comprehensive analysis of thermal boundary conductance (TBC) for beyond-graphene materials. Previously [2D Mater. 6 (2019) 025019] we have shown that the TBC depends strongly on the overlap of available phonon modes in the long-wavelength regime and found selection criteria for choosing the best substrate for TBC. Here we use first-principles calculations and phonon interface transport modeling to calculate the TBC of beyond-graphene 2D materials, such as; silicene, germanene, BAs, InAs, and blue and black phosphorene, on amorphous and crystalline substrates. Our results show the TBC for these 2D materials on amorphous SiO$_2$ (a-SiO$_2$) falls between 20-50 MW.m$^{-2}$K$^{-1}$. A trend emerges that 2D materials with lower ZA branch frequencies have higher TBCs when placed on a-SiO$_2$. Our results provide selection criteria for 2D materials that improve interfacial heat transport in 2D devices with amorphous and crystalline substrates.
Spatially-Resolved Phonon Hydrodynamic Flow from First Principles

GEORGIOS VARNAVIDES (Presenter), Massachusetts Institute of Technology MIT, ADAM JERMYN, Center for Computational Astrophysics, Simons Foundation, Flatiron Institute, POLINA ANIKEEVA, Massachusetts Institute of Technology MIT, PRINEHA NARANG, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Material hydrodynamic regimes are characterized by numerous scattering events, each of which conserves quasi-momentum and thus doesn't oppose the flow of carriers. Recent observations of non-resistive carrier transport in two-dimensional materials suggest that hydrodynamic flow can occur over a wide range of temperatures. In thermal transport, hydrodynamic flow manifests itself in two separate phenomena: the wavelike propagation of heat, termed second sound, and parabolic heat profiles, reminiscent of classical incompressible fluid pipe flow. Theoretical efforts to characterize and predict such phenomena are often restricted to momentum-space, effectively assuming spatial homogeneity. However, hydrodynamic flow exhibits strong real-space signatures. In this talk, we extend previous work and solve the phonon Boltzmann Transport Equation using both spatial and momentum resolution. We present ab initio calculations of hydrodynamic phenomena in real-space in experimentally-realizable geometries.


Microscopic thermal transport mechanisms in Tl$_3$VSe$_4$: lattice phonons or localized oscillators?

YI XIA (Presenter), KOUSHIK PAL, JIANGANG HE, Northwestern University, VIDVUDS OZOLINS, Applied Physics, Yale University, CHRISTOPHER MARK WOLVERTON, Northwestern University — Recently, crystalline Tl$_3$VSe$_4$ was experimentally reported to exhibit an ultralow lattice thermal conductivity ($\kappa_l$) of 0.3±0.05 W/mK at 300 K [Science 360, 1455 (2018)]. Understanding of the underlying thermal transport mechanism has been deemed nontrivial, which requires a complex scenario that involves two channels: lattice phonons and localized oscillators. However, the observed Raman spectra, specific heat, and temperature dependence of $\kappa_l$ only reveal features characteristic of phonons in an ordered crystalline compound. To resolve this conundrum, we investigate the heat transfer in Tl$_3$VSe$_4$ by combining a first-principles density-functional theory based framework of anharmonic lattice dynamics with the Peierls-Boltzmann transport equation for phonons. Specifically, we include contributions of the three- and four-phonon scattering processes to the phonon lifetimes as well as the temperature-dependent anharmonic renormalization of phonon energies. We reveal the dominant thermal transport mechanism by explicitly evaluating both diagonal (particle-like propagation) and off-diagonal (wave-like tunneling) terms of the heat current operator.

*Toyota Research Institute (TRI)
U.S. Department of Energy under Contract No. DE-SC0015106
National Science Foundation Grant DMR-1611507
10:24AM L44.00009: Violation of the Wiedemann-Franz law in graphene: plasmon contribution to the heat conductivity  LARS FRITZ (Presenter), Physics, Utrecht University — It is well established that close to the Dirac point in graphene the Wiedemann-Franz law is violated. Using a microscopic Boltzmann approach we first show that a theory of electrons and holes cannot quantitatively account for the heat conductivity observed in experiment. We argue that the missing heat conductivity is due to plasmons which make a sizeable contribution in the vicinity of the Dirac point.

10:36AM L44.00010: Influence of Adsorbed Liquid Monolayer Ordering on the Kapitza Resistance at Solid/Liquid Interfaces*  HIROKI KAIFU (Presenter), SANDRA TROIAN, Applied Physics, Caltech — Applications ranging from small scale avionics control to AI computing platforms are ever more reliant on high density integrated chips prone to thermal runaway. Thermal extraction is now the limiting factor in information processing and so conventional air cooling is being displaced by microscale liquid cooling systems, which are more efficient due to the higher heat capacity of liquids. In this work, we use non-equilibrium MD simulations to examine thermal transport across solid/liquid (S/L) interfaces in quiescent fluids, as quantified by the Kapitza resistance. While previous studies have focused on interfacial behavior mediated by liquid density stratification, wettability and solid crystalline symmetry, we instead examine the influence of in-plane ordering within the first few liquid monolayers adsorbed at the solid surface. The characteristics of these proximal layers are tuned by varying the depth and repulsive distance characterizing the intermolecular potential. Our results, some intuitive and some not, yield general correlations between the Kapitza jump and measures of interfacial commensurability influenced by the structure and collective response of such monolayers.

*HK gratefully acknowledges support from a 2019 NASA Space Technology Research Fellowship.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L45 DCOMP GDS DSOFT DPOLY: Emerging Trends in Molecular Dynamics Simulations and Machine Learning II  706 - Ken-ichi Nomura, University of Southern California - Tag(s): Focus

8:00AM L45.00001: Deep Learning for molecular simulation and spectra calculation* [Invited] LINFENG ZHANG (Presenter), Princeton University — I will discuss some mathematical perspectives of model representation and exploration of \textit{ab initio} data for generating reliable deep learning-based models that represent the interatomic potential energy surface and electronic information of complex systems. This gives us an unprecedented opportunity to perform large-scale molecular simulation and extract direct experimental observables, such as the infrared and Raman spectra. I will show how these methodologies help us understand the complex nature of water in a large region of its thermodynamic phase diagram.

*This work is partially supported by the Center Chemistry in Solution and at Interfaces (CSI) funded by the DOE Award DE-SC001934.
Molecular dynamics (MD) simulations rely on accurate numerical integrators such as Verlet method to model the equations of motion to generate a set of trajectories for a finite ensemble of particles. The design of MD simulations are constrained by the available computation power and must use small enough timestep to avoid discretization errors. Multiple timestep methods have been developed to mitigate this situation but are generally constrained by specific applications.

We introduce and develop recurrent neural networks (RNN) based Integrators (“surrogate”) for learning MD dynamics of physical systems generally simulated with Verlet solvers. The RNN surrogate, trained on trajectories generated using Verlet integrator, learns to propagate the dynamics of few-particle systems with multiple timestep values that are orders of magnitude higher compared to the typical Verlet timestep. Different pair interaction potentials including spring potential and Lennard-Jones potential are investigated. Prospects for extending the approach to simulate a large number of particles are outlined.

*This work is supported by the National Science Foundation through award 1720625.

Correlated quantum-chemical methods for condensed matter systems, such as the random phase approximation (RPA), hold the promise of reaching a level of accuracy much higher than that of conventional density functional theory approaches. However, the high computational cost of such methods hinders their broad applicability, in particular for finite-temperature molecular dynamics simulations. We propose a method that couples machine learning techniques with thermodynamic perturbation theory to estimate finite-temperature properties using correlated approximations [1]. We apply this approach to compute the enthalpies of adsorption in zeolites and show that reliable estimates can be obtained by training a machine learning model with as few as 10 RPA energies. This approach paves the way to the broader use of computationally expensive quantum-chemical methods to predict the finite-temperature properties of condensed matter systems.


*Work supported through the COMETE project co-funded by the European Union under the program FEDER-FSE Lorraine et Massif des Vosges 2014-2020.*
9:00AM L45.00004: Neural Network Potentials for Twisted Few-Layer Materials*  EMINE KUCUKBENLI (Presenter), EFTHIMIOS KAXIRAS, Harvard University — Few-layer materials twisted at small angles are experimentally shown to host non-trivial electronic structure such as superconductivity or strongly-correlated insulating state. It is also theoretically demonstrated that in twisted bilayer graphene, the prototypical system for this class of materials, characteristics of the band structure is significantly affected by the atomic relaxation that occurs due to the twist. Since small twist angles result in large Moiré patterns, atomistic simulation of these systems from first principles is computationally costly, and empirical potentials are needed. However, the development of such interatomic potentials is also challenging due to the very different energy and length scales of inter- and intralayer interactions. Furthermore, the changes in atomic positions and energy due to the twist is only a small fraction of the typical length and energy scales, imposing a tight accuracy requirement on the potential design. In this talk we present our attempt at developing such a potential via neural networks, and how the challenges highlighted above translate into practical steps during training and testing. Finally we examine the performance of the neural network potential and its transferability.

*This work is supported by DoE Award DE-SC0019300.

9:12AM L45.00005: Development of reliable neural network potential for metal–semiconductor interface reaction: case study for Ni silicidation  WONSEOK JEONG (Presenter), DONGSUN YOO, KYUHYUN LEE, SEUNGWU HAN, Seoul National University — Molecular dynamics using classical interatomic potentials can provide valuable information at the atomistic scale. However, when the simulation involves chemical reactions of bond breaking and forming along with mixed bonding characters, it is challenging to develop an accurate force field for the system and sometimes practically impossible. In this respect, the machine-learning potentials are highly anticipated since they are based on flexible mathematical structures with no pre-fixed form. In this presentation, we discuss the process of constructing a reliable neural network potential (NNP) for a challenging metal–semiconductor interface reaction, with example of thermally activated Ni silicidation. We present a systematic way to build up the training set that can describe the interface reaction. We also introduce some of the techniques we utilized for higher reliability and efficiency, including Gaussian density function weighting, principle component analysis training etc. In order to obtain the prediction uncertainty for certain local configurations, we adopt replica NNPs that are trained directly on the atomic energy of the reference NNP. Finally, we suggest the underlying mechanism of abnormal crystal phase growth from ultra-thin Ni film silicidation.
9:24AM L45.00006: Linearized machine learning potential with high-order rotational polynomial invariants for multi-component systems  ATSUTO SEKO (Presenter), ISAO TANAKA, Kyoto Univ — Machine-learning potential (MLP) providing an accurate description of the structure-energy relationship and its potential applications are of growing interest. Such an approach is based on a linearized MLP framework, which was successful in constructing accurate MLPs in a variety of elemental metals [1]. Also, the introduction of group-theoretical high-order rotational polynomial invariants can contribute to systematically derive MLPs with high predictive power for a wide range of structures, including extreme structures [2]. The present study proposes a formulation of linearized MLP extended to multi-component systems involving high-order rotational invariants. We also show its applications to several binary alloy and ionic systems such as Ti-Al system. For each system, we obtain MLPs with high predictive power and Pareto frontier MLPs for the computational cost versus the accuracy.


9:36AM L45.00007: Transfer learning of neural network potentials for reactive chemistry* JASON GOODPASTER (Presenter), University of Minnesota — Large, condensed phase, and extended systems impose a challenge for theoretical studies due to the compromise between accuracy and computational cost in their calculations. Machine learning methods are an approach to solve this trade-off by leveraging large data sets to train on highly accurate calculations using small molecules and then apply them to larger systems. In this study, we are developing a method to train a neural network potential with high-level wavefunction theory on targeted system of interest that are able to describe bond breaking. We combine density functional theory calculations and higher level ab initio wavefunction calculations, such as CASPT2, to train our neural network potentials. We first train our neural network at the DFT level of theory. Using an adaptive active learning training scheme, we retrained the neural network potential to a CASPT2 level of accuracy. We demonstrate the process as well as report current progress and performance of this neural network potential for molecular dynamic simulations.

*This research was carried out within the Nanoporous Materials Genome Center, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences under Award DE-FG02-17ER16362.
9:48AM L45.00008: Insights about accelerated dynamics calculations of the acid $pK_a$ beyond biasing the coordination number collective variable  CARLOS WEXLER (Presenter), JIASEN GUO, Univ of Missouri - Columbia, ALBERTO ALBESA, Univ Nacional de La Plata — Knowing the dissociation constant $K_a$ of a weak acid is fundamental to understand many chemical and physical processes. Theoretical calculation of the $K_a$ remains a challenge. The use of accelerated methods such as metadynamics has shown promise for numerical computation of $K_a$ with explicit solvent molecules. In the most common approach, a single collective variable (CV) representing the coordination number of the proton donor group yields results that are in reasonable agreement with experiments, however there remains questions as to whether the configuration space of the deprotonated state was sufficiently sampled given the small typical simulation box. We studied the deprotonation of acetic acid using the ReaxFF in simulation boxes of varying sizes and observed significant size dependence of $\Delta G$ when biasing with a single CV representing the coordination number of the acetate oxygen atoms. However, biasing with an additional CV describing the $H_3O^+$ and acetate anion distance results in a virtual elimination of the size dependence. The improvement is due to accelerated sampling of the deprotonated configuration state.

10:00AM L45.00009: Multitask machine learning of collective variables for enhanced sampling of reactive molecular dynamics*  LIXIN SUN (Presenter), SIMON BATZNER, JONATHAN VANDERMAUSE, YU XIE, BORIS KOZINSKY, School of Engineering and Applied Science, Harvard University — Ability to discover reactions and predict their rates is key to understanding many computational physics, biology and chemistry problems. Enhanced sampling techniques, such as metadynamics and umbrella sampling, use a low-dimensional reaction coordinate / collective variable (CV) space to accelerate sampling for slow reactions. However, their efficiency relies on the choice of CVs, which requires intuition and many trial-and-error tests.

In this work, we propose a multi-task machine learning algorithm to learn collective variables (CVs) from short MD trajectories and transition path sampling, which preserves the information on state labels and potential energies. We show that the algorithm can accurately measure reaction progress and identify the slow motion of the system. It offers a unified dimensionality reduction framework that integrates different learning objectives and can be applied to a wide variety of reactive systems, including Muller-Brown potential model and alanine dipeptide.

*This work was supported by the Integrated Mesoscale Architectures for Sustainable Catalysis funded by DOE under Award # DE-SC0012573. And it used resources of the National Energy Research Scientific Computing Center, a DOE Facility operated under Contract No. DE-AC02-05CH11231.
10:12AM L45.00010: Exploring Cucurbituril-Fentanyl Binding (and Beyond) with Parallel Biasing Methods*  
ANNE LEONHARD (Presenter), JONATHAN K. WHITMER, University of Notre Dame — The physics underlying drug delivery, molecular separation, and detection of harmful agents relies in many cases on microscopic binding events. There is a critical need for information about these processes, in particular from molecular simulations which can be used to pre-screen molecules and materials. Binding events can be simple, such as gas molecules adsorbing onto surfaces, or complex, such as protein-ligand interactions. Here, we discuss new techniques for computing the binding free energy of small organic molecules to cucurbituril (CB) macrocycles (specifically, cucurbit[7]uril with fentanyl) as both a test case of intermediate complexity, and one of great potential application in sensing and remediation platforms. The system exhibits multiple potential binding conformations, rendering computational study of CB–fentanyl binding difficult with standard methods. Parallel biasing metadynamics is used to enhance sampling in this system along multiple important structural and dynamic degrees of freedom, without restricting the movement between bound states. We compare our results to experiment and discuss the general applicability of the parallel biasing scheme to alternate systems.

*ACL would like to acknowledge funding from a NSF-GRFP fellowship.

10:24AM L45.00011: Neural Network Interatomic Potentials for Water*  
ALBERTO TORRES (Presenter), Instituto de Física Teórica, Universidade Estadual Paulista (UNESP), LUANA PEDROZA, Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, ALEXANDRE R ROCHA, Instituto de Física Teórica, Universidade Estadual Paulista (UNESP) — Water is the most important liquid on Earth. And difficult to describe theoretically, due to a delicate balance of weak and strong interactions tuned by entropic effects. High level ab initio calculations, such as Coupled Cluster (CC), can do the job, but albeit highly accurate their application is limited to systems with a few molecules due to their computational cost, not being amenable to simulate liquid water. Recent developments in density functional theory (DFT), i.e. new functionals and better description of van der Waals interactions, have made it possible to describe water with reasonable accuracy, and a good cost/accuracy compromise. Yet, even with DFT it is difficult to perform simulations on large systems at long time scales. Artificial Neural Networks (ANN) force fields have been shown to be able to yield accurate (on par with the method they were fitted to) results with low cost. In this work we employ ANNs to represent the water potential surface with DFT- and CC-quality, and compare ANNs trained at different levels of theory to discuss the accuracy of different methods in describing macroscopic properties of water under different conditions including nuclear quantum effects.

*Supported by FAPESP (2018/12545-5, 2017/02317-2) and NCC/GridUNESP.
10:36AM L45.00012: Anharmonicity in a linear chain of Lennard-Jones atoms  ADRIAN DE LA ROCHA (Presenter), JORGE MUNOZ, University of Texas, El Paso — Atoms in solids move in the force fields of their vibrating neighbors and these vibrations give rise to thermodynamics. In many systems it is enough to use the Taylor expansion of the potential energy up to second order to derive most of their thermodynamic properties, but higher order (anharmonic) terms are necessary to predict quantities that depend on scattering rates, such as thermal conductivity. Here we present a study of the anharmonicity that arises from atoms in a linear chain interacting via the Lennard-Jones potential and a test run of a dynamic mean field theory in which the atoms only see a harmonic potential but the stiffness of the potentials depends on the configuration of the system which is determined using a machine learning classifier.

10:48AM L45.00013: Hunting FOX: Using Fragments to Sniff Out Drug Leads for Antibiotic Discovery*  RACHAEL MANSBACH (Presenter), Los Alamos National Laboratory, INGA V LEUS, JITENDER MEHLA, University of Oklahoma, CESAR A LOPEZ, Los Alamos National Laboratory, JOHN K WALKER, Saint Louis University, VALENTIN V RYBENKOV, University of Oklahoma, NICOLAS W HENGARTNER, Los Alamos National Laboratory, HELEN I ZGURSKAYA, University of Oklahoma, S GNANAKARAN, Los Alamos National Laboratory — Drug discovery faces a potential crisis. Due a dwindling "obvious" search space, productivity is declining. This has led to the idea of "drug repurposing," in which data on drugs that have failed clinical trials are reused. We approach drug repurposing by introducing an algorithm—which we term "Hunting FOX" for "Hunting Fragments Of X"—that combines a fragment-based representation with traditional machine learning to identify the most important submolecules correlating with an activity of interest. We validate our approach on the problem of drug permeation through the highly-impermeable outer membrane of P. aeruginosa. We show that Hunting FOX is able to recapitulate a set of relevant fragments with understandable physicochemical properties. By using coarse-grained molecular dynamics, we show a possible mechanism behind fragment-based permeation enhancement. We also fit a predictive classifier using the identified fragments and verify its predictions experimentally. Overall, we have developed a novel algorithm of great use in improving outcomes for drug discovery and validated it as applied to the design of antibiotics that can permeate Gram-negative bacteria.

*This work was supported by NIAID/NIH grant R01AI136799. RAM acknowledges a Los Alamos Director's Postdoctoral Fellowship.

Wednesday, March 4, 2020 8:00 AM - 10:48 AM

Session L46 GMAG DCOMP DCMP: Magnetism and Magnetoelectrics: Molecule-Based and 2D Materials  708 - Vivien Zapf, Los Alamos Natl Lab - Tag(s): Focus
8:00AM L46.00001: σ-Dimerization of organic radicals as mechanism for strongly hysteretic magneto-structural phase transitions* [Invited] MICHAEL SHATRUK (Presenter), Florida State Univ — In this contribution, we present a few systems of σ-dimerizing organic radicals, which provide examples of magneto-structural phase transitions that occur with a large thermal or photochemical hysteresis window. In each case, the dimerization causes drastic structural changes that underlie a substantial energy barrier for the conversion between the diamagnetic σ-dimer phase and the paramagnetic π-radical phase. We demonstrate that in the case of dithiazolyl radicals the existence of such energy barrier allows photo-generation of paramagnetic state with remarkable thermal stability. In the case of N-oxyl radicals that exist as a rotationally disordered plastic crystalline phase at room temperature and dimerize into a long-range ordered crystalline phase upon cooling, the barrier to the intra-dimer bond breaking causes a large thermal hysteresis, which exhibits high sensitivity to applied pressure. We will also discuss general requirements for observing such transitions for other organic radicals.

*This research was supported by the National Science Foundation (award CHE-1464955).

8:36AM L46.00002: Controlling the Kinetics of Spin Transitions through Heterostructure Elasticity* JOHN CAIN (Presenter), WANHONG HE, Chemistry, University of Florida, JERRY L. ZHANG, Physics, University of Florida, DANIEL R. TALHAM, Chemistry, University of Florida, MARK W MEISEL, Physics and NHMFL, University of Florida — An often overlooked feature of spin transitions is the significant volume change associated with altered metal-ligand bonding between the two spin states. Recent examples of exploiting the strain developed during a spin transition include integration into hybrid materials to influence electrical, optical, or magnetic properties. These applications all require the spin transition material to physically couple to other components; however, an interface with another material can strongly influence the behavior of the spin transition material, especially as sizes approach the nanoscale. Our lab has shown these interfaces can dramatically influence the kinetics of solid-state spin transitions. For example, the rate of the light-induced spin transition in Rb$_x$Co[Fe(CN)$_6$]$_y$ (RbCoFe-PBA) increases by several orders of magnitude when RbCoFe-PBA is used as the core of a core-shell particle, relative to uncoated RbCoFe-PBA. A theoretical electroelastic model was used to guide chemical alterations, allowing the mechanism to be probed experimentally with nuclear inelastic scattering.

*Supported by the NSF via DMR-1904596 (DRT) and DMR-1708410 (MWM). A portion of this work was performed at the MagLab, which is supported by NSF DMR-1644779 and the State of Florida.
8:48AM L46.00003: Microscopic theory of spin-crossover phase transition and magnetolectric coupling* JIE-XIANG YU (Presenter), DIAN-TENG CHEN, JIE GU, JIA CHEN, JUN JIANG, LONG ZHANG, XIAOGUANG ZHANG, Department of Physics, Center for Molecular Magnetic Quantum Materials and Quantum Theory Project, University of Florida, VIVIEN ZAPF, National High Magnetic Field Lab, Los Alamos National Lab, HAI-PING CHENG, Department of Physics, Center for Molecular Magnetic Quantum Materials and Quantum Theory Project, University of Florida — The molecular magnet Mn(taa) is one of the earliest studied spin-crossover system where the spin can transit from a low-spin state to a high-spin state around 45 K. Very recently, the magnetolectric coupling was observed in Mn(taa) and a microscopic theory is needed. Here, we investigated the atomistic origin of the phase transition and magnetolectric coupling in spin-crossover system Mn(taa) via first-principles calculations and Monte Carlo simulations. By constructing a molecular-scale Hamiltonian, we discovered that the Jahn-Teller-induced intermolecular strain interaction is the key factor in both the spin-crossover phase transition and magnetolectric behaviors. Our work leads to a first theory that goes beyond the mean field approximation.

*This work was supported as part of M2QM, an EFRC funded by the U.S. DOE, BES under Award No. DE-SC0019330. Computations were done using the utilities of NERSC, XSEDE under Grant No. TG-PHY170023, and UFRC.

9:00AM L46.00004: Observation of magnetolectric, spin-lattice, and electron-phonon coupling in multiferroic (NH$_4$)$_2$[FeCl$_5$(H$_2$O)] KENDALL HUGHEY, University of Tennessee, Knoxville, JISOO NAM, MINSEONG LEE, Ulsan National Institute of Science and Technology, AMANDA CLUNE, KENNETH R O’NEAL, AVERY BLOCKMON, University of Tennessee, Knoxville, WEI TIAN, Oak Ridge National Laboratory, MYKHAYLO OZEROV, National High Magnetic Field Laboratory, VIVIEN ZAPF, Los Alamos National Laboratory, JUN HEE LEE, Ulsan National Institute of Science and Technology, JANICE LYNN MUSFELDT (Presenter), University of Tennessee, Knoxville — We bring together pulsed-field polarization techniques, magnetoinfrared spectroscopy, and lattice dynamics calculations to uncover the high magnetic field coupling mechanism of polarization and magnetic field in (NH$_4$)$_2$[FeCl$_5$(H$_2$O)] and to explore the structural distortions that this system undergoes through various magnetic phases and across the magnetic quantum phase transition. High-field polarization is quenched by the quasicollinear to collinear sinusoidal magnetic transition. Strikingly, spin-lattice coupling across the magnetic quantum phase transition reveals that nearly all low-frequency vibrations modulate magnetic exchange via hydrogen- and halogen-bonding interactions. An analysis of combined techniques demonstrates that magneto-infrared is sensitive to both spin-phonon and electron-phonon coupling.
Magneto-optical Detection of Chirality Induced Spin Selectivity in 2D Chiral Hybrid Organic-Inorganic Perovskites*  
ZHENGJIE HUANG (Presenter), Physics, North Carolina State University, BRIAN BLOOM, ZHENI NIKOLAEVA GEORGIEVA, Chemistry, University of Pittsburgh, ERIC VETTER, Physics, North Carolina State University, DAVID WALDECK, Chemistry, University of Pittsburgh, DALI SUN, Physics, North Carolina State University — The Chirality-Induced Spin Selectivity (CISS) effect, an appealing 'spin filtering' effect arising from the chirality of materials has been demonstrated in various organic systems. The recent convergence of chiral molecules with metal halide frameworks gives rise to a new family of chiral systems: 2D chiral hybrid organic-inorganic perovskites (2D-chiral-HOIPs). This class of materials possesses both the implanted chirality and the excellent photovoltaic properties, making it a promising platform that bridges opto-spintronic studies and the CISS effect. Here we show the observation of light-induced CISS effect in the 2D-chiral-HOIPs detected by a magneto-optical measurement. It shows that the incident light changes the Kerr response of the ferromagnetic layer attached to the chiral-HOIP layer. The change of Kerr signal follows a linear relation with respect to the applied magnetic field, of which the sign of the slope depends on the chirality of the HOIPs. Our results pave a new route for employing 2D-chiral-HOIPs for future opto-spintronic applications.

*Work at NC State was supported by the NC State-Nagoya Collaboration Grant. Device preparation was partially supported by ECCS-1933297. B.B and Z.N.G. were supported by Department of Energy Grant No. ER46430.

Theoretical design of two dimensional magnetoelectrics*  
SHUAI DONG, LING-FANG LIN (Presenter), Southeast University — Achieving magnetoelectric two-dimensional (2D) materials should enable numerous functionalities in nanoscale devices. Until now, however, predicted 2D magnetoelectric materials are very few and with coexisting yet only loosely coupled (type-I) ferroelectricity and magnetism [1]. Based on physical analysis and by using density functional theory calculations, a type-II multiferroic MXene Hf$_2$VC$_2$F$_2$ monolayer is predicted. For multiferroic MXene Hf$_2$VC$_2$F$_2$ monolayer, its ferroelectricity originates directly from its magnetism [2]. The noncollinear 120° Y-type spin order generates a polarization perpendicular to the spin helical plane. Remarkably, the multiferroic transition is estimated to occur above room temperature. Our investigation should open the door to a new branch of 2D materials in the pursuit of intrinsically strong magnetoelectricity.


*Work was supported by National Natural Science Foundation of China (Grant Nos. 11834002 & 11674055)
Gate tunability of 2D antiferromagnet magnon modes

XIAO-XIAO ZHANG (Presenter), University of Florida, LIZHONG LI, KIN FAI MAK, JIE SHAN, Cornell University — The recently discovered atomically-thin magnetic crystals provide a unique playground to develop new approaches to manipulate magnetism. Rapid progresses have been made that demonstrate the potentials of utilizing 2D magnets to construct novel spintronics devices. However, their spin dynamics, which are crucial for microscopic understanding and determine the fundamental limit of spin manipulation, still remain elusive due to the difficulty to characterize these micron-sized samples with conventional microwave techniques. In this talk, we will show how we can access and probe the collective spin-wave excitations in an antiferromagnetic bilayer CrI3, which allows us to extract magnetic anisotropy and exchange energy. In particular, we will demonstrate the gate tunability of magnon frequencies, which is unique for the 2D magnet system.

2D ferromagnetism in porphyrin-based semiconductors

*ARTEM PIMACHEV, ROBERT D NIELSEN, Univ of Wyoming, ANRI KARANOVICE, Virginia Tech, YURI DAHNOVSKY (Presenter), Univ of Wyoming — We study an environmentally stable 2D ferromagnetic semiconductor with applications in biomedicine, solar cells, spintronics, and energy and hydrogen storage. We describe the electronic, transport, optical, and magnetic properties of a π-conjugated micropore polymer with three iron atoms placed in the middle of an isolated pore. We study how these properties change when bonded with CO, CO$_2$, and O$_2$. This material exhibits strong Fe-localized d$_{z^2}$ bands with a direct bandgap of 0.28 eV. The material is a ferromagnet of an Ising type with long-range exchange interactions with a very high magnetic moment per unit cell, m = 6 μB. The estimated exchange integral is calculated to be about J$_{nn}$ = 25 meV. The binding of CO, CO$_2$, and O$_2$ modifies the d$_{z^2}$ bands of the Fe ions with varying indirect bandgaps with values between 0.269 - 0.626 eV, 0.039 - 0.434 eV, and 0.291 - 0.347 eV for CO, CO$_2$, and O$_2$, respectively. Both the absorption coefficient and conductivity have large modifications to the xy-components. The material remains ferromagnetic with the magnetic moment per unit cell decreasing to 4, 2, and 0 μB for gases attached to one, two, and three Fe ions per unit cell, respectively.

*This acknowledge a grant (No. DMR-1710512) from the US National Science Foundation
10:00AM L46.00009: Low-Damping Ferromagnetic Resonance in Electron-Beam Patterned, High-Q Vanadium Tetracyanoethylene Magnon Cavities* ANDREW FRANSON (Presenter), Physics, The Ohio State University, NA ZHU, Electrical Engineering, Yale University, SETH KURFMAN, MICHAEL CHILCOTE, Physics, The Ohio State University, DENIS CANDIDO, Physics and Astronomy, University of Iowa, KRISTEN S. BUCHANAN, Physics, Colorado State University, MICHAEL FLATTÉ, Physics and Astronomy, Yale University, HONG X TANG, Electrical Engineering, Yale University, EZEKIEL JOHNSTON-HALPERIN, Physics, The Ohio State University — Integrating patterned, low-loss magnetic materials into microwave devices and circuits presents many challenges due to the specific conditions that are required to grow ferrite materials, driving the need for flip-chip and other indirect fabrication techniques. The low-loss ($\alpha=3.98 \times 10^{-5}$), room-temperature ferrimagnetic coordination compound vanadium tetracyanoethylene ($V[\text{TCNE}]_x$) is a promising new material for these applications that is potentially compatible with semiconductor processing. Here we present the deposition, patterning, and characterization of $V[\text{TCNE}]_x$ thin films with lateral dimensions ranging from 1 micron to several millimeters. We employ electron-beam lithography and liftoff using an aluminum encapsulated PMMA/P(MMA-MAA) copolymer bilayer on sapphire. Growth occurs in an argon atmosphere at 30 mTorr and 50 °C. Films patterned via this method maintain low-loss characteristics down to 25 microns with only a factor of 2 increase down to 5 microns. A manifold of thickness and radial confined spin wave modes reveals the quality of the patterned films. This work establishes the versatility of $V[\text{TCNE}]_x$ for applications requiring highly coherent magnetic excitations ranging from microwave communication to quantum information.

*Support from EFRI Grant No. EFMA-1741666.

10:12AM L46.00010: Two-dimensional magnetic coordination polymers: tuning the surface and the magnetic properties. SAMUEL MAÑAS-VALERO (Presenter), EUGENIO CORONADO, Univ de Valencia — Magnetic two-dimensional (2D) materials have emerged recently with examples of inorganic monolayers like antiferromagnets (FePS$_3$) [Nano Letters 16, 7433, 2016; 2D Materials 3, 031009, 2016] and highly unstable ferromagnets such as CrI$_3$ [Nature 546, 270, 2017] or Fe$_3$GeTe$_2$ [Nature Materials 17, 778. 2018].

To overcome the present unstabilities of 2D magnetic materials, we take advantage of layered molecular magnets since, thanks to the chemical design, it is feasible to bring new magnetic scenarios as well as to overcome the present unstabilities of 2D magnetic materials. Here [Nature Chemistry 10, 1001, 2018 and unpublished data] we present a pre-synthetic method based on coordination chemistry that affords the isolation of crystalline molecular monolayers. The concept is illustrated using layered coordination polymers formed by reacting various benzimidazole derivatives with ferrocene. By the election of the proper ligand and the metal source, it is possible to tune the surface properties as well as the magnetism. Moreover, the magnetic order of the flakes is probed by its integration into membranes. Therefore, these new 2D molecular materials are exceptional candidates for studying the magnetism in the 2D limit, as well as for developing membranes for selective molecular sensing.
A New Mercury-based Cation Radical Salt: α-(BEDT-TTF)$_2$Hg(SeCN)$_2$Cl$^*$

ALYSSA HENDERSON (Presenter), KAYA WEI, JOHAN VAN TOL, RACHAEL RICHARDSON, KOMALAVALLI THIRUNAVUKKUARASU, THEO SIEGRIST, Natl High Magnetic Field Lab, JOHN A SCHLUETER, National Science Foundation — BEDT-TTF [BEDT-TTF = bis(ethylenedithio)tetrathiafulvalene, henceforth referred to as ET] cation radical salts continue to serve as important physical representations of various theoretical quantum systems. The arrangement of ET radical cations in these materials have dramatic effects on their physical properties. Here we report the synthesis of the new α-(ET)$_2$Hg(SeCN)$_2$Cl salt. Single crystals, crystallizing in the monoclinic space group $P2_1/n$, were prepared through the use of electocrystallization.\(^1\) The two dimensional crystal structure is characterized by layers of ET radical cations separated by dimerized Hg(SeCN)$_2$Cl$^-$ anions. The synthesis, structure, and magnetization, heat capacity, electron-spin-resonance, and Raman measurements are reported.


*J.A.S. acknowledges support from the Independent Research/Development program while serving at the NSF. Work carried out at the NHMFL was supported by the NSF under grant DMR-1644779 and the State of Florida. A.H., L.D. and T.S. acknowledge funding from the NSF under grant DMR-1534818 and DMR-1849539. Use of the APS, a DOE Office of Science User Facility at ANL, was supported under Contract No. DE-AC02-06CH11357
10:36AM L46.00012: Magneto-elastic coupling in multiferroic metal-organic framework [(CH$_3$)$_2$NH$_2$]Co(HCOO)$_3$  KOMALAVALLI THIRUNAVUKKURASU (Presenter), RACHAEL RICHARDSON, Florida A&M University, ZHENGGUANG LU, National High Magnetic Field Laboratory, NAN HUANG, Department of Materials Science and Engineering, University of Tennessee Knoxville, DMITRY SMIRNOV, National High Magnetic Field Laboratory, DAVID MANDRUS, Department of Materials Science and Engineering, University of Tennessee Knoxville — Metal-organic frameworks (MOFs) are a class of nanoporous compounds where organic groups are used in combination with transition metal ions to obtain multifunctional materials. The family of MOFs comprised of methylammonum (A= (CH$_3$)$_2$NH$_2$) and metal (B=Co, Cu, Fe, Mn, Ni) cations with a formate (X=HCOO$_3$) anion are very interesting because of their multiferroic properties [1]. Therefore, several efforts have been made to understand the exchange interactions in these materials including magnetization at magnetic fields up to 60 T and infrared spectroscopy at fields up to 35 T [2,3]. Concurrently, we performed Raman spectroscopy on [(CH$_3$)$_2$NH$_2$]Co(HCOO)$_3$ at magnetic fields up to 31T to probe the magneto-elastic coupling. Also, the effect of hydrostatic pressure on the magnetic-elastic coupling in this system was explored. We will discuss our investigations and its implications.

References:

This work has been performed at the user facilities in the National High Magnetic Field Laboratory (NHMFL), Tallahassee. The NHMFL is supported by the NSF through NSF/DMR-1644779 and the state of Florida. The project is also funded by DoN HBCU/MI program award # N000141713061.

L46.00013: High throughput ab initio screening for magnetic two dimensional materials
XUE JIANG (Presenter), Dalian University of Technology — Quantum information and spintronics devices, based on searching and manipulating magnetism, open up new questions in the studies of two dimensional materials. In this talk, I will present our theoretical design on few new types of 2D ferromagnetic materials (MBene, CrSBr, K2N, and 2D MOFs). They are shown robust ferromagnetism coupling, high Curie temperature (Tc), and large magnetic anisotropy energy (MAE). Many strategy have also been introduced to tailor their magnetic behavior, such as chemical functionalization, isoelectronic substitution, non-stoichiometry, strain, and metal decoration.

This work was supported by the National Natural Science Foundation of China (11874097) and the Fundamental Research Funds for the Central Universities of China (DUT19LK12).
**8:00AM L47.00001: Strain effects on bulk α-RuCl$_3$ and α-RuCl$_3$/graphene bilayer**  SANANDA BISWAS (Presenter), YING LI, DAVID KAIB, KIRA M. RIEDL, STEPHEN WINTER, Goethe University Frankfurt, JOHANNES KNOLLE, Department of Physics, Technical University Munich, ROSER VALENTÍ, Goethe University Frankfurt — α-RuCl$_3$ has gained considerable attention recently, being the ‘proximate’ Kitaev spin liquid candidate. We discuss the effect of electronic proximity of α-RuCl$_3$ to graphene which gives rise to an insulator to metal transition in α-RuCl$_3$ with the Fermi energy located close to the bottom of the upper Hubbard band of the t$_{2g}$ manifold. These results suggest the possibility of realizing metallic and even exotic superconducting states. Moreover, we show that in the strained α-RuCl$_3$ monolayer, the Kitaev interactions are enhanced compared to the unstrained bulk structure. Furthermore, we investigate the thermal expansion and magnetostriction coefficients of bulk α-RuCl$_3$ via *ab initio* based methods.

*This project was supported by the Deutsche Forschungsgemeinschaft (DFG) through grant VA117/15-1.

**8:12AM L47.00002: Magneto-oscillations in the Thermal Conductivity of Kitaev Magnet RuCl$_3$**  PETER CZAJKA (Presenter), TONG GAO, JINGJING LIN, Princeton University, MAX HIRSCHBERGER, RIKEN, ARNAB BANERJEE, PAULA LAMPEN-KELLEY, JIAQIANG YAN, DAVID MANDRUS, STEPHEN E NAGLER, Oak Ridge National Laboratory, N. PHUAN ONG, Princeton University — RuCl$_3$ has been the subject of much intrigue and controversy due to it’s status as a possible realization of Kitaev’s honeycomb model and it’s exotic physics. Much of this attention has focused on the half-integer quantized thermal hall conductivity reported by Kasahara et al [1]. Here, we report a striking new observation in the system’s thermal transport physics. When cooled below 4K, RuCl$_3$ exhibits strong magneto-oscillations in its longitudinal thermal conductivity. Additionally, the thermal conductivity follows a butterfly-shaped hysteresis loop that also displays oscillations. We discuss possible explanations for this surprising effect and provide updates on our attempts to reproduce the half-integer quantized thermal hall conductivity reported by Kasahara et al.


*This research was supported by the Department of Energy (DE-SC0017863), the Gordon and Betty Moore Foundation’s EPIQS initiative through grants GBMF4539, and by the US National Science Foundation (grant DMR 1420541).*
8:24AM L47.00003: Kitaev-Γ-Heisenberg exchange in Ni$^{3+}$ honeycomb magnet NaNi$_2$BiO$_{6-δ}$

ALLEN SCHEIE (Presenter), Oak Ridge National Lab, COLLIN LESLIE BROHOLM, Physics and Astronomy, Johns Hopkins University, KATE ROSS, Physics, Colorado State University, PANAGIOTIS PETER STAVROPOULOS, Physics, University of Toronto, ELIZABETH SEIBEL, Chemistry, Princeton University, JOSE RODRIGUEZ-RIVERA, National Institute of Standards and Technology, JOEL TANG, Chemistry, Johns Hopkins University, YI LI, Physics and Astronomy, Johns Hopkins University, HAE-YOUNG KEE, Physics, University of Toronto, ROBERT J. CAVA, Chemistry, Princeton University — We present experimental and theoretical evidence for bond-dependent Kitaev-Γ-Heisenberg exchange in honeycomb Ni$^{3+}$ magnet NaNi$_2$BiO$_{6-δ}$. Heat capacity and neutron diffraction reveal a low-temperature ordered magnetic state for $T < 4.8$ K with $(1/3, 1/3, 0.15(1))$ order. In-plane magnetic correlations match the 120° ordered state of the Kitaev-Γ-Heisenberg exchange. Electron spin resonance and density functional theory reveal a uniform 3+ valence in Ni intermediate between a $S=3/2$ and $J=1/2$ state. DFT shows that covalent bonding between oxygen and Bi produces an enhanced spin orbit coupling in Ni$^{3+}$, which allows for strong bond-dependent exchange. The ordering wave vector, in-plane magnetic correlations, missing entropy, spin state, and superexchange pathways are all consistent with bond-dependent Kitaev-Γ-Heisenberg exchange interactions in NaNi$_2$BiO$_{6-δ}$.

*This work was supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331, and Gordon and Betty Moore foundation under the EPIQS program GBMF4532.

8:36AM L47.00004: Intermediate magnetic phase of the proximate Kitaev system in the in-plane magnetic field

BEOM HYUN KIM (Presenter), Korea Institute for Advanced Study, SHIGETOSHI SOTA, TOMONORI SHIRAKAWA, RIKEN Center for Computational Science, YOUNG-WOO SON, Korea Institute for Advanced Study, SEIJI YUNOKI, RIKEN Center for Computational Science — a-RuCl$_3$ is the antiferromagnetic insulator with a zigzag order which is believed to be proximate to the Kitaev spin liquid. Its magnetic continuum excitation likely resulted from fractionalized Majorana fermions has been evidently observed in recent experiments. The zigzag long-range order can be suppressed and an intermediate phase, a possible quantum spin liquid, can emerge in between the zigzag phase and parallelly polarized phase when the magnetic field is applied. A few theories have attempted to explain the origin of intermediate magnetic phase in the presence of magnetic field. However, they have failed to manifest the intermediate phase in the in-plane external field observed by some experiments.

In the study, we verify that a simple magnetic model with a ferromagnetic Kitaev interaction and antiferromanetic third nearest neighbor Heisenberg interaction ($K$-$J_3$ model) can give successfully the intermediate phase in the in-plane magnetic field. Based on both exact diagonalization and density matrix renormalization group methods, we investigate the magnetic phase diagram of $K$-$J_3$ model in the in-plane magnetic field and demonstrate that the intermediate phase can occur when the field direction is perpendicular to the displacement vector between the nearest neighboring spins.
8:48AM L47.00005: Analysis of the high-field evolution of magnetic excitations in α-RuCl₃*

DAVID KAIB (Presenter), STEPHEN WINTER, ROSER VALENTI, Goethe University Frankfurt — The antiferromagnetic order of α-RuCl₃ can be suppressed by an in-plane magnetic field of approximately 7.5 tesla. Above this critical field, a rather unconventional field-dependence of the magnetic excitations has been reported. More recent Raman and terahertz spectroscopy experiments went up to significantly higher fields [1, 2]. We theoretically analyze these and compare the response of realistic anisotropic models. To this end we discuss different scattering mechanisms for the Raman response. We find that the Fleury-Loudon mechanism (usually discussed as the “two-magnon mechanism”) can explain the strikingly strong intensity of the single-magnon in the Raman spectra, as a consequence of strong Kitaev and anisotropic couplings. Our study firmly establishes the partially-polarized quantum disordered character of the high-field phase.


This work was done in collaboration with A. Sahasrabudhe, S. Reschke, R. German, T. C. Koethe, J. Buhot, D. Kamenskyi, C. Hickey, P. Becker, V. Tsurkan, A. Loidl, S. H. Do, K. Y. Choi, M. Grüninger, Z. Wang, and P. H. M. van Loosdrecht.

*Deutsche Forschungsgemeinschaft (DFG) through grant VA117/15-1

9:00AM L47.00006: Half-integer quantized thermal Hall conductance without out-of-plane magnetic field in a chiral spin liquid state of α-RuCl₃

YUICHI KASAHARA (Presenter), TAICHI YOKOI, SIXIAO MA, SHIGERU KASAHARA, Department of Physics, Kyoto University, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, University of Tokyo, NOBUYUKI KURITA, HIDEKAZU TANAKA, Department of Physics, Tokyo Institute of Technology, JOJI NASU, Department of Physics, Yokohama National University, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo, CIARAN HICKEY, SIMON TREBST, Institute for Theoretical Physics, University of Cologne, YUJI MATSUDA, Department of Physics, Kyoto University — Kitaev quantum spin liquid (QSL) displays the fractionalization of quantum spins into Majorana fermions. In magnetic fields, the emergence of Majorana edge current is predicted to manifest itself in the form of half-integer quantized thermal Hall plateau, which has recently been reported for two-dimensional honeycomb material α-RuCl₃ [1]. While the conventional electronic Hall effect requires a perpendicular magnetic field, we find that the thermal Hall plateau appears even for a magnetic field with no out-of-plane components. In addition, the topological Chern number determined by the sign of the quantized thermal Hall conductance is consistent with that expected in the pure Kitaev spin liquid. These results demonstrate that the Kitaev interaction is primarily responsible and that the non-Abelian topological order persists even in the presence of non-Kitaev interactions in α-RuCl₃.

New Kitaev Magnet with Compelling Thermodynamic Evidence of Proximity to the Kitaev Spin-Liquid*  
FARANAK BAHRAMI (Presenter), Boston College, WILLIAM LAFARGUE-DIT-HAURET, University of Liège, OLEG I. LEBEDEV, Laboratoire CRISMAT, ROMAN MOVSHOVICH, Los Alamos National Laboratory, HUNG-YU YANG, DAVID BROIDO, Boston College, XAVIER ROCQUEFELTE, Chemistry, University of Rennes 1, FAZEL TAFTI, Boston College — Kitaev magnets are widely studied in search of quantum spin-liquid (QSL) ground states and Majorana excitations. Recent theoretical studies predict two potential signatures of a QSL at finite temperatures: a scaling behavior of thermodynamic quantities and a two-step release of the magnetic entropy. Here, we successfully synthesized a new Kitaev magnet, Ag$_3$LiIr$_2$O$_6$ with both signatures in our AC magnetic susceptibility, magnetization and heat capacity measurements. In this new quaternary oxide, despite the existence of a large Weiss temperature, there is no evidence of long-range order in our DC magnetic susceptibility and heat capacity measurements. Based on our DFT calculations, a mixing between silver d and oxygen p orbitals enhances the spin-orbit coupling within the honeycomb layers suggesting a closer proximity to the QSL in Ag$_3$LiIr$_2$O$_6$ compared to known Kitaev magnets, α-Li$_2$IrO$_3$ and Na$_2$IrO$_3$.

*NSF-DMR-1708929

Quasiparticle Relaxation Dynamics in the Kitaev Hyperhoneycomb β-Li$_2$IrO$_3$*  
PETER KISSIN (Presenter), ALEJANDRO RUIZ, PETER KIM, MAX POORE, ANANYA RAI, University of California, San Diego, MAYIA A VRANAS, JAMES ANALYTIS, University of California, Berkeley, ALEX FRANO, RICHARD AVERITT, University of California, San Diego — We study quasiparticle relaxation dynamics in single crystals of the three dimensional Kitaev hyperhoneycomb β-Li$_2$IrO$_3$ (LIO) using time-resolved optical pump-probe spectroscopy (OPPS). OPPS is extremely sensitive to subtle changes in the low energy electronic structure and the emergence of new quasiparticles, which can be missed with other probes. For LIO, we show that the photoinduced change in reflectivity is sensitive to several distinct phases upon varying temperature, photoexcitation intensity, and magnetic field applied along the crystallographic b axis. We observe large differences in the relaxation dynamics in the incommensurate spiral phase at low applied fields as compared to the field-induced zig-zag phase at fields above 2.8 Tesla. In addition, OPPS is sensitive to the recently discovered bulk high temperature phase transition at approximately 100 Kelvin. By tracking the evolution of quasiparticle dynamics within this new phase as a function of temperature and field, our results shed light on the nature of this phase as well as its relationship to the known low temperature phases.

*Research supported by ARO W911NF-16-1-0361.
9:36AM L47.00009: A rare-earth Kitaev material candidate YbCl$_3$*  

EVE EMMANOUILIDOU (Presenter), JIE XING, Department of Physics and Astronomy and California Nano Systems Institute, University of California, Los Angeles, CA 90095, USA, HUIBO CAO, Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, CHAOWEI HU, JINYU LIU, Department of Physics and Astronomy and California Nano Systems Institute, University of California, Los Angeles, CA 90095, USA, DAVID E GRAF, National High Magnetic Field Laboratory, 1800 E. Paul Dirac Drive, Tallahassee, FL 32310, USA, ARTHUR RAMIREZ, Department of Physics, University of California, Santa Cruz, CA 95064, USA, GANG CHEN, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China, NI NI, Department of Physics and Astronomy and California Nano Systems Institute, University of California, Los Angeles, CA 90095, USA —

Most of the searches for Kitaev materials deal with 4d/5d magnets with spin-orbit-coupled $J = \frac{1}{2}$ local moments such as iridates and $\alpha$-RuCl$_3$. Here we propose a new Kitaev material candidate YbCl$_3$. We perform thermodynamic, ac susceptibility and angle-dependent torque measurements on a YbCl$_3$ single crystal. We find that the Yb$^{3+}$ ion exhibits a Kramers doublet ground state that gives rise to an effective spin $J_{\text{eff}} = \frac{1}{2}$ local moment with likely strong anisotropic exchange interactions. The compound exhibits short-range magnetic ordering at around 1.20 K followed by long-range ordering at 0.60 K. These orderings can be suppressed by in-plane and out-of-plane magnetic fields, resulting in a quantum critical point at around 6 and 10 T, respectively. Furthermore, the non-monotonic decrease of Neel temperature under out-of-plane magnetic fields and the 99.8% of ground state entropy release across the short-range ordering, strongly suggest that YbCl$_3$ is a close realization of a Kitaev system.

*Work at UCLA was supported by NSF DMREF-1629457. Work at UCSC was supported by DOE DE-SC0017862. Work at NHMFL is supported by NSF/DMR-1644779 and the State of Florida. G. C. acknowledges MOST Grant 2016YFA0301001 and 2016YFA0300500. H. C. acknowledges US DOE BES Early Career Award KC0402010.
Field-angle-resolved specific heat measurements in the Kitaev material α-RuCl₃

OHEI TANAKA (Presenter), RYUHEI HARASAWA, YUTA MIZUKAMI, Department of Advanced Materials Science, University of Tokyo, MARCIN KONCZYKOWSKI, Laboratoire des Solides Irradiés, Ecole Polytechnique, NOBUYUKI KURITA, HIDEKAZU TANAKA, Department of Physics, Tokyo Institute of Technology, EUN-GOOK MOON, Department of Physics, KAIST, YUICHI KASAHARA, YUJI MATSUDA, Department of Physics, Kyoto Univ, KENICHIRO HASHIMOTO, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, University of Tokyo — Recently, 4d⁵ or 5d⁵ honeycomb materials with strong spin-orbit coupling have attracted great attention as a candidate for realizing a Kitaev quantum spin liquid (QSL). However, most of the candidate materials show magnetic orders at low temperatures. Indeed, α-RuCl₃, one of the most promising candidates, also exhibits a zigzag antiferromagnetic order below \( T_N \) (~ 7 K). However, the magnetic order of this material can be suppressed by applying a critical magnetic field \( H^* \) of 7.5 T parallel to the honeycomb plane. Recent thermal transport measurements, as well as spectroscopic studies such as inelastic neutron scattering, suggest the emergence of spin fractionalization into Majorana fermions in the field-induced QSL phase. Here, we report specific heat measurements under in-plane magnetic fields up to 7 T on electron-irradiated α-RuCl₃ single crystals, in which a systematic suppression of \( T_N \) and \( H^* \) was observed. We find a remarkable six-fold oscillation in the field-angle dependence of the specific heat at low temperatures above \( H^* \). This result is consistent with the field-angle dependence of the Majorana gap expected in the Kitaev QSL.

Ruthenium Substitution in Beta-Lithium Iridate

MAYIA VRANAS (Presenter), University of California, Berkeley, ALEJANDRO RUIZ, Physics, Univ of California - San Diego, BENJAMIN FRANDSEN, Physics, Brigham Young University, ARANI ACHARYA, VIKRAM NAGARAJAN, GILBERT LOPEZ, NITYAN NAIR, University of California, Berkeley, NICHOLAS BREZNAY, Physics, Harvey Mudd College, ZAHRUL ISLAM, Physics, Argonne National Laboratory, ALEX FRANO, Physics, Univ of California - San Diego, JAMES ANALYTIS, University of California, Berkeley — In the Kitaev model, orthogonal bond-directional exchange interactions have been proposed to give rise to quantum spin liquid ground state with fractional Majorana excitations. However, the candidate honeycomb materials described by this model order at low temperatures. Nonetheless, external perturbations, such as applied magnetic field, pressure, and chemical substitution, have been shown to change the strengths of the magnetic interactions and alter their ground state. Additionally, recent work in beta-lithium iridate has shown a hidden magnetic anomaly at T~100K which may be connected to the Kitaev-like behavior in the material. In this work, we present thermodynamic, resonant X-ray diffraction, and muon spin relaxation studies on ruthenium-doped beta-lithium iridate (\( \beta-Li_2Ru_xIr_{1-x}O_3 \)). We describe how the addition of magnetic impurities on the iridium sites suppresses the incommensurate phase and gives rise to an anisotropic spin glass. Additionally, we discuss the impact that these impurities have on the high-temperature phase.

*The authors would like to acknowledge UC LEADs and the UC President's Postdoctoral Fellowship Program.
10:12AM L47.00012: Confinement of fractional excitations in the 3D Kitaev magnet β-Li$_2$IrO$_3$  
YIPING WANG (Presenter), Boston College, ALEJANDRO RUIZ, Physics, university of California San Digo, JAMES ANALYTIS, Physics, University of California Berkerley, KENNETH BURCH, Boston College — Kitaev quantum spin liquid (QSL) is a highly frustrated state in topological magnets with excitations from fractional particles. In candidate materials like RuCl$_3$ and A$_2$IrO$_3$ (A = Na, Li), there is always an ordered state below Tc. However, the transition from spin liquid like fractional excitations to the magnons of the ordered state is still unclear. Here, we report the Raman scattering result on three-dimensional magnet β-Li$_2$IrO$_3$. We identified the polarization and temperature dependence of the magnons and fractional excitations in Raman. This provides first direct evidence for confinement of fractional excitations into magnons in a kitaev system, which so far has only been observed in quasi-1d systems.

10:24AM L47.00013: Evolution of magnetic phases in beta-Li2IrO3 under high magnetic fields*  
VIKRAM NAGARAJAN (Presenter), University of California, Berkeley, KIMBERLY MODIC, Max Planck Institute, JOHN SINGLETON, MUN K. CHAN, Los Alamos National Laboratory, KEVIN WANG, JAMES ANALYTIS, University of California, Berkeley — The Kitaev model describes a honeycomb net of Ising spins where each bond direction exchange-couples an orthogonal component of spin. Remarkably, this model is exactly solvable and predicts a quantum spin liquid ground state. Within the past decade, several materials have been theorized to realize the Kitaev model in their magnetic interactions. One of these materials is beta-Li2IrO3, which crystallizes in a 3D "hyperhoneycomb" structure. While this material does not possess a quantum spin liquid ground state, it contains a variety of interesting magnetic phases that coexist at intermediate temperature. In this talk, we describe how these phases evolve under strong magnetic fields using the state-of-the art technique of resonant torsion magnetometry.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE 1752814. This work was also supported by the Gordon and Betty Moore Foundation EPIQS Initiative through Grant No. GBMF4374.
High-resolution RIXS as a probe of Kitaev Magnetic Excitations in β-Li$_2$IrO$_3$

ALEJANDRO RUIZ (Presenter), ANTHONY ALLEN, University of California, San Diego, VIKRAM NAGARAJAN, Argonne National Lab, JAKE KORELEK, SLAC National Accelerator Laboratory, MARY UPTON, JONGHO KIM, Argonne National Lab, NICHOLAS BREZNAY, Physics, Harvey Mudd College, JAMES ANALYTIS, Physics, University of California Berkeley, DIEGO M CASA, Argonne National Lab, ALEX FRANO, University of California, San Diego — Spin-orbit entangled Mott insulators with strong bond-directional interactions have been proposed as a possible venue for the realization of the Kitaev honeycomb model. Most candidate materials, however, order at low temperatures due to the presence of additional spin coupling interactions. Nonetheless, a wealth of theoretical and experimental work has shown that the Kitaev term is the dominant magnetic exchange. The 3D Kitaev material β-Li$_2$IrO$_3$ hosts nearly degenerate states below 38K when a magnetic field is applied along a Kitaev direction: an incommensurate spiral (INC) and a commensurate field-induced ‘zig-zag’ phase (FIZZ). Most recently, a high-temperature magnetic anomaly was revealed at 100K using thermodynamics and muon relaxation techniques. In this work, we used a high-resolution RIXS spectrometer (FWHM=10meV) to measure the low-energy spin excitations in β-Li$_2$IrO$_3$ under a 2T applied field. We have identified magnon branches near each q-vector and the closing of a gap at the FIZZ q-position with the applied field. More importantly, we have observed a broad continuum of magnetic excitations centered around 35meV, which is unaffected by the low-temperature ordered states, and whose integrated intensity is constant up to 100K and continuously decreases above that.

Anomalous, Anisotropic and Extended Nonlinear Susceptibility in a-RuCl$_3$

BELLAVE SHIVARAM (Presenter), LUDWIG FW HOLLEIS, Univ of Virginia, JOSEPH PRESTIGIACOMO, Naval Research Laboratory, ZHIJE FAN, Univ of Virginia, SATOSHI NISHIMOTO, IFW Dresden, Germany, JIAQIANG YAN, ARNAB BANERJEE, Oak Ridge National Laboratory, MICHAEL OSOFSKY, Naval Research Laboratory, JEROEN VAN DEN BRINK, IFW Dresden, Germany, GIA-WEI CHERN, Univ of Virginia, DAVID MANDRUS, University of Tennessee, STEPHEN E NAGLER, Oak Ridge National Laboratory — In proximate Kitaev a-RuCl$_3$, we establish a radically new behavior of the nonlinear susceptibility hitherto not established. For T < T$_c$ and B || ab-plane, a dual nonlinear response is observed. The high field response above 2 T yields a third order nonlinear susceptibility which peaks near T$_c$ = 7.5 K, reminiscent of behavior in a classical 2D antiferromagnet, but with a large positive value for lowest T. The low field response, for B less than 2T - on the other hand, is positive quadratic and shows a rapid rise below T$_c$. This dual response vanishes for T beyond T$_c$ where the nonlinear response is dominated by only the cubic term. This term is significantly > 0 and turns negative only for a temperature T > 50 K >> T$_c$. Classical Monte Carlo (CMC) simulations capture the observed quadratic response, albeit only near T$_c$. The CMC however fail to reproduce the large quadratic term at low T.. This discrepancy indicates inadequacy of current models and points to the importance of multi-spin correlations in a-RuCl$_3$. For B || c-axis, we measure no dual response with only the cubic term being apparent. We also compare our results with exact diagonalization calculations performed on 16 x 16 cluster.

*The work at ORNL and the University of Tennessee were supported by the Department of Energy.
Motivated by recent discoveries of the coexistent phenomena of superconductivity and ferroelectricity in doped SrTiO$_3$ [1,2], we investigated the feasibility of ferroelectric (FE) superconductivity in which superconductivity coexists with a FE-like order. By analyzing an electron-lattice coupled model for a two-dimensional superconductor, we show that the FE superconductivity is realized through two different mechanisms that rely on the intrinsic spin-orbit coupling [3]. First, the FE superconducting state is stabilized by the ferroelectricity-induced Lifshitz transition in low carrier density regimes. Second, the FE superconducting state is stabilized under a Zeeman magnetic field owing to the suppression of the Pauli depairing effect in the FE phase. Furthermore, we show that the FE superconductivity in SrTiO$_3$ is strongly affected by the multiorbital effect of $t_{2g}$ electrons [4]. Then, we predict a topological Weyl superconducting state in the FE superconducting phase of bulk SrTiO$_3$.

8:12AM L48.00002: Capillary waves on ferroelastic domain walls as a pairing mechanism in strontium titanate*

DAVID PEKKER, Physics and Astronomy, University of Pittsburgh, C STEPHEN HELLBERG, Naval Research Laboratory, ANTHONY TYLAN-TYLER, JEREMY LEVY (Presenter), Physics and Astronomy, University of Pittsburgh — While it has long been known that strontium titanate is a superconductor, with a transition temperature of ~300 mK, the pairing mechanism that leads to superconductivity remains a mystery. We gather insight from recent experiments on superconductivity in the two-dimensional gas formed in lanthanum aluminate/strontium titanate heterostructures. These experiments provide evidence that superconductivity is localized to the edge of the electron gas, which is also associated with a ferroelastic domain wall between an out-of-plane deformation associated with the high electron density region and an in-plane deformation associated with the electron poor region. While the energy scales associated with bulk ferroelastic domains are quite large, on the order of 100 K, we show that capillary waves on domain walls can have much lower energy scales. Further, we argue that these capillary waves are strongly coupled to charge, making them a compelling candidate for an intermediate boson that mediates pairing interaction. We put these notions together in a model of ferroelastic domain walls that supports electron pairing.

*JL acknowledges a Vannevar Bush Faculty Fellowship (ONR N00014-15-1-2847). DP and JL acknowledge NSF (PHY-1913034).

8:24AM L48.00003: Unconventional High Temperature Superconductivity in Cubic Zinc-blende Transition Metal Compounds*

QIANG ZHANG (Presenter), KUN JIANG, YUHAO GU, JIANGPING HU, Institute of Physics, Chinese Academy of Sciences — Recently, we have identified a key character, called high temperature superconductivity "gene", which separates the cuprates and iron-based superconductors from other transitional metal compounds, and proposed some candidates for unconventional superconductivity. All of them are quasi-two dimensional. Here we propose a three dimensional candidate, transition metal compounds in a cubic zinc-blende lattice with electronic filling d^7. We argue that upon doping, this electronic environment can be one of `genes" to host unconventional high temperature superconductivity with a time reversal symmetry broken d+id pairing symmetry. With gappless nodal points along the diagonal directions, this state is a direct three dimensional analogue to the two dimensional B1g d-wave state in cuprates. We suggest that such a case may be realized in electron doped zinc-blende CoN.


*Q. Zhang acknowledges the support from the International Young Scientist Fellowship of Institute of Physics CAS (Grant No. 2017002) and the Postdoctoral International Program (2017) from China Postdoctoral Science Foundation.
Superconducting pairing in non-pseudospin electron bands

KIRILL SAMOKHIN (Presenter), Brock University — We develop the symmetry classification of superconducting gap functions in electron bands that do not transform like the pure spin-1/2 states under the crystal point group operations. Generalizing the commonly used Ueda-Rice prescription, we define the Bloch bases in twofold degenerate bands with spin-orbit coupling in a way which satisfies all symmetry and continuity requirements. These bases are used to construct general multiband pairing Hamiltonians in centrosymmetric crystals. Focusing on single band pairing, several exceptional cases are identified in which the triplet superconducting gap function does not transform under the point-group operations as a pseudovector, with a significant impact on the nodal structure.

*Supported by a Discovery Grant 2015-06656 from the Natural Sciences and Engineering Research Council of Canada.

A microscopic picture of pseudogap phase related to charge fluxes

XIN LI (Presenter), Harvard University — Pseudogap phase in unconventional superconductors is mysterious. Previously, our work disclosed a new relation that the strength of apical charge flux in different families of cuprate superconductors obtained from our computation is correlated with the superconducting transition temperatures reported in previous experiments [1]. A microscopic picture about how such flux can further modulate the in-plane hopping of individual charge carrier was also proposed [1].

In this talk we further discuss an important emergent behavior of such charge fluxes in cuprate superconductors [2]. We use a combination of DFT simulations and theoretical modeling to quantitatively describe how such emergent behavior controls the hopping of charge carriers to give the observed pseudogap phenomena. Simulations of ARPES and resistivity are further compared with experiments. We hope that this new picture of pseudogap phase will shed light on the understanding of more complicated phenomena in the phase diagram of unconventional superconductors.


*Dean's competitive fund at Harvard University
9:00AM L48.00006: Multiband Superconductivity: Anisotropy, Scattering and Bound States

TOM SAUNDERSON (Presenter), Univ of Bristol, GABOR CSIRE, Catalan Institute of Nanoscience and Nanotechnology (ICN2), JAMES F ANNETT, Univ of Bristol, BALAZS UJFALUSSY, Hungarian Acad. of Science, MARTIN GRADHAND, Univ of Bristol — First principles modeling of phonon mediated s-wave superconductors has been largely successful for bulk crystals [1], however, the incorporation of impurities in such theories will be much harder. This problem becomes particularly relevant as impurities affect the superconducting state and magnetic impurities are pair breaking and lead to bound states [2]. Such states are a possible source of Majorana Fermions [3]. Here we present the implementation of the Bogoliubov-de Gennes (BdG) equation into a Green's function (KKR) first principles method [4]. This method is ideal to model impurities and interfaces without the need of artificial supercells. We parameterize the pairing potential but solve the BdG equation self-consistently incorporating microscopic electronic properties of real materials. Our method allows us to investigate the rich complexity of gap anisotropy on the Fermi surface and also how real magnetic and non-magnetic impurities interfere with the superconducting state.


*T. Saunderson acknowledges funding via EPSRC EP/L015544/1

9:12AM L48.00007: Using unsupervised machine learning to predict critical temperatures of superconductors

BENJAMIN ROTER, SASA DORDEVIC (Presenter), Univ of Akron — We use the superconductors from the SuperCon database to construct element vectors and then perform unsupervised learning of critical temperatures. Only the chemical composition of superconductors is used in this procedure. No physical predictors (neither experimental nor numerical) of any kind are used. We archive $R^2=0.93$ which is comparable and in some cases higher than similar estimates using other artificial intelligence techniques. Based on this machine learning model, we predict several new superconductors with high critical temperatures. We also discuss the factors that impede the learning process and suggest possible ways to fix them.
9:24AM L48.00008: Superconducting Neural Networks for Faster Machine Learning
ALEXANDRA DAY (Presenter), ALEXANDER WYNN, EVAN GOLDEN, Massachusetts Institute of Technology MIT — Next-generation neural networks have the potential to deliver advanced performance and higher processing speeds for applications in machine learning and artificial intelligence. MIT Lincoln Laboratory is investigating the feasibility of a superconducting neural network to support faster and lower-energy computing. We will present a conceptual framework for a superconducting neural network and its related benchmarks, along with simulation results for simple circuits.

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9:36AM L48.00009: Novel Magnetoelectric Effects in Gyrotropic Superconductors and a Case Study of Transition Metal Dichalcogenides*  
WENYU HE (Presenter), KAM TUEN LAW, Hong Kong University of Science and Technology — In this work, we classify superconductors according to their magnetoelectric response. Among all the noncentrosymmetric superconductors, only superconductors with gyrotropic point groups have non-zero magnetoelectric response such that a supercurrent can induce a finite spin magnetization. We call these superconductors gyrotropic superconductors. Importantly, the general form of the magnetoelectric response is dictated by the point group symmetry and lead to novel magnetoelectric effects. Novel magnetoelectric effects of several noncentrosymmetric superconductors, including superconductors with chiral lattice symmetry and atomically thin superconducting transition metal dichalcogenides are discussed. Using a newly discovered monolayer 2H-structure NbSe2 as an example, we further show that how an unconventional magnetoelectric response can be induced by strain in superconductors with non-gyrotropic point groups.

*W.-Y. He and K. T. Law are thankful for the support of HKRGC through C6026-16W, 16324216, 16307117 and 16309718. K. T. Law is further supported by the Croucher Foundation and the Dr. Taichin Lo Foundation.
9:48AM L48.00010: Resonant study of the vortex state in LSCO cuprates up to 35 T.*
ARKADY SHEKHTER (Presenter), ALI BANGURA, Natl High Magnetic Field Lab, ANDREAS RYDH, stockholm university, KIMBERLY MODIC, Max Planck Dresden, GREGORY SCOTT BOEBINGER, Natl High Magnetic Field Lab, BRAD J RAMSHAW, Cornell, ROSS MCDONALD, Los Alamos Natl. Lab — We used a newly developed resonant probe of elastic moduli to explore the phase diagram of the vortex state in LSCO cuprates near critical doping x=0.20, up to 35 T. The elastic anomaly at the vortex melting transition—jump down upon entry into the vortex solid—is consistent with a second order phase boundary. The magnitude of the jump, ~0.1 GPa at 20 T is consistent with expected magnitude $\sim H^2/8\pi$ of elastic moduli of the vortex lattice. We also observe a second thermodynamic anomaly at around 5T in the vortex-solid state that is weakly dependent on temperature and field orientation that appears to have dynamic origin. Finally, we will discuss magnetotrophic coefficient measurements in the same system.

*NSF through DMR-1157490

10:00AM L48.00011: Four-fold anisotropy of the parallel upper critical magnetic field in a layered d-wave superconductor at T = 0  
ANDREI LEBED (Presenter), Univ of Arizona — It is well known that a four-fold symmetry of the parallel upper critical magnetic field disappears in the Ginzburg-Landau (GL) region in quasi-two-dimensional (Q2D) d-wave superconductors. Therefore, it has been accurately calculated so far as a correction to the GL results, which is valid close to superconducting transition temperature and is expected to be stronger at low temperatures. As to the case T=0, some approximated methods have been used, which are good only for closed electron orbits and inappropriate for the open orbits which exist in a parallel magnetic field in Q2D superconductors. For the first time, we accurately calculate the four-fold anisotropy of the parallel upper critical magnetic field in a Q2D d-wave superconductor at T=0, where it has the highest possible value. Our results are applicable to Q2D d-wave high-Tc and organic superconductors.
Recently we discovered three laws [1] of electronic thermal conductivity (ETC) in HTSCs via dipolon theory [2-5]. Previously, the dipolon theory predicted first of all two new high energy kinks which were observed later on experimentally. Here we present three corollaries to the three laws of ETC. First corollary: For HTSCs for which \( \Delta(0) = \alpha T_C \), the peak of the ETC is at \( T^{(p)} = 0.4\alpha T_C \). Second corollary: If the superconducting energy gap is destroyed, the peak of the ETC disappears. Third corollary: The peak of the ETC is not due to the reduction of the scattering rate though it enhances the ETC and shifts the peak dependent on the variation of the scattering rate with temperature. These along with three laws [1] explain clearly the origin and behavior of ETC in HTSCs.

(4) R. R. Sharma, Physica \( \text{C 468} \), 190 (2008).
**10:24AM L48.00013: Detecting superconductivity out-of-equilibrium**

SEBASTIAN PAECKEL
(Presenter), Insitut fuer Theoretische Physik, Georg-August Universitaet Goettingen, BENEDIKT FAUSEWEH, Theoretical Division, Los Alamos National Laboratory, ALEXANDER OSTERKORN, Insitut fuer Theoretische Physik, Georg-August Universitaet Goettingen, THOMAS KOEHLER, Department of Physics and Astronomy, Uppsala University, DIRK MANSKE, Quantum Many-Body Theory, Max-Planck-Institut für Festkörperforschung, SALVATORE MANMANA, Insitut fuer Theoretische Physik, Georg-August Universitaet Goettingen — Recent pump-probe experiments on underdoped cuprates and similar systems suggest the existence of a transient superconducting state above \( T_c \). This poses the question how to reliably identify the emergence of long-range order, in particular superconductivity, out-of-equilibrium. We investigate this point by studying a quantum quench in an extended Hubbard model and by computing various observables, which are used to identify (quasi-)long-range order in equilibrium. Our findings imply that, in contrast to current experimental studies, it does not suffice to study the time evolution of the optical conductivity to identify superconductivity. In turn, we suggest to utilize time-resolved ARPES experiments to probe for the formation of a condensate in the single- and two-particle channel.

*Deutsche Forschungsgemeinschaft (DFG) Research Unit FOR 1807 (project P7)
Deutsche Forschungsgemeinschaft (DFG) through SFB/CRC1073 (projects B03 and B07)
European Union's Horizon 2020 research and innovation program under grant agreement No. 758935

**10:36AM L48.00014: Computational Simulations of the Cooling of Type II Superconductors Using a Material Specific Formulation of the Ginzburg Landau Equations**

AIDEN HARBICK
(Presenter), William & Mary College, ALDEN PACK, BRAEDON JONES, MARK TRANSTRUM, Brigham Young University — Superconducting Radio Frequency (SRF) cavities play a fundamental role in particle accelerators. Efficient operation depends on expelling magnetic flux from the cavity, and any residual flux that remains trapped after cooling below the critical temperature can have a significant impact on performance. Experimental evidence suggests that cooling protocols can have a strong impact on subsequent performance. To better understand this phenomenon, we use time-dependent Ginzburg-Landau theory implemented as finite-element simulations. We adapt the theory to allow spatial variation of material-specific parameters along with realistic temperature dependencies. We report on numerical experiments for different configurations of pinning sites and cooling protocols and discuss implications for SRF cavity design and operation.

*This work was supported by the US National Science Foundation under Award OIA-1549132, the Center for Bright Beams.*
10:48AM L48.00015: Hall anomalies and vortex charge in layered superconductors*  DANIEL AROVAS (Presenter), University of California, San Diego, ASSA AUERBACH, Physics, Technion, Israel Institute of Technology — The Hall anomalies in the flux flow regime are associated with moving vortex charge (MVC) in the superconducting layers, which are screened by immobile charges in neighbouring dopant layers. The MVC depends on the logarithm of the magnetic field, and proportional to the doping dependent superfluid stiffness and interlayer dielectric constant. The MVC is shown to add to the Hall conductivity by reformulating Flux Flow transport theory as a current response to applied electric and magnetic field, without the use of vortex forces or complex relaxation rates. MVC curves are extracted from experimental resistivities of hole and electron doped cuprates. These are fit to theory using measured London penetration depths, and a reasonable value of interlayer dielectric constant.

*We gratefully acknowledge support from the US-Israel Binational Science Foundation.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L49 DCMP: Superconducting Proximity Effect and Josephson Junctions III  Mile High Ballroom 1B - Keith Taddei, Oak Ridge National Lab

8:00AM L49.00001: Novel superconducting effects in multiterminal Josephson junctions, Part 1*  ANDREW SEREDINSKI (Presenter), ETHAN ARNAULT, TREVYN LARSON, LINGFEI ZHAO, Department of Physics, Duke University, HENGMING LI, Department of Physics and Astronomy, Appalachian State University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, NIMS, FRANCOIS AMET, Department of Physics and Astronomy, Appalachian State University, IVAN BORZENETS, Department of Physics, City University of Hong Kong, GLEB FINKELSTEIN, Department of Physics, Duke University — We present comprehensive transport measurements of multiterminal graphene Josephson junctions. We have previously found that the coupling between different pairs of contacts results in nontrivial distribution of supercurrent across the device. Here, we isolate supercurrent mediated entirely by continuum contributions with energies above the superconducting gap. We also characterize the superconducting behaviors induced by out-of-plane magnetic fields and RF radiation.

*Transport measurements conducted by E.G.A. and T.L. were supported by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under Award No. DE- SC0002765. E.G.A., A.S. and L.Z. performed lithographic fabrication and characterization of the samples with the support of NSF awards ECCS-1610213 and DMR-1743907. G.F. was supported under ARO Award W911NF16-1-0122. H.L. and F.A. acknowledge the ARO Award W911NF-16-1-0132. I.V.B. acknowledges City U New Research Initiatives/Infrastructure Support from Central (APRC):9610395, and the Hong Kong Research Grants Council (ECS) Project: 9048125.
8:12AM L49.00002: Novel superconducting effects in multiterminal Josephson junctions, Part 2*  
ETHAN ARNAULT (Presenter), ANDREW SEREDINSKI, TREVYN LARSON, LINGFEI ZHAO, Duke University, HENGMING LI, Physics, Appalachian State University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Lab, NIMS, FRANCOIS AMET, Physics, Appalachian State University, IVAN BORZENETS, Physics, City University of Hong Kong, GLEB FINKELSTEIN, Duke University — We present comprehensive transport measurements of multiterminal graphene Josephson junctions. We have previously found that the coupling between different pairs of contacts results in nontrivial distribution of supercurrent across the device. Here, we isolate supercurrent mediated entirely by continuum contributions with energies above the superconducting gap. We also characterize the superconducting behaviors induced by out-of-plane magnetic fields and RF radiation.

*Transport measurements conducted by E.G.A. and T.L. were supported by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under Award No. DE-SC0002765. E.G.A., A.S. and L.Z. performed lithographic fabrication and characterization of the samples with the support of NSF awards ECCS-1610213 and DMR-1743907. G.F. was supported under ARO Award W911NF16-1-0122. H.L. and F.A. acknowledge the ARO Award W911NF-16-1-0132. I.V.B. acknowledges City U New Research Initiatives/Infrastructure Support from Central (APRC):9610395, and the Hong Kong Research Grants Council (ECS) Project: 9048125.

8:24AM L49.00003: Radio-frequency response of a graphene Josephson junction based superconducting oscillator circuit*  
SUBHAMOY GHATAK, JOYDIP SARKAR (Presenter), PRATAP ADAK, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research (TIFR), BISWAJIT DATTA, Materials Department, University of California, Santa Barbara, SUPRIYA MANDAL, LUCKY N. KAPOOR, KISHOR V SALUNKHE, SUMAN KUNDU, R VIJAY, MANDAR M DESHMUKH, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research (TIFR) — Ballistic transport in a graphene-based Josephson junction provides a great opportunity to realize different superconducting quantum circuits. Such circuits are tunable by various externally controllable knobs like - doping, electric field, magnetic field; hence, they can have the potential to be used as superconducting qubits over the existing ones which do not have such variety of tunability. We have devised a superconducting oscillator circuit, employing graphene-based Josephson junction. The analogous electrical circuit is a simple parallel LC oscillator, where the oscillator frequency is tunable through magnetic flux variation and carrier density modulation in graphene. The response of a Josephson junction as an inductor and its non-linearity is vital. The readout of the device involves coupling of an external RF signal to the oscillator through a reflection based measurement. Such a response can be promising for the future direction of graphene-based quantum devices.

*We acknowledge funding support from the Department of Atomic Energy and the Department of Science and Technology of India.
8:36AM L49.00004: Gate Controlled Anomalous Phase Shift in Al/InAs Josephson Junctions*
WILLIAM MAYER (Presenter), MATTHIEU DARTAILH, JOSEPH YUAN, KAUSHINI S WICKRAMASINGHE, Center for Quantum Phenomena, New York University, ENRICO ROSSI, Department of Physics, William & Mary, JAVAD SHABANI, Center for Quantum Phenomena, New York University — In a standard Josephson junction the current is zero when the phase difference between superconducting leads is zero. This condition is protected by parity and time-reversal symmetries. However, the combined presence of spin-orbit coupling, and in-plane magnetic field breaks these symmetries, which can lead to a finite supercurrent even when the phase difference is zero. This is the anomalous Josephson effect which can be characterized by the corresponding anomalous phase shift. We report the observation of a tunable anomalous Josephson effect in Al/InAs Josephson junctions measured via a superconducting quantum interference device. By gate controlling the density of InAs, we are able to tune the spin-orbit coupling in the Josephson junction. This gives us the ability to tune the anomalous phase using both in-plane magnetic field and gate voltage. We observe anomalous phase shifts larger than expected from theory for our material parameters. These results open new opportunities for superconducting spintronics, and new possibilities for realizing and characterizing topological superconductivity.

*This work is supported by DARPA Topological Excitations Grant No. DP18AP90000 in Electronics (TEE) program and NSF dmr 1836687. ER acknowledges support from NSF, ONR and ARO.

8:48AM L49.00005: Superconductivity induced in InSb nanowires from new thin film superconductors
BOMIN ZHANG (Presenter), Physics, Univ. of Pittsburgh, MIHIR PENDHARKAR, IEE, UC Santa Barbara, PO ZHANG, HAO WU, AZARIN ZARASSI, Physics, Univ. of Pittsburgh, CONNOR DEMPSEY, JOON SUE LEE, SEAN HARRINGTON, IEE, UC Santa Barbara, GHADA BADAWY, SASA GAZIEGOVIC, ROY OP HET VELD, JASON JUNG, MARCEL VERHEIJEN, Applied Physics, Eindhoven Univ. of Technology, MOIRA HOCEVAR, Institute Neel, CEA Grenoble, ERIK BAKKERS, Applied Physics, Eindhoven Univ. of Technology, CHRIS J PALMSTROM, IEE, UC Santa Barbara, SERGEY M FROLOV, Physics, Univ. of Pittsburgh — Previous research on superconductor-semiconductor nanowire devices focused heavily on aluminum and niobium alloys. Here we study superconductivity from new thin film superconductors in InSb nanowires. We observe hard superconducting gap and quantized conductance plateau at zero field. The magnetic field evolution of superconducting gap and of supercurrent are studied. New super-semi hybrid structures offering larger critical field and increased energy gap, as compared to aluminum, are interesting as they provide a powerful platform to study topological superconductivity, spin-orbit and Zeeman effects in Superconductor-Semiconductor Josephson Junctions.
9:00AM L49.00006: Magnetic field and flux driven 0-π phase transition in a spinful Josephson junction  ALEXANDER WHITICAR (Presenter), ANTONIO FORNERI, FELIX PASSMANN, ABHISHEK BANERJEE, ASBJORN DRACHMANN, Center for Quantum Devices, Microsoft Quantum Lab – Copenhagen and Niels Bohr Institute, University of Copenhagen, TIANTIAN WANG, CANDICE THOMAS, SERGEI GRONIN, GEOFF C GARDNER, MICHAEL MANFRA, Department of Physics and Astronomy and Station Q Purdue, Purdue University, CHARLES MARCUS, Center for Quantum Devices, Microsoft Quantum Lab – Copenhagen and Niels Bohr Institute, University of Copenhagen — The coexistence of magnetism and superconductivity in a Josephson junction can lead to a 0-π phase transition. Quantum dots (QDs) can serve as spin impurities that can be controllably coupled to a superconductor (S). Here, we probe the Andreev spectrum of a hybrid S-QD-S Josephson junction by performing tunneling spectroscopy with a weakly coupled normal lead. We identify a gate-voltage-induced transition from singlet to doublet ground state, where the Andreev spectrum develops a π-phase shift. We demonstrate control of the 0−π transition using superconducting phase difference across the junction and an external magnetic field. We identify parity transitions by measuring zero-bias crossings induced by a magnetic field, phase difference, and gate voltage. This research was supported by Microsoft and the Danish National Research Foundation.

9:12AM L49.00007: A Mesoscopic Spectrometer Based on the Josephson Effect*  JOËL GRIEßMAR, FABIEN LAFONT, RAMIRO RODRIGUEZ (Presenter), VINCENT BENZONI, LÉO PEYRUCHAT, JEAN-LOUP SMIRR, CAGLAR GIRIT, Flux Quantum Lab, CNRS USR 3573, Collège de France, Paris, France — A key element of mesoscopic topological systems, such as hybrid semiconductor-superconductor circuits, are Andreev Bound States, single quasiparticles localized at superconducting weak links. The characteristic transition energy of these states is twice the superconducting gap (90 GHz in Al). Conventional microwave techniques allow probing these states but only in a limited bandwidth. We implement a new broadband spectrometer operating at frequencies up to 180 GHz, with a 2 MHz linewidth and a minimal theoretical sensitivity of 5 kHz, based on the Josephson effect which converts a DC voltage to microwave oscillations at a frequency proportional to this voltage. Conveniently the absorption of the emitted photons is measured in the spectrometer DC current-voltage characteristic. Using a symmetrical SQUID biased at half a flux quantum allows decoupling the spectrometer from parasitic environmental modes. We demonstrate this spectroscopy technique by detecting the plasma frequency, near 100 GHz, of an RF-SQUID, fabricated both on- and off-chip, inductively coupled to the spectrometer.

*Project funded by IDEX grant ANR-10-IDEX-0001-02 PSL, Paris Programme Emergence(s) Grant and the ERC under the European Union's Horizon 2020 research and innovation programme (grant agreement 636744)
Graphene Josephson junctions in high in-plane magnetic field

TOM Dvir (Presenter), QuTech, Delft University of Technology, Ayelet Zalic, The Racah Institute of Physics, The Hebrew University of Jerusalem, Kenji Watanabe, Takashi Taniguchi, Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba 305-0044, Japan, Hadar Steinberg, The Racah Institute of Physics, The Hebrew University of Jerusalem — In recent years, there is a growing interest in graphene as the main ingredient in Josephson junctions (JJs). The ability to control the concentration and the sign of the charge carriers allows the fabrication of bipolar JJ with critical currents that can be varied in three orders of magnitude in the same device. Also, using clean graphene allows studying the interplay between quantum Hall effect and superconductivity. The study of graphene JJs in high magnetic fields was so far limited by the response of the host superconductor to the application of field. We fabricate JJs using ultra-thin NbSe$_2$ as the superconductor, allowing us to apply very high in-plane magnetic fields without significantly affecting the superconducting gap. We show that such JJs, NbSe$_2$-graphene-NbSe$_2$, are highly transparent, and survive to in-plane fields up-to 8T. Due to the two-dimensional nature of the system, the interaction of the in-plane field with the system occurs only with the spin degree of freedom, imitating S-ferromagnet-S JJs, with effective exchange energy determined by the external field.

*This work was funded by a European Research Council Starting Grant (No. 637298, TUNNEL), an Israeli Science Foundation grant 1363/15, and BSF grant 2016320. T.D. and A.Z. received Azrieli Fellowships.

Interference of chiral Andreev edge states in a multi-terminal Josephson junction

Lingfei Zhao (Presenter), Ethan Arnault, Andrew Seredinski, Trevyn Larson, Duke University, Hengming Li, Appalachian State University, Kenji Watanabe, Takashi Taniguchi, Advanced Materials Laboratory, NIMS, Francois Amet, Appalachian State University, Gleb Finkelstein, Duke University — We study the interference effects of chiral Andreev edge states (CAES) in a multiterminal Josephson junction operated in the quantum Hall regime. On well quantized QH plateaus, we observe CAES interference in the form of voltage fluctuations downstream from the grounded superconducting contact. We have previously attributed this interference to successive electron-hole conversion along the quantum Hall-superconducting interface. Here, we show that these fluctuations also exist in the Hall voltage, indicating a second order effect whereby the downstream particle experiences an additional electron-hole conversion along more than one superconducting contact. These observations indicate the potential for coherent control of the chiral Andreev edge states.

*L.Z. and E.G.A. are supported by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under Award No. DE-SC0002765. A.S. acknowledge the support of NSF awards ECCS-1610213 and DMR-1743907. T.L., and G.F. acknowledge the support of ARO Award W911NF-16-1-0122. H.L. and F.A. acknowledge the ARO under Award W911NF-16-1-0132.
9:48AM L49.00010: Proximity effects in superconducting heterostructures*  
BALAZS UJFALUSSY (Presenter), GABOR CSIRE, Wigner Research Centre for Physics, KYUNGWHA PARK, Virginia Tech — The overlayer of metallic thin films on top of an s-wave superconducting substrate is studied by the numerical solution of the fully relativistic Kohn-Sham-Bogoliubov-de Gennes equations via multiple scattering methods. We briefly describe the methodology which allows for a material-specific calculation of the Andreev band structure. We discuss the relation of the effective pair interaction, the anomalous charge density and the induced superconducting gap in heterogeneous systems. Taking Au/Nb films as an example, we also show how surface and interface states behave in such systems and study the formation of the superconducting gap in one-dimensional impurity systems.

*BME Nanotechnology FIKP grant

10:00AM L49.00011: Visibility of a topological qubit quantum dot measurement  
ALEKSEI KHINDANOV (Presenter), University of California, Santa Barbara, DMITRY I. PIKULIN, Microsoft Research — Topological superconductor-quantum dot-topological superconductor (TS-QD-TS) system is of current interest for topological quantum computing, being a proposed platform for detecting Majorana zero modes (MZMs) and for measuring a topological qubit state. Here, using perturbation theory we derive expression for Josephson energy in this system, with a particular emphasis on a term associated with a coupling of the QD to quasiparticle continuums in each TS, arising in the fourth order. Furthermore, we study how 1/f flux noise, typical for SQUID-type devices, interferes measurement visibility of the qubit. We find that even though coupling of the QD to quasiparticle continuums does not directly affect measurement outcomes, the flux noise might considerably decrease the signal to noise ratio. We calculate experimental parameter values for which the effect is minimized and a best signal to noise ratio can be achieved.

10:12AM L49.00012: Domain wall based spin-triplet Josephson junction and SQUID  
EKTA BHATIA (Presenter), NISER, ANAND SRIVASTAVA, JAMES DEVINE STONEMAN, NADIA A STELMASHENKO, ZOE BARBER, JASON ROBINSON, Material Science and metallurgy, University of Cambridge, KARTIK SENAPATI, NISER — Spin-singlet Cooper pairs convert to spin-triplet Cooper pairs on passing through a magnetic non-collinear structure at superconductor(S)/ferromagnet(F) interface [1]. In this context, the generation of triplet supercurrents through intrinsic ferromagnetic domain walls, which are naturally occurring non-collinear magnetic structure, was proposed theoretically in the last decade [2]. However, an experimental demonstration has been lacking in the literature, particularly due to the difficulty in accessing a single domain wall which is typically buried between two domains in a ferromagnetic material. In this report, by pinning a magnetic domain wall at the barrier of a nanoscale S/F/S planar junction, we have been able to demonstrate the predicted long-range triplet supercurrent due to a domain wall. The spin-triplet current was measured over a ferromagnetic barrier width exceeding 70 nm. Using the same concept of domain wall pinning at the Josephson junction barrier, we have also demonstrated a planar Nb/Ni/Nb triplet SQUID device.

10:24AM L49.00013: Unconventional magnetic flux response of Josephson junctions with a weak link made from alternating normal and ferromagnetic interlayers*  IVAN P NEVIRKOVETS, MIKHAIL BELOGOLOVSKII (Presenter), Department of Physics and Astronomy, Northwestern University — We present the first systematic study of critical current-vs-external magnetic flux dependences in Josephson junctions with a weak link formed by alternating normal (N=Al) and ferromagnetic (F=Ni or Py) nominally identical nm-thick films coupled to superconducting (S=Nb) electrodes. In contrast to the well-known Fraunhofer-type behavior for conventional Josephson trilayers, the S/(NF)ₙ/S hybrids with n > 5 (with or without an ultra-thin Al-oxide barrier) have revealed anomalous patterns. In the most samples, with increasing magnetic flux, the supercurrent underwent periodic, constant-amplitude modulation resembling that in SQUIDs, see preliminary data [1]. The oscillatory pattern was superposed on a background supercurrent having much larger oscillation period in an externally applied magnetic field. We explain the origin of the non-Fraunhofer critical current curves as being associated with a special type of diffusive charge trajectories confined to the edges of the periodic (NF)ₙ weak link. The Josephson devices in the surface-dominated transport regime can be exploited for nanoscale low-field detection.


*Belogolovskii's research at the NWU was supported by the Fulbright Visiting Scholar Program.

10:36AM L49.00014: Enhanced triplet pairing in magnetic junctions with s-wave superconductors  CHENGHAO SHEN (Presenter), State Univ of NY - Buffalo, THOMAS VEZIN, Ecole Polytechnique, JONG E HAN, IGOR ZUTIC, State Univ of NY - Buffalo — A common path to Majorana fermions and topologically-protected quantum computing relies on spin-triplet superconductivity[1]. While spin-triplet pairing is elusive in nature and even common spin-triplet candidates, such as Sr₂RuO₄, could support alternative explanations[2], proximity effects in heterostructures can overcome these limitations. Specifically, a common expectation is that robust spin-triplet superconductivity in magnetic junctions should rely on highly spin-polarized magnets or complex magnetic multilayers[3]. Instead, we predict that the interplay of interfacial spin-orbit coupling and the barrier strength in simple magnetic junctions with s-wave superconductors can lead to nearly complete spin-triplet superconducting proximity effects when magnets have only a small spin polarization[4]. We show that this enhanced spin-triplet regime is characterized by a huge increase in conductance magnetoanisotropy[4-6], orders of magnitude larger than in the normal state.

The current-phase relationship of Josephson junctions is often assumed to be a sinusoid. However, this is not always the case. In order to directly measure the current-phase relationship of junctions with a range of characteristics, including both SIS and SNS junctions, we fabricated Josephson junctions having $\text{Nb}_x\text{Si}_{1-x}$ barriers with varied Nb concentration. We constructed a superconducting SQUID-sensor-based circuit to extract their current-phase relationships. SIS-like junctions had the expected near-sinusoidal current-phase relationship, but the current-phase relationship gained additional harmonics as the barriers became less insulating. Thus, SNS-like junctions with normal barriers and high Nb content had sawtooth-like current-phase relationships. This deviation is likely due to additional Andreev reflections. The effects of this non-sinusoidal current phase relationship were observed in current-voltage characteristics through the appearance of non-integer Shapiro steps. Additionally, the same techniques were applied to Si-Mn nanocluster junctions to measure the changes in the current-phase relationship caused by the dynamic tuning of the critical currents of these junctions.

*This work is partially funded by NIST and the IARPA SuperTools Program.
8:00AM L50.00001: Late time dynamics of dynamical correlation functions and out of time ordered correlators* JONATHON RIDDELL (Presenter), McMaster Univ, ÁLVARO ALHAMBRA, Perimeter Institute, LUIS GARCIA-PINTOS, University of Maryland, ERIK SORENSEN, McMaster Univ — In this talk we study the universal properties of different types of dynamical quantities in time, for large classes of systems. First we investigate two-point correlation functions—also known as dynamical response functions in closed non-integrable many-body quantum systems. We show that for a large class of models these correlation functions factorize at late time, proving dissipation emerges from unitary dynamics. We similarly show that the fluctuations around the late time are bounded by the purity of the thermal ensemble. For auto-correlation functions we provide an upper bound on the timescale for which they equilibrate to this late time factorization. We then move onto study the late time dynamics of fermionic models in the presence of disorder for out of time ordered correlators. Focusing on the Aubry-André model we derive universal late time behavior for the OTOC in the extended regime of the model. These fermionic results are then used to extend the discussion to equilibration in finite time for all quadratic models in the extended regime.

*This research was supported by NSERC and enabled in part by support provided by (SHARCNET) (www.sharcnet.ca) and Compute/Calcul Canada (www.computecanada.ca).

8:12AM L50.00002: Self-averaging in many-body quantum systems out of equilibrium* LEA SANTOS (Presenter), MAURO SCHIULAZ, Yeshiva Univ, E. JONATHAN TORRES HERRERA, Benemérita Universidad Autónoma de Puebla,., FRANCISCO PÉREZ-BERNAL, Universidad de Huelva — Despite its importance to experiments, numerical simulations, and the development of theoretical models, self-averaging in many-body quantum systems out of equilibrium remains underinvestigated. Usually, in the chaotic regime, self-averaging is just taken for granted. The numerical and analytical results presented here force us to rethink these expectations. They demonstrate that self-averaging properties depend on the quantity and also on the time scale considered. We show analytically that the survival probability in chaotic systems is not self-averaging at any time scale, even when evolved under full random matrices. We also analyze the participation ratio, Rényi entropies, the spin autocorrelation function from experiments with cold atoms, and the connected spin-spin correlation function from experiments with ion traps. We find that self-averaging holds at short times for the quantities that are local in space, while at long times, self-averaging applies for quantities that are local in time. Various behaviors are revealed at intermediate time scales.

*This work is supported by the NSF Grant No. DMR-1603418.
**Measurement-induced entanglement dynamics in many-body localizable systems**

OLIVER LUNT (Presenter), ARJEET PAL, Univ Coll London — In this work we explore the interplay of two types of entanglement transition: the many-body localization (MBL) transition, where eigenstates go from volume law to area law, and measurement-induced transitions, where recent work has demonstrated that the late-time entanglement entropy of random circuits can collapse from volume to area law above a finite critical measurement rate [1-3]. Whereas previous studies have focused mainly on random quantum circuits, here we focus on Hamiltonian dynamics. Many-body localizable systems exhibit at least two phases with distinct dynamical properties: the thermal and the localized phases. In this work, we investigate the effect of measurements on the entanglement dynamics of these phases.


**Quantum Impurity Far from Equilibrium: Quantum Transport Through a Dissipative Resonant Level Using DMRG**

XIN ZHANG (Presenter), THOMAS BARTHEL, HAROLD U BARANGER, Duke University — Using time-dependent matrix product state techniques, we study the quantum transport properties of a dissipative resonant level model, in which a quantum impurity is coupled to two leads and a bosonic bath. Experimentally, this model can be realized by coupling a quantum dot with resistive leads [1]. We focus on the far-from-equilibrium steady states. The non-linear I-V curves and their scaling behavior are presented for different dissipation strengths in the case of both symmetric and asymmetric coupling. In the symmetric setup, a quantum critical point of the two-channel Kondo class is present [2]. To probe properties of the quasiparticle excitations, which can be measured with tunneling spectroscopy, we study the spectral function and shot noise.

[1] HT Mebrahtu, et al., Quantum phase transition in a resonant level coupled to interacting leads, Nature (2012);

*We acknowledge support from the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under Award No. DE-SC0005237 (X.Z. and H.U.B.), and Award No. DE-SC0019449 (T.B.).
8:48AM L50.00005: Role of non-linear susceptibilities in non-equilibrium transport through an N-level Anderson impurity model away from half-filling

YOSHIMICHI TERATANI (Presenter), AKIRA OGURI, Osaka City Univ — We study non-equilibrium SU(N) Kondo effect that occurs in quantum impurity systems at low-temperatures T and low-bias voltages eV. We expand the differential conductance up to terms of order T^2 and (eV)^2 at arbitrary electron fillings, using an extended version of the Fermi-liquid theory for the Anderson impurity model. The coefficients for these terms are determined by the linear and non-linear susceptibilities defined with respect to the equilibrium ground state [1,2]. We calculate these susceptibilities using the NRG for N=2, 4, and 6 in a wide range of electron fillings N_d, varying the impurity level position ε_d. The results show that contributions of the three-body susceptibilities on the transport coefficients increase as N_d deviates away from half-filling, especially near the fillings of N_d = 1 and N_d = N-1. We also employ a large N approach, i.e., the 1/(N-1) expansion with a scaling that keeps (N-1)U constant [3]. We find that the 1/(N-1) results and NRG results are in good already at N=4 and 6.


9:00AM L50.00006: Hamiltonian dynamics of a sum of interacting random matrices*

MATTEO BELLITTI (Presenter), SIDDHARDH MORAMPUDI, CHRISTOPHER LAUMANN, Boston Univ — In ergodic quantum systems, physical observables have a non-relaxing component if they "overlap" with a conserved quantity. In interacting microscopic models, how to isolate the non-relaxing component is unclear.

We compute exact dynamical correlators governed by a Hamiltonian composed of two large interacting random matrices, H=A+B.

We analytically obtain the late-time value of 〈A(t)A(0)〉; this quantifies the non-relaxing part of the observable A.

The relaxation to this value is governed by a power-law determined by the spectrum of the Hamiltonian H, independent of the observable A.

For Gaussian matrices, we further compute out-of-time-ordered-correlators (OTOCs) and find that the existence of a non-relaxing part of A leads to modifications of the late time values and exponents.

Our results follow from exact resummation of a diagrammatic expansion and hyperoperator techniques.

*The authors acknowledge support from the NSF through grant PHY-1752727. This work was performed in part at the Aspen Center for Physics, which is supported by National Science Foundation grant PHY-1607611, and at the Galileo Galilei Institute in Florence.
9:12AM L50.00007: Universal Dynamics of Stochastically Driven Quantum Impurities*
WILLIAM BERDANIER (Presenter), University of California, Berkeley, JAMIR MARINO, Harvard University, EHUD ALTMAN, University of California, Berkeley — We show that the dynamics of a quantum impurity subject to a stochastic drive on one side and coupled to a quantum critical system on the other display a universal behavior inherited from the quantum critical scaling. Using boundary conformal field theory, we formulate a generic ansatz for the dynamical scaling form of the typical Loschmidt echo and corroborate it with exact numerical calculations in the case of a spin impurity driven by shot noise in a quantum Ising chain. We find that due to rare events the dynamics of the mean echo can follow very different dynamical scaling than the typical echo for certain classes of drives. Our results are insensitive to irrelevant perturbations of the bulk critical model and apply to all the microscopic models in the same universality class.

*WB is supported in part by the Hellman Foundation and by the DARPA DRINQS program (award D18AC00014). JM is supported by the European Union’s Framework Programme for Research and Innovation Horizon 2020 under the Marie Sklodowska-Curie Grant Agreement No. 745608 (‘QUAKE4PRELIMAT’). This collaboration was started during the KITP program ‘The Dynamics of Quantum Information’, and it has been supported in part by the National Science Foundation under Grant No. NSF PHY-1748958.

9:24AM L50.00008: Non-Equilibrium Dynamics of the SYKq=∞ Model  STEFAN KEHREIN
(Presenter), Institute for Theoretical Physics, University of Goettingen — The Sachdev-Ye-Kitaev model is a paradigm for quantum many-body systems without a quasiparticle description. Its non-equilibrium dynamics after a quench was investigated in Ref. [1], where certain quenches to the q=∞ model could even be solved analytically. In this talk these analytical results are extended to arbitrary quenches to the q=∞ SYK model. Remarkably one always finds instant thermalization.


9:36AM L50.00009: Using charge- and spin-specific local integrals of motion to explore entanglement growth in the disordered Fermi Hubbard model*  RACHEL WORTIS (Presenter), BRANDON LEIPNER-JOHNS, Trent University — The Fermi Hubbard model has both charge and spin degrees of freedom at each site. We explore the coupling of the dynamics in these two channels in the presence of disorder. In particular, we write the Hamiltonian in terms of charge- and spin-specific local integrals of motion, and compare the strengths of the coupling constants linking integrals of motion of the same species (charge-charge and spin-spin) with those linking charge and spin. This provides an avenue to understanding the wide range of time scales which appear in the dynamics.

*Supported by NSERC of Canada.
9:48AM L50.00010: Scalable probes of measurement-induced phase transitions* DAVID HUSE (Presenter), MICHAEL GULLANS, Princeton University — Measurement-induced phase transitions are a recently uncovered class of critical phenomena that occur when many-body unitary dynamics are interspersed with measurements at a tunable rate. We uncover a local order parameter for such measurement-induced criticality (MIC) equal to the average entropy of a single reference qubit initially entangled with the system. Using this order parameter, we identify scalable probes of MIC that are immediately applicable to advanced quantum computing platforms. We test our proposal on a 1+1-dimensional stabilizer circuit model that can be classically simulated in polynomial time. We determine bulk and surface critical exponents of MIC for such models and find that they are very close, or equal to those of 2+0-dimensional critical percolation. Developing scalable probes of MIC in more general models may be a useful application of noisy-intermediate scale quantum (NISQ) devices, as well as point to more efficient realizations of fault-tolerant quantum computation.

*Research supported in part by the DARPA DRINQS program. D.A.H. was supported in part by a Simons Fellowship.

10:00AM L50.00011: Higher-order and fractional discrete time crystals in clean long-range interacting systems* ANDREA PIZZI (Presenter), Univ of Cambridge, JOHANNES KNOLLE, Technical University Munich, ANDREAS NUNENKAMP, Univ of Cambridge — Discrete time crystals are periodically driven systems characterized by a response with periodicity $nT$, with $T$ the period of the drive and $n>1$. Typically, $n$ is an integer and bounded from above by the dimension of the local (or single particle) Hilbert space, the most prominent example being spin-1/2 systems with $n$ restricted to 2. Here we show that a clean spin-1/2 system in the presence of long-range interactions and transverse field can sustain a huge variety of different 'higher-order' discrete time crystals with integer and, surprisingly, even fractional $n>2$. We characterize these non-equilibrium phases of matter thoroughly using a combination of exact diagonalization, semiclassical methods, and spin-wave approximations, which enable us to establish their stability in the presence of competing long- and short-range interactions. Remarkably, these phases emerge in a model with continuous driving and time-independent interactions, convenient for experimental implementations with ultracold atoms or trapped ions.

*A.P. acknowledges support from the Royal Society. A.N. holds a University Research Fellowship from the Royal Society and acknowledges additional support from the Winton Programme for the Physics of Sustainability.
10:12AM L50.00012: Time dependent, external perturbations of Hubbard clusters with explicit many electron interactions and their implications  GAYANATH FERNANDO, ADIL-GERAI KUSSOW (Presenter), Univ of Connecticut - Storrs, KALUM PALANDAGE, Physics, Trinity College — We examine the effects of harmonic and other time dependent external perturbations on a many electron system using exact diagonalization and Lanczos method for Hubbard clusters in our search for time crystal and other behaviors such as precursors to superconducting states. It is possible to open time dependent breathing modes of the Hubbard Hamiltonian by exposing the cluster to electromagnetic radiation. The analysis based on exact solutions of the Heisenberg equation demonstrates that it is possible to reach highly populated states with localized pairs of electrons having opposite spins (related to possible superconductivity). Since the system is principally time dependent in the pre-thermalization regime, it can be treated as an example of a time crystal.

10:24AM L50.00013: Flow Renormalization and Prethermal Regimes of Periodically-Driven Quantum Systems  MARTIN CLAASSEN (Presenter), Center for Computational Quantum Physics, Simons Foundation Flatiron Institute — One of the most fascinating aspects of non-equilibrium physics is that a quantum system pushed out of equilibrium can exhibit markedly different dynamics when probed on different time scales. We develop a flow renormalization approach for periodically-driven quantum systems, for which a rigorous relation between "flow time" and real time can be established. In this formalism, the dynamical problem is recast in terms of a flow towards an attractive thermal fixed point, while narrowly avoiding a series of unstable fixed points that determine distinct transient dynamical regimes at intermediate times. We show that a unique choice of flow permits relating flow-time and real-time evolution via analytic continuation, and study the appearance of long-lived prethermal regimes in Floquet Hubbard models and spin chains.
10:36AM L50.00014: Flow equation approach to periodically driven quantum systems*
MICHAEL VOGL (Presenter), University of Texas at Austin, PONTUS LAURELL, Oak Ridge, AARON BARR, GREGORY A FIETE, University of Texas at Austin — We present a theoretical method to generate highly accurate time-independent Hamiltonians governing the finite-time behavior of time-periodic systems. The method exploits infinitesimal unitary transformation steps, from which renormalization group-like flow equations are derived to produce effective Hamiltonians. The method has a range of validity reaching into frequency regimes that are usually inaccessible by high frequency expansions. Our approach is demonstrated for many-body Hamiltonians and offers an improvement over the more well-known Magnus expansion and the rotating frame approximation. We show how the method relates to the rotating frame approximation and how it can be used to approximately transform to a rotating frame when the exact transformation isn't tractable. We compare our approximate results to those found via exact diagonalization.

*We gratefully acknowledge funding from Army Research Office Grant No. W911NF-14-1-0579, NSF Grant No. DMR-1507621, and NSF Materials Research Science and Engineering Center Grant No. DMR-1720595. We acknowledge the Texas Advanced Computing Center (TACC) at The University of Texas at Austin for providing computing resources. GAF acknowledges support from a Simons Fellowship.

10:48AM L50.00015: Fermi-liquid corrections to non-equilibrium Keldysh vertex functions for an Anderson impurity model. AKIRA OGURI (Presenter), YOSHIMICHI TERATANI, Department of Physics, Osaka City Univ, RUI SAKANO, ISSP, The university of Tokyo — We study in detail the residual interaction between quasi-particles that plays an essential role in the non-equilibrium transport through quantum dots under finite bias voltage $eV$. Specifically, Fermi-liquid corrections to the vertex functions, which can be related to the collision integral for the Anderson impurity model, are calculated away from half-filling up to linear terms with respect to $\omega$, $\omega'$, and $eV$ at zero temperature $T=0$. Here, $\omega$ and $\omega'$ correspond to the energies of two interacting quasi-particles. The expansion coefficients are obtained by extending the recent developments [1,2], using the Ward-Takahashi identity for the Keldysh current vertex functions. We also discuss low-energy behavior of nonlinear current noise in the Fermi-liquid regime using the numerical renormalization group approach.


Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L51 DCMP: Optical Spectroscopy of 2D Materials Mile High Ballroom 1D -
Yunqiu (Kelly) Luo, Cornell University
Monolayer transition metal dichalcogenide (TMD) semiconductors have garnered interest due to their direct band gap, strong excitonic effects, and valley optical selection rules. Organic semiconductors also host strongly bound excitons and allow for broadly tunable emission energies. Together, heterointerfaces of a molecular semiconductor adsorbed on a monolayer TMD are characterized by interesting effects including enhanced Raman scattering. These Raman enhancements are poorly understood but are attributed to different charge transfer mechanisms [1], [2], [3]. Here, we study a system of monolayer 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) on WSe₂, chosen for its type-II band alignment. We performed low temperature Raman and photoluminescence spectroscopy and observe a large enhancement of the PTCDA Raman signal compared to monolayer PTCDA on SiO₂. The behavior of this Raman scattering is explored through electrostatic doping of the TMD and excitation energy dependence. Control over the Raman enhancement would yield new understanding of the Raman enhancement phenomena in these systems.


*Funded by NSF grant No. ECCS-1708562
**8:12AM L51.00002: Dark Excitons in Monolayers of Molybdenum based Transition Metal Dichalcogenide**  
CEDRIC ROBERT (Presenter), Institut National des Sciences Appliquees de Toulouse, PIOTR KAPUSCINSKI, Institute of Experimental Physics, Faculty of Physics, University of Warsaw, ALEX DELHOMME, LNCMI Grenoble, BO HAN, Institut National des Sciences Appliquees de Toulouse, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, BERNHARD URBASZEK, XAVIER MARIE, Institut National des Sciences Appliquees de Toulouse, CLEMENT FAUGERAS, MAREK POTEMSKI, LNCMI Grenoble — Excitons with binding energies of a few hundreds of meV drive the optical properties of Transition Metal Dichalcogenide (TMD) monolayers. One can expect that the optoelectronic properties will change drastically whether the spin-forbidden dark excitons lie below or above the bright excitons. This exciton fine structure splitting was accurately determined recently for WS2 and WSe2 monolayers using various experimental techniques [1-5]. In contrast the energy of the dark exciton in MoS2 ML has not been measured yet though this was the first member of the TMD family to be established as a direct gap semiconductor in the monolayer form. Here we have performed magneto-photoluminescence experiments on MoS2 monolayers encapsulated in hexagonal Boron Nitride (hBN) with a magnetic field oriented along the monolayer plane. The high quality of the investigated samples allowed us to determine accurately the bright-dark energy splitting. We have performed similar measurements for other MoX2 monolayers (X=Se or Te) encapsulated in hBN. The different contributions to the exciton fine structure will be discussed.


**8:24AM L51.00003: Effect of many-body interactions on the valley-selective optical Stark in WS2**  
PAUL CUNNINGHAM (Presenter), United States Naval Research Laboratory, AUBREY T. HANBICKI, Laboratory for Physical Sciences, University of Maryland, THOMAS L REINECKE, KATHLEEN M MCREARY, BEREND THOMAS JONKER, United States Naval Research Laboratory — Breaking the valley degeneracy in monolayer transition metal dichalcogenides through the valley-selective optical Stark effect can be exploited for quantum valleytronic operations such as coherent manipulation of valley superposition states. The strong light-matter interactions that give rise to the optical Stark effect have historically been described by a two-level dressed-atom model, which assumes non-interacting particles. While this model works well far from resonance where the Rabi frequency is larger than the exciton formation rate, here we show experimentally that it does not apply for excitation near resonance in monolayer WS2. Instead, our observations are well described by an excitonic model of the optical Stark effect that includes many-body Coulomb interactions. We observe a blue-shift due to the valley-selective optical Stark effect for excitation both below and above resonance, confirming the prediction from this theory that repulsion between virtual excitons dominates the light-matter interactions for photoexcitation detuned from resonance by less than the exciton binding energy. We expect our findings to be general to low-dimensional semiconductors that support bound excitons and other many-body Coulomb interactions.
8:36AM L51.00004: Direct Observation of Gate-Tunable Dark Trions in Monolayer WSe$_2$*

TIANMENG WANG (Presenter), ZHIPENG LI, Rensselaer Polytechnic Institute, ZHENGUANG LU, Natl High Magnetic Field Lab, MANDEEP KHATONIAR, The City College of New York, ZHEN LIAN, Rensselaer Polytechnic Institute, YUZE MENG, Nanjing University, MARK BLEI, Arizona State University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, STEPHEN A MCGILL, Natl High Magnetic Field Lab, SEFAATTIN TONGAY, Arizona State University, VINOD M MENON, The City College of New York, DMITRY SMIRNOV, Natl High Magnetic Field Lab, SUFEI SHI, Rensselaer Polytechnic Institute — Spin-forbidden intravalley dark excitons in tungsten-based transition-metal dichalcogenides (TMDCs) have attracted intense research interest. It has been discovered that tungsten-based TMDCs such as WSe$_2$ and WS$_2$ have a unique bandstructure, in which the spin-orbit coupling also induces the splitting of the conduction band. The resulted ground state of the exciton, however, is a spin-triplet state as the spin-forbidden dark exciton. We show that we can control the dark exciton electrostatically by dressing it with one free electron or free hole, forming the dark trions. The existence of the dark trions is suggested by the unique magneto-photoluminescence spectroscopy pattern of the monolayer WSe$_2$ device. And the existence of the dark trions is unambiguously demonstrated by directly resolving the radiation angle of the dark trions through back focal plane imaging. The dark trions possess binding energy of $\sim$15 meV, and inherit the long lifetime and large g-factor from the dark exciton. The dark trions open the door to new possibilities of valleytronics and excitonic applications.

*We thank Dr. Lei Shi and Shengnan Miao for helpful discussions. We acknowledge support from AFOSR, through Grant No. FA9550-18-1-0312. and support from ACS PRF, through Grant No. 59957-DNI10.

8:48AM L51.00005: Spin-allowed quantum emission from strain confinement in monolayer semiconductors

LEO YU (Presenter), MINDA DENG, JINGYUAN LINDA ZHANG, Stanford Univ, SVEN BORGHARDT, BEATA KARDYNAL, Peter Grünberg Institute, Forschungszentrum Jülich, JELENA VUCKOVIC, TONY F HEINZ, Stanford Univ — Here we demonstrate quantum emitter behavior from strained monolayer MoSe$_2$. Exciton confinement has been achieved using strain associated with causing the monolayer to conform to a nanoscale indentation prepared in the substrate. By sufficiently reducing the lateral scale of the confinement, we have achieved single quantum emitter behavior, with the A exciton feature showing a drop in linewidth to below 0.2 meV at cryogenic temperatures, in an emission 70-meV redshifted from the bulk A exciton feature of the unstrained monolayer. The quantum emitter characteristics of these confined excitons has been demonstrated directly by $g(2)$ measurements. Unlike recent demonstrations of quantum emitters in monolayer WSe$_2$, the exciton involved for our MoSe$_2$ samples has a spin aligned configuration. This was demonstrated by Zeeman measurements indicating a g factor of 4, and was also reflected in the relatively short, 0.2 ns measured photoluminescence lifetimes. Our approach has the potential for creating spin-allowed quantum emitters that can be arbitrarily located laterally and tuned by the engineered strain properties.
Propagation of excitons in TMDC monolayers with suppressed disorder
KOLOMAN WAGNER (Presenter), JONAS ZIPFEL, JONAS D. ZIEGLER, University of Regensburg, RAUL Perea causin, Roberto Rosati, Samuel Brem, Chalmers University of Technology, MARVIN KULIG, University of Regensburg, Takashi Taniguchi, Kenji Watanabe, National Institute for Material Science, Tsukuba, Ermin Malic, Chalmers University of Technology, Mikhail Glazov, Ioffe Institute Saint Petersburg, Alexey Chernikov, University of Regensburg — Coulomb-bound electron-hole pairs, or excitons, dominate the electro-optical properties in single layers of semiconducting transition metal dichalcogenides (TMDCs) and their heterostructures. In these 2D systems, excitons can move freely across large distances. We study exciton propagation by directly monitoring their spatial behavior in single layers of TMDCs by spatially- and time-resolved photoluminescence microscopy. In high-quality boron nitride encapsulated samples with strongly suppressed disorder, we find very efficient diffusion at low excitation densities and a strongly non-linear behavior at high densities. Single layers of encapsulated TMDCs provide a highly promising platform to explore exciton transport phenomena, including low-temperature conditions with suppressed phonon-scattering and manipulation of spin-valley polarized excitations.

9:24AM L51.00008: Polarizability of finite-bandwidth two-dimensional electron gas  KAVEH KHALIJ (Presenter), University of Minnesota, TOBIAS STAUBER, ICMM, CSIC, Madrid, TONY LOW, University of Minnesota — The two-dimensional electron gas (2DEG), characterized by its parabolic electron energy dispersion, has been the subject of intense research for more than half a century. The main fuel to this interest has been its simplicity and physical relevance to describe the low energy behavior of most known 2D electronic systems, up to a point where any deviation from a 2DEG behavior (such as what was observed in graphene) has been pinpointed as anomalous and receives extra attention. Following this, here, we ask what would happen to the polarizability if we restrict the parabolic energy dispersion to a finite bandwidth (FBW), for which the 2DEG behavior would then be a natural limit (i.e. allowing for the bandwidth to be infinite). We discuss the polarizability of the FBW-2DEG, in dynamical and static limits, as the key physical quantity to obtain elementary excitation spectra, collective modes, charged impurity-limited transport properties, and spin-spin exchange interaction.

9:36AM L51.00009: Quasiparticle and optical properties of monolayer C$_3$N*  ZHAO TANG (Presenter), WEIYI XIA, State Univ of NY - Buffalo, YABEI WU, WENQING ZHANG, Department of Physics, Southern University of Science and Technology, PEIHONG ZHANG, State Univ of NY - Buffalo — Highly ordered honeycomb structure carbon nitride (C$_3$N) is an emerging 2D material that has attracted much interest recently. The (indirect) band gap of this material has recently be predicted to be about 1.5 eV [1]. In this work, we present fully converged GW+BSE results for monolayer C$_3$N. The calculated the GW band gap of monolayer C$_3$N is about 1.5 eV, an ideal value for electronics applications. Detailed investigations of the band-edge electronic states suggest a strong band edge absorption. Our fully converged GW+BSE calculation predicts an optical gap about 1.9 eV, with an excitonic binding energy of 0.7 eV.

[1] 2D Mater. 6, 015018 (2019)

*This work is supported in part by the NSF (Grant No. DMR-1506669 and DMR-1626967).
Hyperbolic plasmon polaritons are uncommon light-matter modes in materials at the extreme of anisotropy — where metallic and dielectric characters coexist along different crystallographic directions. Using Kramers-Kronig analysis and finite-difference time-domain simulations, we have identified a new quasi-two-dimensional material, palladium cobaltate ($\text{PdCoO}_2$), that is expected to support low-loss hyperbolic plasmon polaritons at infrared frequencies. Simulations are consistent with the polariton dispersion calculated from the complex reflection coefficient. The large optical anisotropy can be recognized by the order of magnitude difference between the in-plane and out-of-plane plasma frequencies. Scanning near-field optical microscopy can be used to study these light-matter modes. However, because hyperbolic polaritons travel inside the material and reflect off the surfaces, observing them requires a thin layer (50-150 nm) of $\text{PdCoO}_2$ with smooth surfaces. This presents a challenge to an experimental demonstration of hyperbolic modes in $\text{PdCoO}_2$ since the material does not exfoliate readily from flux-grown single crystals and forms twin domains in films grown by molecular beam epitaxy. Efforts to isolate flat, thin flakes of $\text{PdCoO}_2$ for near-field measurements will be presented.

Directional shift current and dipole selection rules in the layered semiconductor $\text{BC}_2\text{N}^*$

We study the shift-current optical response in a noncentrosymmetric polytype of the quasi-2D layered semiconductor $\text{BC}_2\text{N}$ [1]. Employing a recently developed first-principles Wannier-interpolation technique [2] implemented in the latest release of Wannier90 [3], we find that the photoconductivity exhibits two distinctive features at the band edge. First, it ranks among the largest bulk nonlinear responses reported to date, and peaks in an energy range suitable for optical manipulation. Secondly, it is strongly anisotropic, due to the vanishing of particular tensor components not foretold by phenomenological symmetry arguments; this is a consequence of dipole selection rules imposed by mirror symmetry, which imply that the relative parities between valence and conduction bands are key for determining the directionality of the band-edge response. The implications of the dipole selection rules should apply to a broad class of nonlinear responses.


*Work funded from Grant No. FIS2016-77188-P from Spanish Ministerio de Economía y Competitividad, and EU's H2020 program by MSCA grant Agreement PhotoNow No 839237.
10:12AM L51.00012: First-principles calculations for high-harmonic generation in two-dimensional materials: from single atomic layer to thin films* SHUNSUKE YAMADA (Presenter), KAZUHIRO YABANA, Center for computational sciences, University of Tsukuba — We present first-principles studies on high-harmonic generation (HHG) in thin materials using the time-dependent density functional theory (TDDFT). HHG in reflected and transmitted waves from a thin film exposed to intense light pulses is modulated from the bulk optical response by light propagation effect and surface effect. We have developed a real-time simulation method combining the time-dependent Kohn-Sham and the Maxwell equations for describing the microscopic dynamics of electrons and electromagnetic field in a thin film. This method can take into account both the propagation and surface effects. Using our method, we investigate the dependencies of HHG on the light intensity, polarization, and film thickness for semiconductor films. We discuss the mechanism of HHG signal growth in reflected and transmitted waves.

*This research was supported by JST-CREST under grant number JP-MJCR16N5.

10:24AM L51.00013: Quasiparticle and optical properties of hexagonal boron nitride: from monolayer to bulk* WEIYI XIA (Presenter), State Univ of NY - Buffalo, WEIWEI GAO, University of Texas at Austin, PEIHONG ZHANG, State Univ of NY - Buffalo — Hexagonal boron nitride (h-BN), an emerging building block for van der Waals heterostructures, has become a research focus in recent years. Interesting, some of the most fundamental aspects of this material are still not fully understood. For example, there are still debates on whether the fundamental band gap is direct or indirect, for both monolayer and bulk h-BN. To the best of our knowledge, the quasiparticle band gap of few-layer h-BN has not been accurately determined. In this talk, we will present fully converged GW+BSE results for monolayer, bilayer and bulk h-BN, aiming to resolve some of the controversies and illustrate the effects of dielectric screening and interlayer interaction on the quasiparticle and optical properties of this material.

*This work is supported in part by the NSF (Grant Nos. DMR-1506669 and DMR-1626967).

10:36AM L51.00014: Optical Absorption and Emission of Two-Dimensional Tetracene Crystals SEONGHYUN KOO (Presenter), SUNMIN RYU, Pohang Univ of Sci & Tech — Organic crystals have received much attention because of their unique properties different from inorganic crystals such as mechanical flexibility and high quantum yield of luminescence. Although various organic solids are used in many industrial applications, the electronic structures of low-dimensional forms are far from being understood not only because their van der Waals interactions between molecules are intractable but also because it has been a challenge to prepare such crystalline systems with sufficient stability. In this work, we present absorption and emission spectroscopy on single and few-layer tetracene (Tc) layers sandwiched between two-dimensional (2D) inorganic crystals including graphene and hexagonal BN. Tc deposited by thermal evaporation formed flat films with thickness of multiples of its minimum (~1.3 nm) and long-range order confirmed by polarized spectroscopy. Vibrational progressions and Davydov splitting observed in the absorption and emission spectra revealed significant deviation from their bulk counterparts, which suggests distinctive crystalline structures and dielectric environments of 2D Tc. We will also discuss structural details and excitonic dynamics probed by time-resolved spectroscopy.
**10:48AM L51.00015: Low efficiency of the exciton-phonon scattering involving large momentum transfer in 2D-TMDC**  HANZ YECID RAMÍREZ (Presenter), School of Physics, Universidad Pedagógica y Tecnológica de Colombia (UPTC) — Atomically thin transition metal dichalcogenide sheets are among the most promising systems for efficiently controlled emission of quantum light. However, like in all solid-state based emitters, temperature is a critical parameter to have into account, because of the ever present decoherence induced by phonons. In this theoretical work, the effects of the transferred momentum on the exciton-phonon interaction is studied. As a main result, the inefficiency of this coupling for scattering involving large phonon momentum is found, as consequence of the localization of the exciton wave function in the reciprocal space. This feature may favor robustness of the high quality optical activity of these low dimensional systems, along significant temperature ranges.

*This work was funded by the Research Division of Universidad Pedagógica y Tecnológica de Colombia, and the Ministry of Science and Technology of Taiwan.

**Wednesday, March 4, 2020 8:00 AM - 10:36 AM**

**Session L52 DCMP: Semiconductor Films and Interfaces** Mile High Ballroom 1E - Daniel Dougherty, North Carolina State University

**8:00AM L52.00001: A novel surface reconstruction of the TiO₂ Anatase (001) surface from machine learning**  MAXIMILIAN AMSLER (Presenter), ULRICH ASCHAUER, University of Bern — Surfaces of semiconductors often exhibit reconstructions that can significantly influence their physical and chemical properties. Especially for catalysts, studying the surface structures at the atomic scale is crucial to gain a better understanding of the catalytic activity and, ultimately, to design improved materials. Atomistic simulations can provide insight, but *ab initio* structure predictions are rather challenging due to the large supercells required to model 2D surfaces. To alleviate this issue, we use a machine-learned interatomic potential trained on DFT data in conjunction with a sophisticated structure prediction method to explore low-energy reconstructions of the TiO₂ Anatase (001) surface. We identify a new surface reconstruction that is comparable in energy with the well-known (001)-1x4 ad-molecule model and could explain the recently discovered experimental structures from STM imaging.
8:12AM L52.00002: Theoretical investigation of the GaN (0001) surface reconstruction

FATIMA ALQUAITI (Presenter), ALEXANDER DEMKOV, University of Texas at Austin — Using density functional theory we study the surface reconstruction of GaN (0001). We compare energetics of the 2x2 and root 3 by root 3 R30 GaN (0001) surface structures and find them to be energetically equivalent. In addition, we systematically compare the results found when using the local density approximation and the generalized gradient approximation. We also consider Ga and La ad-atoms on Ga (0001), and determine the corresponding potential energy surfaces and diffusion rates and compare them with those previously computed for Eu, Ce, and Gd. In addition, similarly to the cases of Eu, Ce, and Gd, the La ad-atom exchange with a surface Ga atom is found energetically favorable and with a much smaller barrier of 0.15 eV. This may indicate a path to forming intermetallic LaGa$_2$ through the surface exchange reaction.

*The work at the University of Texas at Austin is supported by the National Science Foundation under grant DMR-1507970.

8:24AM L52.00003: Two-dimensional overlayers of Au and Ag on the Ge(111) surface: insights from first-principles calculations

SHREE RAM ACHARYA (Presenter), Physics, Univ of Central Florida, SHIRLEY CHIANG, Physics, University of California, Davis, TALAT S. RAHMAN, Physics, Univ of Central Florida — Experimental observations using low-energy electron microscopy (LEEM) of Au overlayers on the Ge(111) surface have revealed two-dimensional Ge(111)-Au(√3×√3)R30° structure as the only ordered structure being irrespective of Au coverage and sample temperature [1] while Ag overlayers form a number of structures on the same range of coverages and temperatures [2]. The charge density distribution analysis is performed using the density functional theory to see the variation in binding of Ag and Au on the Ge surface taking the thermodynamically stable √3 structures which shows that the Au atoms form strong covalent bond with Ge atoms (height = 0.56 Å) than bond between Ge atoms whereas the Ag atoms does not share charge with the Ge atoms indicating that they are trapped at height 0.73 Å inside the cage of the strong Ge-Ge bond. We will compare the electronic and vibrational structures of additional overlayer structures and strain on those systems to trace the reason behind such a difference in observed structures.


*Work supported by NSF DMR-1710306 (SRA, TSR); NSF DMR-1710748 (SC).
8:36AM L52.00004: 3D atomic mapping of rutile-TiO2(110) supported Vanadium oxide catalyst using X-ray Standing Wave excited XPS*  
ANUSHEELA DAS (Presenter), YANNA CHEN, Northwestern University, TIEN-LIN LEE, Diamond Light Source Limited is United Kingdom's national synchrotron and is a leading scientific facility in the world. They host facilities supporting cutting edge research, KVLV NARAYANACHARI, MICHAEL J BEDZYK, Northwestern University — XSW excited XPS was used to study atomic-scale structure of 1/2 monolayer vanadium oxide catalyst supported on rutile TiO2(110) single crystal. The experiments were performed at I09 beamline at the Diamond Light Source. Collecting V 2p, O 1s and Ti 2p XPS signals as we scanned across a Bragg peak at different stages of a redox reaction allowed tracking of surface sites for chemically distinct V atoms, important for understanding their catalytic behaviour. V5+ and V4+ 2p XPS peaks were found to be separated by 1.4 eV and were found to have different XSW coherent fraction and position. Summation of these Fourier components for 5 symmetry inequivalent hkl Bragg peaks generates a chemical state sensitive 3D atomic map of vanadium. These results give us unique insights into this as well as other related oxide supported catalysts.

*Northwestern University (NU) Institute for Catalysis in Energy Processes under DOE Grant DE-FG02-03ER15457, NU MRSEC program (NSF DMR-1121262), NU Center for Hierarchical Materials Design program under NIST Grant 70NANB14H01.

8:48AM L52.00005: Combinatorial Synthesis of a New II-IV-N2: MgSnN2*  
ANN GREENAWAY (Presenter), AMANDA L LOUTrIS, KAREN HEINSELMAN, National Renewable Energy Laboratory, CELESTE MELAMED, REKHA SCHNEPF, Colorado School of Mines, MARSHALL TELLEKAMP, National Renewable Energy Laboratory, RACHEL WOODS-ROBINSON, University of California, Berkeley, RACHEL SHERBONDY, Colorado School of Mines, DYLAN BARDGETT, STEPHAN LANY, STEVEN CHRISTENSEN, ADELE TAMBOLI, National Renewable Energy Laboratory — Nitrides with novel compositions are an emerging research topic in basic energy science, with applications in optoelectronics, catalysis, and magnetism. Ternary semiconductors are underexplored and have unique properties, such as transitions between cation ordered and disordered structures, which may be exploited to modify properties in a single composition. We demonstrate combinatorial co-sputtering of a new II-IV-N2, MgSnN2, in a phase-pure wurtzite structure across a range of cation compositions and from 200 to 400 °C. Below 200 °C, a metastable rocksalt phase is observed which is a potential wide bandgap, high dielectric constant material. Ellipsometry reveals an optical absorption onset at ~2 eV for the wurtzite phase, suggesting tuning via cation disorder from the predicted bandgap of 2.5 eV; disorder is confirmed by synchrotron x-ray diffraction. Finally, we demonstrate epitaxial growth via combinatorial co-sputtering on GaN. Based on this work, MgSnN2 is a target for fundamental exploration of novel nitride properties as well as a candidate for future device applications.

*Work funded by a Director’s Postdoctoral Research Fellowship (LDRD) at NREL and by the Office of Science, Basic Energy Sciences, Material Sciences and Engineering Division.
9:00AM L52.00006: Temperature-Dependent Spectroscopy of Rutile Tin Dioxide*  
HAWAZIN ALGHAMDI (Presenter), Physics Department, Howard University, BENJAMIN CONCEPCION, Physics Department, George Mason University, SUGATA CHOWDHURY, PRABHAKAR MISRA, Physics Department, Howard University — The present spectroscopic investigation focuses on rutile tin dioxide (SnO₂) in powder form. Raman spectroscopy with laser excitation at 780 nm has been used to characterize the different vibrational modes of SnO₂. Thermal effects on the vibrational features in the Raman spectrum have been studied in the range 30 – 170 °C. We have demonstrated a red-shift in the Raman spectra as the temperature increases for both A₁g (634 cm⁻¹) and B₂g (775 cm⁻¹), while E₉ (475 cm⁻¹) exhibited little change. FT-IR spectra have been obtained in order to study the IR-active vibrational modes for tin dioxide: Sn-O stretching vibration at 467.36 cm⁻¹ and Sn-O-Sn asymmetric vibration at 569.37 cm⁻¹. X-ray diffraction (XRD) spectra have been recorded to confirm the rutile structure of tin dioxide. Scanning Electron Microscope (SEM) images have provided information regarding the size of the spherical grain particles. Molecular Dynamic simulation (MD) has been utilized to study the various vibrational modes at different temperatures using the LAMMPS software.

*Financial support from the REU Site in Physics at Howard University (NSF Award# PHY-1659224) is gratefully acknowledged.

9:12AM L52.00007: First-Principles Theory for Schottky Barrier Height*  
DMITRY SKACHKOV (Presenter), XIAOGUANG ZHANG, HAI-PING CHENG, University of Florida — The physics of Schottky contact is very challenging and there are exist only simple empirical models for Schottky barrier. In current work we are developing the first-principles theory for the Schottky barrier height. Our method based on density functional theory and consists of calculation of evanescent states in the gap of the semiconductor based on complex band structure of the semiconductor surface, following by calculation of the induced charge in the bulk of semiconductor. Next we find iteratively an equilibrium between the induced charge and the electrostatic potential. The method is tested on the GaAs(111) – graphene system.

*US Department of Energy Basic Energy Sciences Energy Frontier Research Centers under Grant No. DE-SC0019330
**9:24AM L52.00008: Targeted High-Throughput Growth and Automated Phase Mapping of the Novel Semiconductor Zn$_2$SbN$_3$ Using the Analysis Package COMBItgor**

ALLISON MIS (Presenter), Colorado School of Mines, ELISABETTA ARCA, Lawrence Berkeley National Laboratory, GEOFF BRENNECKA, Colorado School of Mines, ADELE TAMBOLI, National Renewable Energy Laboratory — High-throughput materials discovery has boomed in the past decade through the pairing of combinatorial growth methods and automated characterization routines. However, much of the data collected must still be processed manually, creating a bottleneck, notably for phase identification and phase space mapping. In this work, we will present semi-automated phase identification and targeted sputter growth of the novel semiconducting material Zn$_2$SbN$_3$, to date the only reported crystalline antimony nitride in which Sb functions as a cation with a positive oxidation state. This ternary nitride has a predicted effective electron mass of (0.15-0.19m$_e$) and direct band gap of 1.7 eV that may be tunable with cation disorder. X-ray diffraction patterns were run through an automated fitting routine, the fit parameters of which were fed into routines for the creation of phase maps, tracking thin-film texturing, and directed growth through the use of fit variables as proxies for properties like optical absorption. This work will present an expanded understanding of this unique and promising material as well as a widely-applicable add-on to the free, open-source data handling and analysis package COMBItgor.

*Funding provided by the CoorsTek Fellowship program.

**9:36AM L52.00009: Transition-metal nitride semiconductors**

BAIWEI WANG (Presenter), Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, POOMIRAT NAWARAT, KIM LEWIS, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, PANOS PATSALAS, Department of Physics, Aristotle University of Thessaloniki, DANIEL GALL, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute — Semiconducting transition-metal nitride alloys emerge as a new category of semiconductors that are stable in hostile environments and are compatible with conventional semiconductor device processing. We report on the epitaxial growth and the electrical and optical properties of Ti$_{1-x}$Mg$_x$N, Ti$_{1-x}$Mg$_x$C$_{0.2}$N$_{0.8}$, and (Ti$_{0.5}$Mg$_{0.5}$)$_{1-x}$Al$_x$N on MgO(001) and (Ti$_{1-x}$Mg$_x$)$_{0.25}$Al$_{0.75}$N on Al$_2$O$_3$(0001). X-ray diffraction reciprocal space mapping is used to quantify composition dependent lattice parameters and critical thicknesses for strain relaxation. Ti$_{0.5}$Mg$_{0.5}$N is a new semiconductor with a bandgap of 0.7-1.7 eV. Reducing the Mg-content in Ti$_{1-x}$Mg$_x$N to $x < 0.5$ leads to a tunable plasmonic response that extends from infrared to visible (930 - 470 nm). The substitutional addition of Al and C on anion and cation sites, respectively, reduces the free carrier density: (Ti$_{0.5}$Mg$_{0.5}$)$_{1-x}$Al$_x$N layers show a negligible density of states at the Fermi level and a blue-shift of the absorption edge from 1.8 to 2.1 eV for $x = 0 - 0.4$. Ti$_{1-x}$Mg$_x$C$_{0.2}$N$_{0.8}$ exhibits a metal to semiconductor to insulator transition as $x$ increases from 0.3 to 0.4 to 0.5. Wurtzite-structure (Ti$_{1-x}$Mg$_x$)$_{0.25}$Al$_{0.75}$N(0001) layers have a measured bandgap that increases from 5.1 to 5.2 to 5.9 eV for $x = 0.0, 0.5$ and $1.0$. 
9:48AM L52.00010: Unpinning the relationship between pinning factor and electronegativity by calculating Schottky barrier heights from first principles* NICOLE HALL (Presenter), ISMAILA DABO, Pennsylvania State University — We calculate the Schottky barriers that develop at the interface between a metal and semiconductor. These barriers govern the current-rectification ability of Schottky diodes and the electrical response of metal-semiconductor field effect transistors. A model that accounts for the alignment of the electronic levels across the metal-semiconductor interface and the long-range polarization within the space charge region enables us to predict the heights of the barriers as a function of the electronic offsets, including the effects of charge trapping and Fermi-level pinning. We validate our computational predictions against experimental measurements [1], providing a detailed understanding of trends in the pinning factor, i.e., the change in the Schottky barrier height as a function of the metal work function. The resulting model provides a comprehensive first-principles approach to simulate the characteristics of semiconductor-metal junctions under bias.


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10:00AM L52.00011: Ultrafast Electron Diffraction of Monoclinic GaTe and the Dynamic Breaking of Friedel's Law* QINGKAI QIAN (Presenter), Department of Electrical Engineering, The Pennsylvania State University, University Park, PA 16802, United States, XIAOZHE SHEN, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA, LANXIN JIA, School of Physics, Nanjing University, Nanjing 210046, China, RENKAI LI, JIE YANG, DUAN LUO, XIJIE WANG, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA, SHENGXI HUANG, Department of Electrical Engineering, The Pennsylvania State University, University Park, PA 16802, United States — GaTe is a low-symmetry layered materials with strong anisotropy, which has been widely studied in recent years. Various applications, such as photodetectors, nonlinear optics and thermoelectric devices, have been demonstrated based on GaTe. Here the electron-phonon coupling and the lattice dynamics of GaTe are studied by ultrafast electron diffraction (UED). Besides the Debye-Waller effect caused by the incoherent electron-phonon coupling, we observed a coherent breathing phonon mode in GaTe. Different from the LA breathing modes of high-symmetry 2D materials, the displacement direction of the LA breathing phonon modes in GaTe has deviated incommensurately from the stacking lattices. In-phase and out-of-phase oscillations of diffraction intensities are observed for each Friedel pairs, which in fact break the Friedel's law dynamically. This dynamic breaking of Friedel's law can be explained by the wobbling of the crystal lattice and the Ewald sphere, and the related study can be used as a reference for UED characterization of other low-symmetry thin films.

*The UED work was conducted at SLAC MeV- UED, which is supported in part by the DOE BES SUF Division Accelerator & Detector R&D program, the LCLS Facility, and SLAC under contract Nos. DE-AC02-05-CH11231 and DE-AC02-76SF00515.
Temperature dependent X-ray studies of negative thermal expansion (NTE) ScF$_3$ thin films under strain

AMANI JAYAKODY (Presenter), ZHIWEI ZHANG, Univ of Connecticut - Storrs, ZHIHAI ZHU, Massachusetts Institute of Technology, HOPE R WHITELOCK, University of Colorado, JOSEPH I BUDNICK, JASON N HANCOCK, BARRETT O WELLS, Univ of Connecticut - Storrs —

Bulk Scandium trifluoride (ScF$_3$) is known for a pronounced negative thermal expansion (NTE) over a wide range of temperature, from 10 K to 1100 K. The structure of ScF$_3$ can be described as an ABX$_3$ perovskite with an empty A-site. Growing films of ScF$_3$ allows for tuning the lattice constant, the thermal expansion, and the construction of devices based upon differential thermal expansion. We have investigated the growth of ScF$_3$ films on oxide and fluoride substrates using pulsed laser deposition (PLD). We have found growth routes for producing films with very good epitaxy and stability. Curiously, diffraction studies show narrow Bragg peaks along the principal crystallographic directions but substantial broadening for peaks along other directions, presumably associated with accommodating drastic differentials in thermal expansion. This report describes the temperature dependent X-ray studies of epitaxial NTE ScF$_3$ thin films grown epitaxially on a strongly positive thermal expansion (PTE) substrate.

A revised three-dimensional electron gas model to describe surface plasmonic phenomena*

JIANTAO KONG (Presenter), Rutgers University, Camden — The long wavelength limit negative slope of the surface plasmon dispersion curve (for simple metals such as alkali) has been experimentally [1] and theoretically [2] investigated for a long time. Yet there is no universally accepted theory. On the other hand, the traditional 3D electron gas model such as Lindhard function [3] is successful in explaining many bulk properties, but not much attempt in literature has been made to account for the surface effects. We worked on the traditional 3D electron gas model, modifying the electron self-energy [4] with a correction due solely to surface, and produced the negative slope naturally from simple calculation. In other words, a revised 3D electron gas model can predict and describe surface plasmonic phenomena by itself.


*This work has been supported by the new faculty start-up fund of Rutgers, the State University of New Jersey, Camden.
L52.00014: Low energy excitons in GaN film under strong magnetic fields  YI WANG, School of Physics, Peking University, LIUYUN YANG, XINQIANG WANG, State Key Laboratory of Artificial Microstructure and Mesoscopic Physics, School of Physics, Peking University, CHANGLI YANG, Daniel Chee Tsui Laboratory, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, CAS, CHI ZHANG (Presenter), SKLSM, Institute of Semiconductors, CAS — We investigate magneto- far-infrared (FIR) transmission on a 100 μm thick GaN film, which is grown on a Si/HR-GaN substrate. Under zero magnetic (B) fields, we observe three absorption peaks, which are located at the energy of 30.6 meV (Peak I), 34.7 meV (II), and 40.0 meV (III), respectively. Under perpendicular B-fields, small energy shifts of the three absorption peaks (I, II, III) are all linear to B. Meanwhile, peak II splits into two distinct peaks, with a distance about 0.08 meV/T in between. And three distinct splits are observed around Peak III with a distance of about 0.11 meV/T between neighbor peaks. We propose that the patterns of the absorption can be attributed to the low energy excitons in GaN under strong magnetic fields.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L53 DMP DCOMP: 2D Semiconductors: Magnetism Mile High Ballroom

1F - Rui He, Texas Tech Univ - Tag(s): Focus

8:00AM L53.00001: Stacking dependent 2D magnetism [Invited] SHIWEI WU (Presenter), Fudan Univ — In van der Waals layered materials, the symmetries and functionalities could be controlled by modifying the stacking order through rotation and translation between the layers. Whereas most previous work has focused on the electronic and optical properties associated with the van der Waals stacking, the recent discovery of magnetism in 2D materials, achieved through both mechanical exfoliation and molecular beam epitaxy (MBE), provides an exciting opportunity to explore the effects of stacking order on a material's magnetic properties. In this talk, I will present two of our recent studies in this direction. 1) By discovering a giant nonreciprocal second harmonic generation from layered antiferromagnetism in mechanically exfoliated bilayer CrI3, we revealed the underlying C2h symmetry, and thus monoclinic stacking order in bilayer CrI3, providing crucial structural information for the microscopic origin of layered antiferromagnetism. 2) By using the molecular beam epitaxy to grow monolayer and bilayer CrBr3 and in situ characterization with a spin-polarized scanning tunneling microscopy and spectroscopy, we observed that while individual CrBr3 monolayer is ferromagnetic, the interlayer coupling in bilayer depends strongly on the stacking structure and can be either ferromagnetic or antiferromagnetic. Thus, the direct correlation between stacking order and interlayer magnetism pave the way for manipulating 2D magnetism.
8:36AM L53.00002: Electronic properties of magnetically ordered topological semimetals.*
[Invited] ADAM KAMINSKI (Presenter), Physics and Astronomy, Iowa State University — Magnetic topological semimetals are new and exciting field of research. In this talks we will present ARPES studies of several magentically ordered topological systems, where magnetic ordering allows to tune and control the topological features leading to observation of novel groundstates.

*Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358. Research was partially supported by CEM, a NSF MRSEC, under Grant No. DMR-1420451.

9:12AM L53.00003: Probing magnetic orders and stacking patterns in bilayer CrI$_3$ by theoretical Raman scattering LIANGBO LIANG (Presenter), Oak Ridge National Lab — Chromium triiodide (CrI$_3$), a 2D van der Waals magnet, has been extensively studied due to its fascinating properties. Within each layer spins are ferromagnetically coupled with strong out-of-plane anisotropy, but between layers the spin ordering can be manipulated between ferromagnetic (FM) and antiferromagnetic (AFM) ordering by numerous ways, such as stacking pattern and applied electric/magnetic field. For bilayer CrI$_3$, the interlayer spin ordering is closely connected to the stacking configuration, such as the common hombohedral and monoclinic patterns. Using density functional theory, I carried out a systematic study on a variety of possible stacking patterns in bilayer CrI$_3$, where for each stacking both interlayer FM and AFM spin orders were considered. The calculations found that different stacking patterns and magnetic orderings lead to different symmetries and interlayer coupling strengths, which can alter Raman optical selection rules, phonon frequencies, and Raman intensities. This highlights the intricate interactions between stackings, spins, and phonons in 2D magnets. I will present a Raman spectra map of bilayer CrI$_3$ with different stacking patterns and spin orderings under both linearly and circularly polarized light for guiding experimental identification.
**9:24AM L53.00004: Imaging domains and defects in the stacking of few-layer and twisted CrI$_3$**

ARIANA RAY (Presenter), Physics, Cornell University, YU-TSUN SHAO, YANG XU, NIHIL SIVADAS, TINGXIN LI, ZEFANG WANG, Applied and Engineering Physics, Cornell University, JIE SHAN, Physics, Cornell University, KIN FAI MAK, DAVID ANTHONY MULLER, Applied and Engineering Physics, Cornell University — Different lateral shifts of the stacked monolayers in CrI$_3$ lead to different magnetic ground states, with a rhombohedral-symmetry stacking resulting in ferromagnetic layer ordering, and a monoclinic-symmetry stacking leading to antiferromagnetic layer ordering. Here we explore the structural arrangements found as the CrI$_3$ thickness is systematically reduced to the monolayer limit using 4D-STEM electron diffraction and atomic resolution imaging. We find that CrI$_3$ flakes from bilayer to 50 nanometer thickness remain in a monoclinic stacking when cooled to 95 K. However, the monoclinic group allows for multiple variants -- arising from 120 degree stacking rotations both in-layer and between neighboring CrI$_3$ layers -- and we observe a rich assortment of stacking orders and domains, as well as moirés. We show that these stacking rotations can change as a function of temperature. The observed vertical superposition of monoclinic variants in few-layer to bulk CrI$_3$ flakes may present as an overall three-fold symmetry to macroscopic-averaged measurement, but can be recognized by atomic resolution imaging.

*Research supported by PARADIM DMR-1539918, AFOSR MURI FA9550-18-1-0480, CCMR DMR-1719875.

**9:36AM L53.00005: Raman spectroscopy studies of spin-lattice coupling in bilayer CrI$_3$**

WENCAN JIN (Presenter), University of Michigan, HYUN HO KIM, University of Waterloo, ZHIPENG YE, GAIHUA YE, Texas Tech University, BOWEN YANG, University of Waterloo, SHANGJIE TIAN, HECHANG LEI, Renmin University of China, ADAM TSEN, University of Waterloo, RUI HE, Texas Tech University, LIUYAN ZHAO, University of Michigan — CrI$_3$ has been shown to be a layered antiferromagnet in its few-layer form. Upon the application of a moderate out-of-plane magnetic field, the layered antiferromagnetic state can be switched to a fully spin-polarized state. Among the few-layer CrI$_3$ system, bilayer CrI$_3$ is of particular interest because the coupling between its crystal structure and magnetic ordering can give rise to unique magneto-optical effects such as magnetic circular dichroism, nonreciprocal second harmonic generation, and deviation of Raman selection rules. In this talk, we will present Raman spectroscopic evidence of spin-lattice coupling in bilayer CrI$_3$. We will show that spin-lattice coupling in bilayer CrI$_3$ manifests itself in both first-order and higher-order Raman modes. The results of temperature and magnetic field dependence measurements will be discussed.

*Supported by NSF Career Grants No. DMR-1760668 and No. DMR-1749774.
9:48AM L53.00006: Topological spin waves in 2D CrI$_3$: an itinerant fermion description*  
ANTONIO COSTA, International Iberian Nanotechnology Laboratory (INL), DANIEL LR SANTOS, CEFEDET, NUNO PERES, JOAQUIN FERNANDEZ-ROSSIER (Presenter), International Iberian Nanotechnology Laboratory (INL) — We present a theory of spin waves in ferromagnetic CrI$_3$ monolayers based on the calculation of the renormalized spin susceptibility, computed using an extended multi-orbital Hubbard model obtained from first-principles calculations. Our theory includes the multi-orbital nature of Cr and I atoms, as well as their spin orbit coupling and yield the spin waves as poles from the spin susceptibility tensor. For monolayers, theory reproduces the spin wave dispersion measured with inelastic neutron scattering, with a gap at the Dirac point compatible with a topological origin. We have computed the spin waves for a ribbon and find in-gap chiral edge states that provide further back-up to this scenario. Importantly, our approach goes does not require to define spin Hamiltonian, and can be applied to a wide class of magnetic 2D materials.

*JFR acknowledges funding from FCT UTAPEX/NTec/0046/2017

10:00AM L53.00007: Magneto-optical properties of CrI$_3$, CrBr$_3$ and CrCl$_3$ monolayers: chemical trends and excitonic effects*  
ALEJANDRO MOLINA-SANCHEZ (Presenter), GONÇALO CATARINA, International Iberian Nanotechnology Laboratory, DAVIDE SANGALLI, Istituto di Struttra della materia (ISM), CNR, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory — Chromium trihalides (CrI$_3$, CrBr$_3$ and CrCl$_3$) are a prominent family of isostructural insulating layered materials in which ferromagnetic order has been observed down to the monolayer. Here we provide a comprehensive computational study of the magneto-optical properties useful to probe ferromagnetic order of monolayers, magnetic circular dichroism and magneto-optic Kerr effect. We combine density functional theory calculations and many-body perturbation theory. We solve the Bethe-Salpeter to obtain the excitonic states and to calculate the optical absorption and Kerr angle spectra. We compare the magneto-optical response of the chromium trihalides series. We find strong excitonic effects on the optical response. Moreover, the Kerr angle spectrum is governed by the spin-orbit coupling of the ligand atoms (I, Br or Cl) and is a fingerprint of the degree of magnetic anisotropy of these compounds.

*A. M.-S. acknowledges the Marie-Curie-COFUND program Nano TRAIN For Growth II (Grant Agreement 713640). J. F.-R. acknowledges funding from FCT, project UTAPEX/NTec/0046/2017.
10:12AM L53.00008: Evidence of the polaronic character of excitons in a two-dimensional ferromagnet* ZHIPENG YE (Presenter), GAIHUA YE, RUI HE, Texas Tech University, HYUN HO KIM, BOWEN YANG, ADAM TSEN, University of Waterloo, Canada, WENCAN JIN, JASON SHIH AN HORNG, HUI DENG, KAI SUN, LIUYAN ZHAO, University of Michigan — Studies of exciton dynamics in two-dimensional (2D) transition metal dichalcogenide (TMDC) semiconductors have led to discoveries of a variety of fascinating properties for optoelectronic applications. It has been known that exciton dynamics can be strongly affected by lattice vibrations through electron-phonon (e-ph) coupling. The recently discovered 2D ferromagnetic semiconductor, CrI$_3$, provides a new platform to explore exciton physics beyond the well-studied 2D TMDC semiconductors because of its localized orbitals, intrinsic long-range ferromagnetic order, and strong e-ph coupling. Here we use linear absorption spectroscopy to identify the exciton resonance transitions in bilayer CrI$_3$. We further use resonant micro-Raman spectroscopy to explore the electron-phonon coupling in bilayer CrI$_3$. Temperature and magnetic field dependence of e-ph coupling in bilayer CrI$_3$ will be discussed.

*Supported by NSF CAREER Grants No. DMR-1760668 and No. DMR-1749774.

10:24AM L53.00009: Switching 2D Magnetic States via Pressure Tuning of Layer Stacking TIANCHENG SONG (Presenter), ZAIYAO FEI, MATTHEW A YANKOWITZ, ZHONG LIN, QIANNI JIANG, KYLE HWANGBO, QI ZHANG, BOSONG SUN, University of Washington, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, MICHAEL MCGUIRE, Oak Ridge National Laboratory, DAVID E GRAF, National High Magnetic Field Laboratory, TING CAO, JIUN-HAW CHU, DAVID COBDEN, University of Washington, CORY DEAN, Columbia University, DI XIAO, Carnegie Mellon University, XIAODONG XU, University of Washington — The physical properties of two-dimensional van der Waals crystals can be sensitive to the interlayer coupling. For 2D magnets, theory suggests that the interlayer exchange coupling strongly depends on layer separation, while the stacking arrangement can even change the sign of the interlayer magnetic exchange, thus drastically modifying the ground state. Here, we demonstrate pressure tuning of magnetic order in the 2D magnet CrI$_3$. We probe the magnetic states using tunneling and scanning magnetic circular dichroism microscopy measurements. We find that the critical field for the spin-flip transition can be more than doubled by hydrostatic pressure. In bilayer CrI$_3$, pressure induces a transition from layered antiferromagnetic to ferromagnetic phases. In trilayer CrI$_3$, pressure can create coexisting domains of three phases, one ferromagnetic and two antiferromagnetic. The observed changes in magnetic order can be explained by changes in the stacking arrangement. Such coupling between stacking order and magnetism provides ample opportunities for designer magnetic phases and functionalities.
10:36AM L53.00010: Uncovering two-dimensional intrinsic ferromagnetism from host antiferromagnet via super-exchange interaction modulation*  FANG ZHANG (Presenter), Institute of Applied Physics and Materials Engineering, University of Macau, XINGQIANG SHI, Department of Physics, Southern University of Science and Technology of China, STEVEN LOUIE, Department of Physics, University of California, Berkeley, ZI KANG TANG, Institute of Applied Physics and Materials Engineering, University of Macau — Two-dimensional ferromagnetic semiconductors have been gaining great attention as they incorporate low-dimensionality, ferromagnetism and semiconductivity, which are promising for next-generation multifunctional spintronics. Here, we report an effective strategy to design ferromagnetic single crystals based on our previous extended super-exchange theory for polyvalent anion materials, e.g. CrOCl. We reveal that the magnetic order of one specific super-exchange cation-anion-cation path in CrOCl prototype is directly related to all anions' valence state. Choosing suitable anions (A_1=VIIA, A_2=VA element) in sites, all super-exchange paths are tuned into strongly ferromagnetic, leading to designed materials are intrinsic ferromagnets companied with high Curie temperatures. On the basis of the explored strategy and first-principles calculations, two stable monolayers CrIP and CrIAs are predicted to be ferromagnetic half-metal and semiconductor, respectively. The Curie temperature, estimated by Monte Carlo simulation using Heisenberg model, is as high as 1050 K and 655 K.

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10:48AM L53.00011: Exotic magnetism in 2D Ni-based halides  SILVIA PICOZZI (Presenter), DANILA AMOROSO, PAOLO BARONE, CNR-SPIN, Consiglio Nazionale delle Ricerche — Driven by the increasing enthusiasm towards long-range magnetic order in two-dimensional materials (2D) (such as CrI3 and CrGeTe3), we carry out simulations based on density functional theory (DFT) for halides, focusing in particular on Ni-(VII)2 (VII = Cl, Br, I) monolayers. In addition to standard analysis of structural and electronic properties, we put special emphasis on the magnetic properties, in terms of magnetic moments, Heisenberg exchange coupling (including anisotropic and off-diagonal terms in the exchange tensor) and magnetic anisotropy energy. Moreover, starting from DFT results and mapping total energies on model spin Hamiltonians, we perform Monte-Carlo simulations to investigate the ground-state magnetic ordering and trends at finite temperatures and upon magnetic fields. Our predictions suggest a particularly rich phase diagram for Ni iodide and bromide monolayers, with exotic non-collinear spin configurations and complex topological transitions.

Wednesday, March 4, 2020 8:00 AM - 10:36 AM

Session L54 DCMP: Computational Studies of Topological Materials Mile
High Ballroom 2A
8:00AM L54.00001: Time-reversal-invariant Weyl semimetals indicated by symmetry indicators and invariants  
YUTING QIAN, JIACHENG GAO, Chinese Academy of Sciences, Institute of Physics, ZHIDA SONG, Department of Physics, Princeton University, SI-MIN NIE (Presenter), Department of Materials Science and Engineering, Stanford University, ZHIJUN WANG, HONGMING WENG, ZHONG FANG, Chinese Academy of Sciences, Institute of Physics — For the time-reversal(TR)-breaking centrosymmetric systems, an odd number of all the even/odd parity occupied bands, at eight inversion-symmetry-invariant (ISI) momenta, indicates the appearance of Weyl points in the systems. Here, based on the first-principles calculations and symmetry analysis, we demonstrate that, for the TR-preversing noncentrosymmetric systems with S4 symmetry, the Weyl semimetal phase can be characterised by the nonequality between an invariant \( \eta \) and an S4 indicator \( z_2 \). By applying it, we find that some candidates can be ideal Weyl semimetals in a noncentrosymmetric space group with S4 symmetry. Our first-principles calculations show that four pairs of Weyl points are located in the \( k_{x,y} = 0 \) planes, being right at the charge neutrality level. An effective model has been built and captures the nontrivial topology in these materials. Our strategy to find the Weyl points by using symmetry indicators and invariants opens a new route to search for Weyl semimetals in TR-invariant systems.

8:12AM L54.00002: Topological crystalline insulator: from symmetry indicators to material discovery  
TAY-RONG CHANG (Presenter), XIAOTING ZHOU, National Cheng Kung University, CHUANG-HAN HSU, VITOR MANUEL PEREIRA, National University of Singapore, ARUN BANSIL, Northeastern University, SYUYANG XU, Harvard University, HSIN LIN, Academia Sinica, LIANG FU, Massachusetts Institute of Technology — Topological crystalline insulators (TCIs) are insulating electronic phases of matter in which the nontrivial topology is driven by crystalline symmetries. Recent theoretical advances have proposed new rotational-symmetry-protected TCI states that are expected to show unique topologically protected boundary modes. The surface normal to the rotational axis in these TCIs features "unpinned" Dirac surface states whose Dirac points are located at generic \( k \) points. Also, due to the "higher-order" bulk-boundary correspondence, such a 3D TCI supports 1D helical edge states. However, to date, rotational-symmetry-protected TCIs have remained elusive in real materials. We systematically examine the topological properties of the TCI states in \( \text{Ca}_2\text{As} \). On both the top and side surfaces, we show the presence of topological surface states protected independently by rotational and mirror symmetries [1]. We also discuss the van der Waals material \( \alpha\text{-Bi}_4\text{Br}_4 \) and the pristine bulk bismuth and show that these materials harbor TCI states protected purely by rotation symmetry [2,3], even though these materials have been long thought to be topologically trivial.

Emergent dual topology in the three-dimensional Kane-Mele Pt$_2$HgSe$_3$

ANTIMO MARRAZZO, NICOLA MARZARI, École Polytechnique Fédérale de Lausanne, MARCO GIBERTINI (Presenter), Department of Quantum Matter Physics, University of Geneva — Recently, the very first large-gap Kane-Mele quantum spin Hall insulator was predicted to be monolayer jacutingaite (Pt$_2$HgSe$_3$), a naturally-occurring exfoliable mineral. The stacking of quantum spin Hall monolayers typically leads to a (0;001) weak topological phase, which does not protect the existence of surface states on the (001) surface. Unexpectedly, recent ARPES experiments revealed the presence of surface states dispersing over large areas of the 001-surface Brillouin zone. Such 001-surface states have been shown to be topologically protected by a non-zero mirror Chern number, associated with a nodal line gapped by spin-orbit interactions. Here, we extend the two-dimensional Kane-Mele model to bulk jacutingaite and unveil the microscopic origin of the gapped nodal line and the emerging crystalline topological order. By using maximally-localized Wannier functions, we identify a large non-trivial second nearest-layer hopping term that breaks the standard paradigm of weak topological insulators. Complemented by this term, the predictions of the Kane-Mele model are in remarkable agreement with recent experiments and first-principles simulations, providing an appealing conceptual framework also relevant for other layered materials made of stacked honeycomb lattices.

Doping induced topological phase transition in Bi: The role of quantum electronic stress*

KYUNG-HWAN JIN (Presenter), University of Utah, HAN WOONG YEOM, Pohang University of Science and Technology, FENG LIU, University of Utah — Charge doping is an essential means to tailor materials' properties. However, besides moving the Fermi level, charge doping is generally not expected to induce topological phase transition (TPT). Surprisingly, using first-principles calculations, here we demonstrate an electron doping induced TPT in bulk Bi from a higher-order topological insulator (HOTI) to a TI. The underlying mechanism is revealed to be driven by an electron doping induced quantum electronic stress (QES), which in turn induces a highly anisotropic lattice expansion to close/reopen the small energy gap in Bi band structure. Our finding significantly resolves an outstanding controversy concerning the topological characterization of bulk Bi among existing experiments and theories, and explains the physical origin of the topologic order in Bi (111) thin films. It sheds new lights to fundamental understanding of topological properties of small band gap materials in relation to doping and QES.

*This work is supported by DOE-BES under Grant No DE-FG02-04ER46148.
Possibility of topological properties in 2D cadmium chalcogenide (CdX, X = S, Se, and Te) buckled honeycomb monolayer on substitutional doping*  

SUTAPA CHATTOPADHYAY, ANJALI KSHIRSAGAR (Presenter), Univ of Pune — Two-dimensional honeycomb monolayers doped with tin atoms are designed from (111) surface of bulk zinc blende structures of cadmium chalcogenides using first principles density functional theory based calculations. On relaxation the buckled honeycomb monolayer shows signature of band inversion between Sn and Cd orbital at the zone center (Γ point) deep in the valence band and high above in the conduction band. The band inversion, due to hybridization, stays even after inclusion of spin-orbit coupling. The systems were chosen with an intention to exploit the possibility of d-d band inversion. CdSnS has s-s band inversion but CdSnSe and CdSnTe monolayers do show band inversion involving d states. The calculated phonon spectra confirmed the stability of all the systems studied. The details of the electronic structure bring out the importance of s-d band inversion. We also report the topological invariants and analysis of edge state properties and band structure of these materials in ribbon geometry. Such systems can be useful for technological application in the Spintronic domain.

*Authors acknowledge financial support from DST Nanomission Council, Government of India (DST/NM/NS- 15/2011(G))

The electronic and topological properties of plumbene by first-principles calculations*  

YUE LI (Presenter), ZHONGQIN YANG, Fudan Univ — Combining tight-binding (TB) models with first-principles calculations, we investigate the electronic and topological properties of plumbene. “Constructive” coupling effects of topological states are found in the plumbene, causing the system being a normal insulator, opposite to topologically nontrivial states formed in the other group IVA monolayers. Based on this mechanism, several schemes are raised to produce a globally topological state in the plumbene. Interestingly, after the edge modification in the nanoribbon structure, the plumbene can own low-dissipation tunable edge states with good conduction performance despite the topologically trivial behavior.

*This work was supported by the National Natural Science Foundation of China under Grants No. 11574051, No. 11874117, No. 11604134, and No. 11747137, and the Natural Science Foundation of Jiangsu Province (China) with Grants No. BK20170376. All the calculations were performed at the High Performance Computational Center (HPCC) of the Department of Physics at Fudan University.
9:12AM L54.00007: Topological States in \(\beta\)-PbO\(_2\)?  SHARAD MAHATARA (Presenter), BORIS KIEFER, New Mexico State Univ — The electronic properties of \(\beta\)-PbO\(_2\), have been controversial for over a century. Experiments find metallic behavior, attributed to its defect structure, to indirect semiconducting for stochiometric samples, with a gap of 0.61 eV. Theory leads to similar ambiguities, and predicts this phase to be metallic (PBE, HSE06) or the opening of too small a bandgap (HSE06). An area where this inconsistency is significant, is when a material property depends on the electronic structure in the vicinity of the Fermi energy, such as topological states. In our work, we use a self-consistent DFT+U approach and find stochiometric \(\beta\)-PbO\(_2\) to be an indirect semiconductor with a band gap of \(\sim\)0.8 eV, similar to experiment. The larger bandgap requires strains of \(\sim\)4% to drive \(\beta\)-PbO\(_2\) into a nodal line semimetallic state, which is not protected under the application of spin-orbit-coupling. Moreover, our surface computations do not show any topologically protected states near the Fermi energy. Therefore, our results show that in contrast to previous computations \(\beta\)-PbO\(_2\) is a topologically trivial material, consistent with experiment. Differences to previous work can be attributed to our more accurate description of the optical properties of bulk \(\beta\)-PbO\(_2\).

9:24AM L54.00008: Mode-Selective Spontaneous Oscillation of Bandgap in Dirac Wedge Semimetals  ZHIGANG SONG (Presenter), Lawrence Berkeley National Laboratory —

This article studies the time-dependent behavior of semimetal \(\text{Zr}_3\text{AgX}_3\text{F}_{20}\) [\(X=\text{Cd and Hg}\)], \(\text{M(MoS)}_3\) and \(\text{M(MoSe)}_3\) [\(\text{M}=\text{Li, Na, K, Rb, Tl, In, I}\)] using time-dependent density functional theory. The results show half-occupied Dirac wedge bands. Due to the one-dimensional character, the materials oscillate in a selective mode at a finite temperature. The wedge bands couple to such a phonon mode, resulting in spontaneous oscillation in a rigid period. Especially, the bandgap periodically closes and opens in a large scale, supporting a pulsed current even under a constant biased voltage. Besides, these systems might be long sought time crystals in condensed matters.
9:36AM L54.00009: Application of Convolutional Neural Network to Quantum Percolation in Topological Insulators*  
TOMI OHTSUKI (Presenter), TOMOHIRO MANO, Phys. Division, Sophia Univ — Quantum material phases such as Anderson insulator, diffusive metal, Weyl/Dirac semimetal as well as topological insulators show specific wave functions both in real and Fourier spaces. These features are well captured by convolutional neural networks, and the phase diagrams have been obtained, where standard methods are not applicable. One of these examples are the cases of random lattices such as quantum percolation. Here we study the topological insulators with random vacancies, namely the quantum percolation in topological insulators, by analyzing the wave functions via convolutional neural network. The vacancies in topological insulators are especially interesting since peculiar bound states are formed around the vacancies. We show that only a few percent of vacancies derives topological phase transition. The results are confirmed by independent calculations of localization length, density of states, and wave packet dynamics.

Reference:  

*JSPS KAKENHI Grant Nos. JP17K18763, 19H00658.

9:48AM L54.00010: Predicting Topological Properties of Quantum Materials via Statistical Methods*  
THOMAS MERTZ (Presenter), KARIM ZANTOUT, ROSER VALENTI, Goethe University Frankfurt — We discuss the topological phases of correlated and non-correlated (insulating) quantum materials using a statistical method that explores the entire phase space. Based on model systems we draw fundamental conclusions and discuss the predictive power of this method when applied to real materials.

*We thank the German Research Foundation (Deutsche Forschungsgemeinschaft) for financial support.

10:00AM L54.00011: Strong-coupling superconductivity and pseudogap in topological flat bands: a quantum Monte Carlo study  
JOHANNES HOFMANN (Presenter), EREZ BERG, Weizmann Institute of Science, DEBANJAN CHOWDHURY, Physics, Cornell University — We study a two-dimensional model of an isolated narrow topological band at partial filling with local attractive interactions. Exact quantum Monte Carlo calculations show that the ground state is a superconductor with a critical temperature that scales linearly with the interaction strength. We also find a broad pseudogap regime at temperatures above the superconducting phase that exhibits strong pairing fluctuations and a tendency towards electronic phase separation. We discuss the possible relevance of superconductivity in this unusual regime to the Physics of flat band Moiré materials, and as a route to designing higher temperature superconductors.
Role of van der Waals interactions in topological insulators: bulk, surface and interfaces*  

KARUNYA SHAILESH SHIRALI (Presenter), WILLIAM A SHELTON, ILYA VEKHTER, Louisiana State University, Baton Rouge — It is well-known that van der Waals interactions (vdW) play an important role on structural properties of the prototypical 3D topological insulators Bi$_2$Se$_3$ and Bi$_2$Te$_3$. However, systematic investigations of different implementations of vdW interactions using density functional theory are lacking. We have performed a comprehensive comparison using both semi-empirical (DFT+D2, DFT+D3, Tkatchenko-Scheffler) and first principles (Langreth-Lundqvist DF, SCAN-rVV10) vdW methods in bulk and surface calculations for these materials, treating structural and electronic properties on equal footing. We find that semi-empirical methods, especially D2 produce structural parameters, electronic dispersion, and the Dirac velocity of the surface state close to the experimental values, while other methods exhibit serious problems when applied to Bi$_2$Se$_3$ and Bi$_2$Te$_3$. We attribute these differences to the importance of the long range $r^{-6}$ tail of the vdW interaction, and we discuss its relevance for the properties of topological interfaces.

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Portions of this research were conducted with high performance computing resources provided by Louisiana State University

Topological Phases in Hydrogenated Group 13 Monolayers  

RANJAN BARIK (Presenter), RITESH KUMAR, ABHISHEK SINGH, Indian Institute of Science — The topological phases of matters have been a rapid exposed field of research due to its possible applications in spintronics and fault-tolerant quantum computing. Recently, the 2D sheet of gallium (gallenene), a group 13 element, has been synthesized, for which topological properties remain undefined. Using an effective k.p model, symmetry analysis and group theoretical approach with first-principles calculations we studied the topological properties of hydrogenated gallenene (gallenane) and other group 13 elements. Without the inclusion of spin-orbit coupling (SOC) all hydrogenated group-13 sheets that are aluminane, gallenane, indinane and thallinane become nodal line semimetal (NLSM). Interestingly, gallenane under SOC and with 2.6% tensile strain evolves to quantum spin Hall insulator with an energy gap of 28 meV, which makes it promising for room temperature applications. Aluminane preserved its topology even in the presence of SOC due to feeble strength of it. Indinane and thallinane are trivial semimetals under SOC. These findings could offer a new direction in topological research.

J. Phys. Chem. C, 2019, 12342, 25985-25990
**L54.00014: Robust descriptor for high-throughput discovery of alloyed topological insulators based on artificial intelligence**

GUOHUA CAO (Presenter), Wuhan University, RUNHAI OUYANG, LUCA GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, HUIJUN LIU, Wuhan University, CHRISTIAN CARBOGNO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, ZHENYU ZHANG, ICQD, University of Science and Technology of China — Significant advances have been made in predicting new topological materials using high-throughput empirical descriptors or symmetry-based indicators. To date, these approaches have been applied to materials in existing databases, and are severely limited to systems with well-defined symmetries, leaving a much larger materials space unexplored. Using tetradymites as a prototypical class of examples, we uncover a novel two-dimensional descriptor by applying an artificial intelligence (AI) based approach for fast and reliable identification of the topological characters of a drastically expanded range of materials, without prior determination of their specific symmetries and detailed band structures. By leveraging this descriptor that contains only the atomic number and electronegativity of the constituent species, we have readily scanned over four million alloys in the tetradymite family. Strikingly, nearly two million new topological insulators are identified, revealing a much larger territory of the topological materials world. The present work also attests the increasingly important role of such AI-based approaches in modern materials discovery.

*Supported by NSFC and MOST.

**Wednesday, March 4, 2020 8:00 AM - 10:36 AM**

**Session L55 DCMP: One Dimensional Topological Systems** Mile High Ballroom 2B

**8:00AM L55.00001: Mesoscopic Conductance Fluctuations in Class D Superconducting Wires**

DANIIIL ANTONENKO (Presenter), Skolkovo Institute of Science and Technology, PAVEL OSTROVSKY, Max Planck Institute for Solid State Physics, MIKHAIL SKVORTSOV, Skolkovo Institute of Science and Technology — We study disordered superconducting wires (length L) of class D via supersymmetric sigma-model approach in the critical regime between topological and trivial phases, where delocalization happens and average conductance scales as $G \sim L^{-1/2}$ [1]. In order to calculate the variance of conductance $\text{var } G$ in the diffusive regime we introduce $n=2$ sigma-model and apply the method of transfer-matrix Hamiltonian, studying Laplace-Beltrami operator on the rank two symmetric superspace. We use Iwasawa decomposition to construct eigenbasis on this supermanifold, which appears to consist of three-parametric and one-parametric subsets, with the latter closely related to the eigenfunctions on the $n=1$ sigma-model manifold. Our approach allows to find $\text{var } G$ at arbitrary lengths in the diffusive region with the crossover from the perturbative weak-localisation regime at $L \ll \xi$ to the regime of a very broad conductance distribution at $L \gg \xi$, where $\xi$ is the correlation length of the wire. Also, we account to the possible back/forward channels imbalance, which is described by a Wess-Zumino-Witten term in the sigma-model action.

Majorana bound states from textured chiral magnets* STEFAN REX (Presenter), IGOR GORNYI, ALEXANDER MIRLIN, Karlsruhe Institute of Technology — Non-collinear magnetism combined with superconductivity can support the formation of localized Majorana bound states.

We discuss a hybrid system consisting of a conventional superconductor exchange-coupled to a magnetic layer with Dzyaloshinskii-Moriya interaction (DMI). DMI systems are capable of developing complex magnetic textures spontaneously without a need for external microscopic control of the spin. Experimentally observed textures comprise skyrmions, spin spirals, and topological defects at domain walls.

We investigate theoretically in which cases Majorana modes can be expected in the hybrid system, and support our findings with numerical results. In particular, skyrmion-vortex pairs are highlighted as a candidate composite structure for the creation and individual control of localized Majorana bound states [PRB 100, 064504 (2019)]. Thus, the hetero-systems that we study represent an exciting new platform in the pursuit of topological braiding operations.

*The work was supported by the Deutsche Forschungsgemeinschaft via the Grants MI 658/9-1 (joint DFG-RSF project) and MI 658/7-2 (Priority Programme 1666 “Topological Insulators”). I.V.G. acknowledges support by the Russian Science Foundation through Grant No. 17-12-01182.

Topological Phases in a One-dimensional Majorana-Bose-Hubbard Model* ANANDA ROY (Presenter), JOHANNES HAUSCHILD, FRANK POLLMANN, TU Munich — Majorana zero modes (MZM-s) occurring at the edges of a 1D, p-wave, spinless superconductor, in absence of fluctuations of the phase of the superconducting order parameter, are quintessential examples of topologically-protected zero-energy modes occurring at the edges of 1D symmetry-protected topological phases. In this work, we numerically investigate the properties of the topological phase in the presence of phase-fluctuations using the density matrix renormalization group (DMRG) technique. To that end, we consider a one-dimensional array of MZM-s on superconducting islands at zero temperature. We show that the system can be in either a Mott-insulating phase, a Luttinger liquid (LL) phase of Cooper-pairs or another gapless phase. The latter phase can be viewed as a LL of charge-e bosons where nonlocal string correlation functions decay algebraically. These nonlocal correlation functions, together with correlation functions of the Cooper-pair creation operators, distinguish the different phases of the model. We map the system to an interacting model of spins coupled to rotors and use DMRG to characterize the different phases and the phase-transitions.

*Funding through the Alexander von Humboldt Foundation and ERC Grant no. 771537 is acknowledged.
8:36AM L55.00004: Boundary-induced dynamics and quantum memory effect of 1D and 2D topological systems  CHIH-CHUN CHIEN (Presenter), University of California, Merced, YAN HE, Sichuan University — The dynamics after a change of the boundary condition for selected 1D and 2D topological systems are analyzed. We consider the 1D Su-Schrieffer-Heeger (SSH) model and Kitaev model transforming from periodic to open boundary condition and the 2D Chern insulator (CI) and topological quadrupole insulator (TQI) transforming from a cylinder or Mobius strip to open boundary condition. In all the cases, we found the occupation of the topological edge states reaches a steady-state value after the transformation is completed in absence of any external dissipation mechanism. The steady-state value depends on the ramping rate of the boundary condition. The dependence of the steady-state occupation of the topological edge states on the ramping rate thus exemplifies one kind of quantum memory effect, which originates from the trapping of excitations due to the localized nature of the edge states. The mechanism suggests that this type of quantum memory effect may be universal in topological systems with localized edge states.

8:48AM L55.00005: Interaction Driven Floquet Engineering of Topological Superconductivity in Rashba Nanowires  MANISHA THAKURATHI (Presenter), University of Waterloo, PAVEL ASEEV, DANIEL LOSS, JELENA KLINOVAJA, Department of Physics, university of Basel — We analyze, analytically and numerically, a periodically driven Rashba nanowire proximity coupled to an s-wave superconductor [1] using bosonization and renormalization group analysis in the regime of strong electron-electron interactions. Due to the repulsive interactions, the superconducting gap is suppressed, whereas the Floquet Zeeman gap is enhanced, resulting in a higher effective value of g-factor compared to the non-interacting case [2]. The flow equations for different coupling constants, velocities, and Luttinger-liquid parameters explicitly establish that even for small initial values of the Floquet Zeeman gap compared to the superconducting proximity gap, the interactions drive the system into the topological phase and the interband interaction term helps to achieve larger regions of the topological phase in parameter space.


9:00AM L55.00006: Almost strong 0, π edge modes in clean, interacting 1D Floquet systems*  DANIEL YATES (Presenter), New York Univ NYU, FABIAN H.L. ESSLER, University of Oxford, ADITI MITRA, New York Univ NYU — Certain periodically driven quantum many-particle systems in one dimension are known to exhibit edge modes that are related to topological properties and lead to approximate degeneracies of the Floquet spectrum. A similar situation occurs in spin chains, where stable edge modes were shown to exist at all energies in certain integrable spin chains. Moreover, these edge modes were found to be remarkably stable to perturbations. Here we investigate the stability of edge modes in interacting, periodically driven, clean systems. We introduce a model that features edge modes that persist over times scales well in excess of the time needed for the bulk of the system to heat to infinite temperatures.

*This work was supported by the US Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0010821
9:12AM L55.00007: Rigorous results on topological superconductivity with particle number conservation* MATTHEW LAPA (Presenter), MICHAEL LEVIN, University of Chicago — Most theoretical studies of topological superconductors and their unpaired Majorana fermions rely on a mean-field (or Bogoliubov-de Gennes) approach to describe superconductivity, which violates particle number conservation (PNC). Recently, however, A.J. Leggett and others have argued that this violation of PNC may pose a serious conceptual problem for Majorana-based quantum computation. To resolve this issue, reliable results on number-conserving models of superconductivity are essential. As a first step in this direction, we use rigorous methods to study a number-conserving toy model of a topological superconducting wire. We prove that this model exhibits many of the desired properties of the mean-field models, including a finite energy gap in a sector of fixed total particle number, and the existence of long range “Majorana-like” correlations between the ends of the wire. These results show that many of the remarkable properties of mean-field models of topological superconductivity persist in more realistic models with number-conserving dynamics.

*Kadanoff Center for Theoretical Physics at the University of Chicago, Simons Foundation "Ultra-Quantum Matter" collaboration

9:24AM L55.00008: Braiding Floquet Majorana Modes in One-Dimensional Topological Superconductors* BILL TRUONG (Presenter), TAMI PEREG-BARNEA, KARTIEK AGARWAL, McGill University — It is well-known that braiding Majorana zero modes in one-dimensional (1D) topological systems is a challenge since the modes hybridize when they are within proximity of each other. Recent developments have indicated that braiding in 1D can be accomplished through periodic driving. In our work, we study a 1D $p$-wave superconductor modelled as a Kitaev chain with the driving achieved by periodically modulating the parameters of the system. This Floquet system gives rise to Majorana edge modes of both zero and $\pi$ quasienergy. We numerically implement the adiabatic protocol developed in Ref. [1] to braid the Floquet Majorana zero modes, using the Floquet Majorana $\pi$ modes as an auxiliary degree of freedom. We consider the inclusion of interactions and disorder into the system and demonstrate the robustness of the protocol by examining quantities such as the exchange operator.


*This work was supported by the Natural Sciences and Engineering Research Council of Canada.
9:36AM L55.00009: Universal delocalization transition in 1D chiral Floquet topological insulators*  PRATIK SATHE (Presenter), ALBERT BROWN, FENNER HARPER, RAHUL ROY, University of California, Los Angeles — Periodically driven systems of non-interacting fermions, also known as Floquet topological insulators, exhibit novel topological characteristics distinct from those of static systems. In the case of 1D Floquet topological insulators with chiral symmetry (class AIII), the dynamical topological nature can be understood through studying the time evolution operator U(t) evaluated close to the midpoint of a driving period, i.e. U(T/2). We investigate the localization properties at this special point, for flat-band, two-step Floquet drives. Specifically, for topologically non-trivial disordered drives, we show that the localization length of eigenstates of U(T/2 - epsilon) diverges as epsilon approaches 0 as a power law with exponent nu = 2, and argue that this property is universal for this class of AIII models.

*P.S., A.B., F.H. and R.R. acknowledge support from the NSF under CAREER DMR-1455368 and the Alfred P. Sloan Foundation.

9:48AM L55.00010: Experimental study of 1D Su-Schrieffer-Heeger edge modes in a water-wave channel  ADAM ANGLART, PAWEL OBREPALSKI, KEI KUSUMI, Physique et Mecanique des Milieux Heterogenes (PMMH), AGNES MAUREL, Institut Langevin, ESPCI, PHILIPPE PETITJEANS, Physique et Mecanique des Milieux Heterogenes (PMMH), VINCENT PAGNEUX (Presenter), Laboratoire d'Acoustique de l'Universite du Maine — The main objective of this work is to experimentally investigate the topologically protected edge-states and band gaps in a water waveguide with periodic geometry. One of the representations of the topological states, provided by the Su–Schrieffer–Heeger model (SSH) [1], is applied to describe the observed phenomena [2]. A waveguide with step periodic width as well as corresponding rectangular tank with constant width are examined using Confocal Displacement Sensors allowing the measurement of water surface displacements. 2D numerical simulations are carried out in order to verify the SSH model and experimental data. The obtained results show that this very simple setup exhibits all the properties of the SSH model with an excellent agreement to the water-wave systems.

References
10:00AM L55.00011: Path integral for spin-1 chain in the entangled basis  JUNG HOON HAN
(Presenter), Physics, Sungkyunkwan University — We develop path-integral formulation of spin-1
Haldane chain in the entangled, matrix product state (MPS) basis. Whereas the conventional path
integral approach is founded on spin-based coherent states as the basis, we here adopt a new
basis consisting of bond-based coherent states. The Affleck-Kennedy-Lieb-Tasaki (AKLT)-type
ground state is obtained as the saddle point solution of the newly developed action. Small
fluctuations around the saddle point are developed in terms of conventional gradient expansion.
Ways to compute various correlation functions based on the effective action will be discussed.
While certain crude approximations have to be made to proceed with the calculation, it appears
that features of spin gap in the spin-1 chain seems nicely captured at the mean-field level by the
path integral written in the entangled basis. This work was done in collaboration with Jin-Tae Kim,
Rajarshi Pal, and Jin-Hong Park at SKKU.

10:12AM L55.00012: Detecting one-dimensional interacting topological phases by edge-
state pinning*  SHUN-CHIAO CHANG (Presenter), PAVAN HOSUR, Univ of Houston — In density
matrix renormalization group (DMRG) simulations, edge states are often identified by computing
edge-edge or bulk-edge two-point correlation functions. Since this approach involves computing
the square of the local order parameter, very large systems at high precision are required to
obtain reliable results when the order parameter is small, which is true, for instance, near a
phase boundary. Moreover, the computational cost of this method increases drastically with the
bulk entanglement. In this work, we propose and demonstrate an efficient method for detecting
the topological edge states with DMRG. That is, we study edge states by pinning one edge with
appropriate fields and observing the corresponding local order parameter of the other edge. The
method is validated here for antiferromagnetic Heisenberg model, the simplest realization of the
Haldane phase. It would be interesting to study other one-dimensional topological phases using
this method.

*This work was supported by the Department of Physics, College of Natural Sciences and
Mathematics and the University of Houston.

10:24AM L55.00013: Generalized bulk-edge correspondence for non-hermitian topological
phases*  KEN-ICHIRO IMURA (Presenter), YOSITAKE TAKANE TAKANE@HIROSHIMA-U.AC.JP,
Hiroshima Univ — In a recent paper [1] we have established that the idea of bulk-edge
correspondence in the hermitian limit can be generalized to non-hermitian topological systems.
But strictly speaking, the proof given there was limited to the regime of weak (perturbative) non-
hermiticity. Here, we deepen the idea of the generalized bulk-edge correspondence proposed in
Ref. [1] and give a more general proof valid also in the non-perturbative non-hermitian regime.


*JSPS KAKENHI Grant No. 15K05131, 18H03683

Wednesday, March 4, 2020 8:00 AM - 10:48 AM
8:00AM L56.00001: Topology and the doped Kondo Heisenberg model** JULIAN MAY-MANN (Presenter), RYAN LEVY, EDUARDO FRADKIN, BRYAN CLARK, University of Illinois at Urbana-Champaign, RODRIGO B SOTO, Departamento de Física, Pontificia Universidad Católica de Chile, GIL YOUNG CHO, Korea Institute for Advanced Study — In previous works, it has been proposed that the doped Kondo Heisenberg model is topological and hosts Majorana zero modes. These Majorana zero modes correspond to solitons of the gapped spin sector of the model. We have investigated this claim on the lattice using DMRG, and found no evidence for these proposed zero modes. In light of this, we revisit the original claims that the model is topological using bosonization. We discuss how this continuum analysis fits with the numeric data and the lattice model.

**Julian May-Mann is supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE – 1746047

8:12AM L56.00002: Fermionic multichannel dynamical large-N approach to Kondo lattice model** JIANGFAN WANG, YUNG-YEH CHANG (Presenter), CHUNG-HOU CHUNG, Natl Chiao Tung Univ — We establish a novel theoretical framework to study the quantum phases and phase transitions of a two-dimensional Kondo Heisenberg lattice model based on the dynamical large-N approach to the multichannel pseudofermion representation of the model with $\text{Sp}(N) \times \text{SU}(K)$ symmetry with $N$ and $K$ being number of spin flavors and Kondo screening channels, respectively. This approach captures the heavy electron Fermi liquid state when $\text{SU}(K)$ symmetry is broken with Kondo hybridization in terms of Bose-condensed holons, and a spin-liquid metallic state with gaped fermionic spinons when the anti-ferromagnetic coupling dominates. A self-consistent Green’s function method is used. The global phase diagram and the thermodynamic properties of the spin liquid state share close resemblance to CePdAl, a heavy-fermion systems with magnetic frustration.

**This work is supported by the MOST (Grant NO.: 107-2112-M-009-010-MY3), the NCTS of Taiwan, R.O.C. (C.-H. C.)
Kondo effect due to a hydrogen impurity in graphene: A multichannel Kondo problem with diverging hybridization*  ZHENG SHI (Presenter), Dahlem Center for Complex Quantum Systems and Physics Department, Freie Univ Berlin, EMILIAN NICA, Department of Physics, Arizona State University, IAN AFFLECK, Department of Physics and Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia — We consider the Kondo effect arising from a hydrogen impurity in graphene. Approximating the C-H covalent bond as infinitely strong and the Hubbard interaction to be present only on the three nearest neighbors of hydrogen impurity, we obtain a Kondo model with three $Z_3$-symmetric impurity spins and three conduction channels, two of which support a diverging local density of states $\propto 1/|\omega| \ln^2(\Lambda/\omega)$ near the Dirac point $\omega \to 0$. When the particle-hole (p-h) symmetry breaking at the impurity is not too strong, numerical renormalization group shows that the ground state is either a p-h symmetric spin-1/2 doublet with ferromagnetic impurity spin correlations, or a p-h asymmetric spin singlet with antiferromagnetic impurity spin correlations. This behavior is inherited by the Anderson model containing the hydrogen impurity and all four carbon atoms in its vicinity.

*We acknowledge support by NSERC Discovery Grant 04033-2016 and the Canadian Institute for Advanced Research.

Magnon Bose-Einstein Condensation and Superconductivity in a Frustrated Kondo Lattice*  JED PIXLEY (Presenter), PAVEL VOLKOV, Department of Physics and Astronomy, Center for Materials Theory, Rutgers University, SNIR GAZIT, Racah Institute of Physics, The Hebrew University, Jerusalem — Magnetically frustrated Kondo lattices are considered to be one of the most promising platforms for the realization of novel types of metallic quantum criticality. Motivated by the recent experiments on the heavy fermion compounds with a nonmagnetic valence bond solid (VBS) ground state of the localized spins, such as YbAl$_2$C$_3$, we study a one-dimensional two-leg spin ladder model with a VBS ground state doped with itinerant fermions. Using field theory techniques and precise density matrix renormalization group calculations, we provide a solution of the model as a function of the Kondo coupling and magnetic field. We demonstrate that the magnetic field-driven transition to an easy-plane antiferromagnet (known as magnon Bose-Einstein condensation (BEC) in the insulating limit) is stable in the presence of a Fermi sea and its universality class is unchanged, while the critical field decreases as a function of Kondo coupling. We also find that spin fluctuations in the VBS phase can drive unconventional superconducting correlations. Finally, we argue that, depending on the filling of conduction electrons, the magnon BEC transition can remain stable in a metal also in dimensions two and three.

*PV is supported by Rutgers CMT Postdoctoral Fellowship
8:48AM L56.00005: Magnetic Doublon Bound States in the Kondo Lattice Model* ROMAN RAUSCH (Presenter), University of Kyoto, MICHAEL POTTHOFF, I. Institute for Theoretical Physics, University of Hamburg, NORIO KAWAKAMI, University of Kyoto — We present a novel pairing mechanism for electrons, mediated by magnons. These paired bound states are termed magnetic doublons. Applying numerically exact techniques (exact diagonalization and the density-matrix renormalization group, DMRG) to the Kondo lattice model at strong exchange coupling J for different fillings and magnetic configurations, we demonstrate that magnetic doublon excitations exist as composite objects with extremely weak dispersion at excitation energies of the order of $3J/2$ above the ground state. They are highly stable, support a novel "inverse" colossal magnetoresistance and potentially other effects like metastable superconductivity, or cooling via quantum distillation.


* R.R. would like to thank the Japan Society for the Promotion of Science (JSPS) and the Alexander von Humboldt Foundation.

Computations were partially performed at the Yukawa Institute for Theoretical Physics, Kyoto. We gratefully acknowledge the support by the Deutsche Forschungsgemeinschaft within the SFB 925 (project B5), by the Cluster of Excellence Advanced Imaging of Matter EXC 2056 (project ID 390715994), as well as by JSPS KAKENHI (grant No. JP15H05855, JP18H01140, JP19H01838).

9:00AM L56.00006: Competing Energy Scales and Quasiparticle Dynamics in a Driven Kondo Impurity System* CHEN-YEN LAI (Presenter), Los Alamos Natl Lab, QIMIAO SI, Rice University, JIAN-XIN ZHU, Los Alamos Natl Lab — The ultrafast pump-probe techniques are used to probe the elementary excitations and its energy scale in materials. Recent study [Nat. Phys. 14 1103 (2018)] shows the collapse and revival of the Kondo correlations from terahertz reflectivity measurement. Here we propose a model study as a proof of principle to first determine the corresponding Kondo energy scale by using the matrix product state to simulate the Fermi-Bose-Anderson impurity model, which is a good starting model for the study of Kondo lattice model. In equilibrium, the model displays a quantum critical point that captures the competition between RKKY interaction and Kondo coupling in the underlying system. As a laser pump pulse is applied to the system, our nonequilibrium simulations show that the driven system exhibits qualitatively different response, which is related to the competing energy scales. Our results benchmark the competing energy scales in a Kondo impurity system and provide new insight on the behavior of the critical quasiparticle in heavy fermion compounds.

* This work was carried out under the auspices of the U.S. DOE NNSA under Contract No. 89233218CNA000001, and was supported by the LANL LDRD Program. Work at Rice was supported by the NSF (DMR-1920740) and the Robert A. Welch Foundation (C-1411).
9:12AM L56.00007: Universality in the ferromagnetic strong coupling regime of the Kondo model out of equilibrium*  
ADRIAN CULVER (Presenter), NATAN ANDREI, Rutgers University, New Brunswick — We present a nonperturbative method for calculating the time-dependent many body wavefunction following a local quench and use it to find new results in and out of equilibrium in the universal strong ferromagnetic regime of the Kondo model. The method addresses the general problem of calculating $e^{-iHt}\Psi$, where the initial state $\Psi$ is a free N-particle state (such as a Fermi sea) and $H$ is a many body Hamiltonian which is switched on at $t=0$. While the method may be of wider applicability, we have so far focused on one dimensional models of quantum dots attached to linearized leads. The method yields the exact many body wavefunction of the two lead Kondo model following the quench. In the strong ferromagnetic regime, we find a new universal scale $T_K = D \exp[3\pi^2 \rho J / 8]$ and the surprising result that the steady state conductance $dI/dV$ reaches the unitarity limit asymptotically at large voltage or temperature.

*Research supported by NSF Grant DMR 1410583.

9:24AM L56.00008: Comparing Different Refermionizations of Multichannel Kondo Hamiltonians  
ALEKSANDAR LJEPOLA (Presenter), Univ of Cincinnati, NAYANA SHAH, Washington University in St. Louis, C. J. BOLECH, Univ of Cincinnati — Following a critical revision of the procedures for bosonization and debosonization of theories with boundaries [1,2] we consider novel alternative schemes to arrive at refermionized Hamiltonians for the standard multichannel Kondo model. We compare them order by order using Green-function based perturbative expansions and discuss the results on the basis of symmetries and decoupled dynamical sectors of the original theory.


9:36AM L56.00009: Various Fermi liquid phases on the Kondo - Heisenberg model at quarter filling  
HEE SEUNG KIM (Presenter), HYEOK-JUN YANG, SUNGBIN LEE, KAIST — Motivated by exotic phases emerged from Kondo insulators, we study transport properties of electronic system under Kondo and Heisenberg interactions. Particularly, we focus on the Kondo - AF (antiferromagnetic) Heisenberg model on a honeycomb lattice at quarter filling. By using paraton mean-field theory, we construct generic mean-field phase diagram and investigate distinct Fermi liquid phases. In strong Kondo coupling limit, due to quarter filling condition, half of localized moments form Kondo singlet and the others develop triangular lattice with AF Heisenberg interaction which yields spin liquid phase. To investigate the low-energy excitation properties, we evaluate transport coefficients of mobile electrons and fractionalized quasiparticles respectively. Even though mobility of charge carriers is suppressed, Fermi liquid behavior is verified arose from neutral low-energy excitations.
9:48AM L56.00010: Emergent non-Fermi liquid phenomena in itinerant electron systems with multipolar local moments

ADARSH PATRI (Presenter), ILIA KHAIT, YONG-BAEK KIM, Univ of Toronto — Recent experiments on cubic heavy fermion systems with multipolar local moments offer a new avenue for the discovery of novel spin-orbital entangled quantum ground states. In this talk, we theoretically investigate the fate of the multipolar Kondo effect, where the local moment does not carry any dipole moment, but only quadrupolar and octupolar moments. Using perturbative renormalization group methods, we discover a number of non-Fermi liquid ground states, which are characterized by an absence of well-defined quasiparticles and singular power-law behaviours in physical properties. This work lays a novel ground for the identification of emergent non-Fermi liquid phases in many heavy fermion materials.

*NSERC of Canada, Canadian Institute for Advanced Research, and Center for Quantum Materials at the University of Toronto.

10:00AM L56.00011: Global phase diagram of a Kondo Hund impurity model and the destruction of Fermi-liquid theory

YILIN WANG (Presenter), Brookhaven National Laboratory, ELIAS WALTER, SEUNG-SUP LEE, KATHARINA M STADLER, JAN VON DELFT, Ludwig Maximilian University of Munich, ANDREAS WEICHESELBAUM, Brookhaven National Laboratory, GABRIEL KOTLIAR, Rutgers University, New Brunswick — In many correlated materials, notably the Hund metals, the Landau Fermi-liquid coherence scale $T_{FL}$ is found to be very small. In this Letter, we interpret its smallness in terms of proximity to quantum critical points (QCPs): We use the numerical renormalization group (NRG) to compute the global phase diagram of the simplest three-channel spin-orbital Kondo impurity model capturing the essential physics of Hund metals. When the spin or spin-orbital Kondo couplings are tuned into the ferromagnetic regimes, we find quantum phase transitions to a singular Fermi-liquid or a novel non-Fermi-liquid phase, signalling the existence of QCPs, while $T_{FL}$ is suppressed to zero. The new non-Fermi-liquid phase shows frustrated behavior involving alternating overscreenings in spin and orbital sectors, with universal power laws in the spin ($\omega^{-1/5}$), orbital ($\omega^{1/5}$) and spin-orbital ($\omega^1$) dynamical susceptibilities. These power laws, and the NRG eigenlevel spectra, can be fully understood using conformal field theory arguments, which also clarify the nature of the NFL phase.
Dynamical Kondo effect and Kondo destruction in effective models for quantum-critical heavy fermion metals

**Ang Cai** (Presenter), **Haoyu Hu**, Rice University, **Kevin Ingersent**, University of Florida, **Silke Buehler-Paschen**, Vienna University of Technology, **Qimiao Si**, Rice University — Kondo destruction that results in a sudden reconstruction of Fermi surface at the quantum critical point arises in certain heavy-fermion metals [1,2,3,4]. In the Kondo-destroyed phase, the static Kondo singlet amplitude vanishes and, thus, a well-defined Kondo resonance is lost, but the Kondo singlet correlations remain at nonzero frequencies. We elucidate the dynamical Kondo effect in Bose-Fermi Kondo/Anderson models which unambiguously exhibit a Kondo-destruction QCP [5]. We demonstrate that the dynamical Kondo effect is important for the stability of Kondo-destruction quantum criticality and provides understanding of the enhanced effective mass in the Kondo-destroyed phase.


*Work supported by the NSF (DMR-1920740) and the Robert A. Welch Foundation (C-1411)

Multiorbital Hund's coupled impurity in the mixed valence regime

**Victor Drouin-Touchette** (Presenter), **Elio Koenig**, **Yashar Komijani**, **Piers Coleman**, Rutgers University, New Brunswick — Motivated by the relevance of Hund's coupling in iron-based superconductors, we revisit the problem of a multiorbital Anderson impurity with Hund’s interaction. Using large-N and Schwinger boson techniques, we study the ground state and thermodynamic properties of this system in both integer and mixed valence regimes. The physics is characterized by the interplay of Hund's coupling, which tends to form large moments by aligning the spins of the impurity, and the Kondo effect, which leads to the low-temperature screening of the moments. In the integer valence regime, we confirm the formation of large moments, which eventually become screened at an exponentially reduced Kondo temperature due to the so-called Schrieffer effect, and compare to previous renormalization group studies [1]. In the mixed valence regime, the Hund's coupling gives rise to interesting physics: we explore the presence of a non-Fermi-liquid ground state and the possibility that the large moments can generate retarded on-site pairing correlations for the conduction electrons.


*We acknowledge support by the DOE, Basic Energy Sciences grant DE-FG02-99ER45790, and the Quebec FRQNT.
Numerical renormalization group method for computing four-point correlation functions

SEUNG-SUP LEE (Presenter), FABIAN KUGLER, JAN VON DELFT, Ludwig Maximilian University of Munich — Four-point correlation functions commonly appear in various contexts of the theory of strongly correlated systems, including diagrammatic extensions of dynamical mean-field theory (DMFT). Here we develop the numerical renormalization group (NRG) method for computing four-point correlation functions in quantum impurity systems. First, we derive the Lehmann representation for general four-point functions (i) in imaginary Matsubara frequencies, (ii) on the real-frequency axes at zero temperature, and (iii) on the Keldysh contour. By using the complete basis of energy eigenstates constructed within NRG, four-point functions can be computed at arbitrarily low temperatures. We present results for paradigmatic models, including the effective quantum impurity model arising in DMFT treatments of the Hubbard model.

S.-S.L., F.K., and J.v.D. were supported by the Deutsche Forschungsgemeinschaft under Germany’s Excellence Strategy – EXC-2111–390814868; S.-S.L. further by Grant. No. LE3883/2-1. F.K. acknowledges funding from the research school IMPRS-QST.

Fractionalized Fermi liquid in square-lattice Kondo-Heisenberg model

YUNG-YEH CHANG (Presenter), CHUNG-HOU CHUNG, Natl Chiao Tung Univ, ALEXEI TSVELIK, Condensed Matter Physics and Materials Science Division, Brookhaven National Lab — The Kondo-Heisenberg model on a (un-frustrated) square lattice is studied via a controlled large-N (Sp(2N)) approach to demonstrate on a general ground the existence of a peculiar metallic state so-called “fractionalized Fermi liquid (FL*)” with unbroken translational symmetry and a Fermi surface volume not controlled by the total electron density. Close to half-filling, we show that the nesting of Fermi surface favors the Kondo hybridization to form between conduction electrons and local resonant-valence-bond spin-liquid fermions, which stabilizes FL* state with well-defined quasiparticle and gapped spinon excitations. The system develops an ordered phase at ground state (charge density wave or pair density wave superconducting). Our result generalizes the FL* state previously proposed in Phys. Rev. Lett. 90, 216403 (2003), which is restricted to frustrated Kondo lattice systems.

This work is supported by the MOST Grant NO. 107-2112-M-009-010-MY3, the NCTS of Taiwan, R.O.C. (C.-H. C.), Office of Basic Energy Sciences, Material Sciences and Engineering Division, U.S. Department of Energy (DOE) under Contract No. DE-SC0012704 (A.M.T.).
8:00AM L57.00001: Complementary logic inverters based on polarity-controllable MoS$_2$ fin-shaped and v-shaped field effect transistors* CHE-YU LIN, National Cheng Kung University, PO-CHUN CHEN, National Taiwan Normal Univ, MING-CHENG CHEN, MING-YANG LI, LAIN-JONG LI, Taiwan Semiconductor Manufacturing Company, KAI-SHIN LI, Taiwan Semiconductor Research Institute, YANNWEN LAN (Presenter), National Taiwan Normal Univ — Integration of high performance $n$-type and $p$-type field-effect transistors with complementary device operation in the same kind of layered materials is highly desirable for pursuing low power and flexible next-generation electronics. In this work, we show a well-mannered growth of MoS$_2$ between two electrodes on silicon oxide with fin-shaped and v-shaped structure. In the fin-shaped case, both $n$-type and $p$-type MoS$_2$ can be integrated by using a traditional implantation technique. In the v-shaped case, the device can alternately operate either as a $p$-type or an $n$-type semiconductor in the identical one. The proposed device is built with an adjustable threshold voltage ($V_{th}$), which can be varied by adding a layer of plasma-oxidized dielectric at the top gate structure. Consequently, the $V_{th}$ shifts and the top gate structure switch from the typical $n$-type to $p$-type while $n$-type behaviour remains in the application of bottom-gate voltages. In both cases, we have accordingly demonstrated the complementary logic inverters based on the polarity-controllable behavior. Our results provide evidence for complementary 2D materials operation in the same materials, a promising avenue for the development of high-density complementary 2D electronic devices.

*MOST, Taiwan 108-2112-M-003-010-MY3

8:12AM L57.00002: Device simulation study of ion-gated ambipolar transition-metal dichalcogenide transistors* AKIKO UEDA (Presenter), Spintronics Research Center, National Institute of Advanced Industrial Science and Technology (AIST), YIJIN ZHANG, Max Planck Institute for Solid State Research, HIROSHI IMAMURA, Spintronics Research Center, National Institute of Advanced Industrial Science and Technology (AIST), YOSHIHIRO IWASA, Department of Applied Physics and Quantum-Phase Electronics (QPEC) Center, The University of Tokyo — Ion gating is known as a powerful tool to access electronic functionalities with low voltage operation. Though many interesting experimental studies have been reported, the device simulation had never been performed before. In this work, we developed a two-dimensional layer transistor model based on the drift-diffusion method for an ionic liquid (IL) as a gate dielectric. We reproduced the transport characteristics of the ion-gated WSe$_2$ transistors reported in several experiments and explained the transport mechanism using the band profile and spatial distribution obtained by the calculation. In particular, the simulation explains the ambipolar behavior with the gate voltage comparable to the band gap energy, as well as the formation of p-n junctions in the channel reported in several experimental papers. The simulation clearly shows that the ambipolar behavior becomes possible by the dramatic change of the potential profile at the contacts. The developed model is highly advantageous for exploring the functionalities and design ideal devices for ion-gated transition-metal dichalcogenide transistors.

*This research was supported by Grant-in-Aid for Scientific Research (A) (no. 19H00653) and Grant-in-Aid for Scientific Research (C) (no. 19K05201) from JSPS.
8:24AM L57.00003: Hybrid Transfer of 2D materials: An approach towards a wrinkle and contaminations free transfer of 2D materials grown on metallic substrates for van der Waals heterostructures and large scale industrial applications.*  SAJITH WITHANAGE (Presenter), THARANGA NANAYAKKARA, U. KUSHAN WIJEWARDENA, ANNIKA KRIISA, RAMESH MANI, Georgia State University — There has been much recent interest in transferring 2D materials on to non-conducting surfaces. One approach was to pick-up graphene grown by the CVD method using a flake of hexagonal boron nitride (hBN) to have a contamination-free dry transfer. [1] But this kind of transfer technique can be only used in small-scale device fabrication for laboratory use since the scale limitations of the hBN flakes and the limited supply of hBN flakes with low thicknesses. Here, we report a hybrid transfer technique that combines wet and dry transfer processes using polymer support resulting in wrinkle and contamination-free high mobility 2D materials. Thus, we detail the transfer process, conditions for a successful transfer and the quality of CVD grown graphene. The transferred graphene layers are characterized by various methods, and the results of the study are reported.


*This work was supported by the NSF under Grant No. ECCS-1710302.

8:36AM L57.00004: Magnetotransport studies in hybrid 2D/0D nanostructures  ETHEL PEREZ-HOYOS (Presenter), YUNQIU (KELLY) LUO, ABHILASHA DEHANKAR, JINSONG XU, DANIEL PHARIS, ROLAND KAWAKAMI, JESSICA WINTER, EZEKIEL JOHNSTON-HALPERIN, Ohio State Univ - Columbus — We introduce a device fabrication strategy that takes advantage of stacking techniques developed for van der Waals heterostructures to construct hybrid 2D/0D composite magnetic nanostructures, with potential application in the study of spin and charge disorder as well as magnetic-proximity effects. The structures in this study are comprised of superparamagnetic iron oxide nanoparticles (SPIONs) and monolayer graphene. The SPIONs are deposited first using a Langmuir-Blodgett technique, yielding rafts of highly ordered nanoparticles (Fig.1b). Characterization via magnetic force microscopy (MFM) reveals magnetic order at multiple length scales and SQUID magnetometry identifies both glassy antiferromagnetic and ferromagnetic response. Single graphene monolayers are mechanically stacked on the SPIONs layer, and characterized via low temperature magneto-transport. Initial measurements show good electron mobility in the graphene layer and indications of exchange coupling between the graphene and the SPIONs layer. Measurements in the quantum Hall regime will be discussed.

ABRAR ALHAZMI (Presenter), MALAK ALBOGAMI, OALAIYAN ALOLAIYAN, MOHAMMED R AMER, King Abdulaziz City Sci & Tech — Layered 2D materials have recently attracted attention due to their unique electrical and optical properties. In particular, Germanium Sulfide (GeS) which has been predicted to exhibit high mobility. However, few research work reported in the literature on GeS devices and they exhibit high contact resistance. The origin of this contact resistance is still not clear. Here, we investigate the electron transport of pristine GeS field effect transistors. A high contact resistance was observed. Various methods were used to overcome this issue including thermal, electrical annealing, and 2D heterojunction contact. Both annealing methods did not yield any improvement in the measured $I/V_{ds}$. However, we observe an anomalous negative differential resistance (NDR) with low contact resistance and $n$-type conductivity when black phosphorus (BP) are deposited between GeS and S/D electrodes. This NDR is uncontrollable in ambient and insensitive to gate voltage. We believe this NDR is caused by chemical reaction between GeS and degraded BP where the measured electrical conductivity leads to chemical doping, causing the observation of conductivity switch from $p$-type for pristine GeS, to $n$-type for GeS with degraded BP contacts. Further investigations are needed to characterize the origin of this NDR.

**9:00AM L57.00006: Contact Doped Multi-layer Tungsten Diselenide Field Effect Transistors**

INYONG MOON (Presenter), SUNGWON LEE, Sungkyunkwan Univ., MINSUP CHOI, Columbia Univ., WON JONG YOO, Sungkyunkwan Univ. — According to the conventional transistor process including the silicon semiconductor device, it is the common practice to heavily dope contact regions under the metallic electrodes by using the ion implantation technique so as to minimize contact resistance. In this study, we demonstrate a contact doping technique applied to the ultra-thin (2~5 nm) tungsten diselenide (WSe$_2$) channel formed in field effect transistors (FET) by applying the selective oxidation process to the contact regions. Using our devices that underwent the contact doping, we were able to achieve high performance $p$-type FET electrical properties with an on/off ratio of $10^8$, a field effect mobility of 180 cm$^2$/Vs and a contact resistance of 1 kΩμm. Importantly, Schottky barrier heights (SBH) and Fermi level pinning factors of the contact doped WSe$_2$ FET were measured by employing various work function metals (In, Ti, Au, Pd) as the electrodes. We were able to derive the relationship between the Schottky barrier heights and the contact resistances very reliably.

*This work was supported by the National Research Foundation of Korea (NRF) as the Basic Science Research Program (2018R1D1A1B07044712), the Global Research Laboratory (GRL) Program (2016K1A1A2912707) and the Global Frontier R&D Program (2013M3A6B1078873).*
The so-called Boltzmann Tyranny defines the fundamental thermionic limit of the subthreshold slope (SS) of a metal-oxide-semiconductor field-effect transistor (MOSFET) at 60 mV/dec at room temperature and, therefore, precludes the lowering of the supply voltage and the overall power consumption. Adding a ferroelectric dielectric as a negative capacitor to the gate stack of a MOSFET may offer a promising solution to bypassing this fundamental barrier. Meanwhile, two-dimensional (2D) semiconductors, such as atomically thin transition metal dichalcogenides (TMDs) due to their low dielectric constant, and ease of integration in a junctionless transistor topology, offer enhanced electrostatic control of the channel. In this talk, we will review the recent progress on negative capacitance field-effect transistors (NC-FET) and ferroelectric field-effect transistors (Fe-FET) using TMDs as the transistor channels. [1,2] More importantly, a new device concept, which we call as ferroelectric semiconductor field-effect transistor (FeS-FET), was proposed and experimentally demonstrated. [3] In this novel FeS-FET, a 2D ferroelectric semiconductor \( \alpha-\text{In}_2\text{Se}_3 \) is used to replace conventional semiconductor as channel. \( \alpha-\text{In}_2\text{Se}_3 \) is identified due to its proper bandgap, room temperature ferroelectricity, the ability to maintain ferroelectricity down to a few atomic layers and the feasibility for large-area growth.


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**9:48AM L57.00008: 2D Heterostructure Devices** [Invited] ROMAN GORBATCHEV (Presenter), Manchester — Selected by Focus Topic Organizer (Deji Akinwande)
10:24AM L57.00009: New Approaches and Observations in Scaled Contacts for 2D FETs
ZHIHUI CHENG (Presenter), Duke University & Purdue University & NIST, HATTAN ABUZAID, Electrical and Computer Engineering, Duke University, YIFEI YU, Materials Science and Engineering, North Carolina State University, SHREYA SINGH, Electrical and Computer Engineering, Duke University, LINYOU CAO, Materials Science and Engineering, North Carolina State University, CURT RICHTER, Physical Measurement Laboratory, National Institute of Standards and Technology, AARON FRANKLIN, Electrical and Computer Engineering, Duke University — Atomically thin 2D crystals are promising channel materials for extremely scaled field-effect transistors (FETs). For devices at the scaled regime, both channel and contact length must be scaled, with channel length being the distance from source to drain contacts and contact length being the length of the source/drain covering the 2D semiconductor channel. Contacting 2D materials at these scaled contact lengths (< 30 nm) has rarely been pursued or studied in depth. Moreover, the device community has not yet determined how contacts can be scaled down without causing significant degradation in device performance; i.e., how long is the transfer length, below which current crowding effects appear? Here, we demonstrate new measurement approaches and results for determining the transfer length of MoS\textsubscript{2} FETs by physically scaling the contact length. We found that, contrary to previous reports, top contacts can be scaled to ~20 nm without obvious degradation in transistor performance. Our data from measurements of over 100 devices with different contact lengths statistically imply that contact resistance variation increases in the scaled contact regime. Our work illustrates the impact of current crowding in scaled contacts and the ultimate scalability of metal-2D contact interfaces.

10:36AM L57.00010: Ultrasensitive molecular interaction in MoS\textsubscript{2}-graphene hybrid structure via electrostatic control
RAHUL TRIPATHI (Presenter), ABHA MISRA, Indian Institute of Science — Following the discovery of graphene, other 2D materials such as TMDs offer great potential for future sensing devices because of the high surface-to-bulk ratio. Moreover, electronic transport in vertically stacked atomically thin heterojunctions of 2D materials are extremely sensitive to the surrounding atmosphere, thus allowing their exploration in molecular sensing applications. We report the fabrication of designed vdW interfaces of few-layer graphene and MoS\textsubscript{2} in vertical heterojunction and evaluation of electrical and molecular interaction. The few-layer MoS\textsubscript{2}-graphene with vertically stacked hybrid shows a non-linearity in the drain current due to barrier formation at the interface that can be modulated by an external electric field. The hetero p-n junction between MoS\textsubscript{2} on graphene reveals superior molecular interaction with a high sensitivity of 18\% at 10 ppb level of nitrogen dioxide in transfer characteristics near accumulation region at room temperature. We further observed that the recovery time of the device can be tuned using the switching behavior of the device depicting an overall superior sensing capability leading to an excellent advancement in sensing devices. Our findings offer significant insight into the MoS\textsubscript{2}-graphene heterostructure for molecular interaction.
10:48AM L57.00011: Monolayer-Bulk Black Phosphorus Natural Heterojunction Tunnel Field-Effect Transistor for Low Power Switches  
SEUNGHO KIM, SUNGJAE CHO, GYUHOMYEONG, WONGIL SHIN, HONGSIK LIM, BORAM KIM, TAEHYEOK JIN (Presenter), KAIST, SUNGJIN CHANG, NNFC, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS — Transistor down-scaling by Moore's law over fifty years enabled today's information technology, but fundamental limits have ended Moore's law [1]; Transistors require at least 60 mV switching voltage for each 10-fold current increase (subthreshold swing (SS) 60 mV/dec). Alternative tunnel field-effect transistors (TFETs) are widely studied to achieve a sub-thermionic SS and high I$_{60}$ (current where SS becomes 60 mV/dec) [2]. Heterojunction (HJ) TFETs bear promise to deliver high I$_{60}$, but experimental results do not meet theoretical expectations due to interface problems in the HJs constructed from different materials. Here, we report a natural HJ-TFET with spatially varying layer thickness in black phosphorus (BP) without interface problems. We achieved record-low average SS over 4–5 decades of current, SS$_{ave_{4dec}}$ ≈ 22.9 mV/dec and SS$_{ave_{5dec}}$ ≈ 26.0 mV/dec with record-high I$_{60}$ (= 0.65–1 μA/μm), paving the way for the application in low power switches.


Wednesday, March 4, 2020 8:00 AM - 10:00 AM

Session L58 DCP DCOMP DPOLY DCMP: DFT and Beyond VII  
Mile High Ballroom

3B - Alberto Vela, CINVESTAV-IPN - Tag(s): Focus

8:00AM L58.00001: Quasiparticle Energies and Excitation Energies from Ground State DFT Calculations  
[Invited] WEITAO YANG (Presenter), Duke University — The perspectives of fractional charges and fractional spins provide a clear analysis of the errors of commonly used density functional approximations (DFAs). These errors, the delocalization and static correlation error, of popular DFAs lead to diversified problems in present-day density functional theory calculations. To achieve a universal elimination of these two errors, we developed a localized orbital scaling correction (LOSC) framework. The LOSC-DFAs lead to systematically improved results, including the dissociation of ionic species, single bonds, multiple bonds without breaking space or spin symmetry, the band gaps of molecules and polymer chains, the energy and density changes upon electron addition and removal, and photoemission spectra. Comparison of experimental quasiparticle energies for many finite systems with calculations from the GW Green function approach and LOSC shows that LOSC orbital energies achieve slightly better accuracy than the GW calculations with little dependence on the semilocal DFA, supporting the use of LOSC DFA orbital energies to predict quasiparticle energies. This leads the development of the Quasiparticle Energy DFT (QE-DFT) approach to the calculations of excitation energies of the N-electron systems from the ground state DFA calculations of the (N - 1)-electron systems. Results show good performance of QE-DFT for valence excitations with commonly used DFAs with or without LOSC, for Rydberg states only with the use of LOSC-DFA, and the accurate description of conical interactions. This highlights a new and simplest pathway to describe excited states.
We present an efficient self-consistent first-principles computational approach that extends the density functional theory plus on-site interaction (DFT+U) method further to include inter-site Hubbard Coulomb interaction (V). The extended DFT+U +V method is suitable to calculate electronic structures of periodic systems with various interactions with disparate spatial ranges. It has been known that typical computational methods for DFT+U and DFT+U+V require additional set of computations to obtain U and (or) V. In this presentation, we suggest a scheme to compute the Hubbard parameters self-consistently and ab initio without additional computations for a set of parameters of U and V. A few examples of calculations of energy bands for semiconductors and insulators will also be presented.

DFT calculations of defects in transition-metal oxides constitute a challenging task, often requiring advanced methods to ensure a reasonable description of the electronic structure and large supercells to mimic the dilute defect concentration. Several contradicting DFT results were reported for oxygen vacancies (V\text{O}) in SrTiO\text{3} (STO) and were often related to the peculiar properties of STO, which is a d\text{0} transition metal oxide with mixed ionic-covalent bonding. Here, for the first time, we apply the extended Hubbard DFT+U+V approach, including on-site (Ti-3d) as well as inter-site (Ti-3d and O-2p) electronic interactions, to study oxygen-deficient STO with Hubbard U and V parameters computed self-consistently via density-functional perturbation theory. The negligible additional cost of DFT+U+V compared to standard DFT enables the treatment of large supercells, yet the obtained structural and electronic properties agree well with hybrid-functional calculations and experiments. As such, DFT+U+V results in a bandgap and crystal field splitting for STO in good agreement with experiments. In turn, the description of the electronic properties of V\text{O} is improved, with formation energies much less dependent on the cell size compared to DFT+U and in excellent agreement with experiments.
9:00AM L58.00004: Spectral function database for correlated materials using beyond-DFT methods*  SUBHASISH MANDAL (Presenter), KRISTJAN HAULE, KARIN M RABE, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, United States — While DFT or DFT+U methods give quite accurate results for structural parameters in most materials, correct predictions of excited-state properties, even at a qualitative level, and other properties of correlated materials, usually require beyond-DFT methods. The existing materials databases, constructed in the spirit of the Materials Genome Initiative, are built almost exclusively by the DFT method and are thus very often making incorrect predictions for correlated materials. Various beyond DFT methods, such as meta-GGA, hybrid functionals, GW approximation, or dynamical mean-field theory have been developed to describe the electronic structure of correlated materials, but it is unclear how accurate these methods are when applied to a given strongly correlated solid. It is thus of pressing interest to compare their accuracy as applied to different categories of materials, and at the same time, to build the database of beyond-DFT calculations. We discuss a systematic study of these methods on a few training sets of correlated materials such as binary transition-metal oxides, Fe-pnictides & chalcogenides, and transition-metal dichalcogenides, and we compare theoretical predictions with experimental photoemission data, where available.

*NSF DMREF DMR-1629059 & NSF DMREF DMR-1629346.

9:12AM L58.00005: Assessment of excited-state molecular geometries with optimally-tuned range-separated hybrid functionals  BERNHARD KRETZ (Presenter), DAVID ALEXANDER EGGER, Department of Physics, TU Munich — Computational modelling of photochemical processes (e.g., for photocatalysis) requires accurate descriptions of excited-state structural dynamics of the involved molecules. Often, the starting point of such investigations are geometries optimized for the lowest-lying excited state, as obtained in time-dependent density functional theory (TD-DFT) or high-level wave-function methods. While calculations based on TD-DFT are computationally very efficient, they often do not reach the accuracy of computationally more expensive wave-function methods[1]. However, the recently developed class of optimally-tuned range-separated hybrid (OT-RSH) functionals promises to reduce the gap in accuracy[2]. Here, we assess the precision of excited-state geometries obtained with TD-DFT and OT-RSH for a selection of organic molecules. Our focus lies on structural parameters (e.g., bond lengths, bond angles, etc.) of the lowest-excited singlet states, which we compare to high accuracy wave-function data from literature to benchmark our results.

9:24AM L58.00006: Kohn-Sham Density Functional Theory with Complex, Spin-Restricted Orbitals: Accessing a New Class of Densities without the Symmetry Dilemma  JOONHO LEE (Presenter), MARTIN P HEAD-GORDON, University of California, Berkeley — We show that using complex, spin-restricted orbitals in Kohn-Sham (KS) density functional theory allows one to access a new class of densities that is not accessible by either spin-restricted (RKS) or spin-unrestricted (UKS) orbitals [1]. We further show that the real part of a complex RKS (CRKS) density matrix can be nonidempotent when the imaginary part of the density matrix is not zero. Using CRKS orbitals shows significant improvements in the triplet-singlet gaps of a benchmark set, called TS12, for well-established, widely used density functionals. Moreover, it was shown that RKS and UKS yield qualitatively wrong charge densities and spin densities, respectively, leading to worse energetics. We demonstrate that representative modern density functionals show surprisingly no improvement even with a qualitatively more accurate density from CRKS orbitals. To this end, our work not only provides a way to escape the symmetry dilemma whenever there exists a CRKS solution, but also suggests a new route to design better approximate density functionals.


9:36AM L58.00007: "Implementation of imaginary time dependent density functional theory to periodic and noncollinear systems"*  JOHN MCFARLAND (Presenter), Florida State Univ — Recently an alternative to the SCF method for calculating the DFT electronic ground state was proposed that evolves the DFT wave function in imaginary time [1]. One benefit of this new method is that the DFT wave function is guaranteed to lower its energy and eventually reach the ground state with a sufficiently small time step. This avoids the problems in SCF that hinder convergence such as charge sloshing, which can necessitate fractional level filling. We extend imaginary time dependent density functional theory to periodic systems using a modification of the DFT package Quantum ESPRESSO, with the option of noncollinear and DFT+U calculations. We discuss some of the technical aspects of this as well as example systems which converge with this modification but have difficulty with standard implementations of SCF.


*This work was supported in part by the U.S. National High Magnetic Field Laboratory, which is funded by NSF DMR-1157490 and the State of Florida.
PyProcar: A Python library for electronic structure pre/post-processing

UTHPALA HERATH (Presenter), PEDRAM TAVADZE, Physics and Astronomy, West Virginia University, XU HE, ERIC BOUSQUET, Materials Theory, University of Liege, SOBHIT SINGH, Department of Physics and Astronomy, Rutgers University, FRANCISCO MUNOZ, Department of Physics, University of Chile, ALDO H ROMERO, Physics and Astronomy, West Virginia University — We present PyProcar, a Python package providing graphical representations for electronic structure calculations including band structures and Fermi surfaces as a function of atomic and/or s, p, d, f – orbital projected wavefunctions. This is compatible with DFT codes which output band and projection information in the PROCAR format, as done by the VASP and ABINIT codes. PyProcar is particularly suitable for studying atomic effects into the band structure, Fermi surface and spin texture. Aside from spin, orbital and atom projected band structures and Fermi surfaces, PyProcar plots Fermi surfaces which map colors to properties such as the electron velocity, electron-phonon mean path and effective mass. Another existing feature refers to the band unfolding of supercell calculations into predefined unit cells. PyProcar can be conveniently used in either a stand-alone command line mode or a library mode easily accessible through the Python packaging index (pip) and performs tasks with simple commands.

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Wednesday, March 4, 2020 8:00 AM - 10:36 AM

Session L59 DMP: MnBi2Te4 and Related Compounds: Bulk Properties

Mile High Ballroom 3C
Anti-site disorder and competing magnetic ground states of Mn$_{1-x}$Sb$_{0.67}$Te$_4^*$

YAOHUA LIU (Presenter), XIAOPING WANG, JIAQIANG YAN, Oak Ridge National Lab — Intrinsic magnetic topological insulators (TIs) provide a fertile playground to pursue exotic quantum states of matter at ambient conditions, such as the quantum anomalous Hall effect. MnBi$_2$Te$_4$, with the stacking of septuple-layers, has been recently predicted as the first instance of an antiferromagnetic TI, which has triggered intensive studies on related materials. The as-grown MnBi$_2$Te$_4$ is heavily electron-doped and substituting Bi with Sb is expected to fine-tune the Fermi level with little disturbance on the magnetic structure. Interestingly, we have found that the end compound MnSb$_2$Te$_4$, isostructural to MnBi$_2$Te$_4$ at room temperature, can host two dissimilar magnetic ground states with different magnetic wavevectors but similar ordering temperatures from magnetic measurements and single-crystal neutron diffraction (SCND) experiments. Energy-dispersive X-ray spectroscopy and SCND show Mn vacancies and Mn-Sb anti-site disorder in both cases. To explain the results, we consider a model where the sign of the effective inter-septuple-layer coupling becomes sensitive to the Mn-defect concentration on the Sb site.

*This research used resources at SNS, a DOE Office of Science User Facility operated by the ORNL and was partially supported by U.S. DOE, Office of Science, BES, MSED.

Native defects in Antiferromagnetic Topological Insulator MnBi$_2$Te$_4^*$

ZENGLE HUANG (Presenter), Department of Physics and Astronomy, Rutgers University, New Brunswick, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, WEIDA WU, Department of Physics and Astronomy, Rutgers University, New Brunswick — The coupling of topological electronic states and magnetism can lead to various exotic phenomena such as quantum anomalous Hall effect, axion insulating state, etc. Recently, single crystals and thin films of MnBi$_2$Te$_4$ have been successfully synthesized and it has been shown to be a promising candidate of antiferromagnetic topological insulator [1, 2]. It is crucial to understand and control the defects in this material as they affect its electronic and magnetic properties. In this talk, I will present our study of the native defects in single-crystalline MnBi$_2$Te$_4$ using scanning tunneling microscopy (STM). We identify the dominant defects, Mn$_{Bi}$ antisites in the second layer of Bi, which may impact the magnetic properties of MnBi$_2$Te$_4$ [3, 4, 5]. In addition, we observe another interesting defects with pronounced defect states near the conduction band edge.


*This work is supported by NSF DMR-1506618.
Magnetism in MnBi$_2$Te$_4$ and related compounds

JIAQIANG YAN
(Presenter), ANDREW MAY, MICHAEL MCGUIRE, YAOHUA LIU, BRIAN SALES, Oak Ridge National Lab — MnBi$_2$Te$_4$ has been extensively investigated recently as the first intrinsic antiferromagnetic topological insulator. This compound also shows a strong correlation between structural, magnetic, and transport properties. In this talk, I will present our work on how the stacking of septuple (MnBi$_2$Te$_4$) and quintuple (Bi$_2$Te$_3$) layers, chemical doping, high pressure, and antisite defects affect the magnetic properties. I will also discuss how these results can guide us fine-tuning the magnetism for desired topological phenomena.

*Work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

MnBi$_{2n}$Te$_{3n+1}$: from intrinsic antiferromagnetic to ferromagnetic topological insulators

NI NI (Presenter), University of California, Los Angeles — Magnetic topological insulators provide an important materials platform to explore emergent quantum phenomena. Recently, MnBi$_2$Te$_4$ was discovered to be the first material realization of a van der Waals (vdW) antiferromagnetic topological insulator (TI). In the two-dimensional (2D) limit, at a record high temperature of 4.5 K, MnBi$_2$Te$_4$ manifests the QAH effect in the forced ferromagnetic state above 12 T [1]. To realize the QAH effect at lower fields or even zero field, it is essential to search for ferromagnetic TIs or antiferromagnetic TIs with lower saturation fields. By reducing the interlayer magnetic exchange interaction through our rational design of the natural heterostructure consisting of the building blocks of [MnBi$_2$Te$_4$] septuple layers and [Bi$_2$Te$_3$] quintuple layers, I will show that this family of materials can be tuned from antiferromagnetic to ferromagnetic, providing a superior material platform to investigate various emergent phenomena arising from the interplay between magnetism and band topology [2,3].


*Work at UCLA was supported by DOE, Office of Basic Energy Sciences under Award Number DE-SC0011978.
8:48AM L59.00005: Ferromagnetic van der Waals compound MnSb\(_{1.8}\)Bi\(_{0.2}\)Te\(_4\)  YANGYANG CHEN, YA-WEN CHUANG (Presenter), SENG HUAT LEE, YANGLIN ZHU, KEVIN HONZ, YINGDONG GUAN, YU WANG, KE WANG, ZHIQIANG MAO, Pennsylvania State University, COLIN HEIKES, PATRICK QUARTERMAN, National Institute of Standards and Technology, PAWEL ZAJDEL, University of Silesia, JULIE ANN BORCHERS, WILLIAM RATCLIFF, National Institute of Standards and Technology, JUN ZHU, Pennsylvania State University — The coexistence of topology and magnetism in the same material offers the possibility to realize novel quantum phenomena such as the quantum anomalous Hall effect. Van der Waals magnetic compounds in the form of MnSb\(_x\)Bi\(_{2-x}\)Te\(_4\) are promising candidates. In this work, we show that a Sb-rich composition MnSb\(_{1.8}\)Bi\(_{0.2}\)Te\(_4\) exhibits a ferromagnetic ground state below a Curie temperature of 26 K, in contrast to antiferromagnetic states found in previous studies of this compound family. Magneto-transport measurements are performed on flakes that are ~100 nm thick and prepared in an argon atmosphere. At low temperature, pronounced hysteresis is observed in magnetic field sweeps of \(R_{xy}\) and \(R_{xx}\). A remnant magnetization of \(M_0 = 0.6 \mu_B/Mn\), is extracted from bulk magnetization measurements. The presence of a major ferromagnetic phase is further confirmed by neutron diffraction studies. An excess signal beyond the conventional anomalous Hall effect is observed at \(T < 12\) K. We discuss the implications of our results.

9:00AM L59.00006: Stability subtlety of layered magnetic topological insulator MnBi\(_2\)Te\(_4\)*  JINLIANG NING (Presenter), Physics and Engineering Physics, Tulane University, YANGLIN ZHU, ZHIQIANG MAO, Department of Physics, Pennsylvania State University, JIANWEI SUN, Physics and Engineering Physics, Tulane University — Ab initio description of two dimensional magnetic materials (2DMM) thermodynamics faces great challenges, due to the coexistence of different kinds of chemical bonding, as well as coupling between charge, lattice, and spin degrees of freedom. As an illustration of such challenges, we investigated the metastability of a layered magnetic material MnBi\(_2\)Te\(_4\), which hosts the intrinsic quantum anomalous Hall effect but the crystal itself is hard to synthesize. We calculated the reaction free energy of Bi\(_2\)Te\(_3\)+MnTe→MnBi\(_2\)Te\(_4\), considering electron, vibration and magnetic contributions based on state-of-the-art SCAN+rVV10\(^1\) total energy calculations. We found MnBi\(_2\)Te\(_4\) to be stable only within a short high temperature range, consistent with experiments. Fundamental interactions including SOC effect, vdW interaction, 2D weak magnetism and lattice vibration all contribute subtly to the high-temperature stability of MnBi\(_2\)Te\(_4\), which exemplify that interplay of topology and magnetism can contribute to the stability of the material hosting it. These findings and methods pave a way for future high throughput discovery of novel 2DMM.


*This study was supported by DOE DE-SC0014208.
9:12AM L59.00007: Magnetic structure evolution in the Mn(Bi,Sb)$_2$Te$_4$ family of intrinsic magnetic topological insulators  COLIN HEIKES (Presenter), PATRICK QUARTERMAN, National Institute of Standards and Technology, YANGYANG CHEN, YA-WEN CHUANG, SENG HUAT LEE, YANGLIN ZHU, KEVIN HONZ, YINGDONG GUAN, YU WANG, Physics, The Pennsylvania State University, KE WANG, Materials Research Institute, The Pennsylvania State University, ZHIQIANG MAO, JUN ZHU, Physics, The Pennsylvania State University, PAWEL ZAJDEL, Institute of Physics, University of Silesia, JULIE ANN BORCHERS, WILLIAM RATCLIFF, National Institute of Standards and Technology — The Mn(Bi,Sb)$_2$Te$_4$ family of intrinsic magnetic topological insulators has been predicted to be an ideal platform to realize a high temperature quantum anomalous Hall state, an axion insulating state, as well as a variety of other non-trivial band topologies. The strong coupling between the magnetic ordering in these compounds and the details of their band structure makes understanding their magnetic structure and its evolution with chemistry and magnetic field critical for understanding these exotic states. Our prior work has demonstrated that the field driven spin canting in MnBi$_2$Te$_4$ drives the measured intrinsic anomalous Hall effect in that compound but there are many questions to be addressed about the details of the evolution of the magnetic phase diagram in this system as the Bi atoms are replaced with Sb [1]. Prior magnetometry and magnetotransport shows a clear bulk magnetic behavior change with increased Sb content, but the microscopic details of this evolution are unclear [2]. We will present structural and magnetic neutron scattering measurements and other magnetic characterization of the Mn(Bi,Sb)$_2$Te$_4$ family of compounds to clarify this evolution.


9:24AM L59.00008: Single Crystal Study of Magnetic Topological Material MnBi$_{2x}$Te$_{3x+1}$.  
JOSHUA WAKEFIELD (Presenter), TAKASHI KURUMAJI, TAKEHITO SUZUKI, JOSEPH G CHECKELSKY, Massachusetts Institute of Technology MIT — MnBi$_2$Te$_4$ has emerged as the first stoichiometric antiferromagnetic topological insulator [1]. In thin flakes, MnBi$_2$Te$_4$ has shown remarkable properties including the quantum anomalous Hall (QAH) effect [2]. We investigate the single crystal growth and transport properties of other members of the MnBi$_{2x}$Te$_{3x+1}$ family and find both temperature and low field dependent crossovers from A-type antiferromagnetism to ferromagnetism in MnBi$_4$Te$_7$, suggesting MnBi$_4$Te$_7$ as another candidate for QAH effects in zero external field. We discuss the anomalous Hall response in relation to the magnetic structure, and dependence of the transport properties on angle of the external magnetic field.

MnBi$_{2n}$Te$_{3n+1}$

LEI DING (Presenter), Neutron Scattering Division, Oak Ridge National Laboratory, CHAOWEI HU, Department of Physics and Astronomy and California NanoSystems Institute, University of California, FENG YE, ERXI FENG, Neutron Scattering Division, Oak Ridge National Laboratory, NI NI, Department of Physics and Astronomy and California NanoSystems Institute, University of California, HUIBO CAO, Neutron Scattering Division, Oak Ridge National Laboratory — We present a systematic investigation of the crystal structure and magnetism of van der Waals topological insulators MnBi$_{2n}$Te$_{3n+1}$ (n = 1, 2) using single-crystal neutron diffraction, where emergent quantum phenomena have been recently observed. We show unambiguously that MnBi$_{2}$Te$_{4}$ orders antiferromagnetically below 24 K featured by a magnetic symmetry $R_f$-3c while MnBi$_{4}$Te$_{7}$ is antiferromagnetically below 13 K with a distinct magnetic space group $P_c$-3c1. They both present antiferromagnetically coupled ferromagnetic layers with spins along the c-axis. Further, we put forward a stacking rule for the crystal structure of an infinitely adaptive series MnBi$_{2n}$Te$_{3n+1}$ with the building unit of [Bi$_2$Te$_3$]. This enables us to draw that a two-dimensional magnetism limit might be realized in the derivatives. Our work may promote the theoretical predictions of exotic quantum states in the series of MnBi$_{2n}$Te$_{3n+1}$.

*The research at Oak Ridge National Laboratory (ORNL) was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Early Career Research Program Award KC0402010, under Contract DE-AC05-00OR22725 and the U.S. DOE, Office of Science User Facility operated by the ORNL.
Large intrinsic anomalous Hall effect in hole-doped ferromagnetic phase MnSb$_x$Bi$_{2-x}$Te$_4$*  

SENG HUAT LEE (Presenter), 2D Crystal Consortium, Materials Research Institute, Pennsylvania State University, University Park, Pennsylvania 16802, USA, YANGLIN ZHU, Department of Physics, Pennsylvania State University, University Park, Pennsylvania 16802, USA, LUJIN MIN, VERLINDE KATRINA, JINGYANG HE, Department of Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania, 16802, USA, DAVID E GRAF, National High Magnetic Field Lab, Tallahassee, FL 32310, USA, RONALD REDWING, Department of Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania, 16802, USA, ZHIQIANG MAO, Department of Physics, Pennsylvania State University, University Park, Pennsylvania 16802, USA — MnBi$_2$Te$_4$, an intrinsic magnetic topological insulator, has recently been predicted to possess a variety of topological quantum states, including quantum anomalous Hall insulator, axion insulator in its 2D thin layers and an ideal Weyl semimetal state in its bulk ferromagnetic (FM) phase$^{1,2}$. Although several interesting properties, including Chern insulator, axion insulator, and anomalous Hall effect (AHE) in its canted antiferromagnetic phase have been observed, the predicted FM Weyl state remains elusive$^{3-5}$. In this talk, we will report our magnetotransport studies on MnSb$_x$Bi$_{2-x}$Te$_4$. We will show when the Sb concentration is tuned to be close to a critical concentration where carrier density reaches a minimum, the FM phase under a high field range exhibits a large intrinsic AHE with the anomalous Hall angle reaching 5%. Moreover, the carrier mobility also reaches a maximum at the critical concentration. All these features are possibly associated with the long-sought ideal Weyl state.

3Y. Deng et al., arXiv:1904.11468
4C. Liu et al., arXiv:1905.00715

*The study at PSU 2DCC-MIP is supported by NSF Cooperative Agreement No. DMR-1539916.
10:00AM L59.00011: Quantum Oscillations in Intrinsic Magnetic Topological Insulator MnBi$_{2-x}$Sb$_x$Te$_4$*

QIANNI JIANG (Presenter), ZAIYAO FEI, TIANCHENG SONG, University of Washington, JIAQIANG YAN, Oak Ridge National Laboratory, PAUL MALINOWSKI, ZHAOYU LIU, University of Washington, DAVID E GRAF, National High Magnetic Field Laboratory, XIAODONG XU, JIUN-HAW CHU, University of Washington — The recently discovered first intrinsic antiferromagnetic (AFM) topological insulator (TI) MnBi$_2$Te$_4$ is expected to possess various exotic quantum states including axion insulator and quantum anomalous Hall effect. The band structure portrayed by ARPES measurements reveals nontrivial topology, but claims regarding the surface states are still controversial. When Bi is substituted by Sb, the material crosses a bulk charge neutrality point, from being electron-doped to hole-doped. By applying a magnetic field, it is possible to realize a magnetic Weyl semimetal phase by switching the AFM phase to the FM phase through a metamagnetic transition at B ~ 6T. Here, we present Shubnikov–de Haas oscillations of both electron and hole-doped MnBi$_{2-x}$Sb$_x$Te$_4$ in the FM state and trace its evolution as a function of chemical doping, providing the first measurement of the band structures of MnBi$_{2-x}$Sb$_x$Te$_4$ in the FM state.

*This work is supported as part of Programmable Quantum Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under award DE-SC0019443.

10:12AM L59.00012: Optimization of the intrinsic magnetic topological insulator MnBi$_2$Te$_4$ and transport study

FENGQI SONG (Presenter), Nanjing Univ — Magnetic topological insulators (MTIs) offer a combination of topologically nontrivial characteristics and magnetic order and show promise in terms of potentially interesting physical phenomena such as quantum anomalous Hall (QAH) effect. However, the understanding of their properties and potential applications have been limited due to a lack of suitable MTIs. Here, we grow single crystals of Mn(Sb,Bi)$_2$Te$_4$ to search for intrinsic MTIs. We perform angle-resolved photoemission spectroscopy, transport measurements, and first-principles calculations to investigate the band structure, transport properties, and magnetism, as well as the evolution of their topological properties. We find that there exists an optimized MTI zone in the Mn(Sb,Bi)$_2$Te$_4$ phase diagram, which could possibly host a high-temperature QAH phase. We also report the reserved anomalous Hall effect (AHE) in the MnBi$_2$Te$_4$ thin film. By employing the top/bottom gate, a negative AHE loop gradually decreases to zero and changes to a reversed sign. The reversed AHE exhibits distinct coercive fields and temperature dependence from the previous AHE. It reaches the maximum inside the gap of the Dirac cone. The reversed AHE is attributed to the competition of intrinsic Berry curvature and extrinsic skew scattering.
Magnetotransport properties in MnBi$_{2n}$Te$_{3n+1}$

**CHAOWEI HU** (Presenter), JINYU LIU, SCOTT MACKEY, NI NI, University of California, Los Angeles — Recently, magnetic topological insulators MnBi$_{2n}$Te$_{3n+1}$ were discovered, where quantized anomalous hall resistance was observed in the two-dimensional limit of MnBi$_2$Te$_4$ at a record high temperature of 4 K under 12 T, providing an important material platform to explore emergent quantum phenomena such as quantized anomalous Hall effect and Majorana modes, etc. MnBi$_{2n}$Te$_{3n+1}$ family is made of alternating one septuple [MnBi$_2$Te$_4$] and (n-1) quintuple [Bi$_2$Te$_3$] layers, where the interlayer magnetic couplings are tuned systematically with increasing n. In this talk, we will show our recent results on the magnetotransport properties in MnBi$_{2n}$Te$_{3n+1}$, shedding light on the interplay between magnetism and band topology.

*Work at UCLA was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0011978.

Intrinsic magnetic topological states in MnBi$_2$Te$_4$ family

**JING WANG** (Presenter), Fudan Univ — Here, we first predict the tetradymite-type compound MnBi$_2$Te$_4$ and its related materials host topologically nontrivial magnetic states. The magnetic ground state of MnBi$_2$Te$_4$ is an antiferromagnetic topological insulator state with a large topologically non-trivial energy gap (0.2 eV). It presents the axion state, which has gapped bulk and surface states, and the quantized topological magnetoelectric effect. It has several advantages over the previous proposals on realizing the topological magnetoelectric effect. The intrinsic magnetic and band inversion further lead to quantum anomalous Hall effect in odd layer MnBi$_2$Te$_4$ thin film with combined inversion and time-reversal symmetry breaking, which has been recently observed in experiments. The high quality intrinsic MnBi$_2$Te$_4$ together with other magnetic/superconducting 2D materials provides fertile ground for exploring exotic topological quantum phenomena.

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Pressure-tuned interlayer coupling of the magnetic topological insulators MnBi$_2$Te$_4$(Bi$_2$Te$_3$)$_n$ (n=1,2)

**JIFENG SHAO** (Presenter), XIAO-MING MA, JINGYUAN LI, YICHEN SUN, RUI'E LU, MENG ZENG, YIJIE HAO, CHANG LIU, QIHANG LIU, YUE ZHAO, Southern University of Science and Technology — Magnetic topological insulators with nontrivial topological band structure and broken time-reveal symmetry provide an ideal platform for exploring exotic quantum phenomena, such as quantum anomalous Hall effect (QAHE), axion insulator state and Majorana mode. Recently, MnBi$_2$Te$_4$ was discovered as the first intrinsic antiferromagnetic topological insulator. However, due to the large antiferromagnetic interlayer coupling, strong external magnetic field is needed to fully polarize the magnetic moment to achieve QAHE. By inserting one or two Bi$_2$Te$_3$ layers into the adjacent MnBi$_2$Te$_4$ septuple layers, the antiferromagnetic interlayer coupling can be greatly reduced. Using hydrostatic pressure to further modulate the interlayer interaction, we study the transport properties of the MnBi$_2$Te$_4$(Bi$_2$Te$_3$)$_n$ (n=1,2) bulk crystals and investigate the pressure tuned interlayer coupling in detail.
8:00AM L60.00001: Towards Material realizations of 2D Topological Superconductivities in \( \text{Pb}_{1-x}\text{Bi}_x \) Systems* [Invited] WEI QIN (Presenter), University of Science and Technology of China — New material realization of two-dimensional (2D) topological superconductors (TSCs) can provide new platforms for experimentally detecting and manipulating Majorana quasiparticles, which in pairs serve as an exotic entity for nonlocal encoding of quantum information [1]. In this talk, I will focus possibilities of realizing 2D intrinsic topological superconductivity in a new material family, namely atomic-layer-thin \( \text{Pb}_{1-x}\text{Bi}_x \) alloys. Based on first-principles calculations, three nearly energetically degenerate structural configurations of the prototypical system \( \text{Pb}_3\text{Bi} \) grown on a Ge substrate are identified and labeled respectively as \( T_1, H_3 \) and \( T_4 \) [2]. All three structures possess large Rashba energy band splittings and van Hove singularities (VHS) in the density of states. With proper tensile strains, \( H_3 \) and \( T_4 \) configurations are demonstrated to have nontrivial band topology characterized by topological edge states. To investigate the superconductivity, an effective formalism that respects hexagonal symmetry, Rashba splitting, VHS and electron-electron interactions is developed with parameters obtained from first-principles calculations. Our renormalization group analysis shows that a chiral \( p \)-wave superconducting phase dominates over other competing orders. Given these results, we identify hole-doped \( \text{Pb}_3\text{Bi}/\text{Ge}(111) \) as an appealing platform for realizing intrinsic 2D topological superconductivity [3].

*Supported by NSF of China

8:36AM L60.00002: Volkov-Pankratov states in two-dimensional topological superconductors DAVID ALSPAUGH (Presenter), DANIEL E SHEEHY, Louisiana State University, Baton Rouge, MARK OLIVER GOERBIG, PASCAL SIMON, Laboratoire de Physique des Solides, Université Paris-Sud — We study the in-gap states that appear at the boundaries of two-dimensional topological superconductors. While the massless chiral Majorana quasiparticles are guaranteed to arise by the bulk-edge correspondence, we find that they could be accompanied by massive Volkov-Pankratov (VP) states which are present only when the interface is sufficiently smooth. These predictions can be tested in an s-wave superconductor with strong Rashba spin-orbit coupling placed on top of a magnetic domain wall. We calculate the spin-resolved local density of states of the VP states about the band inversion generated by a magnetic domain wall and find that they are oppositely spin-polarized on either side of the topological phase boundary. We also demonstrate that the spatial position, energy-level spacing, and spin polarization of the VP states can be modified by the introduction of in-plane electric fields.
8:48AM L60.00003: Unconventional superconductivity in a doped quantum spin Hall insulator*  DOMENICO DI SANTE (Presenter), XIANXIN WU, MARIO FINK, WERNER R HANKE, RONNY THOMALE, Institut für Theoretische Physik und Astrophysik, University of Würzburg — A monolayer of jacutingaite (Pt$_2$HgSe$_3$) has recently been identified as a novel quantum spin Hall insulator. By first-principles calculations, we study its Fermiology in the doped regime and unveil a type-I and type-II van Hove singularity for hole and electron doping, respectively. We find that the common link between the propensity for a topological band gap at pristine filling and unconventional superconductivity at finite doping roots in the longer ranged hybridization integrals on the honeycomb lattice. In a combined effort of random phase approximation and functional renormalization group, we find chiral d-wave order for the type-I and odd-parity f-wave order for the type-II regime.


*This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258499086 – SFB 1170 (Project B06) and by the Dresden-Würzburg Center for Topological Quantum Matter Research (ct.qmat).

9:00AM L60.00004: Majorana zero modes by engineering topological kink states in two dimensional electron gas  SHUGUANG CHENG, Department of Physics, Northwest University, China, JIE LIU, Department of Applied Physics, School of Science, Xi’an Jiaotong University, China, HAIWEN LIU, Center for Advanced Quantum Studies, Department of Physics, Beijing Normal University, China, HUA JIANG (Presenter), School of Physical Science and Technology, Soochow University, China, QING-FENG SUN, XINCHENG XIE, International Center for Quantum Materials, School of Physics, Peking University, China — Majorana zero modes (MZMs)–bearing potential applications for topological quantum computing are verified in quasi-one-dimensional (1D) Fermion systems, including semiconductor nanowires, magnetic atomic chains, planar Josephson junctions. However, the existence of multibands in these systems makes the MZMs fragile to the influence of disorder. Moreover, in practical perspective, the proximity induced superconductivity may be difficult and restricted for 1D systems. Here, we propose a flexible route to realize MZMs through 1D topological kink states by engineering a 2D electron gas with antidot lattices, in which both the aforementioned issues can be avoided owing to the robustness of kink states and the intrinsically attainable superconductivity in high-dimensional systems. The MZMs are verified to be quite robust against disorders and the bending of kink states, and can be conveniently tuned by varying the Rashba spin-orbit coupling strength. Our proposal provides an experimental feasible platform for MZMs with systematic manipulability and assembleability based on the present techniques in 2D electron gas system.
Transport properties of Majorana-Josephson interferometer

**CHANG-AN LI** (Presenter), **JIAN LI**, School of Science, Westlake University, **SHUN-QING SHEN**, Department of Physics, The University of Hong Kong — We study the transport properties of Majorana-Josephson interferometer, which is consisted of a two-terminal quantum anomalous Hall insulator strip with two superconducting bars grown over it, to showcase the interference nature of chiral Majorana modes. In this Majorana-Josephson interferometer, the interference effect is caused by a Majorana valve between two topological superconductors that form a Josephson junction. Its transport observables exhibit interference patterns depending on the Josephson phase as well as the junction length. We also show that the interference patterns are robust against weak disorder while strong dephasing effect destroys them. Interestingly, a Majorana-Josephson interferometer can work as two effectively separated Mach-Zennder interferometers, and it is even able to detect the Z2 phase of quantum vortices in topological superconductors. Experimental observation of these interference patterns will probe the topological superconducting phase in related systems and may pave a path for their further manipulations in topological quantum computation.

*C.A.L. and J.L. acknowledges support from NSFC under Project 11774317. S.Q.S. were partially supported by the RGC, UGC, Hong Kong under Grant No. 17301717.*

Josephson Interferometry of Zig-Zag Junctions Demonstrating Enhanced Localization

**ANDREW SAYDJARI** (Presenter), **ANDREW PIERCE**, **HECHEN REN**, **MICHAEL KOSOWSKY**, Harvard University, **CHRISTOPHER AMES**, **MARTIN STENHO**, **LAURENS W MOLENKAMP**, University of Wurzburg, **AMIR YACOBY**, Harvard University — Josephson junctions on mercury telluride quantum wells combine strong spin-orbit effects, s-wave superconductivity, and arbitrary lithographic design. This platform facilitates both the study of induced superconductivity in the quantum well and topological states in quasi-1D systems. While zero bias peaks have been observed in these quasi-1D systems, small topological gaps and poor confinement of the 0-D topological states makes their assignment as Majorana fermions challenging. Recent theoretical work suggests an order of magnitude enhancement in the topological gap and localization when the Josephson junction is fabricated in a zig-zag geometry [1]. In this work, we provide the first characterization of zig-zag geometry junctions and demonstrate enhanced localization of electrons within the junction.


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9:36AM L60.00007: Magnetic Skyrmion Induced Topological Superconductivity
ERIC MASCOT (Presenter), DIRK KLAUS MORR, Univ of Illinois - Chicago — Magnetic skyrmions are a stable topological spin texture found in magnetic materials with Dzyaloshinskii-Moriya interactions. These skyrmions are highly controllable and can be written and deleted using spin polarized currents [1] and varied in size from 1 nm to 100 nm [2] by controlling material properties such as thickness or doping [3].

Here, we investigate magnet-superconductor heterostructures in which the presence of a magnetic skyrmion lattice gives rise to the emergence of topological superconductivity. We demonstrate that tuning between different topological phases can be achieved by varying the size of the skyrmions, the magnetic exchange coupling, and the chemical potential. We also show that the presence of magnetic skyrmions gives rise to a characteristic spatial structure of chiral Majorana edge modes, and of the induced superconducting triplet correlations, which can be probed experimentally.


*This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-FG02-05ER46225.

9:48AM L60.00008: Tuning Shiba states hybridization on proximitized superconducting surface
HAO DING (Presenter), YUWEN HU, Princeton University, SILAS HOFFMAN, University of Basel, MALLIKA RANDERIA, Princeton University, OINDRILA DEB, JELENA KLINOVAJA, DANIEL LOSS, University of Basel, ALI YAZDANI, Princeton University — Magnetic atoms on a superconductor induce in-gap Shiba states that can be hybridized to create a topological superconducting phase when placed in one-dimensional chains, with Majorana zero modes (MZMs) localized at their ends. Here we study magnetic Gd adatoms deposited on the surface of epitaxially grown Bi(110) thin films on a superconducting Nb(110) surface using a dilution refrigerator scanning tunneling microscope (STM). Our spectroscopic measurements show a hard superconducting gap of 1.5 meV on Bi surface and the presence of Shiba states near Gd atoms. By manipulating Gd atoms with the STM tip, we find the Shiba states start hybridizing once two Gd atoms are closer than Fermi wavelength of Bi(110) surface states (~ 20 Å), which indicates the critical role of RKKY interaction mediated by Bi electrons. Through systematically changing the configurations of two Gd atoms, we show the hybridization can be dramatically strengthened as the distance between Gd atoms decreases. Our work provides a promising platform for realizing MZMs because it allows fine control over Shiba states hybridization.

*This work is supported by grants from the ONR, Moore foundation, NSF-DMR, and NSF-MRSEC.
10:00AM L60.00009: RKKY-induced magnetic transition for pairs of magnetic atoms on proximitized superconducting surface* YUWEN HU (Presenter), HAO DING, Department of Physics, Princeton University, SILAS HOFFMAN, Department of Physics, University of Basel, MALLIKA RANDERIA, Department of Physics, Princeton University, OINDRILA DEB, JELENA KLINOVAYA, DANIEL LOSS, Department of Physics, University of Basel, ALI YAZDANI, Department of Physics, Princeton University — An atomic chain with helical spin texture proximitized by an s-wave superconductor can harbor topological superconductivity that gives rise to Majorana zero modes (MZMs) localized at its both ends. Understanding the exchange interaction between magnetic atoms on a superconducting surface is the key to realizing helical spin chains and MZMs. Here we use atomic manipulation to build magnetic Gd dimers on proximitized superconducting Bi(110) surface with a dilution refrigerator scanning tunneling microscope (STM). By measuring the in-gap Shiba states induced by magnetism of Gd dimers, we find the magnetic ground state of Gd dimers changes from out-of-plane ferromagnetic to in-plane antiferromagnetic and then to in-plane ferromagnetic phase as a function of the distance between two Gd atoms. The Shiba states splitting behavior in the in-plane ferromagnetic state suggests the exchange interaction between two Gd atoms is dominated by RKKY interaction. Finally, by taking magnetic anisotropy, spin-orbit coupling and RKKY interaction into account, we propose a theoretical model that can describe this system.

*This work is supported by grants from the ONR, Moore foundation, NSF-DMR, and NSF-MRSEC.

10:12AM L60.00010: Topological superconductivity of adatom chains as probe for unconventional pairing ANDREAS KREISEL (Presenter), Institute for Theoretical Physics, University of Leipzig, TIMO HYART, International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, BERND ROSENOW, Institute for Theoretical Physics, University of Leipzig — Chains of magnetic atoms on the surface of s-wave superconductors, have been established as a laboratory for the study of Majorana bound states. In such systems, the breaking of time reversal due to magnetic moments makes the system a one-dimensional topological superconductor. However, in unconventional superconductors even non-magnetic impurities can induce in-gap states since scattering of Cooper pairs changes their momentum but not their phase. Here, we propose a novel paradigm for creating topological superconductivity, which is based on an unconventional superconductor with a chain of non-magnetic impurities on its surface. The system can be driven into the topological phase by tuning magnitude and direction of an external Zeeman field. We show that the topological energy gap can approach the minimum of the bulk energy gap. We develop a general mapping of films with impurity chains in multiband superconductors to one-dimensional lattice Hamiltonians. This allows us to illustrate the feasibility of our proposal in the case of the material Sr$_2$RuO$_4$, and to demonstrate that the study of impurity chains can be employed as a diagnostic tool for the nature of the pairing symmetry. This enables to distinguish competing proposals for the pairing symmetry in Sr$_2$RuO$_4$. 
10:24AM L60.00011: New classification of topological superconductors in 1D magnetic groups*  JINYU ZOU, Huazhong University of Science & Technology, ZHIDA SONG, Princeton University, GANG XU (Presenter), Huazhong University of Science & Technology — Topological superconductors (TSCs) with Majorana zero modes (MZMs) and their potential application in topological quantum computation have become an important area in condensed matter physics. Their topological classification with crystalline symmetries is an important and useful question for finding the possible TSC materials. We have classified the TSC phase in 1D system with local crystalline time reversal symmetry (LCTRS), where the time reversal symmetry (TRS) is broken, but the combination of TRS with some local crystalline symmetry is preserved. The LCTRS $M_x T$ or $C_{2z} T$ will lead to an effective BDI symmetry class which has a $Z$ classification. The case of LCTRS $C_{4z} T$ ($C_{6z} T$) are not included in the Altland and Zirnbauer (AZ) symmetry classes, and exhibit the $Z (Z + Z)$ classification TSC phase with the robust MZMs protected by the unitary chiral symmetry, which is different from the previously studied TSCs in BDI, DIII and D classes. We also present a minimal BdG Hamiltonian with $C_{4} T$ or $C_{6} T$ symmetry to illustrate the novel TSC phase.

*The authors thank the support from the MOST and NSFC, the Thousand Young Talents Program, and cooperation with Princeton University.

10:36AM L60.00012: Topological Superconductivity Intertwined with Broken Symmetries*  HUI-KE JIN (Presenter), Zhejiang Univ, YI ZHOU, Institute of Physics, DONG-HUI XU, Department of Physics, Hubei University — Recently the superconductor and topological semimetal PbTaSe2 was experimentally found to exhibit surface-only lattice rotational symmetry breaking below Tc . We exploit the Ginzburg-Landau free energy and propose a microscopic two-channel model to study possible superconducting states on the surface of PbTaSe2 . We identify two types of topological superconducting states. One is time-reversal invariant and preserves the lattice hexagonal symmetry while the other breaks both symmetries. We prove that for a C3v lattice with spatial inversion symmetry breaking and strong spin-orbit coupling, the time reversal symmetry must be broken and the only way to lead a nematic superconductor is the mixing of 1D and 2D irreducible representation superconducting states.

*National Key Research and Development Program of China (No.2016YFA0300202), National Natural Science Foundation of China (No. 11774306, No. 11704106), the Strategic Priority Research Program of Chinese Academy of Sciences (No. XDB28000000), Chutian Scholars Program in Hubei Province.
**8:00AM L61.00001: Electronic Nematicity in FeSe** [Invited] MING YI (Presenter), Rice University — Superconductivity emerges in proximity to a nematic phase in most iron-based superconductors. It is therefore important to understand the impact of nematicity on the electronic structure. Orbital assignment and tracking across the nematic phase transition proved to be challenging due to the multiband nature of iron-based superconductors and twinning effects. Here we report a detailed study of the electronic structure of fully detwinned FeSe across the nematic phase transition using angle-resolved photoemission spectroscopy. We clearly observe a nematicity-driven band-reconstruction involving dxz, dyz and dxy orbitals. The nematic energy scale between dxz and dyz bands reach a maximum of 50meV at the Brillouin zone corner. We are also able to track the dxz electron pocket across the nematic transition and explain its absence in the nematic state. Our comprehensive data of the electronic structure provide an accurate basis for theoretical models of the superconducting pairing in FeSe.

**8:36AM L61.00002: Evolution of soft phonons in FeSe under pressure** ADRIAN MERRITT (Presenter), Physics, University of Colorado, Boulder, FRANK WEBER, ANNA BOEHMER, KAUSHIK SEN, JOHN-PAUL CASTELLAN, THOMAS WOLF, Institute for Solid State Physics, Karlsruhe Institute of Technology, SOFIA MICHAELA SOULIOU, European Synchrotron Radiation Facility, AHMET ALATAS, AYMAN SAID, Advanced Photon Source, Argonne National Laboratory, WENLI BI, University of Alabama - Birmingham, RAFAEL FERNANDES, University of Minnesota, DMITRY REZNIK, Physics, University of Colorado, Boulder — FeSe, as the simplest iron-based superconductor (Fe-SC), is of great interest for furthering our understanding of the Fe-SC materials. It shares a common tetragonal-to-orthorhombic phase transition at 90 K with many of the Fe-SCs, and becomes superconducting at 9 K, but in contrast displays no magnetic order. Previous studies have shown an enhancement of the superconducting transition temperature with increasing pressure, with a maximum of 37 K at approximately 6.3 GPa, and magnetic order concurrent with the structural transition above 1.6 GPa. Here we present IXS measurements of TA phonon dispersion from which we can extract the nematic correlation length. The phonon renormalization effects observed in our experiments have important implications for nematicity and superconductivity. This includes a significant reduction in the phonon softening at the high-pressure structural-magnetic transition and a new phonon hardening effect at the superconducting transition. We will discuss the implications of these results in the context of pressure- and doping-dependence in the Fe-SCs.

*DOE, Office of Basic Energy Sciences, Office of Science, Contract No. DE-SC0006939 (AM & DR) European Synchrotron Radiation Facility, Grenoble, France Advanced Photon Source, Argonne National Laboratory, USA*
8:48AM L61.00003: Observation of intra-unit-cell nematic order in epitaxial bilayer FeSe films on SrTiO$_3$(001)  

HUIMIN ZHANG (Presenter), Department of Physics and Astronomy, West Virginia University, ZHUOZHI GE, Department of Physics, University of Wisconsin-Milwaukee, QIANG ZOU, Department of Physics and Astronomy, West Virginia University, MICHAEL WEINERT, Department of Physics, University of Wisconsin-Milwaukee, LIAN LI, Department of Physics and Astronomy, West Virginia University — Epitaxial FeSe thin films provide an ideal platform to probe the interplay of superconductivity and nematicity, due to the absence of long-range magnetic order. Here, we systematically investigate the nematic order in high quality bilayer FeSe/SrTiO$_3$ films grown by molecular beam epitaxy. Using low temperature scanning tunneling microscopy/spectroscopy, we observe features associated with Se atoms to be elongated along the Fe-Fe lattice direction within a specific energy window, demonstrating symmetry breaking from fourfold to twofold. Detailed analysis of Fourier transformation of the STM images reveals that the intensity of Fe Bragg peak breaks rotational symmetry within each Fe unit cell, indicative of an intra-unit-cell nematicity. Our results provide critical information on nematicity in Fe-based superconductors, an essential element in understanding superconducting transition in these materials.

*This research is supported by DOE (DE-SC0017632).

9:00AM L61.00004: Phonon spectroscopy in FeSe using high-resolution inelastic x-ray scattering  

NAOKI MURAI (Presenter), Materials and Life Science Division, J-PARC Center, Japan Atomic Energy Agency, TATSUO FUKUDA, Materials Sciences Research Center, Japan Atomic Energy Agency, MASAMICHI NAKAJIMA, Department of Physics, Osaka University, MITSUAKI KAWAMURA, Institute for Solid State Physics, The University of Tokyo, DAISUKE ISHIKAWA, Japan Synchrotron Radiation Research Institute, SETSUKO TAJIMA, Department of Physics, Osaka University, ALFRED BARON, RIKEN SPring-8 Center — We report an inelastic x-ray scattering investigation of phonons in FeSe superconductor. Comparing the experimental phonon dispersion with density functional theory (DFT) calculations in the non-magnetic state, we found a significant disagreement between them. Improved overall agreement was obtained by allowing for spin-polarization in the DFT calculations, despite the absence of magnetic order in the experiment. This calculation gives a realistic approximation of the disordered paramagnetic state of FeSe, in which strong spin fluctuations are present. We will discuss the current state of our analysis relating magnetism to the phonon dispersion.
9:12AM L61.00005: Room temperature local nematicity in FeSe superconductor* ROBERT KOCH (Presenter), Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, TATIANA KONSTANTINOVA, Department of Physics and Astronomy, Stony Brook University, MILINDA ABEYKOON, Photon Science Division, Brookhaven National Laboratory, AIFENG WANG, CEDOMIR PETROVIC, YIMEI ZHU, EMIL BOZIN, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, SIMON J L BILLINGE, Columbia University, Department of Applied Physics and Applied Mathematics — We report pair distribution function measurements of the iron-based superconductor FeSe above and below the structural transition temperature. Structural analysis reveals a local orthorhombic distortion with a correlation length of about 4 nm at temperatures where an average tetragonal symmetry is observed. The analysis further demonstrates that the local distortion is larger than the global distortion at temperatures where the average observed symmetry is orthorhombic. Our results suggest that the low-temperature macroscopic nematic state in FeSe forms from an imperfect ordering of orbital-degeneracy-lifted nematic fluctuations which persist up to at least 300 K.

*This work was supported by U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (DOE-BES) under contract No. DE-SC0012704. X-ray PDF measurements were conducted on beamline 28-ID-1 of the National Synchrotron Light Source II, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Brookhaven National Laboratory under Contract No. DE-SC0012704.

9:24AM L61.00006: Observation of layer-dependent \(d_{xz}/d_{yz}\) band splittings in the nematic phase of FeSe/SrTiO\(_3\) films XILIANG PENG (Presenter), Institute of Physics, Chinese Academy of Sciences, KUN JIANG, Boston College, XIANXIN WU, University of Wurzburg, YONGHAO YUAN, Tsinghua University, YAOBO HUANG, Shanghai Synchrotron Radiation Facility, TIAN QIAN, Institute of Physics, Chinese Academy of Sciences, WEI LI, Tsinghua University, JIANGPING HU, Institute of Physics, Chinese Academy of Sciences, ZIQIANG WANG, Boston College, YUJIE SUN, HONG DING, Institute of Physics, Chinese Academy of Sciences — The effect of interlayer coupling on physical properties of layered materials such as iron-based superconductors is an interesting question. Here, we use angle-resolved photoemission spectroscopy to directly observe the electronic structure of FeSe films with different layers grown on SrTiO\(_3\)(001) substrates by \textit{in situ} molecular beam epitaxy. We find two distinct layer-dependent band splittings in the Brillouin zone center and corner, respectively. In the Brillouin zone corner, the band splitting caused by the nematic phase decreases with the increase in the number of layers. On the contrary, the degeneracy of \(d_{xz}/d_{yz}\) bands in double-layer FeSe is lifted in multi-layer films and the band splitting in the Brillouin zone center becomes larger with the increase of film thickness. The results of double-layer FeSe grown on SrTiO\(_3\) favor the proposal of \(d\)-wave nematic order. Our layer-dependent experiments provide limitations for the theoretical study of the nematic phase in FeSe and shed insights for the study of the interplay between nematicity and superconductivity.
9:36AM L61.00007: Nematicity from spin correlations in iron-based superconductors*
RONG YU (Presenter), YIMING WANG, Department of Physics, Renmin University of China, WENJUN HU, Department of Physics and Astronomy, University of Tennessee, Knoxville, QIMIAO SI, Department of Physics and Astronomy, Rice University — Electronic nematic order has been the topic of considerable interest in the area of iron-based superconductors. Motivated by recent experimental works, we study the connection between nematic order and magnetic fluctuations. We show, based on a symmetry analysis, that the spin correlations in the system allow for a variety of nematic orders, in particular an unusual $B_{2g}$ nematicity. Using qualitative considerations as well as microscopic calculations, we discuss the types of magnetic fluctuations that stabilize this $B_{2g}$ nematicity and how our proposed mechanism provides a natural understanding of the recent experimental observations in the heavily hole doped iron pnictides (Rb,Cs)Fe$_2$As$_2$. We also discuss the effects associated with the nematic transition.

*This work has been supported by the National Science Foundation of China, Grant No. 11674392, Ministry of Science and Technology of China, National Program on Key Research Project, Grant No. 2016YFA0300504 (R.Y. and Y.W.) and by the DOE BES Award # DE-SC0018197 and the Robert A. Welch Foundation Grant No. C-1411 (W.H. and Q.S.)

9:48AM L61.00008: Spin nematicity in the local-moment Fe-chalcogenide KFe$_{0.8}$Ag$_{1.2}$Te$_2$ YU SONG (Presenter), University of California, Berkeley — Iron-based superconductors appear in the vicinity of a nematic quantum critical point, and due to the presence of spin, orbital and charge degrees of freedom, nature of the nematic order has been the focus of research in recent years. One route to address this question is to look for clues in related materials that exhibit similar physics. In semiconducting KFe$_{0.8}$Ag$_{1.2}$Te$_2$, an analogue of the archetypical iron pnictide BaFe$_2$As$_2$, we found simultaneous stripe-type magnetic order and nematic order below $T_{S,N}=$35 K, with striking similarities between the two systems. Above $T_{S,N}$, a sizable spin anisotropy develops under a small strain and increase upon cooling towards $T_{S,N}$, indicative of a divergent nematic susceptibility. Since the magnetic susceptibility of KFe$_{0.8}$Ag$_{1.2}$Te$_2$ is well described by the Curie-Weiss law with $S\approx$1, it is a local-moment magnet with orbital degeneracy. The similarities between nematic orders in KFe$_{0.8}$Ag$_{1.2}$Te$_2$ and BaFe$_2$As$_2$ suggest our findings to be relevant for iron-based superconductors, and establish KFe$_{0.8}$Ag$_{1.2}$Te$_2$ as a model system to investigate electronic nematicity in the localized limit.
Exploring the electronic structure of BaFe$_2$As$_2$ using resonant Raman scattering

RUDOLF HACKL (Presenter), ANDREAS BAUM, Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, YING LI, Institute for Theoretical Physics, Goethe University Frankfurt, NENAD LAZAREVIC, Center for Solid State Physics and New Materials, Institute of Physics Belgrade, DANIEL JOST, Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, JIUN-HAW CHU, Department of Physics, University of Washington, IAN FISHER, Geballe Laboratory for Advanced Materials & Dept. of Applied Physics, Stanford University, ROSER VALENTI, Institute for Theoretical Physics, Goethe University Frankfurt, IGOR MAZIN, Code 6393, Naval Research Laboratory — Iron-based materials are characterized by the competition of various phases including magnetism, nematicity, and superconductivity. The interrelation of these instabilities is a key question of both materials science and theoretical modelling. In this study we present light scattering data on twin-free BaFe$_2$As$_2$ as a function of the energy of the incident photons. The phonon intensities display an anisotropy for the polarizations oriented along either the ferro- or the antiferromagnetically ordered direction. This anisotropy makes the fully symmetric As phonon to appear in crossed polarizations. The anomalous intensity and the anisotropy of the spectral weight increase substantially in the blue-green spectral range. The experimental results are analyzed using density functional theory. Qualitative agreement between model calculations and experiment is found if the magnetic order is properly taken into account. The anomalies are fully developed only in the presence of long range magnetic order and are not directly linked to nematicity. Rather they are a high-energy phenomenon indicating that magnetism and nematicity are interrelated.

We acknowledge support by the DFG, the Serbian Ministry of Education, the DAAD, by BaCaTeC, the DOE, the NRL and by the AvH Foundation.

Hidden antiferro-nematic order in BaFe$_2$As$_2$ and NaFeAs above $T_S$

SEIICHIRO ONARI (Presenter), HIROSHI KONTANI, Physics, Nagoya University — In some Fe-based superconductors such as BaFe$_2$As$_2$ and NaFeAs, $C_4$ symmetry breaking emerges at $T^*$, which is tens of Kelvin higher than the structural transition temperature $T_S$ [1,2]. In this "hidden nematic state" below $T^*$, the orthorhombicity is very tiny. To explain this long-standing mystery, we propose the emergence of antiferro-bond order with antiferro wavevector $q=(0,\pi)$ at $T^*$, by solving the linearized density-wave equation based on the vertex correction theory [3,4]. This antiferro-bond order originates from the inter-orbital nesting between the $d_{xy}$-orbital hole-pocket and the electron-pocket, and naturally explains the pseudogap, band-folding, and tiny nematicity linear in $T^*-T$.

Quantum Critical Enhancement of Nematic-Resistivity Anisotropy in Underdoped Ba(Fe\textsubscript{1-x}Co\textsubscript{x})\textsubscript{2}As\textsubscript{2}\* SHUA SANCHEZ (Presenter), PAUL MALINOWSKI, University of Washington, JONG WOO KIM, PHILIP RYAN, APS, Argonne National Labs, JIUN-HAW CHU, University of Washington — The proportionality constant between the thermodynamic order parameter of a symmetry breaking phase and its associated transport coefficient often contains important information about the underlying electronic structure of a material. For instance, the anomalous Hall effect has been used to probe the Berry curvature of the band structures. Here we show how the proportionality constant between resistivity anisotropy and orthorhombicity in the nematic ordered phase is directly related to the elastoresistivity coefficient measured above the phase transition temperature. Using this relation, we discovered that this proportional constant increases significantly as doping approaches optimal, indicating the enhanced coupling between nematicity and conducting electrons near the quantum critical point.

*This work is supported by the Air Force Office of Scientific Research Young Investigator Program under Grant FA9550-17-1-0217.

Non-linear elasto-Hall measurements in iron-based superconductors\* PAUL MALINOWSKI (Presenter), QIANNI JIANG, ZHAOYU LIU, YUE SHI, SHUA SANCHEZ, JIUN-HAW CHU, University of Washington — It is well established that a rotational symmetry breaking electronic nematic phase is ubiquitous in the phase diagrams of iron-based superconductors and that anisotropic strain is a uniquely powerful in-situ probe of electronic anisotropy in these systems. In addition to the long-held belief that magnetic/nematic fluctuations are essential to understanding the pairing mechanism of the high $T_c$ superconductivity, they also drastically modify the normal state properties, evidenced by non-Fermi liquid behavior and strongly temperature dependent transport coefficients. In this work, we present the observation of the non-linear elasto-Hall effect in Co doped and P doped BaFe2As2. Our measurement reveals a large quadratic term of the Hall coefficient as a function of B2g anisotropic strain. For the optimally doped composition, the nonlinear elasto-resistivity diverges as temperature decreases. Combined with elastoresistivity, our result provides crucial insight into how nematicity and nematic fluctuations couple to conducting electrons.

*This work was mainly supported by NSF MRSEC at UW (DMR-1719797) and the Gordon and Betty Moore Foundation’s EPiQS Initiative, Grant GBMF6759 to J.-H.C.
Investigation of nematic phase in LaFeAsO

SOONSANG HUH, YOUNSIK KIM (Presenter), WONSHIK KYUNG, JONGKEUN JUNG, Seoul Natl Univ, SAICHARAN ASWARTHAM, BERND BUECHNER, IFW Dresden, CHENGXIAO DONG, JIANGPING HU, Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, SOOHYUN CHO, DAWEI SHEN, Shanghai Institute of Microsystem and Information Technology (SIMIT), Chinese Academy of Sciences, JONATHAN DENLINGER, Advanced Light Source, Lawrence Berkeley National Laboratory, CHANGYOUNG KIM, Seoul Natl Univ — The nematic phase is believed to play a key role in iron based superconductor (IBSC), but it is not fully understood. LaFeAsO, known to have nematic phase but its electronic structure is not well understood, is a good system to get new clues about the nematic phase. To investigate the electronic structure of LaFeAsO nematic phase, we performed angle resolved photoemission spectroscopy (APRES) experiment. We report temperature dependent band splitting behavior between $d_{xz}$ and $d_{yz}$ hole band near $\Gamma$ and $M$ point.

*This work was supported by the Institute for Basic Science in Korea (Grant No. IBS-R009-G2)

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L62 DMP: Electron Transport in Nanostructures I — Mile High Ballroom 4C

- Jia Li, Brown University - Tag(s): Focus

Ultrafast and Cooperative Light-Matter Coupling [Invited] JUNICHIRO KONO (Presenter), Rice Univ — Recent experiments have shown that light and matter can mix together to an extreme degree, entering previously uncharted regimes of light-matter interactions [1]. This talk will summarize a series of experiments we have performed in such regimes. We will first describe our observation of ultrastrong coupling (USC) of a 2D electron gas with high-Q THz cavity photons in a quantizing magnetic field, demonstrating a record-high cooperativity [2]. The electron cyclotron resonance peak exhibited splitting into the lower and upper polariton branches with a magnitude that is proportional to the square-root of the electron density, a hallmark of cooperative vacuum Rabi splitting (VRS), known as Dicke cooperativity. Additionally, we have obtained evidence for the vacuum Bloch-Siegert shift [3], a signature of the breakdown of the rotating-wave approximation. The second part of this talk will present microcavity exciton polaritons in a thin film of aligned carbon nanotubes [4] embedded in a Fabry-Pérot cavity. This system exhibited cooperative USC with unusual continuous controllability over the coupling strength through polarization rotation [5]. Finally, we have generalized the concept of Dicke cooperativity to show that it also occurs in a magnetic solid in the form of matter-matter interaction [6]. Specifically, the exchange interaction of $N$ paramagnetic Er$^{3+}$ spins with an Fe$^{3+}$ magnon field in ErFeO$_3$ exhibited a VRS whose magnitude is proportional to $N^{1/2}$. Our results provide a route for understanding, controlling, and predicting novel phases of condensed matter using concepts and tools available in quantum optics. 1. P. Forn-Díaz, L. Lamata, E. Rico, J. Kono, and E. Solano, Revi. Mod. Phys. 91, 025005 (2019). 2. Q. Zhang et al., Nat. Phys. 12, 1005 (2016). 3. X. Li et al., Nat. Photon. 12, 324 (2018). 4. X. He et al., Nat. Nanotechnol. 11, 633 (2016). 5. W. Gao et al., Nat. Photon. 12, 362 (2018). 6. X. Li et al., Science 361, 794 (2018).
**8:36AM L62.00002: Anomalous Dirac Plasmons in 1D Topological Electrides**  JIANFENG WANG  (Presenter), Beijing Computational Science Res Ctr, XUELEI SUI, Tsinghua University, SHIWU GAO, Beijing Computational Science Res Ctr, WENHUI DUAN, Tsinghua University, FENG LIU, University of Utah, BING HUANG, Beijing Computational Science Res Ctr — Plasmon opens up the possibility to efficiently couple light and matter at sub-wavelength scales. In general, the plasmon frequency, intensity and damping are dependent of carrier density. These dependencies, however, are disadvantageous for stable functionalities of plasmons and render fundamentally a weak intensity at low frequency, especially for Dirac plasmon (DP) widely studied in graphene. Here we demonstrate a new type of DP, emerged from a Dirac nodal-surface state, which can simultaneously exhibit density-independent frequency, intensity and damping. Remarkably, we predict realization of anomalous DP (ADP) in 1D topological electrides, such as Ba$_3$CrN$_3$ and Sr$_3$CrN$_3$, by first-principles calculations. The ADPs in both systems have density-independent frequency and high intensity, and their frequency can be tuned from terahertz to mid-infrared by changing the excitation direction. Furthermore, the intrinsic weak electron-phonon coupling of anionic electrons in electrides affords an added advantage of low phonon-assisted damping and hence a long lifetime of the ADPs. Our work paves the way to developing novel plasmonic and optoelectronic devices by combining topological physics with electride materials.

**8:48AM L62.00003: Ultrafast terahertz microscopy down to the atomic scale**  TYLER COCKER  (Presenter), SPENCER AMMERMAN, VEDRAN JELIC, NICHOLAS J BRESLIN, Physics and Astronomy, Michigan State University — Recent developments have allowed terahertz (THz) scanning probe microscopy to achieve unprecedented simultaneous temporal and spatial resolutions. Included in the arsenal of THz microscopy techniques are terahertz scanning tunneling microscopy (THz-STM), which reveals the ultrafast response of a tunnel junction with atomic resolution [1-3], scattering-type scanning near-field optical microscopy (s-SNOM), which reveals the local dielectric function [4-6], and terahertz emission nanoscopy, which reveals local contrast in THz fields generated at the sample surface [7,8]. In this talk I will show examples of the types of experiments that can be done with each technique, including atomically resolved THz-STM snapshot imaging of local electron densities.


*Department of Defence Office of Naval Research Division 312
9:00AM L62.00004: Boltzmann treatment of nanoscale inhomogeneous electrical conduction  
RYAN MESCALL (Presenter), Physics, Yale, PHILIP ALLEN, State Univ of NY - Stony Brook —  
Small distance scales (e.g. boundaries of small samples) destroy the propagating electron quasiparticles that Boltzmann transport theory needs. Our model retains propagating single particle electrons, but generates nanoscale inhomogeneities by introducing nanoscale source terms in the Boltzmann equation of a macroscopic homogeneous metal. We solve the equations in Fourier space for electron distribution functions arising from charge input $\sim \exp(iqx)$. Fourier transformation allows computation of fields the $E(x)$, $V(x)$, and $n(x)$ corresponding to currents $j(x)$ derived from a realistic charge input from discrete electrodes. We study the ballistic to diffusive crossover as the sample size and electrode size are varied on distance scales comparable to the electron mean free path.

9:12AM L62.00005: Hydrodynamic effects of ballistic electron jets in high-mobility GaAs/AlGaAs  
ADBHUT GUPTA (Presenter), JEAN J HEREMANS, Virginia Tech, SAEED FALLAHI, GEOFF C GARDNER, MICHAEL MANFRA, Purdue University — The influence of a ballistic electron jet, injected through a lithographic aperture, is experimentally investigated through nonlocal resistance measurements over a distance $L$ from the injection point, in a 2D electron system in a high-mobility GaAs/AlGaAs heterostructure over a temperature range $4 \text{ K} < T < 40 \text{ K}$, at zero magnetic field. The geometry consists of various mesoscopic apertures separated by $L$ ranging from $1.3 \text{ μm}$ to $20.5 \text{ μm}$ such that the jet can be injected from any aperture and the nonlocal potential induced by the current distribution can be measured at any other aperture. The measured nonlocal resistance exhibits a non-monotonic behavior as $T$ is increased, leading to negative values (up to $L = 12.8 \text{ μm}$) in an intermediate $T$ range. This $T$ range lies in the hydrodynamic regime of transport where electron-electron interactions can lead to momentum exchange between the ballistic jet and the surrounding electron fluid, resulting in a depletion of electrons in vicinity of the main jet and extraction of electrons from the nearby detector aperture. The experimental results are compared to the predictions of theoretical models based on Boltzmann transport equations.

9:24AM L62.00006: On the Nonphysical Solutions to the Wigner Equation Used in Electronic Transport  
MAKBULE KUBRA ERYILMAZ (Presenter), SINA SOLEIMANIKAHNOJ, IRENA KNEZEVIC, Electrical and Computer Engineering, University of Wisconsin-Madison — The Wigner transport equation is gaining traction as a useful tool for modeling quantum electronic transport in semiconductors. However, nonphysical results are known to occur in numerical implementations and are often related to violation of the Heisenberg uncertainty principle when finite-difference techniques are employed. In this study, we analyze the role of boundary conditions in the behavior of the solutions to the Wigner equation for the example of a finite-sized one-dimensional nanostructure with a potential barrier in the middle and connected to reservoirs of charge. We discuss the cases in which artefacts occur and propose a boundary condition scheme that alleviates potential issues stemming from charge injection into a finite-sized simulation domain.

*DOE DE-FG02-08ER46532, DOE DE-SC0020138

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*This work was supported by DOE BES DE-SC0008712 and UW ECE Splinter Professorship.
Quantum-dot–insulator–superconductor junctions coupled to a microwave resonator

VASILII SEVRIUK (Presenter), MATTI SILVERI, MIKKO MOTTONEN, QCD Labs, Aalto University — Quantum dots are finding more and more important applications in the modern electronics. Recent works related to the electron tunneling between a quantum dot and superconducting lead [1,2] inspired us to theoretically study the system consisting of quantum-dot–insulator–superconductor (QIS) junctions coupled to the microwave resonator. For this purpose, we adapted the theory developed before for the so-called quantum-circuit refrigerator [3-6], which is based on normal-metal–insulator–superconductor junctions. We demonstrate that the current running through the QIS junctions can lead to a negative damping rate at the microwave resonator and discuss the possibility to use such a system as a narrow-band amplifier and a microwave laser.


*This research was financially supported by European Research Council Consolidator Grant and by Academy of Finland Grants and its Centre of Excellence in Quantum Technology.

Multiple perfectly transmitting states of a discrete level at strong coupling

ÉTIENNE JUSSIAU (Presenter), University of Rochester, ROBERT S. WHITNEY, Univ. Grenoble Alpes, CNRS, LPMMC, ANDREW N JORDAN, University of Rochester — We analyze the transport properties of a discrete level between two reservoirs with a band structure. We focus on the case where the level is strongly coupled to the reservoirs, the coupling parameter is typically of the order of the energy scales of the band structures. In the absence of interactions, this system has an exact solution and the nonlinear Lamb shift can be derived. As expected, the Lamb shift has the effect of pushing the perfectly transmitting state (the reservoir state that flows through the discrete level without reflection) out of resonance with the discrete level, and can possibly turn it into a bound state. However, we show that additional pairs of perfectly transmitting states may appear due to the nonlinear Lamb shift when the coupling exceeds a critical value. The transmission function of the discrete level then resembles that of a multi-level system. Even in situations where the energy of the discrete level is outside the reservoirs' band, a perfectly transmitting state can be created inside the band if the coupling is strong enough. We propose observing the bosonic version of this physics in microwave cavities, and the fermionic version in the conductance of a quantum dot coupled to 1D or 2D reservoirs.
10:00AM L62.00009: Development of single-electron and single-electron-pair sources in LaAlO$_3$/SrTiO$_3$ nanostructures* YANG HU (Presenter), YUHE TANG, DENGYU YANG, YUN-YI PAI, JIANAN LI, Univ of Pittsburgh, HYUNGWOO LEE, JUNG-WOO LEE, CHANG-BEOM EOM, University of Wisconsin–Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — A source of single electrons can be realized by coupling quantum dots with tunnel barriers [1]. The 2D electron gas at the LaAlO$_3$/SrTiO$_3$ interface can be patterned using conductive atomic force microscope (c-AFM) lithography [2], which has been used to create quantum dots and single electron transistors [3]. We aim to use this technique to create an on-demand single-electron source by sketching quantum dots and applying out-of-phase excitation across the dot array. We discuss results for a triple-dot device and their associated electron tunneling phenomenon and issues related to the individual tunabilities of the dots. These devices may have application to quantum computation and simulation, and could also provide a robust standard for the electric unit ampere.


*JL acknowledges a Vannevar Bush Faculty Fellowship, funded by ONR (N00014-15-1-2847). C-BE acknowledges support from NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-4046).

10:12AM L62.00010: Electron transfer in thermally heterogeneous environments GALEN CRAVEN (Presenter), Los Alamos National Laboratory, ABRAHAM NITZAN, University of Pennsylvania — Electron transfer is a fundamental process that drives many physical, chemical, and biological transformations, as well as playing a ubiquitous role in the development of electronics and technologies for energy conversion. Recent advances in temperature measurement and control at the nanoscale allow thermal gradients and heat flow to be addressed at the molecular level, making it possible to observe electron transfer across thermal gradients. In this talk, I will discuss the development of a theoretical framework to describe electron transfer between donor and acceptor sites, where each site has a different local temperature. The transfer of charge across the resulting thermal gradient is found to be coupled with an energy transfer mechanism that may alter heat conduction between sites. Application of the developed theory suggests that emergent relations connecting thermal and electronic currents can be utilized to control energy conversion between redox molecular motifs, at molecule-metal interfaces, and in molecular junctions.
10:24AM L62.00011: Suppression of ballistic effects in the ultra-pure delafossite PtCoO$_2$ via high-energy electron irradiation* PHILIPPA MCGUINNESS (Presenter), ELINA ZHAKINA, VERONIKA SUNKO, Max Planck Institute for Chemical Physics of Solids, MARCIN KONCZYKOWSKI, Ecole Polytechnique, SEUNGHYUN KHIM, MARKUS KOENIG, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids — PtCoO$_2$ is a layered oxide delafossite material which has a hexagonal, single-band Fermi surface. This ultrapure metal is extremely conductive, with a low-temperature mean free path of up to 5 μm [1]. Due to these properties, novel low-temperature ballistic effects have been demonstrated in the magnetoresistance of micron-scale ultrapure delafossite devices [2]. To determine the sensitivity of the ballistic behavior to disorder, we have used 2.5 MeV electron irradiation to introduce point-defect impurities into PtCoO$_2$ microstructures. This reduces the mean free path and therefore suppresses the ballistic phenomena. Surprisingly, these effects remain, in a weaker form, at an impurity level significantly higher than would be expected from the usual limits of the ballistic regime.


*The authors acknowledge support from the Max Planck Society. PM and VS thank EPSRC for PhD studentship support through grant number EP/L015110/1. The irradiation was performed at LSI at the Ecole Polytechnique and was supported by the EMIR network.

10:36AM L62.00012: Single electron occupation in a bilayer graphene double quantum dot
CHRISTIAN VOLK (Presenter), LUCA BANSZERUS, SAMUEL MÖLLER, EIKE ICKING, 2nd Institute of Physics, RWTH - Aachen, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, CHRISTOPH STAMPFER, 2nd Institute of Physics, RWTH - Aachen — Graphene quantum dots (QDs) are an attractive platform for hosting spin qubits since the low nuclear spin densities and weak spin-orbit interaction in graphene promise long spin coherence times. Physically etched graphene QDs have been studied for about a decade. However, the influence of disorder, in particular the edge disorder prevented a precise control of the number of confined charge carriers.

We study an electrostatically gated bilayer graphene double QD (DQD) embedded in hexagonal boron nitride. Finger gates modulate the potential landscape along a one-dimensional channel confined by split gates and enable the formation of a DQD.

We control the number of charge carriers on each of the QDs from the few-electron regime down to the last. Tunnel coupling and capacitive interdot coupling increase with the QD occupation, leading eventually to the formation of a single QD. Furthermore, we can form a DQD in the low electron/hole occupation. Finite bias spectroscopy reveals the excited state spectrum of the first electrons in the DQD.

The precise control of the electron occupation is a key requirement for making such a device a suitable building block for spin qubit devices. The measured interdot tunnel coupling on the order of 2 GHz is in a regime compatible with spin qubits.
10:48 AM L62.00013: Coulomb drag between a carbon nanotube and monolayer graphene
SAMVEL BADALYAN (Presenter), Center for Graphene Research, Frisco, Texas 75035, USA, ANTTI-PEKKA JAUHO, Center for Nanostructured Graphene, Technical University of Denmark, 2800 Kongens Lyngby, Denmark — We study Coulomb drag in a system consisting of a carbon nanotube and monolayer graphene. Within the Fermi liquid theory we calculate the drag resistivity and find that the dimensional mismatch of the system components leads to a dependence of the drag rate on the carrier density, temperature, and spacing, which is substantially different from what is known for graphene double layers. We identify new features of the drag dependence on the electron density, which allows us to control their relative contribution to the drag resistivity.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L63 DMP DCMP FIAP: First Principles Approaches to Defects Mile
High Ballroom 4D - Joel Varley, Lawrence Livermore Natl Lab - Tag(s): Focus

8:00 AM L63.00001: First principles study of defect properties of II-VI photovoltaic materials
[Invited] SUHUAI WEI (Presenter), Beijing Computational Science Research Center — First-principles study of photovoltaic materials plays an important role in developing solar cell technologies because it can provide useful physical insights, fresh perspective and new design principles for developing innovative solar cell materials with high solar power conversion efficiency and reduced cost. Similar to other semiconductors, one of the most important issues in solar cell absorber materials are to control the defects, either for introducing charge carrier, improving charge transport, or reducing non-radiative carrier recombination. For example, a good solar cell material should have good defect properties, that is, it can be easily doped such that charge carriers can be created to generate the required electric field and has less defect-induced recombination centers such that it has high carrier life time and minority carrier mobility, so photo-generated charge can be easily collected. In this talk, using II-V thin-film solar cell absorber materials Cd(Te,Se), Cu(In,Ga)Se$_2$ (CIGS) and Cu$_2$ZnSnS$_2$ (CZTS) as examples, I will discuss how theoretical first-principles studies can be used to better understand and optimize the solar cell performance.
First-Principles Study on the Defect Physics of Ternary Chalcopyrite ZnGeP$_2$ through Hybrid Functional

MENGLIN HUANG (Presenter), SHANSHAN WANG, SHIYOU CHEN, East China Normal University — Zinc germanium diphosphide (ZnGeP$_2$) is a chalcopyrite semiconductor that can be used for infrared frequency conversion applications. It is believed that the intrinsic defects are responsible for the defect-related absorptions and emissions observed in experiments, and the performance of the corresponding device is also limited by those defects. Here we study the defect physics in ZnGeP$_2$ using the density functional theory (DFT) calculations with a hybrid functional. We will firstly present the result of phase stability, which differs significantly from the previous result calculated by semi-local DFT. Ge$_{Zn}$, Zn$_{Ge}$, Ge$_{P}$, P$_{Ge}$ antisites are the dominant point defects among all the Fermi level range and growth conditions. Under Zn-rich condition, the Fermi level is about 0.6 eV above valence band maximum (VBM), which shows the p-type conductivity, while under Ge-poor condition, the Fermi level is located at the middle of the band gap, consistent with the experiment results. We will also discuss the result of calculated optical transition that is related to photoluminescence peak and the possible impurities and defect complexes.

Dimensionality-suppressed chemical doping in 2D semiconductors: the cases of phosphorene, MoS$_2$, and ReS$_2$ from first-principles

JI-HUI YANG (Presenter), Department of Physics, Fudan University — In spite of great appeal of two-dimensional (2D) semiconductors for electronics and optoelectronics, to achieve required charge carrier concentrations by means of chemical doping remains a challenge, due to large defect ionization energies (IEs). Here by decomposing the defect IEs into the neutral single-electron defect level, the structural relaxation energy gain, and the electronic relaxation energy cost, we propose a conceptual picture that the large defect IEs are caused by two effects of reduced dimensionality. While the quantum confinement effect (QCE) makes the neutral single-electron point defect levels deep, the reduced screening effect (RE) leads to high energy cost for the electronic relaxation. The first-principles calculations for monolayer, few-layer, and bulk black phosphorus (BP), MoS$_2$, and ReS$_2$ do demonstrate the general trend. Based on the gained insight into defect behaviors, strategies can be envisaged for reducing defect IEs and improving charge carrier doping. Using BP monolayer either embedded into dielectric continuum or encapsulated between two h-BN layers, as practical examples, we demonstrate the feasibility of increasing the screening to reduce the defect IEs and boost carrier concentration.
9:00AM L63.00004: **First-principles study of defect physics in a photovoltaic semiconductor Cu$_2$ZnGeSe$_4$**  
LELE CAI (Presenter), SHIYOU CHEN, East China Normal University — Cu$_2$ZnGeSe$_4$ is of interest for the development of next-generation thin-film photovoltaic technologies. The additional number of elements in Cu$_2$ZnGeSe$_4$ increases the flexibility of material properties relative to binary and ternary semiconductors. However, a variety of intrinsic lattice defects are formed that have a significant impact on its photovoltaic performance. Here we study the intrinsic point defects in Cu$_2$ZnGeSe$_4$ using the density functional theory calculations with both the generalized gradient approximation and the hybrid functional. Examination of the thermodynamic stability of Cu$_2$ZnGeSe$_4$ shows that the stable chemical potential region for the formation of stoichiometric compound is small. Under Zn-poor condition, the shallow acceptor, Cu$_Zn$ antisite is the dominant defect with the lowest formation energy, accounting for the observed p-type conductivity, while in a Ge-rich condition, the Fermi level is close to the middle of band edge because of the lower formation energy of Zn$_{Cu}$. We will discuss the effects of these defects on the photoelectric properties of Cu$_2$ZnGeSe$_4$.

9:12AM L63.00005: **First principles calculations of phonons and Raman and infrared spectra in ZnGeGa$_2$N$_4$.**  
AMOL RATNAPARKHE (Presenter), WALTER LAMBRECHT, Case Western Reserve University — ZnGeN$_2$ is a semiconductor compound closely related to GaN. They have similar band gaps and are closely lattice matched but have a large band-offset, which enables new capabilities in heterostructure and alloy band structure engineering. Recently, a well-defined crystal structure with space group Pmn2$_1$ was proposed for the 50% compound ZnGeGa$_2$N$_4$ which satisfies the local octet rule around each N [PHYSICAL REVIEW MATERIALS2, 114602 (2018)]. Here, a first-principles study of the phonons in this material is presented. The calculations are performed using the density functional perturbation theory within the ABINIT software. The phonon frequencies at the Brillouin zone center and their symmetry analysis, as well as various associated parameters, will be presented: Born effective charge tensors, oscillator strength tensors, dielectric constants. The infrared and Raman spectra have been calculated for various scattering configurations. The phonon density of states and phonon dispersion curves will also be reported.

*This work is supported by the National Science Foundation.*
9:24AM L63.00006: Energy landscape of vacancy-related defects in silicon: a comprehensive picture from DFT and GW  GABRIELA HERRERO-SABOYA (Presenter), CEA de Bruyeres-le-Chatel, LAYLA MARTIN-SAMOS, CNR-IOM Democritos, ANNE HEMERYCK, LAAS-CNRS, NICOLAS RICHARD, CEA de Bruyeres-le-Chatel — Vacancy related point-like defects are one of the most common degrading centers in silicon-based technology. They have been the subject of extensive studies both experimental and theoretical. However, a comprehensive theoretical model capable of explaining experimental evidence is often missing. By means of first principles calculations we revisit structural, optical and electronic properties of these common point defects in silicon. Guided by simple theoretical models, we are able to perform accurate simulations, including many-body-perturbation corrections based on the GW approximation, in close quantitative agreement with the experiment. Going beyond the common total energy approach allows us to predict the electronic activity and the low temperature dynamics of such centers. At higher temperatures, vacancies become mobile centers, forming more complex systems and/or contributing to the diffusion of impurities. Starting from experimentally proposed mechanisms, we are able to theoretically characterize activation energies of such technologically relevant processes.

9:36AM L63.00007: Charged Defects in TiO$_2$ Anatase: A Comparative Study of Hybrid DFT, GW and BSE to Explore Optical Properties  POOJA BASERA, SASWATA BHATTACHARYA (Presenter), Indian Inst of Tech-New Delhi — Titanium dioxide (TiO$_2$) anatase is one of the most abundant, functionally versatile oxide materials. However, owing to its large bandgap, the photoabsorption efficiency is limited only in the UV region. Doping-mediated modulation is one of the most pragmatic approaches in the pursuit to improve the photocatalytic and solar energy conversion efficiencies of TiO$_2$. We report here using state-of-the-art hybrid density functional and \textit{ab initio} atomistic thermodynamics, the thermodynamic (meta-) stability of different non-metal dopants X (X= N, C, S, Se) as a function of charge state at realistic temperature and pressure. Knowing the most stable defects, we aim an accurate theoretical estimation of the optical properties of doped TiO$_2$. To do this, we have used many body perturbation theory viz. one particle Green's function (GW) method and higher order Green's function techniques Bethe-Salpeter Equation (BSE). Our calculations reveal the highly anisotropic nature of the doped TiO$_2$. The n-type doped TiO$_2$ is optically active in both x, z direction, whereas the p-type doped TiO$_2$ is optically inactive along z-direction. The most evident hallmark of the doped system is the appearance of absorption peaks at low energy below 3 eV, to give rise visible-light absorption.
**9:48AM L63.00008: The Barrier to the Small Polaron Formation in Metal Peroxides**

SHUAISHUAI YUAN (Presenter), ZI WANG, MAXIMILIAN L. F. BARON, KIRK H BEVAN, McGill Univ — Polaron formation is the process by which free electrons (or holes) in a material find a lower energy localized state by distorting their surrounding host lattice. Since polaron formation involves changes in both electronic and atomic coordinates, a deeper understanding of polaron formation promises to open up new avenues towards tailoring the physical properties of materials. Ab initio studies have predominantly focused on studying stabilized small polaron states and their hoping physics, while less investigation has been devoted to the equally important process of polaron formation. In this work, we provide ab initio insights into the polaron formation process and focus on exploring the physical origins of the barrier to polaron formation. We utilize the HSE06 hybrid functional to study small polaron formation in four similar metal peroxides, which exhibit a wide range of polaron formation barriers heights. Our results show that polaron hybridization with the conduction band minimum (CBM) plays a significant role in determining the magnitude of a polaron formation barrier. Moreover, by satisfying the generalized form of Koopmans’ theorem, we are able to show that the degree of hybridization is directly correlated with the electronic relaxation delay during polaron formation.

**10:00AM L63.00009: Machine learned defect and impurity levels in perovskite halides and CdTe**

ARUN KUMAR MANNODI KANAKKITHODI (Presenter), FATIH G SEN, MICHAEL TORIYAMA, MICHAEL J DAVIS, MARIA CHAN, Argonne Natl Lab — Electronic levels introduced by impurities and intrinsic defects in the band gap of semiconductors affect optoelectronic performance. Predictions of these defect levels are possible, but expensive, using first principles density functional theory (DFT), and chemical trends are often not easily available. In this talk, we will describe using machine learning (ML) trained on DFT data for defect levels in hybrid perovskite halides [1] and CdTe [2] photovoltaic materials. Relevant descriptors, relative performance of different ML approaches, and insight from resultant ML models will be discussed.


*We acknowledge funding from the USDOE: SunShot program under Contract No. DE-EE-005956; Argonne National Laboratory LDRD program and the Center for Nanoscale Materials under Contract No. DE-AC02-06CH11357; computational resources of the National Energy Research Scientific Computing Center under Contract No. DE-AC02-05CH11231.*
A quantitative understanding of the electronic excited states of point defects in semiconductors and insulators is crucial for identifying defects detrimental to device performance, as well as those that have attractive properties for quantum applications. In particular, transition metal impurities in semiconductors have been widely studied in both contexts. One of the key limitations for a first-principles description of such systems is that transition metal excited states often involve correlated low-spin multiplets that require a multideterminant treatment. This is beyond the capabilities of density functional theory (DFT), which is the workhorse for computational studies of point defects. Using Fe in GaN and AlN as an example, we address this issue by treating the defect as a correlated subspace embedded in the lattice. The defect structure is obtained from hybrid-functional DFT calculations, and the subspace is isolated via Wannierization. The dielectric screening effects from the surrounding lattice to the local defect Coulomb interactions is accounted for using the constrained RPA approach. Finally, the many-body problem within the subspace is solved exactly. We compare our results to previous calculations using constrained DFT, and experimental measurements.

We employed an experimentally motivated Monte Carlo simulation to calculate the conductance as a function of charged dopant concentration to investigate the non-linear evolution of the resistivity with annealing time in oxygen deficient thin films. The model consists of an N x N square lattice with hydrogenic atoms placed at each lattice site. The valence electrons are bound to their respective lattice site via a harmonic potential, and electrons at different sites are allowed to interact via a screened Coulomb potential. At each Monte Carlo step, electrons attempt to change their position slightly, and in addition attempt to transition between conducting and non-conducting states. We found nonlinear dependence of the resistance as a function of dopant concentration. The dopants act as electron traps where they lower the energy of nearby electrons and increase the energy requirement to transition to the conducting state. As more dopants are added, this effect increases, further suppressing the conductivity. This would indicate that the inclusion of the charged dopants advances the percolative evolution of such a phase transition.

*Project Funded By the US Air Force
10:36AM L63.00012: Formation energies of charged defects in 2D materials - a new perspective

ANDREW O'HARA (Presenter), Department of Physics and Astronomy, Vanderbilt University, BLAIR TUTTLE, Department of Physics, Penn State Behrend, XIAOGUANG ZHANG, Department of Physics, University of Florida, SOKRATES T PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — Formation energies of defects in semiconductors play a major role in understanding a wide range of properties. Supercell schemes have been widely used for calculations. For charged defects, a divergence in the potential arises from the periodic Coulomb interactions and, in the “jellium” approach, is removed by setting the average electrostatic potential to zero. A posteriori corrections are typically used to determine the infinite-supercell limit. For 2D materials, where unscreened Coulomb tails are present in the vacuum regions, additional complications arise. In this work, we present an alternative formalism based on statistical mechanics, which dictates that supercells are naturally neutral: “charged defects” are merely ionized, by trading carriers with the energy bands (charge neutrality of the crystal is an essential ingredient of the statistical mechanics of electrons in semiconductors). We show that the jellium approach can be derived from the statistical-mechanics-backed theory by invoking approximations with unknown consequences. We report density-functional-theory calculations showing that the differences between the two methods are especially large in 2D materials, e.g., h-BN, where they can be of order 1 eV. Convergence rates are excellent.

*DOE Grant DE-FG-02-09ER46554

10:48AM L63.00013: Origin of n-type conductivity of monolayer MoS2

AKASH SINGH (Presenter), ABHISHEK SINGH, Indian Institute of Science — Monolayer MoS2 is a promising two-dimensional material for electronic and optoelectronic devices. As-grown MoS2 is an n-type semiconductor, however, the origin of this unintentional doping is still not clear. Here, using hybrid density functional theory (DFT), we carried out an extensive study of often observed native point defects i.e., VS, VMo, VS2, VMoS3, VMoS6, MoS2, and S2Mo and found that none of them cause n-type doping. Specifically, S vacancy (VS), which has been widely attributed to n-type conductivity, turns out to be an electron compensating centre. We report that hydrogen, which is almost always present in the growth environments, is most stable in its interstitial (Hi) and H-S adatom forms in MoS2 and acts as a shallow donor provided the sample is grown under S-rich condition. Furthermore, they have high migration barrier (in excess of 1 eV), which would ensure their stability even at higher temperature and hence, lead to n-type conductivity.

*The authors thank Materials Research Centre and Supercomputer Education and Research Centre, Indian Institute of Science for the computational facilities. This work was supported by the India-Korea Joint Programme of Cooperation in Science and Technology. Akash Singh acknowledges the DST-Inspire fellowship (1F150954).
8:00AM L64.00001: Probing inhomogeneous superconductivity and magnetism in complex oxide heterostructures with scanning SQUID* [Invited]  HILARY NOAD (Presenter), Max Planck Institute for Chemical Physics of Solids — Complex oxide heterostructures offer unique opportunities for engineering electronic and magnetic systems, combining functionalities of their constituent materials and, in some cases, exhibiting emergent properties. The reduced dimensionality and broken inversion symmetry at interfaces can make them particularly sensitive to local variation in the crystal lattice. A key problem is to disentangle the intrinsic properties of heterostructures from those of ordered states stabilized by defects or other sources of inhomogeneity. I will discuss two studies which used scanning superconducting quantum interference device (SQUID) microscopy, a local magnetic probe, to investigate the effects of intrinsic or controlled inhomogeneity in complex oxide heterostructures. In the first, we imaged superconductivity in lanthanum aluminate/strontium titanate (LAO/STO) and delta-doped STO heterostructures. Spatial motifs in our measurements demonstrate that different orientations of structural domains with respect to the symmetry-breaking interface result in different superconducting transition temperatures. While LAO and STO are both nonmagnetic in the bulk, many experimental probes have found signatures of magnetism in LAO/STO heterostructures, with local measurements showing that magnetism, when present, is inhomogeneous. In our second study, we investigated oxygen vacancies as a proposed mechanism for the magnetism by measuring samples with differing oxygen content, placing tight limits on magnetism, even in the most strongly reduced samples.

*This work was supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-76SF00515.
It is possible to reveal otherwise hidden electronic properties in 2D oxide interfaces, namely LaAlO$_3$/SrTiO$_3$, by using local probes instead of traditional bulk measurements. For example, scanning single electron transistor microscopy has shown enhanced transport along ferroelastic domain boundaries [1]. Furthermore, Frenkel et al. have demonstrated that the local application of pressure to the interface of LaAlO$_3$/SrTiO$_3$ can reveal ferroelastic domain boundaries [2]. Here we detail our efforts to reveal electron transport in “sketched” LaAlO$_3$/SrTiO$_3$ nanostructures [3] using a modified vacuum AFM at room and low (T < 25 K) temperatures.


8:48AM L64.00003: Dependence of LaAlO$_3$/SrTiO$_3$ Electron Pairing Strength on Crystallographic Orientation* ADITI NETHWEWALA (Presenter), Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, Department of Materials Science and Engineering, University of Wisconsin-Madison, JIANAN LI, MEGAN BRIGGEMAN, YUZE ZHANG, TIANYI WANG, Department of Physics and Astronomy, University of Pittsburgh, JUNG-WOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — Recently, it has been shown that superconductivity at the LaAlO$_3$/SrTiO$_3$ interface is essentially 1D in nature, and that the pairing mechanism appears to be linked to the boundaries of naturally formed X, Y and Z ferroelastic domains in SrTiO$_3$ [1]. Here, we investigate the nature of the pairing mechanism in LaAlO$_3$/SrTiO$_3$ nanostructures by examining the electron pairing strength with respect to the crystallographic direction. We write 1D, cross-shaped electron waveguides or “nanocrosses” [2] at the LaAlO$_3$/SrTiO$_3$ interface using conductive atomic force microscope (c-AFM) lithography. The c-AFM lithography and device geometry together defines the X, Y and Z domain boundaries across the nanocross at low temperatures. A sinusoidal dependence is observed as the nanocross is rotated with respect to the crystallographic direction. This characteristic angular dependence helps to constrain and sharpen our understanding of the pairing mechanism at the interface and the role of ferroelastic domain structure.


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9:00AM L64.00004: Transport properties of non-reciprocal 1D quantum channels at the LaAlO$_3$/SrTiO$_3$ interface*  YUZE ZHANG (Presenter), TIANYI WANG, MEGAN BRIGGEMAN, Univ of Pittsburgh, HYUNGWOON LEE, JUNGHOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin - Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — Abstract: Complex oxide heterostructures exhibit many interesting phenomena [1] that can be controlled on the nanoscale using a conductive atomic force microscope (c-AFM) lithography technique [2]. We create chiral 1D superlattices at the LaAlO$_3$/SrTiO$_3$ interface by adding a periodic modulation to an electron waveguide device. These nanostructures support quantized ballistic transport of electrons and electron pairs, as well as oscillatory transport behavior indicating an engineered spin orbit interaction [3]. These experiments represent a first step toward engineering properties in 1D quantum wires and can be regarded as a building block for more complex quantum systems.


*JL acknowledges a Vannevar Bush Faculty Fellowship (ONR N00014-15-1-2847) and NSF (PHY-1913034). C-BE acknowledges NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-4046).

9:12AM L64.00005: Nanoscale control of the metal-insulator transition in free-standing LaAlO$_3$/SrTiO$_3$ membranes*  MUQING YU (Presenter), Univ of Pittsburgh, KITAE EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, DENG YU YANG, Univ of Pittsburgh, JUNGHOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — By combining 2D materials such as graphene into layered van der Waals heterostructures, new types of designer materials with unique and emergent properties have been realized [1]. We describe a method for achieving free-standing single-crystal LaAlO$_3$/SrTiO$_3$ membranes by etching away a sacrificial SrRuO$_3$ layer underneath SrTiO$_3$. LaAlO$_3$/SrTiO$_3$ membranes are transferred to a sapphire substrate, and we use conductive AFM lithography [2] to achieve nanoscale control the insulator to metal transition at the LaAlO$_3$/SrTiO$_3$ interface. Nanoscale conductive channels created at room temperature remain conductive at two Kelvin. These results demonstrate the capacity to create LaAlO$_3$/SrTiO$_3$ membranes that can be integrated with other materials and reversibly patterned at nanoscale dimensions.


*JL acknowledges a Vannevar Bush Faculty Fellowship, funded by ONR (N00014-15-1-2847). C-BE acknowledges NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-4046)
9:24AM L64.00006: Influence of Temperature on LaAlO$_3$/SrTiO$_3$ Nanowire Lifetimes Under Ambient Conditions*

AARON GREENBERG (Presenter), PHILIP SHENK, JOSEPH ALBRO, MUQING YU, Univ of Pittsburgh, CHANG-BEOM EOM, University of Wisconsin - Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh —

The discovery of a tunable 2DEG at the interface of LaAlO$_3$/SrTiO$_3$ has spurred interest in LaAlO$_3$/SrTiO$_3$, which exhibits numerous interesting properties. Using a conductive AFM lithography technique, we can create novel devices at the interface of LaAlO$_3$/SrTiO$_3$ by locally confining the 2DEG to zero or one dimension [1]. However, in ambient conditions, an appreciable degradation of device lifetime occurs [2]. Previously, the decay rate of such devices was characterized as a function of humidity and pressure; however, its dependence on temperature has yet to be determined. Here we describe experiments detailing efforts to quantify the device lifetimes as a function of temperature under otherwise ambient conditions, which will aid in the creation of new, more complex devices.


9:36AM L64.00007: Surface Acoustic Wave Generation and Detection on LaAlO$_3$/SrTiO$_3$*

DENGYU YANG (Presenter), YUN-YI PAI, YUHE TANG, MUQING YU, YANG HU, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNG-WOO LEE, KITAE EOM, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh —

We aim to generate and detect surface acoustic waves (SAW) in LaAlO$_3$/SrTiO$_3$ heterostructures. Using a well-developed conductive-AFM lithography technique [1], we “sketch” interdigitated transducers (IDT) on LaAlO$_3$/SrTiO$_3$ “canvases”, which convert electronic signals into SAW and vice-versa. Two sets of IDTs are written on the structure to function as a generator and detector. SAW can be used to generate dynamic potentials based on piezoelectric properties of LaAlO$_3$/SrTiO$_3$, and have the potential to drive electrons through nanostructures, a property that could be useful for quantum information applications.


*JL acknowledges a Vannevar Bush Faculty Fellowship (ONR N00014-15-1-2847), and the Office of Naval Research (N00014-16-1-3152). C-BE acknowledges NSF DMREF (DMR-1629270), AFOSR (FA9550-15-1-0334), and AOARD (FA2386-15-1-0406).
Creating nano-scale “vias” in LaAlO$_3$/SrTiO$_3$ for integration of nanostructures

CARL WILSON (Presenter), ADITI NETHWEWALA, ERIN SHERIDAN, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — The 2D electron gas (2DEG) at the LaAlO$_3$/SrTiO$_3$ interface exhibits a wide range of gate-tunable properties like superconductivity, magnetism, and spin orbit coupling [1]. Furthermore, the interface can be patterned with nanoscale dimensions using c-AFM lithography [2] and integrated with other 2D materials such as graphene [3]. While the surface of LaAlO$_3$/SrTiO$_3$ is only 1.2 nm from the interface, improved coupling of particles on the surface with the interface requires closer proximity. Here, we discuss methods to create nanoscale holes or “nano vias” in LaAlO$_3$/SrTiO$_3$ with the goal of integrating nanomaterials directly to interface while maintaining interfacial conductivity. These nano vias will allow us to study the effect of local coupling between the 2DEG at LaAlO$_3$/SrTiO$_3$ interface and a wide variety of interesting nanomaterials such as colloidal quantum dots or graphene nanoribbons.


Interface band engineering in LaAlO$_3$/SrTiO$_3$ heterostructures

MICHAEL SING (Presenter), JUDITH GABEL, PHILIPP SCHEIDERER, MICHAEL ZAPF, MARTIN STÜBINGER, University of Wurzburg, Germany, CHRISTOPH SCHLUETER, Deutsches Elektronensynchrotron DESY, Hamburg, Germany, TIEN-LIN LEE, Diamond Light Source, UK, RALPH CLAESSEN, University of Wurzburg, Germany — Novel two-dimensional electron systems at the interfaces of oxide heterostructures such as LaAlO$_3$/SrTiO$_3$ recently have attracted much attention as they display intriguing properties which may be exploited in future electronic devices. A key requirement for such applications is the controllability of the electronic interface properties such as the valence band offset. We demonstrate that these properties can be effectively engineered in LaAlO$_3$/SrTiO$_3$ by virtue of the oxygen vacancy concentration. By angle-dependent hard x-ray photoelectron spectroscopy, we derive a complete band diagram of the heterostructure dependent on the oxygen vacancy concentration which is adjusted during the photoemission experiments by means of synchrotron light irradiation and simultaneous oxygen dosing. The dielectric constant of the SrTiO$_3$ substrates and its strong non-linear dependence on the electric field prove to be essential for the band arrangement of the LaAlO$_3$/SrTiO$_3$ heterostructures. The comprehensive analysis of the band situation at the LaAlO$_3$/SrTiO$_3$ heterointerface as a function of the oxygen vacancy concentration can reconcile the contradicting results of previous photoemission studies.
**10:12AM L64.00010: Character of the insulator-metal transition at the LaAlO$_3$/SrTiO$_3$ interface**  
DANIEL BENNETT, Univ of Cambridge, EMILIO ARTACHO (Presenter), Nanogune, DIPC, Ikerbasque & Univ of Cambridge, NICHOLAS C. BRISTOWE, Physical Sciences, Univ of Kent — Under a film of lanthanum aluminate (LAO) on strontium titanate (STO) a two dimensional metal appears after a critical thickness, as a response to the electrostatic energy build-up originated by the polar discontinuity at the interface. The character of the transition has not been much explored given the discrete character of the controlling parameter, the film thickness. However, an applied electric field across the film for a thickness close to the transition will drive the transition as well, the character of the transition becoming relevant, not only fundamentally but for possible applications, too. A phenomenological mean-field theory predicts a continuous transition, while a saturating discontinuous one has been assumed in other contexts. We will present a theoretical analysis showing a richer phenomenology than expected so far, with the possibility of either continuous or discontinuous transitions, including a situation in which there is a second discontinuous transition with a jump in carrier concentration after an earlier continuous metal-insulator one.

*Funded by EPSRC - UK

**10:24AM L64.00011: Giant nonreciprocal charge transport in noncentrosymmetric LaAlO$_3$/SrTiO$_3$ interfaces**  
DAESEONG CHOE (Presenter), MI-JIN JIN, Ulsan National Institute of Science and Technology, SHIN-IK KIM, HYUNG-JIN CHOI, Korea Institute of Science and Technology, JUNHYEON JO, INSEON OH, JUNGMIN PARK, HOSUB JIN, Ulsan National Institute of Science and Technology, HYUN CHEOL KOO, BYOUNG-CHUL MIN, SUK-MIN HONG, Korea Institute of Science and Technology, HYUN-WOO LEE, Pohang University of Science and Technology, SEUNG-HYUB BAEK, Korea Institute of Science and Technology, JUNG-WOO YOO, Ulsan National Institute of Science and Technology — Electrons confined at an interfacial quantum well of a LaAlO$_3$/SrTiO$_3$ associated with broken inversion symmetry show various exotic condensed matter phases and rich spin-orbitronic functionalities. This two-dimensional polar conductor may exhibit directional propagation of itinerant electrons, *i.e.* the leftward and rightward currents differ from each other, when time-reversal symmetry is further broken. This potential rectification effect generally was displayed to be very weak due to the fact that kinetic energy is much higher than energies related to symmetry breakings producing weak perturbation. Here, we present giant gate-tunable nonreciprocal charge transport in the LaAlO$_3$/SrTiO$_3$ conductive oxide interface, where the electrons are confined at two-dimension with low Fermi energy. The coefficient $\gamma$ indicating the magnitude of nonreciprocal response, was estimated to be as high as $\sim 10^2$ T$^{-1}$A$^{-1}$, which is about 3 order of magnitude higher than those reported for noncentrosymmetric conductors. The observed behavior of nonreciprocal response in LaAlO$_3$/SrTiO$_3$ is related to comparable energy scales among kinetic energy, magnetic field and spin-orbit interaction, which opens a promising route to improve nonreciprocal response and its functionalities in the emerging spin-orbitronics.
High-mobility two-dimensional hole gas at the SrTiO$_3$ interface formed by depositing an ultrathin metal film at room temperature*  

SHINGO KANETA (Presenter), Department of Electrical Engineering and Information Systems, The University of Tokyo, LE DUC ANH, Institute of Engineering Innovation, The University of Tokyo, MASASHI TOKUNAGA, Institute for Solid State Physics, The University of Tokyo, MUNETOSHI SEKI, HITOSHI TABATA, MASAAKI TANAKA, Department of Electrical Engineering and Information Systems, The University of Tokyo, SHINOBU OHYA, Institute of Engineering Innovation, The University of Tokyo — Despite intensive studies on the two-dimensional electron gas (2DEG) at the SrTiO$_3$ (STO) interface [1], forming a 2D hole gas (2DHG) at the STO interface is extremely difficult [2], although both are essential for the realization of high-speed oxide-based electronics. Here, we demonstrate a very simple method to realize a 2DHG with an ultrahigh mobility of 24,000 cm$^2$V$^{-1}$s$^{-1}$ at an STO interface. The 2DHG is obtained by depositing a sub-nm-thick Fe layer (thickness $t \leq 0.2$ nm) on STO substrates at room temperature in an ultrahigh vacuum chamber. The Fe layer is oxidized and becomes insulating amorphous FeO$_x$. Magnetotransport measurements reveal the existence of high-mobility carriers in the STO side, and the carrier type changes from a pure p-type ($t \leq 0.2$ nm) to n-type ($t > 0.3$ nm) by varying the Fe thickness. In a p-type sample ($t = 0.1$ nm), the Shubnikov - de Haas oscillation is clearly observed in out-of-plane magnetic field but disappears in in-plane field. These results clearly demonstrate the 2D nature of the high-mobility hole carriers.


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Shubnikov-de Hass oscillations to the quantum limit in (111) oriented SrTiO$_3$ interface 2D electron gas*  

ZIQIAO WANG, AUTUMN B HELTMAN, SHALINI KUMARI, QI LI (Presenter), Pennsylvania State University, SHALINEE CHIKARA, ALEXEY SUSLOV, Florida State University, FEDOR BALAKIREV, JOHN SINGLETON, Los Alamos National Lab. — The (111) surface of perovskite oxide SrTiO$_3$ has a hexagonal structure, similar to topological insulator Bi$_2$Se$_3$. Existence of topological states has been predicted in this system and high mobility two-dimensional (2D) electron gases at interfaces provide a promising platform to study these properties. We created a 2D electron gas at SrTiO3 (111) interfaces with high mobility over 15000 cm$^2$V$^{-1}$s$^{-1}$ at low temperatures. Utilizing interface engineering, we have achieved relatively low carrier density of 1.3x10$^{13}$ cm$^{-2}$. Longitudinal magnetoresistance shows clear Shubnikov-de Hass (SdH) oscillations at low temperatures and high magnetic fields at both 35 T (DC field) and 60 T (pulsed field). In the low carrier density sample, we have observed the lowest Landau level at magnetic field around 20 T, which shifts to higher fields with higher carrier densities. More strikingly, a linear magnetoresistance (LMR) behavior appears at high magnetic field beyond the quantum limit. Temperature and angular dependence of the quantum oscillations as well as the LMR will be discussed.

*Work at Penn State is supported in part by DOE DE-FG02-08ER46531 and NSF DMR-1905833. National High Magnetic Field Lab. is supported by DMR-1644779 and State of Florida.
8:00AM L65.00001: Stabilization of Crystalline Phase in Organo-metal Halide Perovskite Quantum Dots via Surface Manipulation*  WILLIAM DELMAS (Presenter), ALBERT DIBENEDETTO, University of California, Merced, EVAN VICKERS, JIN ZHANG, Department of Chemistry and Biochemistry, University of California Santa Cruz, SAYANTANI GHOSH, University of California, Merced — Size tunability of semiconducting quantum dots (QDs) is their most attractive characteristic, which allows modulation of their optical and electronic properties. In the case of organo-metal halide perovskite (OMHP) QDs, surface functionalization is one of the routes that offers a unique way to vary the size in a highly precise manner. In this study we use temperature dependent static and dynamic spectroscopy to investigate the effect of four different surface modification protocols on in CH$_3$NH$_3$PbBr$_3$ OMHP QDs using conductive aromatic ligands. Our results indicate that functionalization methods affect quantum yield (QY) based on how well the different ligands passivate the surface states, while simultaneously altering the contribution of those states to the energy landscape that allows us to arrest the structural phase transition of the QDs from tetragonal/cubic to orthorhombic at low temperatures. Further, these ligands allow charge delocalization around the benzoic positions, which improves inter-particle energy transfer efficiency in QD films based on the conjugation state of the ligands. The synthesis of phase stable and high QY QDs that form conducting films is a significant development that will find use in diverse applications.

*This work was funded by NASA grant NNX15AQ01A.
8:12AM L65.00002: Advanced material system for the design of an intermediate band solar cell: type-II CdTe quantum dots in a ZnCdSe matrix*  

VASILIOS DELIGIANNAKIS (Presenter), GEHAN RANEPURA, The City College of New York, MILAN BEGLIARBEKOV, CUNY Graduate Center, IGOR KUSKOVSKY, Queens College, MARIA C TAMARGO, The City College of New York — Photovoltaics based on intermediate band (IB) absorption have the potential to overcome the Shockley-Quiesser limit and maintain a large $V_{oc}$. Quantum dots (QDs) or impurities can be used to form the IB. We propose a material system of submonolayer CdTe QDs embedded a ZnCdSe matrix that is optimum for the formation of an ideal IB and has other advantages to materials previously considered. Some unique attractive features of this material are its binary composition, simplifying growth; the absence of a deleterious interfacial layer, in spite of the lack of common ion; and the presence of strain, which allows for strain engineering of the IB. A superlattice structure of alternating QD and spacer layers is analyzed by X-ray diffraction (XRD) and photoluminescent (PL) spectroscopy. Simple arguments are used, following continuum elastic theory, to deduce the size of the dots and the strain within the superlattice from XRD data. Results of structural and optoelectronic characterization of both active layer and full device structures, using XRD, PL, photocurrent and contactless electro-reflectance measurements will be presented. The results suggest that the optimized materials are very well suited for potential high-efficiency IB solar cells.

*NSF CBET 1512017, NSF HRD-1547830

8:24AM L65.00003: Photo-induced current enhancement in core-shell type quantum dot FET*  

SUNAO SHIMIZU (Presenter), CRIEPI, KEIICHIRO MATSUKI, Waseda University, KAZUMOTO MIWA, CRIEPI, DANIELE BRAGA, Fluxim AG, SHIMPEI ONO, CRIEPI — Low dimensional materials are promising candidates to provide unique electronic properties; among them, quantum dots (QDs) and their hybrid systems are considered highly feasible because of the tunability of physical and chemical properties by material design. Here we report the fabrication of CdSe/CdS core-shell QDs-based field effect transistors (FETs) and its application to photo FET operations under UV light irradiation. The thin films of CdSe/CdS QDs were fabricated on SiO2/Si substrates in order to perform field effect experiments. The UV light irradiation dramatically changed the transfer characteristics for the thin films, the thickness of which ranges from ~20 nm to ~200 nm. We will discuss the thickness and the gate voltage dependence of the photo-induced current enhancement in the core-shell QDs-based FET in detail.

*This work was supported by JSPS KAKENHI Grant Number JP17H02928.
8:36AM L65.00004: Infrared Optical-Field-Driven Luminescence in Quantum Dots  IBRAHIM BOULARES (Presenter), Combat Capabilities Development Command, US Army Research Laboratory, JIAOJIAN SHI, Department of Chemistry, Massachusetts Institute of Technology, BLAIR CONNELLY, Combat Capabilities Development Command, US Army Research Laboratory, KEITH ADAM NELSON, Department of Chemistry, Massachusetts Institute of Technology — A recent study on CdSe-CdS core-shell colloidal quantum dots (QDs) showed that extreme electric fields from ultrafast THz-frequency electromagnetic pulses alone can produce QD luminescence [1, 2]. Unlike multi-photon absorption, which occurs at much higher optical frequencies, such emission was shown to be associated with large energy shifts of the absorption edge (more than 25%) – much like electro-luminescence (EL) driven by a quasi-DC field. While details of the mechanism of THz driven-EL are still under investigation, the effects of high optical electric fields of mid- to long-wavelength infrared (IR) radiation on the optical properties of QDs remain largely unexplored. To expand our understanding of the responses of QDs to extreme optical fields, we investigated the interaction of visible bandgap QD materials with sub-picosecond infrared-frequency pulses in the 3.5 to 12 micron wavelength range, at electric field levels that exceeded 1 MV/cm. We observed significant luminescence, resulting in up-conversion of the IR light to visible wavelengths, throughout the IR range that we explored. Preliminary results suggests similar EL induced by strong THz and IR fields.


8:48AM L65.00005: Exciton Fine Structure in Lead Salt Quantum Dots  SERGUEI GOUPALOV (Presenter), Jackson State Univ, IVAN AVDEEV, MIKHAIL NESTOKLON, Ioffe Institute — Lead chalcogenide quantum dots (QDs) have attracted significant scientific and technological interest as their photoluminescence (PL) is tunable by the size change over a wide infrared wavelength range. Electron and hole states in bulk lead chalcogenides are highly degenerate leading to the 64-fold degenerate exciton states. In quantum dots (QDs), the 64-fold degeneracy of the excitons is lifted by the valley mixing and by the electron-hole exchange interaction. We thoroughly investigate the relative importance of the inter-valley, spin-orbit, and electron-hole exchange couplings for the splittings and calculate the resulting exciton fine structure in the framework of the empirical tight-binding method. The dependence of the exciton fine structure on QD size and shape is analyzed. The calculated exciton fine structure allows one to explain the temperature dependence of the PL lineshapes observed in recent single QD experiments on PbS/CdS core/shell colloidal nanocrystals.
9:00AM L65.00006: Atomic and Electronic Structure of Epitaxial Necking in Quantum Dot Super Lattice  MAHMUT SAMI KAVRIK (Presenter), University of California San Diego, WONHEE KO, JORDAN HACHTEL, Oak Ridge National Lab, CAROLINA QIAN, ALEX ABEISON, University of California Irvine, HARSHIL KASHYAP, SCOTT UEDA, University of California San Diego, AN-PING LI, JUAN IDROBO, Oak Ridge National Lab, MATT LAW, University of California Irvine, ANDREW KUMMEL, University of California San Diego — Quantum coupling between periodic nanocrystalline structures manifests novel mesoscale properties such as mini-band formation, which may induce high carrier mobility\(^1\). Colloidal PbSe quantum dots (QDs) can self-assemble into 3D superlattices and are a promising material system to realize these synergistic properties. In this work, the electronic structures of these systems are investigated with advanced metrology and the modulation of electronic band structure in QD epi-SL by the formation of epitaxial neck between the QDs were observed. Experiments revealed unexpectedly large zero conductance (band) gap formation (~1.1 eV) when the STS probe was located between the QDs, while a smaller band gap of ~0.7 eV was observed when probing the body of the QD, as expected. Monochromated STEM-EELS were performed on the monolayer epi-SL and the band gap modification as a function of the electron probe position studied which shown a high onset for the energy loss when the electron probe was positioned on the QD neck, while a smaller onset was observed when the probe was directly on the QD. It is hypothesized that the epitaxial necks between the QDs confines the electron (hole) wave functions, thereby forming large band gaps on the epitaxial necking regions.

9:12AM L65.00007: Advances in Colloidal Quantum Dot Superlattice Charge Transport*  HENRY TRAVAGLINI (Presenter), University of California, Davis —

Colloidal quantum dot (QD) superlattices are an attractive class of materials for next generation electronic devices due to the manifold methods to tune their fundamental properties, including atomic composition, size, shape, and surface functionalization. However, due to their massive surface area to volume ratio and various structural disorder, defects have prevented the realization of a QD superlattice that shows true band-like transport properties. We report on novel superlattice fabrication techniques and characterization techniques, which show a dramatic increase of mobility without the use of electrochemical gating. We use scanning photocurrent microscopy to provide a means of extracting accurate minority carrier diffusion lengths as a function of temperature. We show a significantly improved minority carrier diffusion length and external quantum efficiency compared to amorphous QD lattices. We conclude by discussing our results in the context of rigorous signatures of band-like transport in generic superlattices.

*This work was supported by the U.S. National Science Foundation Grant DMR-1710737 and the UC Laboratory Fees research program.
Zero field splitting of heavy-hole states in Ge quantum dots

GEORGIOS KATSAROS (Presenter), JOSIP KUKUCKA, LADA VUKUSIC, HANNES WATZINGER, Institute of Science and Technology Austria, FEI GAO, TING WANG, JIANJUN ZHANG, Institute of Physics, Chinese Academy of Sciences, KARSTEN HELD, Technical University of Vienna — Holes have gained increasing interest in the past few years as spin qubit candidates since their strong spin-orbit coupling allows full electrical control of the hole spins [1-4]. Despite the fact that a hole is simply a missing electron, their spins are behaving strikingly different than their electron counterparts. While the electron spin does not correlate with the direction of motion, for holes in semiconductors there is a strong coupling between the momentum and the hole pseudospin.

For heavy-hole (HH) states confined in two dimensions, the pseudospin points in the direction of strong confinement. This implies that such HHs should show a zero field splitting (ZFS). By performing cotunnelling spectroscopy, we measure a ZFS of up to 55μeV for the excited triplet states confined in a Ge hut wire quantum dot with an even hole occupation. The evolution of the triplet states both for perpendicular and parallel magnetic fields is in very good agreement with an anisotropic spin Hamiltonian.

References:

Thermoelectric transport properties of coupled quantum dots

ROBERTO FRANCO PE?ALOZA (Presenter), Departamento de Física, Universidad Nacional de Colombia, Bogotá - Colombia, JOHN ALEJANDRO LANDAZABAL RODRIGUEZ, Departamento de Ciencias Naturales, Escuela Tecnológica Instituto Técnico Central, Bogotá-Colombia, JERESON SILVA VALENCIA, Departamento de Física, Universidad Nacional de Colombia, Bogotá - Colombia, EDWIN ER RAMOS, Departamento de Física, Universidad de los Andes, Bogotá - Colombia, MARCOS FIGUEIRA, Instituto de Física, Universidade Federal Fluminense, Niterói-RJ, Brazil — We study thermoelectric properties of coupled quantum dots (QDs), employing the impurity Anderson model (IAM), taking into account strong, but finite electronic correlation in each QD, and a Green's functions approximation with a many-body character [1,2]. We consider two geometrical configurations: two identical immersed QDs in a quantum wire (QW), taking the first QD in different regimes (different energy values) and the second one in the symmetric condition of the IAM; the second geometrical configuration describes a first QD side coupled to a QW for different QD energy values, a second QD in the symmetric condition is immersed in the QW.

Employing linear response theory we compute the electric (G) and thermal (K) conductances, thermopower (S), and the product between the thermoelectric figure of merit and the temperature (ZT) [2] for different temperatures and regimes of the first QD, studying too the validity of the Wiedemann-Franz law and the quantum scattering process and analysing its possible relation with the ZT improves conditions. We obtain specific conditions that enhance ZT (ZT >4) and that would be tested for experimental work.

9:48AM L65.00010: Entropy measurements in mesoscopic circuits: opportunities and limitations

TIM CHILD (Presenter), OWEN SHELLEY, Physics and Astronomy, University of British Columbia, NIKOLAUS GEORGE HARTMAN, Station Q, Purdue University, SILVIA LÜSCHER, JOSHUA FOLK, Physics and Astronomy, University of British Columbia, SAEED FALLAH, Physics and Astronomy, Purdue University, GEOFFREY C. GARDNER, Materials Engineering, Purdue University, MICHAEL MANFRA, Physics and Astronomy, Purdue University — Recently, Hartman et al. demonstrated the capability to measure the entropy of a quantum dot (QD) containing only a few electrons[1] by detecting shifts in the charge state of the dot with temperature, dN/dT. While the measurement technique in Hartman et al. achieved a high level of accuracy, it lacked versatility because it required the system to be in a weakly coupled state that is thermally broadened, and therefore that charge transitions have the standard cosh^2 line-shape of classic Coulomb blockade theory. Here, we show that integrating the dN/dT signal instead of fitting to a particular line-shape enables an entropy measurement of any transition[2], independent of the transition line-shape or even whether the entropy change occurs in the QD itself or another part of the system that is directly coupled to the dot. We demonstrate an entropy measurement for QDs throughout the range from weak to strong coupling to a reservoir. The QD is also sensitive to changes in entropy of other parts of the system, illustrating the potential for this method to be used to measure the entropy of more complex and interesting systems.


*Microsoft, CFI, NSERC, SBQMI, and CIFAR.

10:00AM L65.00011: Measured phase shift using quantum dot interferometer in Kondo regime

YUJIE ZHANG, Keio Univ, RUI SAKANO, Institute for Solid State Physics, University of Tokyo, MIKIO ETO (Presenter), Keio Univ — Phase measurement was reported by the transport through an Aharonov-Bohm ring with an embedded quantum dot, so-called quantum dot interferometer, with three terminals in the Kondo regime [1]. To evaluate how precisely the phase is measured, we theoretically examine the transport through a double quantum dot (DQD) in parallel, as a tractable model for the interferometer. One of the DQD is in the Kondo regime while the other is transparent with a large line width. We report (i) the formulation of transport through the DQD in terms of Keldysh Green functions for three-terminal setup. The conductance at zero temperature is exactly given using the Bethe Ansatz solution. We find that the Kondo temperature changes with a magnetic flux penetrating the ring. (ii) For the conductance as a function of gate voltage (Coulomb peaks), we show a crossover from an asymmetric shape of Fano-Kondo resonance to a symmetric Kondo plateau with an increase in the number of conduction channels in the leads. (iii) The phase locking at \( \pi/2 \) can be measured around the center of Kondo valley in some conditions for the tunnel couplings between the DQD and three leads, although the measured phase is slightly deviated from the Friedel sum rule.

10:12AM L65.00012: Evidence of quantum phase transition in double charge Kondo quantum dots* WINSTON POUSE (Presenter), DAVID GOLDHABER-GORDON, Stanford Univ, ANDREW MITCHELL, Physics, University College Dublin, GERGELY ZARAND, Theoretical Physics, Budapest University of Technology and Economics, CATALIN PASCU MOCA, Physics, University of Oradea, ULF GENNSER, Centre national de la recherche scientifique — The Kondo effect is one of the simplest many body phenomena, in which a single magnetic impurity couples to a continuum of states. Adding a second impurity coupled to the first has been suggested to provide insight into heavy fermion systems. Implementing such impurities in nanofabricated systems with tunable parameters has proven to be a powerful way to compare experiments to theoretical predictions. Recent experimental work demonstrated a new way to realize this type of physics: the charge on a hybrid metal-semiconductor quantum dot coupled to a quantum hall edge state acts as a pseudospin [1]. We build off this design to create a two impurity configuration, with a competition between a dot-dot Kondo interaction and a dot-lead Kondo interaction. We believe this yields a novel quantum critical state. In our device, we controllably tune the various interaction strengths to explore the distinct phases. We provide evidence of a phase transition via transport measurements, with an enhanced conductance when the interaction strengths are comparable.


*Research supported by the U.S. DoE under contract DE-AC02-76SF00515. Early research supported by NSF award 1608962. WP supported by the SGF Fletcher Jones Foundation Fellowship.

10:24AM L65.00013: Majorana bound state in the continuum: Coupling between Majorana bound state and quantum dot mediated by continuum* JUAN RAMOS ANDRADE (Presenter), PEDRO ORELLANA, Physics Department, Federico Santa Maria Technical University, EDSON VERNEK, Physics Institute, Federal University of Uberlândia — In this work, we consider a single-level quantum dot (QD) and a Majorana bound state (MBS) placed at the end of a topological superconducting nanowire (TSW). Both are coupled to the continuum and do not have a direct connection between them. We addressed the behavior of MBS leaking phenomena and its consequences into the QD physics in the non-interacting and Coulomb blockade regime. By employing Green's function formalism via the equation of motion procedure, we calculate the physical quantities of interest. Our results show that the leakage of the MBS into the continuum state is achieved and can alter the physics of Coulomb blockade in the system through continuum-mediated coupling between MBS and QD. As a main consequence, we found a robust and non-trivial mechanism to accomplish a bound state in the continuum in the system.

*J.P.R.-A is grateful for the funding of FONDECYT Postdoc. Grant No. 3190301 (2019). P.A.O. acknowledges support from FONDECYT Grant No. 1180914. E.V. thanks the Brazilian agencies CAPES, CNPq and FAPEMIG for support.
10:36AM L65.00014: Spherical topological-insulator nanoparticles: Quantum size effects and optical transitions*  
LEI YANG (Presenter), Perimeter Inst for Theo Phys, MAX GOLDWATER CHRISTIE, ULRICH ZUELICKE, MICHELE GOVERNALE, ALEXANDER SNEYD, Victoria University of Wellington — We investigate the interplay between band inversion and size quantization in spherically shaped nanoparticles made from topological-insulator (TI) materials. A general theoretical framework is developed based on a continuum-model description of the TI bulk band structure subjected to a hard-wall mass confinement. Analytical results are obtained for the wave functions of single-electron energy eigenstates and the matrix elements for optical transitions between them. Quantized levels in TI nanoparticles can be labeled by angular momentum quantum numbers \( j \) and \( m = -j, -j+1, \ldots, j \). Additionally TIs possess a doubling of energy-level degeneracy due to different parity eigenstates with eigenvalues \((-1)^{j\pm1/2}\). The existence of energy eigenstates having the same \( j \) but opposite parity enables optical transitions where \( j \) is conserved, in addition to those adhering to the familiar selection rule where \( j \) changes by \( \pm 1 \). We treat intra- and inter-band optical transitions on the same footing and establish ways for observing unusual quantum-size effects in TI nanoparticles. Our theory also provides a unified perspective on multi-band models for charge carriers in semiconductors and Dirac fermions from elementary-particle physics.

*LG was supported by a Vanier CGS. MGC was supported by a VUW SRS.

10:48AM L65.00015: Flexible manipulation of quantum dots by single-pulse optical vortices*  
GUILLERMO FEDERICO QUINTEIRO (Presenter), Departamento de Física, Universidad Nacional del Nordeste, PABLO I TAMBORENEA, Departamento de Física, Universidad de Buenos Aires, M HOLTKEMPER, D. E. REITER, T. KUHN, Institut fur Festkörpertheorie, Universität Münster — Optical vortices (OV) are light fields with surprising properties, such as orbital angular momentum (AM), strong longitudinal components, and more, that can be exploited to control matter in new ways. Here we show that a single-pulse of an OV with the right parameters --degree of focusing, polarization, orbital AM, etc-- can precisely manipulate the electronic state of semiconductor quantum dots (QD) [1, 2]. Our models demonstrate the possibility of creating: i) heavy-hole excitons with arbitrary orbital AM, and ii) light-hole excitons with zero band+spin AM, with or without orbital AM. Such states can be named "envelope-forbidden" (i) or "spin-forbidden" (ii), since they cannot be excited by Gaussian light beams. In addition, we present potential applications to quantum technology: spin-forbidden states allow sub-picosecond spin flips of an extra electron charging the QD or the encoding of information on dark excitons, while envelope-forbidden states allow for the generation of currents that can produce magnetic fields at the nanoscale.


*G. F. Q. thanks the ONRG for financial support thought NICOP grant N62909-18-1-2090.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM
8:00AM L66.00001: Actuating and probing a single-molecule switch at femtosecond timescales*

DOMINIK PELLER, LUKAS Z KASTNER, THOMAS BUCHNER, CARMEN ROELCKE, FLORIAN ALBRECHT, RUPERT HUBER, JASCHA REPP (Presenter), Department of Physics, University of Regensburg, Germany — Accessing ultra-fast non-equilibrium phenomena is enabled by terahertz (THz) scanning tunneling microscopy [1] (THz-STM) through combining STM with lightwave electronics. In THz-STM, the electric field of a phase-stable single-cycle THz waveform acts as a transient bias voltage across an STM junction. These voltage transients may result in a net current that can be detected by time-integrating electronics. The recent development of this lightwave STM has enabled the combined femtosecond and sub-angstrom resolution in observing matter [2].

We now demonstrate the first combined femtosecond and sub-angstrom access in the control of matter. Ultrafast localized electric fields in lightwave STM enable exerting atom-scale femtosecond forces to selected atoms. By shaping atomic forces on the intrinsic timescale of molecules, coherent atomic motion can now be excited. Utilizing this coherent structural dynamics, we can modulate the quantum transitions of a single-molecule switch by up to 39%. We directly visualize the coherent excitation of the switch in the first femtosecond single-molecule movie [3].

To resolve the impact of coherent control of the single-molecule switch, alongside, we introduce single-shot action spectroscopy in lightwave STM as the first concept resolving individual path-selective reaction events of a single molecule in space and time. With this novel concept, we detect the outcome of every single laser shot and further separate the statistics of the two inverse reaction paths.

Our results open a new chapter in the control and observation of reactions of individual molecules directly on the relevant ultrafast and ultrasmall scales.

References

*Financial support from the Deutsche Forschungsgemeinschaft (DFG) through SFB 1277 (Project B02) and Research Grant HU1598/3 is gratefully acknowledged.
One major appeal of STM investigations is the unique combination of atomic scale manipulation capabilities with the excellent spectroscopic insight into the electronic structure of 2D materials; providing quasi-static information due to limited preamplifier bandwidth. However, access to the time-domain would enable additional measurement modalities, ranging from the investigation of charge and spin dynamics to the mechanical motion of nanostructures. Despite the early demonstrations by Nunes and Freeman, the widespread implementation of pump-probe methods has remained elusive due to instrumental hurdles. Here we introduce a versatile, straightforward, and affordable setup to achieve nanoseconds time-resolution with minimal changes to an existing STM system [1]. Our setup consists of a dual-channel arbitrary waveform generator, a transfer switch, and a lock-in amplifier. We demonstrate its plug-and-play capability on a field-trip, providing immediate access to the spin-excitation of a magnetic molecule. We further expand our setup to match requirements for pulsed ESR excitations.


*Funding from the Swiss National Science Foundation under project number PP00P2_176866 is appreciated.
9:12AM L66.00003: Single-atom qubits on a surface: pulsed electron spin resonance in a scanning tunneling microscope* [Invited]  KAI YANG (Presenter), IBM Research - Almaden — Recently, the ability to drive electron spin resonance (ESR) of individual atoms using a scanning tunneling microscope (STM) provides a major step forward in sensing and manipulating magnetism at the atomic scale. In the first part, I will describe the implementation of continuous-wave ESR in STM [1], which has allowed the measurement of the magnetic interaction between individual atoms [2–5] as well as the detection and control of nuclear spins [6, 7]. Next, I will talk about coherent spin rotations of individual atoms on a surface with control at the nanosecond timescale, using all-electric pulsed ESR in STM. By modulating the atomically-confined magnetic interaction between the STM tip and surface atoms [8, 9], the large oscillating electric field in the STM junction induces quantum Rabi oscillations between spin-up and spin-down states in as little as ~20 nanoseconds [10]. Ramsey fringes and spin echo signals allow us to understand and improve quantum coherence. I will also show the coherent operations on the coupled-spin states of engineered atomic dimers. Coherent control of spins arranged with atomic precision provides a solid-state platform for quantum simulation of many-body systems.


*We acknowledge financial support from the Office of Naval Research.
Resolving fast dynamics through measurement in the frequency domain* [Invited] RICCARDO BORGANI (Presenter), DAVID HAVILAND, KTH Royal Inst of Tech — The advent of multifrequency lock-in amplifiers has made possible the development of AFM methods that are explicitly designed to exploit the nonlinear nature of the tip-surface interaction. These methods capture information in the frequency domain with high signal-to-noise ratio through measurement of intermodulation between two or more drive tones.

Intermodulation electrostatic force microscopy (ImEFM) [1] is an open-loop alternative to Kelvin-probe force microscopy (KPFM), where the potential of the surface is obtained from a measurement of four frequency components of the force which fall within the cantilever resonance.

We have recently developed a time-resolved variant of ImEFM [2], where the cantilever drive intermodulates with a series of voltage pulses on the sample to produce force components at multiple frequencies around resonance. Measuring these force components we reconstruct dynamic processes in the material with time resolution of 30 nanoseconds, despite of the limited bandwidth (~500 Hz) of the cantilever resonance.

Intermodulation conductive AFM (ImCFM) [3] measures the current-voltage characteristic (IVC) at every pixel of an AFM scan with a speedup of four orders of magnitude in comparison to the traditional time-domain methods. Frequency-domain analysis allows for complete separation of the galvanic current from displacement current in the tip-sample capacitance. The technique also maps the voltage dependence of the tip-sample capacitance, allowing for the investigation of phenomena such as quantum capacitance.


*This work is supported by the Swedish Research Council (VR) and the Knut and Alice Wallenberg Foundation.

Sebastian Loth Invited Talk [Invited] —

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Twisted bilayer graphene (TBG) with a rotational misalignment (twist) angle close to the magic value of 1.1°, features isolated flat electronic bands. These bands form a strongly correlated electronic system that exhibits a range of quantum phases, including superconductivity, ferromagnetism, and correlated insulating states. In this talk, I will present the latest results from our lab on magic-angle graphene obtained using scanning tunneling microscopy/spectroscopy (STM/STS) and transport measurements [1,2]. The local spectroscopy data shows that the flat bands get highly deformed when aligned with the Fermi level. Near half-filling of the bands, we observe the development of gaps originating from correlated insulating states, while near charge neutrality, we find a regime featuring an enhanced flat band splitting that can be described within a model predicting a strong tendency towards nematic ordering. In the second part of the talk, I will discuss transport measurements using novel stack geometry showing the existence of superconductivity in the absence of insulating states. Our findings provide a basis for a microscopic understanding of correlated quantum phases in twisted bilayer graphene.

We acknowledge support from NSF (DMR-1753306 and DMR-1744011) and the Gist-Caltech memorandum of understanding program.

[2] Superconductivity without insulating states in twisted bilayer graphene stabilized by monolayer WSe2
Van der Waals bilayers with an interlayer twist are an excellent platform towards achieving gate-tunable electronic flat bands. A number of emergent phases driven by electron-electron interactions have been observed when tuning the Fermi level through these flat bands. I will present atomically-resolved doping-dependent scanning tunneling spectroscopy studies of two graphene-based systems with emergent correlated phases due to flat bands – magic angle twisted bilayer graphene (tBG) and ABCA graphene, a simple system with a flat band without a moire potential. Our spectroscopy shows that magic angle tBG features two flat bands separated by 40-55 meV. Correlated states emerge when tuning the Fermi level through an individual flat band with minimized bandwidth suggesting the importance of maximized electronic correlations at the magic angle. We measure the correlated insulator gap at half filling and show evidence of nematicity near half-filling in magic angle tBG. I will then show that twisted double bilayer graphene (tDBG) features a fundamentally different moire pattern than tBG, hosting rhombohedral (ABCA) stacking sites. At tiny tDBG angles this creates micron-scale ABCA graphene domains, a robust platform to stabilize the ABCA graphene. Our spectroscopy reveals that ABCA graphene hosts a flat band of 3-4 meV half-width (versus 9-10 meV in magic angle tBG). The unprecedentedly narrow electronic band enhances electronic correlations inducing a correlated gap at charge neutrality making ABCA graphene a model graphene-based correlated system with no moire superlattice potential or integer fillings. Finally, I will show that ABCA graphene hosts topological surface helical edge states which can be turned on and off with gate voltage.
9:12AM L67.00003: Charge order and broken rotational symmetry in magic-angle twisted bilayer graphene* [Invited] JINHAI MAO (Presenter), YUHANG JIANG, University of Chinese Academy of Sciences, XINYUAN LAI, KRISTJAN HAULE, EVA ANDREI, Rutgers University — Bilayer graphene can be modified by rotating (twisting) one layer with respect to the other. The interlayer twist gives rise to a moiré superlattice that affects the electronic motion and alters the band structure. Near a ‘magic angle’ of twist, where the emergence of a flat band causes the charge carriers to slow down, correlated electronic phases including Mott-like insulators and superconductors were recently discovered by using electronic transport. These measurements revealed an intriguing similarity between magic-angle twisted bilayer graphene and high-temperature superconductors, which spurred intensive research into the underlying physical mechanism. Essential clues to this puzzle, such as the symmetry and spatial distribution of the spectral function, can be accessed through scanning tunnelling spectroscopy. Here we use scanning tunnelling microscopy and spectroscopy to visualize the local density of states and charge distribution in magic-angle twisted bilayer graphene. Doping the sample to partially fill the flat band, we observe a pseudogap phase accompanied by a global stripe charge order that breaks the rotational symmetry of the moiré superlattice. Both the pseudogap and the stripe charge order disappear when the band is either empty or full. The close resemblance to similar observations in high-temperature superconductors provides new evidence of a deeper link underlying the phenomenology of these systems.

*NSF-DMR 1708158 (Y.J.), DOE-FG02-99ER45742 (E.Y.A. and J.M.), National Key R&D Program of China (grant number 2018YFA0305800; J.M.), NSF-DMR 1709229 (K.H.)
9:48AM L67.00004: Spectroscopic signatures of many-body correlations in magic-angle twisted bilayer graphene* [invited] YONGLONG XIE (Presenter), Harvard University — The discovery of superconducting and insulating states in magic-angle twisted bilayer graphene (MATBG)\textsuperscript{1,2} has ignited considerable interest in understanding the nature of electronic interactions in this chemically pristine material. The transport properties of MATBG as a function of doping are similar to those of high-transition-temperature copper oxides and other unconventional superconductors\textsuperscript{1-3}, which suggests that MATBG may be a highly interacting system. However, there is no direct experimental evidence of strong many-body correlations in MATBG. In this talk, I will present the unusual spectroscopic characteristics found on MATBG, obtained using a scanning tunneling microscope, and describe how these correlated features allow us to establish a more concrete connection between MATBG and high-T\textsubscript{c} cuprates beyond the phenomenological resemblance of their transport phase diagrams\textsuperscript{4}.


*This work has been primarily supported by the Gordon and Betty Moore Foundation as part of the EPIQS initiative (GBMF4530) and DOE-BES grant DE-FG02-07ER46419. Other support for the experimental work was provided by NSF-MRSEC programmes through the Princeton Center for Complex Materials DMR-142054, NSF-DMR-1608848, ExxonMobil through the Andlinger Center for Energy and the Environment at Princeton, and the Princeton Catalysis Initiative.

10:24AM L67.00005: Spectroscopy and Correlation Effect at Magic Angle [invited] BIAO LIAN (Presenter), Princeton University — The twisted bilayer graphene (TBG) near the magic angle develops topological flat electron bands at low energies, and exhibits both superconducting and correlated insulating phases at low temperatures. The STM spectroscopy measurements of magic angle TBG shows that the differential tunneling conductances dI/dV at both low and relatively high temperatures have a strong dependence on the doping density in the flat bands. We show that the Hartree Fock mean field theory with spontaneous spin/valley polarization and strain effect fails to capture the spectroscopy at the magic angle. Instead, we show that charge correlation effects beyond the mean field theory are significant for explaining the spectroscopy data, and can be demonstrated in the exact diagonalization of a phenomenological Hubbard model. We also discuss the possible effects of phonon-mediated electron interaction. Lastly, we talk about the effects of the TBG band topology on the Hofstadter butterfly and the interacting phases.

Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L68 DBIO: The Many Dimensions of Evolution Four Seasons 4 - Mikhail Tikhonov, Washington University, St. Louis - Tag(s): Invited, Undergrad Friendly
8:00AM L68.00001: The ecology and evolution of collective behavior [Invited] DEBORAH GORDON (Presenter), Biology, Stanford University — Ant colonies operate without central control, using feedback from simple olfactory interactions to regulate their activities. There are more than 14K species of ants in every habitat on Earth, using diverse stochastic algorithms, producing different feedback regimes, in different environments. These algorithms have evolved to fit the dynamics of particular environments, including energy flow, stability, and the threat of rupture. Harvester ants in the harsh but stable conditions of the desert, regulate foraging effort according to current food availability and humidity, using excitable dynamics based on the rate of contact inside the nest between returning and outgoing foragers. The feedback system sets a default of inactivity unless conditions are favorable. For turtle ants in the trees of the tropical forest, high humidity makes activity easy but competition is high. Their trail networks are constrained to follow the network of vegetation. They use the rate of deposition of a volatile pheromone to build and maintain a distributed routing network in heterogeneous environments, based on design principles that differ from the shortest paths commonly studied in ants and in network science. The feedback system sets a default of persistent activity unless conditions are unfavorable. The diversity of ants provides opportunities to learn how collective behavior evolves to fit diverse environmental dynamics.

8:36AM L68.00002: Attack of the clones: what causes population structure in bacteria and how can we use it? [Invited] WILLIAM HANAGE (Presenter), Epidemiology, Harvard T. H. Chan School of Public Health — In most pathogenic bacteria, the population is made up of multiple distinct lineages or ‘clones’ which are associated with properties like virulence or drug resistance. For the most part, this structure has been taken for granted and its root causes not been examined. We have recently shown, using the pneumococcus as a model organism, that we can explain which clones are present in a community with a simple model of negative frequency dependent selection operating on a subset of the genome: namely the accessory genome of loci not present in all isolates of the species. Moreover, we can use this to predict the consequences of removing some clones, for instance through vaccination. This can be achieved either through a game theory approach using the replicator equation, or through quadratic programming to determine how the equilibrium properties of the population as a whole can be restored by altering the proportions of each clone. Finally the existence of clones offers an opportunity to use emerging DNA sequencing technologies to rapidly detect them in clinical samples, which could be useful for detecting and responding to drug resistant threats.

*National Insitutes of Health (NIH) R01 AI106786 and the Bill & Melinda Gates Foundation GCGH GCE OPP1151010
9:12AM L68.00003: Evolutionary dynamics in large microbial communities [Invited]  BENJAMIN GOOD (Presenter), Stanford Univ — Microbial communities drive important biochemical cycles, from the ocean to the soil to the human gut. High rates of cell turnover endow these communities with an enormous potential for rapid evolutionary change – e.g., billions of new mutations are produced within a single gut microbiome every day. Despite the potential importance of these effects, we currently know very little about the evolutionary dynamics that take place in large microbial communities, and how these dynamics might deviate from our single-species intuition. In this talk, I will describe our recent efforts to address this question using data from the human gut microbiome. I will show how population genetic analysis of sequenced fecal samples can help us quantify the typical timescales of within-host evolution, and how this might constrain the ability of a community to adapt to fluctuating environmental conditions.

9:48AM L68.00004: Microbial interactions across time and space * [Invited]  BRITT KOSKELLA (Presenter), University of California, Berkeley — There is great interest in explaining microbial diversity, but a critical first step that is often downplayed is understanding the spatial and temporal scales that are relevant to the system. In this talk I discuss the relative importance of interactions among bacteria and phage viruses, between bacterial strains and species within a microbiome, and between a host and its symbionts to emphasize the role of evolution and coevolution in shaping diversity across scales. I focus primarily on the plant phyllosphere as a model system to explore these interactions both in natural, ecologically complex, and simple experimental systems.

*National Science Foundation, Winkler Faculty Fund
 Phenotypic heterogeneity between genetically identical cells permits growth with lethal levels of formaldehyde stress* [Invited] JESSICA A LEE, SIAVASH RIAZI, Biological Sciences, University of Idaho, SHAHLA NEMATI, Physics, University of Idaho, JANNELL V BAZURTO, Biological Sciences, University of Idaho, ANDREAS E VASDEKIS, Physics, University of Idaho, BENJAMIN J RIDENHOUR, CHRISTOPHER H REMIEN, Mathematics, University of Idaho, CHRISTOPHER MARX (Presenter), Biological Sciences, University of Idaho — Scientists tend to appreciate microbes for their simplicity and predictability: a population of genetically identical cells inhabiting a uniform environment is expected to behave in a uniform way. However, counter-examples to this assumption are frequently being discovered, forcing a re-examination of the relationship between genotype and phenotype. In most such examples, bacterial cells are found to split into two discrete populations, for instance growing and non-growing. Here, we report the discovery of a novel example of microbial phenotypic heterogeneity in which cells are distributed along a gradient of phenotypes, ranging from low to high tolerance of a toxic chemical. Furthermore, we demonstrate that the distribution of phenotypes changes in different growth conditions, and we use mathematical modeling to show that cells may change their phenotype either randomly or in a particular direction in response to the environment. Our work expands our understanding of how a bacterial cell's genome, family history, and environment all contribute to its behavior, with implications for the diverse situations in which we care to understand the growth of any single-celled populations.

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Wednesday, March 4, 2020 8:00 AM - 11:00 AM

Session L70 DPOLY DSOFT: Vitrimers and Associative Networks 208 -
Christopher Evans, University of Illinois at Urbana-Champaign - Tag(s): Focus
8:00AM L70.00001: Microscopic Theory of the Role of Strong Attractions on the Local Dynamics and Elasticity of Associating Copolymer Liquids  
ASHESH GHOSH (Presenter), KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — We construct a microscopic liquid state theory for how attractions between sticky groups regularly co-polymerized in a chain backbone affect local structure and dynamics of unentangled polymer liquids. Based on the bare attractive interaction and single-chain structure as input, PRISM integral equation theory is combined with activated dynamics approaches that capture caging and physical bond formation to study emergent high frequency elasticity and local relaxation processes. The dynamic free energies and corresponding sticker and non-sticker barrier hopping timescales that define the coupled bond breakage and cage escape processes are predicted within a 2-step dynamical scenario that applies in the strong attraction regime. The first step involves non-sticker hopping (alpha process) which is perturbed due to physical bonds between sticky segments that act as pinning constraints. After the non-sticker hops, the dynamical constraints and friction experienced by the sticky groups are renormalized and activated bond-breaking defines the second step. We present representative results for structure and dynamics as a function of sticker fraction, strength and range of the attraction, density, and temperature. Connections between dynamics and equilibrium properties are identified.

8:12AM L70.00002: LINEAR VISCOELASTICITY AND FLOW OF SELF-ASSEMBLED VITRIMERS: THE CASE OF A POLYETHYLENE/DIOXABOROLANE SYSTEM  
RALM RICARTE (Presenter), Florida State Univ, FRANÇOIS TOURNILHAC, MICHEL CLOÎTRE, Molecular, Macromolecular Chemistry, and Materials, ESPCI Paris, LUDWIK LEIBLER, Gulliver, ESPCI Paris — We investigated the linear viscoelasticity of a polyethylene (PE) vitrimer that has cross-linkable dioxaborolane maleimide grafts. Strong interactions between the PE backbone and grafts cause the molten vitrimer to macro- and microphase separate into hierarchical structures. Small-amplitude oscillatory shear, stress relaxation, and creep measurements were used for characterization. Graft functionalized PE (which does not contain cross-linker, but still self-assembles) had a terminal relaxation time that was two orders of magnitude larger than neat PE. When cross-linker was added to form the vitrimer, the material exhibited a higher melt strength but did not achieve steady-state flow within 8 hr. The soluble graft-poor portion of PE vitrimer had similar flow behavior as neat PE, but its flow activation energy was twice as large. Conversely, the insoluble graft-rich fraction behaved as a viscoelastic solid that relaxed very little over 8 hr. Blend experiments suggested the interface between the graft-rich and graft-poor phases of PE vitrimer also influenced relaxation. These findings indicate that self-assembly/associative cross-linking interplay greatly impacts the rheology and, consequently, processability of vitrimers.
Effect of salt on viscoelasticity and conductivity in vitrimers and dynamic networks

8:24AM L70.00003: BRIAN JING (Presenter), CHRISTOPHER EVANS, University of Illinois at Urbana-Champaign — Polymer networks with associative dynamic bonds (vitrimers) have been investigated as recyclable and self-healing materials. We have developed vitrimers made from polyethylene glycol, dynamic boronic ester crosslinks, and added Li salt that function as Li-ion conductors. These networks were studied over a range of Li:ethylene oxide (Li:EO) ratios to understand the effect of salt concentration on conductivity and viscoelasticity. The storage modulus decreases from 10 to 0.5 MPa at room temperature with added salt, attributed to boron-anion interactions which decrease the number of elastically active boron centers (supported by $^{11}$B NMR analysis). The temperature dependent moduli also show a crossover of $G'$ and $G''$ which occurs at ~100 °C (at 1 Hz) in a neutral system and drops by 85 °C with added salt. Conductivities up to $3 \times 10^{-4}$ S/cm were measured (solvent-free) at 90 °C, and go through a maximum which is attributed to the competition of added salt and increasing Tg. The networks can also be dissolved in water back to monomer and recover conductivity after damage due to the dynamic bonds. Finally, we discuss how these vitrimers transition to dissociative networks with added salt due to anion-boron interactions which lead to non-Arrhenius stress relaxation times.

Understanding the Self-healing of Reversible Polymer Networks through Molecular Dynamic Simulation*

8:36AM L70.00004: ZHIQIANG SHEN (Presenter), HUILIN YE, YING LI, Univ of Connecticut - Storrs — Hydrogels with reversible crosslinking motifs exhibit extraordinary short healing time and high healing strength. However, the understanding about the self-healing behavior of reversible polymer network is limited. Especially, the key problem about relation between the microscopic evolution of polymer networks and the macroscopic stress-strain behaviors during the self-healing process remains largely elusive. In this work, a molecular dynamics / Monte Carlo hybrid coarse-grained model is developed to investigate the relaxation and self-healing behaviors of polymer networks with reversible crosslinking. We systematically investigate the shelf-healing process of the polymer network with a fracture. It is found that the polymer chains at the fracture interface can diffusive through the interfacial gap and form new crosslinking bonds, resulting the recovery of polymer network mechanical strength. We found that the healing time is both determined by the dwelltime of the dynamic bond and relaxation of the polymer chains. Our simulations provide a direct relation between dynamic bond and the self-healing process, which might provide an insight for the design of smart self-healing polymers.

*NSF-CMMI-#1762661
Collaborative Research: Interfacial Self-healing of Nanocomposite Hydrogels
8:48AM L70.00005: Role of Dynamic Bonds on Crystallization in Polyethylene Vitrimers
BHASKAR SOMAN (Presenter), CHRISTOPHER EVANS, University of Illinois at Urbana-Champaign —
Crystallization of linear polyethylene (PE) has been extensively investigated for decades. Here, we
study the effects of dynamic bonds on the crystallization in PE vitrimers by preparing networks
with exactly 8, 10, and 12 carbons (C₈-C₁₂) between dynamic boronic ester crosslink points. The
C₁₂ networks crystallize immediately upon cooling, while C₈ networks only show evidence of
crystallization after waiting multiple weeks at 20 °C. The C₁₀ networks show intermediate initial
crystallization. Samples were aged at room temperature for 30 days, and in all cases, monotonic
increase in melting temperature (Tₘ) is observed which is attributed to dynamic bonds allowing
local rearrangements of network strands in the amorphous regions or at the crystal-amorphous
interface. A control sample of linear PE shows instant crystallization and no substantial long term
Tₘ evolution. Initial melting temperatures are analyzed in the Hoffman-Weeks framework, and
reasonably predict the long-time Tₘ of orthorhombic crystal. Upon aging, a transition in the
morphology is observed via wide-angle x-ray scattering and the time required for the transition
tracks with dynamic bond density. Finally, we demonstrate that step annealing can result in PE
networks with Tₘ approaching 100 °C.

9:00AM L70.00006: Tuning vitrimer mechanics with prepolymer and crosslinker structure*
JULIA KALOW (Presenter), Northwestern University — Dynamic covalent polymer networks in which
the topology is reconfigured through associative exchange reactions are known as vitrimers.
These materials hold promise as repairable and recyclable thermosets and elastomers. A
hallmark of vitrimers is the Arrenhius relationship between viscosity and temperature; the
activation energy for stress relaxation is often used to describe the energetics of the
reconfiguration process. However, the mechanistic interpretation of this activation energy and its
relationship to the associative exchange event are often unclear. We combine physical organic
approaches and mechanical characterization to correlate the activation energy for stress
relaxation to molecular reactivity and macromolecular structure. This study is enabled by the use
of crosslinks that exchange via a catalyst-free conjugate addition/elimination pathway.

*This material is based upon work supported by the National Science Foundation under grants
no. CHE-1901635 and CHE-1832256.

9:12AM L70.00007: Catalyst and Architecture Effects in Polyester Dynamic Covalent
Materials [Invited] CHRISTOPHER BATES (Presenter), University of California, Santa Barbara —
Polyester networks that include dynamic covalent bonds have attracted significant attention as
materials with tunable plasticity. This talk will discuss the role of catalyst strength and building
block architecture on dynamic covalent polyester exchange kinetics and mechanical properties.
To do so, we introduce a versatile synthetic platform that provides good control over network
connectivity through formulation and precursor design. The fundamental insights described
herein expand the utility of crosslinked polyesters by broadening the range of accessible material
properties.
9:48AM L70.00008: Recycling of Poly(thiourethane) Thermosets Enabled by Thiourethane Bonds  SIJIA HUANG (Presenter), MACIEJ PODGORSKI, XUN HAN, CHRISTOPHER BOWMAN, University of Colorado, Boulder — Recycling of polyurethanes is an inviable process due to the harsh reprocessing conditions and high risk of side reactions. Constructing polymer networks incorporating covalent dynamic bonds becomes an attractive strategy in the design of recyclable materials. Here, we report findings on the dynamic nature of thiourethanes, and their application as a new class of recyclable analogs of urethane materials. A series of small molecule experiments was initially conducted to determine equilibrium constant and reverse reaction kinetic constant for the thiourethane reaction. Furthermore, incorporating those thiourethane moieties into a cross-linked network resulted in thermoset materials that can be facilely depolymerized to liquid oligomers. The resultant oligomers can be recrosslinked back to thiourethanes without any loss of performance nor properties (peak stress of 30 MPa with Young's modulus of 1 GPa). Moreover, the increase in value that thiourethane network can undergo when upcycled to the thiol oligomer enables a potential pathway to build materials with properties that exceed its pristine material. Overall, this reprocessing strategy may advance many global sustainability goals, and is applicable to other low-cost commodity materials.

10:00AM L70.00009: Rheology and Rupture of Partial Vitrimer  SHENGQIANG CAI (Presenter), University of California, San Diego — Polymer network with dynamic covalent bonds, also known as vitrimer, exhibit interesting mechanical behaviors which are very different from conventional polymers. Because of the bond exchanging reactions, vitrimers have shown great potential as excellent recyclable polymers with self-healing capability. Our recent experiments have shown that the mechanical properties of a vitrimer such as fracture toughness and stress relaxation can be greatly tuned by selectively mixing the polymer chains with dynamic covalent bonds and routine covalent bonds (referred as partial vitrimer), while the self-healing capability of the polymer can be still maintained. To quantitatively understand the stress relaxation of the partial vitrimer, we developed a simple rheological model for it with certain combinations of spring and dashpot. We have also developed a simple energy argument to explain the rupture phenomenon of vitrimer under different mechanical loading conditions.
10:12AM L70.00010: Investigation of viscoelastic behavior over wide temperature range in PDMS vitrimers  LAURA PORATH (Presenter), CHRISTOPHER EVANS, University of Illinois at Urbana-Champaign — We have prepared vitrimers of poly(dimethyl siloxane) containing dynamic boronic ester bonds to investigate the viscoelastic properties of dynamic networks with extremely low T_g. The stress relaxation times and frequency dependent behavior are probed over a > 200 °C window and show the anticipated Arrhenius behavior at temperatures ranging from 180 to 40°C. The relaxation times here are independent of network strand molecular weight, which varies from 550-11,000 g/mol. We consider this temperature range to be a reaction-limited regime far above T_g, where bond exchange kinetics dominate macroscopic relaxation. Below 40°C, non-Arrhenius behavior emerges, and the apparent activation energy decreases. Time-temperature-superposition of frequency sweeps shows that the flow regime is thermorheologically simple, while the modulus of the plateau regime increases with increasing temperature, which is consistent with a preserved network architecture. As stress relaxation times speed up by orders of magnitude, the rubbery plateau modulus increases, which leads to a strategy for decoupling dynamics from mechanics. Our studies point to the importance of measuring vitrimer properties over a broad temperature window to understand the full range of response in this class of dynamic network.

10:24AM L70.00011: Intrinsically reprocessable, self-healing elastomers  LIHENG CAI (Presenter), Univ of Virginia — Conventional elastomers formed by solely permanent, chemical crosslinks are not reprocessable, which causes environmental burden to the society. By contrast, networks crosslinked by solely reversible, physical bonds are reprocessable and self-healable. The physical bonds, however, are much weaker than chemical crosslinks, limiting the strength of the resulted polymer networks. Here, we propose a concept that exploits the self-assembly of block copolymers integrating strong physical associations and weak reversible hydrogen bonds to create an intrinsically reprocessable, self-healing elastomer. We find that the reversible bonds promote the formation of ordered nanostructures, which, in turn, result in unique macroscopic mechanical properties. Our results provide insights on the development of intrinsically reprocessable, self-healing elastomers.
10:36AM L70.00012: Melt Recyclable Shape Memory Elastomers through Main Chain Association* 

DANIEL KRAJOVIC (Presenter), MITCHELL ANTHAMATTEN, University of Rochester — Shape memory (SM) elastomers can undergo triggered actuation from metastable, deformed states to permanent shapes, offering diverse applications. Covalently crosslinked, semicrystalline SM networks are capable of storing large amounts of elastic energy (>3 MJ/m$^3$) with full recovery, however, these materials cannot be melt-processed or recycled. Here, we demonstrate that replacing covalent crosslinks with hydrogen bond interactions can enable fully melt recyclable SM elastomer with little performance loss. Two high molecular weight poly(caprolactone)s with interchain hydrogen bonding groups have been synthesized and show excellent strain fixation and shape recovery both before and after shredding, melt-pressing, and reannealing. Dynamic mechanical analysis reveals a stiffness plateau that persists to temperatures above the shape-triggering temperature. Stress relaxation studies suggest chain disentanglement is the primary relaxation mode. Disentanglement is sluggish just above the trigger temperature and is much faster at higher temperatures where plastic flow can occur. The role of the polymers’ hard segment associative strength and a first-cycle training effect are under continued investigation.

*Funding was provided by NSF under Grant ECCS-1530540.

10:48AM L70.00013: Leveraging the Stability of Ionic Liquids in Processing Polyampholytes 

DAVID DELGADO (Presenter), Northwestern University, JIAN PING GONG, Global Station for Soft Matter, Global Institution for Collaborative Research and Education, Hokkaido University, KENNETH R SHULL, Northwestern University — Double network gels composed of polyampholytes have been shown to have both tough and strong properties due to both inter and intra electrostatic bonding. Upon deformation, the weaker bonds break and dissipate energy allowing the gel to be load bearing despite retaining up to 90% water. While these gels are suited for bulk applications such as the knee or achilles heel, it remains a challenge to fabricate thin films that can coat non-planer surfaces such as the hip joint. Traditional polyelectrolyte processing has used salt to screen bonds and move across the polyelectrolyte coacervate continuum. Upon evaporation of water, however, this salt can recrystallize and disrupt film morphology. In this work, an ionic liquid composed of choline chloride and urea is used to dissolve and rapidly deposit double network gels. Moreover, in contrast to salt processing, the ionic liquid is stable at ambient conditions. Finally, rheological studies and phase diagrams are presented to understand the interplay between ionic liquid, polyampholyte, and water.

Wednesday, March 4, 2020 8:00 AM - 9:30 AM

Session L71 APS: Tutorial for Authors and Referees (8:00am - 9:30am)
8:00AM L71.00001: Tutorial for Authors and Referees (8:00am - 9:30an) — Editors from Physical Review Letters and Physical Review will provide information and tips for our less experienced referees and authors. This session is aimed at anyone looking to submit to or review for any of the APS journals, as well as anyone who would like to learn more about the authoring and refereeing processes. Topics for discussion will include advice on how to write good manuscripts, similarities and differences in writing referee reports for PRL and PR, and other ways in which authors, referees, and editors can work together productively. Following a short presentation from the editors, there will be a moderated discussion.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M01 DAMOP DCMP: Non-Equilibrium Physics with Cold Atoms and Molecules, Rydberg Gases, and Trapped Ions 103 - Vito Scarola, Virginia Tech - Tag(s): Focus

11:15AM M01.00001: Probing quench dynamics across a quantum phase transition into a 2D Ising antiferromagnet [Invited] WASEEM BAKR (Presenter), Princeton — Strongly interacting dynamics of quantum magnets is a frontier area of many body physics, and Prof Bakr's results are some of the most exciting in the area.

11:51AM M01.00002: Dynamics of a hole in a quantum antiferromagnet ANNABELLE BOHRDT (Presenter), Tech Univ Muenchen, FABIAN GRUSDT, Physics Department, Ludwig-Maximilians-Universität München, MICHAEL KNAP, Tech Univ Muenchen, JAYADEV VIJAYAN, PIMONPAN SOMPET, GUILLAUME SALOMON, JOANNIS KOEPSELL, SARAH HIRTHE, IMMANUEL FELIX BLOCH, CHRISTIAN GROSS, Max-Planck-Institut for Quantum Optics, Garching — Understanding the properties of a single mobile hole doped into an antiferromagnet allows one to reveal the interplay of spin and charge degrees of freedom. This constitutes a crucial step in the theoretical description of the Fermi-Hubbard model and by extension, strongly correlated cuprate compounds. We experimentally study the dynamical deconfinement of spin and charge excitations in real space in one dimensional Fermi-Hubbard chains of ultracold atoms. Using space- and time-resolved quantum gas microscopy, we track the evolution of the excitations through their signatures in spin and charge correlations. We numerically study the real-time dynamics of a single hole created in the ground state of the t−J model on a square lattice. Initially, the hole spreads ballistically with a velocity proportional to the hopping matrix element. At intermediate to long times, the hole propagates again ballistically but with a velocity proportional to the spin exchange coupling, showing the formation of a magnetic polaron. We provide an intuitive explanation of this dynamics in terms of a parton construction.
12:03PM M01.00003: Many-Body Dephasing after Quantum Quench with a Trapped Ion Quantum Simulator  
LINGZHEN GUO (Presenter), Max Planck Inst for Sci Light, HARVEY B KAPLAN, WEN LIN TAN, ARINJOY DE, GUIDO PAGANO, University of Maryland Department of Physics and NIST, FLORIAN MARQUARDT, Max Planck Inst for Sci Light, CHRISTOPHER ROY MONROE, University of Maryland Department of Physics and NIST — We investigate many-body dephasing in the 1D transverse-field Ising chain with long-range power-law interactions. We work in a regime where the properties of the system are closely related to the integrable Hamiltonian with global spin-spin coupling, which enables analytical predictions even for the long-time non-integrable dynamics. We study the dependence of temporal fluctuations of the average magnetization as a function of the system size. Using the eigenstate thermalization hypothesis (ETH), we are able to give an analytical expression for the temporal fluctuations. We also show the first experimental observation of persistent temporal fluctuations after a quantum quench. The measured fluctuations are exponentially suppressed with increasing system size, which is consistent with our theoretical predictions.

12:15PM M01.00004: Subdiffusion and Heat Transport in a Tilted 2D Fermi-Hubbard System*  
ELMER GUARDADO-SANCHEZ, ALAN MORNINGSTAR (Presenter), BENJAMIN M SPAR, PETER T BROWN, DAVID HUSE, WASEEM S BAKR, Princeton University — We study the late-time effective hydrodynamics of an isolated cold-atom Fermi-Hubbard system subject to an external linear potential (a “tilt”). We do this by observing the decay of prepared initial density waves as a function of wavelength \( \lambda \) and tilt strength and find that the associated decay time \( \tau \) crosses over as the tilt strength is increased from characteristically diffusive to subdiffusive with \( \tau \propto \lambda^4 \). In order to explain the underlying physics we develop a hydrodynamic model that exhibits this crossover. For strong tilts, the subdiffusive transport rate is set by a thermal diffusivity, which we are thus able to measure as a function of tilt in this regime. We further support our understanding by probing the local inverse temperature of the system at strong tilts, finding good agreement with our theoretical predictions.

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**12:27PM M01.00005: Reservoir engineering and many-body decoherence in the quantum Ising model**

LINCOLN CARR (Presenter), DANIEL JASCHKE, Physics Dept., Colorado School of Mines, INES DE VEGA, Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-University Munich — We present quantitative predictions for quantum simulator experiments on Ising models from trapped ions to Rydberg chains and show how the thermalization, and thus decoherence times, can be controlled by considering common, independent, and end-cap couplings to the bath. We find (i) independent baths enable more rapid thermalization in comparison to a common one; (ii) the thermalization timescale depends strongly on the position in the Ising phase diagram; (iii) for a common bath larger system sizes show a significant slowdown in the thermalization process; and (iv) finite-size scaling indicates a subradiance effect slowing thermalization rates toward the infinite spin chain limit. We find it is necessary to treat the full multi-channel Lindblad master equation rather than the commonly used single-channel local Lindblad approximation to make accurate predictions on a classical computer. This method reduces the number of qubits one can practically classical simulate by at least a factor of 4, in turn showing a quantum advantage for such thermalization problems at a factor of 4 smaller qubit number for open quantum systems as opposed to closed ones. Thus, our results encourage open quantum system exploration in noisy intermediate-scale quantum technologies.

*Funded by NSF.

**12:39PM M01.00006: Spin squeezing dynamics and large-spin analogues in an optical lattice clock**

MICHAEL PERLIN (Presenter), ANA MARIA REY, JILA — Spin squeezing has been studied for decades as a means to overcome the so-called standard quantum limit for measurement precision. Despite numerous proof-of-principle experiments, however, spin squeezing has yet to push the state-of-the-art in any practical sensing application. We summarize a recent proposal to generate spin squeezing dynamics of two-level Sr-87 atoms in a 3D optical lattice clock, a world-class measurement system. Our proposal combines interactions and spin-orbit coupling to generate spin-squeezed states that are robust to typical sources of experimental noise. We then discuss generalizations of our protocol to the case of multilevel fermions with SU(n)-symmetric interactions, which have been experimentally realized with nuclear spin degrees of freedom. We show how the multilevel generalization of interactions, spin-orbit coupling, and external driving fields can be treated in a simple, unified form. Finally, we discuss prospects to explore the rich dynamics of interacting multilevel systems, such as multilevel spin squeezing and SYK-like models that may feature fast scrambling behavior.

*This work is supported by AFOSR grant FA9550-18-1-0319; the AFOSR MURI grant; DARPA ARO grant W911NF-16-1-0576; NSF grant PHY-1820885; JILA-NSF grant PFC-1734006; and NIST.
12:51PM M01.00007: Dynamic instabilities and universal relaxation in quantum spin systems  JOAQUIN RODRIGUEZ NIEVA (Presenter), Stanford University, SARASWAT BHATTACHARYYA, Oxford, DRIES SELS, EUGENE DEMLER, Harvard University — The presence of symmetries and conservation laws can have striking manifestations in the dynamic behavior of interacting quantum systems. I will discuss manifestations of SU(2) symmetry on the universal dynamics of Heisenberg ferromagnets driven out of equilibrium. In particular, I will address the emergence of universal phenomena at two different timescales. Firstly, I will discuss the long-time thermalization behavior of a non-equilibrium incoherent population of magnons, and show that the distribution function can exhibit self-similar behavior in the prethermal regime[1]. Secondly, I will present a new mechanism for dynamic instabilities in a spin spiral state occurring at short timescales, and which originates from the symmetry-constrained quasiparticle interactions[2]. These two seemingly distinct phenomena provide new links between symmetries and universal phenomena occurring at different timescales.

1:03PM M01.00008: Non-local emergent hydrodynamics in a long-range quantum spin system* ALEXANDER SCHUCKERT (Presenter), IZABELLA LOVAS, MICHAEL KNAP, Technical University of Munich — Generic short-range interacting quantum systems with a conserved quantity exhibit universal diffusive transport at late times. We show [1] how this universality is extended by effective classical Lévy flights in the presence of long-range couplings that decay algebraically with distance as r^{-\alpha} for 0.5<\alpha\leq1.5. We investigate this phenomenon in a long-range interacting XY spin chain at infinite temperature by employing non-equilibrium quantum field theory and semi classical phase-space simulations. We find that the space-time dependent spin density profiles are self-similar, with scaling functions given by the stable symmetric distributions. Hence, autocorrelations show hydrodynamic tails decaying in time as t^{-1/(2\alpha-1)}. We also extract the associated generalized diffusion constant, and demonstrate that it follows the prediction of Lévy flights; quantum many-body effects manifest themselves in an overall time scale depending only weakly on \alpha. Our findings can be verified with current trapped ion experiments.
*Support: Max Planck Gesellschaft through IMPRS-QST; Technische Universität München – Institute for Advanced Studies funded by the German Excellence Initiative and the EU-FP7 under grant agreement 291763
Nonequilibrium dynamics and transport in the frustrated two bath spin boson model

RON BELYANSKY (Presenter), SETH P WHITSITT, REX LUNDGREN, YIDAN WANG, ALEXEY V GORSHKOV, University of Maryland, College Park — The spin-boson model, describing a single two-level system coupled to an Ohmic bath of harmonic oscillators, is a paradigmatic model of open quantum systems. It has been used to understand the connection between quantum dissipation and classical friction and has been applied to a wide range of phenomena ranging from quantum impurity problems to quantum information, biological systems, and state of the art superconducting circuits experiments. In this work, we use numerical and analytical methods to study the dynamics of a generalized spin boson model where the spin is coupled to two independent Ohmic baths via non-commuting operators. It has already been shown that the two competing baths lead to peculiar effects, namely the absence of the phase transition and the coherent to incoherent crossover in the spin dynamics, both of which are well-known features of the single bath system. Here, we explicitly show how the frustration leads to reduced decoherence in the spin dynamics following a quantum quench. We also study the single-particle transport properties of a quasi 1D realization of the model and show asymmetrical features in the intra- and inter-bath elastic and inelastic scattering.

Unravelling open quantum systems on a NISQ Computer

FRANCESCO PETRUCCIONE (Presenter), ILYA SINAYSKIY, Univ of KwaZulu-Natal, KYUNGDEOCK PARK, JUNEOO KEVIN) RHEE, Korea Advanced Institute of Science and Technology — It is well-know that the simulation of the stochastic Schrödinger equations unravelling the typical master equations describing the dynamics of open quantum systems is a very useful computational tool. Here, we show how such unravellings can be simulated on a NISQ computer. The quantum algorithm maintains the cost of initial state preparation constant via quantum forking. Quantum forking creates an entangled state in which a single copy of a quantum state is encoded and evolves under independent quantum processes in each subspace, thereby allowing parallel unravelling from one wave function. A protocol for implementing a generic non-Hermitian evolution using quantum circuit elements is described. The algorithm is applied to the simulation of Markovian master equations describing quantum neural networks.

Linear response theory for the OTOC and entropy growth in dissipative systems

XIN CHEN (Presenter), Tsinghua University — We formulate the linear response theory to calculate the out-of-time ordered correlator (OTOC) and the entropy growth for dissipative systems, i.e. systems suddenly coupled to a thermal bath, which helps to understand the behavior of the information scrambling in the early stage. In addition, we also discuss the linear response of the OTOC to a perturbation for systems that are constantly coupled to a thermal bath and reaches the non-equilibrium static state. Particularly, we illustrated those calculations in the Dicke model.
1:51PM M01.00012: Prethermal non-equilibrium phases in classical systems  BINGTIAN YE (Presenter), FRANCISCO MACHADO, NORMAN YAO, University of California, Berkeley — High-frequency driven quantum systems exhibit long-lived prethermal regimes, where the dynamics are described by effective static Hamiltonians. The existence of such prethermal regime allows exotic non-equilibrium phases to emerge. However, generalizing these phenomena to classical many-body systems remains challenging. In our work, we elucidate the nature of the prethermal regime in classical spin systems. We first demonstrate that the chaotic nature of the classical evolution places an obstacle to define an effective prethermal Hamiltonian: for an initial state, any small error in the dynamics becomes exponentially magnified over time. While such obstacle is inevitable for a single classical trajectory, an effective description can still arise when considering the evolution of an ensemble of states. This then allows us to extend the properties of quantum prethermal dynamics to classical systems. In particular, we prove the existence of an emergent symmetry in the prethermal regime, and utilize this symmetry to generate novel non-equilibrium phases such as classical prethermal discrete time crystals (CPDTC). Finally, we will present an analytical framework as well as numerical demonstration of CPDTC.

2:03PM M01.00013: Engineering generalized Gibbs ensembles with trapped ions  FLORENTIN REITER (Presenter), Institute for Quantum Electronics, ETH Zurich, FLORIAN LANGE, Institute for Theoretical Physics, University of Cologne, SHREYANS JAIN, MATT GRAU, JONATHAN P HOME, Institute for Quantum Electronics, ETH Zurich, ZALA LENARCIC, Department of Physics, University of California, Berkeley — Generalized Gibbs ensembles (GGEs) have been introduced to describe stationary expectation values of local observables in integrable models with macroscopically many conservation laws. Recent advances showed that GGEs also describe more realistic nearly integrable systems which are weakly driven and open. In this case, integrability breaking perturbations determine the parameters of GGE. By tuning the coupling to the environment, it is thus possible to stabilize a broad range of tailored GGEs. Here we pave the way for the first experimental observation of GGEs in a nearly integrable driven-dissipative setup with trapped ions. We present an implementation scheme for a particular choice of Lindblad operators and suggest experimental observables which detect that a GGE approximately describes the stabilized steady-state. To engineer single-, as well as two-body dissipation, we use a combination of couplings which can be engineered in an array of microtraps. We assess the performance of our implementation scheme and discuss the resources required to observe a deviation from a thermal ensemble in an experiment.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M02 DAMOP: Optomechanics  105 - Srivatsan Chakram, University of Chicago
11:15AM M02.00001: Efficient bidirectional piezo-optomechanical transduction between microwave and optical frequency*  Wentao Jiang (Presenter), Christopher J Sarabalis, Yanni D Dahmani, Rishi Patel, Felix M Mayor, Timothy Mckenna, Raphael Van Laer, Amir Safavi-Naeini, Stanford Univ — Efficient interconversion of both classical and quantum information between microwave and optical frequency is an important engineering challenge. The optomechanical approach with gigahertz-frequency mechanical devices can be extremely efficient due to the large optomechanical response of common materials and wavelength-scale localization of mechanical energy. However, existing demonstrations suffer from combination of low optical quality factor, low electrical-to-mechanical transduction efficiency, and low optomechanical interaction rate. Here we demonstrate an on-chip piezo-optomechanical transducer that systematically addresses all these challenges to achieve nearly three orders of magnitude improvement in conversion efficiency. Our modulator demonstrates acousto-optic modulation with $V_\pi = 0.02$ V. We show bidirectional conversion efficiency of $10^{-5}$ with 3.3 μW red-detuned optical pump, and 5.5% with 323 μW blue-detuned pump. Further study at mK temperatures is required to understand how the efficiency and added noise are affected by reduced mechanical dissipation, thermal conductivity and capacity.

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11:27AM M02.00002: Piezoelectric optomechanics in a 3D microwave cavity: A route to microwave to optical transduction*  Hugh Ramp (Presenter), Physics, University of Alberta, Krishna Balram, Kartik A Srinivasan, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, John Davis, Physics, University of Alberta — Numerous examples of microwave to optical transduction have been demonstrated for optomechanical systems. In most cases, the piezoelectric effect allows for microwave-mechanical coupling either through direct capacitive stimulation or by creating surface acoustic waves using interdigitated capacitors. Here, we inject a microwave signal into a 3D microwave cavity where a GaAs optomechanical crystal has been placed at the electric field maxima. This allows the microwave cavity to stimulate the GHz-frequency mechanical breathing mode in the optomechanical crystal through the piezoelectric effect, which is then read out using the telecom optical mode. The GaAs optomechanical crystal is a good candidate for low-noise microwave to optical transduction, as it has been previously cooled to the mechanical ground state $n = 0.7 \pm 0.4$ phonons in a dilution refrigerator [1]. Moreover, the 3D microwave cavity architecture used in this experiment can be naturally extended to couple to superconducting qubits.


*The University of Alberta; the Natural Sciences and Engineering Research Council, Canada (Grants No. RGPIN-04523-16, No. DAS-492947-16, and No. CREATE-495446-17); Quantum Alberta; and the Canada Foundation for Innovation.
Fractal-like mechanical resonators with soft-clamped fundamental mode* SERGEY FEDOROV (Presenter), ALBERTO BECCARI, NILS JOHAN ENGELSEN, MOHAMMADJAFAR BEREYHI, ROBIN GROTH, TOBIAS J. KIPPENBERG, Ecole Polytechnique Federale de Lausanne — Self-similar structures occur naturally and have been employed to engineer exotic physical properties. We show that acoustic modes of a fractal-like system of tensioned strings can display increased mechanical quality factors due to the enhancement of dissipation dilution. We describe a realistic resonator design in which the quality factor of the fundamental mode is enhanced by as much as two orders of magnitude compared to a simple string with the same size and tension. Our findings can open new avenues in force sensing, cavity quantum optomechanics and experiments with suspended test masses.

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Manipulation of geometric nonlinearity to probe nonlinear damping in 2D NEMS PARMESHWAR PRASAD (Presenter), AKSHAY NAIK, Indian Institute of Science — Nonlinearity is inherent in nano mechanical (NEMS) devices. NEMS with high geometric aspect ratio are prone to these nonlinearities. Understanding the role of nonlinearities in the NEMS devices is essential to harvest the maximum benefit from them. In the current work, we probe the nonlinear damping by manipulating the effective Duffing (cubic) nonlinearity using electrical means. We take advantage of tuning of the nonlinearities with strain to minimize the effect of duffing non-linearity thus enabling the study of the effect of nonlinear damping. We use this technique to study the effect of non-linear damping in parametric oscillation regime in 2D material based NEMS resonators.
12:03PM M02.00005: Piezo-optomechanics in lithium niobate on silicon-on-insulator for microwave-to-optics conversion

RAPHAEL VAN LAER (Presenter), WENTAO JIANG, CHRISTOPHER J SARABALIS, RISHI PATEL, FELIX M MAYOR, TIMOTHY MCKENNA, AGNETTA CLELAND, EDWARD A WOLLACK, PATRICIO ARRANGOIZ-ARRIOLA, JEREMY WITMER, AMIR SAFAVI-NAEINI, Stanford Univ — Cryogenic microwave qubits are globally pursued to build a compelling quantum technology. Major efforts are underway to scale up these processors, inching closer to useful tasks beyond the reach of classical technology. However, it is currently infeasible to connect the qubits well beyond a single refrigerator, limiting their use outside the laboratory. Microwave-to-optics converters are uniquely placed to tackle this challenge. One of the leading approaches exploits electro-opto-mechanics, but even cutting-edge systems suffer from excessive dissipated energy per qubit that is converted between microwaves and optics. This dissipated energy sets an upper bound on the quantum communication rate in a severely power-constrained cryo-environment. Here, we take first steps to greatly reduce this dissipated energy by combining a strongly piezoelectric material - lithium niobate (LN) - with a leading optomechanics and photonics platform - silicon-on-insulator (SOI). This hybrid LN-on-SOI platform leverages the best properties of both materials. We observe efficient piezo- and opto-mechanical interactions involving tightly confined GHz mechanics, establishing an intriguing path towards low-energy conversion between microwaves and optics.

*Marie-Curie-665501, NSF ECCS-1808100, ARO/LPS CQTS
12:15PM M02.00006: Gallium Phosphide as a Piezoelectric Platform for Quantum Optomechanics*  
ROBERT STOCKILL (Presenter), MORITZ FORSCH, Kavli Institute of Nanoscience, Department of Quantum Nanoscience, Delft University of Technology, 2628 CJ Delft, Netherlands, GREGOIRE BEAUDOIN, Konstantinos Pantzas, Isabelle Sagnes, Rémy Braive, Centre de Nanosciences et de Nanotechnologies, CNRS, Université Paris-Sud, Université Paris-Saclay, C2N, 91767 Palaiseau, France, Simon Groeblacher, Kavli Institute of Nanoscience, Department of Quantum Nanoscience, Delft University of Technology, 2628 CJ Delft, Netherlands — Piezoelectric materials expand the capabilities of optomechanical devices to include native electromechanical interaction, enabling conversion between microwave-frequency modes and low-loss optical telecom bands. Specifically, the combination of high-cooperativity interfaces and ground-state occupation of the mechanical mode allows for transduction of a quantum state. While cryogenically cooled piezoelectric optomechanical devices have demonstrated sub-phonon occupation [1], absorption induced heating has prevented the observation of non-classical behaviour. Here, we fabricate and operate an on-chip optomechanical device made from gallium phosphide [2], realising high-cooperativity interaction with a long-lived 3-GHz mechanical mode which remains in the ground state. We observe non-classical correlations between state-projecting photons and the confined mechanical mode, establishing GaP as a piezoelectric platform for noise-free quantum-state conversion between microwave and optical carriers. [1] Ramp et al. PRL 123 93603 (2019) Forsch et al. Nat. Phys. (2019) [2] Stockill et al. PRL 123 163602 (2019)


12:27PM M02.00007: Optomechanical Quantum State Tomography*  
RISHI PATEL (Presenter), Timothy McKenna, ZhaoYou Wang, Jeremy Witmer, Wentao Jiang, Edward A Wollack, Christopher J Sarabalis, Pieter-Jan C. Stas, Raphael Van Laer, Amir Safavi-Naeini, Stanford Univ — We generate and characterize heralded quantum states of a mechanical resonator with a single added phonon. Our system consists of an optomechanical crystal cavity operated at about 10 millikelvin. We perform continuous wave sideband asymmetry measurements using single photon counters to calibrate the temperature of a 4 GHz mechanical mode. Photon and phonon pairs are generated using a continuous wave laser blue detuned from the optical cavity resonance. A detected photon at the cavity resonance frequency heralds the addition of a phonon to the mechanical mode; we characterize the generated states by continuously measuring the output cavity field, and performing tomography to determine the Husimi Q function describing the state of the mechanical oscillator.

*R.P. acknowledges support from the NSF Graduate Research Fellowship Program (grant number: DGE-1656518).
PIETIKÄINEN (Presenter), ONDREJ CERNOTIK, RADIM FILIP, Palacky Univ — In optomechanics we are often dealing with squeezing and backaction-evasion schemes that use two-tone driving. In general the time development of this kind of time-dependent Hamiltonian has to be solved from the master equation. Optomechanical system typically have large thermal noise which makes solving the master equation difficult, especially for steady state.

We introduce a method to solve the dynamics of a time-periodic system, by using the Floquet approach to write the dynamics in the form of a Lyapunov equation. With the Floquet method, we can transform a periodic linear differential equation into a time-independent linear system. After which, for the time-independent Hamiltonian that is quadratic in the canonical operators, the time development can be expressed in the form of a Lyapunov equation, which can be solved efficiently.

We demonstrate this method in an optomechanical system with dissipative generation of squeezing. We show that we can include the counter-rotating terms ignored in the rotating-wave approximation. The method is also useful with levitating particles in an amplitude modulated trapping field.

SERGEY FEDOROV, ALBERTO BECCARI, MOHAMMADJAFAR BEREYHI, NILS JOHAN ENGELSEN (Presenter), TOBIAS J. KIPPENBERG, Ecole Polytechnique Federale de Lausanne — We experimentally investigate the thermal noise properties of a room-temperature, membrane-in-the-middle optomechanical cavity in the regime of nominal quantum cooperativity approaching one. We show that with resonant laser drive, the intra-cavity amplitude noise is dominated by thermal noise up-converted by nonlinear cavity transduction of the laser-cavity detuning. This noise conversion process sets a limitation on the observability of quantum features of the optomechanical interaction, which is not specific to membrane in the middle setups.

*This work was supported by the Swiss National Science Foundation under grant no. 182103 and the Defense Advanced Research Projects Agency (DARPA), Defense Sciences Office (DSO), under contract no. D19AP00016 (QUORT). A.B. acknowledges support from the European Union’s Horizon 2020 research and innovation program under the Marie Sklodowska-Curie grant agreement no. 722923 (OMT). N.J.E. acknowledges support from the Swiss National Science Foundation under grant no. 185870 (Ambizione)
1:03PM M02.00010: Phonon-Counting Experiments with Superfluid Helium Optomechanics
YOGESH PATIL (Presenter), JIAxin YU, SEAN FRAZIER, KALE G JOHNSON, Yale University, SÉBASTIEN GARCIA, KONSTANTIN OTT, JAKOB REICHEL, Laboratoire Kastler Brossel, ENS-Universite PSL, CNRS, Sorbonne Universite, JACK G E HARRIS, Yale University — Superfluid Helium is a very good platform for quantum optomechanics owing to its extremely low optical and mechanical losses. In a device consisting of a Fabry-Perot cavity filled with superfluid helium, each acoustic mode of the helium is optomechanically coupled to a single optical mode of the cavity [1]. In previous work we used such a device to measure an acoustic mode's Gaussian quantum fluctuations [2]. Here we describe new measurements in which we have incorporated single-photon detectors (and multiple cascaded optical filters) to record individual sideband photons, each of which is associated with the creation (or annihilation) of a single phonon in the acoustic mode. We will describe the prospects for using this approach to prepare and characterize non-Gaussian states of the acoustic mode.


1:15PM M02.00011: Pulsed quantum processing of two mechanical elements  SHLOMI KOTLER (Presenter), GABRIEL PETERSON, FLORENT LECOCQ, KATARINA CICAK, RAYMOND W SIMMONDS, JOSE AUMENTADO, JOHN TEUFEL, Physics Measurement Lab, National Institute of Standards and Technology — High quality mechanical elements have been shown to be a viable candidate for storage of quantum information. To become useful as processing elements, one has to be able to initialize the mechanics to a pure state, generate interactions with other mechanical elements and measure the resulting state with high efficiency. While each of these capabilities has been demonstrated separately, integrating it to a single device requires reconciling the different resulting constraints. Here we design, fabricate and measure a microwave resonator coupled to two separate mechanical resonators (drums). We use spatial addressing as well as frequency and time domain multiplexing to individually address the drums using microwave pulses. This allows us to perform ground state cooling, simultaneous readout and a two-mode coupling gate between the mechanics. Our work is a stepping stone on the path to information processing with multi-mechanical arrays.
1:27PM M02.00012: Lifetime and Coherence Measurements of an Optomechanical Quantum Memory* ANDREAS WALLUCKS (Presenter), IGOR MARINKOVIC, BAS HENSEN, ROBERT STOCKILL, SIMON GROEBLACHER, Delft University of Technology — Recent experiments have achieved quantum control of so-called nanobeam optomechanical crystals, which possess engineered mechanical resonances in the Gigahertz regime that can be addressed optically from the conventional telecom band. Here we discuss the prospects of such nanobeams with ultra-long lived mechanical modes to act as optical quantum memories. We demonstrate the heralded preparation of a single phonon Fock state which can be stored up to 2 ms while preserving the non-classicality. We further study the coherence of the memory using a superposition state of vacuum with a Fock state and find a quantum coherence time of 15 microseconds. Measurements of the mechanical frequency noise in the classical regime show a clear power dependence, allowing us to reach coherence times exceeding 100 microseconds. The protocol used in these experiments is directly applicable to existing quantum repeater architectures.

*This work is supported by the Foundation for Fundamental Research on Matter (FOM), the European Research Council, and by the Netherlands Organization for Scientific Research (NWO/OCW), as part of the Frontiers of Nanoscience program.

1:39PM M02.00013: Towards cavity quantum circuit electromechanics with millimiter-sized silicon nitride membranes* SARWAN PEITER (Presenter), ADRAIN SANZ MORA, GARY STEELE, Delft University of Technology — Many everyday use appliances consist of hybrid setups, i.e., devices that rely on a close-knit interfacing between different physical elements, each of which can carry out a given task in a complementary way. Interfaces with mechanical membranes and superconducting circuits play an active role in today's research towards a new generation of hybrid devices, the dynamics of which may be prominently ruled by quantum mechanics. Crucial to succesfully harness the quantized dynamics of such devices is their isolation from environmental noise sources. For the millimiter sized membranes we use in our circuits this even requires isolation from the acoustic noise present in the dilution refrigerators wherein they are usually hosted. Based on a systematic characterization of the noisy acoustic signals disturbing our electromechanical circuit we design different methods to suppress them, including an original mass-spring system that enables keeping our device freely suspended inside the fridge. Using these adjustments, and a phononic bandgap shield to minimize acoustic radiation loses of the membrane itself, we prove feasible ground state cooling of the membrane's fundamental mode of vibration.

*Funded by ERC
1:51PM M02.00014: Low-temperature diamond optomechanics*  
JEFF CADY (Presenter), University of California, Santa Barbara, RISHI PATEL, AMIR SAFAVI-NAEINI, Stanford University, ANIA JAYICH, University of California, Santa Barbara — Diamond mechanical devices have the potential to serve as a hybrid platform for facilitating quantum interactions between photons, phonons, and the spin and orbital degrees of freedom of embedded defect qubits, such as nitrogen-vacancy (NV) centers, which can couple to mechanical motion via crystal strain. Recent experiments [1,2] have demonstrated hybrid mechanical systems in diamond consisting of nanofabricated mechanical resonators that host coherent NV centers. However, an outstanding challenge to reaching the high-cooperativity regime in these systems, where such applications as phonon-mediated spin-spin interactions and NV-assisted mechanical cooling become realizable, is the demonstration of long-lived, high-strain mechanical modes near their ground state of motion. As a step toward this goal, we design and fabricate single-crystal diamond optomechanical crystals which host GHz-scale mechanical modes with large zero-point strain and characterize them at 6K in a closed-cycle cryostat. We observe optomechanically-driven phonon lasing, optomechanically-induced transparency, and laser cooling of the mechanical motion in these devices.


*NSF CAREER Award DMR-1352660
NSF Award QIS-1820938

2:03PM M02.00015: Magnomechanical cross-correlation thermometry*  
CLINTON POTTS (Presenter), Univ of Alberta, VICTOR BITTENCOURT, SILVIA G VIOLA KUSMINSKY, Max Planck Institute for the Science of Light, JOHN DAVIS, Univ of Alberta — The development of hybrid quantum technologies has driven a need for low-temperature environments such as dilution refrigerators. In these cryogenic environments, accurate thermometry can be difficult to implement, expensive, and often requires calibration to an external reference. We propose a thermometric measurement of a hybrid system consisting of phonons coupled via the magnetostrictive interaction to magnons within a ferromagnetic sphere. Our approach is based on a cross-correlation measurement which is calibration-free and low temperature compatible. We demonstrate the ability to distinguish thermomechanical motion from the magnon induced back-action. Furthermore, the spectrum of back-action driven motion can be used to scale the thermomechanical motion, providing a direct measurement of the phonon temperature, independent of experimental parameters.

*The University of Alberta; the Natural Sciences and Engineering Research Council, Canada (Grants No. RGPIN-04523-16, No. DAS-492947-16, and No. CREATE-495446-17); and Mitacs Globalink.

Wednesday, March 4, 2020 11:15 AM - 1:39 PM

Session M03 GSCCM: Materials in Extremes: Equation of State and Phase Diagrams 107 - Patricia Kalita, Sandia National Laboratories - Tag(s): Focus
11:15AM M03.00001: Multiphase EOS Table for Gallium*  CARRIE PRISBREY (Presenter), CHRISTINE J WU, Lawrence Livermore Natl Lab — We developed the first LLNL multiphase equation of state (EOS) for Gallium (Ga) covering a wide range of density (10^-7-10^3 g/cc) and temperature (1-10^9K). The EOS includes three known solid phases (I, II and III) and one Ga liquid. The EOS table accurately reproduces available experimental Hugoniot, isotherms and isobar data, as well as observed phase boundaries. We demonstrate that there is a significant uncertainty in predicted phase boundaries beyond the range of existing experimental observations, since they are highly sensitive to small changes in the free energy differences between the neighboring phases. EOS model uncertainty and variations will also be explored in this study.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

11:27AM M03.00002: MgO at Multi-Megabar Pressures: Benchmarking the Equation of State and B1–B2 Transition Using Auxiliary-Field Quantum Monte Carlo*  SHUAI ZHANG (Presenter), Laboratory for Laser Energetics, University of Rochester, FIONN MALONE, MIGUEL A MORALES, Lawrence Livermore National Laboratory — Studying materials at up to multi-megabar pressures is important for understanding the interiors of exoplanets and testing equation-of-state (EOS) models. However, it remains challenging to both experiments (e.g., B1–B2 transition pressure, \( P_{tr} \), for MgO is uncertain by 130 GPa) and theory [two-parameter (zero-pressure bulk modulus \( K_0 \) and its pressure derivative \( K'_0 \)) EOS is subject to >10% uncertainties for compression ratio >1.5, and prevalent density-functional-theory (DFT) computations can be biased by the exchange-correlation functional]. Advances in quantum Monte Carlo (QMC) have shown remarkable successes for solids. In this work, we develop and apply auxiliary-field (AF) QMC to benchmark the EOS and \( P_{tr} \) of MgO. In contrast to DFT predictions that vary by ~3% in equilibrium volume (\( V_0 \)), ~6% in \( K_0 \) of B1 MgO, and ~30 GPa in \( P_{tr} \), AFQMC can anchor all the three quantities with significantly reduced uncertainties, thereby providing an accurate and practical approach to benchmark materials properties at such extreme conditions.

*This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856 and by DOE Computational Materials Sciences Program and Center for Predictive Simulation of Functional Materials.
11:39AM M03.00003: The body-centered cubic Fe phase under extreme conditions: Observed yet unnoticed.* ANATOLY BELONOSHKO (Presenter), Department of Physics, KTH Royal Institute of Technology — The recently disclosed mechanism of the body-centered cubic Fe stabilization under extreme pressures and temperatures allows for a new interpretation of a number experimental observations. The high-PT bcc Fe is stabilized by a liquid-like self-diffusion. This means that Fe at high pressure and temperatures is in many respects similar to liquid. Such similarity is confusing to some experimentalists and makes them to interpret solid-solid hcp-bcc transition as melting. I will demonstrate that a number of experimental data sets get a better explanation in terms of the hcp-bcc transition rather than in terms of hcp-liquid transition. The new interpretation removes a number of controversies concerning the extreme part of Fe phase diagram. I will show that in a number of experiments the bcc Fe was observed yet remained unnoticed because of the unexpected properties of the emerging high-PT Fe bcc phase.

*Support from Swedish Scientific Council (Vetenskapsrådet) is gratefully acknowledged.

11:51AM M03.00004: Experimental observations on microstructure of iron and other metals at high pressures and temperatures* [Invited] ROSTISLAV HRUBIAK (Presenter), Argonne Natl Lab — Materials subjected to high pressure (P) and high/low temperature (T) treatments in the diamond anvil cell (DAC) often exhibit complexity and inhomogeneity, on length scales ranging from nanometers to tens of microns. A recently developed ability to perform detailed spatially resolved characterizations of the inhomogeneity under high P, or in the high P-T treated samples, has allowed to unlock some of the complexity and to gain an understanding of several of emerging physical phenomena in high pressure sciences.

One of the examples discussed here will be the crystal structure of iron (Fe) in the Earth’s inner core, which remains debated. Experimental evidence, based in part on spatially resolved microstructure analysis, shows a bcc-Fe appearing at P-T conditions approaching the Earth’s inner core. Recent results on the microstructure and phases of compressed zirconium metal will be discussed as well.

*This work was performed at HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA’s Office of Experimental Sciences. The APS is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357
12:27PM M03.00005: Assessing the accuracy of first-principles DFT in describing van-der-Waals interactions in energetic molecular crystals at ambient and high pressure conditions  IVAN OLEYNIK (Presenter), KIEN NGUYEN-CONG, University of South Florida — Various density functional theory (DFT) functionals are evaluated in their ability to accurately describe vdW interactions in energetic molecular crystals, which are of critical importance to obtain an accurate isothermal equation of state as well as other basic thermodynamic properties of energetic materials. Equilibrium volumes of seven EM crystals are evaluated using several DFT functionals with or with- out semi-empirical Van der Waals corrections, as well as non-local van der Waals density functionals, and compared with available experimental data. By calculating vibrational spectra of energetic molecular crystals, zero point energy (ZPE) and thermal contributions at finite temperature to cold DFT data, pressure-dependent lattice parameters and equation of state are obtained at experimental temperatures, thus allowing direct quantitative comparison with experiment. Newly developed meta-GGA SCAN functional provides the best description of vdW interactions, and delivers an accurate EOS of EMs in a wide range of pressures and temperatures.

12:39PM M03.00006: Examination of the validity of quantum statistical potentials for carbon  HEATHER WHITLEY (Presenter), Lawrence Livermore Natl Lab, MICHAEL SEAN MURILLO, Michigan State University, LORIN BENEDICT, JOHN I CASTOR, FRANK R GRAZIANI, Lawrence Livermore Natl Lab — In recent years, high power laser facilities, such as NIF, and advanced diagnostics have enabled the determination of detailed properties of dense plasmas over unprecedented regimes. Understanding such plasmas, which may be partially degenerate and/or moderately coupled, represents a major challenge to the plasma physics community. One particular challenge for research in this area is the development of interaction potentials which appropriately incorporate the effects of high electron temperature. We examine the accuracy and applicability of approximate effective potentials in the study of structural and dynamic properties carbon in the partially and fully ionized regimes. The diffractive Coulomb potential is derived from an exact quantum solution for a pair of particles while the fermionic character of the electrons is handled via an effective Pauli potential. We compare computed pressures and internal energies for carbon to an equation of state model that was developed based on path integral Monte Carlo and density functional theory. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-795399
12:51PM M03.00007: Wide-ranged equation of state models for elements from the atom-in-jellium approach*  LORIN BENEDICT (Presenter), DAMIAN SWIFT, THOMAS LOCKARD, PHILIP A STERNE, Lawrence Livermore Natl Lab, MANDY BETHKENHAGEN, University of Rostock, SEBASTIEN HAMEL, ALFREDO A. CORREA, RAYMOND SMITH, CHRISTINE J WU, Lawrence Livermore Natl Lab — We discuss the construction of wide-ranged equation of state models for elements using a DFT-based average-atom model. In our approach, high pressure cold, ion-thermal, and electron-thermal contributions of the free energy are all created from the atom-in-jellium paradigm. In particular, the ionic excitation piece is constructed by computing the restoring force to small displacements of the nucleus within a neutral spherical jellium cell, and the Lindemann criterion is adopted to predict the density-dependent melt curve. We show that with a minimum of fitting to low pressure experimental data (e.g., ambient density, melt temperature at ambient pressure), remarkably accurate wide-ranged equations of state can be generated using this method, as demonstrated by comparing to high pressure experimental data and more sophisticated ab initio predictions.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE- AC52-07NA27344

1:03PM M03.00008: A new multiphase wide range Equation of State for Nickel*  TRAVIS SJOSTROM (Presenter), GIULIA DELORENZI-VENNERI, SVEN PETER RUDIN, Los Alamos Natl Lab — A new equation of state for Nickel has been built and entered in the SESAME database. The EOS was built by Opensesame, based on the multiphase approach. Magnetic effects, derived from the experimental heat capacity, were included by an extra term in the electronic free energy. The solid phase was fitted to available experimental data for thermal expansion, heat capacity and bulk modulus and to data from new DFT calculations of the cold curve and phonon dispersions. The low temperature liquid was calculated, based on the V-T theory approach, from DFT data for the cold curve in the liquid. The high temperature liquid was fitted to new QMD calculations.

*ASC-PEM Program at LANL
1:15PM M03.00009: Update on multi-megabar shockless compression at Sandia’s Z machine (2020)*

JEAN-PAUL DAVIS (Presenter), JUSTIN BROWN, Sandia National Laboratories — Quasi-isentropic, shockless ramp-wave experiments promise accurate equation-of-state (EOS) data of materials in the solid phase at relatively low temperatures and multi-megabar (100’s GPa) pressures. In this range of pressure, isothermal diamond-anvil techniques have limited pressure accuracy due to reliance on theoretical EOS of calibration standards, thus accurate quasi-isentropic compression data would help immensely in constraining EOS models. Multi-megabar shockless compression experiments using the Z Machine at Sandia as a magnetic drive with stripline targets have been performed on many solid materials over the past decade. An update is given on recent results and developments, including experimental techniques, analysis methods, and uncertainty quantification.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

1:27PM M03.00010: High-temperature, high-pressure behavior of lithium fluoride*

KANANI LEE (Presenter), Lawrence Livermore Natl Lab, SARAH M. ARVESON, Geology & Geophysics, Yale University, MINTA C AKIN, NEIL C HOLMES, BRUCE J BAER, HYUNCHAE CYNN, Lawrence Livermore Natl Lab — Lithium fluoride (LiF) is used extensively as optical windows in dynamic compression experiments and is also used as pressure media and thermal insulation in diamond-anvil cell (DAC) experiments. In order to better understand this important high-pressure standard and ubiquitous window material, we present high-temperature isothermal equations of state of LiF below its melting curve as measured in a laser-heated DAC. These measurements complement already measured low-T isotherms [Myint et al., JCP, 2019] performed with resistively-heated DACs and will be used to generate phase-aware, thermally accurate equations of state for LiF. Above its previously determined melting curve [Boehler et al., PRL, 1997], LiF exhibits strong changes in absorption, similar to other alkali halides [Arveson et al., PRB, 2018]. We explore these changes in optical properties and the significant consequences they have for temperature measurements measured spectroscopically.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-795563.

Wednesday, March 4, 2020 11:15 AM - 1:39 PM

Session M06 DLS: Optical Tools, Techniques, Methods, and Theory 113
11:15AM M06.00001: Ultrafast THz Probe of Phonon-Assisted Processes in Photoexcited bulk GaAs  EUGENIO CINQUANTA (Presenter), LORENZO GATTO, CNR - IFN, GABRIELE CRIPPA, Dipartimento di Fisica, Politecnico di Milano, CATERINA VOZZI, CNR - IFN, SALVATORE STAGIRA, Dipartimento di Fisica, Politecnico di Milano — Hot carrier dynamics in semiconductors governs the performances of optoelectronic devices. The out-of-equilibrium distribution of photoinjected carriers relaxes through scattering with the lattice phonons. The main relaxation path can be depicted with an initial hot LO phonon distribution that relaxes through the emission of acoustic phonon. These hot phonon population may lead to the enhancement of two-phonon absorption processes involving optical-acoustic and acoustic-acoustic transitions detectable by time-resolved FIR spectroscopy. By means of Optical Pump - THz probe experiments, we investigated the out-of-equilibrium properties of intrinsic bulk GaAs. By tuning the pump-photon energy it is possible to excite the carriers directly in the Γ and in the higher energy L and X valleys. Independently from the excitation wavelength, we observed a rich transient THz response where a broad Drude-Lorentz complex conductivity is dressed with several sharp Lorentzian features in the 0.5-2.5 THz spectral range. This response is highly fluence-dependent, suggesting a carrier density dependence of the observed behavior. Our outcomes may be related to the enhancement of two-photon absorption processes involving the optical and acoustical out-of-equilibrium phonon distribution.

11:27AM M06.00002: Observations of Group Velocity Dispersion, Raman Scattering, Stimulated Raman, and Spectral Broadening for O-waves and E-waves from a Calcite Crystal Using Femtosecond Laser Pulses  SHAH FAISAL MAZHAR (Presenter), Physics, City College of New York, HENRY MEYER, Electrical Engineering, City College of New York, ROBERT ALFANO, Physics & EE, City College of New York — Group velocity dispersion (GVD), Raman Spectra, Stimulated Raman Scattering (SRS), and Supercontinuum (SC) are investigated for ordinary (O) waves and extraordinary (E) waves from a 2.7 cm thick Calcite crystal. Using 390 fs pulses (~2 μJ pulse energy) at 517 nm, the O-wave produced a stronger sharp SRS peak at 1086 cm⁻¹ and weak SC spectrum in the visible range than E-wave. To explain the salient observation, the difference between Raman cross-section, index of refraction (walk-off), GVD, and the size of nonlinear susceptibility, χ3 for O-waves and E-waves of Calcite are presented.

Multiphoton photoemission spectroscopy of TiO$_2$ and Au/TiO$_2$ surfaces

NAMITHA JAMES (Presenter), HRVOJE PETEK, Department of Physics and Astronomy, Univ of Pittsburgh — TiO$_2$ is a widely investigated metal oxide due to its photocatalytic and photovoltaic applications. Until recently, the ability to probe the ultrafast electron dynamics of this system has been limited to transient absorption experiments. Understanding the photoexcited electron dynamics in TiO$_2$ is vital to extend its applications through a thorough understanding of its electronic structure. TiO$_2$ is known to catalyze reactions upon UV excitation. Photocatalysis in TiO$_2$ can be extended into visible by coupling it with plasmonic metal nanoparticles, which can be very efficient light absorbers in the visible through excitation of their localized plasmon resonance. Au nanoclusters coupled to TiO$_2$(110) have been shown to enhance photocatalytic properties upon visible excitation. By probing the rutile TiO$_2$(110) and Au/TiO$_2$ interface using multiphoton photoemission (mPP) with a tunable ultrashort (~20 fs) laser pulse, we investigate the dynamics of electrons excited in its conduction band. mPP spectra reveal resonances where TiO$_2$ defect state electrons absorb energy to reveal new optical energy levels and transitions between them. Decoration of the surfaces with Au overlayer introduces new resonances, but does not show a plasmonic enhancement of the optical response of Au/TiO$_2$ surfaces.

Exact Theory for Two-Color Laser-Induced Photoemission from a Biased Metal Surface*


*Supported by AFOSR YIP Award No. FA9550-18-1-10061.
12:03PM MO6.00005: Generation and applications of intense terahertz fields produced by multi-color laser pulses interacting with gas plasmas  LUC BERGE (Presenter), CEA, DAM, DIF - 91297 Arpajon - France — Terahertz (THz) pulses are very popular because of their numerous applications, for example in security. Located between microwaves and optical waves in the electromagnetic (EM) spectrum, their spectral domain can be exploited for molecular spectroscopy using the THz waves emitted from plasmas created by two-color femtosecond laser pulses ionizing air. Down-conversion of broadband optical spectra in the plasma produces intense EM radiation suitable for the identification of suspect materials, even remotely. The physical mechanisms involved to create terahertz radiation by laser-matter interaction, such as photocurrents, are here reviewed. The new potentialities offered by ultrafast intense lasers allow the acquisition of many spectral signatures within 20-50 THz broad bandwidths associated to high-field single-cycle THz pulses. We report new features obtained in the framework of the French project ALTESSE, the main objective of which consisted in testing the efficiency of a laser-based terahertz time-domain spectroscopy of various materials, using the air-biased coherent detection (ABCD) method. The last part of this presentation will discuss new perspectives in the production of ultra-intense terahertz pulses from laser-wakefield accelerators in relativistic plasmas.

12:15PM MO6.00006: Periodic Lensing from a One-Component Plasma Imaged by Ultrafast Transmission Electron Microscopy  OMID ZANDI (Presenter), ALLAN EUGENE SYKES, RYAN DEAN CORNELIUS, FRANCIS MARION ALCORN, Department of Chemistry, University of Illinois at Urbana-Champaign, BRYAN REED, Integrated Dynamic Electron Solutions, Inc, RENSKE M VAN DER VEEN, Department of Chemistry, University of Illinois at Urbana-Champaign — Transmission electron microscopy (TEM) has become a powerful technique to study the structure of materials at nanoscale. The temporal resolution of TEM, however, is typically limited by the maximum frame rate of the detector to the ms regime. Ultrafast TEM combines the high temporal resolution of ultrafast laser spectroscopy with the excellent spatial resolution of electron microscopy. The structural and electronic changes in the material are initiated by fs laser pulses followed by similarly short photoelectron pulses to prob the dynamics by imaging, diffraction, or electron spectroscopy. Here, we will present our ultrafast TEM at UIUC, and demonstrate its first application in observation of periodic plasma lensing. We generated a one-component electron plasma (OCEP) by two-photon photoemission from a Cu grid. We directly imaged the subsequent evolution of the OCEP under the influence of an external uniform magnetic field inside the TEM on the ps time scale. The cyclotron oscillations give rise to a periodic lensing effect which maximizes when the OCEP is refocused along the magnetic field. We analytically described the dynamics of OCEP and its time-dependent focal length to extract the number of electrons and their velocity spread. We verified the model by N-body simulations.
12:27PM M06.00007: Attosecond Pulses with Time-Varying Orbital Angular Momentum: The Self-Torque of Light  QUYNH L NGUYEN (Presenter), KEVIN DORNEY, Physics, JILA/University of Colorado Boulder, LAURA REGO, Grupo de Investigación en Aplicaciones del Láser y Fotónica, Departamento de Física Aplicada, University of Salamanca, Salamanca E-37008, Spain, NATHAN BROOKS, CHEN-TING LIAO, Physics, JILA/University of Colorado Boulder, JULIO SAN ROMAN, Grupo de Investigación en Aplicaciones del Láser y Fotónica, Departamento de Física Aplicada, University of Salamanca, Salamanca E-37008, Spain, DAVID E COUCH, ALLISON LIU, Physics, JILA/University of Colorado Boulder, EMILIO PISANTY, MACIEJ LEWENSTEIN, ICFO, Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Av. Carl Friedrich Gauss 3, 08860, LUIS PLAJA, Grupo de Investigación en Aplicaciones del Láser y Fotónica, Departamento de Física Aplicada, University of Salamanca, Salamanca E-37008, Spain, HENRY KAPTEYN, Physics, JILA/University of Colorado Boulder, CARLOS HERNANDEZ-GARCIA, Grupo de Investigación en Aplicaciones del Láser y Fotónica, Departamento de Física Aplicada, University of Salamanca, Salamanca E-37008, Spain, MARGARET MARY MURNANE, Physics, JILA/University of Colorado Boulder — Propagating laser beams with defined orbital angular momentum (OAM) have found applications that enable new paradigms in optical metrology and communication, quantum information, photomechanical manipulation, and super-resolution imaging. To date, however, the generation and application of OAM beams has been largely based on a static interpretation of optical OAM, where OAM is time-independent. We show for the first time that propagating light waves can possess dynamic, time-varying OAM. We exploit the highly non-linear and non-perturbative process of high-harmonic generation to imprint time-dependent OAM onto extreme ultraviolet (EUV) beams. This new photonic property, self-torque (an analogy to mechanical systems that exhibit a self-induced time variation of their angular momentum), manifests as a few-to-sub femtosecond variation of optical OAM states along each pulse in the underlying attosecond pulse train. We confirm that optical self-torque endows unique properties to coherent EUV waveforms, which enable the delivery of optical torque on the natural time and length scales of charge and spin ordering in materials. Ability to sculpt the OAM wavefront of EUV beams also offers exciting potential in imaging, metrology and sensing methods for semiconductor and quantum materials.

12:39PM M06.00008: Direct in-situ single-shot measurements of the absolute carrier-envelope phases of ultrashort pulses*  DUKE DEBRAH (Presenter), GIHAN BASNAYAKE, WEN LI, Wayne State Univ — Many important physical processes such as nonlinear optics and coherent control are highly sensitive to the absolute carrier-envelope phase (CEP) of driving ultrashort laser pulses. This makes the measurement of CEP immensely important in relevant fields. Even though relative CEPs can be measured with a few existing technologies, the estimate of the absolute CEP is not straightforward and always requires theoretical inputs. Here, we demonstrate a novel in-situ technique based on angular streaking that can achieve such a goal without complicated calibration procedures. Single-shot measurements of the absolute CEP have been achieved with an estimated precision of 0.19 radians.

*Research supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under Award # DE-SC0012628.
12:51PM M06.00009: Photoninduced quantum entanglement between remote electron-phonon systems*  KUNIO ISHIDA (Presenter), Utsunomiya Univ, HIROAKI MATSUEDA, National Institute of Technology, Sendai College —
Dynamical control of quantum entanglement by external light is an intriguing problem which is of importance in the study of light-matter interaction as well as quantum information processing. Recent experiments have shown that phonons created between remote samples are entangled by laser pulses[1], which shows that the quantum-mechanical nature of light plays a key role to understand the dynamics of quantum correlation between noninteracting systems. In this paper we discuss the dynamics of entanglement creation in remote electron-phonon systems which is mediated by irradiation of quantized light. A multimode spin-boson model is used to describe photons and phonons coupled with two-level systems[2], and we discuss the quantitative properties of quantum entanglement between photons and/or phonons revealed by numerical calculations.

*This work is partly supported by Research Funding Granted by Utsunomiya University President.

1:03PM M06.00010: Characterization of an ultrastable sapphire optical cavity operated at 10 K*  JOSE VALENCIA (Presenter), ETHAN CLEMENTS, MAY KIM, DAVID B HUME, DAVID LEIBRANDT, National Institute of Standards and Technology — The frequency stability of optical clocks is often limited by the linewidth of the probe laser, where the highest stability cavity-stabilized lasers are dominated by thermal noise in the cavity mirrors [1]. We present an optical reference cavity with a calculated thermal noise limit near Δf/f = 3x10^{-18}, which is compatible with reaching the ultimate stability limit due to quantum projection noise for clocks based on the $^1S_0^0-^3P_0$ transition in $^{27}$Al$^+$ (8 mHz natural linewidth at 267 nm) [2]. The cavity is constructed of single-crystal sapphire with GaAs/AlGaAs crystalline mirror coatings and is operated at 10 K using a closed-cycle cryocooler. We measure environmental and technical noise, including temperature fluctuations and vibrations, and characterize their impact on cavity stability. The cavity stability is found to be near 10^{-16} by comparing to room-temperature ULE cavities.


*This work is supported by the National Institute of Standards and Technology and the Office of Naval Research.
Optical manipulation system for Steady State Microbunching in storage ring. POHSUN WU (Presenter), HAO-WEN LUO, National Tsing Hua University, ALEXANDER WU CHAO, Tsinghua University, CI-LING PAN, National Tsing Hua University, CHUANXIANG TANG, Tsinghua University — Steady State Microbunching (SSMB) is one of the schemes for generation of high average power coherent synchrotron radiation (CSR) in a storage ring. As the first proof-of-principle experiment has succeeded at the MLS storage ring in Berlin, it could be a promising candidate of kW level EUV source for lithography with the advantage of narrow linewidth, high power, collimated and clean beam. To satisfy the requirement of SSMB modulation field, the turn by turn phase must be stable and the field need be as high as ~MV/m over several meters of the modulation length. We have studied the effect on microbunch formation and maintenance of turn by turn phase with arbitrary phase jitter with noise spectrum from a commercially available relatively high-power continuous wave laser with a MW level enhancement cavity. The cases of synthesized field by multicolor laser field and adiabatic modulation are also considered. Compare with single color scheme under the same power, the microbunch length of 2-color scheme can be three times smaller while 3-color scheme can be six times smaller. Thus we can generate CSR at shorter wavelength with shorter microbunch length.

This work is supported in part by MOST grant 108B0174I4.

Investigating High Harmonic Generation Beam Dynamics with Ptychographic Lensless Imaging* DAVID SCHMIDT (Presenter), LOGAN Z RAMLET, ALEX WILHELM, DAVID GOLDBERGER, DANIEL ADAMS, CHARLES G DURFEE, Colorado Sch of Mines — High Harmonic Generation (HHG) allows for tabletop EUV coherent light sources and attosecond pulses that can be used to probe material properties. While the process is relatively straightforward to implement, the beam quality of the harmonics is difficult to measure and control. A first step to realizing a tunable and fine controlled HHG setup is the ability to measure these quantities without having to change the setup drastically. Ptychography is a computational imaging technique that has already been used with HHG to reconstruct images of unique specimens. In this work, we shift the emphasis in computational imaging from reconstructing the specimen to understanding the details of the EUV light generated through HHG. Reconstructed harmonic beam profiles can then be propagated back to their generation point in the system to examine how they formed. Using this knowledge, we can optimize the factors affecting the HHG process and learn to control them.

We acknowledge funding from the United States Air Force MURI grant FA9550-16-1-0121.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M07 DQI: Superconducting Qubits: Josephson Junction-based Amplifiers and Parametric Devices II 102 - Nicolas Roch, Institut Neel
**11:15AM M07.00001: Boardband Tunable Phase Shifter for Microwaves**  JINLI ZHANG
(Presenter), MIKKO MOTTONEN, TIANYI LI, ROOPE KOKKONIEMI, KUAN YEN TAN, CHENGYU YAN, WEI LIU, Aalto University — Recently, we introduced a magnetic-flux-tunable phase shifter for propagating microwaves based on three equidistant SQUIDs operating at a single frequency. Here, we report the phase tunability with unit transmission in a frequency range from 6 to 6.28 GHz. Tunability at different frequencies suggests accurate and practical control of the phase. Our results offer a promising path to tune the phase of microwave signal in waveguides with magnetic-flux bias in quantum computation and quantum communication applications.

**11:27AM M07.00002: Phase noise of a Josephson parametric oscillator**  GOPIKA LAKSHMI Bhai (Presenter), SHOTARO SHIRAI, HIROTO MUKAI, Physics, Tokyo Univ of Science, Kagurazaka, YU ZHOU, RIKEN, VIVISHEK SUDHIR, Massachusetts Institute of Technology, JAW-SHEN TSAI, Physics, Tokyo Univ of Science, Kagurazaka — Josephson parametric amplifiers are acquiring a renewed interest in the quantum information community for implementing single-shot readout, and creating entangled photons and squeezed vacuum states. When these parametric amplifiers are driven above an instability threshold, the average number of coherent output photons increases resulting in parametric oscillation. Here we present the results on the experimental study of the phase diffusion properties of such an oscillator by measuring the phase noise spectrum.

*This research is supported by the NEDO IoT project and the JST CREST project in Japan.

**11:39AM M07.00003: A Josephson Maser Via Three-Wave Coupling**  MARIA MUCCI (Presenter), XI CAO, CHENXU LIU, RYAN KAUFMAN, DAVID PEKKER, MICHAEL JONATHAN HATRIDGE, Physics and Astronomy, University of Pittsburgh — In superconducting quantum information systems, we require coherent light to drive quantum elements such as qubits and quantum amplifiers. This is traditionally achieved by filtering hot, room temperature light sources through 60-80dB of increasingly cold attenuators. A cryogenic maser operated in the 5-10GHz range, if it could be controlled without an external microwave drive, would be ideal for such coherent drives. Instead of a three-level atom, we present a joint system of a single qubit and a three-wave mixing resonator, realized in a transmon and SNAIL (Superconducting Nonlinear Asymmetric Inductive eLement), respectively. We take advantage of the SNAIL’s parametric gain process and large engineered loss to rapidly invert the transmon’s population and drive masing in a superconducting cavity. We will present the project's preliminary experimental results, as well as plans to implement the parametric drive via a dc-biased junction for an all-dc controlled, cryogenic quantum light source.

*Work Supported by: NSF, ARO, LPS, and the Kauffman Foundation.
11:51AM M07.00004: Engineered frequency combs in a multimode Josephson network

SAEED KHAN (Presenter), HAKAN TURECI, Princeton University — We investigate the dynamics of a microwave-driven Josephson junction capacitively coupled to an arbitrary multimode linear network. Under specific symmetry conditions, we show that the classical phase diagram simplifies, and may be determined semi-analytically for an arbitrarily large network. The resulting system admits unstable regimes with emergent frequency combs akin to its single mode counterpart [1], with the latter being recently realized in superconducting circuits [2]. The multimode network enables further control over comb properties via its tunable parameters. The coherence of the combs is found to be determined by the intrinsic nonlinearity of the Josephson junction, but is also controllable via network parameters. We also clarify the connection and identify important differences between the network here which consists of a single Kerr nonlinear mode that ultimately delocalizes over the linear network due to the coupling, and standard multimode Kerr combs that have been well-studied in optical systems. The system provides a highly-engineerable platform for frequency comb generation, especially suited to realization within the superconducting circuit architecture.

[2] Pinlei Lu et al., in preparation

12:03PM M07.00005: Theory of an on-chip Josephson quantum micromaser

DAVID PEKKER (Presenter), CHENXU LIU, MARIA MUCCI, XI CAO, MICHAEL JONATHAN HATRIDGE, Univ of Pittsburgh — Solid-state superconducting qubit systems are one of the most promising systems to achieve quantum computing. One of the shortcomings of this architecture is the lack of an on-chip coherent microwave source. To solve this problem, we explore the feasibility of building a Josephson micromaser powered by tunable superconducting transmon qubit(s) (which serve as an artificial three-level atom). Specifically, we explain how to engineer a system composed of two qubits (one a conventional transmon, the other a transmon with a SNAIL element) to construct an element that behaves like a 3-level atom coupled to a dissipative bath. We construct a master equation description of the maser and estimate its properties, like its coherence time, and their dependence on the pump power, pump noise, cavity widths, etc. Finally, we note that the possibility for highly non-linear devices in the microwave regime allow our maser to generate quantum (i.e. non-Gaussian) light.

*NSF, ARO, LPS, and PQI
12:15PM M07.00006: Microwave Isolation through Adiabatic Mode Conversion in Superconducting Coupled Transmission Lines  MAHDI NAGHILOO (Presenter), KAIDONG PENG, YUFENG YE, KEVIN O'BRIEN, Massachusetts Institute of Technology MIT — Non-reciprocal devices are essential for isolating superconducting quantum circuits from the noisy electromagnetic environment while allowing measurement and control. For the past decade, ferrite-based circulators and isolators have been predominantly used to protect superconducting quantum circuits, but major limitations associated with large permanent magnets motivate a non-ferrite and scalable solution. Here we discuss a new scheme that utilizes adiabatic mode conversion in coupled nonlinear Josephson junction transmission lines to realize broadband isolation without magnetic elements, allowing integration with current superconducting qubit technology. We report on progress toward implementing this device.

12:27PM M07.00007: Design of a Josephson Travelling Wave Photon Detector  YUFENG YE (Presenter), KAIDONG PENG, MAHDI NAGHILOO, KEVIN O'BRIEN, Massachusetts Institute of Technology MIT — High-fidelity and wide bandwidth single microwave photon detection remains a challenge for quantum information experiments. Here, we investigate a new design for the Josephson travelling wave photon detector[1,2], a circuit QED based detector which promises high fidelity, non-destructive, and broadband detection of microwave photons. In this design, the broadband detection relies on nonlinear interactions between signal and probe photons in coupled transmission lines. We engineer a cross-Kerr interaction using both quartons and transmons to eliminate self-Kerr and enhance the readout efficiency. By measuring a phase shift on the probe photons, we can deduce the signal photon number with high fidelity.


12:39PM M07.00008: Experimental studies of flux solitons in reversible logic gates  LIUQI YU (Presenter), WALTRAUT WUSTMANN, KEVIN OSBORN, The Laboratory for Physical Sciences, University of Maryland, USA — Reversible digital logic gates can provide a fundamental advantage in energy efficiency compared to industrial gates which are irreversible. Here we design and measure 1-bit gates implemented in superconducting circuits. The gate consists of Long Josephson junctions (LJJs) connected by a circuit interface. The gate interface includes large shunting capacitors, which is key for the resonant conservative dynamics in the gates. The dynamics of the scattering process, originally discovered in full numerical simulation, is understood using collective coordinate analysis [1,2]. Depending on the interface parameters, the gate dynamics realize different gate operations that may preserve or change the fluxon polarity, as an Identity or NOT gate. The LJ circuit layout uses niobium trilayer short junctions with connecting wiring for inductors. We plan to experimentally study how well a fluxon can travel ballistically towards the gate, and scatter to another LJ with the designed change in flux polarity (bit state).

12:51PM M07.00009: Drive-induced renormalization of Kerr nonlinearity in superconducting circuits* ALEXANDRU PETRESCU (Presenter), Université de Sherbrooke, BAPTISTE ROYER, Department of Physics, Yale University, ALEXANDRE BLAIS, Université de Sherbrooke — Josephson-junction-based amplifiers are now ubiquitously used in high-fidelity qubit readout. In a three-wave mixing parametric amplifier, a cancelation of the Kerr interaction is required. In satisfying this requirement, an important limitation is that available theory does not fully explain the dependence of the Kerr nonlinearity on drive power. We propose a perturbative expansion based on unitary transformations to calculate drive-induced corrections to Kerr interactions, with possible applications to current experiments.

*This work was undertaken thanks in part to funding from NSERC and the Canada First Research Excellence Fund.

1:03PM M07.00010: Observation of the AC Stark shift and idler-resonance in two-tone measurements of a Josephson resonator* FATEMEH FANI SANI, DANIEL BOTHNER, INES C. RODRIGUES, GARY STEELE (Presenter), Delft University of Technology — We report on the behaviour of a nonlinear Josephson cavity driven by two microwave signals. Using a single tone, the cavity exhibits the expected Duffing response of the device at high powers. For two-tone measurements, we use a strong pump at frequency $f_p$ and simultaneously measure the cavity with a weak probe. For $f_p > f_c$ (cavity frequency), a Lorentzian response of the cavity is shifted in frequency, corresponding to the AC Stark-shift of the Josephson resonator. For $f_p < f_c$, we observe an abrupt jump in the shifted cavity frequency and an additional feature in the probe spectrum with net gain, occurring at a frequency mirrored about $f_p$. We attribute this feature to resonance condition of an idler tone, generated by 4-wave mixing, with the cavity frequency, in good agreement with an analytical theory. Our results provide insight into the physics of the driven nonlinear Josephson cavity, and a starting point for exploring the strongly-driven quantum regime.

*Supported by the EU via ERC QOM3D-681476 and ETN HOT-732894
1:15PM M07.00011: Millimeter-Wave Four-Wave Mixing via Kinetic Inductance for Quantum Devices*  ALEXANDER ANFEROV (Presenter), AZIZA SULEYMANZADE, ANDREW ORIANI, JONATHAN SIMON, DAVID I SCHUSTER, University of Chicago — Millimeter-wave superconducting devices offer transformative opportunities for quantum experiments at temperatures above 1K, allowing higher device power dissipation, integration with semiconductor technologies, as well as new avenues for studying light-matter interactions in the strong coupling regime. Using the intrinsic nonlinearity associated with kinetic inductance of thin film materials, we realize four-wave mixing at millimeter-wave frequencies: a key component for superconducting quantum systems. We report on the performance of low-loss planar resonators around 100 GHz, patterned on high kinetic inductance thin films of niobium nitride grown by atomic layer deposition. With two-tone spectroscopy we explore degenerate parametric conversion at single photon powers, paving the way for a new generation of high-frequency high-temperature quantum experiments.

*This research was supported by the Army Research Office under contract W911NF-17-C-0024. Support was provided by the Chicago MRSEC, which is funded by NSF through grant DMR-1420709.

1:27PM M07.00012: Towards the development of a microwave to millimeter-wave quantum frequency converter*  KEVIN MULTANI (Presenter), HUBERT STOKOWSKI, JEREMY WITMER, WENTAO JIANG, RISHI PATEL, NATHAN LEE, MAREK PECHAL, Stanford Univ, EMMA SNIVELY, PAUL B. WELANDER, EMILIO NANNI, SLAC, AMIR SAFAVI-NAEINI, Stanford Univ — Quantum networks of microwave superconducting qubits may require the conversion of photons from microwave frequency to those of higher energy for transmission over thermal channels. An approach pursued across the field is to use a three-wave mixing nonlinearity to convert microwave photons to optical photons, so that optical fibers can be used as links for long-range connections. However, these systems’ conversion rate is inherently limited by optical-loss-induced heating. We pursue conversion between microwave (1-10 GHz) signals to millimeter-wave (mmWave, 50-300 GHz) signals, which has the potential to increase the conversion rate by nearly nine orders of magnitude and allow transmission with low decoherence over tens of meters. This talk will outline our experimental approach to a microwave-mmWave conversion scheme, where high bandwidth and high rate interconnects can be created at the laboratory scale. We design and implement multi-frequency antennae, with two modes in the mmWave frequency band, and one mode in the microwave frequency band. We will present recent experimental results as well as outlining possible applications in quantum sensing.

*Work supported by the U.S. Department of Energy under contract numbers DE-AC02-76SF00515.
1:39PM M07.00013: Fractional harmonic instabilities in a quantum driven non-linear oscillator*  
JAYAMEENAKSHI VENKATRAMAN (Presenter), XU XIAO, YAXING ZHANG, Yale University,  
MAZYAR MIRRAHIMI, INRIA, LUIGI FRUNZIO, MICHEL H. DEVORET, Yale University — The action of  
drives on non-linear modes to engineer parametric processes is ubiquitous in circuit QED. In this  
work, we provide a map in parameter space of the instabilities that are created when the ratio of  
the drive and the mode transition frequencies coincide with rational numbers. With careful  
engineering of system parameters and knowledge of such a map, once could avoid these  
instabilities, particularly at large drive-strengths. Our findings are supported by the bifurcation  
map of the classical analogue of our system where under certain drive conditions there exist a  
manifold of degenerate steady states that would lead to the quantum heating shown in the first  
part of the talk. One could also harness this robust degeneracy and exploit it to generate cat-like  
states which could be used to store and manipulate quantum information. Preliminary  
experimental results will be shown.  

*Work supported by ARO.

1:51PM M07.00014: Dynamical Lamb effect in a superconducting circuit*  
MIRKO AMICO (Presenter), OLEG BERMAN, ROMAN KEZERASHVILI, The Graduate Center, City University of New York —  
The dynamical Lamb effect is predicted to arise in superconducting circuits when the coupling of  
a superconducting qubit with a resonator is periodically switched “on” and “off” nonadiabatically.  
We show that by using a superconducting circuit which allows one to switch between longitudinal  
and transverse coupling of a qubit to a resonator, it is possible to observe the dynamical Lamb  
effect. The switching between longitudinal and transverse coupling can be achieved by  
modulating the magnetic flux through the circuit loops. By solving the Schrödinger equation for a  
qubit coupled to a resonator, we calculate the time evolution of the number of excitations in the  
qubit and the resonator due to the dynamical Lamb effect. The number of excitations created in  
the system is maximum when the coupling is periodically switched between longitudinal and  
transverse using a square-wave or sinusoidal modulation of the magnetic flux with frequency  
equal to the sum of the average qubit and photon transition frequencies.  

*This work is partially supported by the U.S. Department of Defense under Grant No.  
W911NF1810433.
2:03PM M07.00015: Time-Domain Grating with a Periodically Driven Qutrit YINGYING HAN (Presenter), Southern University of Science and Technology, WENXIAN ZHANG, Wuhan University, FRANCO NORI, RIKEN, JIANQIANG YOU, Zhejiang University, XIAOQING LUO, Quantum Physics and Quantum Information Division, TIEFU LI, Tsinghua University — Physical systems in the time domain may exhibit analogous phenomena in real space, such as time crystals, time-domain Fresnel lenses, and modulational interference in a qubit. We report the experimental realization of time-domain grating using a superconducting qutrit in periodically modulated probe and control fields via two schemes: simultaneous modulation and complementary modulation. Both experimental and numerical results exhibit modulated Autler-Townes (AT) and modulation-induced diffraction (MID) effects. Theoretical results also confirm that the peak positions of the interference fringes of AT and MID effects are determined by the usual two-level relative phases, while the observed diffraction fringes, appearing only in the complementary modulation, are related to the three-level relative phase. Further analysis indicates that such a single-atom time-domain diffraction originates from the correlation effect between the two time-domain gratings. Moreover, we find that the widths of the diffraction fringes are independent of the control-field power. Our results shed light on the experimental exploration of quantum coherence for modulated multilevel systems and may find promising applications in fast all-microwave switches and quantum-gate operations in the strong-driving regime.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M08 DQI: NISQ: Noise Resilience, Mitigation, and Characterization 104 - Charles Tahan, Laboratory for Physical Sciences

11:15AM M08.00001: Error-resilient Tensor Network-based Ansatz for a Noisy Quantum Computer* UNPIL BAEK (Presenter), WILLIAM HUGGINS, BIRGITTA K WHALEY, University of California, Berkeley — Quantum computers can approximately prepare the ground states of many physical systems without using an exponential amount of resources. A hybrid quantum-classical algorithm, such as the variational quantum eigensolver (VQE), is a promising candidate for simulating electronic structures on a near-term device. Simulating complex systems with VQE, however, poses serious challenges because of limited qubit coherence times and non-negligible error rates within near-term devices. To tackle this challenge, we integrate the geometric structure of Deep Multiscale Entanglement Renormalization Ansatz (DMERA) circuits with the low-cost verification of fermionic parity symmetry to simulate ground states of the Fermi-Hubbard model. Requiring only a gate depth logarithmic in the total system size and a number of qubits independent of the system size, this protocol enables us to study larger systems than are possible for approaches with different ansatzes. Results for the Fermi-Hubbard model indicate that the protocol effectively leverages the ability of near-term devices to simulate complex lattice models.

*This work was supported by a Quantum Algorithms Focused Award from Google LLC.
(Presenter), PATRICK J COLES, Los Alamos National Laboratory — In this work, we study how machine learning can be applied to formulate noise-aware circuit compilations that can be executed on near-term quantum hardware to produce reliable results. We will demonstrate that experimentally derived noise models can be used to go beyond naive circuit compilations for several example quantum algorithms. There are two inputs to our Noise-Aware Circuit Learning (NACL) method: a task, and a noisy gate alphabet. The task is defined by either a set of classical training data or a desired output quantum state or unitary. The output of NACL is a quantum gate sequence that optimally accomplishes the inputted task in the presence of the inputted noise model. Neither an ansatz nor the circuit depth of the gate sequence is an input to NACL. This is because NACL optimizes over the circuit structure and depth, which is in the spirit of task-oriented programming. We implement NACL for several different problems, such as computing state overlap, preparing multi-body entangled states, and implementing the quantum Fourier transform. In each case, we find that our overall figure-of-merit is significantly lower for NACL than for standard methods of circuit compilation.

*The authors acknowledge support from LDRD program at LANL and U.S. DOE, Office of Science, ASCR.

11:39AM M08.00003: Noise-Resilient Quantum Dynamics Using Symmetry-Preserving Ansatzes  MATTHEW OTTEN (Presenter), CRISTIAN CORTES, STEPHEN K GRAY, Argonne Natl Lab — We describe and demonstrate a method for the computation of quantum dynamics on small, noisy universal quantum computers. This method relies on the idea of ‘restarting’ the dynamics; at least one approximate time step is taken on the quantum computer and then a parameterized quantum circuit ansatz is optimized to produce a state that well approximates the time-stepped results. The simulation is then restarted from the optimized state. By encoding knowledge of the form of the solution in the ansatz, such as ensuring that the ansatz has the appropriate symmetries of the Hamiltonian, the optimized ansatz can recover from the effects of decoherence. This allows for the quantum dynamics to proceed far beyond the standard gate depth limits of the underlying hardware, albeit incurring some error from the optimization, the quality of the ansatz, and the typical time step error. We demonstrate this methods on the Aubry-André model with interactions at half-filling, which shows interesting many-body localization effects in the long time limit. Our method is capable of performing high-fidelity Hamiltonian simulation hundred of time steps longer than the standard Trotter approach. These results demonstrate a path towards using small, lossy devices to calculate quantum dynamics.
11:51AM M08.00004: Error Mitigation in Data Driven Circuit Learning*  
KATHLEEN HAMILTON (Presenter), TYLER KHARAZI, VICENTE LEYTON-ORTEGA, RAPHAEL POOSER, Oak Ridge National Lab — Mitigating state preparation and measurement (SPAM) errors has been shown to improve the performance of noisy intermediate scale quantum (NISQ) devices. This talk focuses on the incorporation of matrix-based SPAM error mitigation into data-driven circuit learning for parameterized circuits implementing generative modeling tasks. We discuss how the choice of nonlinear optimization, loss function and the structure of the target distributions can affect the computational cost associated with gradient-based training of densely parameterized quantum circuits trained on NISQ hardware accessed via cloud-based queues.

*This work was supported as part of the ASCR Testbed Pathfinder Program at Oak Ridge National Laboratory under FWP #ERKJ332

12:03PM M08.00005: Preserving Symmetries for Variational Quantum Eigensolvers in the Presence of Noise*  
GEORGE S. BARRON (Presenter), BRYAN T. GARD, ORIEN J ALTMAN, Department of Physics, Virginia Tech, NICHOLAS J. MAYHALL, Department of Chemistry, Virginia Tech, EDWIN BARNES, SOPHIA ECONOMOU, Department of Physics, Virginia Tech — One of the most promising applications of noisy intermediate scale quantum computers (NISQ) is the simulation of molecular Hamiltonians using the variational quantum eigensolver (VQE) algorithm, which has already been demonstrated on small molecules. We show that encoding symmetries of the simulated Hamiltonian at the level of the ansatz used in the VQE provides improvements to both classical and quantum resources. We further verify that these improvements persist in the presence of noise by simulating such variational forms in noisy environments and evaluating their ability to find the correct ground state. To further improve the quality of our results, we implement state of the art error mitigation techniques. Finally, we demonstrate our results in experiment by using IBMQ quantum processors.

*This research was supported by the US Department of Energy (Award No. de-sc0019318, de-sc0019199) and the National Science Foundation (Award No. <a href="tel:1839136">1839136</a>). This research used quantum computing system resources supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research program office. Oak Ridge National Laboratory manages access to the IBM Q System as part of the IBM Q Network.
12:15PM M08.00006: Querying quantum computers with neural networks: precise measurements and noise reduction*  ANTONIO MEZZACAPo (Presenter), ABHINAV KANDALA, IBM TJ Watson Research Center, GUGLIELMO MAZZOLA, IBM Zurich Research Lab, KENNY JING CHOO, University of Zurich, GIACOMO TORLAI, GIUSEPPE CARLEO, Flatiron Institute — In this talk I will introduce neural-network estimators for quantum observables, obtained by integrating the measurement apparatus of a quantum simulator with neural networks. Unsupervised learning of single-qubit measurement data can produce estimates of complex observables free of quantum noise. Precise estimates are achieved for quantum chemistry Hamiltonians, with a reduction of several orders of magnitude in the amount of measurements needed compared to standard estimators. Finally, I will show results on molecular systems obtained using IBM superconducting quantum processors, combining precise measurements with error mitigation strategies.

*IBM Research Frontiers Institute

12:27PM M08.00007: Measurement Reduction in Variational Quantum Algorithms*  ANDREW ZHAO (Presenter), University of New Mexico, ANDREW TRANTER, WILLIAM KIRBY, Tufts University, SHU FAY UNG, California Institute of Technology, AKIMASA MIYAKE, University of New Mexico, PETER LOVE, Tufts University — Variational quantum algorithms are promising applications of noisy intermediate-scale quantum (NISQ) computers. These algorithms consist of a number of separate prepare-and-measure experiments that estimate terms in the Hamiltonian. The number of separate measurements required can become overwhelmingly large for problems at the scale of NISQ hardware that may soon be available. We approach this problem from the perspective of contextuality, and use unitary partitioning to define VQE procedures in which additional unitary operations are appended to the ansatz preparation circuit to reduce the number of terms one needs to measure. This approach may be tuned to hardware specifications in order to use all coherent resources available after ansatz preparation. We investigate this technique for a variety of Hamiltonian classes, in particular the electronic structure Hamiltonian from quantum chemistry. There, we prove that term reduction always scales at least linearly with respect to the number of orbitals, and we supplement this result with numerical studies.

*This work was supported by the National Science Foundation grant PHY-1818914. WMK acknowledges support from the National Science Foundation, award number DGE-1842474.
12:39PM M08.00008: Noise Resilience of Variational Quantum Compiling  KUNAL SHARMA (Presenter), SUMEET KHATRI, Louisiana State University, Baton Rouge, MARCO CEREZO DE LA ROCA, PATRICK COLES, Los Alamos National Laboratory, New Mexico — Variational hybrid quantum-classical algorithms (VHQCAs) are near-term algorithms that leverage classical optimization to minimize a cost function, which is efficiently evaluated on a quantum computer. Recently VHQCAs have been proposed for quantum compiling, where a target unitary U is compiled into a short-depth gate sequence V. In this work, we report on a surprising form of noise resilience for these algorithms. Namely, we find one often learns the correct gate sequence V (i.e., the correct variational parameters) despite various sources of incoherent noise acting during the cost-evaluation circuit. Our main results are rigorous theorems stating that the optimal variational parameters are unaffected by a broad class of noise models, such as measurement noise, gate noise, and Pauli channel noise. Furthermore, our numerical implementations on IBM's noisy simulator demonstrate resilience when compiling the quantum Fourier transform, Toffoli gate, and W-state preparation. Hence, variational quantum compiling, due to its robustness, could be practically useful for noisy intermediate-scale quantum devices. Finally, we speculate that this noise resilience may be a general phenomenon that applies to other VHQCAs such as the variational quantum eigensolver.

12:51PM M08.00009: Quantum Dynamical Complexity and Reliability of Analog Quantum Simulation*  KARTHIK CHINNI (Presenter), PABLO POGGI, IVAN DEUTSCH, University of New Mexico — The NISQ era is characterized by the absence of fully fault-tolerant quantum simulators, which raises a question about the reliability of such devices. To address this, we seek to quantify the reliability of an analog quantum simulator, which doesn't have access to error correction, in the presence of perturbations that make the dynamics quantum chaotic. In doing so we seek to identify the relationship between the robustness of the quantities that we seek to extract from the simulator and the dynamical complexity of the analog evolution. As one measure, we quantify the complexity by the number of variables that one must track to approximately yield the output within a desired accuracy. We address these questions by studying the basic paradigms such as the ground state and the excited state quantum phase transitions in the Lipkin-Meshkov-Glick (LMG) model[1].

References:

*National Science Foundation
1:03PM M08.00010: Exploiting molecular point group symmetries for quantum simulation
KANAV SETIA (Presenter), JAMES D WHITFIELD, Dartmouth Coll, ANTONIO MEZZACAPO, JULIA RICE, MARCO PISTOIA, RICHARD CHEN, IBM — Simulating molecules is believed to be one of the early-stage applications for quantum computers. Current state-of-the-art quantum computers are limited in size and coherence, therefore optimizing resources to execute quantum algorithms is crucial. In this work, we develop a formalism to reduce the number of qubits required for simulating molecules using spatial symmetries, by finding qubit representations of irreducible symmetry sectors. We present our results for various molecules and elucidate a formal connection of this work with a previous technique that analyzed generic Z2 Pauli symmetries.

*KS and JDW are funded by NSF awards DMR-1747426, 1820747. JDW also acknowledges support from the U.S Department of Energy (Award A053685) and from DOE Office of Science, Office of Advanced Scientific Computing Research, under the Quantum Computing Application Teams program (Award 1979657). AM acknowledges support from the IBM Research Frontiers Institute. We acknowledge useful discussions with Sergey Bravyi

1:15PM M08.00011: Quantum-classical simulation of two-site dynamical mean-field theory on noisy quantum hardware
TREVOR KEEN (Presenter), University of Tennessee, Knoxville, THOMAS MAIER, Computational Sciences and Engineering Division, Oak Ridge National Laboratory, STEVEN JOHNSTON, University of Tennessee, Knoxville, PAVEL LOUGOVSKI, Computational Sciences and Engineering Division, Oak Ridge National Laboratory — We report on a quantum-classical simulation of a two-site dynamical mean-field theory (DMFT) calculation. We use IBM's superconducting qubit chip to compute the zero-temperature impurity Green's function in the time domain and a classical computer to fit the measured Green's function. We find that Trotter errors and noise from the quantum chip lead to inaccurate updates to impurity parameters, preventing the DMFT algorithm from converging to the correct solution. To mitigate this issue, we determine the update to the hybridization parameter by integrating the low-frequency peaks in the spectral function. This allows us to iterate the DMFT loop to self-consistency for a strongly Mott insulating system at half-filling.

*This work is supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR) quantum algorithm teams program, proposal number ERKJ333.
1:27PM M08.00012: Nearly Optimal Measurement Scheduling for Partial Tomography of Quantum States* XAVIER BONET-MONROIG (Presenter), Institute Lorentz, Leiden University, RYAN BABBUSH, Google Inc., THOMAS O'BRIEN, Institute Lorentz, Leiden University — Many applications of quantum simulation require to prepare and then characterize quantum states by efficiently estimating k-body reduced density matrices (k-RDMs), from which observables of interest are obtained. Naive estimation of such RDMs require repeated state preparation for each matrix element. However, commuting matrix elements may be measured simultaneously, allowing for a significant cost reduction.

In this work we design schemes for such parallelization with near-optimal complexity in the system size N. We describe a scheme to sample all elements of a qubit k-RDM using only $O(3^k \log^{k-1}(N))$ unique measurements. We detail a scheme to sample all elements of the fermionic 2-RDM using only $O(N^2)$ unique measurements, with $O(N)$-depth measurement circuit. We prove a lower bound of $O(N^k)$ on the number of unique measurements required to directly sample all elements of a fermionic k-RDM, making our fermionic 2-RDM scheme asymptotically optimal. We finally construct circuits to sample the expectation value of a linear combination of $\omega$ anti-commuting 2-body fermionic operators with $O(\omega)$ gates on a linear array.

*Research funded by the Netherlands Organization for Scientific Research (NWO/OCW) NanoFront and StartImpuls programs, and by Shell Global Solutions BV.

1:39PM M08.00013: Extracting state purity of a large system with limited control YARIV YANAY (Presenter), CHARLES TAHAN, Laboratory of Physical Sciences — As superconducting quantum devices with a large number of qubits become feasible, they offer an avenue for quantum simulation of equally large systems. The extraction of global information, such as a state's purity or entropy, remains a challenging prospect, generally requiring independent control of each qubit. Here, we propose a method of extracting the purity with limited control, applied through multiplexed dispersive readout. We consider the required control fidelity, and scaling of the number of measurements with system size.

1:51PM M08.00014: Evaluation of the classical sampling cost for noisy quantum circuits SHIGEO HAKKAKU (Presenter), KEISUKE FUJII, Department of Systems Innovation, Graduate School of Engineering Science, Osaka University — In order to demonstrate quantum computational supremacy, quantum computers are being developed by Google, IBM, and so on. In an actual quantum device, there is a non-negligible amount of noise, which would deteriorate the advantage of quantum computation. Therefore, it is necessary to evaluate overhead for classical simulation of quantum computation with taking the noise effect into account.

Recently, classical simulation algorithms such as stabilizer propagation and Pauli propagation. In this work, we estimate the overhead for classical simulation of noisy quantum circuits in terms of Robustness of Magic (RoM) and stabilizer norm, and compare them.

Specifically, we study simulation costs of the noisy random quantum circuits and Trotterized quantum circuits. We show that the Trotterized quantum circuits can be easily simulatable by adding small noise.
11:15AM M09.00001: Triangular color codes on trivalent graphs with flag qubits
CHRISTOPHER CHAMBERLAND (Presenter), IBM TJ Watson Research Center, ALEKSANDER KUBICA, Perimeter Institute, THEODORE YODER, GUANYU ZHU, IBM TJ Watson Research Center — The color code is a topological quantum error-correcting code with a variety of computationally-valuable and fault-tolerant logical gates. Its two-dimensional version, the triangular color code, may soon be realized with currently available superconducting hardware limited by qubit connectivity. To guide the experimental effort, we thus study the storage threshold of the triangular color code against the circuit-level depolarizing noise. First, we adapt the Restriction Decoder to the setting of the triangular color code and to phenomenological noise. Then, we propose a fault-tolerant implementation of the stabilizer measurement circuits, which incorporates flag qubits. We show how information from flag qubits can be use with the Restriction Decoder to maintain the effective distance of the code. We numerically estimate the threshold of the triangular color code to be 0.2%, which is competitive with the thresholds of other topological quantum codes. Lastly, we prove that using 1-flag stabilizer measurement circuits are enough to recover the full distance of the code.

11:27AM M09.00002: A numerical error threshold for "colorful" quantum computing*
JOSEY HANISH (Presenter), SKYLAR TURNER, University of Texas at Austin, EOIN BLANCHARD, University of Illinois at Urbana-Champaign, NOAH DAVIS, BRIAN LA COUR, University of Texas at Austin — "Colorful" quantum computing was first proposed by Héctor Bombín to realize universal, fault-tolerant quantum computing using 3D color codes, or tetrahedral codes. Unlike the well-studied surface code methods, colorful quantum computing does not require magic state distillation and instead relies on a universal set of transversal gates and measurements. Colorful quantum computing can be realized in either a 3D or a 2D system. In this paper, we numerically test 3D colorful quantum computing's resiliency to noise. In addition to the independent and identically distributed noise that affects the initial state, we must also correct errors that arise as part of the initialization process. We find a threshold for fault-tolerance on the body-centered cubic lattice. This threshold upper-bounds the more experimentally feasible 2D colorful quantum computing scheme and hopefully motivates research into color code methods of quantum computing.

*This work was supported by the Air Force Research Laboratory under Grant No. FA8750-18-1-0042.
11:39AM M09.00003: Reinforcement learning for toric code error correction  MATS GRANATH (Presenter), University of Gothenburg, MATTIAS ELIASSON, DAVID FITZEK, ANTON FRISK KOCKUM, Chalmers — I will present a summary of our efforts to use deep reinforcement learning (DRL) for quantum error correction of the toric code. A convolutional neural network is trained by exploration of the state space consisting of (hidden) error configurations and corresponding (visible) syndromes. No external input to the algorithm is provided apart from the current syndrome and the final success or failure of the correction episode. The trained network outputs action values of Pauli operations on the system given an input syndrome. Initial work on uncorrelated noise has shown that the DRL agent performs on par with the standard minimum weight perfect matching (MWPM) algorithm. For depolarizing noise the algorithm outperforms MWPM for all error probabilities and with a higher error threshold. The progress on extending this framework to deal with arbitrarily biased noise and syndrome measurement errors, as well as the scalability of the approach will be discussed.


11:51AM M09.00004: Qubit surface codes from rotation systems acting on Majorana fermions  [Invited] RAHUL SARKAR, Institute for Computational and Mathematical Engineering, Stanford University, THEODORE YODER (Presenter), IBM TJ Watson Research Center — A rotation system is a combinatorial description of a graph and its embedding in a 2-dimensional manifold defined by two permutations on a set of objects. We instantiate this set of objects with Majorana operators and define a Majorana code by associating stabilizers to vertices and faces of the graph embedding. We show how the resulting Majorana code corresponds to a qubit stabilizer code that generalizes the known constructions of rotated and twisted surface codes. While we obtain similar macroscopic behavior -- for instance, anyon type changing when crossing defect lines -- the microscopic details of our codes can lead to improved code parameters. For instance, we identify the [[5,1,3]] code as the smallest member of a surface code family on the torus. We find other code families (both in the plane and on higher genus surfaces) improving upon the constants in the Bravyi-Poulin-Terhal bound.

12:27PM M09.00005: Considerations for incorporating small logical qubits in digital error correction codes  DAVID RODRIGUEZ PEREZ (Presenter), ELIOT KAPIT, Colorado Sch of Mines — We introduce a hybrid error correction scheme by considering using traditional error correcting codes (e.g. Surface codes) with small logical qubit architectures, namely, the Very Small Logical Qubit (VSLQ). Previous theoretical work has shown that the VSLQ can achieve a linear scaling improvement factor, with a single qubit $T_1$ lifetime of 30 µs having a logical lifetime of up to 3 ms, all while using two high-coherence qubits and two lossy qubits or resonators, using passive error correction. In this talk, we consider using small logical qubits such as the VSLQ as part of a broader measurement-based code, and explore potential advantages and challenges from such a hybrid approach. In particular, given that digital error correction normally does not account for qubit leakage error, we explore the complexity that would be introduced in dealing with the corresponding leakage error from VSLQ logical states, as well as other concerns.

*This work is supported by the NSF grant (PHY-1653820) and ARO grant # W911NF-18-1-0125
Higher-order autonomous quantum error correction

JOSE LEBREUILLY (Presenter), KYUNGJOO NOH, Department of Physics and Applied Physics, Yale University, CHIAO-HSUAN WANG, Pritzker School for Molecular Engineering, University of Chicago, STEVEN GIRVIN, Department of Physics and Applied Physics, Yale University, LIANG JIANG, Pritzker School for Molecular Engineering, University of Chicago — Autonomous quantum error correction (AutoQEC) harnesses engineered coupling to an external reservoir to protect quantum information from decoherence. First-order codes provide protection against a single fault and have simple structures. However, as a counterpart they suffer from the drawback of requiring an engineered dissipation that is typically orders of magnitude stronger than natural dissipation. In this work, we investigate the higher-order case and identify Knill-Laflamme conditions which, if satisfied up to some order $r$, lead to the existence of an AutoQEC protocol providing protection against at most $r$ consecutive errors. Furthermore, we develop a general theoretical framework for analyzing the effective dynamics in the protected code space. Within this framework we show that the effective decay rate decreases exponentially in $r$, exceeding the first-order code performance already for moderate engineered dissipation strengths. Finally, we demonstrate that the AutoQEC scheme can be combined with an error-transparent Hamiltonian so as to perform a unitary quantum computation over time scales which far exceed the physical qubits lifetime.

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Characterization and critical faults of leakage errors on the surface code

NATALIE BROWN (Presenter), Georgia Inst of Tech, ANDREW CROSS, IBM T.J Watson Research Center, KENNETH BROWN, Duke University — Leakage is a particularly damaging error that occurs when a qubit leaves the defined computational subspace. Leakage errors leave qubits ill-defined and limit the effectiveness of quantum error correcting codes. The effects of leakage errors on the surface code has been studied in various contexts. However, the effects of a leaked data qubit versus a leaked ancilla qubit can be quite different. In this paper, we study the effects of data leakage and ancilla leakage separately. We show that data leakage is much less damaging. If leakage errors can be confined to data qubits, and efficiently removed with a minimum overhead leakage reducing circuit (LRC), then the surface code maintains the code distance in the presence of leakage. We also show that the distance damaging fault in the surface code comes from ancilla leakage at a particular point in the syndrome extraction circuit. Because of this critical fault location, if leakage errors are eliminated in this particular part of the circuit, the surface code can maintain its effective distance, regardless of other leakage errors that occur on either ancilla or data qubits. We simulate two physical realizations of these toy models that can be applied to both superconducting and ion trapped architectures.
1:03PM M09.00008: Fault tolerance on near-term trapped-ion logical qubits with a neural-network decoder
DAVID OBANDO VARGAS (Presenter), YEFRY LOPEZ, Physics, Universidad de Costa Rica, MAURICIO GUTIERREZ, Chemistry, Universidad de Costa Rica — A crucial step towards the construction of a fault-tolerant quantum computer is the implementation of a logical qubit with a higher fidelity than its constituent physical qubits. In this context, we perform simulations of three promising distance-3 quantum error-correcting codes: the color, surface, and Bacon-Shor codes implemented on a state-of-the-art ion trap with realistic noise sources. Our goal is to find the break-even point where the logical memory outperforms the physical one. In previous works [1], after each error correction step, a correction was performed based exclusively on the syndromes of that step. We now use the syndromes of all previous error correction steps and employ a neural-network-based decoder, which has the advantage of not discarding the syndrome history and also being flexible to different noise models. For each code, we compare the two correction approaches and find a clear improvement in the logical fidelity when the neural-network-based decoder is used. These results will serve as a useful guide to future experiments.

1:15PM M09.00009: Implementing a Logical Qubit on a Trapped Ion Quantum Information Processor*
LAIRD EGAN (Presenter), MARKO CETINA, MICHAEL L GOLDMAN, ANDREW RISINGER, CRYSTAL NOEL, DAIWEI ZHU, DEBOPRIYO BISWAS, CHRISTOPHER ROY MONROE, University of Maryland, College Park — Under the IARPA Logical Qubit (LogiQ) program, we aim to demonstrate a logical qubit using the Bacon-Shor [[9,1,3]] subsystem code. Towards this goal, we built a universal ion-trap quantum processor capable of individual qubit addressing, sympathetic cooling, and ancilla readout. The Bacon-Shor code consists of 9 data qubits, encoding 1 logical qubit, with stabilizer circuits mapped to 4 ancilla qubits capable of correcting any single qubit error. In this talk, we report on the experimental progress made towards implementation of quantum error correction, including the encoding of the logical qubit and stabilizer readout. Additionally, we will lay out the near-term path for achieving multiple rounds of error correction and the prospects for surpassing the quantum error threshold.

*This work is supported by the ARO with funding from the IARPA LogiQ program, the NSF Practical Fully-Connected Quantum Computer program, the DOE program on Quantum Computing in Chemical and Material Sciences, the AFOSR MURI on Quantum Measurement and Verification, and the AFOSR MURI on Interactive Quantum Computation and Communication Protocols. L. E. is also funded by NSF award DMR-1747426.
1:27PM M09.00010: Environment noise analysis and real-time decoupling feedback control for a Nitrogen-Vacancy center* ARSHAG DANAGEOZIAN (Presenter), NATHANIEL MILLER, PRATIK BARGE, NARAYAN BHUSAL, JONATHAN P DOWLING, Louisiana State University, Baton Rouge — Nitrogen-Vacancy (NV) centers in diamond have shown to be a very promising candidate for applications of quantum information processing. Given that a small percentage of the Carbon atoms in diamond are Carbon 13 isotopes, we consider how the collective nuclear spins of these atoms affect the nuclear spin state of the Nitrogen 15 atom of the NV center, which is used as our computational qubit. We accomplish this by isolating a three level lambda system out of the electronic structure of the NV center and observing the phenomenon of coherent population trapping. The information gained from this observation is used to find the optimum dynamical decoupling pulse sequence that will help us preserve the state of our computational qubit for a set duration of time.

*Airforce Office of Scientific Research, Army Research Office, National Science Foundations

1:39PM M09.00011: Mediator assisted cooling in quantum annealing* MANUEL PINO GARCIA (Presenter), JUAN JOSÉ GARCÍA-RIPOLL, instituto de fisica fundamental, consejo superior de investigaciones cientificas — We show a significant reduction of errors for an architecture of quantum annealing where bosonic modes mediate the interaction between qubits. These systems have a large redundancy in the subspace of solutions, as there are solutions with arbitrarily bosonic occupancies. We explain how this redundancy leads to a mitigation of errors when the bosonic modes work in the ultra-strong coupling regime. Our numerical simulations predict a large increase of qubits coherence for an specific annealing problem with mediated interactions. We provide evidences that error reduction could also occurs in other types of quantum computers with similar architectures.

*Fundación General CISC (Programa Comfuturo) Project PGC2018-094792-B-I00 (MCIU/AEI/FEDER, UE)
Combined continuous error suppression and error correction for quantum annealing

JUAN ATALAYA, BIRGITTA K WHALEY, University of California, Berkeley,
MURPHY YUEZHEN NIU (Presenter), Google — The scheme of Jordan, Farhi and Shor for error suppression during quantum annealing [Phys. Rev. A 74, 052322 (2006)] adds energy penalty terms to an encoded Hamiltonian. The role of these penalty terms is to suppress the occurrence of errors taking the encoded quantum state out of the code space. However, errors can still occur in this scheme, albeit with lowered probability. Here we address the question of whether continuous error correction can enhance the performance of quantum annealing by further correcting the remaining unsuppressed errors. To answer this question we consider the continuous implementation of the three-qubit bit-flip quantum error correcting code, where the error syndrome operators are continuously and simultaneously measured. We show that, under certain conditions, continuous error correction combined with error suppression can lead to significantly improved final ground state fidelities. A notable feature of the combined protocol is that it requires quantum error correction operations which are different from those typically used in the operation of quantum memory under this encoding. We also discuss generalization of these results to other quantum error correcting codes.

*This work is supported by IARPA and ARO grant No. W911NF-17-C-0050.

Continuous error correction for evolution under time-dependent Hamiltonians

SONG ZHANG, Physics, University of California, Berkeley, JUAN ATALAYA, Chemistry, University of California, Berkeley, MURPHY YUEZHEN NIU, Google, ARMAN BABAKHANI (Presenter), Chemistry, University of California, Santa Barbara, JEFFREY EPSTEIN, HERMAN CHAN, Physics, University of California, Berkeley, BIRGITTA K WHALEY, Chemistry, University of California, Berkeley — We analyze the continuous operation of a three-qubit code designed to protect the coherent evolution in the code space due to an encoded Hamiltonian. Quantum error correction here requires fast detection and immediate correction of errors to avoid spurious coherent evolution in the error subspaces. To detect errors in real time, we smooth the output signals from continuous measurement of the error syndrome operators and use a double threshold protocol for error diagnosis, while correction of errors is done as in the conventional code operation. We evaluate the performance of this protocol under bit-flip errors, quantifying this in terms of fidelity and logical error rate. We show that the optimal error detection time that maximizes the final fidelity can be much shorter than that of the conventional operation, suggesting that continuous implementation is suitable for quantum error correction in the presence of encoded time-dependent Hamiltonians.

*This work is supported by Intelligence Advanced Research Projects Activity (IARPA) and Army Research Office (ARO) under Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this work are those of the author(s) and do not necessarily reflect the views of the IARPA and ARO.
11:15AM M15.00001: Intricate instabilities in drying drops  
SRISHTI ARORA, MICHELLE R DRISCOLL (Presenter), Northwestern University — Complex fluid drops dry with a striking variety of patterns, from the ubiquitous coffee ring to a wide range and scale of cracks. Colloidal suspensions are often used in these experiments, and to date, much of this work has been focused on drops with a relatively low volume fraction of particles. The patterns are thought to be controlled by several factors such as surface wetting properties, evaporation kinetics, and particle interactions. Here, we present a study of the drying of a high-volume fraction suspension drop. We work with highly monodisperse silica and polystyrene colloids made in-house and study both the final pattern morphology, as well as the dynamics of crack growth. In this limit of high concentration, we see intriguing structures emerging: a single dimple appears near the center that then connects to growing radial fractures. The patterns we observe depend on both particle size and concentration. Furthermore, even for similarly sized particles, changing the material of the colloidal particle can qualitatively change the morphology of the crack pattern.

11:27AM M15.00002: Droplet traffic in microfluidic networks: Role of droplet collisions and occlusion  
MASOUD NOROUZI DARABAD (Presenter), SIVA A VANAPALLI, MARK W VAUGHN, Texas Tech Univ — The dynamics of droplet flows in microfluidic loop networks are governed by the frequency at which the droplets enter the loop. At low frequencies, droplets always choose the channel with lower hydrodynamic resistance, and droplets interact indirectly through their modifications to resistance of the channels. As the droplet frequency increases, direct droplet-droplet interactions in the junction also contribute to droplet decisions and may force the droplets to the channels with higher hydrodynamic resistance. Collisions are considered the main type of direct interaction between droplets. However, our study suggests that occlusion of the entrance of the channel by droplets also impacts their decisions, even when there is no collision and contact. We study droplet decision rules by use of droplet trajectories and distribution of the droplets in the junction and throughout the network. Also, application of machine learning techniques to identify decision rules and predict the droplet decisions is studied.
11:39 AM M15.00003: Joint effect of advection, diffusion, and capillary attraction on the spatial structure of particle depositions from evaporating droplets*  KONSTANTIN KOLEGOV, Astrakhan State University, LEV BARASH (Presenter), Landau Institute for Theoretical Physics — A simplified model is developed, which allows us to perform computer simulations of the particles transport in an evaporating droplet with a contact line pinned to a hydrophilic substrate. The model accounts for advection in the droplet, diffusion and particle attraction by capillary forces. The parameters chosen correspond to the experiments of Park and Moon [Langmuir 22, 3506 (2006)], where an annular deposition and snakelike chains of colloid particles have been identified. We find that the annular sediment is formed by advection and diffusion transport. The close packing of the particles in the sediment is possible if the evaporation time exceeds the characteristic time of diffusion-based ordering. The chains are formed by the end of the evaporation process due to capillary attraction of particles in the region bounded by a fixing radius, where the local droplet height is comparable to the particle size. At the beginning of the evaporation, the annular deposition is shown to expand faster than the fixing radius moves. However, by the end of the process, the fixing radius rapidly outreaches the expanding inner front of the ring. The snakelike chains are formed at this final stage.

*This work was supported by the Russian Science Foundation (project No. 18-71-10061).

11:51 AM M15.00004: Dynamics and stability of confined levitating droplets  STUART THOMSON (Presenter), MATTHEW DUREY, JOHN W. M. BUSH, RUBEN R. ROSALES, Mathematics, Massachusetts Institute of Technology — Millimetric droplets have been shown to bounce on the surface of a vibrating liquid bath or “walk” by means of self-propulsion through a resonant interaction with their own wave field. When confined to an annular ring, we show that single droplets are observed to exhibit a random walk like behaviour, while the collective dynamics of one-dimensional droplet lattices exhibit canonical features of driven dissipative oscillator systems, namely out-of-phase oscillations and solitary wave propagation. Our experimental results are supported by a stability analysis of an accompanying theoretical model. Some open areas of investigation of potential interest to the dynamical and non-equilibrium systems community will be discussed in conclusion.

12:03 PM M15.00005: Watching Droplets Dry in Wet and Dry Climates  PAUL LILIN (Presenter), PHILIPPE BOURRIANNE, IRMGARD BISCHOFBERGER, Massachusetts Institute of Technology MIT — The drying of sessile droplets of colloidal suspensions with particle volume fraction > 5% leads to the formation of fracture patterns. As water evaporates, a solidification front propagates from the edge of the droplet, leaving behind a thin close-packed deposit that eventually covers the entire wetted area. Evaporation-induced stresses generate radial cracks in the deposit that grow towards the droplet center, defining regular petals. These petals bend out of plane to form a blooming flower. Strikingly, while the distance between the cracks is independent of relative humidity, the bending behavior changes drastically when the relative humidity is increased; the curvature of the petals along their width becomes inverted, and the kinetics of the petal bending is modified. We discuss the relation between these changes in structure and kinetics and the deposit thickness.
12:15PM M15.00006: How air deforms the free surface just before disk impact on a liquid bath  DEVARAJ VAN DER MEER (Presenter), UTKARSH JAIN, ANAÏS GAUTHIER, DETLEF LOHSE, Univ of Twente — When a flat disk impacts onto a liquid bath, a layer of air is trapped between the disk and the free surface, a phenomenon known as air cushioning. The air layer is pushed out radially at increasing speeds, causing the water surface to be lifted up towards the approaching disk. This qualitative observation is traditionally ascribed to Bernoulli suction occurring in the low-pressure region created by the large air velocities in the gap. Here, by means of a novel high-speed imaging technique that uses the free surface as a mirror, we quantitatively measure the time evolution of the free surface profile. We show that, whereas the manner in which the surface below the center of the disk is pushed down is consistent with potential theory, this is not the case for the elevation of the free surface below the disk's edge. Instead, the surface lifting appears to be initiated by a Kelvin-Helmholtz instability occurring under the edge of the approaching disk.

12:27PM M15.00007: Dispersion of magnetic beads in flowing droplets.*  ERIC BROUZES, EVAN LAMMERTSE (Presenter), State Univ of NY - Stony Brook — Microfluidic droplets have proven useful for the manipulation and sample preparation of single-cells. However, the droplet toolkit lacks a robust and high-throughput purification module that can maintain partitions. We have demonstrated a proof-of-principle of magnetic purification from flowing droplets using an external magnetic field to partition beads within droplets before asymmetric splitting. Here, we study the interplay between the opposing effects of the magnetic and viscous forces by systematically reporting bead aggregation as a function of design parameters and droplet velocity. We used image-processing to measure aggregate count, size, and shape, allowing us to discover how the distributions of these parameters correlates with changes in experimental conditions. Data have revealed distinct aggregation regimes, in which either the magnetic attraction or the viscous dispersion forces predominate. We further explored the effect of design parameters on the transitions between these regimes both experimentally and via modeling using the dimensionless Mason number (ratio of viscous to magnetic forces). This knowledge will drive the optimization of our droplet purification module with increased throughput.

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Simons Foundation
12:39PM M15.00008: Computational modeling of droplet spreading and coalescence on fiber rails*  
FANG WANG, ULF SCHILLER (Presenter), Clemson University — Flow phenomena in porous media are relevant in many technological applications including emulsion filtration, gas diffusion membranes, and biomedical implants. Fiber materials can be used as filtration membranes with tailored permeability range and controllable pore size distribution. In this talk, we will present lattice Boltzmann simulations of droplet spreading on fiber rails. The simulation results reveal the dependence of the droplet morphology on the fluid volume, fiber size, and contact angle. The transition from a barrel shaped drop to a liquid column shows hysteresis depending on the capillary pressure. We further present preliminary results on capillary trapping of droplets on fiber rails and coalescence induced detachment. We will outline how the results can be used to determine the critical capillary number between trapping and squeezing. We will discuss how these insights can be used to design functional materials for coalescence filtration and other applications.

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12:51PM M15.00009: Spreading and evaporation of sessile droplets*  
CHLOE LINDEMAN (Presenter), NICHOLAS SCHADE, SIDNEY ROBERT NAGEL, University of Chicago — We measure the contact angle at which a drop of liquid sitting on a solid surface de-pins as a function of both the concentration of solute in the drop and the amount of time the drop has been allowed to sit on the surface. We do this by removing liquid from a drop via a small hole in the substrate. This procedure does not disturb the liquid surface. However, viewing the drop from the side only allows a view of two diametrically opposed points of the contact line which can create artifacts in the drop width data. Instead, we monitor the footprint of the drop from behind the substrate, using total internal reflection, to obtain simultaneous information about the entire contact line. We find that the initial spreading of the drop on the surface for both upright and inverted sessile drops can last for several minutes but is largely independent of the solute concentration. However, during evaporation we find that the de-pinning angle is highly dependent on concentration and on the waiting time.

*We are grateful for support from NSF MRSEC and NSF GRF DGE-1746045.
1:03PM M15.00010: Electric Discharge Mediated Transient Interfacial Dynamics of a Sessile Liquid Droplet: Plethora of Hydrodynamic Features* BHASKARJYOTI SARMA (Presenter), Mechanical Engineering, Indian Institute of Technology Guwahati, SUNNY KUMAR, Chemical Engineering, MaNIT Bhopal, AMARESH DALAL, DIPANKAR NARAYAN BASU, Mechanical Engineering, Indian Institute of Technology Guwahati, DIPANKAR BANDYOPADHYAY, Chemical Engineering, Indian Institute of Technology Guwahati — We experimentally demonstrate a plethora of hydrodynamic features namely jetting, crowning, and bursting, engendered from capturing electrical discharge inside a sessile liquid droplet. The intense electrical energy deposited inside the conducting droplet in a capacitor like configuration designed with a pin-type anode and thin dielectric film-coated plate type cathode. The high-speed experiments reveal the formation of thermal bubbles from the electrodes and their subsequent evolution till collapse as the dominant mechanism underlying the rich hydrodynamics of the droplet. By tuning the properties of the liquid droplet and the electric field, we can tune the intensity of the discharge and ensuing bubble dynamics, thereby enabling the transition from one regime to another. The position of the electrode can also be tuned to alter the dynamics of shape evolution. The bursting phenomena result from the high electric field and/or high conductivity of the droplet, producing numerous micron size secondary droplets. The explored regimes, specifically bursting of a liquid droplet, are highly relevant for many industrial applications involving enhanced mass transfer such as spray generation, tissue ablation to name a few.

*DST SERB, Grant no. EMR/2016/001824, Government of India

1:15PM M15.00011: High density ratio Lattice Boltzmann simulations of immiscible drop collision* NEERU BALA (Presenter), Northumbria university, HALIM KUSUMAATMAJA, Durham university, CIRO SEMPREBON, Northumbria university — The physics and dynamics of a ternary fluid system are of special interest for a variety of practical applications, including combustion engines, ink-jet printing, and oil recovery. For example, recent experiments demonstrated that if fuel and water droplets are colliding in a combustion chamber, the water can be encapsulated by the fuel. This causes micro-explosions and enhances the burning rate of the combustion chamber. In this contribution, I will present a numerical investigation of the collision between two immiscible droplets by employing a high density ratio (~10^3) Free energy Lattice Boltzmann model, which account for the Inertial effects[1]. I mainly focus on the transition from adhesion to bouncing for a wide range of dimensionless numbers (Weber and Ohnesorge number) and Impact parameter by varying relative surface tension, Impact speed, liquid viscosity and drop size.

References:

*Northumbria University

Wednesday, March 4, 2020 11:15 AM - 2:15 PM
11:15AM M16.00001: Algorithm-specific Performance Analysis of Transmon Qubit Devices*
MICHAEL O'KEEFFE (Presenter), MIT Lincoln Laboratory, MORTEN KJAERGAARD, Research Laboratory of Electronics, Massachusetts Institute of Technology, MOLLIE SCHWARTZ, MIT Lincoln Laboratory, GABRIEL SAMACH, AMY GREENE, CHRIS MCNALLY, Research Laboratory of Electronics, Massachusetts Institute of Technology, DANNA ROSENBERG, MIT Lincoln Laboratory, WILLIAM OLIVER, Research Laboratory of Electronics, Massachusetts Institute of Technology, ANDREW JAMES KERMAN, KEVIN OBENLAND, MIT Lincoln Laboratory — Many demonstrations of quantum algorithms exhibit a tradeoff between the accuracy of the algorithm and the fidelity of the circuit that implements that algorithm. In particular, for algorithms that rely on Trotter decomposition to approximate a target unitary, increasing the number of steps reduces the algorithm error. However, in current devices, uncontrolled interactions with the environment and suboptimal control limit qubit coherence and gate fidelity, which ultimately restrict circuit depth. We analyze algorithm performance on transmon qubit devices using simulated, model-based, and experimentally measured process maps for gates, and compare a number of characterization metrics. In the case of a Trotterized algorithm, we determine the optimal operating point and predict the expected performance in good agreement with experiment.

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ALISTAIR MILNE (Presenter), CLAIRE EDMUNDS, CORNELIUS HEMPEL, The University of Sydney, HARRISON BALL, MICHAEL HUSH, ANDRÉ CARVALHO, Q-CTRL, MICHAEL BIERCUK, The University of Sydney — We present a technique for the characterization of noise in oscillator-mediated entangling operations applicable to a range of gate implementations in both trapped ion and superconducting circuit architectures. A major source of error in this class of entangling gates is residual coupling between the system of qubits and the intermediate oscillator modes, often caused by noise on the mode frequencies. In order to characterize this leading source of gate error, we use discrete phase modulation of the field driving the gate to construct sequences of oscillator-phase-space displacements with a band-limited sensitivity to oscillator frequency noise. By displacing the motion of a single trapped $^{171}\text{Yb}^+$ ion, we characterize the sensitivity of these sequences to engineered noise, verifying analytic predictions in the filter function formalism for the observed signal strength. We also perform sensing of intrinsic noise, leveraging tools for spectrum reconstruction based on a singular value decomposition approach developed at Q-CTRL.
**11:39AM M16.00003: Detector Tomography on IBM Quantum Computers and Mitigation of Imperfect Measurement**

YANZHU CHEN (Presenter), MAZIAR FARAHZAD, Stony Brook University, SHINJAE YOO, Brookhaven National Laboratory, TZU-CHIEH WEI, Stony Brook University — We use quantum detector tomography to characterize the qubit readout in terms of measurement POVMs on IBM Quantum Computers IBM Q 5 Tenerife and IBM Q 5 Yorktown. Our results suggest that the characterized detector model deviates noticeably from the ideal projectors. Further improvement on this characterization can be made by adopting two- or more-qubit detector models instead of independent single-qubit detectors for all the qubits in one device. We also find evidence indicating correlations in the detector behavior, i.e. the detector characterization is slightly altered when other qubits and their detectors are in operation. We also discuss how the characterized detectors' POVM can be used to estimate the ideal detection distribution.

*This work was supported by National Science Foundation under grants No. PHY 1620252 and No. PHY 1915165, as well as a SUNY Center-Scale Proposal Planning and Development Grant Program RFP 18-02CSP (No. CSP18035) and a research subcontract No. 358980 from Bookhaven Science Associates, LLC.*

**11:51AM M16.00004: Characterizing mid-circuit measurements with a new form of gate set tomography part 1: Theory**

KENNETH RUDINGER (Presenter), TIMOTHY PROCTOR, ERIK NIELSEN, Quantum Performance Laboratory, Sandia National Laboratories, GUILHEM RIBEILL, MATTHEW WARE, LUKE GOVIA, THOMAS A OHKI, BBN Technologies, KEVIN YOUNG, ROBIN BLUME-KOHOUT, Quantum Performance Laboratory, Sandia National Laboratories — While quantum circuits end with measurements, they can also include measurements in the middle. Such mid-circuit measurements are required for real-time feedforward control applications, such as quantum error correction. Understanding error processes in these mid-circuit measurements will be critical for building next-generation quantum processors. To that end, we extend gate set tomography (GST), a highly accurate and self-consistent protocol for diagnosing quantum gate errors, to be able to also characterize mid-circuit measurements. We will describe this extension and demonstrate its success in simulations.

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12:03PM M16.00005: Characterizing mid-circuit measurements with a new form of gate set tomography part 2: Experiment*  GUILHEM RIBEILL (Presenter), MATTHEW WARE, LUKE GOVIA, BBN Technology - Massachusetts, KENNETH RUDINGER, TIMOTHY PROCTOR, Sandia National Laboratory, THOMAS A OHKI, BBN Technology - Massachusetts — Quantum computers rely on classical electronics for qubit control and readout. An important capability for the implementation of complex algorithms such as quantum error correction is the ability to operate the classical hardware in a feedback loop with the quantum processor. Mid-circuit measurements are the key operation in this type of control scheme, and their efficient and precise characterization will be critical to understanding the performance of algorithms on near-term quantum devices. To that end, we demonstrate the use of an extension to gate set tomography (GST), a highly accurate protocol for diagnosing quantum processes, to characterize intermediate measurements on a superconducting transmon qubit.

*This material is based upon work supported by the U.S. Army Research Office under Contract No: W911NF-14-C-0048. Sandia National Labs is managed and operated by NTESS, LLC, a subsidiary of Honeywell International, Inc., for the U.S. DOE's NNSA under contract DE-NA0003525. Any opinions, findings and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of ARO, DOE, or the US Government This document does not contain technology or technical data controlled under either the U.S. ITAR or the U.S. EAR.

12:15PM M16.00006: A proposed gold standard family of protocols for benchmarking and diagnosing elementary quantum gate operations* KRISTINE BOONE, ARNAUD CARIGNAN-DUGAS, JOEL WALLMAN, University of Waterloo, IAN HINCKS, DAR DAHLEN, Quantum Benchmark, JOSEPH V EMERSON (Presenter), University of Waterloo — We propose a family of randomized benchmarking protocols as a gold standard for assessing and diagnosing error rates on elementary one and two qubit gates. We discuss various advantages of our bespoke family of protocols relative to other standard approaches. These advantages include: reducing the number of single shot experiments and the number of distinct random sequences including; improving the accuracy and convergence of confidence intervals; accommodating arbitrary gates within SU(4); and reliably assessing the error rate and error type associated with individual gates from any universal gate set. Time-permitting, we will report results from implementing these protocols across a variety of leading platforms, including both superconducting qubits and trapped ions.

*NSERC
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12:27PM M16.00007: Efficient learning of quantum noise* [Invited] ROBIN HARPER (Presenter), STEVEN FLAMMIA, Centre for Engineered Quantum Systems, School of Physics, University of Sydney, JOEL WALLMAN, Institute for Quantum Computing and Department of Applied Mathematics, University of Waterloo — Noise is the central obstacle to building large-scale quantum computers. Quantum systems with sufficiently uncorrelated and weak noise could be used to solve computational problems that are intractable with current digital computers. There has been substantial progress towards engineering such systems. However, continued progress depends on the ability to characterize quantum noise reliably and efficiently with high precision. Here I will discuss a newly introduced protocol that completely and efficiently characterizes the qubit error rates of quantum noise. The method returns an estimate of the effective noise with relative precision and detects all correlated errors. I will show how the reconstruction allows the easy visualization of these correlated errors, enabling both the discovery of long-range correlations in the device and the construction of scalable models that describe the noise in the device to arbitrary precision. These properties of the protocol make it exceptionally well suited for high-precision noise metrology in quantum information processors. Our results are the first implementation of a provably rigorous, diagnostic protocol capable of being run on state of the art devices and beyond. These results pave the way for noise metrology in next-generation quantum devices, calibration in the presence of crosstalk, bespoke quantum error-correcting codes, and customized fault-tolerance protocols that can greatly reduce the overhead in a quantum computation.

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1:03PM M16.00008: Long-Sequence Quantum Process Tomography* TAKANORI SUGIYAMA (Presenter), Univ of Tokyo — It is indispensable for development of a quantum computer to further improve accuracy of elemental quantum operations. Details of errors during the operations are useful information for achieving the accuracy improvement. Quantum tomography has a potential to provide such information, but its standard protocols suffer from low reliability due to its high sensitivity against state preparation and measurement (SPAM) errors. Self-consistent quantum tomography such as GST and RSCQT overcomes the low reliability, but it requires too large costs of experiments and data-processing. Here, we propose a new tomographic method with an error amplification, named long-sequence quantum process tomography. We theoretically prove that the error amplification can suppress effects of SPAM errors in arbitrary finite dimensional system, and numerically show that its implementation costs can be practical for one- and two-qubit systems. We also explain how to use the method for characterizing leakage and crosstalk errors, and discuss its practicality beyond two-qubit systems.

*This work was supported by JST PRESTO (JPMJPR1915), JST ERATO (JPMJER1601), and MEXT Q-LEAP (JPMXS0118068682), Japan.
1:15PM M16.00009: Spectral Quantum Tomography*  JONAS HELEN (Presenter), KdV Institute / QuSoft, University of Amsterdam, FRANCESCO BATTISTEL, BARBARA MARIA TERHAL, Delft University of Technology — We introduce spectral quantum tomography, a simple method to extract the eigenvalues of a noisy few-qubit gate, represented by a trace-preserving superoperator, in a SPAM-resistant fashion, using low resources in terms of gate sequence length. The eigenvalues provide detailed gate information, supplementary to known gate-quality measures such as the gate fidelity, and can be used as a gatediagnostic tool. We apply our method to one- and two-qubit gates on two different superconducting systems available in the cloud, namely the QuTech Quantum Infinity and the IBM Quantum Experience. We discuss how cross-talk, leakage and non-Markovian errors affect the eigenvalue data.

*The work by FB and BMT was supported by ERCgrant EQEC No. 682726. JH is funded by STW Netherlands, NWO VIDI, an ERC Starting Grant and by the NWO Zwaartekracht QSC grant.

1:27PM M16.00010: Independent State and Measurement Characterization on Quantum Computers*  JUNAN LIN (Presenter), JOEL WALLMAN, RAYMOND LAFLAMME, University of Waterloo — Correctly characterizing state preparation and measurement (SPAM) processes is a necessary step towards building reliable quantum processing units (QPUs). In this work, we approach this problem by assuming certain structure on SPAM and gate elements, and derive a simple experimental procedure to separately estimate the SPAM error strengths on a QPU. After discussing principles behind the experimental design, we present the protocol along with an asymptotic bound for the uncertainty in the estimated parameters in terms of quantities that can be estimated independently of SPAM processes. We test this protocol on a publicly available 5-qubit QPU and discuss the applicability of our protocol on near-term devices.

*This research was supported by the Government of Ontario and the Government of Canada through CFREF, NSERC and Industry Canada.

1:39PM M16.00011: Extracting Coherence Information From Random Circuits Using “Speckle Purity Benchmarking”  JULIAN KELLY (Presenter), SERGIO BOIXO, ZIJUN CHEN, JOHN M MARTINIS, HARTMUT NEVEN, Google — Budgeting the contributions of coherent and incoherent noise sources is an important component of benchmarking quantum gates. Typically, methods such as Cross Entropy Benchmarking (XEB) or Randomized Benchmarking are used to measure an error-per-gate that includes noise and control errors. These sequences can be extended to quantify the decay of a quantum state due to noise only by measuring the state purity with tomography as described in previous publications. Here, we introduce a method that allows us to extract the same information with exponentially fewer sequences from raw XEB data. We introduce “Speckle Purity Benchmarking” which quantifies the purity via the contrast (or “speckliness!”) of output bitstring probabilities. Pure quantum states generated by the XEB procedure will have high contrast, while incoherent mixtures will have low contrast. Compared to conventional XEB, this procedure can be done with zero information about the actual quantum process. Additionally, this can be scaled to a handful of qubits.
1:51PM M16.00012: Quantum noise spectroscopy for multiaxis noise models*  LEIGH NORRIS (Presenter), Dartmouth Coll, GERARDO A PAZ SILVA, Griffith University, FELIX BEAUDOIN, NanoAcademic Technologies, LORENZA VIOLA, Dartmouth Coll — Characterizing decoherence that arises from coupling to noisy environments is essential for optimized control and error correction strategies in realistic quantum information processors. Motivated by this challenge, quantum noise spectroscopy (QNS) seeks to estimate the spectral properties of noise affecting quantum systems. To date, QNS protocols have largely focused on platforms dominated by dephasing ($T_2$) processes, rendering them inapplicable to systems in which longitudinal relaxation ($T_1$) processes occur on a comparable timescale. To move beyond dephasing-dominated platforms, we extend frequency-comb based QNS to a multi-axis qubit noise model that takes into account both $T_1$ and $T_2$ processes from either classical or quantum environments. Targeted control of the qubit permits a complete spectral reconstruction, including arbitrary cross-axis correlations. Using a novel spherical representation for the noise operators, we show that three noise spectra characterize the reduced dynamics in a regime where the qubit energy splitting is large. This spherical representation enables a straightforward multi-axis extension to QNS protocols based on continuous driving, such as spin-locking.

*Research supported by ARO grant No. W911NF1410682 and MURI grant No. W911NF1810218.

2:03PM M16.00013: Cayley path and quantum computational supremacy: A proof of average-case #P-hardness of Random Circuit Sampling with quantified robustness*  RAMIS MOVASSAGH (Presenter), Quantum Theory and Algorithms, IBM Research — A one-parameter unitary-valued interpolation between any two unitary matrices is constructed based on the Cayley transformation, which extends our work. The entries of the interpolated unitaries are shown to be low-degree rational functions in the parameter, which we proved can be efficiently determined using an extension of the Berlekamp-Welch algorithm. We prove that this path provides scrambled unitaries with probability distributions arbitrarily close to the Haar measure. We then prove the simplest known average-case #P-hardness of random circuit sampling (RCS), which is the task of sampling from the output distribution of a quantum circuit whose local gates are random Haar unitaries, and is the lead candidate for demonstrating quantum supremacy in the NISQ era. We show that a previous work based on the truncations of the power series representation of the exponential function does not provide practical robustness. Explicit bounds on noise resilience are proved, which on a grid of $\sqrt{n} \times \sqrt{n}$ qubits with circuit depth $\sqrt{n}$ is $2^{O(-n^3)}$, and with constant-depth it is $2^{O(-n^2)}$. Improvements to $O(2^{(-n)/\text{poly}(n)})$ would prove the quantum supremacy conjecture, which may be false.

*The Frontiers Foundation and the MIT-IBM collaborative grant

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M17 DQI: Hybrid Systems - Spins, Quantum Dots, Microwaves

203 - Karl Petersson, Niels Bohr Inst - Tag(s): Focus
**11:15AM M17.00001: Long-distance entangling gates between quantum dot spins mediated by a superconducting resonator** [Invited] SOPHIA ECONOMOU (Presenter), Virginia Tech — A recent experimental breakthrough in gate-defined quantum dots (QDs) is the strong coupling between the spin and a superconducting resonator mode, mediated through the orbital degree of freedom. This, along with advances in the control of QD spins, indicate a path toward scalable quantum information processing devices. I will present our work on high-fidelity quantum gates, both between spin qubits in neighboring QDs and between remote QDs coupled through a resonator mode. I will also discuss possible paths to multi-qubit gates and quantum algorithms.

*This research is supported by ARO (grant number W911NF-17-0287).*

**11:51AM M17.00002: Resonant Microwave Mediated Interactions Between Distant Electron Spins** FELIX BORJANS (Presenter), XANTHE CROOT, XIAO MI, MICHAEL GULLANS, JASON PETTA, Princeton University — The ability to transfer quantum states and generate entanglement over distances much larger than qubit length scales is an important step towards maximal parallelism and the implementation of two-qubit gates on arbitrary pairs of qubits. Extending qubit interactions beyond the nearest neighbor is particularly beneficial for spin-based quantum computing architectures, which are limited by short-range exchange interactions. Experimental progress towards achieving long-range spin-spin coupling has so far been restricted to interactions between individual spins and microwave photons [1,2,3]. We demonstrate resonant microwave-mediated coupling between two electron spins that are physically separated by more than 4 mm [4]. Our results imply that microwave-frequency photons may be used as a resource to generate long-range two-qubit gates between spatially separated spins.


*Funded by Army Research Office grant W911NF-15-1-0149 and the Gordon and Betty Moore Foundation’s EPIQS Initiative through grant GBMF4535. Devices were fabricated in the Princeton University Quantum Device Nanofabrication Laboratory.*
Interfacing epitaxial rare earth spins with superconducting circuits for high-sensitivity ESR

NOAH JOHNSON, Pritzker School of Molecular Engineering, University of Chicago, SHOBHIT GUPTA (Presenter), Physics, University of Chicago, YUXIANG PEI, Physics, University of Science and Technology of China, MANISH KUMAR SINGH, Pritzker School of Molecular Engineering, University of Chicago, SUPRATIK GUHA, Argonne National Laboratory, DAVID I SCHUSTER, Physics, University of Chicago, TIAN ZHONG, Pritzker School of Molecular Engineering, University of Chicago, JUN YANG, HAITAO ZHANG, Corning Inc. — Hybrid quantum systems interfacing superconducting circuits with solid-state spin ensembles provide a practical route to realizing long-term microwave quantum memories and high-sensitivity inductive electron spin resonance (ESR) detection [1,2]. Specifically, ensembles of erbium ions are a promising platform for quantum networks and transduction [3] due to their long coherence times and telecom band optical transition at 1.54 μm. We report on pulsed and continuous wave ESR spectroscopy measurements of erbium dopants in Y$_2$O$_3$ [4] performed at millikelvin temperature using a microwave resonator. Using a superconducting low impedance resonator on epitaxially grown thin-film Y$_2$O$_3$ will allow for further increased coupling rates between the cavity photons and electron spins on the order of kHz.


*We acknowledge funding support from the National Science Foundation EAGER award No 1843044, Funder Id: http://dx.doi.org/10.13039/100000001.
This work was supported by a NASA Space Technology Research Fellowship.
High-Speed Quantum Interface with a Quantum Dot Molecule Coupled to a Superconducting Resonator

YUTA TSUCHIMOTO (Presenter), ETH Zurich, ZHE SUN, EPFL, EMRE TOGAN, PATRICK KNÜPPEL, ETH Zurich, AYMERIC DELTEIL, CNRS, STEFAN FÄLT, MARTIN KRONER, KLAUS ENSSLIN, ANDREAS WALLRAFF, WERNER WEGSCHEIDER, ATAC IMAMOGLU, ETH Zurich — Quantum transduction between optical and microwave photons is a key element of quantum networks. An optically-active quantum dot molecule (QDM) has a large electric dipole moment which can couple to microwave (MW) photons in a superconducting (SC) resonator [1]. In our scheme, the following features with a large MW coupling strength realize fast and efficient transduction: (i) a low-Q asymmetric optical cavity encapsulating the QDM ensures high-efficient absorption of incoming optical photons; (ii) fast radiative decay of the QDM finishes the transduction in nanosecond time scales; (iii) the radiative decay channel emits heralding photons upon success of the transduction.

We fabricate an onchip hybrid device consisting of a QDM and a SC resonator and demonstrate a large MW coupling strength. With a modest device improvement, we estimate that a large conversion bandwidth of over 100 MHz with high conversion efficiency is feasible.


*This work is supported by NCCR QSIT (National Centre of Competence in Research, QSIT-Quantum Science and Technology).
On-chip superconducting resonator devices for sensitive spin detection at high magnetic fields.*

GIOVANNI FRANCO-RIVERA (Presenter), JOSIAH COCHRAN, Department of Physics and The National High Magnetic Field Laboratory, Florida State University, LEI CHEN, ZHEN WANG, Center for Excellence in Superconducting Electronics, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Science, Shanghai, China, SYLVAIN BERTAINA, Inst Mat Microelectronique et Nanosciences de Provence, UMR7334, CNRS, Aix-Marseille Universite, Marseille, France, IRINEL CHIORESCU, Department of Physics and The National High Magnetic Field Laboratory, Florida State University — The ability to probe spin-photon interactions using Electron Spin Resonance techniques has gained significant interest given the realization of hybridized states between microwave photons and different spin ensembles.\(^1\)\(-3\) On-chip superconducting resonators provides a way to inductively couple a spin two level system with a resonant electromagnetic mode leading to enhanced sensitivity\(^4\) when compared to traditional 3D resonators. We demonstrate the implementation of λ/4 resonator placed after a coplanar waveguide-to-stripline transition on a 20 nm thick Nb film. Temperature effects on the losses and resonance frequency are studied for bare and spin loaded resonators. A resonance signal at 0.62 T for a spin S=1/2 system is presented, demonstrating the feasibility of such on-chip structures for high magnetic field electron spin detection.


*The National High Magnetic Field Laboratory is supported by the National Science Foundation through NSF/DMR-1644779 and the State of Florida. We acknowledge the Frontier Science Key Programs of the CAS, grant No. QYZDY-SSW-JSC033.
12:39PM M17.00006: Theory of spin-orbit mediated hole spin-photon coupling in lateral 
Ge/SiGe quantum dots* VANITA SRINIVASA (Presenter), Center for Computing Research, Sandia 
National Laboratories, RUPERT M LEWIS, LISA A TRACY, TZU-MING LU, WILL J. HARDY, Sandia National 
Laboratories, MITCHELL BRICKSON, ANDREW D. BACZEWSKI, Center for Computing Research, Sandia 
National Laboratories, DWIGHT R LUHMAN, Sandia National Laboratories — Coupling semiconductor 
spin qubits to microwave photons enables long-range quantum information transfer, and strong 
spin-photon coupling has recently been demonstrated for electron spin qubits in silicon [1, 2]. In 
this context, hole spin qubits in lateral Ge/SiGe quantum dots [3, 4] represent an attractive 
alternative platform without valley degeneracy and with strong intrinsic spin-orbit interaction. We 
present an analytical formulation of heavy hole spin-photon coupling mediated by spin-orbit 
interaction in lateral Ge/SiGe quantum dots. Using this formalism, we derive expressions for 
effective single-photon and three-photon coupling within this system and explore the strengths 
of these interactions in experimentally relevant parameter regimes.


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Energy's NNSA under contract DE-NA0003525. The views expressed above do not necessarily 
represent the views of the DOE or the U.S. Government.
High kinetic inductance superconducting cavity for strong coupling of Si/SiGe qubits

Achieving long range coherent interactions between qubits is a milestone of quantum information. In recent years the field of circuit quantum electrodynamics (cQED) has demonstrated long range coupling between superconducting qubits, quantum dots in various semiconductors systems, and even coupling between hybrid systems. Strong coupling between remote qubits requires that the coupling strength be larger than the decoherence rates of both the microwave cavity and the qubits. The coupling can be enhanced by increasing the impedance of the cavity. There are two possible ways to achieve such a goal: first, by using a superconductor with high kinetic inductance; second, by using an array of Josephson junctions, which constrains the application of an external magnetic field. We present a Si/SiGe quantum dot device that combines a high impedance cavity and low impedance leads to reduce the photon leakage through the DC lines. The resonator is made of NbN, a high kinetic inductance superconductor, while the leads are composed of a thin layer of NbN with a thicker layer of Nb on top to reduce the impedance of the leads. The third harmonic can be used to further enhance the coupling strength between the dots and the resonator, which is important for strong coupling.

Coupling silicon qubits via a high-impedance superconducting resonator

Spin qubits in semiconductors like silicon are widely perceived as an ideal technology platform to realize a quantum computer. Their advantages range from the high integration density and the mature manufacturing technology of classical computers, to their long lifetimes and low error rates. On the other hand, spins in semiconductors are not easy to couple over long distances. For this, optical or microwave photons are much better suited. Here, I will describe our experimental efforts to couple two spin qubits through a superconducting microwave resonator. To enlarge the coupling to the qubit charge dipole, we use a high-kinetic-inductance NbTiN nanowire resonator and achieve a large impedance of about 3 kΩ. The high impedance and kinetic inductance come with microwave engineering challenges (e.g. leakage through the gate fanout) and we discuss several approaches to overcome these. Finally, we demonstrate operation of a device with two silicon double quantum dots coupled to the same resonator. Our work opens up opportunities to adapt very powerful and well-developed techniques from circuit quantum electrodynamics and superconducting qubits to the spin qubit world. These opportunities include long-range coupling of spin qubits, and fast spin readout without charge sensors.
**1:15PM M17.00009: Sensitive spin detection using differential squids and on chip microwave waveguide**

JOSIAH COCHRAN (Presenter), GIOVANNI FRANCO-RIVERA, Department of Physics, Florida State University, LEI CHEN, ZHEN WANG, and IRINEL CHIORESCU, Department of Physics — Sensitive detection of spin resonance is essential for achieving coherent spin qubit control. Recent experiments have involved bifurcation resonators, and artificial atoms, which provide sensitivity over a wide frequency range; however, a broadband device is needed for complex materials. A novel differential squid detection method for spin systems on a microwave waveguide is being developed at NHMFL. This method utilizes a superconducting niobium coplanar strip line broadband microwave device coupled with niobium nano-squid devices. A nano-fabricated planar Dayem bridge squid is placed inside an omega loop for sensitive spin detection while a secondary squid is placed far away from the omega loop in order to measure background fields. The differential measurement of the fields measured by the two squids will result in a cancellation of background fields with the goal of having a more sensitive spin detection.

1 G. Yue et al., APL 202601 (2017).
2 Budoyo et al., PRM 2.1, 011403 (2018).
3 Toida et al., Comm. Phys. 2.1, 33 (2019).

*The National High Magnetic Field Laboratory is supported by the National Science Foundation through NSF/DMR-1644779 and the State of Florida. We acknowledge the Frontier Science Key Programs of the CAS, grant No. QYZDY-SSW-JSC033.*

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**1:27PM M17.00010: From Transistors to Circuit Realization of a 50mK Analog Amplifier in FDSOI Technology For Measuring Quantum-Dots**

LOÏCK LE GUEVEL (Presenter), GÉRARD BILLIOT, CEA-LETI, MARCO L.V. TAGLIAFERRI, CEA-IRIG, MARCos ZURITA, CEA-LETI, SILVANO DE FRANCESCHI, MARC SANQUER, CEA-IRIG, MAUD VINET, CEA-LETI, XAVIER JEHL, ALOYSIUS G.M. JANSEN, CEA-IRIG, GAËL PILLONNET, CEA-LETI — On-chip cryogenic electronics will accelerate the development of silicon-based quantum bits for quantum computing allowing for faster systematic device tests with various materials and geometries. Low-frequency analog characteristics of single FDSOI 28nm MOSFETs and available passive elements were investigated at cryogenic temperature and compared to actual model predictions. The impact on circuit specifications was studied for a transimpedance amplifier (TIA) operating down to 50mK such as the low-temperature increase of the transistor transconductance leading to a times-5 improvement of the bandwidth. This cryogenic TIA was cointegrated with a quantum dot and compared to a commonly used room-temperature measurement method. Finally, we foresee that the bandwidth of 2.6 kHz can be increased by almost two orders of magnitude while maintaining a 1 μW power consumption, compatible with available cooling power at 100 mK.
1:39PM M17.00011: 3D integrated device architecture for hybrid superconductor-semiconductor quantum dot devices*  
FELIX JULIAN SCHUPP (Presenter), XANTHE CROOT, FELIX BORJANS, XIAO MI, Physics, Princeton University, DANNA ROSENBERG, RABINDRA DAS, DAVID K KIM, ALEXANDER MELVILLE, WILLIAM OLIVER, MIT Lincoln Laboratories, JASON PETTA, Physics, Princeton University — Low internal losses in superconducting resonators require optimized fabrication that was developed in the framework of superconducting qubits. Semiconductor spin-qubit experiments in hybrid super-semi cQED involve semiconducting substrates, gate-oxides, dopants or even micromagnets, which may not be compatible with conventional resonator fabrication leading to higher internal losses. Here we present a 3D integrated super-semi architecture with the superconducting resonator chip fabricated in an environment optimized for superconducting qubits and then flip-chip bonded onto a spin-qubit chip fabricated in its own dedicated facility. Compared to previous cQED experiments with semiconductor spins, we demonstrate reduced photon losses in the few-photon regime and with Al gate-electrodes connected to the resonator. Using a perforated ground plane, we achieve Q=74k at an in-plane magnetic field of 100 mT, which is required for spin-photon coupling.

*Sponsored by ARO (W911NF-15-1-014), and the Gordon and Betty Moore Foundation's EPIQS Initiative (GBMF4535), and NSF (DMR-1409556). The devices were fabricated at MIT Lincoln Laboratories and the Princeton University Quantum Device Nanofabrication Laboratory. We acknowledge helpful discussion with Joe Kerckhoff from HRL Laboratories, LLC.

1:51PM M17.00012: Quantum physics with pulses of radiation*  
KLAUS MOLMER (Presenter), Aarhus University — The ability to control quantum systems and apply special superposition states and entangled states of light and matter is pursued with many experimental platforms and forms the basis of strategies for quantum computing, communication and metrology. I shall discuss the interaction of a quantum system with a pulse of quantized radiation. While crucial for multiple effects in quantum optics and for the entire concept of flying and stationary qubits, quantum optics textbooks do not provide a formal description of this foundational and elementary interaction process. I shall present a new (and simple) theoretical formalism [1] that accounts for the interaction of travelling pulses of quantized radiation with a local quantum system such as a qubit, a spin or a multi-level atom in a cavity. Applications of the theory are shown for recent experiments with optical, microwave and acoustic quantum pulses.


*This research was supported by the the Villum Foundation, the European Union FETFLAG program, Grant No. 820391 (SQUARE),and the U.S. ARL-CDQI program through cooperative Agreement No. W911NF-15-2-0061.
Quantum optical characterization of rare earth ion in superconductor quantum memory* OSAMA NAYFEH (Presenter), Naval Information Warfare Center Pacific — There is a need for the implementation of quantum entangled memory devices that can interface to computational qubit devices via efficient transfer of the low coherence time qubit states to the high coherence spin states of optically active ions. We present characterization in the cryogenic regime of a rare earth ion quantum memory we formed from ion implantation of Neodymium ions in superconducting Niobium Nd$^{3+}$:Nb. We examine via spectroscopy in a cryo-magneto-optical probe station, the 4F3/2 to 4I 9/2 transition in the NIR at 903.4 nm as a function of magnetic and microwave field. We quantify the spin echoes to evaluate T1 and T2 coherence times. We find an improvement when entering the superconducting regime of Niobium at 7.5 K. We study the effects of varying the laser excitation intensity and the microwave and magnetic field strengths on key parameters. The results are consistent with an increase of the spin relaxation and are discussed in accordance with theoretical models.

*We acknowledge support of the NIWC Pacific / Office of Naval Research applied research program. The views and conclusions are not to be interpreted as representing the official policies, either expressed or implied, of NIWC PAC or the U.S. Government. Approved for Public Release.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M18 DSOFT: Memory Formation in Matter: From Reading the Past to Designing the Future 205 - Joseph Paulsen, Syracuse University - Tag(s): Invited, Undergrad Friendly

Global Memory From Local Hysteresis and Disorder in a Jammed Solid* [Invited] NATHAN KEIM (Presenter), Physics, Pennsylvania State University, JACOB B HASS, BRIAN KROGER, DEVIN WIEKER, Physics, California Polytechnic State University, San Luis Obispio — Cyclically shearing a soft 2D jammed material can train it with a memory of strain amplitude that can be retrieved later. Using experiments with particles at an oil-water interface, we show that this memory arises from the hysteresis of particles' rearrangements within the material. A stable population of rearrangements is created by training, and disorder ensures that they collectively discriminate among different inputs. These results point to a generic way of encoding memories in hysteresis and disorder, and explain why jammed and dilute suspensions must have different kinds of memory. The behavior in jammed systems is reminiscent of the return-point memory found in ferromagnets and many other systems, but in light of jammed systems' unquenched disorder, it is unexpected.

*This work was supported by NSF DMR-1708870.
11:51AM M18.00002: Memory formation in cyclically deformed glasses* [Invited] SRIKANTH SASTRY (Presenter), MONOJ ADHIKARI, Jawaharlal Nehru Ctr Adv Sci, MUHITTIN MUNGAN, Institut fur angewandte Mathematik, Universität Bonn, IDO REGEV, Jacob Blaustein Institutes for Desert Research,, Ben-Gurion University of the Negev, KARIN ANDREA DAHMEN, Department of Physics, University of Illinois at Urbana-Champaign —

Cyclically shear deformed glasses reach, after a transient regime, periodic orbits involving transitions between basins of energy minima that are visited repeatedly during repeated cycles of deformation, if the amplitude of deformation is not too large. These periodic orbits encode information of their deformation history, and have been shown to retain memory of training at multiple strain amplitudes. Such memory effects, in the presence of plastic rearrangements involved in transitions between basins, is surprising, but appears to be generic. Investigations of the nature of such periodic orbits reveals rich structure, whose analysis permits investigation of the presence or otherwise of features such as return point memory, and suggests protocols by which the encoded information may most efficiently be recovered.

*J. C. Bose Fellowship, DST, India

12:27PM M18.00003: Memories in a jar [Invited] ZORANA ZERAVCIC (Presenter), ESPCI Paris — Self-assembly has emerged as a powerful technique for synthesizing structures on the nano and micro-scale. The basis of this development is the use of biopolymers, like DNA, to design specific interactions between multiple species of components, allowing the spontaneous assembly of complex structures. Inspired by biological systems, where the same set of components can assemble many different complexes, we can design mixtures of shared components that have memory of many distinct structures and are capable of assembling each at will. Moreover, these structures can transition one to another when an appropriate switch is triggered. In this talk I will discuss examples of memories modeled as structures made of DNA coated colloidal particles.

1:03PM M18.00004: Yoav Lahini Invited Talk [Invited] —
NIDHI PASHINE (Presenter), University of Chicago — Disordered materials exist in a rugged energy landscape and become trapped in metastable states that are not a global energy minimum. These far-from-equilibrium systems relax slowly as they search for lower-energy configurations. This aging often leads to material degradation and is thus thought of as undesirable. Here I show how this aging can be directed to produce a final state that has advantageous properties and unique functions not typically found naturally [1]. Aging a system subject to external constraints leaves a memory of how it was aged and creates stresses that direct its evolution [2]. Aging obeys a natural “greedy algorithm”: the material simply follows the path of most rapid and accessible relaxation. During aging, the material modifies stressed regions differently from those under less stress. Our goal is to find out what range of behaviors can be achieved by directed-aging protocols. We do this through experiments and with simulations that use simple models of the aging process in disordered networks. Our experimental networks are laser cut from EVA foam and then aged under external stress. (We can apply heat not only to accelerate the aging process but also to help the material retain a memory of how it was aged after the system has been re-cooled.) Using different applied stresses, we can achieve different functions; a memory of the stress protocol can be read out by measuring the mechanical response of the aged systems. Directed aging provides a pathway for modifying and tuning a material's elastic properties in the non-linear as well as the linear regime without having to control the material at the microscopic level.


*Supported by DOE BES and Simons Foundation.

**Wednesday, March 4, 2020 11:15 AM - 2:15 PM**

**Session M19 FIP: Physics for Development** 207 - R Peterson, University of Colorado, Boulder - Tag(s): Invited, Undergrad Friendly
11:15AM M19.00001: Actions and schemes of support towards developing countries  [Invited]
JOSEPH NIEMELA (Presenter), ICTP — This talk will highlight actions aimed at fostering advanced studies and research in the physical and mathematical sciences in developing countries. An overarching concern is the recurrent problem of scientific isolation that has remained a serious impediment to scientific career growth for those scientists who choose to remain in their home countries. The emphasis will be on programs of the Abdus Salam International Center for Theoretical Physics (ICTP), a category 1 institute of UNESCO that uniquely provides an international forum for the basic sciences for scientists from all UNESCO member states. A wide spectrum of programs has evolved, often with the collaboration of partner institutions and organizations, especially in the case of applied sciences and/or education outreach: A few examples will be drawn from collaborations with the European Physical Society (EPS), through its Physics for Development Group, the International Society of Optics and Photonics (SPIE), and Centro Fermi in Rome. The list of international partners is much longer than this, of course, and working together has proved to be very beneficial, and in some cases crucial, in achieving shared goals.

11:51AM M19.00002: The voice of physics in Africa  [Invited]  JAMES GUBERNATIS (Presenter), Los Alamos Natl Lab — In 2017, the APS's Committee on International Scientific Affairs, in co-operation with the IoP, EPS, ICTP, and SAIP conducted a survey of the state and needs of the physics community in Africa. To bridge communication gaps in and with the African physics community identified by the survey, the APS recently launched the electronically distributed quarterly, The African Physics Newsletter. The launch is timely. A lot is happening in the African physics community. In the past three years, the number of African national physical societies has increased from nine to fifteen. The Abdus Salam International Centre for Theoretical Physics (ICTP) recently opened in Rwanda its first institute in Africa, the East African Institute for Fundamental Physics. In addition, there have been numerous schools, workshops, and conferences. I will highlight several interesting articles that have appeared in the newsletter about these and other events. Subscriptions to the newsletter are free (https://go.aps.org/africanphysics). Recent issues have information about how you can contribute news articles. Whether you are from Africa or just interested in African physics, by subscribing, reading, and especially by contributing, you will be strengthening what has become the voice of physics in Africa.
12:27PM M19.00003: SESAME project in the Middle East: Synchrotron radiation for sciences
[Invited] ESEN ALP (Presenter), Argonne Natl Lab — SESAME is a modern 2.5 GeV electron synchrotron, delivering infrared, ultraviolet, soft and hard x-rays. It is governed by an International Council, and it is funded by its member states. SESAME utilizes its beamlines for general scientific purposes. It has become operational in 2018. Currently three beamlines are dedicated to x-ray absorption spectroscopy, x-ray diffraction and infrared spectroscopy studies. Three additional beamlines are in various stages of development, including a soft-x-ray photoelectron spectroscopy, hard-x-ray tomography and imaging, and a macromolecular crystallography beamlines.

There can be as many as 18 beamlines built at full operations. The beamtime allocation is based on proposal system and it is free of charge for publishable work. Recent examples of published scientific work will be presented.

1:03PM M19.00004: Fundamental physics and accelerator science in developing countries
[Invited] CHRISTINE DARVE (Presenter), European Spallation Source — Education and industrialization are essential to promote positive developments in the least developed countries. The recent evolution of technologies and ICT open the doors to innovative way to support education in developing countries. To enhance the existing African School of Fundamental Physics and Applications (ASP), Massive Open On-line Courses (MOOC) have been prepared and implemented to teach accelerator physics and technologies. The goal of those initiatives is to catalyze the development of world-class institutions through the production of high-quality scientists and engineers to stimulate economic growth and employment creation. Pursuant to this goal, the objective is to produce the next generation of African scientists and engineers by training them in the necessary technical, entrepreneurial and leadership capacities to solve African problems thus contributing to economic and social transformation.
1:39PM M19.00005: Multifunctional Materials for Emerging Technologies [Invited]  FEDERICO ROSEI (Presenter), INRS - Energie et Materiaux — As the age of fossil fuels is coming to an end, now more than ever there is the need for more efficient and sustainable renewable energy technologies. This presentation will give an overview on recent developments in solar technologies that aim to address the energy challenge. In particular, nanostructured materials synthesized via the bottom-up approach present an opportunity for future generation low cost manufacturing of devices [1]. We demonstrate various multifunctional materials, namely materials that exhibit more than one functionality, and structure/property relationships in such systems, including new strategies for the synthesis of multifunctional nanoscale materials to be used for applications in photovoltaics, solar hydrogen production, solar windows and other emerging technologies. [2-23].

References

Wednesday, March 4, 2020 11:15 AM - 1:27 PM

Session M20 DFD GSNP: Turbulence & Nonlinear Dynamics 301 - Joel Newbolt, Harvard University
11:15AM M20.00001: Propagating oscillons in a 1Dim. Faraday experiment JOSE WESFREID (Presenter), PMMH, ESPCI PARIS, SAMANTHA KUCHER, PABLO COBELLI, DF-FCEN, University of Buenos Aires — We present the first experimental evidence of the existence of trains of propagating oscillons or localized structures in a 1D Faraday experiment in water. The fluid layer, contained within a thin annular vessel, is excited with a periodic vertical acceleration. Far beyond the threshold for Faraday instability, we have found the formation of localized structures with high nonlinear profile. In particular, we have observed cases where several structures form and propagate around the annulus at a constant velocity while keeping their relative individual position and amplitude. On the other hand, our experiments show that by phase-modulating the acceleration (driving) field it is possible to generate several individual trains of such structures distributed symmetrically over the annular region.

11:27AM M20.00002: Linearly driven flow on a rotating sphere ROHIT SUPEKAR (Presenter), Department of Mechanical Engineering, Massachusetts Institute of Technology, VILI HEINONEN, KEATON BURNS, JÖRN DUNKEL, Department of Mathematics, Massachusetts Institute of Technology — We investigate a generalized Navier–Stokes (GNS) equation as an analytically tractable minimal model for fluid flows driven by active stresses. The GNS dynamics couple an advective nonlinearity with a generic linear instability and have been shown to permit exact solutions in a stationary 2D spherical geometry. Here, we extend the analysis to actively driven flows on rotating spheres, motivated in part by the complex flow patterns observed in planetary atmospheres. The resulting model generalizes the widely studied barotropic vorticity equation by accounting for internal forcing effects that depend on the flow vorticity itself. We find exact solutions of the GNS equations corresponding to time-independent zonal jets and their superposition with westward propagating Rossby waves. Simulations for large rotation rates confirm that the statistically stationary state is close to these exact solutions. The phase speed of the nonlinear Rossby waves measured in the simulations agrees well with analytical predictions.
11:39AM M20.00003: Numerical Simulations of Gravitational Waves from Early-Universe Turbulence  ALBERTO ROPER POL (Presenter), University of Colorado, Boulder — We perform direct numerical simulations of magnetohydrodynamic turbulence in the early universe and numerically compute the resulting stochastic background of gravitational waves and relic magnetic fields. We obtain kinetic and magnetic energy spectra with greater realism than earlier analytic models. The computed gravitational wave spectra have a new universal form at low frequencies, with more power than suggested by earlier analytical models. The efficiency of gravitational wave production varies significantly with the physical form of the turbulence. For the same amount of turbulent energy, we find that the gravitational wave signal is stronger for irrotational flows than for vortical ones. Our results predict that a signal produced at the electroweak scale is detectable by the planned Laser Interferometer Space Antenna if at least 1% of the total energy density is injected into magnetic fields or turbulent plasma motions.

https://arxiv.org/abs/1903.08585
https://arxiv.org/abs/1807.05479

11:51AM M20.00004: Imaging Fluorescence of He*$_2$ Excimers Created by Neutron Capture in Liquid He II—a New Approach for Turbulent Flow Research*  XIN WEN (Presenter), Department of Physics and Astronomy, University of Tennessee, Knoxville, SHIRAN BAO, Florida State University, LANDEN MCDONALD, University of Tennessee, Knoxville, JOSH PIERCE, Oak Ridge National Laboratory, GEOFFREY L GREENE, Department of Physics and Astronomy, University of Tennessee, Knoxville, MORRIS LOWELL CROW, Oak Ridge National Laboratory, XIN (TONY) TONG, Institute of High Energy Physics, Chinese Academy of Sciences, ANTHONY MEZZACAPPA, Department of Physics and Astronomy, University of Tennessee, Knoxville, RYAN GLASBY, University of Tennessee, Knoxville, WEI GUO, Florida State University, MICHAEL FITZSIMMONS, Oak Ridge National Laboratory — We show unequivocal evidence for formation of He*$_2$ excimers in liquid He II created by ionizing radiation produced through neutron capture. Laser beams induced fluorescence of the excimers. The fluorescence was recorded by a camera at a rate of 55.6 Hz with the ability to determine the location of an event with an uncertainty of 5 microns. The technique enables measurement of turbulence around macroscopic size (liter+) objects or vortex matter in three dimensions under conditions of extreme Reynolds number. Using thermal counterflow techniques we explored excimer flow in cryogenic He.

*Work supported by the Office of Basic Energy Sciences, U.S. Department of Energy, Division of Materials Science and Scientific User Facilities, and ORNL Lab Directed Research and Development, and support from National High Magnetic Field Laboratory, which is supported by the National Science Foundation.
12:03PM M20.00005: Small-scale Energy Transfer in Turbulence*  JAMES CHEN (Presenter), MOHAMAD CHEIKH, State Univ of NY - Buffalo — The dynamics behind the multi-scale energy transfer in turbulent flows is investigated by introducing morphing continuum conservation laws on the basis of the Boltzmann-Curtiss kinetic theory. The resulting conservation laws reveal the existence of small-scale routes for the flow of energy broadening the view on energy cascade (forward or inverse). The comparison of the turbulence characteristic with the reference study indicates that the turbulence features in both frameworks are equivalent at the global and small-scales. The analysis reveals that at the small-scale both forward and inverse energy cascade exist in homogeneous isotropic turbulence while an overall negative energy flux (forward cascade) is present globally.

*This study is supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0154.

12:15PM M20.00006: Optimal perturbations for transient growth in a 3D stratified channel using nonlinear direct-adjoint looping  RITABRATA THAKUR (Presenter), International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, ARJUN SHARMA, Sibley School of Mechanical and Aerospace Engineering, Cornell University, RAMA GOVINDARAJAN, International Centre for Theoretical Sciences, Tata Institute of Fundamental Research — Laminar shear flows often transition to turbulence at Reynolds numbers smaller than that of their first linear instability. The underlying mechanism can be transient algebraic growth, either linear or nonlinear in nature. We obtain the maximum perturbation energy growth in a three-dimensional heated plane channel. A nonlinear technique of direct-adjoint-looping is employed to numerically achieve this. With this technique, we also obtain the initial velocity and temperature perturbation structure that leads to this growth. The energy growth associated with this optimal can be large enough to push the flow to turbulence. We study the effect of varying stratification strengths (gradient Richardson numbers), Reynolds numbers, and target times on the structure of the optimal. We show similarity or the lack thereof between the optimal perturbations for small (linear optimal) and large (non-linear optimal) initial energies.
12:27PM M20.00007: Role of elasticity and solvent viscosity on the center mode instability in pipe Poiseuille flow of Oldroyd-B fluids. INDRESH CHAUDHARY (Presenter), IIT Kanpur, GANESH SUBRAMANIAN, JNCASR Bangalore, VISWANATHAN SHANKAR, IIT Kanpur — A linear stability analysis of pipe Poiseuille flow of an Oldroyd-B fluid has been carried out to investigate the interplay among fluid inertia, elasticity and the ratio of solvent to the total viscosity. The stability has been analyzed for axisymmetric perturbations using pseudospectral and shooting methods. The system is found to be linearly unstable at the Reynolds numbers relatively lower than the values for which the transition to turbulence is typically observed for the Newtonian pipe flows. The system has been analyzed for the vast ranges of the wavelength, Reynolds number, elasticity number and the ratio of solvent to the total viscosity. In the limit of low elasticity, the fluctuations are found to be near the axis in the flow domain; hence we refer to this unstable mode as ‘centre mode’. This unstable mode stabilizes in the UCM limit (absence of solvent). Various scalings among the threshold and critical parameters have been established. Comparisons of the present results with those from the experimental studies in the existing literature have been made to establish theoretical evidence for the instability in viscoelastic flows which can potentially turn the steady laminar base flow into a turbulent one.

12:39PM M20.00008: Turbulence generation through an iterative cascade of the elliptical instability RYAN MCKEOWN (Presenter), Harvard University, RODOLFO OSTILLA MONICO, Mechanical Engineering, University of Houston, ALAIN JACK PUMIR, ENS Lyon, MICHAEL PHILLIP BRENNER, SHMUEL RUBINSTEIN, Harvard University — Turbulent flows are notoriously difficult to study due to the lack of a mechanistic framework that encapsulates how vortices interact, break down, and form new vortices, driving the cascade of energy down to the dissipative scale. We demonstrate the existence of a novel mechanism in which two counter-rotating vortices violently collide and break down, leading to the rapid development of a turbulent energy cascade mediated by iterations of the elliptical instability. We probe the full 3D dynamics of this complex breakdown by conducting both experimental flow visualizations and numerical simulations of colliding vortex rings. The onset of the elliptical instability generates an ordered array of secondary vortex filaments that are perpendicular to the original cores. Adjacent secondary filaments counter-rotate and interact with each other. In the high-Reynolds number limit, we observe another iteration of this instability, whereby even smaller tertiary filaments form in the same manner. The energy spectrum of this breakdown exhibits Kolmogorov scaling, E(k) ~ k^(-5/3), a hallmark of homogeneous isotropic turbulence. Clear evidence of this mechanism of vortex generation has also been recently observed over many length scales in recent numerical simulations of forced turbulence.
12:51PM M20.00009: 3D Visualization of Reconnections in Vortex Ring Collision  JOEL W. NEWBOLT (Presenter), RYAN MCKEOWN, SHMUEL RUBINSTEIN, Harvard University — Vortex interactions appear in many fluid systems, from the wake behind an airplane in flight to that of a ship moving through the water. This is because friction between a fluid and a solid boundary can generate vorticity in the fluid. A simple example is the vortex ring, yet even the interaction between two vortex rings can cause instabilities that break the symmetries of the flow. When two vortex rings of equal size collide head-on at moderate Reynolds number, the rings undergo an instability that brings the two vortex cores together at several points around the circumference of the rings. As the two vortex cores touch, there is an annihilation of the opposing vorticity from each ring which results in reconnection between the original two vortex rings. These reconnections have a complicated 3D structure that is difficult to measure experimentally, leading many studies to focus on numerical simulation. By scanning a laser sheet across the collision of two dyed vortex rings, we are able to reconstruct a tomographic 3D visualization of the vortex ring collision and reconnection as it occurs. This 3D visualization allows for comparison between the structure of reconnections in experiment and the predictions from numerical models.

1:03PM M20.00010: Dynamics and deformation of a vortex during pairing under the influence of external shear  PATRICK FOLZ (Presenter), University of California, San Diego — In general, a given vortex in a real flow may interact with other nearby vortices as well as large-scale background flows such as shear. To better understand the behavior of the vortices in such flows, the dynamics and interactions of a pair of two-dimensional like-signed viscous vortices having a circulation ratio $\Lambda = \Gamma_1/\Gamma_2 = (a_1^2/a_2^2)(\omega_1/\omega_2)$ under the influence of a linear background shear having vorticity $\omega_2$, of strength $\zeta = \omega_5/\omega_2$, with finite viscosity, are investigated numerically. The main flow regimes, pairing and separation, are identified and briefly discussed; this work focuses on vortex-dominated pairings, in which the shear is observed to primarily aid or hinder the onset of detrainment, which precipitates the main convective interaction that results in a single final vortex. During such pairings, the vortices revolve with varying peak-peak distance $b$, such that the strain rate each vortex induces on the other varies in time, while the orientation of this vortex-induced strain rate relative to that of the background shear also varies. This results in a periodic deformation effect. The nature of this effect is examined and discussed. The subsequent pairing outcomes are then outlined and characterized in terms of key parameters.
Two-dimensional (2d) and quasi-2d flows occur at macro- and mesoscale in a variety of physical systems. Examples include stratified layers in Earth's atmosphere and the ocean, soap films and more recently also in dense bacterial suspensions, where the collective motion of microswimmers induces patterns of mesoscale vortices. A characteristic feature of turbulence in 2d and thin fluid layers is the occurrence of an inverse energy cascade. In case of weak large-scale friction the inverse energy cascade results in the formation of large-scale coherent structures, so-called condensates, which can take the form of jets or large-scale vortices. With a view towards atmospheric physics, we study the formation of the condensate in a rotating thin layer with free-slip boundary conditions as function of the amplitude of the forcing, and we quantify the effect of large-scale friction. Direct numerical simulations show that the condensate appears in a first-order non-equilibrium phase transition, with rare transitions occurring towards and away from the condensate state. This clearly distinguishes between 2d dynamics and that of thin fluid layers, as condensate formation 2d turbulence proceeds by means of a second-order non-equilibrium phase transition.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M21 GERA: Energy Related Catalysis and Photo/Thermo effects 302
High throughput theoretical and experimental screening of photocatalysts for water splitting

*JULIAN FANGHANEL (Presenter), QUINN CAMPBELL, Department of Materials Science and Engineering, The Pennsylvania State University, CATHERINE BADDING, Department of Chemistry and Chemical Biology, Cornell University, HUA[I YU WANG, Department of Materials Science and Engineering, The Pennsylvania State University, JARED MONDSCHEIN, Department of Chemistry, The Pennsylvania State University, YIHUANG XIONG, NICOLE HALL, Department of Materials Science and Engineering, The Pennsylvania State University, KRITI SETH, Department of Chemistry, The Pennsylvania State University, ANDRÉS VILLARINO, Department of Chemistry and Chemical Biology, Cornell University, XAVIER QUINTANA, Department of Materials Science and Engineering, The Pennsylvania State University, T[IFFANY RIVERA, Department of Chemistry, The Pennsylvania State University, NATHAN SMITH, MEGAN PENROD, Department of Materials Science and Engineering, The Pennsylvania State University, IURII TIMROV, MATTEO COCOCCIONI, Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne, SENORPE ASEM-HIABLIE, Institutes of Energy and Environment, The Pennsylvania State University, VENKATRAMAN GOPALAN, Department of Materials Science and Engineering, The Pennsylvania State University, HÉCTOR ABRUÑA, Department of Chemistry and Chemical Biology, Cornell University, RAYMOND EDWARD SCHAAK, Department of Chemistry, The Pennsylvania State University, ISMAILA DABO, Department of Materials Science and Engineering, The Pennsylvania State University — We apply a high-throughput computational screening process with feedback from experimental results to identify promising photocatalysts for water splitting. Using an automated linear response framework for predicting Hubbard parameters, we overcome the limitations of local and semilocal density-functional theory calculations in predicting band gaps. From our computational screening, we identify 28 promising photocatalysts, many of which have not been previously reported. We then synthesized some along with chemical derivatives from our selection, for a total of 18 synthesized materials using solid-state synthesis techniques. We report hydrogen production in a number of the materials tested for photocatalysis using gas chromatography; many of which have been previously unreported for water splitting. We further measure cyclic voltammograms, demonstrating high levels of photoactivity in several samples.

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Computations for this research were performed on the Pennsylvania State University’s Institute for CyberScience Advanced CyberInfrastructure (ICS-ACI).
11:27AM M21.00002: High-Throughput DFT of Solar Thermochemical Perovskite Oxides: Comparison of Computed and Experimental Thermodynamics*  BIANCA BALDASSARRI (Presenter), JIANGANG HE, CHRISTOPHER MARK WOLVERTON, Northwestern University — Thermochemical water-splitting (TWS) offers a renewable alternative to fossil fuels by utilizing solar energy for the production of hydrogen via a two-step redox reaction sequence involving a metal oxide. Current and past efforts have been aimed at identifying the best compounds for such reactions based on thermodynamic and kinetic properties. In this context, high throughput density functional theory (HT-DFT) represents an attractive tool for a quick and efficient refinement of the pool of potential candidates. This work concentrates on ABO3 perovskite compounds, conducting a high throughput study of their reduction enthalpy, and selecting a group of 12 compounds for a critical, quantitative comparison with experimental data generated by our collaborators. Building on, and significantly extending, a previous HT-DFT study, we have confirmed the use of high throughput DFT as a reliable method for screening for potential candidates for water splitting reactions, while also demonstrating the importance of choosing the appropriate structure for the compound under investigation. Furthermore, we provided predictions for several promising compounds, highlighting the crucial role played by the B site cation and its oxidation state.

*US Department of Energy, DE-EE0008089.

11:39AM M21.00003: Increased Hydrogen Production of Perovskite Solar Thermochemical Water Splitters by Joint Reduction on A and B Sites  ROBERT BELL (Presenter), SARAH SHULDA, DAN PLATTENBERGER, National Renewable Energy Laboratory & SLAC Linear Accelerator Laboratory, SAI GAUTAM GOPALAKRISHNAN, Princeton, NICHOLAS STRANGE, PHILIP ANTHONY PARILLA, National Renewable Energy Laboratory & SLAC Linear Accelerator Laboratory, EMILY CARTER, University of California, Los Angeles, ANTHONY MCDANIEL, Sandia National Laboratory, ELLEN B STECHEL, Arizona State University, DAVID S GINLEY, National Renewable Energy Laboratory & SLAC Linear Accelerator Laboratory — Oxide based solar-thermochemical hydrogen (STCH) production operates by cyclic creation of oxygen vacancies that then react with steam to produce hydrogen. STCH performance is strongly dependent on both the change in vacancy stoichiometry (��) during cycling (��) and the output gas ratio of H₂/H₂O. Perovskites (ABO₃) have been investigated by controlled synthesis and X-ray adsorption spectroscopy (XAS) as STCH oxides in-part due to their tunable cation-dependent oxygen vacancy enthalpies. Classically, only one site, either A or B, has been responsible for charge compensation of oxygen vacancies. However, in this work we investigate water splitting by computationally designed perovskites expected to possess dual reduction on both A and B sites, which is predicted to increase vacancy formation, and hence performance, through increased formation entropy of vacancies. In-operando X-ray absorption spectroscopy (XAS) results at Ce L-edge and Mn and V K- and L-edges will demonstrate changing oxidation states of A and B site elements. Additional in-operando diffraction and mass loss experiments will correlate and structural changes with cation reduction. This work will demonstrate the effectiveness of dual site reduction as a design criterion for STCH material design.
Photocatalytic Reaction driven by hot electrons on Plasmon-resonant Grating Nanostructures* YU WANG (Presenter), INDU ARAVIND, ZHI CAI, LANG SHEN, Univ of Southern California, GEORGE GIBSON, Physics, University of Connecticut, JIHAN CHEN, BO WANG, HAOTIAN SHI, BOXIANG SONG, Univ of Southern California, ERNEST GUIGNON, Ciencia Inc, NATHANIEL CADY, Nanoscale Science & Engineering, SUNY Polytechnic Institute, WILLIAM PAGE, ARTURO PILAR, Ciencia Inc, STEVE CRONIN, Univ of Southern California — We demonstrate hot electron injection in a Ag-based plasmon resonant grating nanostructure. By varying the incident angle of irradiation, sharp dips are observed in the photoreflectance with p-polarized light when there is wavevector matching between the incident light and the plasmon resonant modes of the grating. With 633nm light, we observe a 12-fold enhancement in the photocurrent between resonant and non-resonant polarizations at incident angles of ±7.6° from normal. At 785nm irradiation, we observe similar resonant profiles to those obtained with 633nm wavelength light but with a 44-fold enhancement factor. Using 532nm light, we observe two resonant peaks (10X enhancement) in the photocurrent at 19.4° and 28.0° incident angles. Finite difference time domain (FDTD) simulations of these grating structures confirm the resonant profiles observed in the angle-dependent spectra of these gratings and provide a detailed picture of the electric field profiles on and off resonance.

*Army Research Office (ARO) Award No. W911NF-17-1-0325 (Y.W.), National Science Foundation (NSF) Award No. CBET-1512505 (L.S.), Air Force Office of Scientific Research Grant No. FA9550-15-1-0184 (I.A), Department of Energy (DOE) Award No. DE-FG02-07ER46376 (Z.C), and ACS-PRF Grant #55993-ND5 (J.C.).

Using density functional theory to evaluate Ca-Ce-M-O (M = 3d transition metal) oxide perovskites for solar thermochemical applications SAI GAUTAM GOPALAKRISHNAN (Presenter), Mechanical and Aerospace Engineering, Princeton University, ELLEN B STECHEL, ASU Lightworks® and the School of Molecular Sciences, Arizona State University, EMILY CARTER, Office of the Chancellor, University of California Los Angeles — Solar thermochemical (STC) processes that use redox-active, off-stoichiometric, transition-metal oxide substrates to split water and/or CO₂ are an efficient way to generate reusable fuels or fuel precursors using concentrated solar flux. However, STC processes require oxides that are thermally stable, tolerate high oxygen off-stoichiometry, and be resistant to adverse phase transformations. In this work, we explore the chemical space of Ca-Ce-M-O (M=3d transition metal) oxide perovskites as potential STC candidates using density functional theory based calculations. Specifically, we use the strongly constrained and appropriately normed (SCAN) functional, with an appropriately determined Hubbard U correction to reduce the self-interaction errors of the highly-correlated 3d and 4f electrons within M and Ce, respectively. While, we consider Ca and Ce on the A site (in an ABO₃ perovskite framework) because of their similar ionic radii and the potential redox-activity of Ce, we consider all 3d transition metals except Zn on the B-site. Subsequently, we evaluate the oxygen vacancy formation energy, electronic properties, and thermodynamic stability of ternary Ca-M-O, Ce-M-O, and quaternary Ca-Ce-M-O perovskites and identify promising candidates that can improve STC efficiencies.
12:15PM M21.00006: Nanoparticle Enhancement of Plasma-driven CO\textsubscript{2} reduction to Higher-order Hydrocarbons  
SISI YANG (Presenter), BOFAN ZHAO, INDU ARAVIND, ZHI CAI, SRIRAM SUBRAMANIAN, MARTIN GUNDERSEN, STEVE CRONIN, Univ of Southern California — By discharging ns high voltage pulses across an insulating substrate containing metal nanoparticles, we observe a significant enhancement in the generation of plasma through local field enhancement on the surface of the nanoparticles. Electromagnetic simulation shows local field enhancement on the order of 10X. Since the plasma is initiated by field emission of electrons, which depends exponentially on the electric field, we believe that this 10-fold increase can result in several orders of magnitude increases in the generation of plasma. By discharging ns high voltage pulses in CO\textsubscript{2}-saturated water, we observe CO\textsubscript{2} reduction to higher-order hydrocarbons. Here, the plasma emission spectra exhibit Swan bands, which correspond to C\textsubscript{2} species, indicating that, in addition to reducing CO\textsubscript{2}, C\textsubscript{2}-species are formed, presenting the exciting possibility of converting a notorious greenhouse gas into an energy dense hydrocarbon fuel. We have also performed cryogenic NMR spectroscopy of various products in water and liquid ion chromatography(IC) ex-situ. Here, we observe clear peaks corresponding to formic acid, and acetic acid, which corresponds to a C\textsubscript{2}-hydrocarbon species. We have also observed the presence of oxalates (i.e., C\textsubscript{2}O\textsubscript{4}^{2-}), which is C\textsubscript{2} species, at approximately 150g/L using IC.

12:27PM M21.00007: Excitonic Effects in Absorption Spectra of Carbon Dioxide Reduction Photocatalysts*  
TATHAGATA BISWAS (Presenter), TARA BOLAND, ARUNIMA SINGH, Arizona State Univ — We study the quasiparticle bandstructure and excitonic properties of 52 selected materials. These materials were recently shortlisted for their potential as a photocatalyst in CO\textsubscript{2} reduction, through rigorous first-principles computation-based screening strategy. Many body perturbation theory within GW approximation has been used to explore the electronic structure of these materials. We use state-of-the-art Bethe-Salpeter formalism to inspect the excitonic effects. A high-throughput computational workflow using the “atomate” package has been used to perform the GW-BSE calculations and analyze the results. We validate our results with 10 previously studied materials found in literature and report the results for 42 promising unexplored materials. Furthermore, our study investigates the suitability of these materials in applications such as CO\textsubscript{2} photo-reduction, efficient solar cells, etc. by examining their absorption spectra and excitonic properties.

*This work used the Extreme Science and Engineering Discovery Environment (XSEDE), supported by National Science Foundation grant number ACI-1548562, through award number TG-DMR150006.
12:39PM M21.00008: Understanding the C1 Selectivity Descriptors in Electrochemical CO2 Reduction for Production of Solar Fuels* MICHAL BAJDICH (Presenter), MICHAEL T. TANG, HONGJIE PENG, PHILOMENA SCHLEXER LAMOUREUX, FRANK ABILD-PEDERSEN, SLAC - Natl Accelerator Lab — Generating solar fuels from carbon dioxide (CO2) and water offers an intriguing opportunity for a carbon-neutral, sustainable, and scalable source of energy. Electrochemical reduction of CO2 is a key reaction for the production of liquid fuels, but it follows a complex reaction network. Even for products with a single carbon atom (C1 products), two bifurcated pathways exist. In this study, we combine evidence from the experiments with a theoretical analysis of energetics to rationalize that not all steps in the reduction of CO2 are electrochemical. This insight enables us to create a selectivity map for two-electron products (carbon monoxide (CO) and formate) on elemental metal surfaces using only two energy descriptors. In the further reduction of CO*, we also find bifurcated pathway one for CHO* and one for COH*. We find Cu to be the only elemental metal capable of reducing CO2 to products beyond 2e− via the proposed COH pathway. Our analysis also rationalizes experimentally observed differences in products between the thermal and electrochemical reduction of CO2 on Cu.

*This material is based upon work performed by the Joint Center for Artificial Photosynthesis, a BES DOE Award # DE-SC0004993 and the use of the computer time allocation at NERSC DOE Award # DE- AC02-05CH11231.

12:51PM M21.00009: CO2 conversion on defect-induced single-layer h-BN* DUY LE (Presenter), TAO JIANG, Department of Physics, University of Central Florida, KATERINA L CHAGOYA, Department of Mechanical and Aerospace Engineering, University of Central Florida, DAVID J. NASH, RICHARD BLAIR, Florida Space Institute, University of Central Florida, TALAT S. RAHMAN, Department of Physics, University of Central Florida — Finding effective heterogeneous catalysts, consisting of abundant elements, for hydrogenation of waste gas carbon dioxide into value added molecules is a challenging task for global energy and sustainability solutions. In this talk, we will present results of a closely coupled computational and experimental effort that shows that reconfiguration of the frontier orbital in defect-laden hexagonal boron nitride (dh-BN) can effectively activate the CO2 molecule for hydrogenation. Our density functional theory (DFT) based calculations of reaction pathways and activation energy barriers demonstrate that activation occurs through back-donation to the π* orbitals of CO2 from frontier orbitals (defect state) of the h-BN sheet localized near a nitrogen vacancy (VN). Subsequently, CO2 is hydrogenated to formic acid (HCOOH) and methanol (CH3OH). These results were experimentally confirmed in a reactor designed to continuously produce defects in h-BN by the application of mechanical force. We find temperature-dependent switchable catalysis with formic acid formation observed at reaction temperatures above 160 °C and methanol formation at lower temperatures (as low as 20 °C).

*This work is supported in part by DOE grant DE-FG02-07ER15842
1:03PM M21.00010: Optimizing Power Output of Graphene Energy Harvesting  FERDINAND HARERIMANA (Presenter), PAUL M THIBADO, Univ of Arkansas-Fayetteville — Free standing graphene has been found to invert its curvature over time by researchers at the University of Arkansas. Recently, they have been working on building a chip for converting kinetic energy from the system to electrical energy by using a variable capacitor principle. In this study we investigate the macroscopic models of graphene energy harvesting (GEH) with the goal of finding the output power optimal conditions. We present a GEH circuit model, which contains a manually-driven variable capacitor in series with a DC voltage source, diodes components for rectification, and a storage capacitor for storing the harvested charge. The DC experiment, however, presents difficulties with measuring efficiency, controlling the frequency, and reaching high voltage limits. Therefore, we design an equivalent AC experiment, in which we replace the DC voltage with an AC source and the variable capacitor with a fixed one. Our power studies reveal that the maximum efficiency of is reached at the maximum power output point, which happens at the time of times the time constant of the circuit.

1:15PM M21.00011: Defect chemistry in La/Sr-based oxyhydrides* ANDREW ROWBERG (Presenter), Materials Department, University of California, Santa Barbara, LEIGH WESTON, Energy Technologies Area, Lawrence Berkeley National Laboratory, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — Oxyhydrides in the series La$_{2-y}$Sr$_y$LiH$_{1+y}$O$_{3-y}$ have attracted interest for solid-state hydrogen electrolytes on account of their high H$^-$ ionic conductivity. Here, we use first-principles calculations to examine the prevalence of native point defects in La$_2$LiHO$_3$ and Sr$_2$LiH$_3$O and connect our results to ionic transport properties. We find that both oxyhydrides have high concentrations of point defects. Sr$_2$LiH$_3$O, in particular, experiences a stabilizing effect from disorder caused by the presence of pairs of compensating species, such as O$_{H^-}$ and V$_{H^+}$, or O$_{H^-}$ and H$_i^{+}$. V$_{H^+}$ serves as the most important point defect for ionic conduction; its presence explains the high conductivity in Sr$_2$LiH$_3$O. We identify O-rich and moderately H-rich synthesis conditions as optimal for ensuring stability and maximizing ionic conductivity.

*This project was supported by DOE and NSF.

MASANORI KANEKO (Presenter), KOICHI YAMASHITA, Kyoto Univ — The visible light region accounts for approximately 40% of the energy of solar radiation. Therefore, tungsten oxide, which is the visible light-driven photocatalysts, has been receiving much attention. It is known that photoexcited tungsten oxide has long-lived photocarriers, which have an important role in photocatalytic reactions. In a recent study, the dynamics of photoelectrons and structural changes of tungsten oxide has been observed by femtosecond transient XAFS. They have found that the electronic state was the first to change followed by the local structure, which was affected within 200 ps of photoexcitation. However, little is known about how the structure changes and how it affects the photocarrier. Therefore, in this study, tungsten oxide was investigated by performing first-principles calculations based on density functional theory and many-body perturbation theory. We discuss the light absorption related by excitation, photoexcited carriers, and structural changes from electronic, optical, phonon, electron-phonon properties, et cetera.

*This research was supported by MEXT as "Priority Issue on Post-K computer"(Development of new fundamental technologies for high-efficiency energy creation, conversion/storage and use).

1:39PM M21.00013: Ab-initio investigation of a novel photocathode: bulk and surface properties of CuFeO₂

MATTEO FERRI (Presenter), SISSA, JOSHUA DAVID ELLIOTT, University of Manchester, MATTEO FARNESI CAMELLONE, STEFANO FABRIS, SIMONE PICCININ, CNR-IOM — Photoelectrochemical (PEC) devices offer the possibility to convert solar radiation into chemical fuels, mimicking the natural process of photosynthesis. Recent experiments have highlighted CuFeO₂ (CFO) as a promising candidate in the role of photocathode [1, 2], yet in spite of these encouraging results, improvement in the catalytic activity and charge separation is required. In this work, we present a theoretical characterization of CFO based on the DFT+U approach and refined with hybrid calculations. We characterized the stability of bulk CFO with respect to other iron and copper oxides in air and in an aqueous environment, coupling DFT with ab-initio thermodynamics. On this basis, we studied the formation energy of native defects of CFO. The low formation energy of a copper antisite defect could be detrimental for the PEC operations of CFO since states inside the energy gap could favour the electron-hole recombination. Based on our thermodynamic screening we focused our investigation on two energetically relevant surfaces. We interfaced these surfaces with water and we performed ab-initio molecular dynamics simulations to determine the alignment between the band edges and the redox potentials of water.

1:51PM M21.00014: Linking Nanoscale Grain Boundary Composition and Energetic Properties in Ceramic Oxides*  
TARA BOLAND (Presenter), ARUNIMA SINGH, PETER REZ, PETER CROZIER, Arizona State Univ — Ceramic oxides are used for a wide variety of technologically relevant applications from electrochemical devices, novel resistive switching devices and oxygen sensors. Applications such as these typically rely upon the ability of oxides to conduct ions efficiently through the lattice. Recent nanoscale compositional characterization of the GB composition has shown different nominal concentrations of solutes could result in orders of magnitude increase in GB ionic conductivity relative to the undoped samples. This study aims to predict the optimal dopants that, when present in high concentrations, increase the ionic conductivity across the GB. Computational modeling is employed using density functional theory to optimize the GB interfacial structure for various GB misorientations in CeO2. This study further develops our understanding of high solute GB composition enabling the development of methods such as selective doping to improve macroscopic ionic conductivity for both the grain and GB.

*The authors would like to acknowledge the National Science Foundation DMR-1308085 for funding and the research computing facilities of SDSC's cluster Comet as well as ASU's cluster Agave for computing resources.

Wednesday, March 4, 2020 11:15 AM - 1:51 PM

Session M22 DBIO DCP DMP DPOLY: Biomaterials IV: Nano and Bioinspired materials 303 - Pupa Gilbert, University of Wisconsin - Madison - Tag(s): Focus

DEBAPRIYA PINAKI MOHANTY (Presenter), School of Industrial Engineering, Purdue Univ, KOUSHIK VISWANATHAN, Department of Mechanical Engineering, Indian Institute of Science, India, ANIRUDH UDUPA, School of Industrial Engineering, Purdue Univ, ANIL CHANDRA, Mechanical Engineering, B M S College of Engineering, India, SRINIVASAN CHANDRASEKAR, School of Industrial Engineering, Purdue Univ — The undesirable effects of plastics on the environment are well-documented. One of the common uses of plastics is in products with short-term uses in the food industry, e.g., cutlery and plastic bags. This has focused interest in finding bio-degradable alternatives for these products that are mechanically, physically and aesthetically equal to if not superior to plastics. Areca palm sheath is a possible plant-based green alternative that can be used in the manufacture of plates and bowls. In fact, it has been in use in India for more than a century despite little knowledge about its mechanical behavior. To advance the use of these materials, it is critical to understand their formability and the nature of diffusion of water through the sheath. In this study, we report on the results of an investigation of their formability. Using measurements carried out on plates and bowls, we show that Areca sheaths are quite deformable and capable of withstanding strains as high as 0.7. The interplay between moisture content and formability is quantified. The formability and failure strains are related to the microstructure e.g., fiber, porosity of the palm sheath. The results show interesting opportunities for creating a wide range of environmentally friendly cutlery and packaging products.
11:27AM M22.00002: Polycarbonate Mold Copying Technique to Fabricate Microengineered Devices for Biophysical Studies  UTKU SONMEZ (Presenter), PHILIP R LEDUC, Carnegie Mellon Univ — Microengineered devices made out of high aspect ratio flexible polymers provide very useful experimental means to study biophysical properties of living entities at various scales ranging from single cells to multicellular small organisms by enabling application of precise forces and deformations. However, fabrication of such devices require expensive and cumbersome mold fabrication procedures which limits appreciation of this technology by experimental biophysicists. Here, we report a novel microfabrication technique that we have developed for benchtop fabrication of microengineered devices outside the cleanroom so that they can be cheaply fabricated with high throughput. The polycarbonate (PC) mold copying technique consists of reverse molding of Polydimethylsiloxane parts fabricated from master molds in order to combine different microstructures into single monolithic PC mold for subsequent flexible polymer microdevice fabrication. We have characterized dimensional fidelity of the microstructures fabricated by this technique and fabricated various microstructures with feature sizes ranging from submicron level to tens of centimeters. Lastly, we used these devices to study fibroblast alignment dynamics, Young's Modulus of Drosophila embryo and cardiomyocyte contractility.

11:39AM M22.00003: The Design and Modeling of Adsorption Based Filters and the Bioremediation of Heavy Metal Contaminated Water*  CHRIS MCCARTHY (Presenter), Mathematics, BMCC City University of New York — I will discuss kinetic models of adsorption, as well as our mathematical models of such filters. These mathematical models have been developed in support of our interdisciplinary lab group and can be used in filter design. Our group conducts research into bio-remediation of heavy metal contaminated water via filtration. The filters are constructed out of biomass, such as spent tea leaves. The spent tea leaves are available in large quantities as a result of the industrial production of tea beverages. The heavy metals bond with the surfaces of the tea leaves (adsorption). I will compare the models’ predictions to data obtained from computer simulations and experimentally by our lab group.

*CUNY Collaborative Incentive Research Grant (Round 12); CUNY Research Scholars Program; BMCC Faculty Development Grant.
11:51AM M22.00004: Reciprocal Control of Hierarchical DNA Origami-Nanoparticle Assemblies*  JOSHUA JOHNSON (Presenter), ABHILASHA DEHANKAR, JESSICA WINTER, CARLOS E CASTRO, Ohio State Univ - Columbus — A major focus in bionanotechnology is interfacing with inorganic materials, such as nanoparticles (NPs), for effective integration and control over emergent functions of composite materials. The structural precision and dynamic capabilities of DNA origami make it ideal to achieve these goals. We present an actuation scheme utilizing NPs as control elements enabling rapid and reversible thermal actuation of DNA origami and higher order assemblies. We demonstrate tunable thermal actuation between open and closed configurations on the timescale of seconds, with evidence that reconfiguration is only limited by heating or cooling rates of the bulk solution. We extend the dynamic capabilities in higher-order assemblies by polymerizing hinges which can achieve micron-scale reconfiguration. Control of NPs at the arrays scale combined with NP based control of hinges at the individual scale serves as a basis for reciprocal control of hierarchical assemblies. We also polymerize hinges side-to-side to create more compact NP arrays, or use a combination of polymerization schemes to assemble expandable 2D NP arrays. These NP-hinge composites serve as a novel basis for creating reconfigurable emergent materials.

*This work is funded by the U.S. Department of Energy under award no. DE-SC0017270.

12:03PM M22.00005: Fiber fluorescence photo thermometry during magnetic heating reveals directional alignment of suspended nanoparticles*  RAHUL MUNSHI (Presenter), Center for the Physics of Biological Function, Princeton University, MUYE HE, Physics, SUNY, Buffalo, IDOIA RUBIO-CASTELLANOS, Química Inorgánica, Facultad de Ciencia y Tecnología, UPV/EHU, KOMAL SETHI, JUNTING LIU, ARND PRALLE, Physics, SUNY, Buffalo — We developed highly sensitive camera-based fiber fluorescence photometry to measure temperature changes of magnetically heated nanoparticles. Temperature changes as small as 20 milli Kelvin were resolved with a temporal resolution of 5 ms, using common fluorophores. Suspensions of various nanoparticles, including synthesized magnetite and core-shell nanoparticles, engineered magnetoferritin and purified magnetosomes, as well as intact magnetotactic bacteria were heated in alternating magnetic fields (AMF). Using prior calibration, nanoparticle surface temperature changes were calculated from fluorescence intensity changes of the attached dyes. From nanoparticle surface temperatures, we determined the limits of concentration scaling of suspension temperature rise. We captured sudden (sub 5 ms) fluorescence changes, corresponding to AMF driven reversible nanoparticle alignment. The orientation of the AMF field lines determines the direction of the relative fluorescence changes. The rate of aggregation is modulated by changing the medium viscosity and depends on field strength and nanoparticle size. Our findings shed light on the implications of Specific Loss Power measurements and the limits of local heat confinement around freely diffusing nanoparticles.

*NIH (NIMH), NSF
**12:15PM M22.00006: Landscapes, nonlinearity, and optimality of ion transport in sub-nanoscale pores**  
SUBIN SAHU (Presenter), JUSTIN ELENEWSKI, CHRISTOPH ROHMANN, IREAP, University of Maryland College Park, MICHAEL ZWOLAK, Biophysics Group, National Institute of Standards and Technology — Biological ion channels evolved to have high transport rates and high selectivity, among other functional characteristics. Synthetic nanoscale pores aim to mimic these properties for applications such as desalination and osmotic power generation.\(^1\) In these systems, ion-ion and ion-channel interactions occur at sub-nanometer distances which entails large electrostatic and dehydration energies.\(^2\) The balance of these energies determines selectivity and permeation rates. Importantly, the susceptibility of transport and selectivity to minute changes in distances—changes on the order of picometers—is enormous resulting in highly-nonlinear behavior. Biological systems can exploit this susceptibility via variations in protein structure that steer the local electrostatic and structural conditions. We demonstrate how this works in a synthetic selectivity filter and discuss how to probe this system, which will help to experimentally quantify optimal transport conditions and will give the foundation for a robust understanding of more complex biological pores.


*S.S. is supported by the Cooperative Research Agreement between UMD & NIST, Award# 70NANB14H209.

**12:27PM M22.00007: Potentiometric Detection of Single Protein Molecules in Solution by Nanoimpact Method**  
POPULAR PANDEY (Presenter), JIN HE, Physics, Florida International University — Nanoscale electrochemical methods based on nanopores and nanoelectrodes have gained enormous popularity for single-entity detection and analysis. This work integrates two aforementioned methods in one nanopipette apex to simultaneously monitor the ionic current and surface potential changes at the nanopore and the nanoelectrode when a protein translocates through the nanopore or collides with the nanoelectrode. In this presentation, I will demonstrate a facile potentiometric method of detecting protein at the single-molecule level in solution based on the nanoimpact events of proteins at the nanoelectrode, which is further supported by molecular dynamics (MD) simulation. Proteins, such as ferritin, hemoglobin, cytochrome-c, and lysozyme are tested to validate the method. When a protein molecule arrives at the vicinity of the electrically floating nanoelectrode, open-circuit potential (OCP) changes are detected at the nanoelectrode. Compared with the ionic current change, the OCP changes can be detected with better signal-to-noise ratio and higher time resolution. The nanopipette based novel potentiometric detection method provides new opportunities to study various biological entities at a single-entity level with close to physiological conditions.
12:39PM M22.00008: Drops: A bio-inspired tool to structure materials [Invited]  ESTHER AMSTAD (Presenter), EPFL — Nature uses drops to build soft materials possessing well-defined structures and locally varying compositions and therefore display exceptional mechanical properties. Inspired by nature, we use emulsion drops as building blocks of macroscopic granular hydrogels with well-defined micrometer-scale structures and locally varying compositions. I will demonstrate the influence of the micrometer-scale structure of these granular hydrogels on their mechanical properties. To render hydrogels responsive and adaptive, we employ selectively permeable capsules fabricated from water-oil-water double emulsions as building blocks. In addition, we use amorphous inorganic biominerals, such as CaCO3, as reagents that can locally change the mechanical properties of these materials.

1:15PM M22.00009: On the interaction of molecular rotors with lipid nanodroplets*  ROBERT ZIOLEK, BETHAN CORNELL, PAUL SMITH, I. EMILIE STEINMARK, KLAUS SUHLING, CHRISTIAN LORENZ (Presenter), Department of Physics, King’s College London — Lipid droplets are cytoplasmic organelles that store neutral lipids (e.g. triacylglycerols & sterol esters) that serve as reservoirs of energy. The neutral lipid core of lipid droplets are bounded by a phospholipid monolayer, which differentiates them from most other organelles that have a bilayer membrane. There are various nano-environments of different viscosities present in these complex organelles, which can be studied with fluorescent molecular rotors. In this presentation, I will present the results of several large-scale classical molecular dynamics simulations in which we investigate the molecular scale interactions of a molecular rotor, BODIPY-C12, with lipid droplets. In doing so, we investigate how the orientation and confirmation of the molecular rotors changes during their adsorption into the interface of the lipid droplets. We investigate how different compositions of the bounding lipid monolayer affect the confirmation and tilt of the molecular rotors. Finally, we will use the results of our simulations to resolve the multi-component signals observed experimentally.

*Simulations were performed with UK’s HEC MCC (EP/L000202/1, EP/R029431/1), the ARCHER UK National Supercomputing Service and the UK MMM Hub (EP/P020194/1).
1:27PM M22.00010: Design of bio-inspired surface topographies via polymer bilayer wrinkling superposition  LUCA PELLEGRINO (Presenter), SEPIDEH KHODAPARAST, JOAO CABRAL, Imperial College London — Naturally occurring patterns on surfaces have evolved to form topological micro- and nano-structures with a variety of functionalities, such as drag reduction, tuneable wetting, anti-microbial resistance and optical effects, often found in insect wings and plant leaves. Wrinkling of bi- and multi-layered materials provides a powerful, versatile, large-surface area patterning methodology to fabricate complex periodic structures with features ranging from 10s of nm to 100s of μm. Here, we investigate the formation of analogous 2D wrinkling patterns in artificial soft materials, built as a superposition of single frequency features. The pattern superposition is achieved sequentially, starting from single frequency wrinkles and generated by stretching a cross-linked elastomer slab that is simultaneously plasma oxidized. The wrinkled surface formed upon the strain release is replicated, then stretched at a specific angle to the first wrinkling step and plasma treated simultaneously to yield a prescribed wrinkling second generation. Specifically, an orthogonal superposition generates checkerboard patterns. Oblique superposition, gives rise to wavy or sand dunes-like patterns with structural characteristics that are independently tunable via changing the plasma experimental parameters.

1:39PM M22.00011: Near-IR Absorbing Quantum Dots Designed to Kill Multidrug-Resistant Pathogens  MAX LEVY (Presenter), JOHN BERTRAM, KRISTEN ELLER, YUCHEN DING, ANUSHREE CHATTERJEE, PRASHANT NAGPAL, University of Colorado, Boulder — Multidrug-resistant (MDR) pathogens infect millions of people in the US, with global predictions of 10 million annual deaths by 2050.\(^1\) New classes of antibiotics are needed to address this global public health crisis. Light-activated quantum dots (QDs) can fill this role by perturbing the bacteria’s biochemical environment using specifically designed optoelectronic properties.\(^1\) Inside bacteria, QDs can be energized by visible light, transferring electrons to \(O_2\) to generate superoxide radicals. We show that low doses of QDs can kill pathogens without harming human cells. CdTe QDs, while effective,\(^2–5\) are limited by the use of visible light for activation. As such, we recently developed two InP QDs which operate with tissue-penetrating near-IR and deep-red light.\(^6\) These heavy metal free QDs kill MDR pathogens without harming human cells. This work has the potential to treat dangerous infections of bacterial pathogens with a low-cost rational approach.


Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M24 GSNP DSOFT DFD: Granular Flows Beyond Simple Mechanical Models I 401 - Abe Clark, The Naval Postgraduate School - Tag(s): Focus
11:15AM M24.00001: Mechanics of Deformation in 3D Granular Materials Using X-ray Measurements* [Invited] RYAN HURLEY (Presenter), CHONGPU ZHAI, Johns Hopkins University, ERIC B HERBOLD, Lawrence Livermore National Lab, STEPHEN HALL, Lund University — Granular materials deform in complex ways, including through particle deformation, local particle rearrangements, inter-particle slip, and particle fracture. Discrete and continuum models have been proposed within the engineering and physics communities to capture the effects of these deformation mechanisms on mechanical and dynamical material properties. For instance, local particle rearrangements have been captured in glassy rheology models and shear transformation zone theories, while particle fractures have been captured in the continuum breakage mechanics framework. A major challenge remains the quantitative validation and calibration of these models using in-situ 3D experimental data.

In this talk, I will discuss our experiments combining in-situ X-ray computed tomography (XRCT) and 3D X-ray diffraction (3DXRD) during the deformation of granular materials. The samples we have studied to-date include tens to over 1,000 spherical and angular particles, each ranging in size from 100 to 400 μm, and each typically composed of single-crystal sapphire or quartz. We have subjected samples to a variety of loading conditions, including uniaxial compression and triaxial compression. XRCT measurements performed periodically during loading provide high-resolution 3D images of the evolving structure of granular materials during deformation. 3DXRD measurements provide the location (with several um precision), the orientation (with 0.05° precision) and the strain tensor (with $10^{-4}$ resolution) in each of thousands of particles, from which the stress tensor of each particle can be computed. I will present examples of prior work studying local particle rearrangements and inter-particle slip. I will also discuss ongoing and future work on the impact of both structure and forces on ultrasound transmission and the quantitative details of local particle rearrangements.

*LLNL's LDRD program (17-LW-009) and JHU's Whiting School of Engineering.

11:51AM M24.00002: Dimensionality and viscosity exponent in shear-driven jamming* PETER OLSSON (Presenter), Department of Physics, Umea University, Sweden — Collections of bidisperse frictionless particles at zero temperature in three dimensions are simulated with a shear-driven dynamics with the aim to compare with behavior in two dimensions. Contrary to the prevailing picture, and in contrast to results from isotropic jamming from compression or quench, we find that the critical exponents in three dimensions are different from those in two dimensions and conclude that shear-driven jamming in two and three dimensions belong to different universality classes.

*Simulations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at HPC2N.
**12:03PM M24.00003: Identification of a universal data collapse in the rheology of granular media**  
SEONGMIN KIM (Presenter), School of Engineering and Applied Sciences, Harvard University,  
KENNETH N KAMRIN, Department of Mechanical Engineering, Massachusetts Institute of Technology —  
We propose a reduced description of nonlocal phenomena in dense granular flows where the shear stress ratio $\mu$ is not locally determined by the inertial number (dimensionless shear rate) $I$. The nonlocal granular fluidity (NGF) model has been proposed to describe nonlocality by introducing an implicit “fluidity” field and its diffusion. A recent study found the fluidity can be roughly expressed by two physical quantities: the particle velocity fluctuations $\delta v$ and packing fraction. Here, we reduce the number of quantities from two to one revealing that only $\delta v$ is needed to explain nonlocality. We perform DEM simulations in many geometries using 3D spheres and 2D discs with various surface frictions. For each granular material, we show there exists a clear constitutive equation that works across geometries, which directly relates three local dimensionless variables: $\mu$, $I$, and the dimensionless granular temperature (dimensionless $\delta v^2$) $\Theta$. It allows us to consider the nonlocal phenomena as the result of various spatial distributions of the granular temperature, a field that is generated, diffuses, and dissipates similar to the implied behavior of the fluidity field in the NGF model. We also demonstrate how this $\mu$-$I$-$\Theta$ relation can be applied in continuum simulations of granular flows.

**12:15PM M24.00004: Nonlocal rheology of dense granular flows: the effect of particle and boundary properties**  
FARNAZ FAZELPOUR (Presenter), ZHU TANG, KAREN DANIELS, North Carolina State University — In granular rheology, one of the most promising recent advances has been the development of nonlocal rheologies, including the nonlocal rheology model proposed by Kamrin and Koval. This model extends a local Bagnold-type granular flow law to include a Laplacian term governing the diffusion of fluidity. It has been observed to successfully capture the dynamics of quasi-2D flows without the need to provide detailed particle dynamics, using a single set of experimentally-determined model parameters. For use as a modeling tool, the next step is to make predictions for particles with any particle shape/material, and to correctly model the response to various boundary conditions. We perform experiments to study particles of three different shapes and three different stiffnesses to explore their influence on the rheological parameters. We find that the nonlocal parameter varies with both particle shape and material, frictional parameter varies primarily with particle shapes, and the local parameter is approximately constant. Finally, we identify how the roughness of the boundary changes both the flow and the interparticle forces using photoelastic force measurements.

*IFPRI, NSF, McDonnell Foundation
Local plastic deformation in sheared highly polydisperse foams

YONGLUN JIANG (Presenter), ERIC WEEKS, Emory University — We simulate the shear of dense two-dimensional foams using the Durian bubble model with a Lees-Edwards boundary condition. In particular, we study highly polydisperse systems with the largest bubble diameters being as much as ten times the smallest diameter. The high polydispersity requires us to rethink the conventional ideas that are applied to study the local plastic deformation of systems with comparable sizes of droplets, such as $D_{\text{min}}^2$ which highlights locally nonaffine motion (Falk & Langer, PRE 1998). We modify the conventional definition of "local" in the calculation of $D_{\text{min}}^2$ to consider the existence of big droplets and study how the "local" rearrangements differ for large and small droplets. More specifically, we find the large droplets follow the mean shear, while the small droplets have significant nonaffine motions and move more erratically. We demonstrate an optimal definition of local that best distinguishes the local nonaffine motions from the bulk shear.

Generalized Granular Resistive Force Theory for Rate-Dependent Intrusions

ANDRAS KARSAI (Presenter), Physics, Georgia Institute of Technology, SHASHANK AGARWAL, KENNETH N KAMRIN, Mechanical Engineering, Massachusetts Institute of Technology, DANIEL I GOLDMAN, Physics, Georgia Institute of Technology — The resistive forces during intrusion into granular media can be described accurately by reduced-order models like Resistive Force Theory, but rate effects may emerge as intrusion speed increase. We demonstrate with both rapid plate drag data and freely locomoting rigid wheel experiments how such rate-dependent dynamics diverge from the quasistatic limit. Additional forces from a continuum momentum balance are sufficient for describing the forces in rapid plate drag, but do not capture the effects of rapid rotational shear in the wheeled locomotion experiments. A frictional flow continuum model captures these phenomena without needing to account for micro-inertial effects such as frictional dependence on grain inertia. Based on the observed physics of the flow model simulation, we propose a modified RFT for arbitrary intruders that reconciles both cases using a geometry-dependent modification and an additional macro-inertial resistance, extending RFT beyond describing quasistatic intruding bodies.

This work was funded by the Army Research Office, Triangle Park.
Stick-slip and intermittent flow dynamics of a single-grain intruder driven through a granular medium with and without basal friction

RYAN KOZLOWSKI (Presenter), Physics Department, Duke University, C MANUEL CARLEVARO, Mechanical Engineering Department, Universidad Tecnologica Nacional, La Plata, KAREN DANIELS, Physics Department, North Carolina State University, LOU KONDIC, Mechanical Engineering Department, Universidad Tecnologica Nacional, La Plata, KAREN DANIELS, Physics Department, North Carolina State University, LUIS A PUGNALONI, Physics Department, Universidad Nacional de La Pampa, JOSHUA SOCOLAR, Physics Department, Duke University, HU ZHENG, Geotechnical Engineering Department, Tongji University, ROBERT P BEHRINGER, Physics Department, Duke University — We report on experiments in which a grain-sized intruder is pushed by a spring through a quasi-2D granular material in an annular geometry. We study intruder dynamics as a function of packing fraction for two types of supporting substrates: a frictional glass plate and a layer of water, which completely removes basal friction. In the presence of basal friction, we observe a novel crossover with increasing packing fraction from intermittent flow to stick-slip dynamics. In intermittent flow, the intruder only occasionally gets stuck by the medium; in stick-slip, the intruder advances via a sequence of distinct, rapid slip events. With lower interparticle friction, the crossover packing fraction shifts to higher values; when basal friction is removed, no crossover to stick-slip dynamics is observed. We characterize the dynamics using statistics of the intruder velocity, the force of the medium on the intruder, and the waiting times between sticking periods. Our results indicate the qualitative importance of basal friction and suggest a possible connection between intruder dynamics in a static material and clogging dynamics in granular flows.

*ARO grant W911NF-18-1-0184; Universidad Tecnologica Nacional grants PID - MAUTNLP0004415 & PID-MAIFIBA0004434TC; COCINET grant RES-1225-17.
1:03PM M24.00008: Intruder dynamics in a 2D granular system: Effects of dynamic and static basal friction

JOSHUA SOCOLAR (Presenter), Physics Department, Duke University, C MANUEL CARLEVARO, Instituto de Fisica de Liquidos y Sistemas Biologicos, CONICET, Argentina, LUIS A PUGNALONI, Departamento de Fisica, Universidad Nacional de La Pampa, CONICET, Argentina, RYAN KOZLOWSKI, Physics Department, Duke University, HU ZHENG, Tongji University, Shanghai, Department of Geotechnical Engineering, LOU KONDIC, Department of Mathematical Sciences and Center for Applied Mathematics and Statistics, New Jersey Institute of Technology — We discuss the results of simulations of an intruder pulled through a 2D granular system by a spring, using a model designed to lend insight into the experimental findings described by Kozlowski et al. [Phys. Rev. E 100, 032905 (2019)]. In that previous study, the presence of basal friction between the grains and the base was observed to change the intruder dynamics from clogging to stick–slip. Here we first show that our simulation results are in excellent agreement with the experimental data for a variety of experimentally accessible friction coefficients governing interactions of particles with each other and with boundaries. We then use simulations to explore a broader range of parameter space, focusing on the friction between the particles and the base. We consider a range of friction coefficients, which are difficult to vary smoothly in experiments. The simulations show that dynamic friction strongly affects the stick–slip behavior when the coefficient is decreased below 0.1, while static friction plays only a marginal role.

*Work supported by US Army Research Office grant W911NF1810184; Keck Foundation; Universidad Tecnologica Nacional grants pidmautnlp0004415 and pidmaifiba0004434TC; CONICET grant RES-1225-17; NSF Grant No. 1521717.

1:15PM M24.00009: Drafting of intruders in dry and fluid-saturated granular beds

BENJAMIN ALLEN (Presenter), ARSHAD KUDROLLI, Clark University — We discuss an experimental study of the drag experienced by two vertical rods as they follow each other around a circular track while being dragged across a granular bed. We systematically measure the drag experienced as a function of rod speed, separation distance, penetration depth, and the properties of the interstitial fluid. As in drafting in air and fluids, we find significant separation effects on the total drag experienced in comparison with that of a single rod [1]. The drag ratio is observed to decrease monotonically as the separation distance is decreased over a scale set by the penetration depth in a dry granular bed essentially independent of their speed. A complex rate-dependence is observed in a liquid-saturated granular bed at separation distances comparable to the penetration depth. A peak in drag is observed when the distance of separation is comparable to the penetration depth which is greater than the drag of experienced at large separation distance. We will discuss our results in light of resistive force theory, and nondimensional inertial and viscous numbers used to characterize granular mediums.


*Supported by NSF-CBET 1805398.
Reduction in Resistive Forces by Directional Air Fluidization in Dry Granular Media

MASON MURRAY-COOPER (Presenter), ANDRAS KARSAI, YASEMIN OZKAN-AYDIN, Georgia Institute of Technology, NICHOLAS NACLERIO, ELLIOT W. HAWKES, Mechanical Engineering, UC Santa Barbara, DANIEL I GOLDMAN, Georgia Institute of Technology — Directional fluidization applies the concept of granular air fluidization to vary the resistive forces locally around an intruder in a granular medium. We fabricated a cylindrical intruder (d = 30mm, length = 30 mm) capable of blowing air through a nozzle at varying flow rates (from 0 to 100 L/min) and angles relative to the direction of intruder motion in dry granular media. Varying the flow rate and angle affects the drag force parallel to the intruder's direction of motion as well as the lift force in the vertical direction. Drag experiments were performed by forcing the intruder horizontally with a robot arm at a low speed (v ~10 mm/s) in 5 cm of dry sand with grain diameters ranging from 0.4-0.8 mm. Multi-axis force data demonstrated a consistent reduction in saturated drag forces that was sensitive to air flow rate but insensitive to blowing angle (BL). Saturated lift forces showed a greater dependence on BL, with more significant reductions coinciding with steeper angles (60 - 90 degree range). These results suggest a scheme for minimizing resistive forces in lift and drag by blowing air downwards and open a door for growing robot navigation in granular media.

Properties of air-fluidized granular media*

MIGUEL ANGELO LOPEZ-CASTANO (Presenter), JUAN FRANCISCO GONZÁLEZ-SAAVEDRA, ÁLVARO RODRÍGUEZ-RIVAS, FRANCISCO VEGA REYES, Departamento de Física, Universidad de Extremadura — We study a 2D granular system of particles interacting via a short-ranged potential, and thermalized homogeneously. This achieved by means of a turbulent air flow. Particles consist of 4 cm diameter ping-pong balls. We will show that, as packing fraction and air current are increased, the system can undergo transitions from gas to liquid, glass, and hexagonal phases.

The particles, placed on a metallic mesh and are subject to an uniform air flow from. This creates vortexes past the spheres, injecting energy. Air flow is adjusted so that particles remain in contact with the mesh, so that the dynamics are purely 2D. The system can be regarded as being under a stochastic white noise.

We perform several series of measurements with varying air flow intensity and density, detecting particle positions through a CV algorithm. We then carry out an analysis on single-particle trajectories and study configurational properties: pair correlation function, and order parameters.

We compare our granular temperature results against other 2D homogeneously driven granular systems.

*Financial support from Spanish Ministerio de Economía y Competitividad Grant No. FIS2016-76359-P and Junta de Extremadura through Grants No. IB16087 and GR18079, partially funded by the European Regional Development Fund.
1:51PM M24.00012: Granular chiral separation  RUO-YU DONG (Presenter), SLAWOMIR LACH, YAROSLAV SOBOLEV, BARTOSZ GRZYBOWSKI, STEVE GRANICK, IBS Center for Soft and Living Matter — Single helical granular particle (~5 mm), when placed in a slowly rotating tube, migrates laterally to different sides dependent on the chirality. First entrained by the rotating tube up to certain height, the particle suddenly starts to slide or roll down, during which process chiral separation is made possible as the particle only rolls at certain particle orientation and thus migrates in one direction exclusively. The intricate interplay between particle shape, which determines a critical slope of rolling, and static friction, which determines a critical slope of sliding, is found responsible for the chiral separation and its efficiency. We corroborate the experimental finding with theoretical predictions and extend the single particle phenomena to multi-particles.

2:03PM M24.00013: Super-Flory scaling in compressed micro-gel packings  AHMED ELGAILANI (Presenter), CRAIG E MALONEY, Northeastern University — We perform multi-body finite element simulations of packings of hydrogel particles immersed in a large solvent bath in 2D at various particle volume fraction, φ using the Flory-Rehner constitutive law to model the mechanics of the hydrogel network. The system becomes rigid with finite osmotic pressure, Π and zero-frequency storage modulus, G, only above the random close packing point. At large enough φ regions of pure solvent are completely eliminated, and we find a qualitative change in the G vs φ curve with a weaker dependence on φ. However, in this dense limit, G exceeds the modulus of a monolithic piece of hydrogel made of the same Flory-Rehner material and continues to increase with φ. This result is surprising as we observe strong inhomogeneous non-affine relaxation which helps to reduce the modulus, however, it is in agreement with experiments which also show super-Flory behavior. Furthermore, we show that the slip at the facets between particles is proportional to the transverse gradient of the applied deformation which strongly screens the stress near facets oriented along the applied shear. Our results on the deformation kinematics during shear suggest new measurements to attempt in experiments and should open the way to quantitative theories to estimate G at high φ.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M25 GSNP DSOFT: Fabric, Knits and Knots I  402 - Michael Dimitriyev, Georgia Inst of Tech - Tag(s): Focus
11:15AM M25.00001: What Can Knitting Machines Make? [Invited] JAMES MCCANN (Presenter), Carnegie Mellon Univ — Industrial knitting machines are used to fabricate many complex 3D objects, including gloves, sweaters, and shaped fiber reinforcement for composites. But what are the limits of these machines? This talk will introduce two of the approaches my group has taken to answering this question.

The first -- top-down -- approach views a knitting machine as a device for shaping, splitting, and merging tubes. This leads to the observation that all manifolds with boundary whose Reeb graph under some smooth function has an upward-planar embedding are machine-knittable. This observation forms the basis of our work on knitting design tools.

The second -- bottom-up -- approach translates low-level machine instructions into a geometric description of intertwined yarns, allowing direct enumeration of structures. The important insight made in this work is that the way the yarn is routed between stitches is as important to model as the way the yarn behaves within stitches.

Taken together, these two views of knitting machine capabilities have enabled us to develop new design and simulation tools for machine knitting.

11:51AM M25.00002: Knitting Machine State Representation Using the Artin Braid Group* JENNY LIN (Presenter), JAMES MCCANN, Carnegie Mellon Univ — Industrial knitting machines are incredibly powerful, flexible machines that are capable of creating a wide variety of shapes and structures using just a few basic operations. However, effectively using these operations to take full advantage of the machine’s capabilities is nontrivial; when creating a machine knitting pattern, the designer must decide how to move loops of yarn around the machine’s hundreds of needles, all while tracking interloop connections and tangles. Furthermore, they should do so in a way that minimizes construction time and error rate.

To enable the computation of optimal machine knitting patterns, we developed an abstraction of the knitting machine state that uses the Artin braid group when describing interstitch relationships. We provide a formulation for each machine operation’s effect on this abstract representation. In addition, we leverage key properties of the braid group when considering the distance between any two machine states. These insights make searching the knitting machine state space for efficient patterns more computationally tractable, and we show several computationally planned patterns.

*This work was support by a grant from Shima Seiki.
12:03PM M25.00003: Mechanics-Based Simulation of Multistable Knitted Fabrics  XIAOXIAO DING (Presenter), CHRISTOPHER RYCROFT, KATIA BERTOLDI, Harvard University — The pattern formation process of a one-dimensional yarn into a two-dimensional sheet of knitted fabric exhibits intricate deformation modes with complex contact description. Given this complexity, we are motivated to develop a mechanics-based predictive model that accounts for mechanical parameters in this mechanics-based process. We first characterize parameters that significantly dominate the pattern formation, such as pretension and boundary conditions on the knitted fabric. Then integrate this with development of a simulation scheme, where yarn-yarn interaction and mechanical forces are computed and cross validated against parametric study on the macroscopic mechanical response of knitted elastic fabrics. Our model is generalized to explore the rich landscape of knitted fabrics as each yarn can be parameterized with varying material properties, enabling the design space for functionality of the fabrics to be enormously enlarged. Projecting forward, we hope to extend this simulation scheme for coupled analysis on functionality and data augmentation for optimization of pattern design for multifunctional knitted fabrics.

12:15PM M25.00004: Constructing a constitutive model of knitted fabric*  MICHAEL DIMITRIYEV (Presenter), KRISHMA SINGAL, ELISABETTA MATSUMOTO, Georgia Inst of Tech — Knitting is an ancient technology wherein yarn is manipulated into an array of slipknots to form fabric. By patterning these stitches in different ways, one can create fabrics possessing a wide array of elasticities and geometries, without needing to change the type of yarn being used. Thus, knitting is a way of programming material properties via a code that describes stitch patterns. However, while there have been mechanical models of aspects of knitted fabric, there is currently no unifying description that models knitted fabric elasticity given a prescribed stitch pattern. To make progress towards this end, we seek a method of generating constitutive relations for a given stitch pattern. Using a geometric framework in which yarn degrees of freedom are modeled as elastic space curves, with stitches held together by contact interactions, we solve for energy-minimizing stitch structures numerically within the unit cell of a given pattern. We then extract the constitutive relations by monitoring the deformation of the stitch given external stresses on the unit cell. This method not only gives us predicted stress-versus-strain relations that compare favorably with experiments but it allows us to probe the role of yarn geometry in determining fabric mechanics.

*NSF: DMR 1847172
12:27PM M25.00005: Stress-Strain Studies of Knitted Swatches  KRISHMA SINGAL (Presenter), MICHAEL DIMITRIYEV, ELISABETTA MATSUMOTO, Georgia Inst of Tech — The properties of a knitted fabric are highly dependent on what stitches the fabric is made of and what patterns they are used in. Different stitches correspond to different linking topologies of the yarn that constrain the yarn configurations and therefore the overall fabric mechanics and shape. Here we examine the relationship between large scale properties of knitted swatches and the small scale yarn shape within each stitch via experiments that probe the elasticity of the swatches while imaging corresponding changes in the shape of the constituent yarn. Under stress, knitted fabric deforms not only as a bulk response, but the yarn-level deformations give rise to nonlinear elasticity. To quantify this shape change we are developing a method for tracking the 3D path of the yarn. By tracking the yarn within the fabric while we measure the stress-strain relationship, we can untangle the effects of curvature, compression, and friction on the emergent nonlinear elasticity of the textile.

12:39PM M25.00006: Emergent yarns and fabrics by twist origami*  JULIEN CHOPIN (Presenter), Physics, Universidade Federal da Bahia, ARSHAD KUDROLLI, Physics, Clark University — A first step to making functionalized fabrics is to spin yarns by twisting together a natural or synthetic soft material with a prescribed structure. We will discuss experiments that demonstrate large spontaneous shape transformations that couple with mechanical response starting with a hyperelastic rectangular sheet which is simply held under tension and twisted around its central long axis. For twists larger than half a turn, the sheet adopts an accordion shape with self-contacts and folds oriented at an angle with respect to the axis of rotation. We reconstruct the 3D shape of the folded sheet using x-ray Computed Tomography and calculate the Gaussian and mean curvature to characterize their morphology. Modeling the full soft elastic sheet undergoing such a large transformation is prohibitively difficult. Thus, we propose an origami starting with an inextensible sheet with a prescribed number of triangular folds corresponding those observed at the onset of transverse wrinkling of the elastic sheet as a starting point to analyze the emergence of the structure. Building on this insight, we then present a string model based on the origami kinematics to explain not only the emergence of the accordion folds but also its torsional response.

*Supported by NSF DMR Grant 1508186
A Study of Two-Periodic Knitted Fabrics using Tangles

SHASHANK MARKANDE (Presenter), ELISABETTA MATSUMOTO, Georgia Inst of Tech — We have previously created a framework to classify and characterize two-periodic stitch patterns of knitted fabrics that is based on knot and link theory. Using this theory, we are able to associate a unique link in three dimensional sphere $S^3$, to every two-periodic stitch pattern of a knitted fabric. In every such link, the subset of loops representing the yarn satisfy ribbonness or forms a ribbon link. A link is said to be ribbon if each of its component loops bound a 2D disk that pierces through itself making a finite number of slit like intersections lying in the interior of the collection of disks. Based on the ribbonness, and different types of yarn-needle moves catalogued in the knitting literature, we are able to describe knittable stitch patterns composed of -- knit and purl with twists, yarn overs, knit or purl two together, knit front back, slip stitch, cable etc. The description uses the notion of a tangle -- a collection of properly embedded arcs inside a euclidean three ball. This set up lets us define operator invariants for two-periodic knitted stitch patterns because tangles can be described using tensor products and composition by contraction of indices.

Untangling the mechanics of the clove hitch knot

TOMOHIKO SANO (Presenter), PAUL GRANDGEORGE, PAUL JOHANNES, Ecole Polytechnique Federale de Lausanne, CHANGYEON BAEK, Massachusetts Institute of Technology, HARMEET SINGH, JOHN MADDOCKS, PEDRO REIS, Ecole Polytechnique Federale de Lausanne — Knots can impart unique mechanical function to filamentary structures, with examples ranging across length scales, including DNA, polymer-chains, shoelaces climbing ropes, tennis racket, and surgical sutures. Still, the predictive understanding of the mechanics of this class of structures is limited. The fundamental challenge arises from the complex interplay between topology, geometry, elasticity, and friction. Here, we focus on the clove hitch knot, which typically attaches a flexible rod/filament/rope to a rigid post. The clove hitch can sustain a remarkably large tension ratio between the two ends of the rod when compared to the simpler strategy of spooling the rod around the rigid post in a helical configuration. In our study, we combine experiments (mechanical testing and X-ray tomography), finite element and a theory based on the Kirchhoff equations. We find that the twist in the rod increases with the ratio of the tensions applied to the two ends. Furthermore, in contrast to helical spooling, the clove hitch loses a significant amount of its tension at the regions of self-contact, thereby enhancing its mechanical performance.

*We acknowledge financial support in the form of Grants-in-Aid for JSPS Overseas Research Fellowship.
A stopper knot tied to the end of a climbing rope prevents it from retracting through a narrow passage in the climber’s belay device. Numerous other applications of stopper knots are found in stringing of tennis rackets, sailing and fishing. If a single-stranded stopper knot meets the requirement of preventing a rope from escaping the system, it is able to unfold its full potential by converting a high-traction force into an insignificant stress state. This sharp tension drop results from the complex interplay of the topology, the tightness of the configuration, and the nontrivial frictional interactions in regions of self-contact of the elastically deformed rod. Existing models in knot theory or Kirchhoff's theory for elastic rods are insufficient to describe this functional behavior due to the importance of finite elastic deformations of the cross-section and frictional interactions. We tackle this problem by performing a combination of mechanical testing and X-ray tomography on a variety of stopper knots. Our experimental data, combined with finite element simulations, allows us to systematically explore the different ingredients at play that conspire to dictate the mechanical performance of stopper knots.

*Supported by the Fonds National de la Recherche, Luxembourg 12439430

Knotted structures play a fundamental role in the dynamics of biological and physical systems, from DNA and polymers to liquid crystals and turbulent plasmas, as well as in climbing, weaving and sailing. Despite having been empirically studied for centuries, the subtle interplay between topology and mechanics in knotted elastic materials remains poorly understood. Here, we combine optomechanical experiments with theory and simulations to analyze the behavior of knots in flexible fibers that change their color in response to mechanical deformations. Exploiting a previously unrecognized analogy with long-range ferromagnetic spin systems, we identify simple counting rules to predict the relative mechanical stability of knots and tangles, in agreement with numerical simulations and experimental measurements for commonly used climbing and sailing knots. The underlying topological principles provide a conceptual foundation for understanding the roles of twist and writhe in untangling processes, and are expected to find broad applications in the description and control of systems with complex entanglements.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M26 DSOFT: Disordered and Glassy Systems 403 - John Crocker, University of Pennsylvania
11:15AM M26.00001: Linking Melt Dynamics with Glass Topological Phases in Ge\textsubscript{x}P\textsubscript{x}Se\textsubscript{100-2x} Ternary*  
AARON WELTON (Presenter), RALPH CHBEIR, SOUMENDU CHAKRAVARTY, PUNIT BOOLCHAND, University of Cincinnati — We have synthesized homogeneous equimolar Ge\textsubscript{x}P\textsubscript{x}Se\textsubscript{100-2x} ternary glasses over a wide range of compositions 0<x<26%. 1.5 gram sized samples in evacuated (5mm ID) quartz tube were alloyed at 960 °C for 10 days. When Raman spectra taken along the 1 inch long melt column became identical the samples were declared to be homogenous. Homogeneity means the variance of Se along the melt column decreased to ~0.1%. Modulated DSC experiments were undertaken and trends in $T_g(x)$, del $C_p(x)$ and the enthalpy of relaxation at $T_g$, del $H_{nr}(x)$, were established. We observe a reversibility window in the 9%<x<18% range fixing the three topological phases; flexible phase 0<x<9%, intermediate phase (IP) 9%<x<18%, stressed-rigid phase 18%<x<26%. The IP of this ternary is the widest of any chalcogenide multicomponent chalcogenide glass system, a feature that could be tied to the existence of the Ethylene like P\textsubscript{2}Se\textsubscript{1/2}\textsubscript{4} local structure besides the QT, Se=P(Se\textsubscript{1/2})\textsubscript{3} and PYR P(Se\textsubscript{1/2})\textsubscript{3} ones. Molar volumes reveal a volumetric window with $V_m(x)$ decreasing in the IP range from the average behavior across all x. Melt fragility index, $m(x)$, measurements show a Gaussian like minimum near $m=15$ in the center of the IP and increasing to $m(x)>20$, both in the flexible (x<9%) and stress-rigid (x>18%)

*DMR 08-53957

11:27AM M26.00002: Local and Extended range molecular structures of (Na\textsubscript{2}O)\textsubscript{x}(P\textsubscript{2}O\textsubscript{5})\textsubscript{100-x} glasses probed by Raman Scattering and Infrared reflectance*  
VAMSHI KIRAN GOGI (Presenter), AVIK MANDAL, CHANDI MOHANTY, RALPH CHBEIR, PUNIT BOOLCHAND, University of Cincinnati — Raman scattering and IR reflectance reveal striking similarities between crystalline (c-) and glassy (g-) NaPO\textsubscript{3}. The c- and g- are each composed largely of chains of $Q^2$ species, a 4-fold P having 2 bridging ($O_b$) and 2 terminal ($O_t$) Oxygen neighbors, and display three vibrational features; an asymmetric stretch (as) of P-O\textsubscript{t} (1300 cm\textsuperscript{-1}), a symmetric stretch (ss) of P-O\textsubscript{t} (1172 cm\textsuperscript{-1}) and a ss of P-O\textsubscript{b} (685 cm\textsuperscript{-1}). There are glaring differences as well, and these come from the fact that ss of P-O\textsubscript{t} and P-O\textsubscript{b} although quite narrow in the c- but are rather broad in the g-, and can be deconvoluted in terms of a triad of modes due to long chains (LC), large rings (LR) and small rings (SR) in the latter. These triad of modes are also observed in IR displaying complementary behavior, with modes of SR and LR, weakly excited in Raman but strongly in IR. These vibrational features are also observed at non-stoichiometric (x ≠ 50%) compositions ranging from 20%<x<61% and have permitted to elucidate the role of glass structure in stabilizing the three Topological phases. In the Intermediate Phase range\textsuperscript{1} (37.5%<x<46%), LC far exceed the count of LR and SR thus promoting the configurational entropy of that phase.


*Supported by NSF grant DMR 08-53957
**M26.00003: Molecular origin of the 7-folds narrowing of the Tg transition upon aging in Se-rich multicomponent glasses**

RALPH CHBEIR (Presenter), SHREERAM J DASH, PUNIT BOOLCHAND, Univ of Cincinnati — The nature of the glass transition temperature in Se-rich (x < 4%) ternary GeₙAsₙSe₁₀₀₋₂ₓ [1] glasses is examined as a function of room temperature aging in Modulated DSC experiments. Our experiments show Tg(x) to increase by 6°C with x displaying a trapezoidal variation in the 0% < x < 4% range, with the enthalpy of relaxation, ΔHnr increasing 4-folds and the width (W) of the glass transition decreasing 7-folds upon RT aging for 8 months. The molecular origin of these changes can be connected with the polymeric Seₙ chains in the fresh glass steadily correlating with each other to become quasi-helical provided n > 8. These features are due to the undercoordinated nature of Se glass rendering compositions x < x_c to be super-flexible when the length of chains exceeds 10 atoms. Parallel results were obtained in the GeₓSe₁₀₀₋ₓ [1] binary, underscoring that these effects are strictly controlled by the topology or network connectedness.


*NSF grant DMR- 08-53957

**M26.00004: Origin of the Raman active 490 cm⁻¹ mode in binary As-S and Ge-S and ternary Ge-As-S glasses from compositional studies and Ab-initio Cluster calculations.**

SOUMENDU CHAKRAVARTY (Presenter), RALPH CHBEIR, BADRIAH ALMUTAIRI, Univ of Cincinnati, SHIBALIK CHAKRABORTY, Intel Corporation, KOBLAR JACKSON, Physics, Central Michigan University, PUNIT BOOLCHAND, Univ of Cincinnati — Raman scattering results on binary As-S and Ge-S and ternary Ge-As-S provide evidence of a mode near 490 cm⁻¹. The fractional scattering strength of the mode in question normalized to the sum of the S₈ (472cm⁻¹) and Sₙ chain (461cm⁻¹) mode reveals evidence of a local maximum near x = 25% in binary AsₓS₁₀₀₋ₓ glasses and near y = 20% in binary GeₓS₁₀₀₋ₓ glasses. These results are most suggestive that the mode in question has a frequency which is tied to the S-S stretch between a pair of AsS₃ pyramids or between a pair of GeS₄ tetrahedra. We have now carried forward NRLMOL calculations on select clusters and results of these will be compared to experiments. Preliminary results place the symmetric stretch mode frequency at 450 cm⁻¹ for a 14 atom cluster of (H-S-As)₂-S-S- (As-S-H)₂.

*NSF grant DMR-08-53957
12:03PM M26.00005: Compositional variation of the Specific Heat $C_p(x)$ in binary Ge$_x$Se$_{100-x}$ melts and glasses across the Intermediate Phase. MATTHEW BURGER (Presenter), RALPH CHBEIR, BERNARD GOODMAN, PUNIT BOOLCHAND, Univ of Cincinnati — We have examined the specific Heat $C_p$ in the glassy state and the metastable liquid state across $T_g$ in binary Ge$_x$Se$_{100-x}$ system in the 19% < x < 26% range of compositions focusing on the Intermediate Phase. The bulk glasses used in the present Modulated DSC study were the ones synthesized by Bhosle et al.\(^1\). Our results show $C_p$(glass) and $C_p$(liquid), each term to display a broad Gaussian-like maximum centered about the mid-point composition, x = 23%, of the Intermediate Phase. We are also investigating the variation of $C_p$(liquid) at higher temperature in the $T_g < T < 550°C$ range to look at any anomalies that could be related to the liquid-liquid transition recently suggested\(^2\).


12:15PM M26.00006: Universal hidden order in amorphous cellular geometries GERD SCHROEDER-TURK (Presenter), Murdoch Univ — Partitioning space into cells with certain extreme geometrical properties is a central problem in many fields of science and technology. Here we investigate the Quantizer problem, defined as the optimisation of the moment of inertia of Voronoi cells, i.e., similarly-sized ‘sphere-like’ polyhedra that tile space are preferred. We employ Lloyd’s centroidal Voronoi diagram algorithm to solve this problem and find that it converges to disordered states associated with deep local minima. These states are universal in the sense that their structure factors are characterised by a complete independence of a wide class of initial conditions they evolved from. They moreover exhibit an anomalous suppression of long-wavelength density fluctuations and quickly become effectively hyperuniform. Our findings warrant the search for novel amorphous hyperuniform phases and cellular materials with unique physical properties. This research was published in M.A. Klatt et al, Nature Communications 10, 811 (2019).
In recent years, bulk-boundary correspondence (BBC) has been one of the hot topics both in solid state physics (topological materials) and high energy theory (holography and gauge/gravity duality).

Our work is the first ever exposition of BBC yet in another domain; soft condensed matter. We for the first time hypothesize and confirm that BBC also holds in soft matter. Instead of studying the bulk nature of LC+aerosil gels–like the classical works of x-ray scattering and heat capacity measurements–we chose to study the surface of these gels using atomic-force microscopy (AFM) techniques where we managed to correlate the surface related parameters with the ones of the bulk. The essence of our study is based on the created randomness which can be systematically controlled. This is the aerosil amount in the gels. Here we study the surface effects as functions of the disorder strengths created in the 8CB+aerosil gels samples. The correspondence between the bulk (order parameter; beta) and the surface parameters (fractal dimensions) are systematically studied as functions of disorder strength (aerosil amount in the samples).

This work is supported by the National Natural Science Foundation of China (Grants No. 11734014)
12:51PM M26.00009: The role of hydrodynamic interactions on the long-time structural fate of dense colloidal suspensions  
MONICA E. A. ZAKHARI (Presenter), JIALUN WANG, GADDEIEL OUAKNIN, ROSEANNA ZIA, Chemical Engineering, Stanford University — The colloidal glass transition presents an intriguing temporal convolution of structural, dynamical, and mechanical effects during aging. This competition simultaneously advances aging and deepens arrest. In this work, we study the mechanics of this competition by considering both the equilibrium and non-equilibrium solidification processes, i.e. crystallization and vitrification, respectively, utilizing large-scale Stokesian dynamic simulations that are massively parallelized. Jumps from liquid into the solid region are executed via controlled volume-fraction quenches, where the speed of the quench is used to modulate the particle dynamics and, consequently, permits toggling between equilibrium and arrested states. We find that the long-time structural fate of the suspension, i.e. a glass or a crystal, is determined during the quench itself and is mechanistically regulated by many-body hydrodynamic interactions.

1:03PM M26.00010: Why phonon scattering in glasses is universally small at low temperatures*  
HERVE M. CARRUZZO, CLARE YU (Presenter), Department of Physics and Astronomy, University of California, Irvine — We present a novel view of the standard model of tunneling two level systems (TLS) to explain the puzzling universal value of a quantity, $C \sim 3 \times 10^{-4}$, that characterizes phonon scattering in glasses below 1 K as reflected in thermal conductivity, ultrasonic attenuation, internal friction, and the change in sound velocity. Physical considerations lead to a broad distribution of phonon-TLS couplings that (1) exponentially renormalize tunneling matrix elements, and (2) reduce the TLS density of states through TLS-TLS interactions. We find good agreement between theory and experiment for a variety of individual glasses.

*This research was primarily supported by the National Science Foundation (NSF) through the University of Wisconsin Materials Research Science and Engineering Center (DMR-1720415).

1:15PM M26.00011: Nearest Neighbor Functions for Stealthy Hyperuniform Many-particle Ground States*  
TIMOTHY MIDDLEMAS (Presenter), SALVATORE TORQUATO, Princeton University — We present new analytical theories backed by simulation for the nearest neighbor functions of disordered stealthy hyperuniform many-particle ground states. Stealthy systems display a variety of ordered and disordered phases, and have been related to novel photonic band gaps in disordered systems. They can also be shown to have optimal transport properties, such as the fluid permeability, trapping constant, and elastic properties. The nearest neighbor functions, which include the probability to find a hole of a certain radius, are intrinsically related to the geometric properties of stealthy systems, such as their bounded hole size and quantizer error. The manner in which these functions approach the critical (bounded) hole size is a fundamental geometrical question (in particular, whether they behave like ordered lattices), and is also related to their thermodynamics. We use insights from simulation and previous analytical work to develop new analytical theories of the core and tail regions of these functions, and comment on their implications for geometric problems and material properties.

*We acknowledge support from NSF Grant No. CBET-1701843, the Taylor Fellowship, and the NSF Graduate Research Fellowship, and the use of resources from Princeton Research Computing.
1:27PM M26.00012: Analytical theory of enhanced logarithmic Rayleigh scattering in amorphous solids*

BINGYU CUI (Presenter), Univ of Cambridge, ALESSIO ZACCONE, University of Milan — The damping or attenuation coefficient of sound waves in solids due to impurities scales with the wavevector to the fourth power, also known as Rayleigh scattering. In amorphous solids, Rayleigh scattering may be enhanced by a logarithmic factor although computer simulations offer conflicting conclusions regarding this enhancement and its microscopic origin. With tensorial replica field strategy, a theoretic derivation based on heterogeneous elasticity suggests that the logarithmic enhancement to Rayleigh scattering of phonons might be ascribed to long-range (power-law) power law decay in spatial elastic disorder in amorphous solids. Further, the density of states (DOS) associated with self-consistent equations of self-energy in the model exhibit power d+1 decay in low frequency regime, supporting the evidence of numerical simulation in sound waves.

*This work was supported by the CSC-Cambridge Scholarship (B.C.) and by the US Army ARO Cooperative Agreement W911NF19-2-0055 (A.Z.).

1:39PM M26.00013: Tracer Transport in Attractive and Repulsive Supercooled Liquids and Glasses*

RYAN C ROBERTS, JACINTA CONRAD, JEREMY PALMER (Presenter), Univ of Houston — The transport of small penetrants through disordered materials with glassy dynamics is encountered in drug delivery and chemical separations. Understanding the influence of matrix structure and fluctuations on penetrant motions remains a challenge. We use event-driven molecular dynamics to investigate the transport of small, hard-sphere tracers in matrices of square-well particles. Short-range attractions between matrix particles give rise to reentrant dynamics in the supercooled regime, in which the liquid's relaxation time increases dramatically upon heating or cooling. Heating results in a repulsive supercooled liquid where relaxations are frustrated by steric interactions between particles, whereas cooling produces an attractive liquid in which relaxations are hindered by long-lived interparticle bonds. Further cooling/heating, or compression, of the supercooled liquids results in the formation of distinct glasses. Our study reveals that tracer transport in these liquids and glasses is influenced by matrix structure and dynamics. The relative importance of each factor varies between matrices and is examined by analyzing mean-square displacements, caging behavior, and trajectories sampled from the isoconfigurational ensemble.

*Welch Foundation (E-1882), NSF (CBET-1705968)
1:51PM M26.00014: Glass Transition in Supercooled Liquids with Medium-Range Crystalline Order  INDRAJIT TAH (Presenter), TIFR Centre for Interdisciplinary Sciences, SHILADITYA SENGUPTA, University of Tokyo, CHANDAN DASGUPTA, Indian Institute of Science, SRIKANTH SAstry, Jawaharlal Nehru Centre for Advanced Scientific Research, SMARAJIT KARMAKAR, TIFR Centre for Interdisciplinary Sciences — The origin of the rapid dynamical slowdown in glass forming liquids in the growth of static length scales, possibly associated with identifiable structural ordering, is a much debated issue. Growth of medium range crystalline order (MRCO) has been observed in various model systems to be associated with glassy behavior. Such observations raise the question of whether molecular mechanisms for the glass transition in liquids with and without MRCO are the same. In this study we perform extensive molecular dynamics simulations of a number of glass forming liquids and show that the static and dynamic properties of glasses with MRCO are different from those of other glass forming liquids with no predominant local order. We also resolve an important issue regarding the so-called point-to-set method for determining static length scales, and demonstrate it to be a robust method for determining static correlation lengths in glass formers.

2:03PM M26.00015: Understanding how the degree of disorder affects structural colors of colloidal packings  MING XIAO (Presenter), ANNA B. STEPHENSON, VICTORIA HWANG, VINOTHAN MANOHARAN, Harvard University — Disordered structures that multiply scatter light sometimes show phenomena such as Anderson localization, structural colors, and super whiteness. We investigate the scattering from dense packings of spherical colloidal particles in a weak multiple scattering region. Using a Monte Carlo framework, we predict the wavelength-dependent reflectance (colors) of simulated packings. To quantify the degree of disorder, we calculate the structure factor. We then explore how variations in the structure factor affect both the reflectance and the angle-dependence of the colors. We find only the first peak of the structure factor determines the feature of the reflectance, which provide guidance to control colloidal packings to tune the colors.

Wednesday, March 4, 2020 11:15 AM - 1:51 PM

Session M27 FIAP GIMS DMP: Optical Spectroscopic Measurements of 2D Materials 404 - Okan Koksal, Cornell University
Monolayer MoS$_2$ has become a very promising two-dimensional materials for photo-related applications. Establishing the impact of individual ambient gas components and chemical dopants on the optical properties of MoS$_2$ is a necessary step toward application development. By using in situ Raman micro-spectroscopy with an environment-controlled reaction cell, the photoluminescence (PL) intensity of CVD-grown MoS$_2$ monolayers is monitored at different intralayer locations under ambient and controlled gas environments, such as N$_2$, O$_2$, H$_2$O, and pyridine. Our study demonstrates that photoreactions with the gaseous environment on MoS$_2$ monolayer flakes should be taken into consideration even upon mild photoirradiation as they strongly impact the flakes' optical properties. The optical properties of MoS$_2$ at the edges are strongly affected by photoirradiation induced reactions with O$_2$ and H$_2$O. We have also studied the effect of the dopant phase of the same dopants – liquid and gaseous – on the optical properties of ML MoS$_2$. The gaseous n-type dopant, i.e. pyridine, completely quenches the PL intensity of ML MoS$_2$, while liquid pyridine preserved 50% of the original PL intensity attributed to its less effective charge transfer to MoS$_2$ than the gaseous counterpart.
11:27AM M27.00002: Imaging strain-localized exciton states in nanoscale bubbles in monolayer transition metal dichalcogenides at room temperature  THOMAS DARLINGTON (Presenter), University of California, Berkeley, CHRISTIAN CARMESIN, MATHIAS FLORIAN, Institute for Theoretical Physics, University of Bremen, EMANUIL YANEV, DEMI AJAYI, JENNY ARDELEAN, Mechanical Engineering, Columbia University, AUGUSTO GHIOTTO, Department of Physics, Columbia University, ANDREY KRAYEV, Horiba Scientific, JEFFREY KYSAR, Mechanical Engineering, Columbia University, ABHAY PASUPATHY, Department of Physics, Columbia University, JAMES C HONE, Mechanical Engineering, Columbia University, FRANK JAHNKE, Institute for Theoretical Physics, University of Bremen, NICHOLAS J BORYS, Department of Physics, Montana State University, P. JAMES SCHUCK, Mechanical Engineering, Columbia University — In monolayer transition metal dichalcogenides (1L-TMD's), applied strain can deterministically create quantum emitters at arbitrary sites on-demand. Despite a robust empirical correlation with strain, the nanoscopic details of these quantum emitters are poorly understood. Here we combine room-temperature nano-optical imaging of excitons in nanobubbles in 1L-WSe$_2$ with atomistic structural models to elucidate how strain induces the nanoscale confinement potentials that give rise to highly localized exciton states in 2D semiconductors. Nano-optical imaging reveals localized excitons on length scales of ~10 nm at multiple sites along the periphery of individual nanobubbles, which is in stark contrast to predictions of continuum strain models. These results agree with theoretical confinement potentials derived from measured topographies of nanobubbles. We reproduce these findings in nanobubbles of low-defect WSe$_2$ and MoSe$_2$, suggesting our results are applicable to excitons in all the semiconducting 1L-TMD's. Our results provide one-of-a-kind insight of how strain-induced confinement—without crystalline defects—can localize excitons on length scales commensurate with exciton size, providing key nanoscale structure-property information for quantum emitter phenomena in 1L-TMD's.

11:39AM M27.00003: Multi-harmonic phonon assisted upconversion in van der Waals heterostructure p-n junction photodiodes  FATEMEH BARATI (Presenter), TREVOR ARP, SHANSHAN SU, ROGER LAKE, NATHANIEL GABOR, Physics & Astronomy, UCR — In atomically thin van der Waals heterostructures, the interaction between electrons and phonons is highly restricted compared to bulk materials, suggesting that precise stacking of atomic layers could be used to manipulate vibrational coupling to photoexcited electron-hole pairs. Here, we report on phonon assisted anti-stokes absorption near the interlayer exciton edge of vdW semiconductor heterostructures composed of 2L-WSe$_2$ and MoSe$_2$. By carefully tuning the chemical potential of the heterojunction, we find highly rectifying I-V characteristics reminiscent of conventional diode behavior. Using advanced photocurrent spectroscopy measurements, we observe a strong photocurrent peak at near-infrared photon energies with several low energy echoes spaced by 30 meV below this feature. These unusual features occur only when device is precisely tuned to the charge neutrality point. We attribute this behavior to multi-harmonic phonon assisted upconversion, a process by which multiple phonons contribute kinetic energy to the electronic ground state to produce an excited state electron-hole pair. It marks the first observation of strong resonant coupling in a semiconductor system and may herald a new generation of precision optical experiments on laser cooling of vdW heterostructures.
Strong-Coupling of Hybrid Quasiparticles in Excitonic-Dielectric Gratings

BHASKAR ABHIRAMAN (Presenter), HUIQIN ZHANG, Electrical and Systems Engineering, University of Pennsylvania, QING ZHANG, Department of Electrical and Computer Engineering, National University of Singapore, JINSHUI MIAO, KIYOUNG JO, STEFANO ROCCASECCA, Electrical and Systems Engineering, University of Pennsylvania, MARK KNIGHT, Northrop Grumman Corporation, ARTUR DAVOYAN, Mechanical and Aerospace Engineering, University of California, Los Angeles, DEEP M JARIWALA, Electrical and Systems Engineering, University of Pennsylvania — Tightly bound exciton states in van der Waals semiconductors such as MX₂ (M= Mo, W; X= S, Se) are promising for optoelectronic applications. However, to-date, strong light-exciton interaction and control of excited states in them has been limited to monolayer samples with external optical cavities. Here, we demonstrate that nanostructured multilayer WS₂ provides an ideal cavity-less and exposed surface platform for exciton-photonics where the WS₂ serves the role of both the cavity and the excitonic medium. We show that by patterning sub-15 nm thick WS₂ into 300 nm wide resonators an avoided crossing of excitons and photon-polaritons with interaction potentials exceeding 410 meV can be engineered with precision. We further observe that inherently strong TMDC exciton absorption may be completely suppressed due to excitation of hybrid photon-exciton states and their interference. By modifying the system with dielectric spacers, we observe a rich platform for coupling and field confinement with bulk and monolayer TMDCs. Our work paves the way to a new class of integrated exciton optoelectronic nano-devices and their applications in light generation and manipulation.

*Supported by: U.S. Army Research Office, Northrop Grumman, NSF and Vagelos Institute for Energy Science and Technology.
12:03PM M27.00005: Ultrafast exciton dynamics in WSe\textsubscript{2} optical waveguides*  AARON STERNBACH (Presenter), Physics, Columbia University, SIMONE LATINI, Max Planck Institute for the Structure and Dynamics of Matter, SANGHOON CHAE, Mechanical Engineering, Columbia University, HANNES HUEBENER, UMBERTO DE GIOVANNINI, Max Planck Institute for the Structure and Dynamics of Matter, YINMING SHAO, LIN XIONG, ZHIYUAN SUN, NORMAN SHI, Physics, Columbia University, PETER KISSIN, Physics, University of California, San Diego, GUANGXIN NI, Physics, Columbia University, DANIEL A RHODES, BRIAN S Y KIM, Mechanical Engineering, Columbia University, NANNFANG YU, ANDREW MILLIS, Physics, Columbia University, MICHAEL M FOGLER, Physics, University of California, San Diego, P. JAMES SCHUCK, Mechanical Engineering, Columbia University, MICHAL LIPSON, Department of Electrical Engineering, Columbia University, XIAOYANG ZHU, Chemistry, Columbia University, JAMES C HONE, Mechanical Engineering, Columbia University, RICHARD AVERITT, Physics, University of California, San Diego, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter, DMITRI BASOV, Physics, Columbia University — We investigated dynamics of excitons in a Van der Waals Semiconducting, WSe\textsubscript{2}, waveguide. We monitored the electric-field profile of waveguided infrared radiation under intense femtosecond photo-excitation in real space and time. Drastic modifications of the complex wavevector of guided radiation were observed. The non-equilibrium energy momentum dispersion relationship implicates excitons in the photo-induced transformations. Unprecedented coherent dynamics of refraction, on the sub-ps timescale, reveal an optical stark-shift of the A-exciton resonance. Our study establishes that excitons enhance the performance of vdW optical modulators providing a tuning knob unavailable in conventional III-V semiconducting platforms. Our transient images and first-principles theoretical calculations establish fundamental limits of excitons in WSe\textsubscript{2} optical modulators.

*Support by Programmable Quantum Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under award DE-SC0019443”, the European Research Council (ERC-2015-AdG694097), the Cluster of Excellence 'Advanced Imaging of Matter' (AIM), the Flatiron Institute, a division of the Simons Foundation, and the Alexander von Humboldt foundation are acknowledged.
**12:15PM M27.00006: Twist-angle dependent optical properties of interlayer excitons in MoSe\textsubscript{2}/WSe\textsubscript{2} heterostructures**

JUNHO CHOI (Presenter), KHA TRAN, Department of Physics, Complex Quantum Systems, and Texas Materials Institutes, University of Texas at Austin, GALAN MOODY, Department of Electrical and Computer Engineering, University of California Santa Barbara, AKSHAY K SINGH, Department of Materials Science and Engineering, Massachusetts Institute of Technology, JIAMIN QUAN, LIUYANG SUN, ROB CLAASSEN, CARTER YOUNG, Department of Physics, Complex Quantum Systems, and Texas Materials Institutes, University of Texas at Austin, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Material Science, XIAOQIN (ELAINE) LI, Department of Physics, Complex Quantum Systems, and Texas Materials Institutes, University of Texas at Austin — We investigate the interlayer excitons in MoSe\textsubscript{2}/WSe\textsubscript{2} heterostructures, mechanically stacked with an accurately controlled twist angle and capsulated by hexagonal boron nitride. Three \textit{R}-stacking style samples with different twist angles are measured by polarization-resolved steady state and time-resolved photoluminescence at low-temperature. We observe multiple resonances of interlayer excitons which we attribute to quantized states in the moiré potential. The recombination dynamics of the interlayer excitons are found to change significantly with a small change in the twist angle.

*We gratefully acknowledge funding from NSF DMR-1720595, NSF DMR-1808042, and Welch Foundation F-1662.

**12:27PM M27.00007: Excitonic spectral features of 1L-WSe\textsubscript{2} with silicon nitride waveguide coupling**

YUEH-CHUN WU (Presenter), Physics, Univ of Mass - Amherst, SARATH SAMUDRALA, ANDREW MCCLUNG, Electrical and Computer Engineering, Univ of Mass- Amherst, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, AMIR ARBABI, Electrical and Computer Engineering, Univ of Mass- Amherst, JUN YAN, Physics, Univ of Mass - Amherst — In this study, we present excitonic spectral features of 1L-WSe\textsubscript{2} coupled to a platform with Silicon nitride (SiNx) waveguides, allowing us to excite and collect signals in different polarizations. In our high quality BN/1L-WSe\textsubscript{2}/BN/SiNx sample, bright neutral exciton, intervalley/intravalley trions, dark exciton, and bi-exciton and exciton-trion states can be clearly resolved, in agreement with previous reports. The dark exciton, which is known to have out-of-plane dipole moment and thus has been elusive in most standard optical measurements, can be selectively enhanced with out-of-plane light waveguide coupling scheme. Moreover, we study the resonance excitation with 1s bright and dark excitons with different polarizations. Interestingly, as we resonantly excite at dark exciton with out-of-plane light, we observe the up-conversion of bright exciton as well as a down conversion feature lying around 25-27meV lower which indicates dark associate states as being reported to be either dark trions or phonon replica of dark exciton in WSe\textsubscript{2}.

*This work is mainly supported by the University of Massachusetts Amherst and NSF ECCS 1509599
**12:39PM M27.00008: The Nature of Trions and Trion-Polaritons in 2D Materials: Theory and Experiments**  
OKAN KOKSAL (Presenter), MINWOO JUNG, CHRISTINA MANOLATOU, GENNADY SHVETS, FARHAN RANA, Cornell University — The traditional picture of trions as bound states of two electrons and hole has been called into question by several recent works \[1,2\]. The traditional model of trions is also inconsistent with coherent trion-polaritons \[3\]. In this work we present a many body description of trions and trion-polaritons that is valid over a wide range of electron densities. In our work, a negatively charged trion, for example, appears as a bound state of a valence band hole, two conduction band electrons, and a conduction band hole. At small electron densities, this 4-body bound state description of trions is found to be approximately correct. The binding of the conduction band hole allows coherent trion-polaritons. At much larger electron densities, bound trion states don’t exist and a many-body screened-exciton description of trions is found to be more accurate. We present experimental results for the evolution of the exciton and trion oscillator strengths and binding energies with the electron density, and also for the trion-polariton dispersion relations, in 2D-MoSe$_2$, and show very good agreements with our theoretical model. [1] Phys. Rev. B, 95, 035417 (2017), [2] Nat. Phys., 13, 255 (2016). [3] Nat. Phys., 14, 130 (2018)

*The research was funded by the NSF EFRI-1741694 and NSF DMR-1120296.

**12:51PM M27.00009: Excitonic Lifetime in CVD-Grown, Few-Layer MoTe$_2$**  
AARON SCHULZETENBERG (Presenter), JAMES JOHNS, University of Minnesota — Two-dimensional semiconductors such as transition metal dichalcogenides (TMDCs) with high binding energy excitons provide an ideal platform to study exciton physics such as exciton-exciton annihilation and chemical defect scattering. The dominant exciton decay mechanisms of chemical vapor deposition (CVD) grown, few-layer MoTe$_2$ are investigated by measuring and statistically analyzing its ultrafast, optical transient reflectivity dynamics under different pump excitation energies, fluences and temperatures. Defect interaction controls the ultrafast exciton decay pathways. Weak intralayer bonding in few-layer, CVD MoTe$_2$ causes it to have a greater defect density than in other mechanically exfoliated 2D transition metal dichalcogenides. Direct charge carrier occupation of trap states is thought to cause an additional transient feature on the A’ exciton which is not present in the absorption spectrum. Additionally, long-term ambient air exposure does not significantly affect few-layer MoTe$_2$ exciton decay time and absorption peak shape, increasing this material’s suitability for many technological applications.
Continuous Wave Sum Frequency Generation and Imaging of Monolayer and Heterobilayer 2D Semiconductors

KAIYUAN YAO (Presenter), EMANUIL YANEV, Columbia University, HSUN JEN CHUANG, MATTHEW ROSENBERGER, naval research laboratory, XINYI XU, THOMAS DARLINGTON, Columbia University, KATHLEEN M MCCREARY, AUBREY T. HANBICKI, BEREND THOMAS JONKER, naval research laboratory, XIAOYANG ZHU, DMITRI BASOV, JAMES C HONE, P. JAMES SCHUCK, Columbia University — Optical nonlinearities in two-dimensional transition metal dichalcogenides (TMDs) are greatly enhanced by excitonic resonances. Here we report continuous-wave second harmonic and sum frequency generation from two-dimensional TMD monolayers and their heterostructures, with pump irradiances several orders of magnitude lower than conventional pulsed experiments. The high nonlinear efficiency originates from above-gap excitons in the band nesting regions, as revealed by wavelength-dependent second order optical susceptibilities quantified in four common monolayer transition metal dichalcogenides. Using sum frequency excitation spectroscopy and imaging, we identify and distinguish one- and two-photon resonances in both monolayers and heterobilayers. Data for heterostructures reveal responses from constituent layers accompanied with nonlinear signal correlated with interlayer transitions. Furthermore, we demonstrate spatial mapping of heterogeneous interlayer coupling by sum frequency and second harmonic confocal microscopy on heterobilayer MoSe$_2$/WSe$_2$.

Second harmonic generation spectroscopy of MoS$_2$/WSe$_2$ heterostructure

JUNGCHEOL KIM (Presenter), HYEONSIK M CHEONG, Physics, Sogang University — Recently, heterostructures of transition metal dichalcogenides (TMDs) have attracted much interest owing to their unique physical properties. One of the most interesting characteristics is the large exciton energy of TMDs. As the electronic band structures of TMD materials are highly dependent on the number of layers, the interlayer interaction between constituent layers in the heterostructure also affects the band structure [1]. Therefore, understanding the changes of exciton states is important to revealing the band structure of the TMD heterostructure. We fabricated MoS$_2$/WSe$_2$ heterostructures by the stamping methods using exfoliated monolayer MoS$_2$ and WSe$_2$. The PL and Raman measurements were carried out to determine the quality of interface in the heterostructures. Finally, using the second harmonic generation spectroscopy, which is a useful experimental method to measure the exciton states in TMD materials [2], we observed a shift of the exciton energy in the heterostructure compare to those in individual constituent layers.

Trion valley relaxation dynamics in monolayer WSe$_2$  

Keisuke Shinokita (Presenter), Xiaofan Wang, Yuhei Miyauchi, Kyoto Univ - Uji Campus, Kenji Watanabe, Takashi Taniguchi, National Institute for Materials Science, Satoru Konabe, Department of Chemical Science and Technology, Hosei University, Kazunari Matsuda, Kyoto Univ - Uji Campus — Valley degrees of freedom of atomically thin materials have received much attention, with potential in future applications of electronics and optoelectronics as emerging valleytronics. The exploration of novel valley-dependent phenomena has been boosted by strongly Coulomb-bounded electrons and holes acting as neutral excitons and charged excitons (trions) with finite Berry curvature in monolayers of transition metal dichalcogenides. However, neutral excitons have been reported to undergo fast intervalley scattering on the order of 10 ps, which blurs observations of valley-dependent phenomena. Here we report the valley relaxation dynamics of the bright state of positively charged excitons (bright positive trions) in monolayer WSe$_2$ through polarization- and time-resolved photoluminescence and femtosecond transient reflection measurements. A long valley relaxation time, exceeding 100 ps, is observed for positive trions at low temperature, which is notably prolonged when compared with the characteristic excitonic valley relaxation time of 10 ps. With increasing temperature, the relaxation time decreases to a few ps. This finding implies that phonon-mediated intervalley scattering is important for the relaxation process of the valley-polarized bright state of positive trions.

Pressure-tunable stacking order in few-layer WS$_2$ revealed by second harmonic generation  

Chengrong Wei (Presenter), Physics, The University of Hong Kong, Huimin Su, Xuefeng Zhou, Shanmin Wang, Jun-Feng Dai, physics, Southern University of Science and Technology — In 2D material, interlayer interaction can be tuning by internal pressure. We experimentally demonstrate a controllable interlayer translation freedom in hBN-encapsulated few-layer WS$_2$ under applying hydrostatic pressure, which is characterized by Raman spectroscopy and the polarization-resolved second harmonic generation (SHG) spectroscopy. The E$_{2g}^1$ and A$_{1g}$ modes of all samples increased with pressure and there is no new peak observed in the Raman spectrum. The SHG patterns in monolayer WS$_2$ have insignificant distortion and the SHG signal in bilayer WS$_2$ is negligible. Meanwhile, SHG patterns in trilayer WS$_2$ show six asymmetric lobes. Such observations suggest that the threefold rotational symmetry is broken under pressure, which origins from a relative sliding between adjacent layers in the zigzag direction. The tunability of translation structural symmetry by using a hydrostatic pressure presented in this work provides a platform to explore novel physical properties in new class of 2D materials.

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M27.00014: Donor-acceptor-pair transitions in suspended monolayer WS$_2$*  YUNKUN WANG

(Presenter), State Key Laboratory for Mesoscopic Physics and Collaborative Innovation Center of Quantum Matter, School of Physics, Peking University, HAILAN LUO, XINGJIANG ZHOU, YUAN HUANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Science, YUNAN GAO, State Key Laboratory for Mesoscopic Physics and Collaborative Innovation Center of Quantum Matter, School of Physics, Peking University — In conventional semiconductors, the donor-acceptor-pair (DAP) transitions could dominate the photoluminescence, when the sample is cooled to low temperature and the excitation is weak. Here we report observation and characterization of DAP transitions in a suspended monolayer WS$_2$ using steady-state and time-resolved photoluminescence spectroscopy. Without substrate induced doping in suspended monolayer WS$_2$, we observed an ultra-broad emission centered at 1.83 eV and with bandwidth of more than 300 meV. The bandwidth is much larger than generally observed bound excitons. These sub-band states show a sub-linear power-law dependence with an index of 0.3 at 12 K. In the DAP transitions, the recombination centers are spatially separated, and their emission energy depends on their relative distances. We observed that the board emission spectra shift to higher energy as the excitation power increased. Time-resolved photoluminescence spectra show the broad emission shifts from higher energy to lower one along the intensity decay. This work provides further deep understanding of trap states and decay channels in transition metal dichalcogenides.

*National Key R&D Program of China 2018YFA0306300

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M28 FIAP: Imaging in Industry 405-407 - Matthew Thompson, BAE Systems - Tag(s): Careers, Industry, Invited, Undergrad Friendly
11:15AM M28.00001: Subterranean Visualization Through Multi-Sensor Fusion* [Invited] JOE MORRIS (Presenter), Lawrence Livermore National Laboratory — We depend upon the subsurface for much of the energy and raw material that enables civilization. Groundwater sources often supply water for agricultural, drinking, and industrial use. However, we remain relatively blind in the subsurface environment. Geological formations can be strongly heterogeneous at all length scales, making it difficult to locate resources. Furthermore, the performance of subsurface engineering is difficult to monitor due to our blindness.

I will describe challenges associated with engineered geothermal systems (EGS) and hydraulic fracturing in shale formations. In both instances, our optimization of an engineered system is impeded by gaps in understanding of the fundamental processes and our inability to monitor and visualize system performance.

I will present sensors that help us image the subsurface. Of note is the recent growth of fiber optic measurements. Leveraging interferometry applied to light pulses sent down a fiber, we infer the state of the fiber along its entire length. However, each sensor technology has strengths and weaknesses. By combining multiple sensors, we can best avoid blind spots. I will discuss examples of multi-sensor fusion in petroleum and EGS field projects where concurrent measurements of velocity, acoustic, chemical, thermal, and resistive properties enable determination of system performance. Today, such projects rely on large teams of scientists and engineers to collect and interpret data and make engineering decisions. Increasing automation through machine learning is showing promise for decreasing the lag between measurement and decision making. I will close by describing a new initiative that seeks to develop a comprehensive platform for integrating data and providing a virtual environment for exploring the subsurface.

*This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

11:51AM M28.00002: How Self-Driving Cars Find Their Way [Invited] COLIN MCCORMICK (Presenter), Georgetown University — Autonomous vehicles such as self-driving cars (SDCs) use sophisticated sensors and complex perception and planning algorithms to navigate in a variety of environments. The sensor systems include lidar, radar and RGB video cameras, while the algorithms include localization, object detection and tracking, and path planning. SDCs have the potential to save thousands of lives when widely deployed, but they face technical, economic and regulatory barriers. Industry is currently investing billions of dollars to develop SDC technology, and it is eager to identify technical talent. Physicists are extremely well suited to work on these technical issues, and have many opportunities to do so. I will describe the basics of SDC technology, give a brief summary of the economic and policy landscape, and highlight ways that physicists can enter this important and interesting field.

12:27PM M28.00003: Augmented Reality in Aerospace [Invited] SHELLY PETERSON (Presenter), Lockheed Martin — TBD
The Role of Physics in Overhead Imaging

Jonathan Edwards, BAE Systems — Basic physics has profound implications for overhead imaging. This presentation will examine illustrative surveillance concepts for defense applications using unmanned and space-based platforms. We focus on two topics where physics plays a crucial role: 1) wide-area drone surveillance, and 2) low-earth orbit (LEO) imaging.

To accommodate drone limitations, sensor concepts minimizing size and weight while maximizing scene coverage and resolution are preferred. One intriguing concept uses composite focal plane arrays (CFPA). CPFAs apply multiple discrete FPAs on a flat surface behind a single optical path. For this technology, we discuss trade-offs for field-of-view and resolution and describe a number of engineering challenges addressed for a realizable system.

Given CFPA ‘big-data’ acquisition, physical principles are invoked to facilitate a key capability – automated object tracking. Here, traditional kinematics permits the tracking of moving entities from a moving platform over a large area.

Cheaper and frequent rocket launches have resulted in a burgeoning ‘small satellite’ market. This has motivated desire for small earth-observing payloads. We discuss critical trade-space drivers including LEO’s high velocity and stringent platform volume bounds. The space environment also presents challenges for analysis using traditional electronics. We discuss the trade-off of cost and reliability that defines LEO operation by examining the impact of the physical radiation environment.
The need for persistent microwave imaging spectrometry of the Earth within 100-200 GHz and with sub-hourly temporal resolution for severe weather monitoring had been identified in 1978 by Staelin et al. in a NASA-sponsored study [1]. The clear need presented in this study has driven the laboratory-level development of large geostationary filled-and synthetic-aperture microwave sounders throughout the past period of more than four decades. However, the recent demonstration of small CubeSat-based imaging microwave spectrometers in this frequency range suggests a new pathway to achieving these goals. The successful launch in April 2019 and subsequent demonstration of the Global Earth Monitoring System (GEMS) GEMS-1 In-orbit Demonstration (IOD) mission using a 118-GHz imaging microwave spectrometer supports this goal. Importantly, however, it enables a scalable constellation framework with the capability to provide temporal Nyquist-sampled microwave imagery of the Earth’s troposphere and lower stratosphere.

GEMS-1 IOD was developed by Orbital Micro Systems in partnership with the University of Colorado’s Center for Environmental Technology and the UK Space Applications Catapult. The GEMS-1 IOD sensor is currently the highest spatial resolution microwave temperature sounding sensor on orbit. The GEMS-1 sensor design, its on-orbit performance, and the pathway to an evolved GEMS constellation capable of meeting and exceeding the severe weather observation requirements set forth over 40 years ago will be discussed.


*OMS is grateful for support in the development of the GEMS constellation by the US Air Force under the Commercial Weather Data Pilot program and Innovate UK / Space Applications Catapult through the In-Orbit Demonstrator (IOD-1) program.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M29 DSOFT DPOLY: Liquid Crystals II: Phases and Transitions
501 - Vianney Gimenez-Pinto, Lincoln University, Missouri
**11:15AM M29.00001: Theory of the splay nematic phase**  
MICHELY ROSSETTO, Universidade Estadual de Maringá, JONATHAN SELINGER (Presenter), Kent State Univ - Kent — Recent experiments have reported a novel splay nematic phase, which has alternating domains of positive and negative splay [1]. To model this phase, researchers have considered a 1D splay modulation of the director field, accompanied by a 1D modulation of polar order. When the flexoelectric coupling between splay and polar order becomes sufficiently strong, the uniform nematic state becomes unstable to the formation of a modulated phase [1,2]. Here, we re-examine this theory in terms of a new approach to liquid crystal elasticity [3], which shows that pure splay deformation is double-splay rather than planar single-splay. Following that reasoning, we propose a structure with a 2D splay modulation of the director field, accompanied by a 2D modulation of polar order, and show that the 2D structure generally has a lower free energy than the 1D structure. We also investigate a generalized flexoelectric coupling between director deformations and tetrahedral order, but still find a lower free energy for the 2D modulation.


*This work was supported by NSF Grant No. DMR-1409658 and by CAPES Finance Code 001.

**11:27AM M29.00002: Twisted topological defect lines in achiral nematic liquid crystal confined in glass capillaries**  
ZHAOFEI ZHENG (Presenter), JOSE X VELEZ, Johns Hopkins University, DANIEL BELLER, Physics, School of Natural Sciences, University of California, Merced, FRANCESCA SERRA, Johns Hopkins University — Chirality occupies a remarkable space in biology and soft matter. In liquid crystals, chirality at the molecular scale propagates to the macroscale in non-trivial ways and can emerge even from achiral components. Here we report that common nonchiral thermotropic liquid crystals confined in square capillary tubes with homeotropic anchoring can show a spontaneous twist during the phase transition from smectic-A to nematic. The chiral structure is transient, but it can be stabilized for a few hours by accurate control of the temperature. We hypothesize that this chiral structure is related to the different rate of change of the twist and bend elastic constants at the phase transition. However, also the shape of the confining capillary plays a key role. In fact, this effect is clearly seen in capillaries, with square cross-section: the edges of the capillary, on the one hand, stabilize disclination lines in the nematic phase, and on the other hand they induce the formation of many defects in the smectic phase.
11:39 AM M29.00003: Phase Transition Triggering in a Liquid Crystal Droplet*  
JAKE SHECHTER (Presenter), Physics, University of Massachusetts - Amherst, NOE ATZIN CANAS, RUI ZHANG, ALI MOZAFFARI, Molecular Engineering, University of Chicago, BENJAMIN A STRAIN, LINDA M OSTER, Physics, University of Massachusetts - Amherst, MANISHA CHAHAR, Chemistry, University of Massachusetts - Amherst, JUAN DE PABLO, Molecular Engineering, University of Chicago, S. THAI THAYUMANAVAN, Chemistry, University of Massachusetts - Amherst, JENNIFER L ROSS, Physics, Syracuse University — Liquid crystals (LCs) are a class of molecules that form a variety of phases easily influenced by external interactions. Of particular interest are rod-like LC molecules confined to a spherical geometry, which have a competition between interfacial tension and elastic deformations. The phase of the liquid crystal inside a droplet can be controlled using surfactants, influencing the boundary conditions, in an oil-in-water emulsion. Here, we test the effects of the surfactant sodium dodecyl sulfate (SDS) on the phase of polydisperse LC droplets in an aqueous background examining different diameter sizes and SDS concentrations. We trigger phase transitions by the increase or decrease of SDS concentration while observing an individual LC droplets held in place using an optical tweezer. The dynamic phase transitions are compared to previous molecular dynamic simulations that predicted the intermediate states of the LC inside the droplets. We observe a hysteresis in the SDS concentration that induces the phase transition from radial to bipolar and back as well as a fluctuation in state when the phase transition starts.

*DoD ARO MURI 67455-CH-MUR “Specifically Triggerable Multi-Scale Responses in Organized Assemblies” to S. Thayumanavan, University of Massachusetts Chemistry.

11:51 AM M29.00004: Nanoparticle Network embedded polymer films formed using liquid crystal transition templating.*  
ALAUNA WHEELER (Presenter), LINDA S. HIRST, University of California, Merced — Our lab recently demonstrated that nanoparticles, well-dispersed in the isotropic liquid crystal (LC) phase, will self-assemble into hollow structures when the LC solvent undergoes cooling through the isotropic-to-nematic (I-N) phase transition. The form and size of the nanoparticle structures can be controlled by varying the nanoparticle concentration and the cooling rate (1). Thus far this process has only been accomplished using 5CB (4’-pentyl-4-Biphenylcarbonitrile) as the LC solvent. In this study we demonstrate that hollow networks of self-assembled nanoparticles can be formed in different nematic LC mixtures, compatible with polymerization. The cooling rate across the I-N phase transition can be used to control the size and density of the network structures. We embed these nanoparticle structures in a thin film by using a polymerizable LC mixture in the formation process and characterize the properties of the film.


*National Science Foundation grant numbers CBET 1507551, DMR 1625733
12:03PM M29.00005: One pot synthesis of hollow colloidal gel* DEVIKA GIREESAN SUDHA (Presenter), JOCELYN OCHOA HERNANDEZ, LINDA S. HIRST, University of California, Merced — Liquid crystal (LC) phase transitions can drive the assembly of dispersed nanoparticles. Hollow microstructures of various morphologies can be created, on cooling through the nematic-isotropic transition temperature (T_{NI}) at different temperature quenches. At high quench rates single compartment hollow capsules are observed. These colloidal capsules frustrate orientational order in the liquid crystal leading to topological defects. These defects stabilize the capsules into a mechanically robust gel. The capsule sizes can be controlled by varying the quench depth. Here we present structural analysis using confocal and fluorescence imaging of these gels for a range of capsule sizes. We also observed continuous tubular network morphologies at lower quench rates. These networks under birefringence show the presence of defect lines and loops. Such one pot synthesis technique leads to the rapid self-assembly of liquid crystal nanocomposites, that may find applications in controlled release, sensing and catalysis.

*The authors would like to acknowledge generous funding from the NSF grant number CBET 1507551. The data in this work was collected, in part, with a confocal microscope acquired through the NSF MRI Award Number DMR-1625733.

12:15PM M29.00006: Intertwined spontaneous helix formation in achiral bent-core liquid crystals* VIKINA MARTINEZ (Presenter), ADAM GREEN, CHEOL PARK, Physics and Soft Materials Research Center, University of Colorado Boulder, MATTHEW GLASER, University of Colorado, Boulder, JOSEPH E MACLENNAN, NOEL ANTHONY CLARK, Physics and Soft Materials Research Center, University of Colorado Boulder — Inspired by several reports of spontaneous helix formation in bent-core smectics, we have investigated the smectic phases of a series of bent-core mesogens with 4-cyanoresorcinol bisbenzoate cores. In PAL30, the homolog with n=14 alkyl tails, we observed an incommensurate, bent-core phase with a single helix incommensurate with the smectic layering [1], a structure broadly analogous to the phase of rod-shaped molecules. In the PAL29, the n=16 homolog, we have confirmed, using both resonant and non-resonant x-ray diffraction, as well as electro-optical methods, the existence of a phase with intertwined helices, similar to the structure recently reported by Salamonczyk and co-workers [2]. Establishing the existence of the intertwined double-helical phase and the single-helical phase in such closely related homologs is an important step in understanding the competing interactions that lead to such exotic phase structures.


*This work was supported by the Soft Materials Research Center under NSF MRSEC Grant No. DMR-1420736. and by NASA Grant Nos. NNX-13AQ81G and NAG No. NNX17AC74G.
12:27PM M29.00007: Transformations Between Different Self-Organized Defect Arrays at the Nematic-Smectic A Phase Transition*  DANIEL BELLER (Presenter), University of California, Merced, AHRAM SUH, MIN-JUN GIM, DONG KI YOON, Graduate School of Nanoscience and Technology, Korea Advanced Institute of Science and Technology (KAIST) — We model transformations in self-organized liquid crystal defect arrays in hybrid-aligned thin films at the nematic-smectic A phase transition. The smectic A phase forms a packing of focal conic domains, while the nematic phase features a square lattice of boojum surface-defects at larger spacing. Heating from smectic A to nematic transforms the focal conic domain packing into a dense array of boojums, which we study through Landau-de Gennes numerical modeling and a connection to graph theory. The reverse transformation upon cooling proceeds through a very different morphological sequence, beginning with a stripe instability which we examine analytically and numerically. The focal conic domain packings that emerge retain a geometric memory of the nematic boojum configuration.

*This work was supported by National Science Foundation Grant No. MRSEC-1420382 and CBET-1437195, and by a grant from the National Research Foundation (NRF), funded by the Korean Government (MSIT) (2017R1E1A1A01072798 and 2017M3C1A3013923).

12:39PM M29.00008: Investigation of Thermal Properties of Itraconazole at Ultra-Fast Rates*  JOHN ZAPATA-HINCAPIE (Presenter), MADHUSUDHAN REDDY PALLAKA, SINDEE L SIMON, Texas Tech Univ — The thermal behavior of itraconazole (ITZ) was studied using a conventional differential scanning calorimeter (DSC) and a flash differential scanning calorimetry (Flash DSC) over five decades of cooling rates. Itraconazole forms a smectic glass and shows two endothermic liquid crystal transitions located at 74 and 90 °C at all cooling rates in DSC. On the other hand, in the Flash DSC, the glass that is formed can have smectic order for the lowest cooling rates, nematic order at intermediate cooling rates, and no ordering (i.e., an isotropic glass is formed) at the highest cooling rates of 1000 K/s. The T_g values obtained in conventional and Flash DSC are similar at comparable cooling rates and can be described by the WLF equation over five decades of cooling rate. No discernible change in the T_g versus cooling rate relationship is evident as different glasses are formed, suggesting that differences in T_g for the three glasses is solely attributable to the different cooling rates and not due to the difference in structures. Additionally, the kinetics of the liquid crystal transformations and the kinetics of structural recovery are followed by annealing at different temperatures ranging from -30 to 92 C.

*The authors are grateful to NSF under the grant CMMI-1662046
12:51PM M29.00009: Coalescence Dynamics of Fluids in Two Dimensions: Merging of Islands in Freely-Suspended Smectic Films*  DUONG NGUYEN, Physics and Soft Materials Research Center, University of Colorado Boulder, KIRSTEN HARTH, Institute of Solid State Physics, Otto-von-Guericke Universitat, AARON GOLDFAIN, CHEOL PARK, JOSEPH E MACLENNAN (Presenter), MATTHEW GLASER, NOEL ANTHONY CLARK, Physics and Soft Materials Research Center, University of Colorado Boulder — Smectic liquid crystal films a few molecular layers thick that are freely suspended in air are used as a model system to study the coalescence of fluids in two dimensions. High-speed video microscopy is used to study the coalescence of islands, thicker, disk-shaped regions of the film bounded by edge dislocations. The early time growth of the bridge connecting the merging islands is essentially linear, while at long times the relaxation dynamics are exponential. The observations are compared with Hopper's classical hydrodynamic model of the coalescence of two infinitely long, fluid cylinders [Journal of the American Ceramic Society 76, 2947 (1993)] and with models appropriate to quasi-two dimensional fluids developed by Mann [Phys. Rev. E 51, 5708 (1995)] and Camley [Biophysical Journal 99, L44 (2010)] to explain their observations of domain relaxation in Langmuir films.

*This work was supported by NASA Grant No. NNX-13AQ81G and by the Soft Materials Research Center under NSF MRSEC Grant Nos. DMR-0820579 and NSF Grant DMR-1420736, and by DLR Grants OASIS-Co 50WM1430 and 50WM1744 and DFG Grant STA 425/40

1:03PM M29.00010: Phase behavior and elastic response of liquid crystal mixtures in atomistic models  JIALE SHI (Presenter), HYTHEM SIDKY, JONATHAN K. WHITMER, University of Notre Dame — In practical applications, liquid crystal devices tend to utilize mixtures of liquid crystal molecules. Liquid crystals mixtures can be formulated to have a broad nematic phase range, elastic responses and dielectric anisotropies which are distinct compared to the components. Elasticity, in particular, is important in determining equilibrium morphologies and material responses. Despite this importance, limited knowledge exists about the connections between microscopic composition and macroscopic elastic response in liquid crystal blends. Here, we apply advanced sampling methods in atomistic models to study both the phase behavior and elastic response of liquid crystal mixture. Our simulation work can help understand the elasticity of liquid crystals mixtures and help to rationally design new liquid crystal mixtures.
Macroscopic sheets of negative order parameter Liquid Crystal Elastomer with high dissipation and auxetic properties*  
DEVESH MISTRY (Presenter), ROSS VOLPE, NICHOLAS TRAUGUTT, CHRISTOPHER YAKACKI, University of Colorado, Denver — Negative Order Parameter (NOP) Liquid Crystal Elastomers (LCEs) offer a route to new LCE actuation modes and the study of previously impossible LC systems.[1-3]

Mistry et. al. reported an acrylate LCE with a strain-induced NOP, coinciding with a negative Poisson's ratio (auxeticity).[1,2] Jampani et. al. reported microfluidic thiol-acrylate NOP LCE shells. [3] Due to the microfluidic synthetic process, there are 2 mechanisms for the development of the NOP state in the LCE shells – the shell wall either anisotropically deswelling or being biaxially strained through osmotic pressure. [4] Results Urayama et. al. suggest the latter method does not lead to NOP states.[5]

However, here we create NOP LCEs via the biaxial straining of polydomain LCEs. Using 2 methods we prepare >2x2 cm sheets of NOP LCEs – large enough for the first characterisation of a NOP LC system. Our NOP LCEs have higher levels of energy dissipation and display auxeticity at significantly lower threshold strain compared to LCEs of conventional ordering.[2]

4. J. Lagerwall *ILCEC Presentation, Einhoven (2019)*
5. K. Urayama *ILCEC Presentation, Einhoven (2019)*

*Lindemann Trust Fellowship
1:27PM M29.00012: Oligomeric odd–even effect in liquid crystals.*  RONY SAHA (Presenter), GRETA BABAKHANOVA, ZEINAB PARSOUZI A.SH, MOJTABA RAJABI, PRABESH GYAWALI, Kent State Univ - Kent, CHRIS WELCH, GEORG H. MEHL, University of Hull, JAMES GLEESON, OLEG D LAVRENTOVICH, SAMUEL N SPRUNT, ANTAL ISTVAN JAKLI, Kent State Univ - Kent — In organic materials, they are usually associated with the number of methylene groups in aliphatic chains. In this work, we unveil multiple signatures of a new odd–even effect in liquid crystals that occurs at the larger scale of molecular moieties that by themselves express liquid crystalline behavior. We demonstrate that oligomeric liquid crystals, with \( n = 1–4 \) number of rigid mesogenic segments connected by flexible aliphatic chains with an odd number of methylene groups, produce an odd–even effect in optical anisotropy and the bend elastic constant of the liquid crystal oligomer. This effect is different from the usual odd–even effects with respect to the parity of carbon atoms in an aliphatic chain and can be understood in term of the average molecular shape and the associations between \( n \)-mers based on the packing of these shapes. We also show that, in spite of the fact that there is no long-range electron density modulation, careful analysis of synchrotron SAXS results can provide important information about the molecular associations in the N and NTB phases that other techniques cannot access.


1:39PM M29.00013: Relative orientation of defects in smectic-C films*  XINGZHOU TANG (Presenter), JONATHAN SELINGER, Kent State Univ - Kent — In a 2D liquid crystal, each topological defect has a topological charge and a characteristic orientation, and hence can be regarded as an oriented particle. Theories predict that the trajectories of annihilating defects depend on their relative orientation [1,2]. Recently, these predictions have been tested in experiments on smectic-C films [3]. Those experiments find curved trajectories that are similar to the predictions, but the detailed relationship between the defect orientations and the far-field director field is different. To understand this difference, we improve the previous theories by adding the effects of elastic anisotropy and nonequilibrium dynamics. We find that the theory with elastic anisotropy gives good agreement with the experiment, and hence can describe the effects of defect orientation.


*This work was supported by NSF Grant No. DMR-1409658.
Tying knots in liquid crystals. The topological nature of knots in fields has fascinated physicists and mathematicians. Experimentally they had been found only as transient features or required complex boundary conditions to exist until recently [1]. Here we present energetically stable, micrometer-sized knots in the chiral background of liquid crystals. These knots are spatially localized and diffusing in all directions. They self-assemble into crystalline lattices with open and closed structures, resembling colloidal particles and atomic nuclei. These knots are robust and topologically distinct from the host medium and can be morphed and reconfigured by weak stimuli under conditions such as those in displays. We use a combination of energy-minimizing numerical modeling and optical imaging to uncover the internal structure and topology of individual knots and the various hierarchical crystalline organizations they form. We further explore the effects of elastic anisotropy and external fields on the stability of these knots.


Computational model of a Maier-Saupe field theory for nematic liquid crystals. We develop a computational model based on a field theory extension of the Maier-Saupe molecular model of a uniaxial, nematic liquid crystal. A tensor order parameter is defined as the second moment of an orientational probability distribution, leading to a free energy that is not convex within the isotropic-nematic coexistence region, and that goes to infinity if the eigenvalues of order parameter become non-physical. An elastic free energy is added which is an expansion in spatial gradients of the order parameter up to third order, allowing for parametric control over the anisotropy and elasticity of the liquid crystal. Computations of the spatial profile of the order parameter are presented for an isotropic-nematic interface in one dimension, a nematic defect in two dimensions, and a tactoid in two dimensions. We compare the simulation results to those given by the Landau de-Gennes free energy.

*This research is funded by the National Science Foundation, Contract No. DMR - 1838977

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M30 DSOFT DPOLY: Soft Mechanics via Geometry II

Rochester Institute of Technology - Tag(s): Focus
11:15AM M30.00001: The topography of tuning [Invited]  ELENI KATIFORI (Presenter), University of Pennsylvania — Allosteric proteins globally adjust their conformation upon binding a ligand in order to control the activity of a distant active site. Inspired by such a system, we explore how mechanical systems achieve a specified complex function such as strain propagation in mechanical networks. We investigate computationally the maximum complexity of a tuned function that can be achieved as a function of network size. Further, we identify the structural features responsible for function in these tuned networks. We show how we can use topographical information to improve the tuning process and how the complexity of the tuned function scales with network size. Using persistent homology, we show that networks tuned to perform such functions develop characteristic features that are similar for different networks that perform the same function, regardless of differences in the local link connectivity.

11:51AM M30.00002: Mechanics of soft fibrous mats with inter-fiber adhesion and friction* CATALIN PICU (Presenter), VINEET NEGI, Rensselaer Polytechnic Institute — Many soft materials of biological and industrial interest are composed from nanofibers and take the form of quasi-two-dimensional mats with stochastic structure. Examples include membranes in the human and animal bodies, geotextiles, non-wovens used in consumer products and tissue scaffolds. We investigate the mechanical behavior of such structures, which is largely controlled by geometry and adhesive and frictional interactions of constituent fibers. We consider two cases: one in which the fibrous mat is stabilized by adhesion, and the other in which fibers interact only frictionally. Both systems exhibit rich non-linear mechanics. We determine the scaling of material properties with the intensity of adhesion, and describe the interplay between frictional interactions and geometry in defining the mechanics of the mat. Stress in these systems is primarily associated with dissipation and exhibits interesting dependence on the network architecture.

V. Negi, R.C. Picu, Soft Matter, 2019, 15, 5951

*Work supported by the NSF through grant CMMI-1634328.

12:03PM M30.00003: Nonlinear Poisson effect in critical mechanical networks* JORDAN SHIVERS (Presenter), SADJAD ARZASH, FRED C MACKINTOSH, Department of Chemical and Biomolecular Engineering, Rice University — Fibrous networks of stiff athermal biopolymers such as collagen, a major structural component of the extracellular matrix, have been shown to exhibit anomalously large apparent Poisson ratios, i.e. significant transverse contraction under small applied longitudinal extension. Here we show that this effect can be understood in the context of a macroscopic mechanical phase transition from a bending-dominated regime to a stretching-dominated regime at a critical applied extension controlled by the network connectivity. We measure this effect using a variety of 2D and 3D model network structures and propose a phase diagram governing the transition as a function of connectivity and strain.

*This work was supported in part by the National Science Foundation (DMR-1826623 and PHY-1427654). J.L.S. acknowledges additional support from the Ken Kennedy Institute Graduate Fellowship and the Riki Kobayashi Fellowship in Chemical Engineering.
12:15PM M30.00004: Shear modulus discontinuity in fiber networks*   SADJAD ARZASH (Presenter), JORDAN SHIVERS, FRED C MACKINTOSH, Department of Chemical & Biomolecular Engineering, Rice University — Fibrous networks such as collagen are common in physiological systems. One important function of these networks is to provide mechanical stability for cells and tissues. It has been shown that athermal coarse-grained models of fibers with bending and stretching interactions can explain the experimental observations. By applying an extensional or shear deformation, subisostatic fiber networks with only central force interactions undergo a phase transition from a floppy to a rigid state. By simulating various network models, we confirm that although the network's stiffness exhibits a discontinuity, the transition is critical in nature. We study the finite-size scaling behavior of this discontinuity in order to identify the corresponding non-mean-field critical exponent in the thermodynamic limit.

*This work was supported in part by the National Science Foundation (Grants DMR-1826623 and PHY-1427654).

12:27PM M30.00005: Shaping curved surfaces using origami.   THÉO JULES (Presenter), Laboratoire de Physique, Ecole Normale Superieure de Lyon, FREDERIC LECHENAULT, Laboratoire de Physique, Ecole Normale Superieure, MOKHTAR ADDA-BEDIA, Laboratoire de Physique, Ecole Normale Superieure de Lyon — In order to understand the full range of equilibrium shapes and mechanical response of origami-based metamaterials, one is led to take into account both the geometrical constraints induced by the crease network and the elasticity of the material. A model example for this is a shell formed by an accordion-like origami, made from a single elastic sheet decorated by a series of parallel creases, crossed by a central longitudinal crease. Surprisingly, while the imprinted crease network does not have a geodesic curvature, the emergent three-dimensional structure is characterized by an effective curvature along the central line. We craft these patterns and scan them using a structured-light 3D-scanner. Our study captures the exotic zoology of face deformations that appear due to kinematic constraints imposed by the crease network, ranging from simple bending to ribbon-like behavior, as confirmed by FEM simulations.
**Non-Hookean Elastic Moduli of 2D Tissue Model**

ARTHUR HERNANDEZ (Presenter), University of California, Santa Barbara, MICHAEL MOSHE, The Racah Institute of Physics, Hebrew University, M CRISTINA MARCHETTI, MARK J BOWICK, University of California, Santa Barbara —

We study the peculiar mechanical response of a discrete vertex model (VM) of 2D epithelia. In the absence of T1 rearrangements, the VM exhibits a transition between a soft and a stiff solid tuned by the target shape index of the cells and associated with the onset of geometric incompatibility. By examining the response to a variety of deformations, we show that the stiff solid phase exhibits nonlinear elastic response that cannot be recast in the framework of conventional Hookean elasticity even in the limit of infinitesimal strain. The soft solid is characterized by floppy modes that can absorb strain. As a result, the linear mechanical response is not fully characterized by two independent Lamé coefficients, as in linear elasticity of a 2D isotropic solid, but depends on the specific imposed deformation. We show that this unconventional mechanical behavior is in agreement with a continuum version of the model developed recently by some of us.

*This work was supported by the NSF through awards DMR-1609208 (M.C.M and A.H.) at KITP under Grant PHY-1748958 (M.J.B.)*

**Geometry and kinetics determine the packing structure on evolving surfaces**

ZHAOYU XIE (Presenter), CHRISTOPHER BURKE, BADEL L MBANGA, Tufts Univ, PATRICK T SPICER, School of Chemical Engineering, University of New South Wales Sydney, TIM ATHERTON, Tufts Univ — We consider the evolution, arrest and jamming of particulate media on an evolving surface. As the shape changes, local regions of compression and rarefaction induce local solidification or melting and, consequently, rich kinetic effects. Here we resolve the relative influence of kinetics and geometry in determining the structure of a model system: the coalescence of Pickering emulsion droplets that can be arrested by the solid particles coated on the surface. By Monte Carlo simulations, we demonstrate that in the quasi-static regime, the geometry still governs the microstructure of these particles, resembling the spherical crystallography regime explored in previous literature. Conversely if the evolution of surface is fast, the kinetics can change the structure at the arrest point depending on the local surface deformation, with jamming fronts that develop from the compressed area. Other surfaces and particles are explored and we propose a new class "metric jamming" to describe the transition to rigidity under shape deformation.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1654283.*
1:03PM M30.00008: Crumple-Origami Transition for Twisting Cylindrical Shells*  
LI-MIN WANG (Presenter), Department of Physics, Natl Tsing Hua Univ, SUN-TING TSAI, Department of Physics and Institute for Physical Science and Technology, University of Maryland, CHIH-YU LEE, Hsinchu Senior High School, PAI-YI HSIAO, JIA-WEI DENG, HUNG-CHIEH FAN CHIANG, Department of Physics, Natl Tsing Hua Univ, YICHENG FEI, Department of Physics and Astronomy, Rice University, TZAY-MING HONG, Department of Physics, Natl Tsing Hua Univ — Origami and crumpling are two extreme tools to shrink a 3-D shell. In the shrink/expand process, the former is reversible due to its topological mechanism, while the latter is irreversible because of its random-generated creases. We observe a morphological transition between origami and crumple states in a twisted cylindrical shell. By studying the regularity of crease pattern, acoustic emission and energetics from experiments and simulations, we develop a model to explain this transition from frustration of geometry that causes breaking of rotational symmetry. In contrast to solving von Karman-Donnell equations numerically, our model allows derivations of analytic formula that successfully describe the origami state. When generalized to truncated cones and polygonal cylinders, we explain why multiple and/or reversed crumple-origami transitions can occur.

*We gratefully acknowledge financial support from MoST in Taiwan under grant 108-2112-M007-011-MY3.

1:15PM M30.00009: Statistical mechanics of nanotubes*  
SIDDHARTHA SARKAR (Presenter), ANDREJ KOSMRLJ, Princeton University — We investigate how thermal fluctuations affect mechanical properties of nanotubes by employing renormalization group procedure. For 2D sheets it was previously shown that thermal fluctuations effectively renormalize elastic constants beyond a characteristic thermal length scale (a few nanometers for graphene at room temperature), where the bending rigidity increases, while the in-plane elastic constants reduce with universal power law exponents. However, the curvature of nanotubes produces new phenomena. Specifically, we find that in the axial direction the in-plane elastic constants stop renormalizing at the elastic length scale (proportional to geometric mean of the radius and the effective thickness of the shell), while in the circumferential direction they continue to renormalize albeit with different universal exponents. On the other hand, the bending rigidity stops renormalizing in the circumferential direction at the elastic length scale. These results were verified with molecular dynamics simulations by measuring the mechanical response to axial loads and external pressure. We also comment on how these temperature dependent properties affect the critical buckling loads for nanotubes.

*Work was supported by the NSF Career award DMR-1752100.
1:27PM M30.00010: Braided biopolymer filament bundles produce topologically protected kinks  VALENTIN SLEPUKHIN (Presenter), University of California, Los Angeles, MAXIMILIAN GRILL, Technical University of Munich, QINGDA HU, ELLIOT BOTVINICK, University of California, Irvine, WOLFGANG WALL, Technical University of Munich, ALEX LEVINE, University of California, Los Angeles — Bundles of stiff filaments are ubiquitous in the living world, found both in the cytoskeleton and in the extracellular medium. These bundles are typically held together by smaller cross-linking molecules. We demonstrate analytically, numerically and experimentally that such bundles can be kinked, i.e., have localized regions of high curvature that appear to be at least long-lived metastable states. We find analytically three possible mechanisms of kink stabilization: the different trapped length of the filaments between two cross-links; the endpoint of the filament in the middle of the bundle; the braiding of the filaments in the bundle. For a high concentration of cross-links, last two effects lead to the topologically protected kinked state. Finally, we explore the transition of the metastable kinked state to the stable straight bundle state both numerically and analytically.

1:39PM M30.00011: Fabrication of supported lipid bilayers of designed shape with micro-printing and replica-molding  MELISSA RINALDIN (Presenter), LUCA GIOMI, DANIELA JUTTA KRAFT, Leiden University — Membrane curvature is a fundamental part of the cellular machinery. In cells, membrane curvature can be generated by different mechanisms, including cytoskeletal scaffolding and lipid and protein sorting. In protein-free systems in vitro, membrane curvature can be artificially obtained by, for example, membrane micro-manipulation, phase separation, and supported lipid bilayers fabrication. However, until now, these methods allowed for studying a restricted range of shapes only. Here, we present a general and facile method to obtain membranes of designed curvature with high precision. By combining 3D micro-printing and replica-molding lithography, we fabricate scaffolds of designed shape and size suitable for lipid coating. We show that the resulting supported lipid bilayers are homogeneous and fluid. We demonstrate their potential by using them for fluorescence after photobleaching and phase separation experiments on curved surfaces. We anticipate that our method will open new possibilities to investigate curvature sensing proteins and, more generally, the role of membrane curvature in biology.
1:51PM M30.00012: Curvature-driven propulsion of floating films: Part 1*  MONICA RIPP
(Presenter), ZACHARIAH SCHRECENGOST, ELIZABETH LAWSON-KEISTER, JOSEPH PAULSEN, Syracuse University — Water striders can propel themselves up a curved liquid meniscus by repositioning their feet to match the curvature of their destination, providing one example of propulsion along an interface due to a mismatch in geometry [1]. How does a highly-flexible elastic solid respond when it is placed on a liquid surface with a curvature different than its own? We find that flat films spontaneously flee highly-curved menisci towards flatter regions, whereas curved shells are attracted to regions with finite curvature. These findings are borne out of experiments where polymer films are released from different initial positions in overfilled petri dishes. Focusing on flat films that are ~1 cm wide and ~100 nm thick, we examine the effects of film thickness, liquid viscosity, and meniscus curvature on the velocity of this motion. Our data across a wide range of parameters are in agreement with a theoretical picture in which the sheet is propelled by its ability to cover progressively more liquid surface area in the regions where it is attracted [2]. We develop this model and its consequences in the next talk. (This is part 1 of a 2-talk series.)


*Support from NSF-DMR-CAREER-1654102 is gratefully acknowledged

2:03PM M30.00013: Curvature-driven propulsion of floating films: Part 2*  ZACHARIAH SCHRECENGOST (Presenter), MONICA RIPP, JORDAN V BARRETT, Syracuse University, VINCENT DÉMERY, Physics, Université de Lyon, JOSEPH PAULSEN, Syracuse University — The remaining pieces of breakfast cereal spontaneously clump together in a cereal bowl due to the interactions of the menisci around each particle. A highly-bendable elastic sheet participates in a very different interaction with the liquid around it. In the previous talk, experimental results were given where a polymer film spontaneously propels itself to a region that more closely matches its intrinsic curvature. These results were interpreted as falling within a geometric framework, where the sheet bends and wrinkles in such a way as to minimize the exposed liquid surface area [1]. Implementing this model is a nontrivial optimization problem, due to the wide variety of configurations available to the sheet and interface. We use Surface Evolver simulations and analytic calculations to study the energetic cost of placing an ultrathin elastic disc on a local topography of arbitrary curvature. We establish scaling laws that relate the total energy to the principal radii of curvature. By estimating the fluid drag forces, we develop theoretical predictions for sheet velocity, which we compare with our experiments. (This is part 2 of a 2-talk series).


*Support from NSF-DMR-CAREER-1654102 is gratefully acknowledged.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M31 DSOFT: Directed Assembly 2: Field Driven 503 - Alex Travesset, Ames Lab
**11:15AM M31.00001: Hyperuniform structures formed by shearing colloidal suspensions**

SAM WILKEN (Presenter), RODRIGO EMIGDIO GUERRA, DAVID J PINE, PAUL M CHAIKIN, New York Univ NYU — Time-reversibility is an essential feature of viscous, creeping flow that is lost when rigid particles suspended in the liquid are forced to collide with each other. In periodically sheared suspensions this loss manifests as a dynamical phase transition between reversible and chaotic particle trajectories characterized by a critical strain amplitude. Repulsive, non-hydrodynamic interactions between colliding particle surfaces have been proposed as the likely source of this broken symmetry, and a toy model that emphasizes particle collisions, called Random Organization\(^1\), qualitatively reproduces the dynamical features of this transition. This model also displays a concomitant structural reorganization characterized by vanishingly small density fluctuations on long length-scales, called hyperuniformity, at criticality\(^2\). Here we show that the particles in periodically sheared suspensions organize into structures with anisotropic short-range order but isotropic, long-range hyperuniform order when oscillatory shear amplitudes approach the critical strain amplitude.


\*This work was supported primarily by the MRSEC Program of the National Science Foundation under Award Number DMR-1420073.

**11:27AM M31.00002: Optimized Large Hyperuniform Binary Dipolar Colloidal Suspensions in Two Dimensions**

ZHENG MA (Presenter), Princeton University, ENRIQUE LOMBA, Instituto de Química Física Rocasolano, SALVATORE TORQUATO, Princeton University — We have developed a protocol to guide experimentalists to fabricate large disordered hyperuniform two-phase system in two dimensions by binary colloidal particles. In our model, colloidal particles are doped such that it induces dipole-dipole interactions when a magnetic field is applied. We show that despite each component is not hyperuniform, there exists an optimal composition that makes the resulting two-phase system effectively hyperuniform. By changing magnetic fields or the doping level/size of particles, the system can self-organize into tunable structures. Our approach provides a general solution for making large hyperuniform materials in labs in an efficient manner.
**Assembly of gold nanoparticles directed by light polarization**

PANUPON SAMAIMONGKOL, ERICH M SEE, Physics, Virginia Tech, CHERYL L PECK, WEBSTER L SANTOS, Chemistry, Virginia Tech, HANS ROBINSON (Presenter), Physics, Virginia Tech — When polarized light is incident on a small metal nanoparticle, the light intensity at the particle surface is enhanced in two opposite polar regions defined by the polarization direction. By functionalizing the nanoparticles with photosensitive ligands, this intensity distribution can be transferred into permanent surface properties, forming two opposite patches on the particle. Using a ligand that photocleaves to reveal a positively charged amine group, we assemble smaller (15 nm diameter) gold nanoparticles onto the larger (80 nm diameter) functionalized patchy particle. Since all areas of the 80 nm particle are exposed to light, binding can take place in any orientation, but is strongly preferential to the direction set by the polarization of the exposing light, resulting in arrays of oriented nanoparticle assemblies. Interestingly, we also see increased particle binding around the equator of the particle, where light exposure was at a minimum. Possibly, this is due to electrostatic bias in the random walk toward the polar regions being absent around the equator, leading to a relative accumulation of the 15 nm particles in this region.

*This work was in part supported by a grant from the National Science Foundation (DMR-1006753)*

**Acoustokinetics: Organizing Soft Matter with Acoustic Holograms**

MOHammed ABDELAZiZ (Presenter), DAVID G GRIER, New York Univ NYU — Factoring the pressure field of a harmonic sound wave into its amplitude and phase profiles provides the foundation for an analytical framework for studying acoustic forces that not only provides novel insights into the forces exerted by specified sound waves, but also addresses the inverse problem of designing sound waves to implement desired force landscapes. These force landscapes could be used to transport and organize matter on scales from microns to millimeters. We illustrate the benefits of this acoustokinetic framework through case studies of purely nonconservative force fields, standing waves, pseudo-standing waves, and tractor beams.

*This work was supported by the MRSEC program of the National Science Foundation through Award Number DMR-1420073.*
**12:03PM M31.00005: Landau theory of complex spherical packing phases**

SARAH DAWSON (Presenter), DUNCAN MCCLENAGAN, ANCHANG SHI, McMaster Univ — The complex spherical packing phases, including the Frank-Kasper $\sigma$ and A15 phases, appear in a diverse array of soft-condensed matter systems. The universality of these novel ordered structures points to some common underlying physics that can be probed by a suitable Landau theory. The stability of several complex phases was investigated in two theories that are often used to study pattern formation: The Landau-Brazovskii and Ohta-Kawasaki models. Unexpectedly, these phases were found to be stable in the former theory and not the latter. Appropriately scaled, these two free-energy functionals favour periodic modulation of the order parameter at a particular wave number, and differ only in the shape of the free-energy about this value. Motivated by this result, we studied how the shape of the free-energy about its optimal wave number can influence the relative stability of the complex phases over the BCC and FCC spherical phases. This talk is concerned with how these results can inform us of the general mechanisms guiding the formation of the complex spherical phases.

*This research is supported by the Natural Science and Research Council (NSERC) of Canada*

**12:15PM M31.00006: Templated assembly of self-propelled particles in targeted micromachines**

ANTOINE AUBRET (Presenter), JEREMIE PALACCI, University of California, San Diego — In this talk, I will show how we can carve non-equilibrium pathways for the controlled self-assembly of active microparticles using light as a tool. We previously demonstrated the light-triggered self-assembly of self-propelled particles in robust geared micromachines [Aubret et al., Nature Physics 2018]. The gears constitute the fundamental components of synchronized micro-machineries, whose dynamics is tuned by the spins of their internal components. Here, we demonstrate a new approach -tempered assembly- which exploits optical forces and the activity of the colloids to create larger ensembles of self-spinning microgears. Thanks to our approach, the chirality of the gears can be selected and changed over time. It allows us to finely examine the interaction between multiple gears depending on their precise arrangement, and to explore the non-equilibrium interaction potential of the gears, which is due to both hydrodynamics and phoretic phenomena. Our study demonstrate the potential of light to manipulate and image the non-equilibrium interactions between dynamical colloidal architectures.

*This material is based on work supported by the National Science Foundation under Grant No. DMR-1554724. J.P. thanks the Sloan Foundation for support through grant FG-2017-9392.*
12:27PM M31.00007: Synchronization of colloidal oscillators  JINZI HUANG, YAOCHENG DESMOND LI (Presenter), ANTOINE AUBRET, JEREMIE PALACCI, University of California, San Diego — Christiaan Huygens invented pendulum clocks and observed ‘an odd sympathy’ that pendulum clocks hanging on the same wall autonomously synchronize with one another. However, the phenomenon was a mysterious until coupling by the wall was shown to be the driving force for the synchronization. Indeed, interactions between dynamical systems promote synchronization, and we aim to study such phenomena on a micro scale by designing colloidal oscillators. Using self-assembly of microswimmers with passive structures, we develop colloidal clocks that oscillate. We show that pairs of microclocks are able to synchronize with each other, in spite of thermal noise, and compare well with a stochastic model. Further, assemblage of clocks are achieved to study how the clocks can achieve synchronicity in situations of spatial frustration.

12:39PM M31.00008: Development of surface composition and ordering during reverse-emulsion assembly of binary colloidal particle mixtures  CHRISTIAN HEIL (Presenter), THOMAS E GARTNER, ARTHI JAYARAMAN, Chemical and Biomolecular Engineering, University of Delaware — Nanoparticle assembly at a fluid-fluid interface is a proven route to precisely engineer materials with controlled optical properties. In this talk, we will present our recent work using coarse-grained Langevin dynamics simulation that mimics reverse-emulsion directed assembly of binary nanoparticle mixtures into supraballs. We model a binary mixture of silica and synthetic melanin particles in implicit solvent within a shrinking spherical confinement to replicate the shrinking reverse-emulsion droplet. The simulation protocol captures the physics of this process by reproducing the experimental observation of melanin and/or smaller nanoparticles enriching the water-octanol interface. For all mixtures, we observe enrichment of the melanin particles at the supraball surface compared to the supraball interior. This enrichment decreases with increasing melanin/silica size ratio. We observe appreciable crystalline ordering only for systems with similarly sized particles. Particle size dispersity, finite assembly timescale, and curvature of the supraball surface all serve to suppress particle ordering. These findings serve as design rules for tailoring the supraballs for structural color applications and improve our fundamental understanding of particle assembly near curved interfaces.
12:51PM M31.00009: Enhanced Diffusion and Magnetophoresis of Paramagnetic Colloidal Particles in Rotating Magnetic Fields  ZACHARY SHERMAN (Presenter), University of Texas at Austin, JULIA L PALLONE, Massachusetts Institute of Technology, RANDALL M ERB, Northeastern University, JAMES SWAN, Massachusetts Institute of Technology — Dispersions of paramagnetic colloids can be manipulated with external magnetic fields to assemble structures and control transport. For fields held steady in time, the structure and dynamics are coupled, which becomes problematic for processes where aggregation competes against particle transport. Rotating the field direction in time drives dispersions out of equilibrium, allowing the structure and dynamics to be tuned independently to enhance transport. Fundamental transport properties, like the diffusivity and magnetophoretic mobility, dictate a suspension's nonequilibrium response and are crucial to understand to design processes utilizing rotating fields. Here, we investigate the transport properties of paramagnetic colloids in rotating magnetic fields using dynamic simulations. We find that self-diffusion is enhanced in rotating fields compared to steady fields, and that the self-diffusivity in the plane of rotation reaches a maximum value at intermediate rotation frequencies that is larger than the Stokes-Einstein diffusivity of an isolated particle. While the magnetophoretic velocity through bulk fluid decreases with increasing rotation frequency, enhanced in-plane diffusion allows for faster magnetophoretic transport through porous materials in rotating fields.

1:03PM M31.00010: Mesoscale simulation approach for dynamics and assembly of deformable objects  TOLUWANIMI BELLO (Presenter), TEJUS SHAISTRY, SANGWOO LEE, PATRICK UNDERHILL, Rensselaer Polytechnic Institute — In concentrated suspensions, surfactant micelles, emulsion droplets, and microgels often form contacts among the objects leading to nonspherical shapes. In this limit, the dynamics and assembly of the suspension depend more on the interfaces between objects than the bulk objects themselves. This type of deformation of domains also occurs in microphase separation of block copolymer systems. We have adapted a mesoscale approach (called vertex models) in order to apply it to the dynamics and assembly of small deformable objects. In this way, we are developing a unifying framework to understand micelles, emulsions, microgels, and block copolymers. In this talk, we will describe the application of vertex models to small deformable objects. In particular, we have quantified the phase diagram of assembly in thin films of particles (2D simulations) and bulk assembly of particles (3D simulations). A balance of thermal fluctuations and deformability leads to an order-disorder transition in both cases. A unique feature of 3D materials is that multiple ordered states are possible. We have quantified their meta-stability and transitions between ordered states. These transformations are well-known in metallic systems, but have only recently been found in experiments with soft materials.
1:15PM M31.00011: Ordering and Interactions of Gold Nanoparticles (AuNPs) with Fractional Surface Coverage of Ligands*  MORGAN E REIK, CHRIS LIEPOLD, SEAN D GRIESEMER, WEI BU, ALEX SMITH, STUART A RICE, JUAN DE PABLO, Binhua Lin (Presenter), University of Chicago — We studied the properties of self-assembled AuNPs monolayers. These monolayers are formed from solutions with varying thiol concentrations. We show that equilibrium between adsorbed thiols on Au cores and thiols in the bulk solution imply fractional coverage of the Au cores. The equilibrium coverage of AuNPs is adequately described by Langmuir adsorption kinetics, and, therefore, we interpret the way in which varying thiol concentration affects the nanoparticle-nanoparticle interactions as a function of surface coverage of the Au core [1]. We also examine the structure and general shape of the ligand envelope as a function of the surface coverage using molecular dynamics simulation and demonstrate that the equilibrium structure of the envelope and the deformation of that envelope generated by interaction between the AuNPs are coverage-dependent, so that the shape, depth, and position of the minimum of the potential of mean force display a systematic dependence on the ligand coverage [2].


*This research was supported by the UChicago MRSEC (NSF/DMR-1420709). NSF's ChemMatCARS is supported by NSF/CHE-1834750.

1:27PM M31.00012: Divine Proportions and the Fractal Dimension of DLCA Aggregates*  Chris Sorenson (Presenter), Kansas State Univ — Aggregation is a non-equilibrium process of fundamental importance for all dispersed particulate systems. Here I present a restricted hierarchical model of diffusion limited cluster-cluster aggregation (DLCA). The model yields an analytical calculation of the fractal dimensions and self-preserving cluster shapes in two and three spatial dimensions in excellent agreement with those found in nature and simulations. Remarkably the shape is described by the Fibonacci series and the divine proportion in two dimensions and d-dimensional generalization of the Fibonacci series and the divine proportion in three and higher dimensions.

*The author is supported by NSF grant AGS 1649783
1:39PM M31.00013: Polydisperse Gold Nanocrystals and Hard Sphere Diameters* XUN ZHA (Presenter), ALEX TRAVESSET, Iowa State University — A fundamental property of nanocrystals is its hard sphere diameter. In this talk, I will provide a critical discussion on how to compute the diameter, why it is important and in what situations determines the nearest neighbor distance through packing considerations. I will then classify polydisperse nanocrystals of the truncated octahedral family and show that it consists of 351 different types within the size range 1-5nm. I will compute the hard sphere diameter and show how it changes with system size for all these cases. Connections with experiments with 16% polydispersity in alkylthiolated gold nanocrystals, which show crystal fractionalization, will also be discussed.

*This work is funded by NSF, DMR-CMMT 1606336 "CDS&E: Design Principles for Ordering Nanoparticles into Super-crystals". This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562. Our project within XSEDE is supported by grant TG-MCB140071.

1:51PM M31.00014: Effect of Water Vapor on the Pair Potential Between Ligated Nanoparticles* MICHAEL MARTINEZ (Presenter), MIAOCHEN JIN, ALEX SMITH, KEVIN SLATER, LINSEY NOWACK, BINHUA LIN, STUART A RICE, University of Chicago — We have carried out all-atom molecular dynamics simulations to illuminate the physical basis for the change in Young’s modulus of a monolayer of dodecane thiol ligated Au nanoparticles discovered by Wang et al.[1] For a water vapor concentration that would generate 80% monolayer coverage of the nanoparticle surface we find that water molecules form large fluctuating “hemispherical” clusters on the nanoparticle surface with the correct macroscopic contact angle. We have constructed AuNP-AuNP potential curves for both wet and dry systems; the difference in the shapes of these curves near their minima is consistent with the change in Young’s Modulus found by Wang et al. [1] The in vacuum all-atom NP ligand conformations and NP-NP potential agrees well with those previously obtained from united-atom simulations.[2] Additionally, both the wet and dry potential energy curves differ significantly between sampled frozen orientations, implying the possibility of variation in the local NP energy in a self-assembled ordered AuNP array.


*Research supported by the University of Chicago MRSEC (NSF Grant No. DMR-1420709)
2:03PM M31.00015: Ligand Structure and Free Energy of Nanoparticles on Substrates*
MATTHEW PHAM (Presenter), ALEX TRAVESSET, Iowa State University — 2D nanoparticle superlattices are commonly assembled on or transferred to solid substrate supports such as silicon wafers, silica, or graphene. In order to better understand nanoparticles in this context, molecular dynamics simulations were carried out to study the nanoparticle-substrate interactions. Simulations were run using HOODLT/HOOMD-blue to analyze the capping ligand vortices and adhesion free energies of substrate supported gold nanoparticles of various sizes grafted with hydrocarbons of various lengths. The relation of this work to nanoparticle superlattices is also discussed.

*This work is funded by NSF, DMR-CMMT 1606336 "CDS&E: Design Principles for Ordering Nanoparticles into Super-crystals". This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562. Our project within XSEDE is supported by grant TG-MCB140071.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M32 DSOFT DPOLY: Physics of Complex Liquid Interfaces 504 -
Gordon Christopher, Texas Tech Univ - Tag(s): Focus
The dependence of the Laplace pressure, $\Delta P = 2\gamma/R$, on alveolar radius, $R$, means that interconnected alveoli are metastable if $\gamma$ is constant. However, while not generally appreciated in the medical literature, but well known in the foam and emulsion stability literature, the dynamic resistance of an interfacial film to compression can reverse the Laplace instability. The dilatational modulus, $\varepsilon = A \partial \gamma / \partial A$, relates the change in surface tension, $\gamma$, to the change in molecular area, $A$, as the interface is compressed at frequency, $\omega$ (ranging from 1-20 radians/second for normal breathing). If the dilatational modulus is large enough, the resistance to interfacial compression can overcome the Laplace pressure so that the gas pressure in the alveolus no longer increases with decreasing radius. For $(2\varepsilon - \gamma) > 0$, the Laplace pressure decreases with decreasing radius and increases with increasing radius, which reverses the Laplace instability, thereby stabilizing the alveoli against collapse. Under normal conditions, lung surfactant generates conditions such that $(2\varepsilon - \gamma) > 0$, and the lung remains stable. However, during Acute Respiratory Distress Syndrome, trauma or disease leads to a dramatic increase in the concentration of albumin and lysophosphatidylcholine, soluble surface-active molecules that compete for the interface with lung surfactant. Using a newly designed capillary microtensiometer, we have found that increasing concentrations of lysophosphatidylcholines, a product of the inflammation induced degradation of phospholipids, causes the dilatational modulus to decrease as $\omega$ decreases, resulting in $(2\varepsilon - \gamma) < 0$, creating conditions that induce the Laplace instability. This suggests a mechanism underlying ARDS which kills 50,000 people each year with no known cure. Increasing the breathing frequency or decreasing the lysophosphatidylcholine concentration can increase the dilatational modulus and may restore proper lung function in ARDS.

*NIH HL-51177, HL-135065, NSF CBET170378

**11:51AM M32.00002: Solutal Marangoni spreading in the presence of pre-deposited insoluble surfactant monolayers** MADELINE SAULEDA (Presenter), STEPHEN GAROFF, ROBERT TILTON, Carnegie Mellon Univ — Marangoni spreading can be used for pulmonary drug delivery. However, endogenous surfactant in the lung may inhibit that spreading. Here we investigate how the density of pre-existing phospholipid monolayers impacts Marangoni flows induced by exogenous surfactants on a thin fluid subphase. A dipalmitoylphosphatidylcholine (DPPC) monolayer is pre-deposited at a predetermined lateral density on an aqueous subphase before depositing a drop of oleic acid, an insoluble surfactant. Talc tracer particles monitor the extent of spreading, and a trans-illumination method is used to measure the temporal evolution of the subphase surface deformation. This reveals the outwardly moving “Marangoni ridge”. As long as the surface pressure of the DPPC monolayer is less than that of an oleic acid monolayer, spreading proceeds until the surface pressures of the monolayers are equal. The final area per molecule of DPPC in the compressed monolayer is thus the same in each case. The trajectory and degree of interface deformation caused by Marangoni flow are altered by increasing initial DPPC concentration. Unlike Marangoni flow on bare subphases, there is surface flow ahead of the Marangoni ridge as the DPPC monolayer is compressed.
12:03PM M32.00003: Exploring the free energy landscape to predict surfactant adsorption isotherm at nanoparticle-water interface  PAOLO DE ANGELIS (Presenter), ANNALISA CARDELLINI, PIETRO ASINARI, Politecnico di Torino — The long-lasting stability of nanoparticle (NP) suspensions in aqueous solutions is commonly reached by the addition of surfactants. However, a tailored prediction of surfactant concentration enabling a well dispersion of NPs is still an ambitious objective (Cardellini et al., 2019). Here, by coupling Steered Molecular Dynamics (SMD) with the Langmuir theory, we predict the adsorption isotherm of Sodium-Dodecyl-Sulphate (SDS) on α-alumina NP. Beyond the design, our results unveil the role of NP curvature and morphology in the adsorption phenomena at solid-liquid interface. First, the Free Energy Landscapes (FELs) obtained via SMD show the dominance of the entropic contribution by increasing the SDS molecules on target bare NP. Second, a thorough analysis on the FELs, clarifies how the enhanced adsorption deviates from a Markovian dynamics in a curved interface. In fact, both NP curvature and morphology promote modification of the thermodynamics state of adsorption with consequent free energy profiles splitting and the identification of specific sites of adsorption. The proposed modelling framework provides physical insights in the surfactant adsorption onto spherical NPs and suggests guidelines to design NP suspensions in aqueous solutions. (De Angelis et. al, accepted on ACScs).

12:15PM M32.00004: Finite-size line tension effects for nanoparticles at the air-liquid surface*  BRUCE LAW (Presenter), Kansas State Univ, HIROKI MATSUBARA, JO OTSUKA, Chemistry, Kyushu University — The line tension of nanoparticles, at the air-liquid surface, can be deduced by examining the variation in surface tension with nanoparticle bulk concentration. The line tension of dodecane thiol ligated Au nanoparticles at the octadecane-air surface (at 30°C) is found to vary with nanoparticle size. This finite-size line tension effect is qualitatively explained by integrating over the van der Waals contributions to the line tension at the three-phase solid-liquid-air contact line [1].


*BML acknowledges partial support for this work from the American Chemical Society Petroleum Research Fund. H.M. appreciates funding for this work from MEXT/JSPS KAKENHI Grant Number JP 17H02943.

12:27PM M32.00005: Adsorption of nanosheet particles to surfactant-laden interfaces*  NISHAT ANJUM (Presenter), YA-WEN CHANG, Texas Tech Univ — It is known that particles with appropriate wettability spontaneously adsorb to neat water-oil interfaces. The combined effect of particles and surfactants at interfaces, however, is still poorly understood. In this work, we show that selected oil-soluble surfactants promote the adsorption of hydrophilic nanosheet particles and enhance bulk oil-in-water emulsion stability. Using microfluidics, we evaluate interface stability against coalescence and the competitive adsorption dynamics of particles versus surfactant for nanosheets of varying degrees of surface activity.

*Texas tech university and ACS PRF
12:39PM M32.00006: What are the effects of processing conditions on the interfacial viscoelasticity of asphaltene interfaces?  GARRETT COLE, GORDON CHRISTOPHER (Presenter), Texas Tech Univ — Stable crude/water emulsions that form during processing result in the formation of the rag layer, which is a major detriment to petroleum processing. The stability of the rag layer is determined by drop resistance to coalescence. Interfacial asphaltenes and other surface active components create viscoelastic interfaces that inhibit coalescence, resulting in stable rag layers. Although, there have been efforts into studying asphaltene interfaces, there are still many open questions regarding their behavior. In particular, the formation pathway of the asphaltene interface on final interfacial elasticity.

We have examined how large amplitude dilatational strains change the interfacial shear viscoelasticity of asphaltene interfaces. We see changes in viscoelastic moduli that depends on how the interface was formed: adsorption, larger single compression, or multistep small compressions. Interfaces that adsorb show larger viscoelastic moduli than single step compression interfaces, but smaller values than multistep compression. Small interfacial expansions result in minimal changes of the interface, but large expansions significantly disrupt surface structure creating weak interfaces. These results shed important light on how processing of these interfaces may affect rag layers.

12:51PM M32.00007: Pore scale, multi phase flow assessment for industrial applications
MATHIAS STEINER (Presenter), RODRIGO NEUMANN, RONALDO GIRO, MICHAEL ENGEL, IBM Research - Brazil — We report progress of our research of flow analysis at nanometer to micrometer scales for industrial applications. For an investigation of oil recovery at pore scale, digital representations of capillary networks in reservoir rocks are derived from data obtained by applying microscopic computer tomography to representative rock samples. The capillary network representations derived from digital rock are used as geometric boundaries for numerical flow simulations of complex fluids containing water, oil, and additives such as polymers or surfactants. The hierarchical, multiphase flow models deployed in the numerical simulations are calibrated at nanometer scale through molecular dynamics simulations. Importantly, the flow simulations are experimentally verifiable by means of a nanofluidic rock-on-chip measurement platform integrated with semiconductor technology. The laboratory method allows extracting physical parameters that determine surface wetting and capillary flow properties at microscopic scales. The methods developed in our research are more generally applicable to problems of fluid flow in porous media. Their combined application will increase accuracy and enable cost and time reduction in permeability assessment for exploration and production of natural resources.
1:03PM M32.00008: 2D to 3D transition of nanoparticles assembled at the liquid interface

YU CHAI (Presenter), ALYSIA LUKITO, Lawrence Berkeley National Laboratory, JAFFAR HASNAI, ANJU TOOR, University of California, Berkeley, WENQIAN FENG, Lawrence Berkeley National Laboratory, YUFENG JIANG, University of California, Berkeley, JOE FORTH, YUNHUI TANG, HONGHAO HOU, TERESA WILLIAMS, RAVI CHANDRA, DONG LI, Lawrence Berkeley National Laboratory, PHILLIP GEISSLER, University of California, Berkeley, BRETT HELMS, THOMAS RUSSELL, PAUL ASHBY, Lawrence Berkeley National Laboratory — With in situ atomic force microscopy (AFM) imaging, the structure of nanoparticles assembled at the water-oil interface is clearly resolved with the nanometer in 3D. The increase in the surfactant concentration in the oil phase leads to the increase in the contact angle of the nanoparticles at the water-oil interface. Unlike the prediction by equilibrium theory, a 2D monolayer to a 3D multilayer transition of nanoparticles is observed at high surfactant concentrations, which is attributed to the co-existence of completed wetted and partially wetted nanoparticles at the water-oil interface. The contact angle change and structural transition of nanoparticles induced by the increase of surfactant concentration is further confirmed macroscopically by the phase-inversion of Pickering emulsions and anomalous compliance of liquid interface. Our study sheds light on the importance of both thermodynamics and kinetics on the assembly of nanomaterials at the liquid interface and also demonstrate the advantage of using in situ AFM to characterize the assembly of nanomaterials at the liquid interface.

1:15PM M32.00009: Co-surfactant based interfacial strategies for the formation and stabilization of multiple nanoemulsions

TANVI SHETH (Presenter), MATTHEW E. HELGESON, University of California, Santa Barbara — There has been significant recent interest in the production of multiple emulsions – i.e., droplets in droplets – of increasingly small size, especially at the nanoscale. However, the energetic cost of stabilizing many highly curved interfaces makes it challenging to produce and stabilize such multiple nanoemulsions. Here, we propose a general method for promoting and stabilizing complex nanodroplet structures by manipulating their interfacial mechanics through co-surfactants of opposing spontaneous curvature. Using asymmetric pairs of ethoxylated co-surfactants, we experimentally show that this strategy induces the preferential formation of droplets with multiple highly curved interfaces and develop a theoretical framework to predict the observed droplet structures. Using neutron spin echo experiments, we measure the equilibrium dynamics of these ultra-low surface tension systems to determine the effective elastic constants of the mixed surfactant membranes. Using the measured elastic constants, we develop equilibrium interfacial free energy models to quantify conditions under which multiple nanoemulsion structures are stabilized, providing a rational means for engineering co-surfactant systems to promote the formation and stability of multiphase nanodroplets.
1:27PM M32.00010: High-speed X-ray Photon Correlation Spectroscopy studies of dynamics in liquid-liquid extraction systems  DINA SHEYFER (Presenter), QINGTENG ZHANG, TROY DAVID LOEFFLER, JYOTSANA LAL, ERIC DUFRESNE, SURESH NARAYANAN, LYNGA SODERHOLM, SUBRAMANIAN SANKARANARAYANAN, ALEC RUSSELL SANDY, MARK ANTONIO, GREGORY BRIAN STEPHENSON, Argonne Natl Lab — X-ray Photon Correlation Spectroscopy (XPCS) and newly available high-speed X-ray detector systems provide a golden opportunity for shedding new light on a problem of both practical and fundamental importance – the dynamics of fluctuations near critical points in complex fluids. Here, we present a high-speed XPCS study of critical fluctuation dynamics in an important class of complex organic fluids designed for chemical separations. In these liquid-liquid extraction systems, an amphiphilic extractant molecule is used to selectively transfer targeted species from an aqueous phase into an organic phase through the formation of nanoscale molecular complexes. The most efficient extraction typically occurs near a critical point where the correlation length of the complexes becomes large. Our XPCS studies reveal the microsecond dynamics of the molecular assemblies both away from and at the critical temperature $T_c$. The observed fluctuation dynamics can be characterized as a function of $Q$ and $T$ using predictions from the theory of critical phenomena. In particular, we see that the dynamic critical exponent $z$ describing the $Q$ dependence of $\tau \sim Q^{-z}$ changes from 2 to 3 as the critical temperature $T_c$ is approached.

1:39PM M32.00011: Tubulation and dispersion of oil by growth of marine bacteria on oil droplets  VINCENT HICKL (Presenter), GABRIEL JUAREZ, University of Illinois at Urbana-Champaign — The activity of bacteria on surfaces exhibits collective behaviors such as active turbulence and active stresses, which result from motility or growth and interactions with the local surroundings. Here, we describe experimental observations on the emergence of tubular structures resulting from the growth and division of rod-shaped bacteria on the liquid interface of oil droplets. Using microfluidics and time-lapse microscopy, we quantify the dimensions and growth rates of individual tubular structures as well as the bulk biofilm formation on hundreds of droplets over 72 hours. We find that the length of tubular structures is comparable to the initial droplet radius and that they are composed of an outer shell of bacteria that stabilize an inner filament of oil. The oil filament undergoes breakup into smaller microdroplets dispersed within the bacterial shell, where the average radius of the dispersion is described by the most unstable Plateau-Rayleigh wavelength. This work provides insight into active stresses at deformable interfaces and improves our understanding of microbial oil biodegradation and its potential influence on the transport of oil droplets in the ocean water column.
1:51PM M32.00012: Effect of polymer topology on the structure and dynamics of block copolymers at Liquid/Liquid Interfaces*  KUN QIAN (Presenter), MESFIN TSIGE, Univ of Akron — The behavior of molecules such as polymers at liquid/liquid interfaces is both scientifically and technologically important and has been the focus of much attention in recent years given the various types of materials that have been successfully assembled at liquid/liquid interfaces. Polymers do assemble in various ordered aggregates at liquid/liquid interfaces and understanding the effect of polymer topology on the overall behavior of a given polymer at surfaces and interfaces and especially at liquid/liquid interfaces is very important. Molecular dynamics simulations using a bead-spring model on representative block copolymer architectures at immiscible liquid/liquid interfaces have been carried out. The results of our detailed investigation on the structure and dynamics of the block copolymers at the interface will be presented and discussed.

*This work has been funded by NSF DMR-1912329.

2:03PM M32.00013: A novel method for interfacial rheology using an indirect interfacial rheometer  IAIN MUNTZ (Presenter), JOB H. J. THIJSSEN, Univ of Edinburgh — We have developed a system for performing interfacial rheology without attaching a probe directly to the interface itself. This indirect rheology is motivated by the applications of Pickering type systems, where rather than shear being applied directly to an interface, one of the continuous phases is sheared. The behaviour of the system as a whole is then governed, in part, by the rheology of that interface.

We use this setup to measure flow curves in a system of poly(methyl methacrylate) particles at a water/dodecane interface. The lack of a direct probe ensures two things: 1) we avoid substantial pre-shearing and 2) the response measured is due to the interface itself and not the probe [1]. In this indirect setup a shear is applied to the upper oil phase using a standard stress controlled rheometer. The response of the interface is then measured by confocal microscopy. A range of rheological behaviour is observed dependent on surface coverage, shear rate and surface structure. The direct visualisation of the interface allows all of these input parameters to be measured and various flow curves can be produced to observe their effect on the rheology of the interface.


Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M33 DSOFT GSNP: Kinetic Theory and Its Applications in the Physical, Biological and Social Sciences 505 - Tag(s): Focus
11:15AM M33.00001: Kinetic theory of defect dynamics in active nematics* [Invited] M CRISTINA MARCHETTI (Presenter), University of California, Santa Barbara — Active nematics are fluids of elongated active agents that exhibit self-sustained flows and liquid crystalline order. Realizations include suspensions of cytoskeletal filaments and motor proteins, epithelial tissue, and vibrated layers of granular rods. At high activity, active nematics exhibit spatio-temporal chaotic, turbulent-like flows with proliferation of topological defects. In this talk I will show that, focusing on the defects as the relevant quasiparticles driving the non-equilibrium dynamics, we can formulate a kinetic theory of the active defect gas and describe the onset of active turbulence as activity-driven defect unbinding. By coarse-graining the kinetic theory, we obtain a hydrodynamic description of the active defect gas.

*This work was supported by NSF award DMR-1609208.

11:51AM M33.00002: Kinetic theory for financial Brownian motion: a microscopic model based on forex data analysis and its mean-field theory* [Invited] KIYOSHI KANAZAWA (Presenter), Univ of Tsukuba — Kinetic theory is a powerful mathematical framework in statistical physics and has been applied to understand physical Brownian motions from their microscopic setups. In light of this success, it is an interesting attempt to extend kinetic theory for various social phenomena beyond physics. In particular, we have focused on its application to financial markets since they exhibit random motions quite similar to physical Brownian motion. In this presentation, we will show our recent kinetic approach (K. Kanazawa et al., PRL 2018; PRE 2018) to financial Brownian motion in the context of high-frequency data analyses. First, we have analyzed trading log data of individual traders, to identify the microscopic dynamics in a forex market. The proposed microscopic model of the financial market is then solved systematically via the kinetic theory: we derive the Liouville equation, the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy, the Boltzmann equation, and the Langevin equation for the financial market as a parallel mathematical program to conventional kinetic theory. Our work highlights the potential power of kinetic theory to understand social phenomena from their microscopic dynamics.

*This work was supported by the Japan Society for the Promotion of Science KAKENHI Grants No. 16K16016.
12:27PM M33.00003: A generalization of the Glansdorff-Prigogine criterion for stability based on information geometry and thermodynamic uncertainty relationships*  
SOSUKE ITO (Presenter), Universal biology institute, The University of Tokyo — To consider the relationship between the excess entropy production and the Fisher information of time, we have generalized the Glansdorff-Prigogine criterion for stability. In information geometry, the Fisher information of time is the speed of a statistical manifold, and then our generalized criterion can be interpreted as a criterion by acceleration (deceleration) of this speed. If this speed is accelerated (decelerated), dynamics is unstable (stable).

Our generalization does work even for chemical kinetics driven by the non-linear master equation (e.g., the autocatalytic reaction), where the Glansdorff-Prigogine criterion does not work well. Moreover, our generalization is connected to the recent progress of thermodynamic uncertainty relationships (TURs), and we can quantitatively discuss the stability of dynamics based on TURs.

*This research is supported by JSPS KAKENHI Grant No. 19H05796 and JST Presto Grant No. JP18070368, Japan.

12:39PM M33.00004: Pattern Selection of Shallow Suspensions of Shrimp  
ANDREA WELSH (Presenter), KRISHMA SINGAL, DIVYA VELIVELA, ELLIE FINCH, MICHAEL BARNHILL, FLAVIO H FENTON, Georgia Inst of Tech — Swarming, a self-organization phenomenon which occurs in many biological systems, can emerge spontaneously, arising without any sort of centralized control or leadership. Many crustaceans, such as brine shrimp, produce swarms, in which individuals cluster together rather than spreading out uniformly in their environment. The motion of these crustaceans is also affected by light due to their phototactic nature. The size and distribution of these swarms are governed by local interactions between individuals but are also affected by the boundaries of the container. We discuss the three-dimensional patterns that can be observed in brine shrimp swarms, specifically of the Great Salt Lake strain of *Artemia franciscana*, at high concentration. We experimentally test the effects of average concentration, temperature, and container size on the basic length and times scales of the patterns, the type patterns selected, and the stability of those patterns. We then discuss the physical mechanism behind the formation and selection of these patterns.
**12:51PM M33.00005: Hydrodynamics of Active Lévy Matter**
ANDREA CAIROLI (Presenter), CHIU FAN LEE, Imperial College London — Collective ordered motion is often modeled within the framework of active fluids, where hydrodynamic descriptions typically rely on microscopic models of active self-propelled particles subjected to alignment interactions and reorientational dynamics. However, single-particle superdiffusion is also widespread in biology as it can represent an optimal search strategy for living organisms. Nevertheless, the collective properties of interacting systems exhibiting such anomalous diffusive dynamics -- denoted here as active Lévy matter -- cannot be captured by current active fluid theories. Here, we formulate the hydrodynamic description of active Lévy matter by coarse-graining a microscopic model of alignment interacting active particles performing superdiffusion manifest as Lévy flights. This theory predicts characteristic disordered and ordered phases. Linear stability analysis suggests that the phase transition can be critical. This analysis highlights the need for more realistic models of active matter integrating both anomalous diffusive motility and inter-particle interactions and suggests that these models can shed new light on the universal properties of active systems.

*Dr. Andrea Cairoli acknolewdges funding of the Royal Commission for the Exhibition of 1851.

**1:03PM M33.00006: Towards a statistical mechanics of chiral active gases**
MING HAN (Presenter), MICHEL FRUCHART, COLIN SCHEIBNER, SURYANARAYANAN VAIKUNTANATHAN, WILLIAM THOMAS MARK IRVINE, JUAN DE PABLO, VINCENZO VITELLI, University of Chicago — Statistical mechanics allows to describe materials near equilibrium using just a few thermodynamic variables. Extending this approach far-from-equilibrium is tempting but often unfeasible. In this talk, we present the footprints of a statistical mechanical treatment of chiral active fluids composed of self-spinning particles. The nature of self-spinning breaks time-reversal symmetry and detailed balance. Nevertheless, such active fluids converge to a non-equilibrium steady state exhibiting Boltzmann statistics with a universal effective temperature determined by the active torques. Beyond exhibiting analogues of common thermodynamic properties, the chiral active gas also displays a dissipation-less odd viscosity in addition to the shear viscosity. Both transport coefficients satisfy a Kubo relation in terms of our effective temperature. We show that the stochastic dynamics of this many body system can be represented as a chiral Brownian motion in shear-stress space. Using this assumption, we derive analytically the full frequency dependence of the viscosities in agreement with simulations.
1:15PM M33.00007: Hydrodynamic memory and driven microparticle transport: hedging against fluctuating sources of energy* SEAN SEYLER (Presenter), STEVE PRESSÉ, Physics, Arizona State University — In a viscous fluid, the motion of an accelerating particle is retained as an imprint on the vorticity field, giving rise to the famous $t^{-3/2}$ decay of the velocity autocorrelation. For nonuniform particle motion at low Reynolds number, this hydrodynamic memory effect is captured by the Basset-Boussinesq-Oseen (BBO) equation, which can be derived from various physical perspectives, including (fluctuating) hydrodynamics and kinetic theory. Moreover, finite-temperature dynamics can be modeled by using fluctuation-dissipation to reincorporate (correlated) thermal noise, turning BBO into a generalized Langevin equation. In this work, we numerically solve the BBO equation to simulate driven microparticles and show that hydrodynamic memory generally reduces transport friction, particularly when driving forces do not vary smoothly. Remarkably, this enables coasting over uneven potentials that otherwise trap particles modeled by pure Stokes drag. Our results are germane to questions surrounding intracellular transport efficiency and, more generally, provide direct physical insight into the role of particle-fluid coupling in microparticle transport.

*Supported by ARO Grant No. W911NF-17-1-0162.

1:27PM M33.00008: Cargo transport by dissipative solitons-director bullets in nematics* BINGXIANG LI (Presenter), RUI-LIN XIAO, SERGIJ V SHIYANOVSII, OLEG D LAVRENTOVICH, Chemical Physics Interdisciplinary Program; Advanced Materials and Liquid Crystal Institute, Kent State Univ - Kent — An alternating current (AC) electric field applied to a uniformly aligned nematic liquid crystal is capable to excite and drive particle-like three-dimensional dissipative solitons, the so-called director bullets [1, 2]. The bullets represent regions of a distorted molecular orientation of broken left-right or head-tail symmetry that propagate perpendicularly to the driving field. Here, we demonstrate that the bullets can be generated around colloidal spheres with both tangential and radial anchoring, dispersed in the nematic. The effect represents a soliton-mediated liquid crystal-enabled electrophoresis, in which the electric field first breaks the quadrupolar symmetry of the director field around the sphere and then drives oscillations of this asymmetric director field to power a directional motion of the sphere dressed in the soliton. The effect can be used to transport microscopic cargo when modes of liquid crystal-enabled electrotokinetics based on static asymmetry are ineffective, which is the case of tangentially anchored inclusions.


*The work was supported by NSF grant DMR-1905053.
1:39PM M33.00009: Brownian motion in confinement  MAXIME LAVAUD (Presenter), Laboratoire Ondes et Matière d'Aquitaine, CNRS, PIERRE SOULARD, PSL Research University : UMR7083, ESPCI, Gulliver, VINCENT BERTIN, DAVID DEAN, Laboratoire Ondes et Matière d'Aquitaine, CNRS, RAPHAEL SARFATI, Department of Chemical and Biological Engineering, Boulder, ELIE RAPHAEL, PSL Research University : UMR7083, ESPCI, Gulliver, YANN LOUYER, THOMAS SALEZ, YACINE AMAROUCHENE, Laboratoire Ondes et Matière d'Aquitaine, CNRS — Brownian motion in confinement is a paradigm for numerous biological situations. Here, we study the diffusion of micrometer-sized beads in water confined between two walls that are separated by a micrometric distance. Using holographic microscopy, we track the particles in three dimensions with a precision approaching the nanometric range. From statistical analysis performed on the individual trajectories, we extract the local diffusion coefficient as a function of the position of the bead in the microcavity. The experimental results are in good agreement with the numerical and analytical predictions — which paves the way towards the study of other situations of confinement, such as soft boundaries.

1:51PM M33.00010: Superdiffusion and diffusion in active matter using a stochastic field theory*  PATRICK UNDERHILL (Presenter), PETER R KRAMER, Rensselaer Polytechnic Institute — One important impact of the out-of-equilibrium nature of active matter is the enhanced fluctuations in the system and the mixing of passive tracers. Interesting properties arise in both small and large concentrations of the active objects. Agent based models can incorporate fluctuations and interactions, but are limited to smaller systems. It can also more difficult to extract physical insight from the results. One of the most successful alternative approaches has been a mean field theory. However, in some situations the mean field theory makes predictions that differ significantly from experiments and direct (agent or particle based) simulations. There are also some quantities that cannot be calculated by the mean field theory. In this talk, we will describe our new approach which uses a stochastic field to overcome the limitations of the mean field assumption. The characteristic superdiffusion observed for passive tracers can be computed along with the longtime diffusivity. We will describe how this enhanced diffusion depends on the characteristics of the active particles and their hydrodynamic interactions.

*We acknowledge support from NSF Grant No. DMS-1211665
M33.00011: Disordered hyperuniform state of circularly swimming algae* MINGJI HUANG (Presenter), Shanghai Jiao Tong Univ, WENSI HU, East China Normal University, SIYUAN YANG, Shanghai Jiao Tong Univ, QUAN-XING LIU, East China Normal University, HEPENG ZHANG, Shanghai Jiao Tong Univ — Active matter comprises of individual units that convert locally stored energy into mechanical motion. Interactions between active units can lead to a wide range of collective phenomena, which do not exist in equilibrium systems. Here we show that density fluctuations in active system can be greatly suppressed. Our experiments are carried out with marine algae (*Symbiodinium voratum*). Cells swim in circles at interface and long-ranged nature of hydrodynamic interactions suppresses density fluctuations; disordered hyperuniform state is observed over a wide range of conditions. Emergence of hyperuniformity can be quantitatively reproduced in a numerical model whose main ingredients are hydrodynamic interactions and uncorrelated random cell motion. Our results demonstrate a new form of collective state in active matter and suggest the possibility to use hydrodynamic flow to assemble active matter into hyperuniform states.

*We acknowledge financial supports of the NSFC (No. 11422427, 11402069), the Program for Professor of Special Appointment at Shanghai Institutions of Higher Learning (No. SHDP201301), the Innovation Program of Shanghai Municipal Education Commission (No. 14ZZ030), and government of Shenzhen (Grant No. KQCX20140521144102503).

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M34 DSOFT GSNP DCOMP: Machine Learning in Nonlinear Physics and Mechanics 506 - Shmuel Rubinstein, Harvard University - Tag(s): Focus

11:15AM M34.00001: Learning the onset of frictional motion [Invited] YOHAI BAR-SINAI (Presenter), Google Research — The onset of frictional motion is a central process in modeling mechanical phenomena, from squeaking hinges to catastrophic earthquakes. The processes involved in it are complex and to a large extent not understood. Specifically, the simple notion of "static friction coefficient" is most probably not a well-defined material parameter, as experiments show that it is variable, even for a single interface under carefully controlled experimental conditions. I will show that, in a well-controlled laboratory setup with detailed interfacial measurements, relatively simple linear models can explain much of the observed variance, indicating that a significant portion of the uncertainty is non-stochastic and is encoded in the frictional interface. In addition, I will discuss recent data-driven efforts in predicting the onset of frictional motion in geophysical faults, i.e. earthquake forecasting, which is a long-standing and very challenging problem. However, the confluence of new kinds of measurements and advances in machine learning offers new and promising directions.
11:51AM M34.00002: Detecting Depinning and Nonequilibrium Transitions with Unsupervised Machine Learning*  DANIELLE MCDERMOTT (Presenter), Pacific Univ, CYNTHIA REICHHARDT, CHARLES REICHHARDT, Los Alamos National Laboratory — Using numerical simulations of a model disk system, we demonstrate that a machine learning generated order parameter can detect depinning transitions and different dynamic flow phases in systems driven far from equilibrium. We specifically consider monodisperse passive disks with short range interactions undergoing a depinning phase transition when driven over quenched disorder. The machine learning derived order parameter identifies the depinning transition as well as different dynamical regimes, such as the transition from a flowing liquid to a phase separated liquid-solid state that is not readily distinguished with traditional measures such as velocity-force curves or Voronoi tessellation. The order parameter also shows markedly distinct behavior in the limit of high density where jamming effects occur. Our results should be general to the broad class of particle-based systems that exhibit depinning transitions and nonequilibrium phase transitions.

*This work was supported by the US Department of Energy through the Los Alamos National Laboratory, the M. J. Murdock Charitable Trust, and the Notre Dame Center for Research Computing.

12:03PM M34.00003: Machine Learning and Benchtop Experiments  SHMUEL RUBINSTEIN (Presenter), Harvard University — Machine learning has generated much recent excitement within the physics community and provides a powerful new tool to analyze and understand many physical systems. However, in the experimental study of complex physical systems, the usage of machine learning is still in its infancy. Specifically, it is not obvious which scientific questions are susceptible to machine learning disruption and, even more interesting, which questions are not? In this talk, I will address our approach to these questions, sharing our attempts to leverage lab models of complex systems for this study. I will discuss our tactics to holistically amalgamate experiments with simulations.

12:15PM M34.00004: Supervised Autoencoder for Inverse Kirigami Design  PAUL HANAKATA, Harvard University, EKIN DOGUS CUBUK (Presenter), Google Inc., DAVID K CAMPBELL, HAROLD S. PARK, Boston University — Recently, machine learning (ML) methods have shown successes in predicting mechanical properties of composite materials as a forward solver. While ML approach is much faster than the conventional physics-based solvers (e.g. molecular dynamics), most current ML techniques need to screen the entire library in order to perform inverse design. Thus, this approach might no longer be practical for a system with a very large design space. Here, we use a supervised-autoencoder (sAE) to perform inverse design in graphene kirigami where predicting ultimate stress or fracture point is known to be difficult due to nonlinear effects arise from the out-of-plane buckling. Unlike the standard autoencoder, our sAE is not only able to reconstruct cut configurations but also to predict mechanical properties of graphene kirigami and classify graphene kirigami with either parallel or orthogonal cuts. Furthermore, we find that by interpolating different configurations the sAE is able to generate new designs consisting of mixed parallel and orthogonal cuts while only being trained with kirigami structures with parallel and orthogonal cuts. This allows us to design and optimize materials in the latent space, which is more efficient than to perform optimization in the original representation.
12:27PM M34.00005: Softness Correlations in Low-Temperature Supercooled Liquids*
RAHUL CHACKO (Presenter), James Franck Institute, University of Chicago, FRANÇOIS P LANDES, AO Team, Laboratoire de Recherche en Informatique, GIULIO BIROLI, Laboratoire de Physique, École normale supérieure, OLIVIER DAUCHOT, Laboratoire Gulliver, École supérieure de physique et de chimie industrielles de la Ville de Paris, ANDREA JO-WEI LIU, Department of Physics and Astronomy, University of Pennsylvania, DAVID REICHMAN, Department of Chemistry, Columbia University — Local structure is known to play a dominant role in determining where structural relaxation occurs [1,2]. This can be quantified using a machine learning approach, yielding a linear model mapping local structure to "softness", a quantity that predicts the propensity of a particle to rearrange [3]. We find that this machine-learned weighted integral of the pair correlation function, when trained on an athermal system relaxing under gradient descent, performs surprisingly well when predicting the dynamics of a supercooled liquid. We use swap Monte Carlo [4] to study the evolution of the spatial correlation of the so defined softness, down to deeply supercooled temperatures. We then compare this length scale to other length scales that have been identified in the literature.


*This work was funded by the Simons Collaboration “Cracking the glass problem” via 454935 (GB), 327939 and 454945 (AJL), 454951 (DR) and 348126 (SRN).

12:39PM M34.00006: Data-driven inference of thermodynamic properties from non-equilibrium stochastic fluctuations YOON JUNG (Presenter), JUNANG LI, NIKTA FAKHRI, Massachusetts Institute of Technology MIT — Living systems are driven out of equilibrium via an input of cellular chemical energy, part of which is dissipated into the environment. For systems that exhibit non-equilibrium steady states, thermodynamic fluctuations encode signatures that can be used to infer properties of the system. For example, model-based approaches can be used to quantify how far the system is from equilibrium by measuring the dissipation rate. Here, we present a data-driven approach for inferring system properties based on scattering transforms. The method utilizes symmetries arising from the stationary nature of stochastic fluctuations which allows solving inverse problems with fewer measurements. The results from simulations and experimental data demonstrate that the proposed approach serves as an effective method to infer system properties from thermodynamic fluctuations in living systems.
12:51PM M34.00007: Inverse learning of material physics through in-situ image data and continuum modeling  HONGBO ZHAO (Presenter), Massachusetts Institute of Technology MIT, BRIAN D STOREY, Toyota Research Institute, RICHARD BRAATZ, MARTIN BAZANT, Massachusetts Institute of Technology MIT — With the availability of microscopic spatio-temporal image data of materials, there is a tremendous amount of hidden information about the material properties. Using a framework of PDE-constrained optimization, we demonstrate that multiple constitutive relations can be extracted simultaneously from a small set of images of pattern formation. Examples include state-dependent properties such as the diffusivity, kinetic prefactor, free energy, and direct correlation function in the Cahn-Hilliard equation, Allen-Cahn equation, or dynamical density functional theory (Phase-Field Crystal Model). Compared to the data-driven modeling approach and the recent work on PDE discovery, our approach provides clear physical interpretability by prescribing a general governing equation while achieving a high expressive power through nonlinear and/or nonlocal (integro-differential) constitutive relations. We demonstrate that the inversion technique can be applied to experimental images of lithium-iron phosphate (LFP) particles. By mapping the evolution of lithium concentration in the particles during charge and discharge, we are able to extract its free energy and reaction kinetics, which are difficult to obtain through traditional electrochemical measurements alone due to phase separation.

1:03PM M34.00008: Using Machine Learning to analyze Defect Annihilation Dynamics in Smectic C films*  MATTHEW GLASER (Presenter), ERIC MINOR, STIAN HOWARD, ADAM GREEN, CHEOL PARK, NOEL ANTHONY CLARK, Physics and Soft Materials Research Center, University of Colorado Boulder — We demonstrate a method for training a convolutional neural network with simulated images for usage in the study of topological defect annihilation in freely-suspended SmC liquid crystal films. Modern machine learning methods require large, robust training data sets to generate accurate predictions. Generating these training sets requires a significant up-front time investment that is often impractical for small-scale applications. Here we demonstrate a ‘full-stack’ computational solution, where the training data set is generated on-the-fly using a noise injection process to produce simulated data characteristic of the experimental system. The experiment requires accurate observations of both the spatial distribution of the defects and the total number of defects at every time step, making it an ideal system for testing the robustness of the trained network. The fully trained network was found to be comparable in accuracy to identifying the defects by hand, with a four-orders of magnitude improvement in time efficiency.

*This work was supported by NASA Grant No. NNX-13AQ81G and NAG No. NNX17AC74G and by the Soft Materials Research Center under NSF MRSEC Grant No. DMR-1420736.
1:15PM M34.00009: Experimental Realization of Reservoir Computing with Wave Chaotic Systems*  SHUKAI MA (Presenter), THOMAS M ANTONSEN, EDWARD OTT, SARTHAK CHANDRA, STEVEN ANLAGE, University of Maryland, College Park — The execution of machine learning (ML) software largely depends on the computing `substrate', which is often not optimized for running ML tasks. The invention of ML-tailored hardware may greatly improve the computing speed and power efficiency. Photonic devices are well-suited for ML due to the parallelism of light. Reservoir computing (RC) is essentially a one-layer neural network (NN) with nonlinear connections, but radically simpler than NN since only the coupling between the reservoir nodes and outputs is trained. Thus RC is well-suited for physical realizations. Here we utilize the complicated wave dynamics inside a chaotic-shaped overmoded electromagnetic cavity containing nonlinear elements to emulate the complex dynamics of an RC. We propose unique techniques to create virtual RC nodes by both frequency stirring and spatial perturbation. The computational power of the wave chaotic RC is experimentally demonstrated with the so-called observer task, where we predict the future evolution of chaotic Rossler y(t) and z(t) time series using the x(t) series as the input. Different tasks are executed with a single RC physical device by simply switching output couplers.

*This work is supported by ONR Grants No. N000141512134, No. N000141912481, and AFOSR COE Grant FA9550-15-10171.

1:27PM M34.00010: Chaotic source separation solved by a tank of water through invertible generalized synchronization*  ZHIXIN LU (Presenter), JASON KIM, DANIELLE BASSETT, University of Pennsylvania — Statistical methods such as independent component analysis and principal component analysis were proposed to separate a set of source signals from a mixed signal by assuming the statistical independence of sources. Here, we focus on chaotic source separation where the sources are chaotic systems. We assume that one has no knowledge about the governing equations of the source signals, and that the mixed signal is simply the sum of the sources. From the perspective of dynamical systems, we propose a supervised learning framework that can solve this problem through an intermediate dynamical system. To demonstrate the power of this framework, we employ a simulated tank of water as the intermediate system, and train it to regenerate chaotic signals from a mixed signal that is the sum of any 2 chaotic trajectories from 6 chaotic systems. We elucidate the underlying mechanism as constructing a nonlinear state-observer utilizing the concept of invertible generalized synchronization. We predict that it is impossible to perfectly separate the chaotic sources if the two sources systems are governed by the same dynamical equations.

*ZL, JZK, and DSB acknowledge support from the Army Research Office (Grafton-W911NF-16-1-0474).
1:39PM M34.00011: The Dependence of Reservoir Computing on System Parameters*
LOUIS PECORA (Presenter), THOMAS L CARROLL, United States Naval Research Laboratory — Reservoir computing (RC) has become an interesting topic for the nonlinear Dynamics field. More so because despite many demonstrations of RC abilities the actual dynamical reasons RCs work is still not well understood. We examined several aspects of RC using fitting and prediction of signals as a benchmark. Among the parameters we explored [1] were network heterogeneity of link weights, existence of symmetries in the networks, variations of node parameters and vector fields, and spectral radius of the network. One important result is that the number of independent signals that can be used from a driven RC is limited and independent of the number of nodes above a certain vertex number.

authors:

*Office of Naval Research

1:51PM M34.00012: Reduced network extremal ensemble learning (RenEEL) scheme for community detection in complex networks*
KEVIN E. BASSLER (Presenter), JIAHAO GUO, PRAMESH SINGH, Department of Physics and TcSUH, Univ of Houston — We introduce an ensemble learning scheme for community detection in complex networks. The scheme uses a Machine Learning algorithmic paradigm we call Extremal Ensemble Learning. It uses iterative extremal updating of an ensemble of network partitions, which can be found by a conventional base algorithm, to find a node partition that maximizes modularity. At each iteration, core groups of nodes that are in the same community in every ensemble partition are identified and used to form a reduced network. Partitions of the reduced network are then found and used to update the ensemble. The smaller size of the reduced network makes the scheme efficient. We use the scheme to analyze the community structure in a set of commonly studied benchmark networks and find that it outperforms all other known methods for finding the partition with maximum modularity.

*This work was supported by the NSF through grants DMR-1507371 and IOS-1546858. Some of the computations were done on the uHPC cluster at the University of Houston, acquired through NSF grant 1531814.
2:03PM M34.00013: Visualizing statistical models in Minkowski space: an analytical coordinate embedding*  HAN KHENG TEOH (Presenter), Cornell University, KATHERINE QUINN, Princeton University, COLIN B CLEMENT, JARON KENT-DOBIAS, QINGYANG XU, JAMES PATARASP SETHNA, Cornell University — Dimensionality reduction techniques are often used to provide a lower dimensional description of high dimensional data. Quinn et. al [1] proposed an intensive isometric embedding, InPCA in visualizing probabilistic models manifold with the Bhattacharyya distance. It was observed that the InPCA manifolds form a hierarchy of cross-sectional spans that shrinks geometrically in Minkowski space, allowing the use of only a few principal components to capture most of the variation. Here, we show that for a large class of multiparameter models that takes the form of exponential families, a different intensive embedding- the isKL embedding, built on symmetrized Kullback Liebler divergence generates an explicitly and analytically tractable embedding in a Minkowski space of dimension equal to twice the number of parameters. In principle, this technique not only offers a great dimensionality reduction, it also allows one to uncover a hidden exponential family that describes an experiment or a simulation if the isKL embedding gives a cutoff after N+N dimensions. We will discuss the optimization of isKL embedding in producing a good visualization with several statistical models.


*This work was supported by ARO W911NF-18-1-0032 and NSF DMR-1719490.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M35 GMAG: Novel Functional Magnetic Materials and Structures 507 - Shinji Miwa, Univ of Tokyo
11:15AM M35.00001: Interplay of local moment and itinerant magnetism in cobalt-based Heusler ferromagnets: Co$_2$TiSi, Co$_2$MnSi and Co$_2$FeSi* GUANHUA QIN (Presenter), University of Missouri, WEI REN, Shanghai University, DAVID SINGH, University of Missouri — Heusler ferromagnets based on Co are important materials for spintronics due to the exceptional combinations of high Curie temperature and strong spin polarization. We investigate the electronic structure, magnetism and spin excitations in the cobalt-based full Heusler compounds, Co$_2$TiSi, Co$_2$MnSi and Co$_2$FeSi using first principles calculations. Co$_2$TiSi and Co$_2$MnSi are half-metals, while Co$_2$FeSi is not. The trends in the Curie temperature of Co$_2$MnSi and Co$_2$FeSi are well reproduced by the calculated spin wave dispersions. Remarkably, Co$_2$TiSi is a very itinerant magnet, while both Co$_2$FeSi and Co$_2$MnSi show local moment behavior regarding the Fe and Mn, while retaining the itinerancy of the Co magnetism. Although our results do not support the half-metallic character proposed for Co$_2$FeSi, consistent with the reported high Curie temperature, we find a very strong positive transport spin polarization, which combined with the large moment, cubic structure and high Curie temperature supports the further investigation of Co$_2$FeSi as a material for spintronic applications.

*Work at the University of Missouri is supported by the Department of Energy, Award Number DE-SC0019114.

11:27AM M35.00002: Effect of V substitution on structural, magnetic, transport and mechanical properties of the half-metal-type Heusler alloy Co$_2$FeGe* RABIN MAHAT (Presenter), SHAMBHU K KC, Physics and Astronomy, University of Alabama, DANIEL WINES, Physics, University of Maryland Baltimore County, SUDHIR REGMI, UPAMA KARKI, Physics and Astronomy, University of Alabama, FATTIH ERSAN, CAN ATACA, Physics, University of Maryland Baltimore County, ARUNAVA GUPTA, Chemistry and Biochemistry, University of Alabama, PATRICK LECLAIR, Physics and Astronomy, University of Alabama — Half-metallic ferromagnets are ideal candidates for spintronic applications due to their ∼100% spin polarization. High Curie temperature $T_c$ is one of the important prerequisite from the application point of view. Co$_2$Fe- based Heusler alloys in L$_{21}$ structure have attracted great interest for this reason. We present a combined experimental and theoretical study of quaternary Heusler alloys Co$_{2-x}$V$_x$FeGe and Co$_2$Fe$_{1-x}$V$_x$Ge (0 ≤ x ≤ 1) as promising candidates for spintronic applications. Single phase microstructures for arc-melted alloys are observed for V substitution for Co from x = 0.25 to x = 0.625, but when V substitutes for Fe only x = 0.25 and 0.375 yield single phase microstructures. All single phase samples show fcc structures with L$_{21}$ ordering, corroborated by X-ray diffraction. Low-temperature saturation magnetic moments agree well with our theoretical results and obey the Slater-Pauling rule, a prerequisite for half metallicity. All alloys are soft ferromagnets with high $T_c$'s, allowing for applications at room temperature and above. Transport measurements are performed to elucidate the electronic structure of the alloys. Relatively high mechanical hardness values are also observed.

*NSF DMREF Grant number 1235396, NSF DMR Grant number 1508680 and NSF DMR Grant number 1726213.
11:39 AM M35.00003: Half-metallicity in CrAl-terminated \( \text{Co}_2\text{CrAl} \) thin film  
JULIANA C. HERRAN, Université de Franche-Comté, RYAN CARLILE, University of Northern Iowa, PARASHU R. KHAREL, South Dakota State University, PAVEL LUKASHEV (Presenter), University of Northern Iowa — Half-metals with high Curie temperature are ideal candidates for applications in spintronics. Many half-metallic materials have been predicted theoretically, and some have been confirmed experimentally. At the same time, in thin-film geometry the electronic structure of these materials may change due to the potential presence of surface/interface states, which could limit practical applications of these materials in nano-size devices. Here, from first principles we study a full Heusler compound, \( \text{Co}_2\text{CrAl} \) in thin film geometry. This material has been studied extensively, and it has been reported that it exhibits half-metallic properties in the bulk. We show that this material retains 100% spin polarization in CrAl-terminated thin film geometry (Co-termination results in destroyed half-metallicity) as well. Moreover, we confirm that under biaxial strain \( \text{Co}_2\text{CrAl} \) retains half-metallicity for a practically feasible range of considered pressure. The magnetic alignment of \( \text{Co}_2\text{CrAl} \) is confirmed to be ferromagnetic, with the non-integer total magnetic moment of Co-terminated cell, and the integer total magnetic moment of CrAl-terminated cell. If confirmed experimentally, these results may have an important impact in spin-based electronics.

11:51 AM M35.00004: Anomalous Hall effect in a two sub-lattice ferrimagnet.  
NISHCHAL THAPA MAGAR (Presenter), DINA MICHEL, NIRMAL GHIMIRE, Department of Physics and Astronomy, George Mason University — The anomalous Hall effect (AHE) is a characteristic of ferromagnets where a finite Hall effect proportional to the magnetization appears in zero external magnetic field. It is now known that the AHE can also arise in non-collinear and non-coplanar antiferromagnets due to spin chirality and in materials consisting of topologically non-trivial electronic structure such as Weyl semimetals. Here we will present the observation of an anomalous Hall effect in a hexagonal ferrimagnet TbMn\(_6\)Sn\(_6\) consisting of two spin sub-lattices due to Mn and Tb ordering. Both spin sublattices order simultaneously above room temperature and show a spin reorientation below 310 K from the basal plane towards c-axis. The AHE that is observed at temperatures well below the spin reorientation temperature does not follow the underlying net magnetization, indicating the formation of a non-coplanar or complex chiral spins textures.
12:03PM M35.00005: Itinerant ferromagnetism and intrinsic anomalous Hall effect in amorphous iron-germanium*  DINAH SIMONE BOUMA, NEAL REYNOLDS (Presenter), University of California, Berkeley, and Lawrence Berkeley National Laboratory, ZHANGHUI CHEN, Lawrence Berkeley National Laboratory, FRANK BRUNI, University of California, Berkeley, BINHUA ZHANG, Fudan University, MICHAEL FLATTÉ, University of Iowa, University of Chicago, and Eindhoven University of Technology, ROBERT STREUBEL, LIN-WANG WANG, Lawrence Berkeley National Laboratory, RUQIAN WU, University of California, Irvine, FRANCES HELLMAN, University of California, Berkeley, and Lawrence Berkeley National Laboratory — The amorphous iron-germanium system (a-Fe$_x$Ge$_{1-x}$) lacks long-range structural order and hence lacks a meaningful Brillouin zone. The magnetization of a-Fe$_x$Ge$_{1-x}$ is well explained by the Stoner model for $x \geq 0.4$, indicating that the local order of the amorphous structure preserves the spin-split density of states of the Fe-3$d$ states sufficiently to polarize the electronic structure despite $k$ being a bad quantum number. Measurements show an enhanced anomalous Hall resistivity relative to crystalline FeGe; comparison to density functional theory calculations of the anomalous Hall conductivity (AHC) resolves its underlying mechanisms. The intrinsic mechanism, typically understood as the Berry curvature integrated over occupied $k$-states but equivalent to the density of curvature (DOC) integrated over occupied energies, dominates the AHC of a-Fe$_x$Ge$_{1-x}$ (0.38 $\leq x \leq$ 0.61). The DOC is the sum of spin-orbit correlations of local orbital states and can hence be calculated with no reference to $k$. This result and the accompanying Stoner-like model for the intrinsic AHC establish a unified understanding of the physics of the anomalous Hall effect in both crystalline and disordered systems.  
D. S. Bouma et al., arXiv:1908.06055, 2019

*Funded by U.S. DOE, Contract No. DE-AC02-05-CH11231 (NEMM, MSMAG)

12:15PM M35.00006: Unusual Friedel and RKKY responses in 3D quadratic band-touching Luttinger semimetals  LOUIS J. GODBOUT (Presenter), SERGUEÏ TCHOUMAKOV, WILLIAM WITCZAK-KREMPA, Universite de Montreal — We study the response of Luttinger semimetals, such as alpha-Sn, HgSe, HgTe, YPtBi and Pr$_2$Ir$_2$O$_7$, to charge and magnetic impurities. In these materials the strong spin-orbit coupling and quadratic band-touching lead to unusual Friedel and Ruderman-Kittel-Kasuya-Yoshida (RKKY) oscillations, as well as an asymmetry in the response upon electron or hole doping. We also examine the magnetic Pauli and Landau susceptibilities, which differ from those of regular metals. These results motivate the study of Kondo physics in Luttinger semimetals, where novel quantum phases can arise due to spin-orbit coupling.
Search for new permanent magnet materials: methodology and applications. OLGA VEKILOVA (Presenter), Physics and Astronomy, Uppsala University — Permanent magnets (PMs) are of vital importance for sustainable industry and in particular, are parts of most of the sources of “green” energy. The theory-assisted search for new PMs, especially those that are free from expensive rare-earth elements, has now become an active field of research. We could recently suggest a number of promising PMs using the ab initio-based analyses and high-throughput approach [1,2]. One of key target properties is the proper ferromagnetic state with high Curie temperature. To be able to effectively describe that, especially in the course of high-throughput calculations, we have introduced a novel theoretical method, combining molecular dynamics with the magnetic state search [3]. The implementation and examples showing the power of the method will be considered.


The Voltage-Controlled Magnetic Anisotropy Effect Under High Electric Field* BOWEI ZHOU (Presenter), MENG XU, PRAVIN KHANAL, YU ZHANG, WEIGANG WANG, Univ of Arizona — The discovery of voltage-controlled magnetic anisotropy (VCMA) effect in perpendicular magnetic tunneling junction (pMTJ) has attracted considerable interests for low-power and high-speed memory application. In a recent DFT study1, the VCMA effect is expected to diverge from commonly observed linear PMA vs E-field relation and exhibit nonlinearity under high E-field. However, limitations of established methods make high E-field unattainable.

Modified TMR method is performed in this work. By using pulsed voltage, on-time can be reduced by at least 2 orders of magnitude, which increases the MTJ breakdown voltage and allows for higher E-field (>800mV/nm). Unexpected magnetoresistance independent of relative FM spin alignment was discovered and attributed to impurity-assisted tunneling. Efforts were made to exclude it from conventional TMR and a nonlinear E-field dependence of PMA can be observed under high bias. Electron doping with different metals as buffer and insertion is carried out and their influence is reported and compared with DFT study.


*This work is supported by NSF ECCS Grant No. 1554011 and the DARPA ERI program (FRANC).
12:51PM M35.00009: Energy-efficient stochastic computing with superparamagnetic tunnel junctions* MATTHEW W DANIELS (Presenter), National Institute of Standards and Technology, ADVAIT MADHAVAN, PHILIPPE TALATCHIAN, ALICE MIZRAHI, IREP, University of Maryland, MARK STILES, National Institute of Standards and Technology — We design an efficient stochastic bitstream generator based on superparamagnetic tunnel junctions, which can produce low energy, truly random bits, in turn drastically reducing cross-correlation. This bitstream generator allows us to address an outstanding issue in stochastic computing: that it has been limited by the inaccuracies introduced by correlations between the pseudorandom bitstreams used in the calculations. This bitstream generator gives us the freedom of not having to design around correlations and allows us to propose a low-energy approach to stochastic computing. To demonstrate the effectiveness of this approach, we incorporate it into an efficient CMOS neural network design. Our simulations of this network reach error rates comparable to recent work in stochastic-computing-based neural networks at nearly an order of magnitude lower energy expenditure.

*AM, AM, PT, and MD acknowledge support from the Cooperative Research Agreement between the University of Maryland and the National Institute of Standards and Technology Center for Nanoscale Science and Technology, Award 70NANB14H209, through the University of Maryland.

1:03PM M35.00010: Atomic scale magnetic and structural imaging by achromatic electron microscopy ZECHAO WANG (Presenter), JING ZHU, Tsinghua University — The atomic-level knowledge of local spin configuration of the magnetic materials is of great importance to predict and control their physical properties, in order to meet the challenges of ever-increasing demands on performance of functional materials. However, it is highly challenging to experimentally characterize magnetic properties of such materials with atomic scale spatial resolution. Here, we show that a combination of electron energy-loss magnetic chiral dichroism (EMCD) and chromatic-aberration-corrected transmission electron microscopy, which can provide element-selective orbital and spin magnetic moments atomic plane by atomic plane. This unique capability, which we demonstrate for Sr\textsubscript{2}FeMoO\textsubscript{6}, opens the door to local atomic level studies of spin configurations in a multitude of materials that exhibit different types of magnetic coupling, thereby contributing to a detailed understanding of physical origins of magnetic properties of materials at the highest spatial resolution. 


1:15PM M35.00011: Electrical transport in FIB-microstructures of single-crystalline Mn$_{1.4}$PtSn

MORITZ WINTER, SANDRA HAMANN, MARC UHLARZ, Dresden High Magnetic Field Laboratory, Helmholtz Zentrum Dresden Rossendorf, JACOB GAYLES, PRAVEEN VIR, MARKUS KOENIG, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, JOACHIM WOSNITZA, TONI HELM (Presenter), Dresden High Magnetic Field Laboratory, Helmholtz Zentrum Dresden Rossendorf — Mn$_{1.4}$PtSn is a half-Heusler compound with tetragonal crystal structure that hosts a D2d symmetry and strong Dzyaloshinskii-Moriya interactions. These are key-ingredients for the possible presence of Antiskyrmion phases. Recently, Antiskyrmions were observed well above room temperature by Lorentz transmission microscopy (LTEM) in polycrystalline nanoscaled ingots of the material [1]. Such a magnetic texture may cause a topological Hall effect (THE) leading to a significant deviation from the expected anomalous Hall effect. Indeed, a topological component of high magnitude was revealed by Hall measurements, conducted on bulk single crystals [2]. It however, only was observed below the spinreorientation transition at T$_{SR} = 160$ K associated with the formation of a non-coplanar spin structure. We investigate transport devices fabricated by the application of focused ion beams (FIB) from high-quality single crystals. Assisted by FIB we are able to conduct experiments on devices with sub-micron feature sizes. Our study of the temperature, field, and thickness dependent transport reveals clear signatures of THE originating from both, the non-coplanar spin structure as well as Antikyrmions, with apparent differences.


1:27PM M35.00012: Valence instability across magnetostructural transition in USb$_2^*$

ZACHARY BRUBAKER (Presenter), Oak Ridge National Laboratory, YUMING XIAO, PAUL CHOW, CURTIS KENNEY-BENSON, JESSE SMITH, Argonne National Laboratory, HYUNCHAE CYNN, CHRISTOPHER REYNOLDS, Lawrence Livermore National Laboratory, NICHOLAS BUTCH, National Institute of Standards and Technology, RENA ZIEVE, University of California, Davis, JASON R JEFFRIES, Lawrence Livermore National Laboratory — Pressure dependent transport measurements on USb$_2$ indicate an abrupt antiferromagnetic–ferromagnetic (AFM–FM) transition near P = 8 GPa, accompanied by a reduction in ordering temperature by more than 100 K. The AFM–FM transition has been the subject of several recent theoretical calculations, though only few experimental probes have been reported. To elucidate the behavior near this magnetic transition, we performed pressure dependent X-ray diffraction and resonant X-ray emission spectroscopy experiments on USb$_2$. The magnetic transition coincides with a tetragonal to orthorhombic structural transition resulting in a 17% volume collapse as well as a transient f-occupation enhancement. The AFM–FM transition width determined from structural and spectroscopic measurements agrees well with previously published transport measurements and suggests a sluggish transition from about 8 to 11 GPa. Except for the enhancement across the transition region, the f-occupation decreases steadily with pressure, demonstrating the multiconfigurational nature of actinide materials.

*This work was performed under LDRD (Tracking Code 18-SI-001) and under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory (LLNL) under Contract No. DE-AC52- 07NA27344.
Effect of Co, Ni, and Co-Ni doping on magnetic and electronic properties of MnBi by first-principles calculations

CHANDANI NANDADASA (Presenter), BIPIN LAMICHHANE, DINESH THAPA, Department of Physics and Astronomy, Mississippi State University, MINYEONG CHOI, YANG-KI HONG, Department of Electrical and Computer Engineering and MINT Center, The University of Alabama, SEONG-GON KIM, Department of Physics and Astronomy, Mississippi State University — While Manganese Bismuth (MnBi) is a well-studied rare-earth free permanent magnetic material, its magnetic and electronic properties in the presence of dopants have not been discovered extensively. We studied the magnetic and electronic properties of MnBi doped with Co, Ni, and Co-Ni using the Generalized Gradient Approximation (GGA) method within Density Functional Theory (DFT). GGA+U method is used to get electronic correlation in 3d electrons in transition metal alloys. We considered both interstitial and substitutional sites in the MnBi lattice when adding Co, Ni, and Co-Ni. The addition of Co, Ni, and Co-Ni into interstitial sites has yielded a significant increase in the magnetization with dopant concentration. However, substitutional doping into Mn site decreased its magnetization with dopant concentration. Our results show that individual Co and Ni doping prefers parallel spin configurations with Mn site while Co-Ni doping prefers both parallel and antiparallel configurations. We further calculated magnetic anisotropy energy (MAE) and magnetic anisotropy constant ($K_u$) of pure MnBi and doped-MnBi. Electronic properties were examined to describe exchange interactions between the dopants and the MnBi lattice.

*NRF of Korea(2015M3D1A1070639) & CCS at Mississippi State University

Kardar-Parisi-Zhang Universality in the Infinite Temperature spin-half Heisenberg Chain

NICHOLAS SHERMAN (Presenter), JOEL MOORE, University of California, Berkeley — There are two simple paradigms of how conserved quantities transport through a system: thermalizing systems with effectively random collisions in the system leading to diffusion, and particles moving freely in a material giving rise to ballistic transport. In the spin-half XXZ model in one dimension, both of these behaviors have been shown rigorously. Recent studies have suggested at the isotropic point of the model, the spin-half Heisenberg model, there is a third behavior at infinite temperature given by the stochastic classical Kardar-Parisi-Zhang (KPZ) universality class. In this work, I computed the dynamical structure factor at infinite temperature using matrix product states for the spin-half Heisenberg, and show that it exhibits the scaling function from the KPZ universality class, strengthening the claim that KPZ dynamics are present in quantum spin systems.
Mechanically Induced Thermal Breakdown in Magnetic Shuttle Structures

OLYA A. ILINSKAYA, SERGEIJ I. KULINICH, ILYA V. KRIVE, B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, ROBERT SHEKHTER, Gothenburg University, HEE CHUL PARK (Presenter), Institute for Basic Science, MATS JONSON, Gothenburg University — A theory of a thermally induced single-electron “shuttling” instability in a magnetic nanomechanical device subject to an external magnetic field is presented in the Coulomb blockade regime of electron transport. The model magnetic shuttle device considered comprises a movable metallic grain suspended between two magnetic leads, which are kept at different temperatures and assumed to be fully spin polarized with antiparallel magnetizations. For a given temperature difference shuttling is found to occur for a region of external magnetic fields between a lower and an upper critical field strength, which separate the shuttling regime from normal small-amplitude “vibronic” regimes. We find that (i) the upper critical magnetic field saturates to a constant value in the high temperature limit and that the shuttle instability domain expands with a decrease of the temperature; (ii) the lower critical magnetic field depends not only on the temperature independent phenomenological friction coefficient used in the model but also on intrinsic friction caused by magnetic exchange forces and electron tunneling between the quantum dot and the leads. The feasibility of using thermally driven magnetic shuttle systems to harvest thermal breakdown phenomena is discussed.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M36 GDS FED: Data Science in the Physics Curriculum

11:15AM M36.00001: Designing curricula for data science based on fundamental skills and competencies informed by expert interviews* [Invited]  DEVIN SILVIA (Presenter), NATHANIEL HAWKINS, BRIAN W O'SHEA, MARCOS DANIEL CABALLERO, Computational Mathematics, Science, and Engineering, Michigan State Univ — With computational modeling and data analysis skills becoming an increasingly integral part of modern scientific work and research, understanding the specific competencies and skills required for individuals to participate in this work is growing more important. Previous efforts have defined these competencies and skills to varying degrees, with recommendations ranging from writing scientific software to designing entire degree programs in data science; however, the existing computational science education literature is incomplete in some ways. Primarily, much of the existing literature lacks a research-based foundation. We conducted a series of semi-structured interviews with experts in academic and industry settings to broadly describe the skills that students need to have in order to participate in work and research in computational science. In this talk, I will present the results of our research and highlight some of the design choices we have made for our introductory computational science course and how those choices connect to our research findings.

*We acknowledge the MSU Department of Computational Mathematics, Science, and Engineering and the MSU College of Natural Science for their generous support of this research.
A university-wide approach to integrative data science education and career paths

Sarah Stone (Presenter), University of Washington — All areas of science, particularly the physical sciences, are experiencing a data revolution that is changing our approaches to discovery. This “data science” transformation is being driven by factors such as advancements in high-throughput instrumentation, new modes of scalable computing, and perhaps most importantly, new breakthroughs in algorithms such as deep learning. Harnessing these advances with a coherent and intentional approach is essential to enabling new discoveries. As such, researchers need access to state-of-the-art data science methods and tools. Moreover, these methods and tools must evolve rapidly, driven by the requirements of discovery. This rate of advancement is currently limited by the “intellectual infrastructure” of trained data science practitioners. At the University of Washington’s eScience Institute, we have developed a university-wide approach to addressing this challenge by developing an integrative education program through formal data science options, now offered by 18 academic units at UW, and informal education programs. We have also supported transformational individuals, in both traditional and non-traditional academic roles, who bridge data science methods development and applied research. As a hub for data science on the UW campus, the eScience Institute has grown and fostered an interdisciplinary community focused on advancing data-intensive research and education across all fields.

In collaboration with: David Beck, University of Washington

A beginner’s guide to using data science for physicists

Trevor David Rhone (Presenter), Physics, Rensselaer Polytechnic Institute — The data revolution is changing the way we live. Exploiting data using data science tools has sparked innovation, spanning areas as diverse as spam filters, driverless cars and image recognition. Data science is rapidly becoming the latest addition to the physicist's toolkit. But, what is data science? Why is it useful? How does it work? This talk provides a beginner’s guide to data science for the inquisitive physicist. We will explore the major aspects of data science and discuss useful applications. In addition, I will provide a step by step guide on how to get started learning data science and share the secret to mastery of this exciting new field.
1:03PM M36.00004: Deep Learning Data Science Competencies to Promote Workplace Readiness [Invited] AMIR SHAHMORADI (Presenter), University of Texas at Arlington — Data science is a rapidly growing field with a 663% increase in the number of job postings for a data scientist between 2013 and 2018. The demand for college graduates who are trained in data science skills spans every field of science. Therefore, undergraduate and graduate programs must be responsive to align their curricula with these dynamic needs. However, the data scientist title is relatively new and formal data science competencies are yet to be defined. In this talk, I will describe our efforts at the University of Texas to 1. determine what these data science technical and soft skill competencies are by analyzing data from national job postings, and 2. systematically investigate how the pattern of required skills varies by co-occurrence, domain of science knowledge, and characteristics of the jobs and employers. Such knowledge can help identify gaps between academic preparation and the skills employers seek by identifying data science competencies employers are requesting within and between domains of science, and then evaluating how well these skills align with science curriculum and finally, predicting the future of job market’s supply versus demand for data science skills.

1:39PM M36.00005: Data Science Tools in the Classroom [Invited] MOHAMMAD SOLTANIEH-HA (Presenter), Boston Univ — Teaching methods for programming and data science-related topics have been evolving faster than ever before. This has been heavily influenced by the fast-growing popularity of cloud-based tools. In this talk, I will provide an overview of tools and techniques that can improve both the learning experience of the students and the instructor’s ability to manage the class and materials. I will discuss the best practices to manage and distribute code and data, as well as the platforms used in a data science project. Among a vast space of competitive solutions, I have decided to use Google products as the primary platform. Google Colaboratory (Colab) will be introduced as a solution to run and share the code. Beyond Colab, I will present an end-to-end data science project on a cloud-based ecosystem, using Google Cloud Platform (GCP). In addition to the essential elements of GCP, I will cover ways to tackle big data problems using Hadoop and Spark, as well as utilizing containerized applications for large scale parallel processing. I will illustrate how I have used GCP in my classes at Boston University and share feedback from the students. Additionally, I will touch on open-source auto-grading tools.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M37 FPS FOEP: Communicating Science to the Public 605 - Richard Wiener, Research Corporation - Tag(s): Invited, Outreach, Undergrad Friendly
11:15AM M37.00001: Joseph A. Burton Forum Award talk: Physics, Truth and the Crisis of Science Denial [Invited] ADAM FRANK (Presenter), Department of Physics and Astronomy, University of Rochester — In this talk I will discuss the current state of relations between Physics (and Science in general) and the non-scientific public. After many years as both a practicing astrophysicist and a science writer/communicator, I have watched as the public perception of science has changed dramatically. Because of critical issues such as climate change, a remarkably large section of the public views science as tainted by "elite" interests rather than as a means of achieving some degree of truth about the physical world. In this talk I will review how this state of affairs came to be, using my own experiences in writing for venues like NPR, The New York Times and elsewhere. The current situation presents great challenges to our community and to the US scientific effort as a whole. I will attempt to articulate both its causes and possible mechanisms with which we can ensure that science maintains its vital role in ensuring the health, welfare and security of the US and global communities.

11:40AM M37.00002: Andrei Sakharov Award talk: Scientific espionage, open exchange, and American competitiveness [Invited] XIAOXING XI (Presenter), Temple Univ — As the federal government warns universities and colleges about the risk of China to academia in the United States, professors, scientists, and students of Chinese ethnic origin are under heightened scrutiny. In 2015, I became a casualty of this campaign despite being innocent. This experience gave me insights into the challenges Chinese scientists face and the immediate threat to the open environment in fundamental research on university campuses. Based on my personal experience and the recent events involving Chinese scientists in the US, I urge the audience to join an increasing number of scientists, university administrators, and professional societies in speaking up to defend liberty, support reaffirmation of NSDD-189 on open fundamental research, and safeguard America’s research enterprise.

12:05PM M37.00003: The role of news journalism [Invited] DENNIS OVERBYE (Presenter), New York Times — tbd
12:30PM M37.00004: The National Academy of Sciences Goes to Hollywood: Employing Creative Engagement Strategies to Connect with Broad Audiences* [Invited]  ANN MERCHANT (Presenter), Office of the Chief Communications Officer, National Academy of Sciences — Entertainment media saturates our lives. According to the Motion Picture Association of America, an average of 600 new movies are created in the United States every year. With the exception of 2009, when the global economic crisis slowed production in Hollywood, the number of movies released in North America has steadily increased since the year 2000. In 2018, a record 878 movies graced U.S. screens.

In 2008 the National Academy of Sciences (NAS) launched The Science & Entertainment Exchange (The Exchange) to connect entertainment industry professionals with top scientists and engineers to create a synergy between accurate science and engaging storylines in both film and television programming. The goal of The Exchange is to use the vehicle of popular entertainment media to deliver sometimes subtle, but nevertheless powerful, messages about science that catalyze more storytelling grounded in authentic science, encourage the depiction of richer, more diverse STEM characters in order to challenge traditional stereotypes, and inspire new media projects driven by science and engineering themes.

Learn more about the ways in which The Exchange has worked closely with the Hollywood community to foster and incubate a collaborative community of scientists, engineers, and entertainment industry professionals to generate science-inspired film, television, and video game projects that have the potential to impact the next generation of scientists and engineers.

*The Science & Entertainment Exchange is grateful to the Alfred P. Sloan Foundation, Howard Hughes Medical Institute, Google, the Simons Foundation, The Walt Disney Company, the Lyda Hill Philanthropies, the Cabot Wellington Family Foundation, and the many individual donors who make our work possible.

12:55PM M37.00005: The art of interviewing scientists [Invited]  IRA FLATOW (Presenter), Science Friday — tbd

1:10PM M37.00006: Panel Discussion [Invited] —

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M38 CSWP: Proactive Ways to Recruit and Retain Women in Physics 607 - Kristen Burson, Hamilton College - Tag(s): Diversity, Education, Invited, Undergrad Friendly
Despite increasing numbers of students graduating with physics and other STEM degrees, the percentage of women earning bachelor’s degrees in physics has stagnated at approximately 20% for the past decade. The drop in representation of women in physics occurs at the high school/college transition. Nearly half of high school physics students are young women, but only one-fifth of physics majors at college entrance are women. Thus, efforts to increase the representation of women in physics need to focus on high school, which is many students’ first and last exposure to physics. STEP UP is a nationwide community with the goal of inspiring young women to pursue physics bachelor’s degrees. We have developed two lessons for use by high school physics teachers: Careers in Physics and Women in Physics. The lessons are grounded in research on physics identity, goal orientation, career intentions, and gender. In this talk, I will give an overview of the project and present results of the pilot study conducted in Fall 2017 and the experimental study conducted in Fall 2018. Learn more about STEP UP and join the movement at http://www.STEPUPphysics.org

*STEP UP* (Supporting Teachers to Encourage the Pursuit of Undergraduate Physics) is funded by the National Science Foundation under Grant Nos. 1720810, 1720869, 1720917, and 1721021.
12:27PM M38.00003: Outcome of the Conferences for Undergraduate Women in Physics
[Invited] PEARL SANDICK (Presenter), University of Utah — The APS Conferences for Undergraduate Women in Physics (CUWiPs) are simultaneous regional conferences designed to help undergraduate students continue in physics by providing them the opportunity to network with other physicists, learn about career options and graduate school, discuss issues associated with underrepresentation in science, and participate in professional development activities. CUWiP attendance has been steadily increasing since the first conference in 2006. In 2019, approximately 2000 undergraduate students attended a CUWiP at one of twelve host sites throughout the US and Canada. The number of attendees has roughly doubled since 2014. In this talk, I'll give an overview of the APS CUWiPs, typical programming, and impact. I'll also discuss the role of the National Organizing Committee and individual host sites, as well as how to apply to host a CUWiP.

1:03PM M38.00004: Julianne Pollard-Larkin Invited Talk [Invited] —

1:39PM M38.00005: Physics – We Have a Problem [Invited] PATRICIA RANKIN (Presenter), University of Colorado, Boulder — Thirty years ago when people asked me why more women did not study physics I did not have a good answer. Now I do. Attempts to increase the percentage of women in Physics go in phases. Early on, the belief was that more female role models would help (they do, but not enough, and intersectionality matters when giving people role models they can see themselves as). Later we went through the “Fix the Women” / “Lean in” stage and the focus was on teaching women the skills (such as negotiation) it was felt they needed to be successful in Physics. I will explain why this approach was not as effective as hoped and why the emphasis has now shifted to looking at processes and policies to make organizations more inclusive not just more diverse. We are now in the “Lean Out” era. This presentation will emphasize research based practice and include some specific suggestions on how to make recruitment less subject to bias.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M39 DCOMP GDS DMP: Machine Learning for Quantum Matter
II 703 - Estelle Inack, Perimeter Inst for Theo Phys - Tag(s): Focus

11:15AM M39.00001: Materials discovery through artificial intelligence [Invited] MURATAHAN AYKOL (Presenter), Toyota Research Institute — New, suitable materials are almost always at the core of new technologies. This endeavor now is spurred by exciting developments at the intersection of artificial intelligence (AI) and materials science. In this talk, I will present new AI tools developed at TRI for end-to-end material discovery systems. Using these tools, codified agents of research can incorporate machine-learning, physics, chemistry, logic or heuristics to make decisions to meet their goals, for example, on which structures to simulate using high-fidelity quantum mechanics. New agent designs can also be simulated a priori, projecting their performance in real-world discovery campaigns. Examples of simulations and executions of stable material discovery campaigns will be shown.
11:51AM M39.00002: Working without data: overcoming gaps in deep learning and physics-based extrapolation [Invited] ISAAC TAMBLYN (Presenter), National Research Council of Canada — Despite its many recent successes, several fundamental issues remain with the application of deep learning to experimental data and first-principles based simulation.

These problems include the ability to extrapolate to unseen experimental conditions, transfer knowledge across length-scales, and the challenge of interpreting results within a physically motivated framework. Other challenges include the lack of a standardized methodology for reporting and understanding model errors as well as the frequent requirement for large quantities of data.

I will outline some of our ongoing efforts to address some of these challenges, with special attention paid to the concept of extrapolation (including the physical conditions of study and across length scales). To explore these ideas, we explore model spin-systems, 2d materials, and optical lattices.

12:27PM M39.00003: Machine learning models of properties of hybrid 2D materials as potential super lubricants* MARCO FRONZI (Presenter), IRCRE, Xi'an Jiaotong University, MUTAZ ABU GHAZALEH, University of Technology Sydney, OLEXANDR ISAYEV, University of North Carolina, DAVID WINKLER, La Trobe University, JOE SHAPTER, Flinders University, MICHAEL J FORD, University of Technology Sydney — The screening of novel materials is an important topic in the field of materials science. Although traditional computational modeling, especially first-principles approaches, is a very useful and accurate tool to predict the properties of novel materials, it still demands extensive and expensive state-of-the-art computational resources. Additionally, they can be often extremely time-consuming. We describe a time and resource-efficient machine learning approach to create a large dataset of structural properties of van der Waals layered structures. In particular, we focus on the interlayer energy and the elastic constant of layered materials composed of two different 2-dimensional (2D) structures, that are important for novel solid lubricant and super-lubricant materials. We show that machine learning models can recapitulate results of computationally expansive approaches (i.e. density functional theory) with high accuracy.

*National Natural Science Foundation of China (No. 51323011), the Australian Government through the Australian Research Council (ARC DP16010130), National Computational Infrastructure (NCI), which is supported by the Australian Government.
12:39PM M39.00004: Charge Density Prediction through 3D-CNN for Fast Convergence of Self-Consistent DFT calculation*  IORI KURATA (Presenter), Univ of Tokyo, CHIKASHI SHINAGAWA, RYOHTO SAWADA, Preferred Networks, Inc. — The electronic charge density plays an important role in understanding the physical properties of quantum materials. Although the charge density can be obtained by solving the Kohn-Sham equation of density functional theory (DFT), one needs to solve a self-consistent equation which takes time until convergence. Recent studies have tried to directly predict the charge density using machine-learning methods, but the target materials are limited to slabs or organic molecules because they only considered local electronic features [1,2,3]. In this study, we propose a machine-learning algorithm to predict the charge densities of crystals using a three-dimensional convolutional neural network (3DCNN). To deal with the periodicity of crystals, we use FFT grid-based representation and a periodic convolution filter. We demonstrate that our model can predict the charge densities of ABO$_3$-type crystalline compounds without solving the self-consistent equation. It will accelerate the high-throughput DFT calculations for materials discovery.


*This work was supported by Preferred Networks, Inc.

12:51PM M39.00005: Data-driven studies of the magnetic anisotropy of two-dimensional magnetic materials*  YIQI XIE (Presenter), TREVOR DAVID RHONE, GEORGIOS TRITSARIS, Harvard University, OSCAR GRÅNÅS, Uppsala University, EFTHIMIOS KAXIRAS, Harvard University — Two-dimensional materials with intrinsic ferromagnetic order are at the forefront of condensed matter research. How many of these materials exist in nature? What is the relationship between their crystal structure and magnetic properties? Remarkably, atomically-thin magnetic structures can exhibit novel spin properties which do not exist in the corresponding bulk materials. We use first-principles calculations, based on density functional theory, and machine learning to study the magnetocrystalline anisotropy of monolayer transition metal trichalcogenides of the form A$_2$B$_2$X$_6$. That is, we created permutations of the chemical composition of the ferromagnetic semiconductor Cr$_2$Ge$_2$Te$_6$. Specifically, we identify trends in their magnetocrystalline anisotropy data. We find that the X site dominates the machine learning prediction of the magnetocrystalline anisotropy of an A$_2$B$_2$X$_6$ monolayer. Our data-driven study aims to uncover physical insights into the microscopic origins of magnetism in reduced dimensions and to demonstrate the success of a high-throughput computational approach for the targeted design of quantum materials with potential applications from sensing to data storage.

*ARO MURI W911NF-14-0247; DOE BES DE-SC0019300; SSF ICA16-0037; XSEDE NSF ACI-1548562; NERSC DE-AC02-05CH11231
1:03PM M39.00006: Robust cluster expansion of multicomponent systems using machine learning with structured sparsity*  ZHIDONG LEONG (Presenter), TECK LEONG TAN, Institute of High Performance Computing — Identifying a suitable set of descriptors for modeling physical systems often utilizes either deep physical insights or statistical methods. In machine learning, a class of methods known as structured sparsity regularization combines both physics- and statistics-based approaches. We present group lasso as an efficient method for obtaining robust cluster expansions (CE) of multicomponent systems, a popular computational technique for modeling the thermodynamic properties of such systems. Via convex optimization, group lasso selects the most predictive set of atomic clusters as descriptors in accordance with the physical insight that if a cluster is selected, so should its subclusters. These selection rules avoid spuriously large fitting parameters by redistributing them among lower order terms, resulting in more physical, accurate, and robust CEs. We showcase these features of group lasso using the CE of bcc ternary alloy Mo-V-Nb. These results are timely given the growing interests in applying CE to increasingly complex systems, which demand a more reliable machine learning method to handle the larger parameter space.

*Funded by the Advanced Manufacturing and Engineering Young Individual Research Grant (AME YIRG) of Agency for Science, Technology and Research (A*STAR) (A1884c0016).

1:15PM M39.00007: Generalizing an Energy Predictor based on Wavelet Scattering for 3D Atomic Systems  PAUL SINZ, MICHAEL SWIFT (Presenter), XAVIER BRUMWELL, KWANG JIN KIM, YUE QI, MATTHEW J HIRN, Michigan State Univ — The dream of machine learning in quantum matter is for a neural network to learn the underlying physics of an atomic system, allowing it to move beyond interpolation of the training set to the prediction of properties that were not present in the original training data. Achieving this ambitious goal will require a method to convert a 3D atomic system into neural-network-friendly features that preserve rotational and translational symmetry, smoothness under small perturbations, and invariance under reordering. The atomic orbital wavelet scattering transform preserves these symmetries by construction, and has achieved great success as a featurization method for machine learning energy prediction. Both in small molecules and in the amorphous Li$_x$Si system, neural networks using wavelet scattering coefficients as features have demonstrated a comparable accuracy to Density Functional Theory at a small fraction of the computational cost. In this work, we test the generalizability of our Li$_x$Si energy predictor to properties that were not included in the training set, such as elastic constants and migration barriers. We also discuss the potential for future improvements in generalizability through automatic training-set expansion based on active learning.
1:27PM M39.00008: Using Machine Learning Models to Predict Higher-Level Quantities from Energy Models*

OLIVIER MALENFANT-THUOT (Presenter), MICHEL COTE, Universite de Montreal — Machine learning methods are now used more and more as a substitute for Density Functional Theory calculations due to their low computational costs. However, in some cases, relevant datasets are not available, and the effort that would be necessary to generate this data suppresses the advantages of using machine learning to speed up the calculations. Furthermore, the process of training a reliable model is not trivial and can also be expensive. For those reasons, we are developing a python package named ML_Calc_Driver\(^1\), which goal is to allow to use portable trained models to make predictions easily. Energy datasets are numerous and, through the use of implemented finite difference workflows, can be used to predict higher-level quantities such as forces, phonon energies, and infrared intensities. As of now, the package is interfaced to use SchNetPack\(^2\) trained models, and more model types can easily be added as our workflows are independent of the actual calculators.

1. https://github.com/OMalenfantThuot/ML_Calc_Driver

*This research was enabled in part by support provided by Calcul Québec (www.calculquebec.ca) and Compute Canada (www.computecanada.ca). Funding was provided by NSERC under Grant No. RGPIN-2016-06666.

1:39PM M39.00009: AI-guided engineering of nanoscale topological materials*

SRILOK SRINIVASAN (Presenter), MATHEW J CHERUKARA, DAVID JASON ECKSTEIN, ANTHONY AVARCA, SUBRAMANIAN SANKARANARAYANAN, PIERRE DARANCET, Argonne Natl Lab — Nanoscale organic materials have long been known to host topologically protected excitations. Inspired by recent progress in classifying topological phases in armchair, cove-edged and chevron graphene nanoribbons, we develop a high-throughput framework based on the computation of the Zak phase and the Z2 invariants using tight-binding and density functional theory to explore the topology of low-symmetry 1D and 2D periodic organic compounds. As of today, we have identified 224,071 new topological nanoribbons using our framework. Training deep neural networks on the graphs of these Hamiltonians, we analyze the graphical features conducive to topological excitations in these systems. We show how this workflow can help the atomic assembly of topologically non-trivial artificial lattices.

*This material is based upon work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357. Work performed at the Center for Nanoscale Materials, an Office of Science user facility, and supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
1:51PM M39.00010: Motif-based machine learning for crystalline materials  HUTA BANJADE (Presenter), Physics, Temple University, SHANSHAN ZHANG, SANDRO HAURI, SLOBODAN VUCETIC, Computer and information Sciences, Temple University, QIMIN YAN, Physics, Temple University — With the development of advanced algorithms and improvements in computational power, machine learning (ML) has been widely successful in predicting various physical and chemical properties of materials. The success of any ML model mainly depends on the good representation of the input data, and there have been surging interests in identifying effective representations for crystalline materials. In this talk, we propose a novel representation of crystalline solid-state materials (such as complex metal oxides) as graphs composed of structure motifs. This motif-based representation serves as input to a graph convolutional network for the learning and prediction of material properties, such as bandgaps and formation energies. Our test results indicate that, when combined with atomic information and related networks, the inclusion of motif information in the network architecture improves the prediction performance, especially for complex oxide materials.

M39.00011: Machine learning powered kinetic energy functional finding in solid state physics  HONGBIN REN (Presenter), Chinese Academy of Sciences, Institute of Physics, XI DAI, Physics, Hong Kong University of Science and Technology, LEI WANG, Chinese Academy of Sciences, Institute of Physics — Kinetic energy functional is crucial to speed up the density functional theory calculation. However, deriving it directly from first principle is challenging, and existing approximations all have significant flaw. In this work, we use machine learning method to build a kinetic energy functional for 1D extended system, our solution combines the dimensionality reduction method with the Gauss process regression, and use a simple scaling trick to generalize the functional to 1D lattice with arbitrary lattice constant. Besides reaching chemical accuracy in kinetic energy calculation, our solution also performs well in functional derivative prediction, and integrating it into the current orbital free density functional theory scheme provide us with expected ground state electron density.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M40 DCOMP DMP: Matter in Extreme Environments IV: Superconductivity  705 - Antonio dos Santos, Oak Ridge National Lab - Tag(s): Focus
11:15AM M40.00001: Room-Temperature Superconductivity in High-Pressure Hydrides: An electronic structure perspective* [Invited] LILIA BOERI (Presenter), Univ of Rome La Sapienza — Conventional Superconductivity near Room Temperature was observed for the first time almost fifty years after its theoretical prediction, when a superconducting critical temperature ($T_c$) of 203 K was reported in sulfur hydride, $\text{SH}_3$.\[1\] $T_c$’s exceeding 200 K have later been reported also in lanthanum and yttrium hydrides.\[2\]

In this talk, I will show how electronic structure methods can be used to understand the material-specific aspects that underlie high-$T_c$ superconductivity in different classes of hydrides,\[3\] and identify strategies to reduce the pressure for high-$T_c$ conventional superconductivity.\[4\]


*I acknowledge funding from the FWF Grant P-30269-N36 Superhydra and Progetto Ateneo Sapienza 2017 and 2018.

11:51AM M40.00002: Design of Ternary Ca-S-H System that are Superconducting Under Pressure YAN YAN (Presenter), TIANGE BI, NISHA GENG, XIAOYU WANG, EVA ZUREK, State Univ of NY - Buffalo — Hydrogen-rich compounds are promising candidates as high pressure superconductors under high compression. Among the most promising hydrides for high temperature superconductivity are those of sulphur and calcium. The high pressure phase transition of S-H system has resulted in the second highest $T_c$ to date, 203 K at 160 GPa, while a $T_c$ of 220-235K has been predicted for $\text{CaH}_6$ at 150 GPa. Here, we present a systematic investigation of Ca-S-H phases with various stoichiometries. We find that $\text{CaSH}_2$, $\text{CaSH}_6$ and $\text{CaSH}_{20}$ are thermodynamically stable at pressures accessible in diamond anvil cells. In these structures hydrogen still exists in its molecular form, and all of these phases are semiconductors with small band gaps. However, an interesting phase with the composition $\text{CaSH}_3$ has been found, which is metastable and metallic, and does not contain any H-H bonds. This unique structure has a $T_c$ up to 46 K at 250 GPa. Analysis of its electronic structure, including the sulphur and hydrogen contributions, reveals a van Hove singularity in the density of states near the Fermi Energy. This feature may be important for the superconductivity. Our approach may pave the way for finding high-$T_c$ superconductors in various ternary hydrides.
Quantum Crystal Structure in the 250 K Superconducting Lanthanum Hydride

ION ERREA (Presenter), University of the Basque Country UPV/EHU, FRANCESCO BELL, Centro de Física de Materiales, LORENZO MONACELLI, La Sapienza, ANTONIO SANNA, Max-Planck Institute of Microstructure Physics, TAKASHI KORETSUME, Tohoku University, TERUMASA TADANO, Research Center for Magnetic and Spintronic Materials, RAFFAELLO BIANCO, Centro de Física de Materiales, MATTEO CALANDRA, Institut des Nanosciences de Paris, RYOTARO ARITA, University of Tokyo, FRANCESCO MAURI, JOSE A. FLORES LIVAS, La Sapienza — Hydrogen-rich materials at high pressures are at the verge of reaching room-temperature superconductivity. Electrical and x-ray diffraction measurements determined a weakly pressure-dependent Tc for LaH10 between 137 and 218 gigapascals in a structure with a fcc arrangement of La atoms. Here we show that quantum atomic fluctuations stabilize in this pressure range a high-symmetry Fm-3m crystal structure consistent with experiments. Even if ab initio classical calculations predict this structure to distort below 230 GPa, the inclusion of quantum effects evidences the Fm-3m as the true ground state. The agreement between the calculated and experimental Tc values further supports this phase as responsible for the 250 K superconductivity. The relevance of quantum fluctuations questions many of the crystal structure predictions made for hydrides within a classical approach that at the moment guide experiments. Furthermore, quantum effects are revealed to be crucial to stabilize solids with extraordinary electron-phonon coupling, reducing the pressures needed for their synthesis.

This research was supported by the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme (grant agreement No. 802533).

High field phase diagram of LaH$_{10}$

DAN SUN (Presenter), Los Alamos National Laboratory, VASILY S MINKOV, PANPAN KONG, ALEXANDER DROZDOV, Max-Planck-Institut fuer Chemie, SHIRIN MOZAFFARI, LUIS BALICAS, National High Magnetic Field Laboratory, MIKHAIL EREMETS, Max-Planck-Institut fuer Chemie, FEDOR BALAKIREV, Los Alamos National Laboratory — Recent research on the hydrogen-rich hydrides pushes the superconducting transition temperature ($T_c$) near the limit of room temperature. In the hydrides family, LaH$_{10}$ keeps the current record of $T_c$ of 250 K. Using a pulsed magnet, we mapped out the phase diagram of LaH$_{10}$ under pressure of 140 GPa. The normal state has a linear temperature dependence and high resistance. $H_{c2}$ has been measured above 60 T. The information on the vortex liquid region, coherence length and density of states are obtained by our measurement, providing valuable information for theoretical and experimental hydride development.

This work was performed at the National High Magnetic Field laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1644779, and the State of Florida.
Effect of pressure on the noncentrosymmetric antiferromagnet CeNiC2

JUN GOUCHI, Institute for Solid State Physics, University of Tokyo, TORU SHIGEOKA, Grad. Sch. of Sci. Eng., Yamaguchi University, YOSHIYA UWATOKO (Presenter), Institute for Solid State Physics, University of Tokyo — Recently, the pressure-induced superconductivity in the CeNiC2 polycrystal has been discovered at 3.5 K around 11 GPa, the highest superconducting transition temperature in a Ce-based heavy-Fermion compound [1]. The intermetallic CeNiC2 crystalizes in orthorhombic structure (space group Amm2) where the lattice lacks the inversion symmetry along c-axis. With decreasing temperature CeNiC2 displays multiple magnetic transitions, an incommensurate antiferromagnetic (iAFM) order at TN1 = 20 K followed by a commensurate AFM order at TN2 = 10 K and a ferromagnetic order at TC = 2 K [2]. In this talk, I will present the pressure phase diagram of CeNiC2 single crystal based on our recent pressure dependence of transport and magnetic data. We observed superconductivity in a narrow pressure range in the vicinity of the vanishing point of TN1. The remarkable coincidence of non-Fermi liquid behavior and the optimal , coupled with moreover, the non-centrosymmetric crystal structure suggest that superconductivity in CeNiC2 is unconventional and exotic in nature.

References

AB3Si3 (A= Na, K, Rb, Cs), the alkali metal borosilicide in sodalite structure with superconductivity under high pressure

MIAO ZHANG (Presenter), EVA ZUREK, Department of Chemistry, State University of New York at Buffalo — Prediction of high-temperature superconductivity in clathrate-like hydrogen cage under high pressure has generated an irresistible interest of searches for clathrate-like superconductors. However, when the pressure is released, atomic hydrogens will decompose into H2, accompanying the disappearance of superconductivity. We herein report the structural and physical properties of AB3Si3 (A= Na, K, Rb and Cs) in clathrate-based sodalite structure, whose frameworks consist of covalent B-Si bonds, by first-principles calculations. Our results show that KB3Si3 and RbB3Si3 are thermally stable within pressure ranges of 6.9-37.0 GPa and 7.3-34.2 GPa, respectively. Phonon calculations confirm that RbB3Si3 is dynamically stable at both ambient and high pressures, while KB3Si3 is not at ambient pressure. Electron-phonon calculations predict that RbB3Si3 possess a Tc of 14.5 K at ambient pressure. Moreover, RbB3Si3 is mechanically stable, and its estimated Vickers hardness values are between 11.8 – 15.2 GPa, which are in good agreement with the ideal strength results.
1:15PM M40.00007: Charge Transfer Induced Band Gap Closure: Trend in Rare Earth Tetrahydrides Discovered under Pressure*  TIANGE BI (Presenter), EVA ZUREK, Chemistry, University at Buffalo — The recent success of the high-pressure synthesis of CaH$_4$ inspired this analysis of a plethora of previously predicted high-pressure rare-earth metal tetrahydrdes: MH$_4$ (M = Ca, Sr, Sc, Y, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu). This type of structure, assuming the space group of $I4/mmm$ and resembling the ThCr$_2$Si$_2$ structure type, contains layers of edge-sharing tetrahedra in the xy plane comprised by the negatively charged atomistic hydrogen layers and molecular H$_2$ layers. When this set of structures are optimized to 0 GPa, while the pressure-induced band broadening is eliminated, the H-H distances within the H$_2$ units are inversely associated with the charges transferred to it, which leads to bandgap closure. The existence of quasi-molecular H$_2$ is stabilized by the electron donation from H$_2$ $\sigma$ bonding state to the vacant metal $d$ states and the back donation from occupied metal $d$ states to the H$_2$ $\sigma^*$ anti-bonding states. The analysis of the electronic properties and stabilization mechanisms of these high-pressure rare earth metal tetrahydrides would potentially benefit the understanding of their exotic physical properties: i.e. superconductivity novel, magnetic behavior.

*NSF (DMR-1827815)

1:27PM M40.00008: Fermiology Study of YBCO* [Invited]  AUDREY GROCKOWIAK (Presenter), WILLIAM A CONIGLIO, STANLEY W TOZER, Florida State Univ — We report on high pressure SdH studies of YBCO6.5 (p=0.1) at He-3 temperatures in pulsed fields to 85 T and 7 GPa at HLD and dc fields of 45 T and pressures of 25 GPa at NHMFL using plastic and metal diamond anvil cells (DACs), respectively, that are coupled with an LC tank circuit based on a tunnel diode oscillator. Our high pressure studies show an enhancement of the superconducting critical field from 24 to 42T between ambient pressure and 6 GPa, which limits the observation of QO to 5 GPa in the 45T Hybrid. Our Fermiology studies clearly show a strongly diverging effective mass at 4.5 GPa along with a local maximum in frequency and superconducting critical temperature, attributed to the effect of various charge orders present in this material. For pressures greater than 15 GPa we are able to measure a critical field of the order of 30T and to measure again QOs. We find that the orbital frequency has increased from 550 T at ambient pressure to 690 T at 15 GP and above. Assuming that the samples are driven by pressure to the overdoped state, those results do not match the reported frequency of 18kT observed for the overdoped analog TI-2201. This indicates that pressure and doping are not playing an equivalent role on the CDWs and the superconducting state as also pointed in other studies, and shows that pressure is a new axis in the YBCO phase diagram which can help understand the interplay between CDWs and superconductivity in this material.

*The National High Magnetic Field Laboratory is supported by National Science Foundation through NSF/DMR-1157490 and DMR-1644779 and the State of Florida. We acknowledge the support of the HLD-member of the European Magnetic Field Laboratory (EMFL).
M40.00009: Superconductivity in Li$_6$P electride* GUOCHUN YANG (Presenter), Department of Physics, Northeast Normal University — Electrides are unique compounds where most of the electrons reside at interstitial regions of the crystal behaving as anions, which strongly determines its physical properties. Interestingly, the magnitude and distribution of interstitial electrons can be effectively modified either by modulating its chemical composition or external conditions (e.g. pressure). Most of the electrides under high pressure are non-metallic, and superconducting electrides are very rare. Here, we report that a pressure-induced stable Li$_6$P electride, identified by first-principles swarm structure calculations, becomes a superconductor with a predicted superconducting transition temperature $T_c$ of 39.3 K, which is the highest among already known electrides. The interstitial electrons in Li$_6$P, with dumbbell-like connected electride states, play a dominant role in the superconducting transition. Our work opens up the interest to explore high-temperature superconductivity in similar binary compounds.

*The author acknowledges the funding supports from the Natural Science Foundation of China under No. 21573037 and 21873017.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M41 GMAG DMP FIAP DCOMP: Spin Phenomena in Nonmagnetic 2D Materials II 707 - Wei Yuan, University of California, Riverside

11:15AM M41.00001: The Electronic Properties of Quasi-One-Dimensional TiS$_3$ and ZrS$_3$
SIMEON GILBERT (Presenter), University of Nebraska - Lincoln, ANDREW J. YOST, Oklahoma State University, MINGXING LI, Brookhaven National Lab, HEMIAN YI, SOLEIL, ALEXEY LIPATOV, TAKASHI KOMESU, University of Nebraska - Lincoln, JOSÉ AVILA, SOLEIL, ALEXANDER SINITSKII, University of Nebraska - Lincoln, JIAN WANG, Canadian Light Source, MARIA ASENSIO, Madrid Institute of Materials Science, PETER A DOWBEN, University of Nebraska - Lincoln — The transition metal trichalcogenides (TMTs) are an emerging class of 2D materials in which 2D sheets are formed by the van der Waals-like bonding of quasi-1D chains. Here we present our work on the electronic properties of two TMTs, TiS$_3$ and ZrS$_3$, including the experimental band structure from nanospot angle resolved photoemission spectroscopy (nanoARPES). The band structures of both TMTs exhibit strong in-plane anisotropy due to their quasi-1D structure. The extracted effective hole mass for both materials is doubled along the chain direction, giving rise to a preferential charge transport direction. Additionally, high resolution nanoARPES measurements show a spin-orbit coupling splitting at the top of the valence band in TiS$_3$. This spin-orbit coupling splitting is expected to increase for heavier TMTs such as ZrS$_3$ and could be utilized to produce a spin polarized surface current.
11:27AM M41.00002: Origin of Magnetism in undoped and Ta doped anatase TiO$_2$ free-standing films  
SONU DEVI (Presenter), THIRUMALAI VENKATESAN, Natl Univ of Singapore — Thin films of anatase titanium dioxide (TiO$_2$) are semiconducting and exhibit signs of room temperature ferromagnetism. However, the role of the surface, substrate and interface in the observed magnetism are controversial. Here, the magnetic properties of two systems, Ta-doped anatase and undoped-anatase have been studied in detail. To avoid the effects from the substrate as well as interface we have fabricated free-standing films using an epitaxial, water-soluble Sr$_3$Al$_2$O$_6$ sacrificial buffer layer. We have found a strong linear correlation between the observed magnetism and Ta-doping, in addition to an intrinsic contribution. The magnetization exhibits a minimum as a function of the oxygen pressure present during film deposition and the result are consistent with a model where Ti interstitials and oxygen vacancies may be responsible for the magnetism at low oxygen pressure while at the high oxygen pressures, Ti vacancies dominate. This study proves that magnetism in anatase TiO$_2$ system is intrinsic and cannot be arising from either the interface or the substrate.

11:39AM M41.00003: Efficient intrinsic spin-to-charge current conversion in an all-epitaxial single-crystal perovskite-oxide heterostructure of La$_{0.67}$Sr$_{0.33}$MnO$_3$/LaAlO$_3$/SrTiO$_3$* 
SHINOBU OHYA (Presenter), DAISEI ARAKI, LE DUC ANH, SHINGO KANETA, MUNETOSHI SEKI, HITOSHI TABATA, MASAAKI TANAKA, Department of Electrical Engineering and Information Systems, The University of Tokyo — The two-dimensional electron gas formed at the interface between insulating perovskite oxides LaAlO$_3$ (LAO) and SrTiO$_3$ (STO) is promising for efficient spin-charge conversion, so-called the (inverse) Edelstein effect (EE). A giant (inverse) EE has been observed in multilayer structures composed of a polycrystalline ferromagnetic layer and LAO/STO; however, the reported temperature dependences of the (inverse) EE are significantly different from each other, and unified understanding of its real mechanism is still lacking. Here, we demonstrate efficient intrinsic spin-to-charge current conversion in an all-epitaxial single-crystal heterostructure of La$_{0.67}$Sr$_{0.33}$MnO$_3$/LAO/STO, which can suppress spin scattering and give us an ideal environment to investigate intrinsic spin-charge conversion. With decreasing temperature to 20 K, the spin-to-charge current conversion efficiency is drastically enhanced to +6.7 nm, which is the largest value among those reported for LAO/STO. Our band-structure calculation well reproduces this behavior and predicts further enhancement by controlling the Fermi level position [1]. [1] S. Ohya et al., arXiv:1906.06016.

*This work was partly supported by Grants-in-Aid for Scientific Research (No. 18H03860), JST CREST (JPMJCR1777), and the Spin-RNJ.
Magnetic proximity effects in vdW heterostructures of layered materials  

JACOB GOBBO (Presenter), RYAN MUZZIO, IGOR PINCHUK, JYOTI KATOCH, SIMRANJEET SINGH, Carnegie Mellon Univ — The van der Waals (vdW) based heterostructures of different layered materials have emerged as a modular solid-state platform to engineer tunable properties in novel quantum systems. The vdW superlattices offer unprecedented flexibility to tune the interfacial interactions at the atomic scale to engineer spin related phenomena in two-dimensional (2D) materials. In this talk, we will present our preliminary results in the direction of probing magnetic proximity effects in vdW based heterostructures of 2D-magnetic systems and transition metal dichalcogenides (TMDs). We will discuss the preparation of high-quality vdW interfaces of 2D-magnets and TMDs in controlled environment. The proximity induced magnetic correlations in otherwise non-magnetic TMDs are probed through variable temperature magneto-transport measurements and will be discussed in this talk.

Magnetic proximity in a van der Waals heterostructure of magnetic insulator and graphene.

BOGDAN KARPIAK (Presenter), Chalmers Univ of Tech, ARON CUMMINGS, Catalan Institute of Nanoscience and Nanotechnology, KLAUS ZOLLNER, University of Regensburg, MARC VILA, Catalan Institute of Nanoscience and Nanotechnology, DMITRII KHOKHRIAKOV, MD ANAMUL HOQUE, ANDRÉ DANKERT, Chalmers Univ of Tech, PETER SVEDLINDH, Uppsala University, JAROSLAV FABIAN, University of Regensburg, STEPHAN ROCHE, Catalan Institute of Nanoscience and Nanotechnology, SAROJ DASH, Chalmers Univ of Tech — By investigating the the van der Waals heterostructures of the ferromagnetic insulator Cr$_2$Ge$_2$Te$_6$ and graphene, we observe an out-of-plane proximity-induced ferromagnetic exchange interaction in graphene$^1$. The perpendicular magnetic anisotropy of Cr$_2$Ge$_2$Te$_6$ results in significant modification of the spin transport and precession in graphene, which can be ascribed to the proximity-induced exchange interaction. Furthermore, the observation of a larger lifetime for perpendicular spins in comparison to the in-plane counterpart suggests the creation of a proximity-induced anisotropic spin texture in graphene. Our experimental results and density functional theory calculations open up opportunities for the realization of proximity-induced magnetic interactions and spin filters in 2D material heterostructures and can form the basic building blocks for future spintronic and topological quantum devices.


*European Union’s Horizon 2020 (no. 785219), EU FlagEra (VR No. 2015-06813), Swedish Research Council (VR No. 2016-03658), Graphene center and the AoA Nano program at Chalmers University of Technology, CERCA Programme/Generalitat de Catalunya, Severo Ochoa program from Spanish MINECO (Grant No. SEV-2017-0706), “La Caixa” Foundation.
12:15PM M41.00006: Novel Exciton Condensation and Lorenz Number in Graphene  SANG-BOO NAM (Presenter), Retired — We present a novel condensation of boson (exciton = electron + hole) in 2 dimension at the temperature $T_c = (6/\pi^2)^{1/2} T_F$ (fermi temperature). At $T_c$, the condensed bosons are to become fermions, electrons to holes, and vice versa. We found the Lorenz number peak value (LNPV) in the case of the elastic scatterings, \[ \frac{L(b)}{L(0)} - 1 = \frac{2bg}{3}, \] \[ L(0) = \frac{(9/4) \zeta(3)}{\ln 2} = 3.895 = 1.183 \left(\frac{\pi^2}{3}\right) \] in the unit of $(k_B/e)^2$, where $b = \text{boson/fermion} = \frac{2gp}{n}$, $g$ and $n$ are the fermion degeneracy and density, respectively, $p$ the optimum density for the condensation, with the temperature full width (the intrinsic nature) for the half LNPV, $Tw = 2(1 - w) T_c$, $w = \left[\frac{1 + b}{2 + b}\right]^{1/2}$. Calculated LNPV and $Tw$ for $g = 4$, account very well, without any parameter, for the data in graphene by Crossno et al, Science 351, 1058 (2016). We found the optimum $2bg/3 = 64/3$, $p = 4 \times 10^9 /\text{cm}^2$, $v_F = 1.03 \times 10^8 \text{ cm/s}$, $T_c = 45 \text{ K}$, and $Tw = 4.5 \text{ K}$ for graphene. We predict the Hall resistance (Rh) peak value and the plasmon frequency square (Ws) dip value, \[ \frac{Rh(b)}{Rh(0)} - 1 = b = \frac{W_s(0)}{W_s(b)} - 1 , \] respectively, with the same $Tw$ as before.

12:27PM M41.00007: Giant spin-layer locking in novel two-dimensional $X_2Bi_2$ (X=Si, Ge, or Sn)  SEUNGJUN LEE (Presenter), YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee Univ - Seoul — In contrast to the general view in spin-orbit interaction, it was reported that even in materials with centro-symmetry may have Rashba spin-orbit coupling (the R-2 effect) resulting in spatial spin splitting. However, not only its underlying fundamental physics been still unclear, but the search for materials emerging the R-2 interaction has also been very limited. Here, we propose novel two-dimensional materials $X_2Bi_2$ (X=Si, Ge, or Sn), which exhibit spin-layer locking with giant Rashba parameter value ($\alpha_R \leq 12.3 \text{ eV nm}$). Our first principles calculations show the top and bottom atomic sublayers in $X_2Bi_2$ produce opposite out-of-plane dipole moments leading to the spin-layer locking phenomenon for in-plane spin moment. We also find that the local orbital angular momentum (OAM) plays a crucial role in determining the R-2 spin splitting. We further suggest possible manipulation strategies for securing the R-2 spin splitting: 1) Strain reinforces the R-2 effect via changing OAM distribution, and 2) layer stacking ensures further spatial spin splitting.
**12:39PM M41.00008: Edgetronic and spintronic applications of carbon phosphide nanoribbon**

LIEMAO CAO (Presenter), YEE SIN ANG, QINGYUN WU, LAY KEE ANG, Singapore University of Technology and Design — Carbon phosphide (CP) monolayer, a hybrid of graphene and phosphorene that simultaneously preserves their high electrical mobility, finite band gap and air stability, has been successfully synthesized in recent experiment. In this work, we study the electronic and transport properties of CP nanoribbons in α-phase with different edge configurations using first-principle density functional theory simulation. We found that Zα-CPNRs can mimic the behaviors of graphene and phosphorene nanoribbon depending on the edge configurations Intriguingly, when the external electric field exceeds a critical value, the charge transport channel becomes strongly localized to only one edge, and the edge localization can be tuned by an external electric field, thus opening up a new device concept of edgetronics. Our findings reveal the potential of CP nanoribbon as a spintronic materials that fuses the strengths of both graphene and phosphorene.


*Singapore MOE Tier 2 Grant (2018-T2-1-007) and A*STAR IRG Grant (IRG A1783c0011).

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**12:51PM M41.00009: Rashba spin splitting and perpendicular magnetic anisotropy of Gd-adsorbed zigzag graphene nanoribbon modulated by edge states under external electric fields**

ZHENZHEN QIN (Presenter), Zhengzhou Univ, GUANGZHAO QIN, University of South Carolina, BIN SHAO, XU ZUO, Nankai University — The one-dimensional (1D) Rashba effect has become much important due to its key role in basic science to realize exotic electronic phenomena, such as Majorana bound states. Similar to the 2D or 3D systems, the modulation of Rashba effect in 1D matrix is the kernel of spintronics for manipulating electron spin. Herein, by investigating the effects of transverse and vertical external electric field (EEF) on the Rashba spin splitting and magnetic anisotropy energy (MAE) of Gd-adsorbed zigzag graphene nanoribbons from first principles, we found that the Rashba spin splitting in such 1D system can be effectively regulated by the transverse EEF. Moreover, perpendicular magnetic anisotropy holds with either transverse or vertical EEF applied, despite obvious modulation of the MAE contributions in k-space as well as the Rashba spin splitting. It is found the modulation of Gd-5dx^2-y^2, dxy by C-p_z orbitals of edge states is the key to manipulating the magnetic anisotropy, which even plays a decisive role on modifying the Rashba spin splitting in such 1D nanoribbon system. Our study introduces a new strategy to manipulate Rashba spin splitting by edge states and provides new insight into the magnetic anisotropy in 1D Rashba system.
1:03PM M41.00010: Observation of Giant Optical Linear Dichroism and Pseudo Critical Slowing Down in van der Waals Zigzag Antiferromagnets  KYLE HWANGBO (Presenter), QI ZHANG, QIANNI JIANG, University of Washington, DI XIAO, Carnegie Mellon University, JIUN-HAW CHU, XIAODONG XU, University of Washington — Two-dimensional antiferromagnetism (AFM) has been a topic of great interest due to its intertwined relationship with various correlated phenomena like unconventional superconductivity and its potential applicability in novel spintronic devices. In contrast to its ferromagnetic counterpart, direct optical probing and study of AFM order is challenging due to the absence of net magnetization and the resulting weak magneto-optical coupling. Here, we report an optical study of an atomically thin zigzag antiferromagnet, FePS$_3$. We observed a large optical linear dichroism associated with the zigzag AFM order. By performing time-resolved polarimetry measurements, we further examined the critical fluctuations of the AFM order parameter, which exhibit a prominent pseudo-critical slowing down behavior near the Néel temperature. Our findings point to a new optical approach to identify zigzag AFM order and study its non-equilibrium dynamics in strongly correlated systems.

1:15PM M41.00011: Ferromagnetism in multilayered graphite nanostructures doped with nitrogen*  ARAM MANUKYAN, CAL State University, Los Angeles, HARUTYUN GYULASARYAN, Physics, Russian-Armenian (Slavonic) University, Yerevan, Armenia, EDUARD SHAROYAN, Laboratory of Solid State Physics, Armenia, Institute for Physical Research, NAS of Armenia, PAUL OYALA, Division of Chemistry and Chemical Engineering,, California Institute of Technology, Pasadena, OSCAR BERNAL, ARMEN KOCHARIAN (Presenter), CAL State University, Los Angeles — Carbon microspheres consisting of multilayered nanographite structures are prepared using solid-phase pyrolysis of metal-free phthalocyanine H$_2$(C$_{32}$N$_8$H$_{16}$). The mean diameter $d=3\pm0.2\mu$m of carbon microspheres have been obtained at pyrolysis $T_{\text{pyr}}=670^\circ\text{C}$, and $t_{\text{pyr}}=30\text{min}$. Morphology and structure of prepared samples at two temperatures $T_{\text{pyr}}$ were investigated by HRTEM, X-ray diffractometry, Raman and XPS spectroscopy. Magnetic properties of samples were investigated using vibrational magnetometer and magnetic fields up to 80 kOe, as well as X-band ESR spectrometer in range of temperature, $T=5$-300K. We found that the temperature dependences of saturation magnetization closely follow the behavior of integrated magnetic resonance intensity. Parameters of ESR spectrum are following g-factor 2.0031, intensity $\sim5\times10^{19}$ spin/g and narrow linewidth of 0.8Oe due to strong exchange. Maximum values of saturation magnetization $M_s\approx0.03\text{emu/g}$ and coercive force $H_c=400\text{Oe}$ have been obtained at 25K. The results suggest that observed ferromagnetism in multilayer graphene can be attributed to nitrogen atoms and zigzag edges.

*This work supported by Russian-Armenian University from Grant #SCS15T-1C249. The work at CSULA supported by the NSF CREST Grant #HRD-1547723 and PREM programs under Grant DMR-1523588.
Modulating electronic and magnetic properties of ferromagnetic Hf2MnC2O2 MXenes*  
EDIRISURIYA SIRIWARDANE (Presenter), Univ of North Dakota, PRAGALV KARKI, University of Oregon, YEN LEE LOH, DENIZ CAKIR, Univ of North Dakota — In this work, density functional theory calculations were carried out to evaluate the electronic and magnetic properties of the uniaxial and biaxial strains applied, and surface defects introduced Hf2MnC2O2 ferromagnetic MXene. The bare Hf2MnC2O2 monolayer is an indirect bandgap semiconductor with a 0.282 eV bandgap. Our calculations show that the semiconductor-to-half-metal phase transition occurs at 7%, and 9% under uniaxial tensile strain in zig-zag and armchair directions, respectively. The same phase transition can be seen at 8% biaxial tensile strain. This ferromagnetic semiconductor can become a metal under small uniaxial and biaxial compressive strains. We are also able to show that the bare Hf2MnC2O2 monolayer contains an easy-plane anisotropy. The anisotropy of the monolayer transforms into an enhanced, easy-axis anisotropy when the O vacancies and the H adatoms are introduced.

*Computer resources are provided by the Computational Research Center at the University of North Dakota (UND) and the Center for Nanoscale Materials (Contract number: DE-AC0206CH11357). A part of this work was supported by UND Early Career Award (Grant number: 20622-4000-02624) and ND EPSCoR through NSF grant #OIA-1355466.

1:39PM M41.00013: Raman signatures on a van der Waals antiferromagnet  
YUJIN CHO (Presenter), University of California, Los Angeles, SUBHAJIT GHOSH, University of California, Riverside, ZHANGJI ZHAO, CHAOWEI HU, JIN HO KANG, University of California, Los Angeles, FARIBORZ KARGAR, University of California, Riverside, NI NI, University of California, Los Angeles, ALEXANDER BALANDIN, University of California, Riverside, CHEE WEI WONG, University of California, Los Angeles — Mixing other exotic properties, such as magnetism or superconductivity, into a topological material has been drawing a lot of researchers’ attention due to its potential as quantum computation and realizing topological phenomena. MnBi2Te4 has been demonstrated to be the first intrinsic antiferromagnetic (AFM) topological insulator (TI) [1]. It consists of Bi2Te3 and Mn-Te bilayer. So far, most studies focused on magnetic properties or electronic structure of the bulk material via magnetic susceptibility, angle-resolved photo-emission spectroscopy, and magnetotransport [2]. When the material comes down to 2D limits, optical Raman spectroscopy becomes advantageous due to its sensitivity and strong layer-dependent characteristic in 2D materials. Raman peaks can also reflect spin interactions that are related to magnetic ordering [3], as well as in-plane magnetic anisotropy. In this project, we will correlate the optical Raman spectrum on MnBi2Te4 with its magnetic transition temperature (~25K) and the in-plane magnetic anisotropy.

Detection of Spin Canting Using Magnetic Field Modulated Microwave Spectroscopy.  

ALEX HOJEM (Presenter), JAMES WAMPLER, IVAN K. SCHULLER, Physics, University of California, San Diego — Magnetic field modulated microwave spectroscopy (MFMMS) is the most sensitive technique for detecting superconducting transitions[1]. While superconducting transitions exhibit a reproducible peak behavior, magnetic transitions can have a range of responses including: slopes, steps and local minima in the temperature dependent MFMMS measurements. Other work has shown that a magnetic response in a similar microwave spectroscopy technique can be caused by spin canting[2]. One system of materials that provides an interesting test case for this is the Ruthenocuprates[3]. These compounds have a ferromagnetic response due to spin canting, above the onset of superconductivity. Here, we show that the temperature and field dependence of spin canting of the Ru-1212 system (RuSr$_2$GdCu$_2$O$_8$) can be determined by comparing the MFMMS to magnetometry and resistance measurements.


*Supported by AFOSR: FA9550-14-1-0202

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M42 GMAG: Spin Transport and Magnetization Dynamics in Ferrimagnets and Antiferromagnets 709/711 - Himanshu Fulara - Tag(s): Focus
11:15AM M42.00001: Decoherence of transverse spin currents in ferrimagnetic CoGd*  
YOUNGMIN LIM (Presenter), BEHROUZ KHODADADI, Physics, Virginia Tech, JIE-FANG LI, DWIGHT D VIEHLAND, Materials Science and Engineering, Virginia Tech, SATORU EMORI, Physics, Virginia Tech — It has been predicted that the coherence length $\lambda_c$ of transverse spin current in antiferromagnetic and ferrimagnetic metals can be much longer than $\lambda_c \approx 1$ nm in ferromagnets. A recent experiment reports $\lambda_c > 10$ nm in ferrimagnetic CoTb alloys [1], although this is rather surprising given the strong spin-orbit coupling in CoTb. Here, we determine $\lambda_c$ in ferrimagnetic Co$_{1-x}$Gd$_x$ alloys with much weaker spin-orbit coupling than CoTb. We perform spin pumping measurements on NiFe/Cu/CoGd trilayers, where a coherent spin current pumped from NiFe decoheres in the CoGd spin sink. The spin sink thickness dependence of Gilbert damping enhancement of the NiFe layer allows us to quantify $\lambda_c$. We demonstrate a maximum of $\lambda_c \approx 4$ nm for the composition of CoGd close to magnetic compensation, indicating partial enhancement of spin coherence due to compensated antiferromagnetic order. We also observe a monotonically decreasing effective spin-mixing conductance with increasing Gd content, suggesting the dominance of Co 3d bands in spin current transport across the interface of the ferrimagnet.


*This research was funded in part by 4-VA, a collaborative partnership for advancing the Commonwealth of Virginia, and the ICTAS Junior Faculty Award.

11:27AM M42.00002: Thermal Hall effect, spin Nernst effect, and spin density induced by thermal gradient in collinear ferrimagnets from magnon-phonon interaction*  
SUNGJOON PARK (Presenter), Department of Physics and Astronomy, Seoul National University, NAOTO NAGAOSA, Department of Applied Physics, The University of Tokyo, BOHM-JUNG YANG, Department of Physics and Astronomy, Seoul National University — We study the thermal Hall and spin Nernst effect in collinear ferrimagnets on a honeycomb lattice with broken inversion symmetry between the nearest neighbors. The broken inversion symmetry allows nearest-neighbor inplane Dzyaloshinskii-Moriya interaction, which has no effect in the linear spin wave theory. However, it induces large Berry curvature in the magnetoelastic excitation spectrum through the magnon-phonon interaction (MPI) to produce spin-polarized thermal Hall current, so that both spin Nernst and thermal Hall currents are produced. Because the MPI does not conserve the spin, we also compute the boundary spin accumulation. Surprisingly, we do not find any asymmetric boundary spin accumulation, which we attribute to spin nonconservation. However, the MPI induces non-vanishing total spin expectation value in the system with armchair edges.

*This work was supported by IBS-R009-D1(SP), Institute for Basic Science in Korea (IBS-R009-D1) (B.-J.Y), Basic Science Research Program through the National Research Foundation of Korea (0426-20190008)(B.-J.Y), POSCO Science Fellowship of POSCO TJ Park Foundation (0426-20180002) (B.-J.Y), U.S. Army Research Office (W911NF-18-1-0137)(SP, B.-J.Y), JST CREST (JPMJCR1874 and JPMJCR16F1)(NN), and JSPS KAKENHI (18H03676 and 26103006)(NN).
11:39AM M42.00003: Electric-Field Control of Strain-Driven Tuning of FMR in the Low-Loss Ferrimagnetic Coordination Compound V[TCNE]_x

SETH KURFMAN (Presenter), ANDREW FRANSON, Ohio State Univ - Columbus, PIYUSH SHAH, GOPALAN SRINIVASAN, MICHAEL PAGE, Materials and Manufacturing Directorate, Air Force National Laboratory, EZEKIEL JOHNSTON-HALPERIN, Ohio State Univ - Columbus — Electric-field control of magnetic resonance has application potential in the design of low-power, compact, high-frequency magnetoelectronic devices, such as microwave filters and circulators. To date, this work has exploited low-loss ferrite materials mechanically coupled to piezoelectric substrates. However, traditional ferrites typically require lattice-matched substrates and extreme growth conditions to produce high-quality material, making on-chip integration while maintaining low damping a significant challenge. Here, we demonstrate electric-field control of the FMR properties of the low-loss ($\alpha = (3.98 \pm 0.22) \times 10^{-5}$), organic-based, room-temperature ferrimagnet vanadium tetracyanoethylene ($\text{V[TCNE]}_{x \approx 2}$) in $\text{V[TCNE]}_x$/piezoelectric composite heterostructures. These structures show shifts in the resonant frequency position by $\sim 50$ MHz, or more than six times the resonant linewidth. These results demonstrate the potential of $\text{V[TCNE]}_x$ to complement traditional ferrites in electrically-controlled magnetoelectronic devices. For example, since $\text{V[TCNE]}_x$ can be deposited on a variety of inorganic substrates, it has the potential to be directly integrated into magnetoelectric devices without the need for flip-chip fabrication techniques.

**NSF Grant No. DMR-1808704

11:51AM M42.00004: Non-local spin transport measurement in TbIG thin films grown by pulsed laser deposition

WEI YUAN (Presenter), JUNXUE LI, VICTOR ORTIZ, YAWEN LIU, JING SHI, University of California, Riverside — Ferrimagnetic insulators (FMIs) attract a lot of attention in spintronics recently. As a medium, FMIs support pure spin current carried by magnon transport over a relatively long distance. In this work, we use nonlocal method to probe spin transport in terbium iron garnet (Tb$_3$Fe$_5$O$_{12}$ or TbIG). We obtain high-quality epitaxial TbIG thin films on the substrates of GGG(111) using a PLD system. After 750 degree Celsius post-growth rapid thermal annealing, clear RHEED patterns demonstrate the single crystal quality of TbIG films, which is further confirmed by X-ray diffraction and atomic force microscopy results. The non-local signal has a sign reversal at 270 K, which corresponds to the compensation temperature of TbIG. Below the compensation temperature, the non-local signal stays approximately constant until a dramatic increase sets in at 50 K, which persists to the lowest temperature of 2 K. We attribute this rapid increase to the spin current transport associated with paramagnetic Tb-spins. We also discuss the temperature dependence of the nonlocal signal in garnets with and without rare-earth moments.

*We acknowledge SHINES, an Energy Frontier Research Center funded by the U.S. Department of energy, Office of Science, Basic Energy Sciences, award no. SC0012670
**12:03PM M42.00005: Anomalous spin Hall angle of a metallic ferromagnet determined by a multiterminal spin injection/detection device**

TOBIAS WIMMER (Presenter), Bayerische Akademie der Wissenschaften, Walther-Meißner-Institut, BIRTE COESTER, Spintronics Device Research Group, Nanyang Technological University, STEPHAN GEPRÄGS, RUDOLF O GROSS, Bayerische Akademie der Wissenschaften, Walther-Meißner-Institut, SEBASTIAN T. B. GOENNENWEIN, Technische Universität Dresden, HANS HUEBL, MATTHIAS K ALTHAMMER, Bayerische Akademie der Wissenschaften, Walther-Meißner-Institut — We report on the determination of the anomalous spin Hall angle in the ferromagnetic metal alloy cobalt-iron (Co$_{25}$Fe$_{75}$, CoFe). This is accomplished by measuring the spin injection/detection efficiency in a multiterminal device with nanowires of platinum (Pt) and CoFe deposited onto the magnetic insulator yttrium iron garnet (Y$_3$Fe$_5$O$_{12}$, YIG). Applying a spin-resistor model to our multiterminal spin transport data, we determine the magnon conductivity in YIG, the spin conductance at the YIG/CoFe interface and finally the anomalous spin Hall angle of CoFe as a function of its spin diffusion length in a single device. Our experiments clearly reveal a negative anomalous spin Hall angle of the ferromagnetic metal CoFe, but a vanishing ordinary spin Hall angle. This work therefore adds new observations to the results reported in Refs. [1,2], where the authors found finite contributions of the ordinary spin Hall angle in the ferromagnetic metals Co and permalloy.


*This work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany’s Excellence Strategy -- EXC-2111 -- 390814868 and project AL2110/2-1.*
12:15PM M42.00006: Investigation of nonequilibrium processes of magnetoelastic waves and evidence of their BEC formation in an antiferromagnetic system* VLADIMIR L SAFONOV, DEREK BAS, Air Force Research Laboratory, YURI V ROSTOVTSEV, JAMES A ROBERTS, Department of Physics, University of North Texas, DIANA BERMAN, Department of Materials Science and Engineering, University of North Texas, MICHAEL E MCCONNEY, MICHAEL PAGE (Presenter), Air Force Research Laboratory — The canted antiferromagnet FeBO$_3$ exhibits strong nonlinear interactions between magnetoelastic waves that can manifest as a variety of interesting phenomena. We show that excited magnetoelastic waves and their quanta, which we refer to as mexons, exhibit a wide range of nonequilibrium nonlinear wave phenomena including mode competition under noisy pumping, full submission to external coherent fields, and evidence of quasi-equilibrium Bose-Einstein condensation (BEC) at room temperature. The mode we suggest as the mexon BEC exhibits extremely high efficiency with a quality factor of $Q \sim 8 \times 10^5$. Remarkably, this behavior occurs in a system that is very near its transition temperature due to the heat generated by microwave pumping. Our results suggest that such systems can be of technological importance due to the uniqueness of the mode quality and ability to modulate external signals, as well as from the standpoint of studying a whole class of nonlinear wave phenomena usually taking place in a wide range of environments and conditions.

*The work was partially supported by the Air Force Office of Scientific Research (AFOSR) Award No. FA9550-15RXCOR198.

12:27PM M42.00007: Elimination of two-magnon scattering for evaluation of intrinsic spin decay length in antiferromagnetic insulator* HIROTO SAKIMURA (Presenter), TAKASHI HARUMOTO, YOSHIO NAKAMURA, JI SHI, School of Materials and Chemical Technology, Tokyo Institute of Technology, KAZUYA ANDO, Applied Physics and Physico-Informatics, Keio University — We present an experimental evaluation of the intrinsic spin decay length in an antiferromagnetic insulator (AFI). A frequently-used sample configuration to study the spin-current propagation in AFIs is a ferromagnet/AFI/heavy-metal trilayer structures, where the ferromagnet and heavy-metal act as spin-current injectors and detectors, respectively. We found that at the ferromagnet/AFI interface, a spin current generated by spin pumping is strongly suppressed by two-magnon scattering enhanced by position-dependent fluctuation of microscopic exchange bias, which is inevitable at ferromagnet/antiferromagnet junctions. By eliminating the two-magnon contribution from the spin transmission signal, we discovered that the characteristic length of spin decay in polycrystalline NiO, a prototypical AFI, was around 100 nm, which is an order of magnitude longer than what was previously believed. Our results provide a new perspective in the emerging field of antiferromagnetic spintronics, especially for the fundamental understanding of spin transport physics in insulators.

*JSPS Grant-in-Aid for Research Fellowship for Young Scientists (DC1) No. JP17J03624
12:39PM M42.00008: Nuclear spin Seebeck effect in antiferromagnets  DEREK REITZ
(Presenter), YAROSLAV TSERKOVNYAK, University of California, Los Angeles — The spin Seebeck effect (SSE) involves transfer of spin angular momentum between a magnet and a metal from internal thermal fluctuations. SSE is usually dominated by electronic, rather than nuclear, spins, since interfacial exchange is much stronger than interfacial hyperfine coupling. At low temperatures, however, electronic magnon thermal occupation numbers are exponentially suppressed, while nuclear spins remain active. The nuclear spins are paramagnetic, weakly polarized in the large hyperfine field of the Neel order. One source for nuclear SSE is interfacial nuclear, metal spin flip-flops, known as Korringa relaxation. Nuclear SSE is then determined by competing rates: thermalization with phonons via hyperfine coupling to electrons in the magnet, and Korringa relaxation into the metal.

12:51PM M42.00009: Topological Hall effect in canted antiferromagnets  JOTARO NAKANE
(Presenter), Physics, Nagoya University, KAZUKI NAKAZAWA, Earth and Space Science, Osaka University, HIROSHI KOHNO, Physics, Nagoya University — The topological Hall effect (THE) is a Hall effect caused by a noncoplanar spin texture, or its spin chirality, in ferromagnetic conductors. This effect is absent in antiferromagnets (AF) due to the cancellation of the two sublattice chiralities. However, if the AF spins are canted, the overall spin chirality, hence the THE, can be finite.

Motivated by a recent experiment [1], we study the THE in a canted AF with textured Neel and uniform moments. Treating the two textures by a spin gauge field, we derive an analytical expression for the topological Hall conductivity (THC). The emergent magnetic field is written as $\nabla \times A$, where A is an emergent vector potential in canted AF. With the obtained THC, we discuss various regimes such as the strong and weak coupling regimes, and large and small canting regimes. In particular, in the strong-coupling large-canting limit, the THC is given by the Berry phase formula ("Bruno formula") multiplied by a reduction factor because of the presence of the Neel moment.

Magnetization dynamics and spin transport in compensated ferrimagnets [invited]  KYUNG-JIN LEE (Presenter), Korea Univ — Spintronics is a multidisciplinary field whose central theme is the active manipulation of electron spins in solid-state systems. The core magnetic system for spintronics research has been ferromagnets since they serve as spin-polarizers/detectors and offer non-volatile memory and logic technologies. Recently, much effort has been expended in employing antiferromagnetic coupled systems as core elements because of their fast dynamics and efficient spin-torque generation. We will discuss the underlying mechanism of fast dynamics of compensated and uncompensated staggered spin moments, driven by magnetic fields or spin torques [1-3]. We will also discuss the increased efficiency of spin torques due the weakened spin dephasing in compensated ferrimagnets [4,5].

References

Thermal spin-Edelstein effect in an antiferromagnetic insulator/normal metal heterostructure*  HANTAO ZHANG (Presenter), RAN CHENG, University of California, Riverside — In an antiferromagnetic insulator with biaxial anisotropy and the Dzyaloshinskii-Moriya interaction (DMI), symmetry ensures a spin-momentum locking similar to that of gapped Rashba electrons. A temperature gradient can generate an interfacial magnon accumulation with a preferred spin polarization, realizing the magnonic counterpart of the spin Edelstein effect. This thermally-driven magnonic spin accumulation can be injected into an adjacent heavy metal and converted into a measurable voltage, which depends monotonically on both temperature and DMI but non-monotonically on the surface-induced magnetic anisotropy. It is found that the overall response coefficient has to be solved under a nontrivial boundary condition regarding spin transmission across the interface.

*This work is supported by MURI of AFOSR with award No. FA9550-19-0307 and subaward No. 24086226-04.
Strain-Tunable Magnetic Anisotropy in Sputtered Thulium Iron Garnet (TIG) Thin Films and TIG/Au/TIG Trilayers*

GILVANIA DA SILVA VILELA (Presenter), Plasma Science and Fusion Center, and Francis Bitter Magnet Laboratory, MIT and Universidade de Pernambuco, HANG CHI, Plasma Science and Fusion Center, and Francis Bitter Magnet Laboratory, and U.S. Army CCDC, MIT and Army Research Laboratory, GREGORY STEPHEN, Department of Physics, Northeastern University, CHARLES SETTENS, Materials Research Laboratory, MIT, PRESTON ZHOU, Department of Electrical Engineering, California Institute of Technology, YUNBO OU, DHAVALA SURI, Plasma Science and Fusion Center, and Francis Bitter Magnet Laboratory, MIT, DON HEIMAN, Department of Physics, Northeastern University, JAGADEESH MOODERA, Plasma Science and Fusion Center, and Francis Bitter Magnet Laboratory, and Department of Physics, MIT — Ferromagnetic insulator thin films have been explored for developing spintronic devices. When combined with quantum materials, the strongly correlated interaction from the proximitized interface results in intense local magnetic fields which modulates them to displaying new interface physical phenomena. We investigate ways to tune the magnetic anisotropy in TIG films by selecting their thickness, substrate, and annealing conditions. When deposited over (111) GGG, they present a negative magnetostriction constant which favors a perpendicular magnetic anisotropy (PMA). While PMA allows high magnetic storage density in hard disk drives, it is required for breaking the time-reversal symmetry in topological insulators (TIs) to aim towards quantized anomalous Hall state in TIs. Controlling the film preparation parameters we observed that TIG films under compressive strain display an in-plane magnetic anisotropy, whereas films under tensile strain demonstrated PMA. These results led to the successful fabrication of TIG/Au/TIG magnon valve structures with independent magnetic switching of each TIG layer.

*This work was supported by ARO (W911NF-19-2-0041 and W911NF-19-2-0015), NSF (DMR 1700137), ONR (N00014-16-1-2657), and CAPES (Gilvania Vilela/POS-DOC-88881.120327/2016-01), FACEPE, CNPq.

Quantum Dynamics of Matrix Product States on Transformed bases*

AMIR MOHAMMADAGHAEI (Presenter), KIRILL SHTENGEL, University of California, Riverside — Numerical simulation of the quantum states under the unitary evolution with generic non-integrable Hamiltonians still remains a challenge. The exact diagonalization (ED) method only works for very small system sizes and methods based on matrix product states (MPS), such as time dependent variational principle (TDVP) fail to capture long time behavior of the systems, such as the diffusion constant, with controlled precision. The main culprit is believed to be the rapid entanglement growth to volume-law in real space cuts. The entanglement blow-up makes the long-times inaccessible for variational ansatz that are designed to represent states with area-law entanglement entropy. In this work, we explore a MPS time evolution but on a set of transformed bases that are local both in real and fourier space. We benchmark this method on the anti-ferromagnetic Heisenberg chain with longer range exchange terms to bring the system out of integrability. We demonstrate the possibility of achieving longer time simulations by comparing the results to exact ED as well as TDVP on real space.

*BSF grant 2016255
11:15AM M43.00001: Computationally driven discovery of new borides in the ternary Li-Ni-B system* [Invited] JULIA ZAIKINA (Presenter), Department of Chemistry, Iowa State University — The crystal structure prediction of multinary inorganic materials is a challenging task given the diversity of potential structures. Experimental validation of the computational predictions is a vital step for accelerated materials discovery, however solid state chemistry synthetic routes lack the predictability of the synthesis outcome. Yet, theoretical predictions of structure and thermodynamic stability of the new ternary phases can yield the desired roadmap for the targeted synthesis. On the other hand, efficient synthesis allows for the fast screening of compositional space, providing timely feedback for the iterative improvement of theoretical predictions. 

Here we report on two novel lithium nickel boride polymorphs RT-LiNiB and HT-LiNiB with layered crystal structures.¹ This family of compounds was theoretically predicted by using the adaptive genetic algorithm (AGA)² and subsequently synthesized by a hydride route with LiH as the lithium source. Unique among the known ternary transition-metal borides, the LiNiB structures feature Li layers alternating with almost planar [NiB] layers. A comprehensive study using a combination of single-crystal/synchrotron powder X-ray diffraction, solid-state NMR spectroscopy, scanning transmission electron microscopy, quantum-chemical calculations, and magnetism revealed on the intrinsic features of these polymorphic compounds. The unique layered structures of LiNiB compounds make them ultimate precursors for preparation of two-dimensional transition-metal borides, MBenes.

*Financial support from the Iowa State University is gratefully acknowledged.
11:51AM M43.00002: Corrosion-resistant magnesium alloy design based on the first-principles calculation  
YAOWEI WANG (Presenter), TIAN XIE, ZHE LUO, HONG ZHU, XIAOQIN ZENG, Shanghai Jiao Tong Univ — Second phase strengthening has been widely used in alloys designs, many of which however have been reported to enhance the galvanic corrosion of magnesium alloys. In this study, a semi-empirical model was proposed based on the first principles calculation to analyze the galvanic corrosion behaviour. Our model is validated in the case of Mg-Ge alloys, which is composed of anode Mg matrix and cathode Mg$_2$Ge second phase. First principles calculations on the hydrogen evolution reaction upon Mg$_2$Ge reveal that the rate-determining step is the hydrogen adsorption, which is extremely energetically unfavored but an inevitable intermediate state. The estimated exchange current of the hydrogen evolution upon Mg$_2$Ge is about 3 orders of magnitude smaller than that on pure Mg, indicating the depressed galvanic corrosion of the Mg-Ge alloys is the result of the low hydrogen exchange current upon Mg$_2$Ge. Moreover, some typical intermetallics, such as MgZn$_2$ and MgSc, were selected to compare the corrosion properties of different Mg alloys, which is in close agreement with the experimental observations. Our model provides a promising perspective for designing better corrosion-resistant magnesium alloys.

12:03PM M43.00003: Automation of the first-principles calculation to search functional materials in high entropy alloys*  
HIORI KINO (Presenter), Natl Inst for Materials Sci, TETSUYA FUKUSHIMA, ISSP, University of Tokyo, TOYOHIRO CHIYO, Natl Inst for Materials Sci — The high entropy alloys attract much attention originally because of strength/hardness. They are potentially also useful as functional materials, such as high Curie temperature and high magnetic moment, and large spin-orbit coupling. However, the difficulty of the research of the high entropy alloys is that there exist too huge number of possibilities for humans to handle. Therefore, it is wise and inevitable to screen materials that have high functionality in the first-principles before executing experiments. We will introduce a newly developed scientific workflow to converge the electric structure self-consistently and to estimate physical properties of random alloys automatically in the first-principles calculation, KKR-CPA. We will also introduce some of the first-principles results, and explain key features for high Curie temperatures and high magnetic moment.

*This work is partially supported by MI^2I.
YING SUN (Presenter), JIAN LV, YU XIE, HANYU LIU, YANMING MA, State Key Laboratory for Superhard Materials, College of Physics, Jilin University — The recent theory-orientated discovery of record high-temperature superconductivity ($T_c \sim 250$ K) in sodalitelike clathrate LaH$_{10}$ [1-4] is an important advance toward room-temperature superconductors. Here, we identify an alternative clathrate structure in ternary Li$_2$MgH$_{16}$ with a remarkably high estimated $T_c$ of $\sim 473$ K at 250 GPa, which may allow us to obtain room-temperature or even higher-temperature superconductivity. The ternary compound mimics a Li- or electron-doped binary hydride of MgH$_{16}$. The parent hydride contains H$_2$ molecules and is not a good superconductor. The extra electrons introduced break up the H$_2$ molecules, increasing the amount of atomic hydrogen compared with the parent hydride, which is necessary for stabilizing the clathrate structure or other high-$T_c$ structures. Our results provide a viable strategy for tuning the superconductivity of hydrogen-rich hydrides by donating electrons to hydrides via metal doping. Our approach may pave the way for finding high-$T_c$ superconductors in a variety of ternary or quaternary hydrides.


CHANG-JONG KANG (Presenter), GABRIEL KOTLIAR, Rutgers University, New Brunswick — We apply material design methodology and find a new indium iodine compound, CsInI$_3$, which is thermodynamically stable but is not reported in Inorganic Crystal Structure Database (ICSD) yet. By using the ab initio evolutionary algorithm, we find several meta-stable structures of CsInI$_3$ and investigate their physical properties. The ideal cubic perovskite structure, which is one of the meta-stable phases, shows the structural instability of the iodine breathing mode at zero temperature. However, the cubic perovskite is eventually stabilized at finite temperature due to the contribution of the phonon entropy. The cubic perovskite shows band inversion above the Fermi level, indicating that it is a topological material. Other meta-stable structures are derived from the cubic perovskite and have two different sizes of indium octahedrons, thereby presenting bond and charge disproportionation. The new compound of CsInI$_3$ presents diverse physics including bond and charge disproportionation, topological nature, and a possible application for photovoltaics, thereby providing an ideal playground for these research fields.
A MoON Race: Computational Design of a Heteroanionic Metal-Insulator Transition Compound Molybdenum Oxynitride.* LAUREN WALTERS (Presenter), NATHAN J SZYMANSKI, DANilo PUGGIONI, JAMES RONDINELLI, Northwestern University — Using symmetry principles and electronic structure calculations we designed a novel metal-insulator transition (MIT) compound MoON. The alpha and beta phase of this material were identified from a set of prototype AB\textsubscript{2} structures based upon energetics, band gap, and the c/a ratio. We show that the \textit{fac} ordering of the polyhedra are important for charge localization, singlet formation, and opening of the band gap. Our density functional calculations show how changes in the electronic band gap are driven by structural distortions, including 1D chain canting and dimer formation. Last we draw parallels between MoON and the well-studied VO\textsubscript{2}, demonstrating that properties such as the c/a lattice parameter ratio could be used for further design and identification of other rutile MIT materials.

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From materials discovery to solar cells: LaYS\textsubscript{3} as a product of the computation/experiment loop ANDREA CROVETTO (Presenter), RASMUS NIELSEN, MOHNISH PANDEY, KARSTEN WEDEL-JACOBSEN, OLE HANSEN, BRIAN SEGER, IB CHORKENDORFF, PETER VESBORG, DTU Physics, Technical University of Denmark — One of the current key challenges in solar photovoltaics and solar-driven water splitting is to identify an efficient, stable, and inexpensive material to be used as a high-band gap (1.6-2.0 eV) absorber in tandem devices. With this purpose in mind, we have computationally screened 705 sulfide perovskites (ABS\textsubscript{3}). Only 15 compounds pass all the screening rounds, which include criteria such as phase stability, suitable band gap, low effective mass, and defect tolerance. The list of 15 compounds includes a number of materials that have not yet been reported experimentally. We have therefore attempted to synthesize some of those novel ABS\textsubscript{3} compounds. Among them, LaYS\textsubscript{3} was experimentally confirmed as a stable and especially attractive high-band gap photoabsorber [1], and it was possible to fabricate some prototype LaYS\textsubscript{3} solar cells [2].

In this contribution, we will use our work on LaYS\textsubscript{3} to reflect upon challenges and opportunities in the much-cherished computation/experiment loop for the discovery new materials. In particular, we will discuss the gaps between measured and calculated properties, and the feedback received from the computational and experimental teams.

Ab initio prediction of Metal Organic Frameworks* JAMES DARBY

(Presenter), Department of Physics, University of Cambridge, MIHAELS ARHANGELSKIS, Faculty of Chemistry, University of Warsaw, ATHANASSIOS KATSENIS, JOSEPH MARRETT, TOMISLAV FRIŠČIĆ, Department of Chemistry, McGill University, ANDREW J MORRIS, Univ of Birmingham — First-principles crystal structure prediction is a well established technique which is routinely used across a diverse range of systems such as periodic solids, interfaces, and encapsulated nanowires. Here we present the first example of ab initio prediction of a Metal-Organic Framework (MOF).

We use the Ab Inito Random Structure Searching\(^1\) method and introduce a new approach for generating trial crystal structures from molecular fragments\(^2\). Our method makes use of molecular symmetries to directly generate structures with molecules on special Wyckoff sites. To test our approach we searched for a selection of Zinc based MOFs with differing ligands and metal coordination. These results are presented alongside a more detailed discussion of the method and its application beyond MOFs.


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Predicting the phase stability of high entropy oxides

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Theoretical and computational methods for accelerated materials discovery

*NIKOLAI A ZARKEVICH (Presenter), DUANE D JOHNSON, Ames Laboratory, Iowa State University — Predicting properties of materials and phase transformation using theoretical and computational multi-scale methods involving artificial intelligence and machine learning is important and highly rewarding. We investigate reliability of the relevant methods, apply them to caloric materials and high-entropy alloys, and demonstrate how theoretical guidance for experiment accelerates materials discovery.

*We acknowledge support by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. Consideration of phase transitions in caloric materials is partially supported by the U.S. DOE, Advanced Manufacturing Office of the Office of Energy Efficiency and Renewable Energy, through CaloriCool(TM). Ames Laboratory is operated for DOE by Iowa State University under Contract No. DE-AC02-07CH11358.
1:39PM M43.00011: Stabilities and electronic structures of XYZ$_2$ thermoelectric materials

LIU KE, CAI XIAOMENG (Presenter), HONG ZHU, Shanghai Jiao Tong Univ — A new class of high-performance thermoelectric materials XYZ$_2$ has been revealed based on high-throughput simulations. But they could also have multiple phase transformations similar to many other high-performance thermoelectric materials like PbTe. Thus, it's important to study the stability and electronic structure of different phases, and how these are related to the chemistry of the compound. The phase stabilities have been assessed by support vector machine methodology. We find compounds with larger X ionic radius have P3m1 space group with X ion in octahedral interstices, while smaller X ionic radius favors a tetrahedral site occupation with a space group of the compound of I-42d. Based on the gradient boosting algorithm, density of states effective mass $m^*_S$ and fermi surface complexity factor $N^*_V*K*$ are identified as important descriptors to enhance $zT$ values. Compounds with larger $m^*_S$ have a flat band to enhance Seebeck coefficient if the X-$s$ (Y-$d$) orbitals have similar energy with Z-$p$ orbital near the VBM. Cu and Ag based compounds with P3m1 space group are benefited from the Y-$d$ orbital contribution to the high $N^*_V*K*$. These results demonstrate altering ionic size and molecular orbitals may be used in strategies to improve the thermoelectric performance of XYZ$_2$ compounds.

1:51PM M43.00012: The analytic metric for geometric series diffraction from icosahedral quasicrystals

ANTONY BOURDILLON (Presenter), emeritus, UHRL — Sharp diffraction patterns show long range order [1] in i-Al$_6$Mn; translational symmetry is seen—by phase-contrast, optimum-defocus imaging—to be hierarchic. The icosahedral diffraction pattern was novel in two ways: that it included five-fold symmetric axes; having moreover diffraction orders in geometric series, imprecisely called Fibonacci. The orders differ from Bragg diffraction which is linear. How does a plane wave X-ray, or electron beam, scatter off the hierarchic structure? The diffraction angles due to scattering from the quasiperiodic solid diverge from Bragg conditions: quasi-Bragg angles are derived from quasi-structure factors with a metric that is derived numerically and analytically. The metric is a conversion factor, $1/(\tau-0.5)$, where $\tau$ is the golden section: the metric harmonizes the incident sine wave with hierarchic scattering (all atoms scatter) while the response occurs in geometric series. The hierarchic structure is represented by triads of golden rectangles, each having principal planes, separated by spaces in geometric series, like the diffraction pattern [2]. [1] Shechtman, D, et al. (1984) Phys. Rev. Lett. 53, 1951, http://dx.doi.org/10.1103/PhysRevLett.53.1951 [2] A.J.Bourdillon, A.J., J. Mod. Phys. 10 [6] 624 (2019), DOI: 10.4263/jmp.2019.106044
2:03PM M43.00013: Elucidating the role of anharmonic effects in understanding oxidation of methane  PREETI BHUMLA (Presenter), SASWATA BHATTACHARYA, Dept of Physics, Indian Institute of Technology Delhi, New Delhi —
In heterogeneous catalysis, materials property changes under operational environment (temperature ($T$), pressure ($p$)). Here we study $T$, $p$ dependence of the composition, structure, and stability of metal oxide clusters using a relevant model system for practical applications: free transition metal (Ni) clusters in a combined oxygen and methane atmosphere. We have employed a robust methodological approach that integrates various levels of theory combined into one multi-scale simulation. To obtain the global minimum structures of the Ni$_4$O$_x$(CH$_4$)$_y$ clusters, an extensive data set is generated using a massively parallel cascade genetic algorithm at the hybrid density functional level. The low energy clusters obtained from GA are further analysed to estimate their free energy of formation at realistic $T$, $p_{O_2}$ and $p_{CH_4}$. By analyzing this large dataset, we show that the conventional harmonic approximation miserably fails to predict thermodynamic stability and capturing the anharmonic effects to the vibration free energy contribution is indispensable. To include the anharmonic vibrational free energy to the configurational entropy, we evaluate the excess free energy of the clusters numerically by thermodynamic integration with ab initio molecular dynamics simulation inputs.

Wednesday, March 4, 2020 11:15 AM - 1:51 PM

Session M44 DCOMP: Heat Transport in Condensed Systems II 704 - Elif Ertekin, University of Illinois at Urbana-Champaign - Tag(s): Focus

11:15AM M44.00001: Coherent phonon manipulation in van der Waals Graphene-MoS$_2$ Hetero-structure  SHIQIAN HU (Presenter), JUNICHIRO SHIOMI, Univ of Tokyo — Generally, the difference in the intrinsic lattice structures of the constituent materials inevitably generates interface disorder during the fabrication process, greatly limiting direct experimental observation of the coherent phonon transport. The flexible integration and atomistic interlayer smoothness of van der Waals hetero-structure provide an ideal platform for the coherent phonon transport manipulation. Thus, in this work, using the non-equilibrium molecular dynamics simulations, we investigate the coherent phonon transport in van der Waals graphene-MoS$_2$ hetero-structure with different stacking order at room temperature. The histogram of the phonon transmissions in different disordered structure exhibits a log-normal distribution, which reveals the localization of the coherent phonons. Furthermore, the optimal stacking order of the graphene and MoS$_2$ is efficiently identified from tens of thousands of candidates by machine learning. The significantly suppressed of the phonon transmission in the low frequency (<5THz) phonons of the optimized structure lead to a significant reduction (~95%) of the thermal conductance compared with the graphite. Finally, the effects of the temperature and strain effect on the graphite and optimized structures are also discussed.
Amorphous-like Thermal Conductivity in Crystalline Solids

Thermoelectric materials (TEs) could play an important role in future energy management through environmentally sound cooling and power generation, e.g., converting waste heat into electricity. Efficient TEs inhibit the propagation of heat (low thermal conductivity, $\kappa$) but conduct electricity well (high power factor). Although $\kappa$ in a given material can be reduced via alloying and nanostructuring, identifying materials with intrinsically low $\kappa$ is still needed. Previously, it has been shown that soft phonon modes due to weakly bonded atoms and $s^2$ lone-pair electrons are common to materials with low-$\kappa$. Here, we predict a series of new materials which are weakly bonded systems with same constituent elements but different stoichiometry either with $s^2$ lone-pair electrons or high mass density. Due to resulting giant phonon anharmonicity and low phonon group velocities, they offer extremely low $\kappa$ (0.3-0.6 W/mK) at 300K approaching those found in the amorphous/disordered regime. In addition to low-$\kappa$, high Seebeck coefficients and high electrical conductivities in these materials may provide a new opportunities for high-efficiency thermoelectrics at room temperature.

*This work was supported by the Office of Naval Research and NRC Research Associateship.

Characterization of Phonon Dynamics and Thermal Environments in FinFET Architectures

Physical device scaling for traditional chip architectures is expected to end by 2021. As a result, alternatives are being aggressively pursued that can meet the increasing computing demands imposed by data-centric computing and sensor networks. Three-dimensional IC architectures are particularly promising due to high levels of integration and enhanced performance. However, increased integration leads to thermal bottlenecks that greatly reduce device performance. To understand the bottlenecks, we use atomistic modeling techniques to characterize the nanoscale phonon dynamics and map the thermal landscape of modern fin field-effect transistors (FinFET). We identify phonon modes of FinFET subcomponents that contribute strongly to thermal transport using a lattice dynamics (LD) framework based on a quasi-harmonic Green-Kubo approximation. In parallel, we generate subcomponent temperature profiles using molecular dynamics (MD) simulations. We establish a relationship between the MD temperature profiles and the corresponding populations of the LD-identified phonon modes using a machine learning algorithm. This relationship is used to predict the full phonon dynamics of the entire FinFET device.

*This project is funded by the National Science Foundation [Award No.: HDR-DIRSE-1940153].
Advances in material science and fabrication techniques enabled the fabrication of samples with nanometric dimensions where it is possible to control the propagation of photons (NIR range) and acoustic-phonons (GHz-THz frequencies) in a single device. In this presentation, I will describe the behavior of a plethora of devices able to control acoustic phonons and the interactions with light and charge at the nanoscale [1-3]. I will introduce some strategies to generate, manipulate and detect ultra-high frequency acoustic phonons both in the time and spectral domains [4-5].

The presented results open a new playground in the control of acoustic vibrations in solids and constitute a new platform to study topological effects, quantum phenomena, and thermal transport properties.

[5] M. Esmann et al., Brillouin scattering in hybrid optophononic Bragg micropillar resonators at 300 GHz, Optica 6, 854, 2019

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12:27PM M44.00005: Complex bond distortion behaviors of anharmonic thermal carriers in van der Waals bonded molecular crystal α-RDX* GAURAV KUMAR (Presenter), PETER W. CHUNG, University of Maryland, College Park — Understanding of phonon properties in molecular crystals is critical due to their influence over, for instance, sensitivity of explosives, and charge separation in organic semiconductors. In particular, hot-spot formation in shocked energetic materials, are known to follow from bond scission events. However, the phonon-mediated mechanisms that promote bond breaking are still unclear. In this work, we examine how distortion of bonds carry heat in van der Waals bonded molecular crystal α-RDX. We rank order the phonons and their distortions to the lattice by their importance as carriers of heat. The motions of the atoms that constitute the bond distortions are determined using the phonon mode energy and mode shapes under the harmonic approximation. We also estimate the thermal conductivity of α-RDX using the Allen-Feldman (AF) harmonic theory. The AF model takes into account the contribution of highly anharmonic diffusive carriers which dominate thermal transport in many molecular crystals. Our preliminary results indicate that the the low frequency modes (< 4 THz) contribute ~90% to the total thermal conductivity as well as ~90% to the total bond strain, among which N-N and N-O bonds were found to exhibit the largest strains and rotations.

*Kulkarni Summer Research Fellowship

12:39PM M44.00006: Ab initio-based scanning Seebeck microscopy simulation of epitaxial graphene on 6H-SiC EUICHEOL SHIN (Presenter), YONG-HYUN KIM, Department of Physics, KAIST — Heat, diffusive and incoherent phenomena, has not been considered as surface scanning means. In spite of those characteristics of heat, the local variation of charge carrier was shown by using coherent electron transport via the temperature difference between tip and sample which is so-called scanning thermoelectric microscopy (SThm). It successfully measured atomic-scale local majority carriers variation at room temperature.

We conducted first-principle scanning Seebeck microscopy (SSM) simulation in order to explain heat-based SThM images. The SSM simulation of freestanding monolayer graphene could successively reproduce the experimental thermoelectric contrast between carbon and void sites at the atomic scale. More importantly, SThM for the supported graphene showed the unique oblique slope of the thermoelectric voltage between A and B sites in graphene unit cell stem from the difference of local charge carrier environment.

Here, SSM simulations for free-standing bilayer graphene and supported monolayer graphene on 6H-SiC are numerically demonstrated. The Seebeck profile of both cases was able to show the opposite results of A and B sites depending on the Fermi energy, and the oblique slope of the previous study could not be explained.
12:51PM M44.00007: First-principles study of enhanced thermal conductivity in ordered AlGaO₃ alloys*  
SAI MU (Presenter), Materials Department, University of California, Santa Barbara,  
HARTWIN PEELAERS, Department of Physics and Astronomy, University of Kansas, CHRIS VAN DE WALLÉ, Materials Department, University of California, Santa Barbara — Monoclinic gallium oxide (Ga₂O₃) has promising applications in high-power and high-frequency electronics due to its wide band gap. However, practical device applications are hampered by its low thermal conductivity. To improve the thermal properties of Ga₂O₃ devices, we propose to alloy Ga₂O₃ with Al₂O₃, forming a low-energy ordered structure at the 50% concentration [1]. We investigate the lattice thermal conductivity of monoclinic Ga₂O₃ and of the ordered AlGaO₃ alloy using the phonon Boltzmann transport equation, with the harmonic and third-order anharmonic force constants calculated from density functional theory. We find that the thermal conductivity of AlGaO₃ is raised by more than 70% compared to Ga₂O₃. The enhancement is ascribed to (1) increased group velocities and (2) reduced anharmonic scattering rates due to the reduced weighted phase space. The findings offer an avenue towards improved heat dissipation from Ga₂O₃ devices.  
The work was supported by the GAME MURI of the Air Force Office of Scientific Research.  


*The work was supported by the GAME MURI of the Air Force Office of Scientific Research.

1:03PM M44.00008: Disentangling mass effects from crystal chemistry in the thermal properties of III-V insulators*  
SABRINA J LI (Presenter), ETHAN RITZ, NICOLE A BENEDEK, Cornell University — B₃As, a III-V insulator, has a thermal conductivity comparable to diamond and a higher thermal conductivity than other cubic III-V boron compounds. The origin of this high thermal conductivity has been attributed to the mass ratio and unique chemical bonding character of B₃As, both of which give rise to specific features in the phonon dispersion curve. We use first-principles density functional theory in combination with the Boltzmann transport equation to systematically explore and disentangle the effects of mass ratio and bonding and chemistry on the thermal conductivity of the entire column of cubic III-V boron compounds, from c-BN to BSb. Our preliminary results and previous work [J. Appl. Phys. 116 073503 (2014)] suggest that although the mass ratio of B₃As may optimally maximize thermal conductivity, there may be a pathway to further increasing thermal conductivity through modifying bonding and chemistry. Our work provides hints regarding the chemical characteristics of high thermal conductivity materials.  

*This work was supported by the National Science Foundation under award DMR-1550347.
1:15PM M44.00009: Precise yet Fast High-Throughput Search for Thermal Insulators
FLORIAN KNOOP, THOMAS A PURCELL (Presenter), MATTHIAS SCHEFFLER, CHRISTIAN CARBOGNO,
Fritz Haber Institute of the Max Planck Society, Berlin — We present a systematic and numerically precise computational search for thermal insulators in material space performed with the FHI-vibes high-throughput framework [1]. FHI-vibes employs a robust metric that quantifies the degree of anharmonicity in the nuclear dynamics via the statistical comparison of first-principles forces with those forces that would act in the harmonic approximation. This enables us to efficiently scan over thousands of materials, including complex oxides and chalcogenides as well as ternary structures like perovskites, and single out strongly anharmonic ones. For these systems, we perform ab initio Green-Kubo simulations to model their thermal-transport properties, thereby naturally including all anharmonic effects [2]. Our strategy allows to avoid redundant calculations and achieve a much higher quality of information than achieved in traditional high-thoughput studies. Besides validating the performed search and analyzing its results, we discuss how big-data analytics techniques can be utilized to further accelerate and guide this search.

[1] https://vibes.fhi-berlin.mpg.de/

1:27PM M44.00010: Optimization of thermal conductivity at interfaces using learning algorithms
*ANNE CHAKA (Presenter), ZEXI LU, MALACHI SCHRAMP, Pacific Northwest National Laboratory — In material science, we are frequently interested in understanding the properties and design implication of material at interfaces. These interfaces can be manipulated to improve the desired characteristics of the bulk material. In this study, we are interested in understanding and optimize the impact of interfacial atomic defects on the thermal transport across a Cu/Si junction. To that end, we developed a reinforcement learning based framework to optimize over a potentially large parameter search. Using this technique allows us to accumulate knowledge of the system of a given type of atoms and store this information into a neural network. In this study, we present our results on optimizing the thermal transport by varying the fraction and length of the interfacial atomic defects using molecular dynamics (MD) simulations with normal mode analysis (NMA) to investigate thermal transport.

*PNNL LDRD CDI Program
1:39PM M44.00011: Valley filtering effect of phonons in graphene with a grain boundary*

XIAOBIN CHEN (Presenter), School of Science, Harbin Institute of Technology, Shenzhen, YONG XU, Collaborative Innovation Center of Quantum Matter and State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University, China, JIAN WANG, Department of Physics and the Center of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China, HONG GUO, Department of Physics, 3600 University, McGill University, Montreal, Quebec H3A 2T8, Canada — Due to their possibility to encode information and realize low-energy-consumption quantum devices, control and manipulation of the valley degree of freedom have been widely studied in electronic systems. In contrast, the phononic counterpart--valley phononics--has been largely unexplored, despite the importance in both fundamental science and practical applications. In this work, we demonstrate that the control of "valleys" is also applicable for phonons in graphene by using a grain boundary. In particular, perfect valley filtering effect is observed at certain energy windows for flexural modes and found to be closely related to the anisotropy of phonon valley pockets. Moreover, valley filtering may be further improved using Fano-like resonance. Our findings reveal the possibility of valley phononics, paving the road towards purposeful phonon engineering and future valley phononics.

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Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M45 DCOMP GDS DSOFT DPOLY: Emerging Trends in Molecular Dynamics Simulations and Machine Learning III 706 - Dvora Perihia, Clemson University - Tag(s): Focus
The Self Learning Kinetic Monte Carlo (SLKMC) method augmented with data analytics for adatom-island diffusion on surfaces* [Invited]

TALAT RAHMAN (Presenter), Department of Physics, University of Central Florida — The Self-Learning Kinetic Monte Carlo (SLKMC) method with its usage of a pattern recognition enabled the collection of a large database of diffusion pathways and their energetics for two-dimensional adatom islands containing 2-50 atoms on fcc(111) metal surfaces [1]. A variety of diffusion mechanisms involving single and multiple island atoms were uncovered in long time (comparable to experiments) KMC simulations. In this talk, I will present results for the diffusion kinetics of two dimensional adatoms islands in homoepitaxial and heteroepitaxial systems. With examples of diffusion of Ag and Pd adatom islands on Ag(111) and Pd(111), and that of Cu and Ni adatoms islands on Ni(111) and Cu(111) [2], I will draw attention to the relative role of lateral interactions and binding energy in the size dependence of island diffusion characteristics. These and a few other descriptors have been the key for application of data driven techniques for the training of predictive models, which we find to yield activation energy barriers that are accurate and obtained with little computational cost. Efforts are also underway to obtain reliable neural network derived interatomic potentials that have accuracy similar to those obtained from density functional theory based calculations. These results are promising for the development of tools for multiscale modeling of morphological evolution of nanostructured systems.


*Work supported in part by grants from NSF and done in collaboration with S. R. Acharya and D. Le
**11:51AM M45.00002: Accelerated Discovery of Dielectric Polymer Materials Using Graph Convolutional Neural Networks**

ANKIT MISHRA (Presenter), Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, PANKAJ RAJAK, Argonne National Lab, EKIN DOGUS CUBUK, Google Inc, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, AJINKYA DESHMUKH, Department of Chemistry, University of Connecticut, Storrs, LIHUA CHEN, Department of Material Science and Technology, Georgia Tech, GREG SOTZING, Department of Chemistry, University of Connecticut, Storrs, YANG CAO, Department of Electrical Engineering, University of Connecticut, Storrs, RAMAMURTHY RAMPRASAD, Department of Material Science and Technology, Georgia Tech, PRIYA VASHISHTA, Mork Family Department of Chemical Engineering and Materials Science, University of Southern California — Polynorbornene (PNB) is an important amorphous polymer system, which has potential applications as a high energy density polymer due to its high breakdown strength with low dielectric loss and high thermal stability. Moreover, electrical properties of PNB can be significantly enhanced by incorporation of defects or synthesis with controlled crystallinity by hydrogenation reaction. However, this process is challenging since it involves experimental synthesis and characterization of combinatorial large number of polymer systems to identify potential candidates. Here, we propose a deep learning-based graph convolutional neural network (GNN) model that can identify polymer systems capable of exhibiting increased energy and power density. The GNN model is trained to predict dielectric constant for a polymer, where the training data for the high frequency dielectric constant of the PNB polymers are computed via ab-initio molecular dynamics simulation. Our model can significantly aid experimental synthesis of potentially new dielectric polymer materials which is otherwise difficult using simplistic statistical procedures.

*This work was supported by the Office of Naval Research through a Multi-University Research Initiative (MURI) under grant number (N00014-17-1-2656).

**12:03PM M45.00003: Deep Learning embedding layers for better prediction of atomic forces in solids**

SIVAN NIV (Presenter), Department of Physical Electronics, Tel Aviv University, GOREN GORDON, Industrial Engineering, Tel-Aviv University, AMIR NATAN, Department of Physical Electronics, Tel Aviv University — The evaluation of atomic forces and total energy is a key challenge for large-scale atomistic simulations of materials. In recent years, machine learning techniques are successfully used to predict potential energies and to derive the atomic forces through the energy gradient. The training data is usually produced by quantum calculations, typically Density Functional Theory (DFT). The direct prediction of atomic forces by deep learning (DL) models was recently demonstrated by us and other groups, it has the advantage of being local and slightly faster while still maintaining state of the art mean absolute error (MAE). A disadvantage is that the predicted forces might be non-conserving. Like models which predict the energy, direct force models should behave well under symmetry operations and permutation of atoms. Here, we show how the use of self-learned embedding layers help to achieve better models for direct prediction of atomic forces. We also examine some sophisticated loss models to assure that the forces are smooth and close to conserving. We demonstrate this by the calculation of phonons in several solids and by the analysis of force derivatives in systems where we move single atoms and compare the DL predicted force derivatives to the DFT results.
12:15 PM M45.00004: A molecular dynamics study of water crystallization using deep neural network potentials of ab-initio quality*  PABLO PIAGGI (Presenter), ROBERTO CAR, Princeton University — We study the crystallization of water into hexagonal ice (Ih) using molecular dynamics simulations. We describe the complex interactions between water molecules using deep neural network potentials[1] and employ state of the art enhanced sampling methods[2] to convert reversibly liquid water into ice Ih. From the simulations we calculate the difference in free energy between these two phases. The ice Ih configurations that emerge contain proton disorder as observed in experiments[3]. The proton disorder has an important contribution to the entropy of the solid[4] that most free energy methods are unable to capture. We assess whether our technique is able to capture it and we study the effect of the interaction potential in the proton disorder.


*P.M.P was supported by an Early Postdoc.Mobility fellowship from the Swiss National Science Foundation. This work was conducted within the center: Chemistry in Solution and at Interfaces funded by the DoE under Award DE-SC0019394.

12:27 PM M45.00005: Machine learning force field using decomposed atomic energies from ab initio calculations*  LIN-WANG WANG (Presenter), Lawrence Berkeley National Laboratory — The development of machine learning (ML) force field from ab initio calculation is currently an intensely studied topic. In this talk, we will present our results using both neural network model and Gaussian process regression to represent such force fields. Examples of one element systems (e.g., Si) and two element systems (e.g., Fe-H) will be represented. We show that the ML force field can reproduce well the density functional theory (DFT) ab initio results. Large scale crystal growth can be simulated using the ML force field. In our ML force field development, we have used not only the atomic forces, but also a special decomposed DFT energy on each atom to carry out the training. We deployed a systematic feature function set to describe the atomic environment of a central atom. We will also present the comparison between the neural network model and the Gaussian process regression model.

*This work is supported by the Director, Office of Science (SC), Basic Energy Science (BES)/Materials Science and Engineering Division (MSED) of the U.S. Department of Energy (DOE) under the Contract No. DE-AC02-05CH11231 through the Theory of Material project.
Machine learning to derive quantum-informed and chemically-aware force fields to simulate interfaces and defects in hybrid halide perovskites  ROSS E LARSEN (Presenter), MATTHEW JANKOUSKY, DEREK VIGIL-FOWLER, AARON M HOLDER, National Renewable Energy Laboratory, K. GRACE JOHNSON, Department of Chemistry, Stanford University — The paradigm for creating materials for energy applications is no longer simply discovering a single material but instead involves combining multiple materials to achieve a desired functionality. Simulating interfaces between disparate materials or entire devices requires large systems, often approximated by classical simulations based on force fields (FFs). The accuracy of such simulations can be questionable because standard FFs may not accurately respond to changing chemical environments near an interface. We demonstrate a machine learning (ML) approach to predict quantum-derived atomic properties (e.g., charge, dipole moment, etc.) from descriptors of the local environment. The properties are used to compute chemically-aware, many-body inter-atomic forces, because the local environment descriptors encode more than just pairwise information. We apply these ML-derived FFs to several all-inorganic halide perovskite systems, CsBX$_3$ (B = Sn, Pb, X = Br, I) with local and extended defects, and to the interfaces between these materials, to correctly capture the anomalous charge and electrostatic multipole dynamics observed in these systems. We report on the MLFFs methods developed, and the resulting materials implications of charge dynamics on halide perovskite functionality.

Active Learning of Coarse Grained Force Fields with Gaussian Process Regression  BLAKE DUSCHATKO (Presenter), JONATHAN VANDERMAUSE, NICOLA MOLINARI, BORIS KOZINSKY, Harvard University — Many physically relevant spatial and temporal scales remain inaccessible with leading MD techniques, especially in soft matter and composite materials. Consequently, it is common practice to replace the all-atom representation with effective beads using coarse graining approaches. However, development of coarse grained force fields is a laborious procedure, and available force fields tend to lose orientation information, making all-atom reconstruction, or fine-graining, difficult. We propose a novel machine learning method for automatically constructing coarse grained force fields by active learning. In addition these force fields contain predictive uncertainty and allow for fine-grain reconstruction. We demonstrate that Gaussian Process Regression can alleviate the need for large initial all-atom trajectories that are generally required for achieving thermodynamically consistent results in the latent space. Moreover, we will discuss the performance of such models in the context of a variety of molecular systems possessing different amounts of rotational symmetry.
1:03PM M45.00008: **External Potential Ensembles to Improve the Learning of Transferable Coarse-Grained Potentials**

KEVIN SHEN (Presenter), KRIS T DELANEY, M. SCOTT SHELL, GLENN H FREDRICKSON, University of California, Santa Barbara — Simulation of complex, heterogeneous molecular systems requires models that are transferable across environmental conditions. However, current bottom-up strategies for parametrizing accurate coarse-grained (CG) models often rely on explicitly targeting the selected thermodynamic quantities (measured from experiments or atomistic simulations), which can be difficult to obtain. We argue that this information limitation can be overcome by coarse graining using thermodynamically informative ensembles, where variables conjugate to the thermodynamic variables of interest are allowed to fluctuate. We demonstrate this approach by using external potential ensembles with the relative entropy optimization to parametrize highly coarse grained models of solvent mixtures from atomistic force fields. The CG models can reproduce the activity coefficient of the atomistic model to within 0.1kT accuracy across the entire composition range, without explicitly measuring and matching chemical potentials during the parameterization process. This approach allows for the efficient transfer of exciting improvements of atomistically detailed models to fast, coarse-grained simulations of macro-scale systems.

*Funded by the BASF California Research Alliance*

1:15PM M45.00009: **Data-driven parameterization of coarse-grained models of soft materials using machine learning tools**

LILIAN JOHNSON (Presenter), FREDERICK PHELAN, National Institute of Standards and Technology — Many advances have been made in coarse-grained (CG) models of polymers to reduce computational effort yet capture the relaxation behavior imparted by hierarchical structure, resulting in two primary classes: “bottom-up” methods which preserve chemical-specificity and “top-down” methods which reproduce physical properties. Here, we combine a bottom-up coarse-grained model with a dissipative potential to obtain a chemically specific, thermodynamically consistent, and dynamically correct model. We parametrize the conservative forces using the iterative Boltzmann inversion (IBI) method to develop a CG force field from short all-atom (AA) simulations to recover AA structure, and thus, thermodynamics. We employ machine learning and filtering techniques to produce smooth distributions that enable automation and rapid convergence to smooth force profiles. We develop a similar approach for parameterization of the dissipative potential to correct the dynamics of the IBI-generated force field. In this method, we match AA diffusivity as a proxy for tuning monomeric friction. We demonstrate this method for oligomers in the melt state. Efforts to develop these methods into complementary automated packages will be discussed.

*LCJ acknowledges support from a NIST NRC Postdoctoral Associateship.*
1:27PM M45.00010: JAX, M.D. End-to-End Differentiable, Hardware Accelerated, Molecular Dynamics in Pure Python  
SAM SCHOENHOLZ (Presenter), EKIN DOGUS CUBUK, Google Inc. — A large fraction of computational science involves simulating the dynamics of particles that interact via pairwise or many-body interactions. These simulations, called Molecular Dynamics (MD), span a vast range of subjects from physics to drug discovery. Most MD software involves significant use of handwritten derivatives and code reuse across C++, FORTRAN, and CUDA. This is reminiscent of the state of machine learning (ML) before automatic differentiation became popular. Here, we bring the substantial advances in software that have taken place in ML to MD. JAX, M.D. is an end-to-end differentiable MD package written entirely in Python that can be just-in-time compiled to CPU/GPU/TPU. JAX MD allows researchers to iterate extremely quickly and lets researchers easily incorporate ML into their workflows. Finally, since all of the simulation code is in Python, researchers can have unprecedented flexibility in setting up experiments. JAX MD also allows researchers to take derivatives through whole-simulations as well as seamlessly incorporate neural networks into simulations. In this presentation we explore the architecture of JAX MD and its capabilities through several vignettes. Code is at github.com/google/jax-md along with a Colab notebook with experiments from the presentation.

1:39PM M45.00011: A neural network interatomic potential for molten NaCl*  
QINGJIE LI (Presenter), Massachusetts Institute of Technology MIT, EMINE KUCUKBENLI, Harvard University, STEPHEN LAM, BORIS KHAYKOVICH, Massachusetts Institute of Technology MIT, EFTHIMIOS KAXIRAS, Harvard University, JU LI, Massachusetts Institute of Technology MIT — Molten salts have been widely exploited for clean energy applications such as molten salt reactor (MSR) and concentrated solar power (CSP) technologies. These applications impose stringent requirements on the choice of molten salts such as excellent thermophysical properties, stability under extreme conditions, tolerance to impurities as well as compatibility with major structural materials. Optimizing/searching appropriate molten salt systems thus calls for a deep understanding of the underlying molecular structures, chemistry and dynamics in a vast salts space. In this talk, we present the application of artificial neural-network (NN) in training accurate interatomic potentials that enable fast evaluations of salt properties on desired time-and length-scales. In particular, we highlight the feasibility of neural-network interatomic potential to accurately predict the short to medium range structures and thermophysical properties of ionic liquids. We also propose a generic strategy to address the short-range interactions that are generally difficult to be learned by artificial NN.

*This work is supported by NEUP project 18-15093.
1:51PM M45.00012: Simulating Aluminum Corrosion Using DFT Trained Deep Neural Network Potentials  
WISSAM A SAIDI (Presenter), Mechanical Engineering & Materials Science, University of Pittsburg, SHYAM DWARAKNATH, Lawrence Berkeley National Laboratory — Current materials challenges necessitate simulations at length and time scales that often exceed the capabilities of the state of the art in density functional theory (DFT). Many effective Hamiltonian methods that can scale beyond these limits, such as cluster expansion, tight-binding, and interatomic potentials, often require a significant amount of expertise to train and employ. Machine learning methods such as deep neural networks exchange expertise for data-volume in what are typically expert-driven processes. Here we demonstrate the power of a deep neural network potential (DNP) to model the stability of various phases and terminations of Al2O3 on Al. This model builds off previous work using DFT to demonstrate that the relative stability of alpha-, gamma-, and amorphous Al2O3 changes with the film thickness, but was limited to one coherency constraint. With our DNP, we are able to find lower strain but less coherent interfaces for all three phases altering the layer thickness at which relative stability shifts. More importantly, we see strong correlations with interface chemistry suggesting that the environment chemical state can play a strong role in the nucleation and early stages of Al2O3 film growth.

2:03PM M45.00013: Tensor-Field Molecular Dynamics: A Deep Learning model for highly accurate, symmetry-preserving force-fields from small data sets*  
SIMON BATZNER (Presenter), LIXIN SUN, Harvard University, TESS E SMIDT, Computational Research Division, Lawrence Berkeley National Laboratory, BORIS KOZINSKY, Harvard University — Simulating the dynamic behavior of molecules and extended materials over large time-scales and with high fidelity has been a long-standing goal in computational physics. Recently, Deep Neural Networks have shown great promise in learning energies and atomic forces from atomistic data, thereby providing access to efficient and accurate interatomic force-fields. However, most existing methods still require the construction of very large reference training sets, consisting of tens of thousands of structures, often computed with expensive first-principles approaches. This provides a challenging bottleneck in the construction of interatomic force-fields, limiting Deep Learning-based approaches to systems for which such large training sets are feasible to generate. We present a framework to learn highly accurate Machine-Learning Force-Fields from small training sets. We show that our proposed method is able to obtain high-accuracy force predictions on a variety of different atomic systems, including organic molecules, bulk solids as well as complex interfaces and discuss the resulting Molecular Dynamics simulations.

*SB and BK acknowledge a generous gift from Bosch Research.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M46 GMAG: Quasi-2D Frustration: Honeycomb Lattice and Other Geometries  
708 - Kate Ross, Colorado State University
11:15AM M46.00001: Topological Quantum Many-Body Scars in Quantum Dimer Models
ALEXANDER SEIDEL (Presenter), Department of Physics, Washington University in St. Louis, JULIA WILDEBOER, Department of Physics, Arizona State University, ANNE E. B. NIELSEN, Max Planck Institute for the Physics of Complex Systems, ONUR ERTEN, Department of Physics, Arizona State University — We construct two-dimensional lattice models with quantum dimer degrees of freedom that violate the eigenstate thermalization hypothesis (ETH) by featuring quantum many-body scars in their excitation spectrum. These scars consist of single exactly known excited eigenstates with atypical (area law) entanglement entropy. We explicitly construct such models for the kagome and checkerboard lattices. We compute entanglement entropy numerically for the surrounding states, and analytically for the scar states themselves. Furthermore, we corroborate the non-integrable nature of these quantum dimer models by studying the statistics of the spacings between consecutive energy levels.

11:27AM M46.00002: Novel Quantum Phase Transition of the Shastry-Sutherland Model
TORU SAKAI (Presenter), HIROKI NAKANO, Graduate School of Material Science, Univ of Hyogo — The Shastry-Sutherland model - the $S = 1/2$ Heisenberg antiferromagnet on the square lattice accompanied by orthogonal dimerized interactions - is studied by the numerical-diagonalization method. Large-scale calculations provide results for larger clusters that have not been reported yet. The present study successfully captures the phase boundary between the dimer and plaquette-singlet phases and clarifies that the spin gap increases once when the interaction forming the square lattice is increased from the boundary. Our calculations strongly suggest that in addition to the edge of the dimer phase given by $J_2/J_1 \sim 0.675$ and the edge of the Neel-ordered phase given by $J_2/J_1 \sim 0.76$, there exists a third boundary ratio $J_2/J_1 \sim 0.70$ that divides the intermediate region into two parts, where $J_1$ and $J_2$ denote dimer and square-lattice interactions, respectively. We report the result from the investigation about this possible novel quantum phase transition in the plaquette singlet phase[1].

11:39AM M46.00003: Antiferromagnetic-to-ferrimagnetic phase transition in frustrated polar magnet CaBaCo$_4$O$_7$  TSUYOSHI OMI (Presenter), YOSHITO WATANABE, NOBUYUKI ABE, YUSUKE TOKUNAGA, Univ of Tokyo-Kashiwanoha, AKIKO NAKAO, KOJI MUNAKATA, CROSS, HAJIME SAGAYAMA, KEK IMSS, TAKA-HISA ARIMA, Univ of Tokyo-Kashiwanoha — Magnetic frustration often plays important roles in multiferroic properties as is exemplified by the electric polarization induced by the spiral magnetic order. CaBaCo$_4$O$_7$ belongs to the orthorhombic space group $Pbn_2_1$. Magnetic Co ions form Kagomé- and triangular- lattice layers, which alternately stack along the $c$-axis. CaBaCo$_4$O$_7$ shows a ferrimagnetic transition at $T_c \sim 60$ K at zero magnetic field. CaBaCo$_4$O$_7$ is a multiferroic material hosting magnetic frustration[1]. It exhibits an electric polarization change of about 17 mC/m$^2$ at the ferrimagnetic transition which is the largest among all the multiferroic materials so far[2]. The specific heat and the electric permittivity of single crystal CaBaCo$_4$O$_7$ exhibits another anomaly at $T_N$~69 K slightly higher than $T_c$ in zero magnetic field, while the origin of the anomaly was not clarified[2].

We investigate the phase transition of CaBaCo$_4$O$_7$. An antiferromagnetic phase is formed between $T_c \sim 60$ K and $T_N \sim 69$ K in our magnetization measurement and single-crystal neutron diffraction measurement. The large electric polarization change in CaBaCo$_4$O$_7$ should be attributed to the antiferromagnetic-to-ferrimagnetic transition.


11:51AM M46.00004: Sign-switching of dimer correlations in SrCu$_2$(BO$_3$)$_2$ under hydrostatic pressure*  SIMON BETTLER (Presenter), LENA STOPPEL, ZEWU YAN, SEVERIAN GVASALIYA, ANDREY ZHELUDEV, ETH Zurich — Magnetic and vibrational excitations in SrCu$_2$(BO$_3$)$_2$ are studied using Raman spectroscopy at hydrostatic pressures up to 34 kbar and temperatures down to 2.6 K. The frequency of a particular optical phonon, the so-called pantograph mode, shows a very strong anomalous temperature dependence below about 40 K. We link the magnitude of the effect to the magnetic exchange energy on the dimer bonds in the Sutherland-Shastry spin lattice in this material. The corresponding dimer spin correlations are quantitatively estimated and found to be strongly pressure dependent. At around $P_2 \sim 22$ kbar they switch from antiferromagnetic to being predominantly ferromagnetic.

*This work was partially supported by the Swiss National Science Foundation, Division 2.
12:03PM M46.00005: Large spin fluctuation in the magnetization process of S=1/2 frustrated square lattice model  TSUYOSHI OKUBO (Presenter), Department of Physics, University of Tokyo — In the frustrated spin systems, a lot of interesting phenomena including non-collinear magnetic orders, magnetization plateaus and spin liquids occur. Such frustrated interactions often appear in geometrically frustrated lattices, such as triangular, kagome or pyrochlore lattices. In addition to these lattice, when we consider further neighbor interactions or combination of ferromagnetic and antiferromagnetic interactions, frustrations can happen even in the square lattice. Motivated by several compounds, we discuss the nature of S=1/2 square lattice Heisenberg magnets with ferromagnetic and antiferromagnetic nearest-neighbor interactions. By means of the infinite tensor product states (iTPS) ansatz, we investigated magnetization process of the models numerically. We show that in the model corresponding to the compound [1], a part of spins reveals very strong spin fluctuation around the half of saturation magnetization. This is because spins connected by strong antiferromagnetic interaction form spin singlet. By varying the interaction strength, we show that such spin fluctuation is related to the 1/2 magnetization plateau stabilized in the vicinity of the model.


12:15PM M46.00006: Quantum Phases Diagram of the Plaquette State of the Shastry-Sutherland Compound SrCu₂(BO₃)₂  SARA HARAVIFARD (Presenter), ZHENZHONG SHI, SACHITH DISSANAYAKE, Duke University, DAVID E GRAF, National High Magnetic Field Laboratory, PHILIPPE R. CORBOZ, Universiteit van Amsterdam, FREDERIC MILA, Ecole polytechnique federale de Lausanne, DANIEL SILEVITCH, THOMAS F ROSENBAUM, Caltech, HANNA DABKOWSKA, McMaster University, CASEY MARJERRISON, Duke University — The Shastry-Sutherland compound SrCu₂(BO₃)₂ features 2D layers of Cu²⁺ S=1/2 spin dimers which are orthogonal to each other. The ground state of the system is determined by the relative strength of the nearest neighbor and next-nearest neighbor interactions, J and J′ respectively. The ratio of J/J′ can be tuned continuously by application of hydrostatic pressure. The ground state changes from a spin dimer singlet state at ambient pressure to an antiferromagnet state at high pressure. At intermediate pressure a novel 4-spin plaquette singlet state has recently been reported. However, the nature of this plaquette state and how it evolves into other phases remains unclear. Here, we report a comprehensive study of the quantum phase diagram of the plaquette state by tuning temperature, pressure, magnetic field, and chemical doping. We mapped out the evolution of the ground states using complementary techniques such as magnetic susceptibility, magnetization and neutron scattering measurements. The results provide insights into the nature of the plaquette state, and also has implications in areas such as studies of deconfined quantum criticality.
We study a fractionally frustrated XY model on the square lattice. This type of frustration is induced by regularly placing a gauge $A_{ij}$ on each link of the lattice, with the requirement that the circulation $\sum_{ij \in \square} A_{ij} = 2\pi f$ where $f$ is a fraction. The model is represented by the Hamiltonian

$$H = -J \sum_{ij} \cos(\theta_i - \theta_j - A_{ij})$$

where $\theta_i$ is the orientation of spin on $i$-th lattice site.

We study (via replica exchange Monte Carlo) how the Berezinskii-Kosterlitz-Thouless(BKT) phase of the conventional ($f = 0$) XY model changes for general fractional $f$.

Ref:


For decades, constrained models with dimer degrees of freedom have been a powerhouse of statistical physics and various branches of theoretical and mathematical physics, in particular aspects of quantum magnetism. For analytic purposes, their utility is usually limited to models defined on planar lattice graphs, where, thanks to a powerful theorem by Kasteleyn, many questions can be answered exactly. Here we present analytic results on a special dimer model on a \{it nonplanar\} checkerboard lattice of interacting dimers, which does not permit for parallel dimers to surround diagonal links. We report exact results on the enumeration of closed packed dimer coverings on finite checkerboard lattices under periodic boundary conditions. Furthermore, we comment on the behavior of the dimer-dimer correlations and find that the correlations between any two dimers vanish identically if their distance is larger than two unit cells. Connections with $\mathbb{Z}_2$ gauge theory, known from planar models, are extended to the present case.
Magnetic structure of the stuffed honeycomb antiferromagnet $\text{GdInO}_3$ 

ERXI FENG (Presenter), Oak Ridge National Lab, XIANGHAN XU, Department of Physics and Astronomy, Rutgers University, EVE EMMANOUILIDOU, Department of Physics and Astronomy, University of California Los Angeles, JAE WOOK KIM, Department of Physics and Astronomy, Rutgers University, YAN WU, LEI DING, ALEXANDER KOLESNIKOV, Oak Ridge National Lab, NI NI, Department of Physics and Astronomy, University of California Los Angeles, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University, HUIBO CAO, Oak Ridge National Lab — Rare-earth indium oxides $\text{RInO}_3$ ($\text{R} = \text{rare earth}$), in which $\text{R}^{3+}$ ions occupy two nonequivalent sites forming a honeycomb lattice with a superimposed triangular lattice (so-called stuffed honeycomb lattice), present an excellent platform to study the combination of two different frustrated lattices. Since the total angular moment $L$ of $\text{Gd}^{3+}$ ion is zero, $\text{GdInO}_3$ is expected as pure spin magnetism and may be considered as a classical Heisenberg spin system in the stuffed honeycomb lattice. A high quality isotope single crystal $^{160}\text{GdInO}_3$ was synthesized for neutron scattering studies to avoid the high neutron absorption of natural Gd. The specific heat measurement shows that the compound exhibits two step magnetic phase transitions at 2.2 K and 1.08 K corresponding to two different antiferromagnetic phases that were characterized by single crystal neutron diffraction. These phases transition may be explained via the order-by-disorder mechanism.

*The research at Oak Ridge National Laboratory (ORNL) was supported by the U.S. Department of Energy (DOE), Office of Science, BES, Early Career Research Program Award KC0402010 and the U.S. DOE, Office of Science User Facility operated by the ORNL.

Frustrated magnetic interactions in an $S=3/2$ bilayer honeycomb lattice compound $\text{Bi}_3\text{Mn}_4\text{O}_{12}(\text{NO}_3)$ 

MASAAKI MATSUDA (Presenter), SACHITH DISSANAYAKE, DOUGLAS L ABERNATHY, Oak Ridge National Lab, YIMING QIU, JOHN COLEY, NIST, NOBUHIRO KUMADA, Univ. of Yamanashi, MASAKI AZUMA, Tokyo Inst. of Tech. — Inelastic neutron scattering study has been performed in an $S=3/2$ bilayer honeycomb lattice compound $\text{Bi}_3\text{Mn}_4\text{O}_{12}(\text{NO}_3)$ at ambient and high magnetic fields [1]. Relatively broad and monotonically dispersive magnetic excitations were observed at ambient field, where no long range magnetic order exists. In the magnetic field-induced long-range ordered state at 10 T, the magnetic dispersions become slightly more intense, albeit still broad as in the disordered state, and two excitation gaps, probably originating from an easy-plane magnetic anisotropy and intrabilayer interactions, develop. Analyzing the magnetic dispersions using the linear spin-wave theory, we estimated the intraplane and intrabilayer magnetic interactions, which are almost consistent with those determined by $\textit{ab initio}$ density functional theory calculations [2], except the third and fourth neighbor intrabilayer interactions. Most importantly, as predicted by the theory, there is no significant frustration in the honeycomb plane but frustrating intrabilayer interactions probably give rise to the disordered ground state.

Observations of antiferromagnetic, antiferroelectric and ferroelastic orderings in honeycomb-lattice Mn$_2$V$_2$O$_7$*  

HUNG-CHENG WU (Presenter), DONG-JIE HSIEH, TSUNG-WEN YEN, PO-JUNG SUN, D. CHANDRASEKHAR KAKARLA, Department of Physics, National Sun Yat-sen University, JIM-LONG HER, Division of Natural Science, Center for General Education, Chang Gung University, Y. H. MATSUDA, Institute for Solid State Physics, University of Tokyo, CHUNG-KAI CHANG, YU-CHUN CHUANG, YEN-CHUNG LAI, National Synchrotron Radiation Research Center, MELISSA GOOCH, LIANGZI DENG, Texas Center for Superconductivity and Department of Physics, University of Houston, KYLE GRANT WEBBER, Department of Materials Science and Engineering, Friedrich-Alexander Universität Erlangen-Nürnberg, CHING (PAUL) W CHU, Texas Center for Superconductivity and Department of Physics, University of Houston — The dielectric and magnetic anomalies were observed in Mn$_2$V$_2$O$_7$ between 275 K and 300 K. Isothermal capacitance-stress hysteresis loop measurements along with crystallographic Aizu notation supported a martensitic phase transition ($T_M$) driven ferroelastic behavior near room temperature. Another dielectric anomaly was also observed near the long-range antiferromagnetic (AFM) ordering temperature ($T_N \sim 16.4$ K) along with noticeable magnetodielectric (MD) coupling below $T_N$, signifying the multiferroic nature of Mn$_2$V$_2$O$_7$. With increasing pressure, the antiferromagnetic ordering ($T_N$) greatly increased, while the ($T_M$) was suppressed. Taking all of these comprehensive research findings into account, we suggest that Mn$_2$V$_2$O$_7$ is a unique multifunctional material with the coexistence of antiferromagnetic, antiferroelectric and ferroelastic orderings.


NMR study on the honeycomb-lattice antiferromagnet Na$_2$Co$_2$TeO$_6$  

WEIQIANG YU (Presenter), ZE HU, Renmin Univ of China, YUAN LI, WEILIANG YAO, Peking University — The honeycomb-lattice magnetic materials have caused a lot of research interests recently, because of possible realization of Kitaev or proximate Kitaev quantum spin liquid in these systems. Na$_2$Co$_2$TeO$_6$, as a new honeycomb-lattice antiferromagnet, has a zigzag magnetic order which can be suppressed by magnetic field. Here we report our NMR studies on Na$_2$Co$_2$TeO$_6$ single crystals, and show rich properties revealed in this system both at zero field and at finite fields.
1:39PM M46.00013: Cooperative liquid-like paramagnetic state in nanoengineered honeycomb lattice*  GEORGE YUMNAM (Presenter), YIYAO CHEN, JIASEN GUO, Univ of Missouri - Columbia, HAILE ARENA AMBAYE, VALERIA LAUTER, Oak Ridge National Laboratory, DEEPAK K SINGH, Univ of Missouri - Columbia — Geometrically frustrated honeycomb structured artificial magnetic lattice has emerged as a testbed to explore the competing physics of energy vs. entropy in a thermally tuned magnetic phase transition. A magnetic honeycomb lattice with competing exchange interactions between Ising moments is theoretically predicted to exhibit disordered magnetic state with macroscopic degeneracy. We demonstrate the realization of a liquid-like magnetic state, comprised of low integer and energetically forbidden high integer magnetic charges, in nanostructured magnetic honeycomb lattice of ultra-small, sub-12 nm, connecting elements. Magnetic charges, related to magnetic moment and interacting via magnetic Coulomb's interaction, act as quantum mechanical entities. Detailed polarized neutron reflectometry measurements on magnetic honeycomb reveal a robust degenerate ground state at low temperature, which remains minimally affected by magnetic field application. Our finding provides a new vista to investigate quantum mechanical phenomena from the perspective of dynamic magnetic charges, instead of magnetic moments, in a classical system.

*The research at MU is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Grant No. DE-SC0014461.

1:51PM M46.00014: Field induced phase transition in the classical honeycomb Gamma model  ZHONGZHENG TIAN (Presenter), ZHIJIE FAN, PREETHA SAHA, GIA-WEI CHERN, Physics, University of Virginia — Recent studies have indicated the importance of the symmetric anisotropic exchange interaction, also called the Γ term, in the so-called Kitaev materials. Moreover, a new type of classical spin liquid was shown to be the ground state of the classical Γ model on the honeycomb lattice [1]. In our previous paper [2], we further demonstrated that thermal order-by-disorder drives the system toward a novel plaquette ordering that spontaneously breaks the lattice translation symmetry. In this work, we study the effects of magnetic field on the plaquette-ordered state. Our extensive Monte Carlo simulations uncover a field-induced phase transition above which the $\sqrt{3}\times\sqrt{3}$ flux order is replaced by a new spin order. We will present our characterization of this intermediate phase and discuss the nature of the phase transitions. [1] I. Rousochatzakis and N. B. Perkins, Phys. Rev. Lett. 118, 147204 (2017). [2] P. Saha, Z. Fan, D. Zhang, and G.-W. Chern, Phys. Rev. Lett. 122, 257204 (2019).

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M47 GMAG DMP: Dynamics of Skyrmions and Chiral Magnetic Textures 710/712 - Sonny H. Rhim, Univ of Ulsan - Tag(s): Focus
In ferromagnet systems, engineered interfaces can give rise to the chiral Dzyaloshinskii-Moriya interaction (DMI) in otherwise symmetric systems. Research has primarily focused on the study of chiral solitons in metallic systems, where heavy metal underlayers provide a large spin-orbit torque and an interfacial DMI. This resulted in extensive research of chiral solitons in ferromagnetic systems. However, damping in metals is generally high, which limits soliton mobility. The low damping and ferrimagnetic dynamics of insulating garnets make them ripe candidates for ultrafast spin textures. Moreover, spin-orbit effects and spin-transport phenomenon from adjacent heavy metal layers have been used to manipulate the magnetisation in these materials. Here, we use a pure spin current from an adjacent Pt overlayer to characterise chiral domain wall motion and DMI in epitaxial iron garnet films with perpendicular magnetic anisotropy. We use the significant interfacial DMI and a large spin-orbit torque to drive chiral domain walls to record velocities of a few thousand meters per second.

11:27AM M47.00002: Universal high-speed dynamics of distorted bubble skyrmions in an uncompensated amorphous ferrimagnet*  
KAI LITZIUS (Presenter), FELIX BUETTNER, ANGELA WITTMANN, Massachusetts Institute of Technology MIT, WEI ZHOU, CHUNG T MA, Department of Physics, University of Virginia, JOACHIM GRAEFE, NICK-ANDRÉ TRAEGER, Max Planck Institute for Intelligent Systems, SIMONE FINIZIO, Swiss Light Source, Paul Scherrer Institut, DANIEL SUZUKI, SIYING HUANG, LUCAS CARETTA, MANTAU HUANG, Massachusetts Institute of Technology MIT, YASSINE QUESSAB, Department of Physics, New York University, HANS NEMBACH, GRANT A RILEY, JUSTIN SHAW, Quantum Electromagnetics Division, National Institute of Standards and Technology, ANDREW KENT, Department of Physics, New York University, GISELA SCHUETZ, Max Planck Institute for Intelligent Systems, JOSEPH POON, Department of Physics, University of Virginia, GEOFFREY BEACH, Massachusetts Institute of Technology MIT — Magnetic skyrmions are topologically stabilized spin configurations that, like domain walls (DWs), can react to external stimuli by collective displacement, which is both physically intriguing and bears promises to realize next generation non-volatile data storage technologies.

Analytical equations of motion describe straight 180° DWs in the one-dimensional (1D) model while rigid, circular bubble domains and skyrmions move according to the Thiele equation. However, DWs and skyrmions are often not perfectly straight or circular.

Here, we study how strongly deformed DWs and bubble skyrmions move in uncompensated ferrimagnetic Pt/CoGd/W in response to current pulses. We find that all 1D spin textures exhibit velocity saturation at ~300 m/s in agreement with the 1D model, while all fully enclosed spin textures, even if significantly distorted, reach >500 m/s. We attribute this significant difference in the dynamics to the topology and the canting of spins in the skyrmion's encircling DWs.

*DARPA TEE program. Devices were fabricated using equipment in the MIT Microsystems Technology Laboratory and the MIT Nanostructures Laboratory.

11:39AM M47.00003: Chiral Edge Currents for ac Driven Skyrmions in Confined Pinning Geometries  
CHARLES REICHHARDT (Presenter), CYNTHIA REICHHARDT, Los Alamos Natl Lab — We show that ac driven skyrmion lattices in a weak pinning channel confined by regions of strong pinning exhibit edge transport carried by skipping orbits while skyrmions in the bulk of the channel undergo localized orbits with no net transport. The magnitude of the edge currents can be controlled by varying the amplitude and frequency of the ac drive or by changing the ratio of the Magnus force to the damping term. We identify a localized phase in which the orbits are small and edge transport is absent, an edge transport regime, and a fluctuating regime that appears when the ac drive is strong enough to dynamically disorder the skyrmion lattice. In some cases, multiple rows of skyrmions participate in the transport due to a drag effect from the skyrmion-skyrmion interactions. The edge currents are robust for finite disorder and should be a general feature of skyrmions interacting with confined geometries or inhomogeneous disorder under an ac drive. Similar effects can occur for skyrmion lattices at interfaces or along domain boundaries for multiple coexisting skyrmion species. The edge current effect provides a new method to control skyrmion motion that has similarities to the emergence of edge currents in chiral active matter systems and gyroscopic metamaterials.
11:51AM M47.00004: Antiferromagnet-based Neuromorphics using dynamics of topological charges*

SHU ZHANG (Presenter), YAROSLAV TSERKOVNYAK, Physics, University of California, Los Angeles — Compared with conventional computers, the human brain is extremely energy efficient and can perform complicated cognitive tasks. Spintronics-based hardware implementations of neuromorphic computing has several advantages, such as low energy dissipation, consistent material platform, and nonvolatile memory. In this work, we propose a new candidate for neuromorphic hardware based on the dynamics of topological charges in an antiferromagnet. The two basic elements—neuron and synapse—are realized and we demonstrate their functionalities that are crucial to form a spiking neural network. A single magnetic domain exhibits binary switch and performs leaky integrate-and-fire as a neuron. A synapse with spike-timing-dependent plasticity is realized by a one-dimensional interacting gas of domain walls, where the synaptic weight is simply the degree of saturation of domain walls. Due to the full compatibility of our artificial neurons and synapses, Hebbian learning can be achieved by simple action rules in the connected system.

*This work is supported by NSF under Grant No. DMR-1742928.

12:03PM M47.00005: Three-dimensional current-induced magnetic hopfion dynamics*

JIADONG ZANG (Presenter), Univ of New Hampshire, YIZHOU LIU, Institute of Physics, CAS — Magnetic hopfions are three-dimensional (3D) topological spin textures characterized by the Hopf invariant. As manifesting by their 3D real-space topologies, magnetic hopfions may exhibit interesting dynamics. Here, we study the current-induced dynamics of a magnetic hopfion in 3D space. The current mainly drives a translational hopfion motion. Depending on the applied current direction, hopfion also shows different moving patterns. We then analyze the equation of motion and find these current-induced dynamics further reflect the 3D nature of hopfion. Such 3D hopfion dynamics may shed light on the study of novel 3D topological spin textures and provides a new pathway to the development of 3D spintronics.

*U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award No.DE-SC0020221
Skyrmions have been suggested for a variety of applications including memory but in particular also non-conventional computing such as probabilistic computing [1]. A key problem for probabilistic computing is that cascading gates propagate undesired correlations. Therefore one needs to reshuffle the signals to keep them uncorrelated. While for many non-conventional computing approaches non-magnetic implementations are most promising, for building a “reshuffler”, skyrmions might be ideally suited due to the low footprint and low power compared to e.g. CMOS implementations [1]. We have studied low skyrmion pinning materials where we can stabilize skyrmions and controllably nucleate and displace them by current pulses due to spin-orbit torques [2]. We find topologically non-trivial N=1 skyrmions that move in the direction of the current pulses. At zero applied current, we find thermally activated skyrmion motion. We track the trajectories of skyrmions and from the dependence of their mean-square-displacement (MSD) on time, we can identify motion by diffusion and obtain the diffusion constant [2]. There is a strong dependence of the skyrmion diffusion parameter on temperature and the skyrmion size. Finally we patterning the reshuffler geometry and ascertain its performance.

Beyond ferromagnetic skyrmions, we are evaluating the efficiency of skyrmion spin structures in antiferromagnets, which have major advantages. In addition to the absence of a skyrmion Hall effect [3], also antiskyrmions can be stabilized for which first indications have been found.


*We thank in particular the ERC, the German Research Foundation and the IEEE Magnetics Society Distinguished Lecturer Program.
NICOLAS VIZARIM (Presenter), CHARLES REICHHARDT, T4, Los Alamos National Laboratory, CYNTHIA REICHHARDT, T1, Los Alamos National Laboratory, PABLO A. VENEGAS, Departamento de Física, UNESP — In this work we simulate the dynamic behavior of skyrmions under the influence of a square lattice of obstacles [1,2]. First, we consider a single skyrmion while varying the size and strength of the obstacles. We find that as the obstacle size is changed, several dynamic phases may appear or vanish. For smaller obstacles, the system exhibits fewer dynamic phases because as the obstacle size is reduced. On the other hand, if the obstacle size is too large, the system may also exhibit fewer dynamic phases due to the reduction in the size of the gaps between the obstacles, which confines the skyrmion motion. Thus, the highest number of dynamic phases appears for intermediate obstacle sizes. Motivated by these results, we consider the behavior of skyrmions of different species [3] under the influence of the square obstacle array. Our preliminary results indicate that is possible to separate the species according to their different skyrmion Hall angles when a driving current is applied.


*This work was supported by the São Paulo Research Foundation (FAPESP), grant: 2018/13198-7

CHRISTINA PSAROUDAKI (Presenter), Physics, California Institute of Technology, DANIEL LOSS, Physics, University of Basel — We investigate the quantum depinning of a weakly driven skyrmion out of an impurity potential in a mesoscopic magnetic insulator. For small barrier height, the Magnus force dynamics dominates over the inertial one, and the problem is reduced to a massless charged particle in a strong magnetic field. The universal form of the WKB exponent, the rate of tunneling, and the crossover temperature between thermal and quantum tunneling is provided, independently of the detailed form of the pinning potential. The results are discussed in terms of macroscopic parameters of the insulator Cu2OSeO3 and various skyrmion radii. We demonstrate that small enough magnetic skyrmions, with a radius of ~10 lattice sites, consisting of some thousands of spins, can behave as quantum objects at low temperatures in the mK regime [1].

1:15PM M47.00009: Thermal Decay of a Single Néel Skyrmion via Helicity Slip in a Nanodisk  
NAVEEN SISODIA, PRANABA MUDULI (Presenter), Department of Physics, Indian Institute of Technology, Delhi — Dynamics of the decay of a single skyrmion confined in a ferromagnetic nanodisk in the presence of stochastic thermal noise are studied using micromagnetic simulations. By analyzing the time-varying oscillations of the in-plane and out-of-plane magnetization under the influence of the thermal field, we identified the presence of two skyrmion eigenmodes with frequencies differing by an order of magnitude— a low-frequency mode associated with gyration of skyrmion core, and a high-frequency breathing mode associated with the oscillations of the skyrmion radius. We show that the thermal fluctuations not only affects the topological charge but also the helicity of the skyrmion, changing the helicity to oscillate around ±π/4—a value which is in between that of the Néel skyrmion and a vortex. We also reveal a phenomenon of helicity slip between +π/4 and -π/4 due to the thermal fluctuations. We explain the helicity slip based on an energy barrier that arises due to a combination of thermally induced deformation of skyrmion and the finite size of the disk.

1:27PM M47.00010: Electron Induced Massive Dynamics of Magnetic Domain Walls*  
HILARY HURST (Presenter), Joint Quantum Institute, National Institute of Standards and Technology, VICTOR GALITSKI, Joint Quantum Institute and Department of Physics, University of Maryland, TERO T HEIKKILÄ, Department of Physics and Nanoscience Center, University of Jyväskylä — We study the effect of conduction electrons on domain walls (DWs) in metallic, ferromagnetic nanowires. Using the Keldysh collective coordinate technique, we show how electrons act as an external bath and derive the Langevin equations of motion for a DW. The DW dynamics is described by two collective degrees of freedom: position and tilt-angle. The coupled Langevin equations therefore involve two correlated noise sources, leading to a generalized fluctuation-dissipation theorem (FDT). The DW response kernel due to electrons contains two parts: one related to dissipation via FDT, and another ‘inertial' part. We prove that the latter term leads to a mass for both DW degrees of freedom, even though the intrinsic bare mass is zero. The resulting equations of motion contain rich dynamical solutions and point toward a new way to control domain wall motion in metals via the electronic system properties. We discuss experimental consequences including two observable signatures of the mass: hysteresis in the DW dynamics and resonant response to ac current.

*H.M.H. acknowledges the support of an NRC Research Assistantship at NIST. V.G. was supported by DOE-BES (DESC0001911) and the Simons Foundation. The work of T.T.H. was supported by the Academy of Finland (project number 317118).
1:39PM M47.00011: Fast, low-power defect-induced polarity switching of a magnetic vortex core* MAHDI MEHRNIA (Presenter), JEREMY N TRIMBLE, Physics, Case Western Reserve University, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory, JESSE BEREZOVSKY, Physics, Case Western Reserve University — The core polarity of a topologically-protected magnetic vortex state is predicted to be extremely stable, and as such is considered as a candidate for non-volatile memory storage. However, here we show that the vortex core (VC) polarity is susceptible to rapid, repeatable switching even under low-amplitude motion. We excite vortices in thin permalloy disks with a magnetic field pulse, and observe the dynamic response using 3D time-resolved Kerr microscopy. In as-fabricated samples, we observe typical gyrations of the VC as it relaxes back to equilibrium. However, we observe a radically altered VC trajectory as prolonged pulsed laser exposure begins to change the VC pinning behavior near the disk center. In this region, the sense of gyration switches multiple times over tens of nanoseconds, indicating highly deterministic switches of the VC polarity that remain clear over >10^6 averaged repetitions. By translating the VC equilibrium position, we can tune the number of switches to zero, or obtain single deterministic switches using field pulses of less than 0.5 mT amplitude and 3 ns duration. Finally, we show simulation results of VC-defect interaction that shed light on this phenomenon.

*O.H. is funded by the US DOE, Office of Science, BES DIV of Materials Sciences and Engineering.

1:51PM M47.00012: Energy Storage in Spin System via Vortices DALTON JONES (Presenter), JI ZOU, YAROSLAV TSERKOVNYAK, University of California, Los Angeles — We formulate an energy-storage concept based on the topological spin textures in magnetic insulators. These textures, such as vortices, are metastable states associated with free energy. Here we propose to store energy in the topological texture of an XY ferromagnetic or antiferromagnetic annulus with easy plane anisotropy. Injecting vortices into the system will establish a net winding texture (energy density) within the bulk as vortices pass through the magnetic system. Once we complete the charging process, we can turn off the vortex conductivity and thus the energy associated with the winding texture is stored.
M47.00013: Current-driving skyrmion motion in inhomogeneous films* XIANG RONG WANG (Presenter), Physics, Hong Kong University of Science and Technology, HUAIYANG YUAN, Physics, Southern University of Science and Technology, XIN GONG, Physics, Hong Kong University of Science and Technology — In this talk, I will discuss current-driven skyrmion motion in disordered films. There are three phases: pinning phase, disorder-boosted transverse motion, and disordered-suppressed transverse motion. I will focus on the origin of the transverse motion boosting. Random potential landscape generate a force on a skyrmion. The force is perpendicular to the current direction when the skyrmion is pinned. The disorder-induced force is opposite to the skyrmion velocity when it is moving. Under a sufficient high current, disorders below a critical strength can boost the transverse skyrmion motion and hinder the longitudinal motion. The boosting comes mainly from the pinning force that is opposite to the driving force of the current. Skyrmions are pinned under a low current and above the critical disorder strength. Both transverse and longitudinal skyrmion motions are hindered at an intermediate current. The phase diagram will also be discussed.

*National Natural Science Foundation of China (Grants No. 11774296 and 11974296) and Hong Kong RGC (Grants No. 16301518, 16301619 and 16300117).

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M48 DCMP: Superconductivity: Materials, Growth, Structure
Mile High Ballroom 1A - Ulrich Welp, Argonne Natl Lab

11:15AM M48.00001: An Investigation into the Characteristics of the Superconductive Phase in Heavily P-doped Germanium KASRA SARDASHTI (Presenter), TRI D NGUYEN, MEHDI HATEFIPOUR, JOSEPH YUAN, WILLIAM MAYER, JAVAD SHABANI, New York Univ NYU — Realization of superconductivity in group IV semiconductors is anticipated to be the key in the scalability of the qubit devices. Such materials are promising candidates for fault-tolerant hybrid semiconductor-superconductor quantum systems due to their high purity and ease of processing. In this study, superconducting Ge is realized via ion implantation of Ga, followed by activation annealing. For all annealing temperatures, transport measurements showed an abrupt normal-superconductor transitions at 2.5–3.5 K, with residual resistances < 50 mΩ at 20 mK. Typical values for critical magnetic fields were about 0.6 to 0.8 T, corresponding to coherence lengths of 20 to 25 nm. Microscopy measurements revealed presence of a 20nm thick polycrystalline Ga-rich Ge layer near the top surface. To localize the superconducting region, implantation energy was reduced. The resulting superconducting layer showed no grain structure in micrometer scale, but Raman measurements confirmed its nanocrystalline nature. By reducing the implantation energy and the annealing temperatures, coherence length only decreased to ~18 nm. To further characterize the superconducting Ge films, strategies for their integration into all-Ge Josephson junctions and transistors will be discussed.
**11:27AM M48.00002: Physical properties of Li-based LiPd$_2$M Heusler compounds (M = Si, Ge, Sn)**

KAROLINA GÓRNICKA, Faculty of Applied Physics and Mathematics, Gdansk University of Technology, GABRIEL KUDEROWICZ, BARTOMIEJ WIENDLOCHA, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, ELIZABETH M. CARNICOM, ROBERT J. CAVA, Department of Chemistry, Princeton University, TOMASZ KLIMCZUK (Presenter), Faculty of Applied Physics and Mathematics, Gdansk University of Technology — We synthesized and studied LiPd$_2$M, M = Si, Ge and Sn, Heusler-type compounds. All three compounds crystallize in the cubic Fm-3m crystal structure with estimated lattice parameters $a = 5.9016$ Å (LiPd$_2$Si), 6.0105 Å (LiPd$_2$Ge) and 6.2642 Å (LiPd$_2$Sn). The compounds were characterized by means of magnetic susceptibility, heat capacity and resistivity. For LiPd$_2$Ge bulk transition was confirmed by a large HC anomaly at $T_c = 1.96$ K. Fitting the HC data yields $\gamma = 5.8$ mJ mol$^{-1}$ K$^{-2}$ and $\Theta_D = 244$ K. The electron-phonon coupling $\lambda_{e-p} = 0.53$ implies weak-coupling superconductivity. Electronic structure, phonons and electron-phonon interaction functions were computed using the density functional theory. LiPd$_2$Ge exhibits the strongest electron-phonon coupling within the studied series, in agreement with the observation of superconductivity. In all the compounds a phonon soft mode is found in the $\Gamma$-K direction, and it is most pronounced in the case of the superconducting LiPd$_2$Ge, which suggests its correlation with the electron-phonon interaction.

*The work at GUT and AGH-UST was supported by the National Science Center (Poland), project 2017/27/B/ST5/03044 and 2017/26/E/ST3/00119, respectively. At Princeton it was supported by the DOE, Division of Basic Energy Sciences, grant DE-FG02-98ER45706.

**11:39AM M48.00003: Layered tin pnictides as a new class of layered superconductors**

YOSUKE GOTO (Presenter), YOSHIKAZU MIZUGUCHI, Tokyo Metropolitan Univ — We report SnPn-based (Pn: pnictogen) materials as a new class of layered superconductors. The crystal structure of these compounds is characterized by two layers of a buckled honeycomb network of SnPn, bound by the van der Waals (vdW) forces and separated by Na ions. Measurements of electrical resistivity and specific heat indicate the bulk nature of superconductivity with transition temperature ($T_c$) of 1.3 K for NaSn$_2$As$_2$ and 2.0 K for Na$_{1-x}$Sn$_2$P$_2$ [1,2]. Recent studies on temperature-dependent magnetic penetration depth and thermal conductivity show that superconductivity of NaSn$_2$As$_2$ is fully gapped s-wave state in the dirty limit. Because there are various structural analogues containing SnPn conducting layers, our results indicate that SnPn-based layered compounds can be categorized into a novel family of layered superconductors. Furthermore, these compounds have also been gaining interest for application as thermoelectric materials and topological materials. In the conference, we will also report our recent progress for the studies on functionalities of SnPn-based layered materials.

11:51AM M48.00004: Interface superconductivity in complex metal-oxide heterostructures

PRIYANKA BROJABASI (Presenter), GUILLAUME HARDY, PATRICK FOURNIER, Universite de Sherbrooke — Interface superconductivity in oxide superstructures (SS) proposes new paths to explore further the mechanism for high-\(T_c\) superconductors allowing the manipulation of their electronic properties, but also discovering novel *artificial* materials [1], e.g., electron transfer from \(\text{LaFeO}_3\) (LFO) to electron-doped \(\text{Sm}_2\text{CuO}_4\) was explored in SS grown by RF sputtering [2]. In the present study, we have grown SS of infinite-layer \(\text{SrCuO}_2\) (SCO) and LFO as well as SS of electron-doped (Sr,Nd)\(\text{CuO}_2\) (SNCO) and LFO by pulsed-laser deposition with various thicknesses and annealing conditions. The coherent growth of SCO/LFO and SNCO/LFO SS has been confirmed by X-ray diffraction. Resistivity and Hall effect measurements confirm superconductivity in selected samples of SNCO/LFO SS, but no superconductivity and little doping by charge transfer has been observed in SCO/LFO SS. However, we observe a strong correlation between the critical temperature and the thickness of the SS subcomponents for SNCO/LFO SS. Our findings indicate that charge transfer may not be playing a significant role behind the superconductivity in these structures.


*We acknowledge the financial support from NSERC, FRQ-NT, CFREF and CFI.

12:03PM M48.00005: Electron-Hole Competition and Structural Response in the Two-Band Superconductor \(\text{Nb}_2\text{Pd}_x\text{Se}_5\) *

JENNIFER NEU (Presenter), DAVID E GRAF, KAYA WEI, Natl High Magnetic Field Lab, ALYSSA GAISER, Chemistry and Biochemistry, Florida State Univ., YAN XIN, Natl High Magnetic Field Lab, THOMAS ALBRECHT-SCHMITT, Chemistry and Biochemistry, Florida State Univ., RYAN BAUMBACH, Natl High Magnetic Field Lab, DAVID J SINGH, Physics, Univ. of Missouri, THEO SIEGRIST, Natl High Magnetic Field Lab — The superconducting properties of \(\text{Nb}_2\text{Pd}_x\text{Se}_5\) are highly dependent on the Pd stoichiometry. We have synthesized single crystals of \(\text{Nb}_2\text{Pd}_x\text{Se}_5\) with \(x\) in the range of 0.68 to 0.96 and have carried out detailed single crystal x-ray structural studies. We observe a pivotal shift in the atomic positions that depend on palladium occupancy at the threshold for superconductivity. We will discuss the crystal growth process, our recent findings of the subtle but profound structural changes, and present the rich spectrum of electronic behavior observed for different Pd occupancy regions. At the threshold Pd stoichiometry for superconductivity, a miscibility gap is apparent, with commensurate change in the electronic transport properties. Electron-hole competition in this two-band system is thought to be responsible for this behavior.

*Work at the Univ. of Missouri was supported by the U.S. DOE, Ofc. of Sci., Ofc. of Basic Energy Sci., DE-SC0019114. KW acknowledges support from the NHMFL through the Jack Crow Postdoctoral Fellowship. AG and TEAS acknowledge support from the U.S. DOE, Heavy Elements Chem. Program, DE-FG02-13ER16414. Part of the work was carried out at the NHMFL, supported by the NSF, NSF/DMR-164779 and the State of FL. JN and TS acknowledge support from the NSF, NSF/DMR-1606952.
Characterizing the penetration depth and coherence length of superconductor-normal superlattices

PATRICK QUARTERMAN (Presenter), National Institute of Standards and Technology, NATHAN SATCHELL, Michigan State University, BRIAN JAMES KIRBY, National Institute of Standards and Technology, REZA LOLOEE, Michigan State University, GAVIN BURNELL, University of Leeds, NORMAN BIRGE, Michigan State University, JULIE ANN BORCHERS, National Institute of Standards and Technology — Ferromagnetic Josephson junctions are a viable candidate for a low power cryogenic memory alternative compared to traditional CMOS technologies. There have been many reports concerning the supercurrent passing through the Josephson junction, including the discovery of spin triplet Cooper pairs in these systems [1]. Previously, we have found that by replacing the bottom Nb layer with a Nb/Al or Nb/Au superlattice, where the Al and Au layers are quite thin, the surface roughness is reduced compared to Nb. This decrease in surface roughness yields improved areal dependence of the critical current [2]. Previously, the effects on the penetration depth and coherence length from the insertion of a thin normal metal between Nb layers have not been fully explored, given that the use of such superlattices in Josephson junctions yielded behavior that was consistent with Nb. In this work, we report on our observation of an increased penetration depth and decreased coherence length in Nb/Al and Nb/Au superlattices utilizing polarized neutron reflectometry and electrical transport, respectively.


Study of electronic properties and mechanical dissipation in epitaxially grown La$_{2-x}$Sr$_x$CuO$_4$ thin films using scanning probe microscopy*

LARISSA LITTLE (Presenter), Harvard University, XUGUANG WANG, Institute of Physics, Chinese Academy of Sciences, WENJIE GONG, DILEK YILDIZ, JASON HOFFMAN, JENNIFER E. HOFFMAN, Harvard University — Understanding interplay between the superconducting dome and adjacent phases is important to better design and manipulate superconductors with high critical temperatures. Here we use the techniques of non-contact atomic force microscopy (nc-AFM) and scanning tunneling spectroscopy (STS) in ultrahigh vacuum to characterize thin films of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO). We grow the LSCO with molecular beam epitaxy and an oxygen plasma source. We produce high quality LSCO (001) samples with precise control over Sr doping level and choose the level of epitaxial strain our films experience by using different substrates (e.g., SrTiO$_3$ or LaSrAlO$_4$). We use nc-AFM to measure excitation and frequency shift as a function of tip distance from the surface and applied voltage bias. These measurements give us insight into the electronic nature of our films, as well as information about how energy dissipates into the sample.

*Work supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319, Gordon and Betty Moore Foundation’s EPIQS Initiative through Grant No. GBMF4536, Office of Naval Research, Grants N00014-18-1-2691 and N00014-19-1-2622. LL supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program.
12:39PM M48.00008: Acoustic Phonon Dynamics and Optical Properties of Bi-2212 Crystals
BRAD MCNIVEN (Presenter), G. TODD ANDREWS, JAMES P. F. LEBLANC, Memo Univ of Newfoundland — Acoustic phonon behaviour and optical properties of bulk Bi-2212 crystals at room temperature were probed using Brillouin light scattering spectroscopy and refined optical contrast methods. Values for the complex refractive index at a wavelength of 532 nm are presented and, along with Brillouin peak frequency shift data, used to determine transverse and longitudinal acoustic phonon mode velocities in these crystals.

12:51PM M48.00009: Electron counting and chemical complexity in the Ta-Nb-Hf-Zr-Ti HEA superconductors
FABIAN VON ROHR (Presenter), Department of Chemistry, University of Zurich, ROBERT J. CAVA, Department of Chemistry, Princeton University — High-entropy alloys (HEAs) are a new class of materials that consist of several principal elements arranged on simple lattices. These structures are stabilized by the high configurational entropy of the random mixing of the elements. The recently discovered Ta-Nb-Hf-Zr-Ti HEA superconductor appears to display properties of both crystalline intermetallics and amorphous materials; e.g., it has a well-defined superconducting transition along with an exceptional robustness against disorder. In this presentation, we will show that the properties of these superconducting HEAs are strongly related to the electron count and that the $T_c$s of these alloys fall between those of analogous crystalline and amorphous materials [1-3]. We find that despite the large degree of randomness and disorder in HEAs, the superconducting properties are nevertheless strongly dependent on the chemical composition and complexity. We argue that HEAs are excellent model systems for understanding how superconductivity evolves from crystals to amorphous solids.

1:03PM M48.00010: Enhancement of Superconductivity in Monolayer NbSe$_2^*$

HEMIAN YI (Presenter), TIMOTHY PILLSBURY, RUN XIAO, FEI WANG, CHENGYE DONG, YIFAN ZHAO, GUANG WANG, LINGJIE ZHOU, LING ZHANG, JOSHUA ROBINSON, MOSES HUNG-WAI CHAN, NITIN SAMARTH, CUI-ZU CHANG, Pennsylvania State University — The superconducting transition temperature of single unit cell FeSe on SrTiO$_3$ (STO) heterostructure is known to be significantly enhanced over that of bulk FeSe, presumably due to a combination of the electron charge transfer from the STO substrate to FeSe and an enhanced electron-phonon interaction across the heterointerface. Here, we explored the possibility of similar physics in monolayer NbSe$_2$ on $n$-type and $p$-type graphene substrates and found that the transition temperature is much higher in the latter heterostructures than in the former ones. The enhancement of superconductivity in monolayer NbSe$_2$ on $p$-type graphene is likely a result of the charge transfer effect. We also studied the temperature dependence of the resistance of NbSe$_2$ under an in-plane magnetic field. The extracted in-plane upper critical field of monolayer NbSe$_2$ overcomes the Pauli paramagnetic limit, suggesting Ising pairing property. We will talk about the properties of monolayer NbSe$_2$ films grown on other oxide substrates.

*This work is supported by the NSF-CAREER awards (DMR-1847811 and DMR-1453924), DOE (#DE-SC0019064), the Alfred P. Sloan Research Fellowship, and NSF 2DCC-MIP (DMR-1539916).

1:15PM M48.00011: MBE synthesis, ARPES and STM characterization of DyBa$_2$Cu$_3$O$_{7-\delta}$ thin films*

ZEBIN WU (Presenter), Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, DANIEL PUTZKY, Max Plank Institute for Solid State Research, ASISH KUNDU, HUI LI, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, GENNADY LOGVENOV, BERNHARD KEIMER, Max Plank Institute for Solid State Research, KAZUHIRO FUJITA, TONICA VALLA, ILYA DROZDOV, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory — Growth and characterization of HTSC cuprate DyBa$_2$Cu$_3$O$_{7-\delta}$ has been achieved in an OASIS system[1], combining together ozone-assisted oxide molecular beam epitaxy (OMBE), angle-resolved photoemission spectroscopy (ARPES), and spectroscopic-imaging scanning tunneling microscopy (SI-STM). Superconducting transition temperature (Tc) of over 80K measured in mutual inductance can be routinely achieved by shuttering via a real-time feedback from RHEED in OMBE. Leveraging on the synergistic capabilities of the instrument, the in-situ grown DyBa$_2$Cu$_3$O$_{7-\delta}$ are transferred in-vacuo into ARPES and SI-STM modules for characterization of their electronic properties. Dispersing quasi-particles are observed in photoemission and superconductivity is confirmed in tunneling spectroscopy.


*This work was supported by the US Department of Energy, Office of Basic Energy Sciences, contract no. DE-SC0012704.
1:27PM M48.00012: Growth and electrical transport properties of (110) YBa$_2$Cu$_3$O$_7$ / (110) PrBa$_2$(Cu$_{0.8}$Ga$_{0.2}$)$_3$O$_7$ heterostructure*  
HOM KANDEL (Presenter), NATHAN D ARNDT, Physics, University of Wisconsin-Parkside, JUNGWOO LI, CHANG-BEOM EOM, Materials Science & Engineering, University of Wisconsin-Madison — We performed pulsed laser-based thin film deposition and study of electrical transport properties on (110)-oriented YBa$_2$Cu$_3$O$_7$ (YBCO)/ (110)-oriented PrBa$_2$(Cu$_{0.8}$Ga$_{0.2}$)$_3$O$_7$ heterostructure for the nanofabrication of Superconductor (S) / Insulator (I) / Superconductor (S) tunneling Josephson junction device which may have many advantages over the conventional low-temperature superconductor-based Josephson junction devices including low cost, cryogenic system simplicity, and high $I_cR_n$ product (with $I_c$ being the junction critical current and $R_n$ the normal resistance). X-ray diffraction pattern (XRD) analysis, atomic force microscopy (AFM), and electrical transport studies were carried out to check the orientation, thickness, roughness, surface morphology, critical temperature ($T_C$), and electrical resistivities of the heterostructures. Here, we report the optimization process for the layer by layer growth, multi-layer epitaxy, thickness control of the superconductor and insulator layers, and the electrical transport properties of the (110) YBa$_2$Cu$_3$O$_7$ / (110) PrBa$_2$(Cu$_{0.8}$Ga$_{0.2}$)$_3$O$_7$ heterostructure.

*This research was supported by WiSys and UW System Applied Research Grant (ARG 2019-2020).
1:39PM M48.00013: Magnetic and superconducting properties of the Ir - rich compounds

MIr₃ (M=Ce, Th and Nd)*

KAROLINA GÓRNICKA (Presenter), Faculty of Applied Physics and Mathematics, Gdansk University of Technology, ELIZABETH M. CARNICOM, Department of Chemistry, Princeton University, DEBARCHAN DAS, Institute of Low Temperature and Structure Research, Polish Acad. of Sci., SYLWIA GUTOWSKA, BARTOMIEJ WIENDLOCHA, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, WEIWEI XIE, Louisiana State University, ROBERT J. CAVA, Department of Chemistry, Princeton University, DARIUSZ KACZOROWSKI, Institute of Low Temperature and Structure Research, Polish Acad. of Sci., TOMASZ KLIMCZUK, Faculty of Applied Physics and Mathematics, Gdansk University of Technology — Recently we have synthesized and studied CeIr₃, NdIr₃ and ThIr₃ compounds that are members of the RE₂m+nT₄m+5n family (m, n > 0). The bulk nature of the superconducting transitions for CeIr₃ and ThIr₃ are evident from the visible anomalies at Tc = 2.5 K and 4.4 K, respectively. The heat capacity experiment revealed that CeIr₃ is a weak-coupling BCS superconductor and ThIr₃ is a moderately coupled type-II superconductor. Theoretical calculations indicate a multi-band character for the Fermi surfaces, with the dominating contribution to the density of states at the Fermi level coming from the 5d states of Ir.

In the case of NdIr₃, our measurements indicate a ferromagnetic ground state with the Curie temperature TC = 10.6 K. The heat-capacity anomaly confirms the bulk nature of the transition, though Cp = 11.7 J mol⁻¹K⁻¹ is lower than expected for J = 9/2 and instead close to that of a J = 1/2 system. This suggests that the Nd ions are subject to a crystalline electrical field that removes spin degeneracy and leaves the Nd ions in a doublet ground state.

*This work was supported by Ministry of Science and Higher Education (Poland) under project DI2016 020546. The work at Princeton was supported by the Department of Energy, Division of Basic Energy Sciences, Grant DE-FG02-98ER45706.
1:51PM M48.00014: Effects of heteroepitaxy on the crystal structure in superconducting DyBa$_2$Cu$_3$O$_{7-x}$ thin films*  DANIEL PUTZKY (Presenter), PADMA RADHAKRISHNAN, GEORG CHRISTIANI, PETER WOCHNER, YI WANG, PETER VAN AKEN, Gennady LOGVENOV, EVA BENCISER, BERNHARD KEIMER, Max Planck Institute for Solid State Research — High-quality DyBa$_2$Cu$_3$O$_{7-x}$ thin films were grown by molecular beam epitaxy (MBE). In contrast to the previous growth by MBE using co-deposition technique, we have employed an atomic-layer-by-layer shuttering sequence with in-situ RHEED feedback. Epitaxial films grown on various oxide substrates have a sharp superconducting transition above 80 K. Scanning-transition electron microscopy (STEM) shows atomically sharp substrate-film interfaces and the absence of stacking faults, unlike films previously grown by pulsed-laser deposition (PLD). We employed synchrotron-based X-ray diffraction (XRD) to determine structural differences imposed by the heteroepitaxy with substrates with varying lattice parameters and crystal symmetry. A particular focus was put on the investigation of twinning which usually occurs in bulk orthorhombic crystal structure. However, in thin films the orthorhombic twinning can be hindered while the films still remain superconducting.

*We thank the Deutsche Forschungsgemeinschaft (DFG) for financial support under Grant No. TRR 80, Project No. G1.

M48.00015: Properties of Superconducting R$_2$O$_2$Bi (R = Y, Er) with Anti-ThCr$_2$Si$_2$-type Structure*  ZHUAN XU (Presenter), Zhejiang University — A new family of bismuth compounds, R$_2$O$_2$Bi (R = Y, Ce and Er etc.) crystallized in the anti-ThCr$_2$Si$_2$-type structure where Bi ions form a square net, has attracted much attention because this family exhibits various interesting ground states including antiferromagnetic (AFM) order, heavy fermion behavior and superconductivity (SC). We have investigated two compounds Ce$_2$O$_2$Bi and Er$_2$O$_2$Bi by measuring transport and magnetic properties, as well as specific heat. While Ce$_2$O$_2$Bi behaves as a Kondo lattice and experiences an antiferromagnetic (AFM) transition at $T_N$ of about 6.7 K, Er$_2$O$_2$Bi is a superconductor with $T_c$ of 1 K. A coexistence of AFM and SC is found. There is a correlation between the oxygen content and $T_c$. This work offers a new candidate material for studying the interplay between SC and 4f electron magnetism.

*The work was supported by the National Key Projects for Research & Development of China (Contract No. 2016YFA0300402) and NSFC.

Wednesday, March 4, 2020 11:15 AM - 1:51 PM

Session M49 DCMP: Superconductivity: Devices and Applications  Mile High Ballroom 1B - Lei Wang, Yale University
11:15AM M49.00001: Development of NbTiN constriction junctions and superconducting quantum interference devices*  ANDREW J MILLER (Presenter), Sandia National Laboratories, CHARLES HARRIS, Sandia National Laboratories, Center for Integrated Nanotechnologies, RUPERT M LEWIS, Sandia National Laboratories, TZU-MING LU, Sandia National Laboratories, Center for Integrated Nanotechnologies — Superconducting Quantum Interference Devices (SQUIDs) have become a leading tool for magnetometry with a wide range of applications. In this work, we investigate the properties of NbTiN SQUIDs created with a patterned constriction junction. The NbTiN film was grown through reactive sputtering, and then patterned using e-beam lithography and ion milling. SQUIDs were fabricated with constrictions as narrow as 50nm across, and loop areas of approximately 1μm². At 250mK, field dependent voltage oscillations were observed up to .3T, with an effective area consistent with the physical dimensions of the device.

*This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

11:27AM M49.00002: Reducing 1/f flux noise in superconducting devices in situ with UV light.* SEAN O’KELLEY (Presenter), Lawrence Livermore Natl Lab, MATTHEW S MARTENS, STEVEN M ANTON, Physics, UC Berkeley, J S BIRENBAUM, DAVID K KIM, JONILYN YODER, MIT-Lincoln Lab, GENE C. HILTON, NIST Bouder, WILLIAM OLIVER, MIT-Lincoln Lab, JOHN CLARKE, Physics, UC Berkeley — Magnetic flux noise with a 1/f power spectrum is pervasive in superconducting devices, and presents a fundamental limit to both the low-frequency energy resolution of dc SQUIDs and the high-frequency coherence of flux-sensitive superconducting qubits. Studies of the scaling of the magnitude of the flux noise with SQUID geometry are consistent with generation of the noise by fluctuating magnetic dipoles on the superconducting surface. Kumar et al. showed that the magnetic dipoles are adsorbed molecular oxygen, and reduced the noise with processes in a room-temperature hermetic sample enclosure. We demonstrate a factor of about three reduction of the 1/f flux noise power spectrum in Nb SQUIDs by applying 240-nm UV light from a Light Emitting Diode at cryogenic temperatures. Subsequent exposure of the SQUIDs to oxygen at atmospheric temperature and pressure restored the flux noise to its original value. Re-exposure to UV at cryogenic temperatures again reduced the flux noise. These results are consistent with molecular oxygen being the source of the noise. Our work demonstrates a practical technique to reduce the flux noise of superconducting devices in situ.

*Funding and support provided by IARPA through the Army Research Office, and LLNL under Contract DE-AC52-07NA27344.
11:39AM M49.00003: Integration of two-dimensional transition-metal dichalcogenide superconductors into superconducting circuits operated at DC and GHz frequencies*

MICHAEL SINKO (Presenter), Carnegie Mellon Univ, OLIVIA LANES, Physics and Astronomy, University of Pittsburgh, SERGIO DE LA BARRERA, Physics, Massachusetts Institute of Technology, DAVID PEKKER, MICHAEL JONATHAN HATRIDGE, Physics and Astronomy, University of Pittsburgh, BENJAMIN HUNT, Carnegie Mellon Univ — Two-dimensional (2D) transition-metal dichalcogenide (TMD) superconductors have unique and desirable properties for integration with conventional superconducting circuits, including the ability to form atomically-flat and clean interfaces with stable tunnel barriers, increased kinetic inductance due to the atomically-thin geometry, and resilience to large in-plane magnetic fields. We created 2D-3D Josephson junction contacts with R=0 and critical currents between 0.15uA-128uA. We study the flux response and observe a Fraunhofer pattern with a frequency proportional to a large fraction of the area of the 2D superconductor. This experimental result is confirmed by our numerical modeling, using the Ginzburg-Landau equation to describe screening currents induced in the flake by the magnetic field. We attribute the large effective area and small distortions of the Fraunhofer pattern to the almost uniform penetration of the TMD by the magnetic field and the distribution of screening currents. We have also embedded these 2D-3D contacts in an RF tank circuit (Q>4000) to measure the kinetic inductance. Our work lays the foundation for the analysis of TMD nano-devices in superconducting circuits.

*Supported by the National Science Foundation PIRE program under award number 1743717

11:51AM M49.00004: A quantum heat switch based on a single driven qubit*  CYRIL ELOUARD (Presenter), University of Rochester, GEORGE THOMAS, JUKKA P PEKOLA, Department of Applied Physics, Aalto University, ANDREW N JORDAN, University of Rochester — With the growing interest to nano and quantum technologies, a lot of attention has been paid to the challenge of controlling the heat currents at the nanoscale. Here we study the photonic heat transfer through a coherently driven qubit coupled to a hot and cold baths and show that such setup behaves as a quantum heat switch. More precisely, the heat flow from the hot bath can be activated or completely suppressed varying the parameters of the drive, its intensity or its frequency. We show the complete suppression of the heat flow is a quantum effect occuring for specific drive parameters and analyze the role of the coherences in the free qubit energy eigenbasis. Such scheme can be tested in state-of-the-art circuit QED setups, e.g. involving a transmon qubit coupled to thermal resistances.

*Work by C.E. and A.N.J. is funded by the US Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under Grant No. DE-SC0017890.
12:03PM M49.00005: Tunable photonic thermal rectification via superconducting qubit

AZAT GUBAYDULLIN (Presenter), BAYAN KARIMI, JORDEN L SENIOR, YU-CHENG CHANG, ALBERTO RONZANI, JOONAS PELTONEN, CHIIDONG CHEN, Aalto University, JOACHIM ANKERHOLD, Institute for Complex Quantum Systems and IQST, University of Ulm, JUKKA P PEKOLA, Aalto University — The intense studies into superconducting circuit quantum electrodynamics (QED) together with the progress in ultrasensitive nanoscale bolometry provide a unique platform for studying heat transport in the quantum limit. On chip integration of superconducting qubits coupled with superconducting resonators together with the tools of ultra-sensitive microwave bolometry have been considered as promising systems to realize such quantum devices as the recently demonstrated heat valve [1] and rectifier [2]. We will present our recent results of the flux-tunable photonic heat transport between thermal reservoirs coupled via a superconducting artificial atom. To study the possibility of manipulating heat currents and the directionality of photonic heat transport, we couple the Xmon qubit to two asymmetric resonators, and implement a flux-tunable wireless quantum thermal rectifier. We will present spectroscopy results of the resonator-qubit-resonator assembly [3].


*This work was supported by the Academy of Finland grant 312057, the Quantum Technology Finland, OtaNano and VTT.

Marie Sklodowska-Curie actions grants 843706,742559 and 766025.

12:15PM M49.00006: Multi-terminal superconducting quantum interference device

HANHO LEE (Presenter), NATALIA PANKRATOVA, ROMAN KUZMIN, KAUSHINI S WICKRAMASINGHE, University of Maryland, College Park, MAXIM G VAVILOV, University of Wisconsin-Madison, JAVAD SHABANI, New York University, VLADIMIR MANUCHARYAN, University of Maryland, College Park — External flux control of the superconducting phase difference is predicted to be a powerful tool to generate and manipulate Majorana bound states in a topological multi-terminal Josephson Junction (JJ). We study multi-terminal superconducting quantum interference devices (SQUID) fabricated from a semiconductor/superconductor (InAs/Al) heterostructure. Such a device consists of superconducting loops connecting some of terminals of a multi-terminal JJ. Due to non-local superconducting coherence, we observe for the first time an effect of “dragging” of the phase difference between one pair of terminals produced by the flux applied through the loop connecting two other terminals. Our ground state measurement implies the existence of novel multi-terminal Andreev bound states (ABS) which depend on more than two superconducting phase differences. Progress in tunneling spectroscopy of such states will also be discussed.
Synthesis of Quantum-Voltage Waveforms with Pulse-Driven High-$T_c$ Josephson Junctions

Josephson Junctions

ADAM WEIS (Presenter), NATHAN E FLOWERS-JACOBS, National Institute of Standards and Technology, STUART BERKOWITZ, Out of the Fog Research, LLC, HORST ROGALLA, SAMUEL P BENZ, National Institute of Standards and Technology — Josephson junctions (JJs) driven by a single-frequency microwave source have been established as quantum-accurate dc voltage standards [1]. Similar JJ devices are biased by patterns of fast pulses to create precise time-varying voltages [2], used for ac voltage standards and pseudo-random voltage noise references integrated into noise thermometry systems. Voltage standards typically use niobium-based JJs, but superconductors with higher-transition temperature, $T_c$, can be an attractive alternative. These high-$T_c$ JJ circuits can have critical currents near 1 milliamp at temperatures between 60 K and 80 K and thus can use compact low-power cryocoolers.

Investigation of high-temperature JJs in quantum voltage devices at NIST has focused primarily on grain-boundary junctions in YBa$_2$Cu$_3$O$_{7-x}$. By driving these high-$T_c$ junctions with pulse codes clocked at microwave frequencies we have demonstrated synthesis of programmable quantum-based voltage waveforms in a miniaturized cryocooler system. We'll also discuss relevant uncertainties, sensitivity of the output to bias currents, and applicability of this waveform-synthesis system to Johnson-noise thermometry.

Demonstration of a circuit-QED maser based on a nanowire Josephson junction*  

WILLEMIJN UILHOORN (Presenter), QuTech and Kavli Institute of Nanoscience, Delft University of Technology, MAJA C CASSIDY, Microsoft Quantum Lab Sydney, University of Sydney, JAMES KROLL, DAMAZ DE JONG, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, DAVID J. VAN WOERKOM, Microsoft Quantum Lab Delft, Delft University of Technology, PETER KROGSTRUP, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen and Microsoft Quantum Materials Lab Copenhagen, LEO P KOUWENHOVEN, Microsoft Quantum Lab Delft, Delft University of Technology — On-chip coherent microwave generation can be achieved by strongly coupling a dc biased Josephson junction to a high quality factor superconducting cavity [1]. The incorporation of a gate-tunable semiconducting nanowire Josephson junction in such a device enables fast control of the junction-cavity coupling and laser emission, paving the way for efficient scalable on-chip microwave control of superconducting qubits.

In these devices, the efficient down-conversion at higher order harmonics stimulates the creation of multiple coherent photons with a single Cooper pair tunneling event, increasing the phase coherence. However, performance is currently limited by incoherent dissipative processes such as quasiparticle poisoning (QPP) that suppress the laser coherence.

Here we report on the quenching of the coherence above the 4th order harmonic. We track the emission dynamics of the 5th order harmonic in time and observe emission blinking due to QPP events with characteristic timescales $T_{\text{poisoning}} = 200 \pm 10 \mu s$ and $T_{\text{unpoisoning}} = 17 \pm 2 \mu s$.

Reference:

*This work was supported by Microsoft Quantum and the Netherlands Organisation for Scientific Research (NWO/OCW) as part of the Frontiers of Nanoscience (NanoFront) program.
12:51PM M49.00009: Epitaxial Josephson junctions for superconducting qubits made by wafer-bonding* ANTHONY MCFADDEN (Presenter), University of California, Santa Barbara, COREY RAE MCRAE, RUICHEN ZHAO, DAVID PAPPAS, NIST, CHRIS J PALMSTROM, University of California, Santa Barbara — State-of-the-art transmons most often utilize Al/AIO_x/Al Josephson junctions (JJs) even though the amorphous AIO_x is known to be defective and lossy. A scalable process to realize epitaxial JJs with low loss barrier dielectrics could improve qubit performance beyond state-of-the-art; however, challenges in materials integration have not yet been overcome. In this work, a wafer-bonding technique is used to realize epitaxial JJ structures utilizing conventional semiconductors for the JJ dielectric. Semiconductors and epitaxial superconductors are grown by molecular beam epitaxy on III-V semiconductor substrates and bonded to low-loss substrates. Selective etching is used to remove the III-V substrate followed by surface cleaning and superconductor regrowth, resulting in epitaxial Al/Semiconductor/Al tri-layers on low loss substrates.

*Laboratory of Physical Sciences, University of MD

1:03PM M49.00010: Confluence of complex surface impedance and critical current studies of model defects in niobium films near critical temperature* COUGAR GARCIA (Presenter), Northrop Grumman & University of Maryland College Park, ALEX SIROTA, Northrop Grumman, BAKHROM ORIPOV, University of Maryland, College Park, NICHOLAS D RIZZO, ANNA HERR, VLADIMIR TALANOV, Northrop Grumman, STEVEN ANLAGE, University of Maryland, College Park — Studying and manipulation of vortex matter is key to understanding fundamental physics of superconducting materials, improving the properties of superconducting devices, and developing new concepts for superconductor applications. Two major approaches to experimentally characterize vortex dynamics are to measure (i) the critical current density or (ii) surface impedance as a function of applied field. In this work we combine both approaches to characterize thin 200 nm Nb films used in superconducting electronic circuits. We measured the vortex pinning constant (2 kN/m^2), viscous drag (~1e-8 N-s/m^2), and depinning frequency (~ 10 GHz) near the critical temperature (~0.85Tc) using a Parallel Plate Resonator technique. In addition, we measured the depairing critical currents (~ 0.75 MA/cm^2 at 0.9Tc) and the pinning force density (~1 MN/m^3 at 0.989Tc) as a function of temperature near Tc. The test results agree well with vortex wiggling experiments using a Scanning SQUID Microscope, and our numerical simulations of vortex potentials and vortex attempt frequencies based on the Ginzburg-Landau model and Kramers theory of escape rate of a Brownian particle from a potential well, respectively.

*Northrop Grumman Corporation
1:15PM M49.00011: 1/B resistance oscillations within the superconducting regime of heterostructure with disordered superconductor*  ASBJORN DRACHMANN (Presenter), ABHISHEK BANERJEE, ANTONIO FORNIERI, ALEXANDER WHITICAR, Center for Quantum Devices and Microsoft Quantum Lab - Copenhagen, University of Copenhagen, CANDICE THOMAS, Department of Physics and Astronomy and Birck Nanotechnology Center, Purdue University, SERGEI GRONIN, Birck Nanotechnology Center and Microsoft Quantum Purdue, Purdue University, TIANTIAN WANG, Department of Physics and Astronomy and Birck Nanotechnology Center, Purdue University, GEOFF C GARDNER, Birck Nanotechnology Center and Microsoft Quantum Purdue, Purdue University, MICHAEL MANFRA, Department of Physics and Astronomy, Birck Nanotechnology Center, Microsoft Quantum Purdue, School of Materials Engineering & School of Electrical and Computer Engineering, P, CHARLES MARCUS, Center for Quantum Devices and Microsoft Quantum Lab - Copenhagen, University of Copenhagen — In-situ growth of Al on top of shallow InAs 2DEG heterostructures gives close to perfect superconducting proximity effect [1]. In recent work, we used anodic oxidation to thin down the Al by oxidizing from the top down, allowing us to create an ultra-thin and disordered Al film with a large perpendicular critical field $B_c > 3$ T on a mesoscopic structure. [2]

For $B > B_c$, the sample resistance rises to >1 kΩ whereas for $B < B_c$, we observe reproducible resistance oscillations of <30 Ω. The oscillations have a 1/B periodicity from which standard SdH analysis yields a density matching closely with the carrier density of the underlying 2DEG. This indicates strong electronic contact between the disordered Al layer and the high mobility InAs 2DEG, creating a novel material system to study disordered 2D superconductivity.

Furthermore, fully oxidizing the Al layer gives rise to quantum Hall effect ($\rho_{xx}=0$) emerging at $B \sim 2.5$ T [2] making this material system a candidate for studying proximitized quantum Hall edge states with close to unity transparency to the superconducting Al, contacting the 2DEG from the top.


*This research was supported by Microsoft and the Danish National Research Foundation
1:27PM M49.00012: Spectroscopy of barrier defects coupled to superconductors in Van der Waals tunneling devices* DEVIDAS T R (Presenter), The Racah Institute of Physics, The Hebrew University of Jerusalem, TOM DVIR, QuTech, Delft University of Technology, ITAI KEREN, HADAR STEINBERG, The Racah Institute of Physics, The Hebrew University of Jerusalem — Superconductor-Quantum Dot (SC-QD) coupling is a subject of an intense research effort. We report on SC-QD devices realized in Van der Waals tunneling heterostructures consisting of transition metal dichalcogenide (TMD) semiconducting barrier and the 2-band superconductor NbSe$_2$. The QDs in our study are naturally occurring defects in the TMD barrier. As reported earlier by Dvir et. al. [1], Andreev Bound states may form due to proximitized defects in an NbSe$_2$-WSe$_2$ system. Here we focus on two device structures. In the first, tunneling through an MoS$_2$ barrier into a graphene-NbSe$_2$ stack reveals zero-energy Kondo features which arise due to the presence of carriers associated with the NbSe$_2$ low-energy band turning normal. In the 2$^{nd}$ device, defect-dot energies are tunable by use of a graphene tunneling electrode which permits the penetration of electric field from an electrostatic gate. This allows the QD to be used as spectroscopic probe to study resonant tunnelling into the superconductor, allowing low-energy spectroscopy of the inner band of NbSe$_2$.

References

*This work was funded by a ERC Starting Grant (No. 637298, TUNNEL), an Israeli Science Foundation grant 1363/15, and BSF grant 2016320.

1:39PM M49.00013: Local measurement of temperature dependent London Penetration Depth in Superconductors using Nitrogen Vacancy Centers in Diamond* KAMAL JOSHI (Presenter), Ames laboratory, Ames, IA, WILLIAM S. SETTERBERG, Macalester College, Saint Paul, MN, NAUFER M NUSRAN, SUNIL GHIMIRE, KYUIL CHO, MAKARIY TANATAR, SERGEY L. BUD'KO, PAUL C CANFIELD, RUSLAN PROZOROV, Ames laboratory, Ames, IA — Local optical magneto-sensing based on nitrogen-vacancy (NV) centers in diamond [1] was used to measure temperature-dependent London penetration depth, $\lambda$ (T), in two different unconventional superconductors, Ba(Fe$_1-x$Co$_x$)$_2$As$_2$ (BaCo122) and YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO). The results are compared with the sensitive bulk measurements of the same samples using tunnel-diode resonator (TDR). Each sample was measured in two orientation to separate the effects of platelet geometry and surface morphology, imaged using SEM. Not only this study compares the absolute numbers from two different techniques, it also allows us to discuss a more realistic picture of the magnetic field penetration into superconducting samples.

*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract #DE-AC02-07CH11358. N.M.N. acknowledges support from the Lab Directed Research and Development (LDRD) program at Ames Laboratory for the implementation of the NV-center optical magnetometry.
We computed the force exerted on a solenoid in a magnetic field, and compared with the experimental results to verify the effect of magnetic moment gradient on exerted force. Based on the concept, a superconducting solenoid thruster driven by geomagnetic field is devised, which has advantages of low energy consumption and propellant-free. To further enhance the force exerted on the solenoid, we replaced an aluminum core with an iron core. Moreover, we placed the solenoid in the geomagnetic field and measured the forces corresponding to different gradients due to variation of cross-sectional area and electric current magnitude. The results demonstrated a proportionality between the force and these two factors, as predicted by the theory. By measuring and calculating the force exerted on a superconducting solenoid at low temperature, we can simulate the condition when such a thruster is used in space. The results showed that the force exerted on a superconducting solenoid at low temperature matched the predicted force relation versus the gradient of varying cross-sectional area and electric current magnitude at room temperature. Therefore, the relation can provide a reference for design of an alternative thruster for space exploration.

* Under NTU-Sinica project: NTU-AS-108L104307

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M50 DCMP: Non-Equilibrium Dynamics

11:15AM M50.00001: Ultrafast magnetic dynamics in insulating YBa$_2$Cu$_3$O$_{6+x}$ revealed by time resolved two-magnon Raman Scattering.*  

DMITRY REZNIK (Presenter), JHIH-AN YANG, NICK PELLATZ, Physics, University of Colorado, Boulder, THOMAS WOLF, Karlsruhe Institute of Technology — Measurement and control of magnetic order and correlations in real time is a rapidly developing scientific area relevant for magnetic memory and spintronics. In these experiments an ultrashort laser pulse (pump) is first absorbed by excitations carrying electric dipole moment. These then give their energy to the magnetic subsystem monitored by a time-resolved probe. A lot of progress has been made in investigations of ferromagnets but antiferromagnets are more challenging. Here we introduce time-resolved two-magnon Raman scattering as a novel real time probe of magnetic correlations especially well-suited for antiferromagnets. Its application to antiferromagnetic charge transfer insulator YBa$_2$Cu$_3$O$_{6+x}$ revealed rapid demagnetization within 90fs of photoexcitation. The relaxation back to thermal equilibrium is characterized by much slower timescales. One of these, which is extremely slow, indicates a novel metastable state hosting trapped charge carriers.

*Work at the University of Colorado was supported by the NSF under Grant No. DMR-1410111
11:27AM M50.00002: Ultrafast charge dynamics in bulk alpha-Fe$_2$O$_3^*$  NASEEM UD DIN (Presenter), VOLODYMYR TURKOWSKI, Physics, Univ of Central Florida, HUNG-TZU CHANG, ALEXANDER GUGGENMOS, MICHAEL ZUERCH, STEPHEN R. LEONE, Chemistry, UC Berkeley, TALAT S. RAHMAN, Physics, Univ of Central Florida — Details of the ultrafast charge dynamics in oxides is crucial for interpretation of recent experimental data and for potential application of such materials in modern technologies. In this talk, we present results for ultrafast charge dynamics in laser pulse-excited antiferromagnet alpha-Fe$_2$O$_3$ obtained with the combined time-dependent density-functional theory and dynamical mean-field theory approach. In particular, we have calculated the time-resolved occupancies of the involved O(p) valence and Fe(d) conduction orbitals and demonstrated that due to strong electron-electron correlations there is delay of a few femtosecond in the charge accumulation in the electron and hole Fe(d) orbitals as compared to the O(p) hole orbitals. The obtained results for the ultrafast dynamics helps explain the attosecond transient absorption spectroscopy data for alpha-Fe$_2$O$_3$ which demonstrate ultrafast modification of the absorption spectra due to ligand-to-metal charge transfer. Our approach can be further extended to treat the femtosecond- and sub-femtosecond resolved dynamics of photoexcitation in strongly correlated materials, specifically, photo-induced insulator-to-metal transitions.

*This work is supported in part by DOE grant DE-FG02-07ER4635 and by AFOSR grant FA9550-15-1-0037.

11:39AM M50.00003: Non-equilibrium dynamics of vibrationally coupled electrons excited by coherent radiation*  JOHN SOUS (Presenter), BENEDIKT KLOSS, Columbia University, DANTE KENNES, RWTH Aachen University, DAVID REICHMAN, ANDREW MILLIS, Columbia University — The non-equilibrium dynamics of matter induced by coupling to light fields have made it possible to induce electronic phases of matter that may not exist at equilibrium, and which can be probed by optical and time-resolved spectroscopy. Transient superconductivity induced in atomic solids as a result of enhancement of atomic vibrations excited by light presents one exciting avenue. Here we employ tensor network methods to simulate the dynamics of a metal driven to a highly excited state at initial time by a pump that excites specific vibrational modes. We study the evolution with time of electronic and vibrational observables and observe non-trivial dynamics of density wave and superconducting correlations.

*Columbia MRSEC and Basic Energy Sciences program of the U.S. Department of Energy under grant DE-SC0018218
High Harmonic Generation and Nonequilibrium Quasiparticle Dynamics in an Unconventional Superconductor with Competing Order* JIAN-XIN ZHU (Presenter), BENEDIKT FAUSEWEH, Los Alamos Natl Lab, WEI ZHU, Westlake Institute for Advanced Study, CHEN-YEN LAI, Los Alamos Natl Lab — A common feature of unconventional superconductors, ranging from high-temperature cuprate, heavy fermion, and recently discovered iron-based compounds, is the close proximity of unconventional superconductivity to an antiferromagnetic phase. The interplay of the unconventional superconductivity with the competing order remains an interesting scientific question. Recently, the ultrafast laser pulse pump-probe technique has become a powerful approach to uncover novel phases and associated quasiparticles dynamics in strongly correlated electron systems. Here we study an effective $t'$-$U$-$V$ Hubbard model which captures the competition between antiferromagnetic spin-density wave (SDW) and d-wave superconducting (DSC) orderings. We show that an ultrafast electromagnetic field can drive the two competing order parameters uniquely depending on different regimes of hole doping. We further elucidate the consequence of the photoinduced electronic states by calculating the high harmonic generation and nonequilibrium momentum-dependent single-particle spectral function.

*This work was carried out under the auspices of the U.S. DOE NNSA (Contract No. 89233218CNA000001) and was supported by the LANL LDRD Program.

Characterization of photoexcited states in the half-filled one-dimensional extended Hubbard model assisted by machine learning KAZUYA SHINJO (Presenter), Tokyo Univ of Science, Katsushika, SHIGETOSHI SOTA, SEIJI YUNOKI, RIKEN, TAKAMI TOHYAMA, Tokyo Univ of Science, Katsushika — Photoinduced nonequilibrium states can provide new insight into dynamical properties of strongly correlated electron systems. One of the typical and extensively studied systems is the half-filled one-dimensional extended Hubbard model (1DEHM). Here, we propose that the supervised machine learning (ML) can provide useful information for characterizing photoexcited states in 1DEHM [1]. Using entanglement spectra as a training dataset, we construct a neural network. Judging from the trained network, we find that bond-spin-density wave (BSDW) order can be enhanced in photoexcited states if the frequency of a driving pulse nearly resonates with a gap. We separately calculate the time evolution of local and non-local order parameters and confirm that the correlation functions of BSDW are enhanced by photoexcitation as predicted by ML. Predicting BSDW demonstrates the advantage of ML to assist characterizing photoexcited quantum states.

12:15PM M50.00006: Negative absolute conductivity in photoexcited metals* GIULIANO CHIRIACO (Presenter), Columbia Univ, ANDREW MILLIS, Center for Computational Quantum Physics, The Flatiron Institute, IGOR L ALEINER, Columbia Univ — We show that in a model of a metal photoexcited by a pump pulse resonant with a phonon mode, the absolute dc conductivity may become transiently negative, depending on the interplay between the electronic structure, the phonon frequency and the pump intensity. The analysis includes the effects of inelastic scattering and thermal relaxation. Results for the time evolution of the negative conductivity state are presented, showing that the associated non-equilibrium physics may persist for long times after the pulse. Our findings provide a theoretical justification for previously proposed phenomenology and indicate new routes to the generation and exploration of intrinsically non-equilibrium states.

*Support was provided by the Basic Energy Sciences Division of the Office of Science of the United States Department of Energy under Grant No. DE-SC0018218 (A.M. and G.C.) and by the Simons Foundation (I.A.).

12:27PM M50.00007: Matrix product state investigations of time-dependent spectral functions after a photoexcitation* CONSTANTIN MEYER (Presenter), SALVATORE MANMANA, University of Gottingen — We study the time-dependent dynamical structure factor after a photoexcitation of a variant of the 1d Hubbard model with a background staggered magnetic field using matrix product state (MPS) techniques. In particular, we use the time-dependent variational principle (TDVP) to investigate the time evolution of the band population, which is a quantity accessible to time-resolved ARPES experiments. Different scenarios for the photoexcitations are discussed, e.g., Peierls-substitution or direct excitation in k-space. Using MPS, we can study in detail the effect of the electron-electron interaction on the redistribution of the band populations in the various photoexcitation setups. An outlook to the relevance of electron-electron interactions on light-harvesting mechanisms in correlated materials is given.

*We acknowledge financial support by SFB/CRC 1073 "Atomic Scale Control of Energy Conversion" (project B03) of the Deutsche Forschungsgemeinschaft (DFG).
12:39PM M50.00008: Field-Driven Correlated Quantum Systems, Bridging the Gap Between the Transient and the Steady State  ERIC DOHNER (Presenter), HERBERT FOTSO, University at Albany, ALEXANDER F KEMPER, North Carolina State University, JAMES FREERICKS, Georgetown University — Correlated quantum systems away from equilibrium have rightfully generated a lot of interest. Computational methods play an important role in understanding these systems but they are constrained by difficulties inherent to correlated systems that are exacerbated away from equilibrium. This prevents a full characterization of the dynamics. Previously, a set of relaxation scenarios were identified when systems initially in equilibrium are suddenly driven by a DC electric field. In particular, for certain parameters both the Hubbard and the Falicov-Kimball models evolve monotonically towards infinite temperature steady states that can be fully characterized by formulating solutions directly in the steady state. In the process these systems evolve through successive quasi-thermal states obeying the fluctuation dissipation theorem. We demonstrate an extrapolation scheme that can be leveraged to extend the characterization of the system from equilibrium to steady state at minimal computational cost. Namely, we extrapolate the monotonic temperature of the system and use the fluctuation dissipation theorem to construct the self-energy beyond the transient. All momentum dependent quantities can then be obtained within the DMFT formalism.

12:51PM M50.00009: Photon echo in the Coloumb glass phase as observed with 2D non-linear THz spectroscopy*  FAHAD MAHMOOD (Presenter), University of Illinois at Urbana-Champaign, DIPANJAN CHAUDHURI, DAVID BARBALAS, Johns Hopkins University, RAHUL NANDKISHORE, University of Colorado Boulder, PETER ARMITAGE, Johns Hopkins University — Phosphorous doped Silicon (P:Si) near the metal insulator transition (MIT) hosts a Coulomb glass phase where charge carriers are localized and have strong long-range Coulomb interactions. Here we perform 2D non-linear THz spectroscopy to study the low energy non-linear electrodynamics of charge carriers in the Coulomb phase. Two time-delayed THz pulses with field strengths on the order of 100 kV/cm are applied sequentially on the sample to extract a 2D spectrum of the non-linear susceptibility of the sample as a function of emission and absorption frequencies. Distinct third-order nonlinear signals are identified in the 2D spectra including a photon echo, the anti-diagonal linewidth of which is used to determine the decoherence time ($T_2$) of excited carriers. This is compared with the energy relaxation time ($T_1$) to understand the interplay between site disorder and long-range interactions as the MIT is approached.

* DARPA DRINQS project FP-017, “Long-term High Temperature Coherence in Driven Superconductors”
1:03PM M50.00010: The quadratically driven nonlinear photonic lattice and its dissipative phase transition: from quantum to classical*  
WOUTER VERSTRAELEN (Presenter), UAntwerpen, RICCARDO ROTA, VINCENZO SAVONA, EPFL, MICHEIL WOUTERS, UAntwerpen — Phase transitions (PT) appear in many flavors. In a Classical PT it results from a competition between energy and entropy, whereas in a quantum PT at zero temperature it results from the competition between non-commuting terms in the Hamiltonian. A quantum PT at finite temperature either vanishes or exhibits a continuous crossover to a classical PT [1]. The fate of a quantum PT at finite dissipation is much less understood.

A paradigmic example of a driven-dissipative system are lattices consisting of nonlinear optical cavities. By driving this system with a two-photon laser, the system retains a $Z_2$-symmetry, that can be spontaneously broken [2].

Here, I show how, using quantum trajectories with a Gaussian ansatz [3], we are able to explore a much larger parameter regime than before. In lattices up to 12x12 cavities we observe a transition from quantum to classical critical behavior, consistent with the interpretation of losses acting as temperature.

This work has been performed in collaboration with Riccardo Rota, Vincenzo Savona and Michiel Wouters.


*I acknowledge FWO travel grant V413119N.

1:15PM M50.00011: Accessing quantum phases in Hubbard honeycomb lattice using an electromagnetic drive*  
UMESH KUMAR (Presenter), SHIZENG LIN, Theoretical Division, T-4, Los Alamos National Laboratory — In the recent past, there has been a great interest in creating novel states of matter under driven conditions, in the condensed matter physics. The Hubbard honeycomb lattice is known to host rich phases [1]. The presence of a periodic drive such as an electromagnetic field in the lattice can be used to tune parameters and to generate new interactions, which can stabilize novel quantum states that is absent in equilibrium. Using Schrieffer-Wolff transformation for the periodically driven system [2] and high-frequency approximation on the drive, we evaluate an effective low-energy Hamiltonian for the Hubbard honeycomb lattice in the presence of drive. We estimate the conditions on the electromagnetic drive that can allow one to tune to different quantum phases, such as transient superconductivity in our model.


*This work was carried out under the auspices of the U.S. DOE NNSA under contract No. 89233218CNA000001 through the LDRD Program.
1:27PM M50.00012: Long-lived coherent states in photo-excited NiO

DENIS GOLEZ (Presenter), Simons Foundation, KONRAD GILMEISTER, Department of physics, Institute of Physics Martin-Luther-Universitat Halle-Wittenberg, NIKOLAJ BITTNER, Department of Physics, University of Fribourg, YAROSLAV PAVLYUKH, Technische Universität Kaiserslautern, Department of Physics, CHENG-TIEN CHIANG, Department of physics, Institute of Physics Martin-Luther-Universitat Halle-Wittenberg, PHILIPP WERNER, Department of Physics, University of Fribourg, WOLF WIDDRA, Department of physics, Institute of Physics Martin-Luther-Universitat Halle-Wittenberg — Charge excitations across electronic band gaps are a key ingredient for transport in optoelectronics and light harvesting applications. In contrast to conventional semiconductors, studies of above-band-gap photoexcitations in strongly correlated materials are still in their infancy.

We will present a combined experimental and theoretical study of the ultrafast dynamics in strongly correlated photo-excited NiO [1]. By combining time-resolved two-photon photoemission experiments and the non-equilibrium extension of dynamical mean-field theory we revealed an ultrafast electronic relaxation (<10 fs) and related photo-induced in-gap states connected with the Hund excitations. Remarkably, the weight of these in-gap states displays long-lived coherent THz oscillations up to 2 ps. The frequency of these oscillations corresponds to the strength of the antiferromagnetic superexchange interaction in NiO and their lifetime vanishes as the Neel temperature is approached. Numerical simulations of a two-band t-J model reveal that the THz oscillations originate from the interplay between local many-body excitations and long-range antiferromagnetic order.


1:39PM M50.00013: Creation of Nonthermal Excited State Populations in a Large U Mott Insulator*

DANIEL NEVOLA (Presenter), Brookhaven National Laboratory, ALEXANDER W BATALLER, ANKIT KUMAR, SAMANVITHA SRIDHAR, JORDAN FRICK, SHAUN O’DONNELL, HARALD W ADE, PAUL MAGGARD, ALEXANDER F KEMPER, KENAN GUNDOGDU, DANIEL DOUGHERTY, North Carolina State University — The ability to tune between thermal and nonthermal populations lies at the heart of quantum control on ultrafast timescales. In this work, we perform time- and angle-resolved spectroscopy on the spin-orbit assisted Mott insulator α-RuCl₃. We demonstrate the ability to tune between thermalized and nonthermalized populations in the upper Hubbard band by tuning the pump energy. These populations are also shown to thermalize and decay on timescales much faster than those predicted by theory.

*Surface characterization (ARPES, 2PPE, and LEED) was funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under award No. DE-SC0010324. 2PPE instrumentation was funded by a UNC-GA ROI award. Theoretical modeling was supported by the National Science Foundation under Grant No. DMR-1752713.
1:51PM M50.00014: Laser pulse driven nonequilibrium dynamics in the Kondo lattice model*  BENEDIKT FAUSEWEH (Presenter), JIAN-XIN ZHU, Los Alamos National Laboratory — Experimental advances in nonlinear optics and ultrafast spectroscopy allow for unprecedented access to nonequilibrium physics of strongly correlated materials. By using this approach, many new and exciting phenomena have been discovered in recent years. They include light-induced superconductivity, the generation of Higgs oscillations, and the dynamical coupling of ferroelectric and ferromagnetic order. Heavy fermion systems are one prototypical class of strongly correlated materials. The interplay between localized magnetic moments and conduction electrons are the driver behind unconventional superconductivity and quantum criticality. The Kondo lattice model is used to describe the emergent phenomena of such systems. By using the powerful time-dependent variational Monte Carlo method, we investigate the nonequilibrium dynamics of the model after strong laser excitation. We demonstrate that the spin and charge fluctuations can be manipulated by varying shape and intensity of the laser pulse in different regimes of electron filling factor. In addition, experimentally measurable quantities are calculated to manifest the dynamics.

*This work was carried out under the auspices of the U.S. DOE NNSA under Contract No. 89233218CNA000001, and was supported by the LANL LDRD Program.

2:03PM M50.00015: Out-of-equilibrium dynamics in a 2D electron system with screened Coulomb interactions*  LILY STANLEY (Presenter), DRAGANA POPOVIC, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ — Considerable experimental evidence suggests that Coulomb interactions are responsible for a variety of phenomena observed in the metallic regime of 2D systems, as well as for glassy behavior near the 2D metal-insulator transition (MIT) and in the insulating regime. To address the fundamental question whether glassy behavior of electrons exists in the absence of long-range Coulomb interactions, we report a study of conductivity relaxations after excitation out of equilibrium, in particular after applying a large change of carrier density $n_s$, over a wide range of temperatures and $n_s$, spanning the 2D MIT. Experiments were performed on strongly disordered thin-oxide Si MOSFETs in which the Coulomb interaction is screened by the nearby metallic gate. The results show differences in the dynamics compared to the case of long-range interactions, and suggest the key role of long-range Coulomb interactions in the existence of glassy behavior of electrons near the 2D MIT in strongly disordered samples.

*Supported by NSF DMR-1707785 and NHMFL via NSF DMR-1644779 and the State of Florida.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M51 DCMP: Optical Studies of 2D Materials and Their Twisted Heterostructures  Mile High Ballroom 1D - Archana Raja, Lawrence Berkeley National Laboratory
11:15AM M51.00001: Fabrication of Single-Photon Emitters in 2D Hexagonal Boron Nitride via Carbon Annealing  YAOZHENG ZHU (Presenter), CHAO LYU, YU YE, Peking Univ — As the most recent addition to the single-photon emitter library, defects in hexagonal boron nitride (hBN) have attracted much attention due to their high brightness at room temperature and stability. These emitters also have the potential to integrate with cavities and photonic waveguides thanks to their 2D hosting system. Here, we developed a new method to activate single-photon emitters in 2D hBN, which is highly desired for their further application. We annealed mechanically exfoliated hBN under mixed atmosphere with methane as carbon source, and our simple one-step annealing process yields a tremendous increase in the concentration of emitters in hBN. With several related experiments, the single defects fabricated by our method are confirmed to be quantum emitters. Some other photophysical properties indicate that the emitters show higher brightness and become more stable after carbon annealing. Our approach to the design of single photon emitters in 2D hBN opens up new avenues for the generation of single photon emitters and their integration in quantum nanophotonic devices.

11:27AM M51.00002: Density functional theory of strain engineering on single photon emitter in hexagonal boron nitride  MEHDI ABDI, Department of Physics, Isfahan University of Technology, SONG LI (Presenter), JYH-PIN CHOU, City Univ of Hong Kong, GERGO THIERING, PÉTER UDVARHELYI, Wigner Research Centre for Physics, Hungarian Academy of Sciences, ALICE HU, City Univ of Hong Kong, MARTIN PLENIO, Institute of Theoretical Physics and IQST, Ulm University, ADAM GALI, Wigner Research Centre for Physics, Hungarian Academy of Sciences — Hexagonal boron nitride has been found as excellent host for color centers as single photon emitters. The complex defect which is a nitrogen vacancy next to a nitrogen antisite (VN\textsubscript{N}B) is regarded as promising candidate due to the nontrivial electronic structure.\textsuperscript{1,2} Here, using density functional theory, we provide detailed investigation of the geometric and electronic evolution of VN\textsubscript{N}B under external strain. The VN\textsubscript{N}B prefers the C\textsubscript{1h} symmetry making the defect as a dynamic Jahn-Teller system.\textsuperscript{3} By lowering the symmetry, the first transition which considered to be a dark state can be activated, inducing the compete between two possible excitation pathways.\textsuperscript{4} The zero phonon line shows non-linear evolution as a function of in plane strain indicating the important role of the out of plane strain between defect atom and its ambient structure. It is predicted that a significantly stronger redshift than blueshift of emission can be realized by applying armchair strain. Our analysis provides insightful understanding of the color centers as single photon emitters.

EMMA REGAN (Presenter), DANQING WANG, CHENHAO JIN, IQBAL UTAMA, University of California, Berkeley, BEINI GAO, Huazhong University of Science and Technology, XIN WEI, University of Chinese Academy of Sciences, SIHAN ZHAO, WENYU ZHAO, University of California, Berkeley, KENTARO YUMIGETA, MARK BLEI, Arizona State University, JOHAN CARLSTROEM, University of California, Berkeley, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, SEFAATTIN TONGAY, Arizona State University, MICHAEL F CROMMIE, ALEX ZETTL, FENG WANG, University of California, Berkeley — Moiré superlattices can be used to engineer strongly correlated phenomena in van der Waals heterostructures, as recently demonstrated in graphene-based systems. Aligned transition metal dichalcogenide (TMDC) heterostructures may also support correlated electronic states, with additional opportunities arising from the strong-light matter interaction and large spin-orbital coupling. Using a novel optical detection technique, we observe correlated electronic phases in semiconducting WSe\textsubscript{2}/WS\textsubscript{2} moiré superlattices. Further, we demonstrate that the spin-valley optical selection rules in TMDCs can be used to optically create and study low-energy spin excitations in the correlated states.

HUAN ZHAO (Presenter), YOUNGHEE KIM, ANDREW JONES, Center for Integrated Nanotechnologies, Materials Physics and Applications Divison, Los Alamos National Laboratory, ANDREI PIRYATINSKI, Theoretical Division, Los Alamos National Laboratory, HAN HTOON, Center for Integrated Nanotechnologies, Materials Physics and Applications Division, Los Alamos National Laboratory — Recently, 2D twisted bilayers with interlayer lattice mismatch and/or rotational misalignment have emerged as a powerful platform for studying unconventional properties such as the interlayer exciton (IX), where electrons and holes located in different monolayers couple to form a bound state. The IXs can further be spatially concentrated into periodic potential minima modulated via the moiré landscape, forming uniform periodic quantum-dot-like emitter array. In this talk, I will introduce optical characterization of 2D heterobilayer transition metal dichalcogenides (TMDCs) interlayer excitons under different configurations of interlayer twisting angles and material selections. 2D heterobilayers with deterministic interlayer twist angle were prepared using a custom-built layer stacking system. Here, we studied the light emission properties with time-resolved photoluminescence (PL), temperature-dependent PL, and magneto-PL. Through the PL studies, we were able to extract key parameters of interlayer excitons such as lifetime, binding energy, valley polarization, etc. These results represent an advance in the understanding of the physics of 2D interlayer excitations and the future implementation of these TMDC materials within tunable light-emitting devices.
12:03PM M51.00005: Anomalous bright narrow interlayer exciton photoluminescence in MoSe$_2$-WSe$_2$ heterostructures*  FATEME MAHDIKHANYSARVEJAHANY (Presenter), Univ of Arizona, MICHAEL KOEHLER, Department of Materials Science and Engineering, University of Tennessee, DAVID MANDRUS, Department of Physics and Astronomy, University of Tennessee, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, OLIVER MONTI, BRIAN J LEROY, JOHN SCHAIBLEY, Univ of Arizona — Van der Waals heterostructures provide a new platform for studying spatially indirect interlayer excitons, where the constituent electrons and holes are located in different layers. These heterostructures are made by stacking two or more two-dimensional materials via a polymer stamping technique. Stacking layers with a lattice mismatch and/or twist angle between layers will form a moiré pattern in real space. This moiré lattice can modulate the exciton energy, resulting in so-called moiré excitons where excitons are trapped at the moiré potential minima. Recent studies on - heterostructures have shown narrow lines in low power photoluminescence(PL), which were attributed to moiré excitons. Optical measurements of our high-quality - heterostructures encapsulated by hBN shows an anomalous bright narrow interlayer exciton PL localized to a small area of the sample. The PL of this structure shows interlayer PL emission whose linewidth is comparable to delocalized interalayer excitons in high quality samples. We will discuss the density and temperature dependence of this bright interlayer exciton PL and how it relates to other recent reports of interlayer moiré excitons in transition metal dichalcogenide heterostructures.

*We thank NSF-DMR 1838378 for the funding.

12:15PM M51.00006: Emergent magnetic field from the moiré of homobilayer 2D semiconductors*  DAWEI Zhai (Presenter), The University of Hong Kong, HONGYI YU, Sun Yat-Sen University (Zhuhai Campus), MINGXING CHEN, Hunan Normal University, WANG YAO, The University of Hong Kong — The spatial texture of internal degree of freedom of electrons has profound effects on material properties. Such texture in real space can manifest as an emergent magnetic field, which is expected to induce interesting transport phenomena. Moiré pattern as a spatial variation at the interface of 2D atomic crystals provides a natural platform for investigating such real space Berry phase effect [1]. Here we study Moiré structures formed in homobilayer TMD due to twisting, uniform strains, and their combinations [2], where electrons can reside in either layer with the layer index serving as an internal degree of freedom. The layer pseudospin exhibits vortex/antivortex textures in the Moiré supercell, which leads to a giant magnetic field. We will show that strain and interlayer bias can be used to engineer the in-plane and out-of-plane layer pseudospin texture, respectively. Therefore, the profile, intensity, and flux of the magnetic field are highly tunable, rendering TMD Moiré structures promising for transport and topological material applications.


*The work is supported by RGC of HKSAR (17306819).
12:27PM M51.00007: Induced spin-orbit coupling in twisted graphene-TMDC heterobilayers: Twistorics meets spintronics

ALESSANDRO DAVID (Presenter), Department of Physics, University of Konstanz, PÉTER RAKYTA, ANDOR KORMANYOS, Department of Physics of Complex Systems, Eötvös Loránd University, GUIDO BURKARD, Department of Physics, University of Konstanz — Transport experiments in graphene deposited on monolayer transition metal dichalcogenide (TMDC) have demonstrated weak antilocalization, Shubnikov-de Haas oscillations, spin lifetime anisotropy, spin Hall effect and Rashba-Edelstein effect [1]. This suggests that spin-orbit coupling (SOC) in graphene is enhanced by the strong intrinsic SOC of the nearby TMDC layer. Setting up a theoretical model of the graphene-TMDC heterobilayer we are able to explain the origin and predict the interlayer twist angle dependence of the induced SOC [2]. We derive the induced valley Zeeman and Rashba type SOC in terms of the TMDC band structure parameters and interlayer tunneling matrix elements. We find that the strength of the induced SOC can be strongly tuned by the twist angle. Provided that the energy of the Dirac point is close to the TMDC conduction band, up to a tenfold increase of the valley Zeeman (at 18 degrees twist angle) and a fourfold increase of the Rashba type induced SOC can be achieved. Moreover, we have extended our model to the case of graphene encapsulated in two TMDC layers, where the induced SOC is also modulated by the additional twist angle.


12:39PM M51.00008: The optical evidence of atomic reconstruction in twisted bilayer MoS$_2$*

JIAMIN QUAN (Presenter), University of Texas at Austin, LUKAS LINHART, Vienna University of Technology, MIAO-LING LIN, Chinese Academy of Sciences, CHUN YUAN WANG, WEI-TING HSU, JUNHO CHOI, CARTER YOUNG, University of Texas at Austin, TAKASHI TANIGUCHI, National Institute of Material Science in Tsukuba, CHIH-KANG SHIH, ALLAN MACDONALD, University of Texas at Austin, PING-HENG TAN, Chinese Academy of Sciences, FLORIAN M LIBLESCH, Vienna University of Technology, XIAOQIN (ELAINE) LI, University of Texas at Austin — In two-dimensional materials, Moiré superlattices formed by stacking two monolayers with lattice constant mismatch or rotational misalignment have been widely used to manipulate their electronic and optical properties. Here, we employ low-frequency Raman measurements and DFT calculations to demonstrate atomic reconstruction in the MoS$_2$ homobilayer with a small twist angle ($\theta$). For $0^\circ < \theta \leq 3.5^\circ$, only interlayer Raman mode of 3R stacking with stable peak position is presented, indicating the overwhelming expansion of stable stacking in small twist angle due to structural relaxation. For $3.5^\circ < \theta \leq 6^\circ$, the small Moiré supercell with weak relaxation results in mixed in-plane and out-of-plane vibrations. The shear mode quickly disappears with an increasing twist angle, while mixed breathing modes are observed. Our work provides a novel strategy to understand and monitor the evolution of structural relaxation in moiré superlattices in two-dimensional van der Waals materials.

*Funding from DOE and a catalyst grant provided by the College of Natural Science at the University of Texas-Austin are gratefully acknowledged.
12:51PM M51.00009: Interlayer Excitons in van der Waals Heterostructures in a Magnetic Field
JINLYU CAO (Presenter), HERBERT FERTIG, Indiana Univ - Bloomington, LUIS BREY, Instituto de Ciencia de Materiales de Madrid-CSIC, Cantoblanco — We investigate particle-hole excitations in bilayer 2D van der Waals heterostructures in a magnetic field. Such systems are interesting because the two constituents of the excitons can reside in band environments of very different Berry’s curvatures. This allows the neutral excitations to carry signatures of the fermionic electronic structures of the individual materials. Moreover, the heterostructures can give rise to a large moiré unit cell. The effective periodicity relaxes momentum conservation so that the exciton dispersion at finite momentum could be detected by light absorption. As an example, we study an MoS$_2$-graphene heterostructure, for which both valleys host Berry’s curvature in only one layer. We consider variational single particle-hole pair wavefunctions, both in terms of the Landau levels and eigenstates of magnetic translation operators. The formalism allows one to identify how wavefunction overlaps determine the exciton state and energy. We show for this heterostructure that the energy disperses remarkably slowly. The impacts of many-body effects and the quasi-periodic tunneling between the layers associated with the moiré pattern on exciton dispersions and light absorption are also considered.

*NSF; Research Corporation; US-Israel Binational Science Foundation

1:03PM M51.00010: Near field study of twisted transition metal dichalcogenide bilayers
SHUAI ZHANG (Presenter), AARON STERNBACH, Department of Physics, Columbia University, BAICHANG LI, Department of Mechanical Engineering, Columbia University, LIN ZHOU, WENJING WU, Department of Chemistry, Columbia University, LIN XIONG, Department of Physics, Columbia University, ESSANCE RAY, NATHAN P WILSON, XIAODONG XIU, Department of Physics, University of Washington, XIAOYANG ZHU, Department of Chemistry, Columbia University, JAMES C HONE, Department of Mechanical Engineering, Columbia University, DMITRI BASOV, Department of Physics, Columbia University — Twistronics has recently emerged as a novel tuning knob to engineer the properties of electrons and excitons in two dimensional van der Waals heterostructures. However, directly probing the properties of vdW heterostructures within a single moiré unit cell remains elusive. In this talk, we utilize near-field optical microscopy to explore twisted transition metal dichalcogenides (TMD) bilayers. The atomically thin vertical p-n junction of WSe$_2$/MoSe$_2$ bilayer is fabricated by mechanical exfoliation and stacking. The type-II band alignment of the WSe$_2$/MoSe$_2$ facilitates electron-hole separation permitting photocurrent measurements at the nanoscale. Features with ~100 nm periodicity are observed and show systematic evolution under electrostatic gating. More experiments are carrying out to conclusively assign these features to the moiré. Our study demonstrates a viable pathway towards probing and manipulating moiré patterned TMD heterostructures at the nanoscale.
1:15PM M51.00011: Floquet-Engineered Topological Flat Bands in Irradiated Twisted Bilayer Graphene* YAN TAO LI (Presenter), HERBERT FERTIG, BABAK H SERADJEH, Indiana Univ - Bloomington — We propose a tunable optical setup to engineer topologically nontrivial flat bands in twisted bilayer graphene under circularly polarized light. Using both analytical and numerical calculations, we demonstrate that nearly flat bands can be engineered at small twist angles near the magic angles of the static system. The flatness and the gaps between these bands can be tuned optically by varying laser frequency and amplitude. We study the effects of interlayer hopping variations on Floquet flat bands and find that lattice relaxation favors their formation. Furthermore, we find that, once formed, the flat bands carry nonzero Chern numbers. We show that at currently known values of parameters, such topological flat bands can be realized using circularly polarized UV laser light. Thus, our work opens the way to creating optically tunable, strongly correlated topological phases of electrons in moire superlattices.

*This work is supported in part by the NSF awards DMR-1350663, DMR-1506263, DMR-1914451, ECCS-1936406, US-Israel BSF grant No. 2016130, the Research Corporation Cottrell SEED Award, the Max-Planck Institute for the Physics of Complex Systems in Dresden, the Aspen Center for Physics via NSF grant PHY-1607611, and the College of Arts and Sciences at Indiana University.

1:27PM M51.00012: Doping-dependence of exciton energies and MCD in TMD moiré superlattices* IGOR BLINOV (Presenter), ALLAN MACDONALD, Physics department, University of Texas at Austin — The long-period pattern formed by two-dimensional crystals that are slightly misaligned or have slightly different lattice constants is known as a moire superlattice. It was recently discovered that the moiré superlattices have a pronounced effect on the electronic properties of many two-dimensional materials. I will discuss the influence of a moiré superlattice on excitons in transition metal dichalcogenide heterostructures. Existing effective boson theories of the moiré excitons do not allow the effect of electron or hole doping to be predicted. I will present a microscopic calculation of the optical response at finite doping, as well as a simple phenomenological model, which captures the main results. When the carriers are valley polarized the optical response exhibits circular dichroism. I will discuss the use of the circular dichroism of the exciton spectrum as a probe of ground state valley polarization.

*Work supported by the Army Research Office (ARO) Grant # W911NF-17-1-0312 (MURI).
1:39PM M51.00013: Excitonic insulator and spin-valley superfluid in twisted bilayer transition metal dichalcogenide* ZHEN BI (Presenter), LIANG FU, Massachusetts Institute of Technology MIT — Recently striking correlated phenomena emerge in twisted bilayer WSe$_2$ -- including a correlated moiré insulating dome at half-filling -- over a range of small twist angles. In this work, we show the half-filling state is an intervalley excitonic insulator, where the electron-hole pairing is strongly enhanced for a certain range of displacement field due to the proximity of a van Hove singularity to the Fermi level. The mean field phase diagram as a function of displacement field, temperature and magnetic field shows a good agreement with the experiment. Furthermore, the excitonic insulator hosts a spin-valley density wave order which can be viewed as a spin superfluid. We propose an all-optical setup to study the superflow of spins in the twisted bilayer transition metal dichalcogenide systems.

*Z.B. is supported through Pappalardo fellowship at MIT. L.F. is supported by DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0018945. L.F. is also partly supported by the David and Lucile Packard Foundation.

1:51PM M51.00014: Dielectric engineering in monolayer WSe$_2$/graphene heterostructures YANG XU (Presenter), CONNOR HORN, Cornell University, NY, USA, DANIEL A RHODES, Columbia University, NY, USA, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Tsukuba, Japan, JAMES C HONE, Columbia University, NY, USA, JIE SHAN, KIN FAI MAK, Cornell University, NY, USA — The strong Coulomb interaction between charge carriers in atomically thin transition metal dichalcogenides (e.g. MoS$_2$, WSe$_2$) is sensitive to the nearby dielectric environment. Here, we investigate the optical response of monolayer WSe$_2$, which is in contact with gate-tunable graphene in van der Waals heterostructures, by optical reflection spectroscopy. We find that both the exciton binding energy and quasiparticle bandgap of WSe$_2$ can be renormalized by the dielectric screening effect. The effect can also be modulated upon the formation of Landau levels in graphene under perpendicular magnetic fields. Furthermore, we directly observe inter-band Landau level transitions of WSe$_2$, which helps to accurately determine the quasiparticle bandgap and effective cyclotron mass in WSe$_2$ as a function of dielectric screening.
HECTOR OCHOA, ANA ASENJO-GARCIA (Presenter), Columbia University — We present a minimal continuum model describing the electronic reconstruction in twisted bilayers of hexagonal boron nitride. The relative twist creates regions of unnatural stacking within the moiré cell, where ions of the same polarity lie on top of each other. The gap is strongly modulated, giving rise to very narrow quasi-bands at relative large twist angles. The absence of a magic angle condition emphasizes the different nature of these flat bands as compared to the case of twisted graphene systems. In particular, changing the parameters of our model we can describe both situations, which are separated by a topological phase transition controlled by inter-band coherences of the envelope wave functions around the moiré zone center. Transitions between these flat bands are manifested as sharp resonances in the optical absorption spectrum. We also evaluate the Hall counter-flow ascribed to the chiral symmetry of the system, which gives rise to different absorption cross sections for right-handed and left-handed circularly-polarized light (circular dichroism).

*This work was supported as part of Programmable Quantum Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under award DE-SC0019443.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M52 DCMP: Surface Studies of Transition Metal Dichalcogenides Mile High Ballroom 1E - Daniel Dougherty, North Carolina State University

SOYEONG KWON (Presenter), YUGYEONG JE, JUNGEUN SONG, EUNAH KIM, BORA KIM, SANG WOOK LEE, DONGWOOK KIM, EWHA Woman's Univ — Understanding the physical properties of metal-semiconductor contacts is crucial for both electrical characterizations and device applications. In this work, MoS$_2$ monolayers were transferred on Au nanostripe arrays. The surface potential distributions of the samples in dark and under light illumination were investigated using Kelvin probe force microscopy, which has a few tens of nm spatial resolution. To explain the surface potential contrast change in dark and light, we proposed the energy band diagrams considering the strain and electronic interaction. Optical micro-reflectivity spectra was also obtained and compared with numerical simulation results. The relationship between the surface potential maps and the optical characteristics of the samples will be discussed in this presentation.
11:27AM M52.00002: Studies of Band Alignment in WS2/MoS2/Al2O3 Heterostructures using Kelvin Probe Force Microscopy  BORA KIM (Presenter), EWHA Woman's Univ, PO-CHENG TSAI, Research Center for Applied Sciences, Academia Sinica, JAYEONG KIM, EUNAH KIM, SOYEONG KWON, SEOKHYUN YOON, EWHA Woman's Univ, SHIH-YEN LIN, Research Center for Applied Sciences, Academia Sinica, DONGWOOK KIM, EWHA Woman's Univ — Two-dimensional (2D) crystals can be assembled into van der Waals (vdW) heterostructures by mechanical exfoliation or chemical vapor deposition. Charge transport and recombination processes are determined by the band alignment in the heterostructures. Therefore, investigation of the band alignment is a crucial step toward the applications of the 2D vdW heterostructures. In this work, we fabricated WS2/MoS2 heterostructures on single crystal Al2O3 wafers, using sulfurization of pre-deposited transition metal layers. The surface potential of the sample in dark and light was measured using Kelvin probe force microscopy, which allowed us to suggest the band diagrams of the vdW heterostructures. The measured Raman spectra of the heterostructures supported the proposed band alignment, considering the electronic interaction at the interface and the interlayer screening effects.

11:39AM M52.00003: Mottness versus unit-cell doubling as the driver of the insulating state in 1T-TaS2  CHRISTOPHER BUTLER (Presenter), MASARO YOSHIDA, TETSUO HANAGURI, CEMS, RIKEN, YOSHIHIRO IWASA, Department of Applied Physics, The University of Tokyo — Recent debate about the nature of the insulating ground state in 1T-TaS2 has largely hinged around the stacking pattern of its quasi-2D charge ordered layers. The stacking determines whether the 3D unit-cell contains one or two ‘Star-of-David’ (SD) clusters, each of which hosts 13 unpaired Ta orbitals. For simple stacking with one SD per cell, the insulating state must be explained by Mott physics, but for stacking with a dimerized pair of SDs per cell, ab initio calculations predict a band insulator [1,2]. We will describe scanning tunneling microscopy measurements [3] showing two distinct terminations of the 3D charge order - the sign of a stacking pattern with two SDs per cell - and determine the inter-layer stacking vectors. We argue that the persistence of a spectral gap even at the surface which breaks the SD dimers is a manifestation of Mottness. We also identify a stacking vector, extrinsic to the natural pattern, which renders the surface metallic. These results help to understand this material's mysterious insulating state, and its potentially useful metal-insulator transitions.

11:51AM M52.00004: Confinement Heteroepitaxy: A Novel Route for Realizing Exotic 2D Materials*  ALEXANDER VERA (Presenter), WILSON YANEZ, NATALIE BRIGGS, TIMOTHY BOWEN, SIAVASH RAJABPOUR, NITIN SAMARTH, JOSHUA ROBINSON, Pennsylvania State University — Advancement of nascent electronic quantum frontiers (spintronics, photonics, and sensing) has been mediated through development of materials platforms with non-trivial band topologies, allowing distinct access to quantum information otherwise lost through decoherence. However, access to the more exotic quantum phenomena within these frontiers still pose a materials challenge due to synthesis difficulties or small windows of performance, which render these routes limited in scalability. We have demonstrated facile synthesis of air-stable, atomically thin, single crystal two-dimensional (2D) metals (gallium, indium, tin, lead, and silver) within a silicon carbide and epitaxial graphene interface through high-pressure intercalation (i.e. confinement heteroepitaxy, or CHet). The non-centrosymmetric nature, coupled with potentially strong spin orbit coupling and superconductivity, in these 2D metals, suggest this novel synthesis route as an avenue for manifesting exotic effects (such as topological superconductivity) due to non-trivial band topology.

*Funding provided by Nothrop Grumman Corp. and the Air Force Office of Scientific Research for this project.

12:03PM M52.00005: Surface Engineering of Monolayer MoS₂ for Atomic Layer Deposition of TiO₂*  JARON KROP (Presenter), CAN ATACA, THEODOSIA GOUGOUSI, Univ of Maryland-Baltimore County — We investigate methods to improve the growth of high-quality TiO₂ films on MoS₂ via atomic layer deposition (ALD). Untreated MoS₂ surfaces are hydrophobic, and as a result, ALD results in discontinuous films that nucleate only on defect sites. Since pristine MoS₂ monolayers have low defect density, argon ion bombardment is used to create sulfur vacancies. The vacancy concentration is monitored in-situ with x-ray photoelectron spectroscopy. We use thiols to passivate the vacancies and act as a seed layer for ALD. However, spontaneous oxidation of the defective MoS₂ layer can occur, and ALD on argon sputtered MoS₂ results in uniform TiO₂ films with and without the thiol treatment. Without thiol treatment, dissociative adsorption of oxygen molecules on the sulfur vacancies may seed the ALD by leaving behind adsorbed atomic oxygen. With density functional theory, we investigate the electronic properties of defective, thiol- and oxygen-passivated sulfur vacancies in MoS₂. Thiol- or oxygen-passivated MoS₂ retains desirable electronic properties. Careful control of the sulfur vacancy concentration followed by functionalization can provide a means of tuning the electronic properties of MoS₂ and providing seed sites for high quality ALD film growth.

*NSF DMR-1726213
NSF ECCS-1407677
Monolayers on Periodic Au Nanostructures  JUNGEUN SONG (Presenter), SOYEONG KWON, EUNAH KIM, BORA KIM, DONGWOOK KIM, EWHA Woman's Univ, SEONGYEON LEE, KIJU YEE, Chungnam National Univ — MoS\(_2\) monolayers were prepared on hexagonal arrays of Au nanotriangles (NTs) and nanoholes (NHs), fabricated by nanosphere lithography. Photoluminescence (PL) and optical reflectivity spectra of the samples on the Au NT and NH arrays were investigated. The surface plasmon excitation and Wood anomaly affected the reflectivity data, which could be clearly explained by numerical simulations. Also, light-induced surface potential change, determined by spatial distribution of the photo-generated charge carriers, was studied using Kelvin probe force microscopy. The comparison of the two kinds of samples on the NT and NH arrays could show us how the periodic metal nanostructures influenced the physical characteristics of the MoS\(_2\) layers.

Scanning tunneling microscopy study of monolayer NbSe\(_2\)*  MENGKE LIU (Presenter), JIA YU, CHIH-KANG SHIH, University of Texas at Austin — Two-dimensional transition metal dichalcogenides (TMD) have received significant interest due to their unique structural and electrical properties. Within the family of TMD materials, NbSe\(_2\) has a 2H phase which is metallic in nature and interestingly exhibits a charge density wave and superconducting phase transition. Naturally occurring bulk NbSe\(_2\) is a 2H phase, however, recently a 1T phase of NbSe\(_2\) was grown by MBE. Intriguingly, this 1T phase exhibits an energy gap and insulating behavior at low temperatures. In this work, we study MBE grown monolayer NbSe\(_2\) using scanning tunneling microscopy and spectroscopy (STM/S). We report both 2H and 1T phases are present in the growth, and whose relative abundance suggests a growth temperature dependence. We further report comparative studies of the electronic properties of both 2H and 1T phases using STM/S.

*This work was supported by National Science Foundation (NSF), DMR-1808751, Welch Foundation, F-1672 and US Airforce, FA2386-18-1-4097.
**12:39PM M52.00008: Thickness Dependent Electronic Structures of Pd Dichalcogenides: A First Principles Study**  
LIANG-YING FENG (Presenter), ROVI ANGELO B. VILLAOS, ZHI-QUAN HUANG, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Natl Sun Yat Sen Univ — Among the family of transition metal dichalcogenides (TMDs), Pd-based TMDs have been one of the less explored materials. In this study, using first-principles calculations, we investigate the electronic properties of PdX$_2$ (X=S, Se, or Te) with respect to film thickness. With regards to the structural stability, the bulk and thin film structures of PdS$_2$ and PdSe$_2$ exhibit pyrite phase, while PdTe$_2$ exhibits 1T phase as their most stable configurations. For the electronic properties, the most stable bulk configurations demonstrate semi-metallic features, while their corresponding monolayer structures for pyrite PdS$_2$ and PdSe$_2$ are insulating with band gaps of 1.399 eV and 1.548 eV, respectively, while 1T PdTe$_2$ remained to be semi-metallic. For the band properties, we observe that all these materials manifest decreasing/closing of indirect band gap with increasing thickness. Moreover, all the stable monolayer band structures exhibit flat bands and diverging density of states near the Fermi level, indicating the presence of van Hove singularity.

*Feng-Chuan Chuang acknowledges support from the National Center for Theoretical Sciences and the Ministry of Science and Technology of Taiwan under Grants No. MOST-107-2628-M-110-001-MY3.*

**12:51PM M52.00009: Electronic Growth Modes in Metal Dichalcogenide Interfaces**  
TIM KIDD (Presenter), EVAN O'LEARY, ANDREW STOLLENWERK, Univ of Northern Iowa — The transition metal dichalcogenides (TMDCs) are a family of materials of great interest for chemical tunability and novel electronic properties. The TMDC surface terminates at a van der Waals gap, making a stable, highly non-interacting growth surface. We have found that this lack of interaction can induce a variety of metals to spontaneously organize into films or nanostructures with strongly preferred heights upon the TMDC surface. The terraces of these features are atomically flat and highly oriented. Their structure can be predicted using only the electronic structure of the metal. This electronic growth differs from previously reported magic height systems in that high temperature annealing enhances growth properties, implying true equilibrium conditions. This process could be extended to a great number of highly 2D materials and open new avenues of research for self-assembled nanostructures with various electronic or spin-based confinement.

*The initial stages of work on Au/MoS$_2$ were supported by funding from National Science Foundation Grant No. DMR-1410496 for the initial stages of research on the Au/MoS$_2$ system. The work performed to refine the Au/MoS$_2$ system and with metals was supported by the grant DE-SC0020334 funded by the U.S. Department of Energy, Office of Science.*
1:03PM M52.00010: Doping WS$_2$ armchair nanoribbons with transition metals* YAN-HONG CHEN, Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan, ROC., CHI-HSUAN LEE, Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan, ROC., SHUN-JEN CHENG, Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan, ROC., CHIH-KAI YANG (Presenter), Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan, ROC — Armchair WS$_2$ nanoribbons are semiconductors with band gaps close to 0.5 eV. When a W atom is replaced by a transition metal, impurity states can have tremendous effect on the overall electronic structures. By using first-principles calculations based on density functional theory, we investigated substitutional of Ti, V, Cr, Mn, Fe, Co for WS$_2$ ribbons of different widths. We found that Fe-doped ribbons have two-channel conduction separately in the middle part of the ribbon and at the edges. Co-doped ribbons are turned in to spin filters, having 100% spin-polarized conductions. These results should be useful for nano-electronic circuit design.

*supported in part by the National Science Council of the Republic of China under grant number MOST 108-2112-M-004-001.

1:15PM M52.00011: Induction of Phase Transition in Transition Metal Dichalcogenides on Metal Substrates* CHI SIN TANG (Presenter), XINMAO YIN, Natl Univ of Singapore, DI WU, Shenzhen University, WEILONG KONG, QIXING WANG, Natl Univ of Singapore, MING YANG, Agency for Science, Technology and Research, MARK B. H. BREESE, Natl Univ of Singapore, WENJING ZHANG, Shenzhen University, ANDRIVO RUSYDI, ANDREW THYE SHEN WEE, Natl Univ of Singapore — Two-dimensional transition metal dichalcogenides (2D-TMDs) possess unique structural phases including the semiconducting 1H and quasi-metallic 1T' phases. They show intriguing optical and electronic properties. 1H to 1T' phase transition processes are important to be utilized for novel device applications. We present a high-yield 1H to 1T' phase transition of monolayer-MoS$_2$ on Cu and monolayer-WSe$_2$ on Au via an annealing-based process. Both experimental and first-principles studies are conducted to study the phase transition mechanism. The 1T' phase yield is increased via interfacial hybridizations enhancement through interfacial binding energy, charge transfer, shorter interfacial spacing, and weaker bond strength.

1:27PM M52.00012: Tuning the Electronic Band Structure of Copper Selenide Cu$_2$Se Thin Films Grown via Molecular Beam Epitaxy* RYAN TREY VAN HAREN (Presenter), TOYANATH JOSHI, DAVID LEDERMAN, Department of Physics, University of California, Santa Cruz — Cu$_2$Se has long been known to be an excellent thermoelectric material whose electronic band structure that is tunable by introducing copper vacancies into the crystal structure. More recently, this compound has been predicted to host topologically-protected surface states. In this work, we will present our successful epitaxial growths of Cu$_{2-x}$Se thin films via molecular beam epitaxy (MBE). Using reflection high energy electron diffraction (RHEED) and x-ray diffraction (XRD) measurements, we will show how we are able to quantify the copper concentration by analyzing the subtle shifts in our observed XRD spectra corresponding to small changes in the lattice spacing due to these copper vacancies and how these vacancies influence electronic transport in the film. In this manner we will demonstrate how we are able to tune the copper vacancies and electronic band structure by precise control of the crystal's growth parameters.

*Funding was provided by the University of California Multicampus Research Programs and Initiatives (grant MRP-17-454963).

1:39PM M52.00013: Fabrication of Copper Selenate Thin Films by Pulsed Laser Deposition* DAVID KING (Presenter), JINKE TANG, UPPALAIHA ERUGU, Physics and Astronomy, University of Wyoming, JOHN ACKERMAN, Chemical Engineering, University of Wyoming — Cu$_2$OSeO$_3$ is a rare material with properties that are highly desirable for spintronic devices: it is an insulating ferrimagnet that also hosts magnetic skyrmions. Previous investigations of Cu$_2$OSeO$_3$ have emphasized single crystals. However, skyrmions are typically more stable in thin films than in bulk materials. Also, thin films are more suitable for device applications than single crystals. In this research, we present results of using pulsed laser deposition (PLD) to fabricate thin films of Cu$_2$OSeO$_3$, specifically accounting for the high disparity in vapor pressure between the reactants CuO and SeO$_2$. Data showing the film's magnetic properties, crystallography, and electrical properties are presented.

*This work was supported by the National Science Foundation (DMR-1710512).
1:51PM M52.00014: Dimensionality-Mediated Semimetal-Semiconductor Transition in Ultrathin PtTe$_2$ Films

MENG-KAI LIN (Presenter), University of Illinois at Urbana-Champaign, ROVIN ANGELO B. VILLAOS, Physics, National Sun Yat-Sen University, JOSEPH HLEVYACK, PENG CHEN, RO-YA LIU, University of Illinois at Urbana-Champaign, CHIA-HSIU HSU, Physics, National Sun Yat-Sen University, JOSÉ AVILA, SynchrotronSOLEIL and Université Paris-Saclay, SUNG-KWAN MO, Advanced Light Source, Lawrence Berkeley National Laboratory, FENG-CHUAN CHUANG, Physics, National Sun Yat-Sen University, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign — Platinum ditelluride (PtTe$_2$), a type-II Dirac semimetal in the bulk form, is made of Te-Pt-Te tri-atomic layers (TLs) loosely bonded together by van der Waals interactions. It remains semimetallic in ultrathin films down to just two TLs, but a further reduction of the film thickness to just a single TL induces a Lifshitz electronic transition to a semiconductor with a sizable gap. This transition is evidenced by experimental mapping of the band structure by angle-resolved photoemission spectroscopy for films of various thicknesses prepared by molecular beam epitaxy on a bilayer-graphene-terminated SiC substrate. Layer-by-layer evolution of the band structure is well resolved, which facilitates absolute layer counting. The measured semiconducting band structure for the single TL is in excellent agreement with theoretical calculations. Our results demonstrate a novel electronic transition at the single-layer, or two-dimensional limit through film thickness control.

2:03PM M52.00015: Structural response of a slit-shaped graphene nanopore to adsorption: Observation by in situ neutron diffraction*

JOSEPH SCHAEPERKOETTER (Presenter), MURR, Univ of Missouri - Columbia, HASKELL TAUB, Physics, Univ of Missouri-Columbia, HELMUT KAISER, MURR, Univ of Missouri - Columbia, ZACHARY BUCK, Physics, Univ of Missouri-Columbia, MATTHEW CONNOLLY, National Institute of Standards and Technology Boulder, CARLOS WEXLER, Physics, Univ of Missouri-Columbia — We have investigated adsorption-induced deformation in graphene oxide framework materials (GOFs) using neutron diffraction at sample pressures up to 140 bar. GOFs, made by solvothermal reaction of graphite oxide (GO) and benzene-1,4-diaboronic acid (DBA), are a suitable candidate for deformation studies due to their narrow (∼1 nm), monodispersed, slit-shaped pores whose width can be measured by diffraction techniques. We have observed, in situ, a monotonic expansion of the slit width with increasing pressure upon adsorption of xenon, methane, and hydrogen under supercritical conditions [1]. We find that the expansion of the three gases can be mapped onto a common curve based solely on their Lennard-Jones parameters, in a manner similar to a law of corresponding states. All scattering measurements were performed on the 2-axis powder diffractometer at the Missouri University Research Reactor (MURR).


*This work was supported by the National Science Foundation Grant No. DGE-1069091.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M53 DMP: Two-Dimensional Magnetism Mile High Ballroom 1F - Tag(s): Focus
Of magnetic van der Waals materials, TMPS3 with TM=transition metal elements have attracted significant attentions as it can exhibit the three fundamental magnetic model of Ising (FePS3), XY (NiPS3) and Heisenberg (MnPS3) Hamiltonian depending on the TM elements. Using these materials, we have studied some of the fundamental theorems of modern magnetism. In addition, we have also investigated how correlation physics plays a role in the optical spectroscopy data. In this talk, I will demonstrate how we can use this unique magnetic property of these materials to learn of the old physics.

A van der Waals metal thiophosphate ferromagnetic semiconductor AgVP$_2$Se$_6$  

YUXUAN PENG (Presenter), XING CHENG, PINGFAN GU, FANGGUI WANG, JIE YANG, WENYUN YANG, YU YE, JINBO YANG, School of Physics, Peking University — The recent realization of two-dimensional (2D) magnetism in van der Waals (vdWs) magnets holds the promise for the low-power spintronic applications. The 2D semiconducting ferromagnets, which remain rare, are special important in developing 2D magnetic devices with new functionalities. Metal thiophosphate (MTP), a multifunctional 2D material system that combines the sought-after properties of complex oxides, is a promising 2D magnet system. Here, we successfully synthesize single crystals of a novel 2D ferromagnetic semiconductor MTP AgVP$_2$Se$_6$ with a bandgap of 2.14 eV at room temperature. Due to the nature of vdWs bonding along the c axis, the magnetic properties of the few-layer AgVP$_2$Se$_6$ with different thicknesses are characterized on the exfoliated samples. The AgVP$_2$Se$_6$ flakes exhibit significant thickness-dependent magnetic properties, and a rectangular hysteresis loop with a large coercive field of 750 Oe at 2 K and an undiminished Curie temperature of 19 K are observed in the 6.7 nm AgVP$_2$Se$_6$ flake. The discovered 2D hard ferromagnet AgVP$_2$Se$_6$ with semiconducting behavior will provide alternative platforms for exploring 2D magnetism and potential applications in spintronic devices.

Tunable defect-induced magnetism in Pt-based dichalcogenides*

PRIYANKA MANCHANDA (Presenter), PRATIBHA DEV, Howard University — The much-sought-after magnetism in two-dimensional (2D) materials is not only important for its potential applications in spintronic and magneto-optical devices, but also due to its impact on our understanding of fundamental principles in solid state physics. In addition, 2D magnetic solids offer a unique opportunity for heterogeneous assembly with potentially new emergent phenomena. Amongst recent reports of magnetic 2D materials, magnetism was experimentally observed in PtSe$_2$ thin films and was attributed to the naturally-occuring Pt vacancies. In this theoretical work, we show that the defect-induced magnetism in the PtSe$_2$ thin films is highly sensitive to: (i) the PtSe$_2$ layer-thickness (ii) defect density, (iii) the strain in the layer, and (iv) substrate choice. These different factors dramatically modify magnetic properties such as, the magnitude of the local moments, strength of coupling, and even the nature of coupling between the moments. The tunability of the magnetic properties in the Pt-based dichalcogenides can be used to design novel devices for magnetoelectric and magneto-optics applications.

*This work is supported by National Science Foundation under grant number DMR-1752840.
12:51PM M53.00005: Atomic-Scale Visualization of Reversible Phase Transformation in 2D Ferroelectric In$_2$Se$_3$  
FAN ZHANG (Presenter), Beijing Academy of Quantum Information Science, Beijing 100193, China;  
Department of physics, Virginia Tech, ZHE WANG, International Center for Quantum Design of Functional Materials, University of Science and Technology of China, LIXUAN LIU, ZHONGYUAN LIU, State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, WENQUANG ZHU, International Center for Quantum Design of Functional Materials, University of Science and Technology of China, CHENGGGANG TAO, Department of Physics, Virginia Tech — Phase transformation in emerging two dimensional (2D) materials is crucial for understanding and controlling the interplay between structure and electronic properties. In 2D In$_2$Se$_3$ synthesized via CVD, we observe that In$_2$Se$_3$ layers with thickness ranging from single layer to ~20 layers stabilize at the $\beta$ phase with a superstructure at room temperature. At around 180 K the $\beta$ phase converts to a more stable $\beta'$ phase that is distinct from previously reported phases in 2D In$_2$Se$_3$. The kinetics of the reversible thermally driven $\beta$-to-$\beta'$ phase transformation is investigated by temperature dependent TEM and Raman spectroscopy, corroborated with the expected minimum-energy pathways obtained from our first-principles calculations. DFT calculations further reveal in-plane ferroelectricity in the $\beta'$ phase. We will also discuss domain boundaries between $\beta'$ phase domains with different orientations. The domain boundary structures are visualized by atomically resolved STM imaging and the localized boundary states are revealed by STS.


1:03PM M53.00006: Anisotropic magnetic properties of novel correlated van der-Waals materials*  
SAICHARAN ASWARTHAM (Presenter), SEBASTIAN SELTER, YULIIA SHERMERLIUK, ANJA WOLTER, BERND BUECHNER, Inst for Festkorper Werkstoffforschung — Layered van der Waals crystals with Weak couplings between individual layers has generated enormous interest in scientific community, because of the presence of long range magnetic order down to monolayer limit. The family of transition metal trichalcogenides (TMTC) belongs to the class of layered van der Waals materials. These TMTCs exhibits many interesting physical properties such as the metal/insulator transition, magnetism, and superconductivity under pressure. Also, when thinned down to the monolayer limit, significant changes in the physical properties have been observed. Most of these properties steam from the strong 2D character associated with the layered crystal structure. Cr$_2$Ge$_2$Te$_6$ is a ferromagnetic insulator whereas Ni$_2$P$_2$S$_6$ & Fe$_2$P$_2$S$_6$ are aniferromagnetic insulators. In this talk, I will discuss about synthesis, physical properties and the tunability of their anisotropic magnetic properties of these novel TMTCs.

*This work was supported by the Deutsche Forschungsgemeinschaft (DFG) through Grant No. AS 523/4-1.
Intrinsic ferromagnetism in quasi two-dimensional chromium telluride nanoplates*  
AMANDA COUGHLIN (Presenter), Department of Physics, Indiana University - Bloomington, YUE YAO, Department of Physics and Astronomy, University of Utah, ZHIPENG YE, Department of Electrical and Computer Engineering, Texas Tech University, HUA GUO, Department of Materials Science and NanoEngineering, Rice University, YAROSLAV LOSOVYJ, Department of Chemistry, Indiana University - Bloomington, HERBERT FERTIG, Department of Physics, Indiana University - Bloomington, JUN LOU, Department of Materials Science and NanoEngineering, Rice University, RUI HE, Department of Electrical and Computer Engineering, Texas Tech University, YAN LI, Department of Physics and Astronomy, University of Utah, SHIXIONG ZHANG, Department of Physics, Indiana University - Bloomington — The recent demonstration of ferromagnetic order in atomically thin crystals has opened many new opportunities to study two-dimensional (2D) magnetism for novel spintronic applications. Most of the 2D magnets realized so far are van der Waals materials. In this talk, we report on the chemical vapor deposition and magnetic studies of thin nanoplates of chromium telluride, a layered magnetic material with a non-van der Waals structure. Bulk magnetization and magneto-optic Kerr effect (MOKE) measurements demonstrate a ferromagnetic order below a $T_c$ of ~ 180 K and a strong magnetic anisotropy with an easy axis along the c-axis. We will discuss how the magnetic properties are influenced by the nanoplate thickness based on MOKE measurement of individual nanoplates. We will also discuss in detail the aging effect at ambient conditions, one of the major challenges of 2D magnets with regards to practical applications.

*This work is supported in part by NSF DMR-1506460, DMR-1760668 and ECCS-1936406

Ferromagnetism in nitrogen-doped graphene*  
MUKUL KABIR (Presenter), ROHIT BABAR, IISER Pune — Metal-free magnetism in graphene has remained a subject of intense research, and many research groups have invested in understanding the roles of doping, structural defects and edge structure in finite-sized nano-flakes. However, a robust long-range magnetic order has remained elusive. In this context, nitrogen-doped graphene is experimentally proposed to be a promising candidate, though the corresponding exchange mechanism endures unclear and is essential to tune further and manipulate magnetism. In this talk, we will systematically discuss the local moment formation and the concurrent interaction between various defect complexes. The importance of adatom diffusion on the differential defect abundance will be elaborated. We will establish that the direct exchange mechanism between the delocalized magnetic moment originating from the $\pi$-electron at the prevalent triazine complex to be responsible for the observed ferromagnetism. We will also discuss the role of B co-doping that further improves ferromagnetism. The present results not only provide the microscopic understanding but also direct to a synthesis strategy towards robust magnetism.

*We acknowledge the Indian Department of Science and Technology through Nano Mission project SR/NM/TP-13/2016.
1:39PM M53.00009: Unraveling the Relationship Between Layer Stacking and Magnetic Order in Nb₃X₈ Systems* ELISABETH BIANCO (Presenter), ISMAIL EL BAGGARI, Cornell University, CHRISTOPHER PASCO, Johns Hopkins University, BERIT GOODGE, Cornell University, TYREL MCQUEEN, Johns Hopkins University, LENA KOURKOUTIS, Cornell University — Niobium halides of form Nb₃X₈ (X=Cl or Br) are cluster-based, 2D materials that exhibit an antiferromagnetic to non-magnetic transition. In Nb₃Cl₈, the loss of magnetic order occurs below 90 K and has been coupled to a layer re-stacking from a 2-layer (α-phase) to 6-layer (β-phase) unit cell. The transition temperature, however, depends strongly on composition with Nb₃Br₈ transitioning at 293 K. While tuning magnetic ordering temperature through composition is appealing, the layer re-stacking mechanism is not understood. Here, we used controlled-temperature cryogenic scanning transmission electron microscopy (cryo-STEM) to study the re-stacking in Nb₃Br₈ with atomic-resolution. Our results reveal a reversible transformation from the α-phase to β-phase at ~250 K upon cooling and the reverse at ~425 K upon heating through a series of intermediate phases. Tracking the emergence of intermediates with electron diffraction and Multislice image simulations provides a clearer picture of favorable stacking configurations for van der Waals Nb₃X₈. Understanding these stacking changes and their effect on magnetic ordering will afford handles for materials with tailored transition temperatures.

*This work is supported by PARADIM, an NSF-MIP (DMR-1539918), and NSF DMR-1429155 & DMR-1719875

1:51PM M53.00010: High mobility in a layered antiferromagnet* SHIMING LEI, JINGJING LIN, YANYU JIA, Princeton University, MASON GRAY, Boston College, TONG GAO, Princeton University, ANDREAS TOPP, MPI for solid state research, FANNY RODOLAKIS, JESSICA L MCCHESENY, Advanced Photon Source, CHRISTIAN R AST, MPI for solid state research, KEN BURCH, Boston College, SANFENG WU, N. PHUAN ONG, LESLIE SCHOO (Presenter), Princeton University — 2D, or ultrathin, magnetic materials are being studied as a new paradigm for device design. Intrinsic magnetic order in atomically thin layered materials has been confirmed only recently. Thus far magnetic 2D materials are mostly insulating or semiconducting; none possesses high electronic mobility. A material that exhibits simultaneously magnetic order and high mobility would enhance development of high-speed spintronic devices. In this talk, I will show how we can use chemical rules to design a material that can combine high mobility and magnetism and also crystallizes in a structure with a van der Waals gap. I will introduce the LnTe₃ family as such highly conducting antiferromagnetic layered materials. In bulk GdTe₃, the mobility reaches more than 60,000 cm²/Vs, [3] which is the highest mobility yet recorded for layered magnetic (ferro or antiferro) materials, and is comparable to non-magnetic, high-mobility materials such as black phosphorous. I will also show GdTe₃ can be mechanically exfoliated to the monolayer limit, which will allow future investigation of the properties in the 2D limit as well as open avenues for future device design.


*DMR-1420541. Arnold and Mabel Beckman foundation.
11:15AM M54.00001: Moving Majoranas across a quantum point contact in 2D topological insulators*  ALESSIO CALZONA (Presenter), BJORN TRAUZETTEL, University of Wurzburg —
Majorana fermions are zero-energy excitations of topological superconductors which obey non-Abelian exchange statistics and are basic building blocks for topological quantum computation. In order to observe and exploit their extraordinary properties, we need to be able to properly manipulate them, for instance, by braiding a couple of them in real space. We propose a setup based on the helical edges of two-dimensional topological insulators (2DTI) which allows for a high degree of tunability by only controlling a handful of superconducting phases. In particular, our setup allows to move the Majoranas along a single edge as well as to move them across two different edges coupled by a quantum point contact. The versatility of the system represents an essential step forward towards probing the non-Abelian exchange statistics of Majoranas.

*We acknowledge support by the Wurzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter (EXC 2147, project-id 39085490).

11:27AM M54.00002: Transport properties of Majorana bound state networks in the Coulomb blockade regime*  JOHAN EKSTRÖM (Presenter), University of Luxembourg Limpertsberg, PATRIK RECHER, Braunschweig University of Technology, THOMAS SCHMIDT, University of Luxembourg Limpertsberg — Topologically protected qubits based on nanostructures hosting Majorana bound states (MBSs) hold great promise for fault-tolerant quantum computing. We study the transport properties of nanowire networks hosting MBSs with a focus on the effects of the charging energy and the overlap between neighboring MBSs in short mesoscopic samples. In particular, we investigate structures hosting four MBSs such as Tjunctions and Majorana boxes. Using a Markovian master equation, we discuss the leading transport processes mediated by the MBSs. Single-electron tunneling and processes involving creation and annihilation of Cooper pairs dominate in the sequential tunneling limit. In the cotunneling regime, Andreev processes are suppressed due to the charging energy and transport is dominated by transitions via virtual intermediate states. Our results show that four-terminal measurements in the T-junction and Majorana box geometries can be useful tools for the characterization of the properties of MBSs with finite overlaps and charging energy.

*JE and TLS acknowledge support by the National Research Fund, Luxembourg under grants ATTRACT 7556175 and CORE 11352881.
PR acknowledges financial support from the Hannover-Braunschweig science cooperation QUANOMET and DFG-EXC 2123, Quantum Frontiers.
11:39AM M54.00003: Josephson radiation from nonlinear dynamics of Majorana modes in topological Josephson junctions*  JIA-JIN FENG, Sun Yat-sen University, ZHAO HUANG, Los Alamos National Laboratory, ZHI WANG (Presenter), Sun Yat-sen University, QIAN NIU, The University of Texas at Austin — Recently, in topological Josephson junctions, the electromagnetic emission with the quantized frequency of eV/h has been experimentally observed as a consequence of the 4π-periodic Josephson effect, showing a phase-sensitive signature of Majorana zero modes. However, experiments show that this nontrivial radiation vanishes above a critical voltage, sharply contradicting previous theoretical results of the standard resistively shunted junction model. We extend this model to include the Majorana dynamics and show a quantitative agreement with the experimental results. Furthermore, we predict a fragment emission line and a chaos regime which can be observed experimentally by altering the junction parameters. We reveal that all these unique features come from the nonlinear dynamics of Majorana zero modes. The fragmental emission line and its vanishment are well explained with a fixed-point portrait, while the chaotic behavior is understood as the result of the bifurcation of fixed points. Our work will inspire more works to examine the structure of the radiation spectrum of topological Josephson junctions, which is wildly presented in experimental devices.

*This work was partially supported by U.S. DOE Office of Basic Energy Sciences E3B5.

11:51AM M54.00004: Signatures of topological ground state degeneracy in Majorana islands  JUKKA VAYRYNEN (Presenter), University of California, Santa Barbara, ADRIAN FEIGUIN, Northeastern University, ROMAN LUTCHYN, University of California, Santa Barbara — We consider a mesoscopic superconducting island hosting multiple pairs of Majorana zero-energy modes. The Majorana island consists of multiple p-wave wires connected together by a trivial (s-wave) superconducting backbone and is characterized by an overall charging energy $E_c$; the wires are coupled to normal-metal leads via tunnel junctions. Using a combination of analytical and numerical techniques we calculate the average charge on the island as well as non-local conductance matrix as a function of a p-wave pairing gap $\Delta_p$, charging energy $E_c$ and dimensionless junction conductances $g_i$. We find that the presence of a topological ground-state degeneracy in the island dramatically enhances charge fluctuations and leads to the suppression of Coulomb blockade effects. Specifically, in contrast with conventional (s-wave) mesoscopic superconducting islands, we find that Coulomb blockade effects are suppressed in Majorana islands regardless of the ratio $E_c/\Delta_p$ or the magnitude of the conductances $g_i$. We also discuss our findings in relation to the so-called topological Kondo effect.
**12:03PM M54.00005: Majorana Bound States at the Superconducting Vortex from Magnetic Skyrmions**

CANON SUN (Presenter), SHU-PING LEE, YI LI, Johns Hopkins University — We show topological superconductivity can arise at the interface of ferromagnetic skyrmion material in proximity to an s-wave superconductor in the presence of strong spin-orbit coupling. We study the Majorana zero modes localized at the interface of the heterostructure and propose a pathway towards a useful platform for the manipulation of Majorana fermions via controlling skyrmions.

*This work is supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331 and in part by the Alfred P. Sloan Research Fellowships.

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**12:15PM M54.00006: Topological superconductivity and Majorana fermions in the heterostructure of EuS island and planar gold surface**

YINGMING XIE (Presenter), KAM TUEN LAW, PATRICK A LEE, Hong Kong University of Science and Technology — In a recent work [1], possible signatures of a pair of Majorana zero-energy modes were found within the platform forming by EuS island and gold wire. In this work, we show the gold wire can be replaced by a large gold surface in this platform. Furthermore, we found the chemical potential step between the EuS island covering region and bare gold surface region are essential for keeping a sizable topological region in the large gold surface case. Our results suggest the feasibility of depositing EuS wires on a large area of gold and simplify the fabrication process further.


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**12:27PM M54.00007: Transmission Amplitude through a Coulomb blockaded Majorana Wire**

MATTHIAS THAMM (Presenter), BERND ROSENOW, Univ Leipzig — We study electronic transport through a Coulomb blockaded superconducting Rashba wire in the co-tunneling regime between conductance resonances. Embedding such a wire into one arm of an electron interferometer allows to study the amplitude for coherent transmission. Varying an external Zeeman field allows to tune the wire into a topological regime, where localized Majorana zero modes are formed at both ends of the wire. In this topological phase, the nonlocal transport through Majorana zero modes is the dominant mechanism and gives rise to a maximum in the transmission amplitude as a function of Zeeman field, whose height is proportional to the wire length. On the other hand, for tunneling through a generic extended state or through a pair of Andreev bound states, the transmission amplitude is independent of wire length. Hence, the Zeeman field and length dependence of the transmission amplitude are unique signatures for the presence of Majorana zero modes.
Parafermion braiding in fractional quantum Hall edge states with finite chemical potential

SOLOFO GROENENDIJK, ALESSIO CALZONA, HUGO TSCHIRHART, EDVIN IDRISOV, THOMAS SCHMIDT (Presenter), University of Luxembourg — Parafermions are non-Abelian anyons which generalize Majorana fermions and hold great promise for topological quantum computation. We study the braiding of $Z_{2n}$ parafermions which have been predicted to emerge as bound states in fractional quantum Hall systems at filling factor $\nu=1/n$ (n odd). Using a combination of bosonization and refermionization, we calculate the energy splitting as a function of distance and chemical potential for a pair of parafermions separated by a gapped region. Braiding of parafermions in quantum Hall edge states can be implemented by repeated fusion and nucleation of parafermion pairs. We simulate the conventional braiding protocol of parafermions numerically, taking into account the finite separation and finite chemical potential. We show that a nonzero chemical potential poses challenges for the adiabaticity of the braiding process because it leads to accidental crossings in the spectrum. To remedy this, we propose an improved braiding protocol which avoids those degeneracies.

*The authors acknowledge support by the National Research Fund, Luxembourg under grants ATTRACT 7556175, INTER 11223315, AFR 11224060 and PRIDE/15/10935404, as well as by Würzburg-Dresden Cluster of Excellence in Complexity and Topology in Quantum Matter.

Entanglement in topological spin Josephson junctions

PEI-XIN SHEN (Presenter), Tsinghua University, SILAS HOFFMAN, University of Basel, MIRCEA T TRIF, Tsinghua University — We study the spin transport through 1D quantum Ising-XY-Ising junctions that emulates topological Superconducting-Normal-Superconducting junctions via Jordan-Wigner transformation. We calculate, both numerically and analytically, the spectrum of Andreev bound states and the resulting $Z_2$ fractional spin Josephson effect from Majorana Fermions. Deep in the topological regime, we identify an effective time-reversal symmetry that leads to $Z_4$ fractional spin Josephson effect in the presence of interactions within junctions. Interestingly, in the lattice model, a hidden lattice time-reversal symmetry is revealed to protect $Z_4$ fractional spin Josephson effect in odd chain sites that persists in the absence of interactions. We also evaluate the resulting spin texture in the presence of the spin currents and highlight the effects of Majorana bound states on the entanglement of neighboring spin within junctions quantified by the concurrence. We propose to use a microwave cavity setup (cQED) for detecting the aforementioned Josephson effects by dispersive readout methods. Our results are relevant for a plethora of spin systems, such as trapped ions, coupled quantum dots, or magnetic impurities on surfaces.

1:03PM M54.00010: Effect of Magnetic Field on Multi-terminal Josephson Junctions  A. BARIS OZGULER (Presenter), University of Wisconsin - Madison, HANHO LEE, VLADIMIR MANUCHARYAN, University of Maryland, College Park, MAXIM G VAVILOV, University of Wisconsin - Madison — Junctions with three or more superconducting terminals gained broad interest as they provide means to study physics and topology in higher dimensions and to braid Majorana fermions for fault-tolerant quantum computation. We study effect of perpendicular magnetic field on Andreev energy levels and critical currents in a 3-terminal Josephson junction with conventional s-wave superconducting leads and a normal 2DEG scattering region. In a 3-terminal junction, currents through two terminals determine the DC Josephson effect which occurs when the two currents are limited by the Critical Current Contour (CCC). We study the Fraunhofer diffraction patterns that manifest itself as oscillations in the diameter and area of the CCC. We show that the oscillations remain in 3-terminal devices but the additional terminal reduces the amplitude of the oscillations. We also show that magnetic field mixes with the superconducting phases in the leads and deforms the ground state energy landscape. We argue that a peculiar modulation of CCC with magnetic flux is the signature of coherent Josephson effect in multi-terminal Josephson junctions.

1:15PM M54.00011: Generic quantized zero-bias conductance peaks in superconductor-semiconductor hybrid structures*  HAINING PAN (Presenter), WILLIAM S COLE, JAY SAU, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland — We show theoretically that quantized zero-bias conductance peaks should be ubiquitous in superconductor-semiconductor hybrids by employing a random matrix model with continuous tuning parameters. We demonstrate that NS junction conductance spectra can be generically obtained in this model replicating all features seen in recent experimental results. The theoretical quantized conductance peaks, which explicitly do not arise from spatially isolated Majorana zero modes, are easily found by preparing a contour plot of conductance over several independent tuning parameters, mimicking the effect of Zeeman splitting and voltages on gates near the junction. This suggests that even stable, apparently quantized, conductance peaks need not correspond to isolated Majorana modes; rather the a priori expectation should be that such quantized peaks generically occupy a significant fraction of the high-dimensional tuning parameter space that characterizes the NS tunneling experiments.

*This work is supported by Laboratory for Physical Sciences and Microsoft.
1:27PM M54.00012: Repulsive interactions enhance the coupling of superconductors to fractional quantum Hall edges  BARAK KATZIR (Presenter), NETANEL LINDNER, Technion - Israel Institute of Technology, ADY STERN, EREZ BERG, Weizmann Institute of Science — We study helical gapless modes arising on the edges of Abelian fractional quantum Hall liquids proximity coupled to a superconductor. This setup can be utilized to create non-Abelian parafermion zero modes if the coupling to the superconductor opens a gap in the helical modes. However, when the coupling to the superconductor is weak it is ineffective and does not open a gap due to the competition with the repulsive interactions stabilizing the fractional quantum Hall liquid. We therefore investigate the possibility for obtaining a gapped phase at strong coupling to the superconductor. To this end, we use an effective wire construction model for the quantum Hall liquid and employ renormalization group methods to obtain the phase diagram of the system. Surprisingly, at strong coupling we find a gapped phase which is stabilized by strong repulsive interactions in the bulk of the quantum Hall fluids. To investigate the possibility for obtaining a gap in the intermediate coupling regime, we identify a duality transformation that maps between the weak coupling and strong coupling regimes. We find conditions on the existence of a gap in the intermediate coupling regime by investigating self-dual points of the model.

1:39PM M54.00013: Survival of the fractional Josephson effect in time reversal invariant topological superconductors  CHRISTINA KNAPP (Presenter), AARON CHEW, JASON F. ALICEA, Caltech — A one-dimensional time reversal invariant topological superconductor (TRITOPS) hosts a Kramers pair of Majorana zero modes at each end. Previous work has established that TRITOPS phases do not enable rigid non-Abelian braiding, even when time-reversal symmetry is preserved throughout: local operators can mix the Majorana Kramers pair, yielding non-universal contributions to the non-Abelian Berry phase. Nonetheless, TRITOPS phases have been predicted to display other topological signatures, including a $4\pi$ periodic fractional Josephson effect. This talk will revisit the fractional Josephson effect and explore to what extent the anomalous periodicity remains robust in the presence of local mixing terms that destroy rigidity of non-Abelian braiding.
1:51PM M54.00014: Presence versus absence of end-to-end nonlocal conductance correlations in Majorana nanowires: Majorana bound states versus Andreev bound states

YI-HUA LAI (Presenter), JAY SAU, Physics, University of Maryland, College Park — By calculating the differential tunneling conductance spectra from the two ends of a Majorana nanowire with a quantum dot embedded at one end, we establish that a careful examination of the nonlocal correlations of the zero bias conductance peaks, as measured separately from the two ends of the wire, can distinguish between topological Majorana bound states and trivial Andreev bound states. In particular, there will (not) be identical correlated zero bias peaks from both ends for Majorana bound states (Andreev bound states), and thus the presence (absence) of correlated zero bias conductance from the two wire ends could imply the presence (absence) of topological Majorana zero modes in the system. We present detailed results for the calculated conductance, energy spectra, and wavefunctions for different chemical potentials at the same magnetic field values to motivate end-to-end conductance correlation measurements in Majorana nanowires.

*This work is supported by Microsoft and Laboratory for Physical Sciences. The authors acknowledge the support of the University of Maryland High Performance Computing Center for the use of Deep Through II cluster for carrying out the numerical work.

2:03PM M54.00015: Dissipative response of a topological Josephson junction at the critical point

VLADISLAV KURILOVICH (Presenter), Yale University, CHAITANYA MURTHY, UCSB, PAVEL KURILOVICH, Yale University, BERNARD VAN HECK, Microsoft, LEONID GLAZMAN, Yale University, CHETAN NAYAK, Microsoft — A semiconducting nanowire proximitized by a superconductor is emerging as a building block of a topological qubit. Magnetic field applied to a proximitized nanowire drives it through the critical point into a topological state. We investigate signatures of this quantum phase transition in the dissipative response of a nanowire Josephson junction. The gap between the ground and excited states vanishes at the transition point. We find, that the low-frequency dissipation may remain weak despite the gap closing; this is markedly different from the conventional transition between the superconducting and normal states. In the absence of phase bias across the junction, the dissipative component of the admittance scales as \( \sigma(\omega) \sim \omega^2 \). At a finite phase bias \( \varphi \) across the junction, \( \sigma(\omega) \sim \varphi^2 \) is frequency-independent in the interval \( \omega \leq \Delta \) (here \( \Delta \) is the value of the proximity-induced gap at zero field). We establish the complete scaling functions for the admittance in the vicinity of the transition. In the presence of a finite gap (i.e., upon detuning from the critical point) the scaling function for \( \sigma(\omega) \) at a finite \( \varphi \) agrees with conventional Mattis-Bardeen formula. However, it is modified substantially and characterized by a much stronger frequency dependence if \( \varphi = 0 \).

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

11:15AM M55.00001: Bulk insulation and surface electrons’ properties of Pb(Bi,Sb)2Te4 Topological Insulator  YUYA HATTORI (Presenter), YUKI TOKUMOTO, KEIICHI EDAGAWA, Univ of Tokyo — In the field of Topological Insulators (TIs), almost all the transport studies are limited to (Bi,Sb)2(Te,Se,S)3 (BSTS)Ts. For now, BSTS-TIs has the largest bulk resistivity and transport properties of surface states have been revealed in detail. However, the utilization of surface states for device application is still a bit difficult for now.
In such context, many theoretical researchers are motivated to find new TIs, and PbBi2Te4 series TIs were discovered. The topological index of Pb-TI is (1;111), which is completely different from BSTS’s (1;000). Also, PbBi2Se4 is considered to have considerably large bulk band gap of 600meV, which is higher than Bi2Se3’s 300meV. However, the single phase and single crystal of PbBi2Te4 series TIs are difficult to grow, which hampers clarification of surface electrons’ nature.
In our study, we fabricated a series of Pb(Bi,Sb)2Te4 TI single crystal from off-stoichiometry mixture. By changing Bi, Sb ratio, we systematically studied the transport properties in order to enhance bulk resistivity. Precise control of Sb concentration made it possible to fabricate bulk insulating samples for the first time in this system. The results of nano-flake transport measurements and STM study to clarify surface electrons’ nature will be presented.

11:27AM M55.00002: Robustness of Helical Edge States Under Proximate Band Reconstruction*  NIELS JOHN (Presenter), BERND ROSENOW, Universität Leipzig, ADRIAN DEL MAESTRO, University of Vermont — We analyze the edge structure of two-dimensional topological insulators described by the Bernevig-Hughes-Zhang model with the help of a self-consistent electrostatic modeling of sample edges, combined with a time-dependent perturbation theory approach. We find that for sufficiently smooth confinement, strongly interacting additional edge states arise under fairly general conditions. While their ground state is spin unpolarized, a spin-exchange coupling between helical and reconstructed edge states can lead to a dynamical spin polarization of the latter. However, we show that spatially random spin-orbit coupling inhibits such dynamical spin polarization and protects the helical edge states against backscattering. Further, we argue that at low electron density, the reconstructed edge states are well described by a Luttinger liquid.

*We acknowledge financial support to DFG grant RO 2247/10-1.

11:39AM M55.00003: Transport properties of a topological system in non-integer dimensions  SONJA FISCHER (Presenter), LARS FRITZ, MIKAEL FREMLING, Univ of Utrecht — In recent years, the subject of topological materials has inspired a very active field of research. A considerable amount of effort was put into investigating the stability of topological edge modes under various kinds of disturbances, such as disorder.
Another less explored avenue is the stability of edge modes under variation of the dimensionality. By putting a topological system on a lattice with fractal geometry and considering and investigating the transport properties we are able to detect the influence of non-integer dimensionality on the topological properites and stability of the system.
11:51AM M55.00004: Probing spin-orbit interactions in monolayer WTe$_2$ edge states
ELLIOTT RUNBURG (Presenter), WENJIN ZHAO, ZAIYAO FEI, JOSHUA MUTCH, PAUL MALINOWSKI, BOSONG SUN, University of Washington, XIONG HUANG, YONGTAO CUI, University of California, Riverside, XIAODONG XU, JIUN-HAW CHU, DAVID COBDEN, University of Washington — Monolayer WTe$_2$ displays edge conduction that is consistent with the material being a two-dimensional topological insulator. The expected helical nature of the edge conduction should limit the conductance between adjacent contacts on an edge to $e^2/h$, and this is consistent with experiments to date. However, the helical nature has not been supported by experiments that probe the form of the Hamiltonian of the edge states. To address this, we investigate the angular dependence of the magnetic field on the conduction of edges and cracks in monolayer WTe$_2$ flakes as a function of gate voltage, temperature, and edge orientation relative to the crystal axes as determined by scanning microwave impedance microscopy.

12:03PM M55.00005: Coulomb Drag in 2D bilayer Topological Insulator systems* KAI-JIE YANG (Presenter), CHAOXING LIU, Pennsylvania State University — InAs/GaSb quantum wells are 2D bilayer topological insulator systems possessing the inverted band structure with the conduction band bottom of the InAs layer below the valence band top of GaSb layer. Recent transport experiment in InAs/GaSb quantum wells has revealed an anomalous high frequency quantum oscillation coexisting with a large resistance when the chemical potential is tuned into the charge neutrality point. The high oscillation frequency (large carrier density) and large resistance (insulating behaviors) are in contradiction with each other and this fact cannot be explained in a single-particle picture, thus motivating us to study the interaction effect of this system. Based on the linear response theory and diagrammatic methods, we carefully investigated the Coulomb drag effect in this 2D topological insulator systems based on the simplified models. Our results shed the light in understanding the anomalous quantum oscillation in 2D bilayer topological insulator systems.

*We acknowledge the support of the Office of Naval Research (Grant No. N00014-18-1-2793), the U.S. Department of Energy (Grant No. DESC0019064) and Kaufman New Initiative research grant KA2018-98553 of the Pittsburgh Foundation.
12:15PM M55.00006: Electrical study of Bi$_2$Te$_3$, Sb$_2$Te$_3$ and (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$ films*  SOORYA SURESH BABU (Presenter), YANG BAI, JAMES ECKSTEIN, University of Illinois at Urbana-Champaign — Bi$_2$Te$_3$ and Sb$_2$Te$_3$ are semiconductors that also behave as topological insulators when they are thin films. The topological properties mean that the surface conducting states have carriers that have spins locked normal to their momentum states. We have studied the growth of thin films grown by molecular beam epitaxy containing Bi$_2$Te$_3$, Sb$_2$Te$_3$ and alloys of (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$. As was discovered earlier$^1$, this allows the chemical potential to be tuned from p-type to n-type by varying the relative composition. We have also grown short period superlattices and thin bilayers of the tellurides to study how this occurs when the binary phases are kept in separate layers. The growth on c-plane sapphire crystallizes into a flatter film when Bi$_2$Te$_3$ is the interfacial layer. Like in the case of alloys, the carrier type in the bilayers can be tuned by modifying layer thickness. In bilayers with different thicknesses we have studied how the conductivity depends on layer thickness.


*This work was supported by the Army Research Offices, the National Science Foundation and the U.S. Department of Energy*

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12:27PM M55.00007: Wide band gap topological insulator via band engineering*  IDO LEVY (Presenter), CODY YOUMANS, THOR A GARCIA, HAIMING DENG, STEVEN ALSHEIMER, The City College of New York, CHRISTOPHE TESTELIN, CNRS, Institut des NanoSciences de Paris, Sorbonne Université, LIA KRUSIN-ELBAUM, POUYAN GHAEMI, MARIA C TAMARGO, The City College of New York — Molecular beam epitaxy (MBE) growth of Bi$_2$Se$_3$ and Sb$_2$Te$_3$ is hindered by a high bulk background doping due to selenium vacancies (n-type) and tellurium anti-sites defects (p-type). In order to explore the unique properties of these topological insulators (TIs), the bulk carriers must be suppressed. We previously presented the growth of TI/TI superlattices (SLs). By growing SLs of Bi$_2$Se$_3$ and Sb$_2$Te$_3$, which have a type III band alignment, a reduction of bulk background doping by more than one order of magnitude, from 1.2x10$^{20}$ cm$^{-3}$ to 8.5x10$^{18}$ cm$^{-3}$ was observed as the period was decreased from 12 nm to 5 nm. We attributed this to the formation of SL bands that create an enhancement of the bulk bandgap. Here we present tight binding calculations, which predict a SL gap of up to 400% larger than the bandgaps of the constituent layers when the SL is grown with the appropriate thicknesses. The calculations also predict the preservation of the Dirac cone, along with these large bandgaps. Measurements of magnetoconductance confirm preservation of the surface states for a SL with period thickness of 5nm. Direct measurement of the bandgaps by FTIR spectroscopy will also be reported.

*This work was supported by NSF Grant Nos. HRD-1547Mo830 and DMR-1420634.*
12:39PM M55.00008: Pb-doped p-type Bi$_2$Se$_3$ thin films via interfacial engineering

JISOO MOON (Presenter), ZENGLE HUANG, WEIDA WU, SEONGSHIK OH, Department of Physics and Astronomy, Rutgers, The State University of New Jersey — Due to high density of native defects, the prototypical topological insulator, Bi$_2$Se$_3$, is naturally n-type. Although Bi$_2$Se$_3$ can be converted into p-type by substituting 2+ ions for Bi, only light elements such as Ca have been so far effective as the compensation dopant. Considering that strong spin-orbit coupling (SOC) is essential for the topological surface states, a light element is undesirable as a dopant, because it weakens the strength of SOC. In this sense, Pb, which is the heaviest 2+ ion, located right next to Bi in the periodic table, is the most ideal p-type dopant for Bi$_2$Se$_3$. However, Pb-doping has so far failed to achieve p-type Bi$_2$Se$_3$ not only in thin films but also in bulk crystals. Here, by utilizing an interface engineering scheme, we have achieved the first Pb-doped p-type Bi$_2$Se$_3$ thin films. Furthermore, at heavy Pb-doping, the mobility turns out to be substantially higher than that of Ca-doped samples, indicating that Pb is a less disruptive dopant than Ca.

*This work was supported by the Gordon and Betty Moore Foundation’s EPIQS Initiative (GBMF4418) and National Science Foundation (NSF) grant EFMA-1542798.

12:51PM M55.00009: Thermoelectric transport in helical edge states via chiral hydrodynamics

XINGHAI ZHANG (Presenter), MATTHEW FOSTER, Rice Univ — We study thermoelectric transport in a 1D helical liquid, as appears at the edge of a 2D topological insulator. We employ semiclassical “chiral hydrodynamics”, which directly incorporates the axial anomaly, and we consider the combination of Rashba-mediated umklapp backscattering and quenched disorder. The conductivity is computed from the balance between umklapp scattering and the anomaly; the results agree with previous bosonization calculations. We also compute the thermoelectric power (TEP) and thermal conductivity. In the clean limit, chiral hydrodynamics gives a TEP equal to the thermodynamic entropy per charge, while the Wiedemann-Franz law is violated for the thermal conductivity by umklapp scattering. In the dirty limit, the electric and thermal conductivities scale the same way with temperature, while the TEP vanishes. We will also discuss results in the nonlinear response regime.

*We acknowledge funding from Welch Foundation under Grant No. C-1809 and NSF CAREER Grant No. DMR-1552327.
1:03PM M55.00010: Proximity-induced quantum anomalous Hall effect in
(Zn,Cr)Te/(Bi,Sb)$_2$Te$_3$/(Zn,Cr)Te heterostructure

RYUTARO YOSHIMI (Presenter), RIKEN, RYOTA WATANABE, University of Tokyo, MINORU KAWAMURA, RIKEN, MASATAKA MOGI, University of Tokyo, ATSUSHI TSUKAZAKI, Tohoku University, XIUZHEN YU, KIYOMI NAKAJIMA, KEI TAKAHASHI, RIKEN, MASASHI KAWASAKI, University of Tokyo, YOSHINORI TOKURA, RIKEN — The quantum anomalous Hall effect (QAHE) is an exotic quantum phenomenon originating from dissipation-less chiral channels at the sample edge. While the QAHE has been observed in magnetically doped topological insulators (TIs), exploiting magnetic proximity effect on the TI surface from adjacent ferromagnet layers may provide an alternative approach to the QAHE by opening an exchange gap with less disorder than that in the doped system. Nevertheless, the engineering of a favorable heterointerface that realizes the QAHE based on the magnetic proximity effect remains to be achieved. Here, we report on the observation of the QAHE in a proximity coupled system of non-magnetic TI and ferromagnetic insulator (FMI). We have designed sandwich heterostructures of (Zn,Cr)Te/(Bi,Sb)$_2$Te$_3$/(Zn,Cr)Te that fulfills two prerequisites for the emergence of the QAHE; the formation of a sizable exchange gap at the TI surface state and the tuning of the Fermi energy into the exchange gap. The efficient proximity coupling in the all-telluride based heterostructure as demonstrated here will enable a realistic design of versatile tailor-made topological materials coupled with ferromagnetism, ferroelectricity, superconductivity, and so on.

1:15PM M55.00011: Franckeite: A new naturally occurring topological insulator*

JUAN PALACIOS (Presenter), Univ Autonoma de Madrid, WENDEL SILVA PAZ, Instituto de Física, Universidade Federal do Espírito Santo, MARCOS MENEZES, RODRIGO CAPAZ, Instituto de Física, Universidade Federal do Rio de Janeiro — Franckeite is a layered material formed by alternating tin disulfide-based Sn(Sb)S$_2$ - pseudohexagonal (H) - and lead sulfide-based Pb(Sb)S - pseudotetragonal (Q) - layers. These layers exhibit different symmetry and periodicity, leading to an incommensurate crystal structure bound by not-so-weak van der Waals interactions between interleaved layers. The electronic properties at large concentration of Sb on the H layer are those of an indirect gap heterostructure (holes and electrons belonging to different layers) [1]. Here we present DFT results on the opposite limit of concentration. For 100% Sn on the H layer, franckeite becomes a topological insulator. This is corroborated by Wilson loop and Z2 number evaluations (the latter when forced into a centro-symmetric structure). We have also evaluated the structural composition of the energetically favorable thinnest possible layer, corresponding this to 0.5Q/H/0.5Q. This layer behaves as a 2D topological insulator, very much like InAs/GaSb quantum wells. [1] Molina-Mendoza et al., Nature Communications 8, 14409 (2017).

*Spanish MICINN through Grant No. FIS2016-80434-P, the María de Maeztu Program for Units of Excellence (MDM-2014-0377), and the European Union Graphene Flagship under Grant Agreement No. 604391 Graphene Flagship.
1:27PM M55.00012: Possible topological protection and superconducting proximity effects in surface states of HfNiSn single crystals* LUCIA STEINKE (Presenter), University of Florida, WILLIAM BAKER, MICHAEL BABB, MASON KLEMM, HARLAN R HARRIS, Texas A&M University, MEIGAN ARONSON, University of British Columbia — Surface states of HfNiSn single crystals were shown to exhibit unconventional properties like nonlocal transport, time-reversal symmetry breaking in the absence of external fields or magnetism, and nonlinear I(V) characteristics indicating electronic correlations [1], possible characteristics of a correlated topological state similar to a quantum Hall system. Oscillations in the magnetoresistance suggest quantum interference with coherence lengths up to 1 μm. The combination of quantum Hall edges or similar chiral one-dimensional states and superconductors is particularly attractive, as such junctions are expected to host the elusive Majorana fermions that could provide a possible platform for topological quantum computing, where the chiral nature of quantum Hall edge states could enable braiding operations. Our first tests of metal deposition on HfNiSn single crystals show promising results, where proximity to superconducting tin or niobium leads to conductance steps of approximately 0.5 e²/h. We further observe a clear disruption of quantum interference patterns at the superconducting transition, and magnetoresistance features associated with the critical field that can be traced up to 80 K.


*This work was supported by the Army Research Office.

1:39PM M55.00013: Influence of electronic band topology on sound waves SANGHITA SENGUPTA (Presenter), MOHAMED NABIL YACINE LHACHEMI, ION GARATE, Physics, Institut quantique de l'Université de Sherbrooke — We present a semiclassical theory of acoustic waves in topologically nontrivial materials. Combining the Boltzmann equation with the dynamical theory of elasticity, we calculate the influence of the electronic Berry curvature on sound velocity and attenuation. We predict signatures of nontrivial electronic band topology in the magnetic-field-dependence of sound propagation and discuss their possible experimental observation.
**1:51PM M55.00014: Thermoelectric Transport Coefficients of a Dirac Electron Gas in High Magnetic Fields**  
VIKTOR KÖNYE (Presenter), MASAO OGATA, Univ of Tokyo  
We study the massive Dirac Hamiltonian in high magnetic fields focusing on the effects of the mass term and we show the main differences that arise compared to massless Dirac fermions. We calculate the thermoelectric transport coefficients based on the formalism developed by Luttinger, and study the transverse components of the electric conductivity, Seebeck, and heat conductivity tensors in high magnetic fields. We prove that the Mott formula and the Wiedemann-Franz law are valid at low temperatures. The magnetic field dependence of measurable quantities strongly depend on the magnetic field dependence of the scattering rate, thus our result relies on the proper treatment of the impurities. We include impurities through the first Born approximation using screened charged impurities as impurity potential. We recovered analytically the experimentally measured linear magnetoresistance in the massless case. The effect of the mass term becomes relevant at high magnetic fields in the quantum limit. We show that in the high field limit the electric conductivity does not change qualitatively in the case of finite mass term. On the other hand we find that the mass term causes significantly different behavior in the Seebeck tensor.

**M55.00015: Epitaxial growth and electronic properties of few-layer stanene on InSb (111)**  
JIANFENG ZHANG (Presenter), XIAOHU ZHENG, RUI-RUI DU, International Center for Quantum Materials, Peking University  
Stanene has been predicted to be a 2D topological insulator with a large band gap, potentially hosting a room-temperature quantum spin Hall effect [1]. Here, stanene with controllable layers has been epitaxially grown on InSb (111) and its electronic properties have been investigated by scanning tunneling microscopy/spectroscopy (STM/STS) and low-temperature magnetotransport experiments [2]. STS results reveal a large band gap on both the wetting layer (~ 0.35 eV) and the subsequently grown single-layer (~ 0.2 eV) stanene. Spectroscopy evidences of edge state with energy inside the band gap, are also observed on the step of stanene film. Furthermore, the magnetotransport results show clear Shubnikov–de Haas oscillations in the bulk state of single-layer stanene. A brief discussion along with the data will be presented.

Reference:  

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**Wednesday, March 4, 2020 11:15 AM - 2:03 PM**

**Session M56 DCMP: Fractional Quantum Hall and Non-Fermi Liquids**

Mile High Ballroom 2C - Andres Felipe Schlief Raether, Max Planck Institute for the Physics of Complex Systems
11:15AM M56.00001: Fractional Quantum Hall Effect from Hilbert Space Algebra and New Approaches for Experimental Realisation  
BO YANG, Nanyang Tech Univ, YING-HAI WU (Presenter), Physics Department, Huazhong University of Science and Technology, ZLATKO PAPIC, Physics Department, University of Leeds — We show that model states of fractional quantum Hall (FQH) fluids for many topological phases can be uniquely determined by the Hilbert space algebra manifested as the classical reduced density matrix constraints, or the local exclusion constraint (LEC). The scheme allows us to identify filling factors, topological shifts and clustering of topological quantum fluids universally without resorting to microscopic Hamiltonians. Elementary excitations of the FQH phases can also be characterised by the LECs. More interestingly, the LEC formalism leads to a new perspective for the FQH model Hamiltonians, which can now be understood as a the von Neumann lattice of local potentials. This suggests a completely new way of experimentally realising the FQH states, including the coveted non-Abelian states (e.g the Moore-Read and Fibonacci states). We show that by tuning the local one-body potential profile, one can effectively tune the individual pseudopotentials (not just two-body, but few-body pseudopotentials) independently, and this can be done in experiments in principle. (related arXiv papers: Bo Yang, arXiv: 1901.00047, Bo Yang, Ajit Balram, arXiv:1907.09493, Bo Yang, Ying-Hai Wu, Zlatko Papic, arXiv:1907.12572)

11:27AM M56.00002: Parton construction of particle-hole-conjugate Read-Rezayi parafermion fractional quantum Hall states*  
AJIT COIMBATORE BALRAM (Presenter), Institute of Mathematical Sciences, MAISSAM BARKESHLI, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, MARK RUDNER, Niels Bohr International Academy and the Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen — The fractional quantum Hall (FQH) effect encompasses a wide range of quantum many-body phases which are characterized by exotic topological orders. Among these, the Read-Rezayi (RR) states harbor parafermionic excitations, whose non-Abelian braiding properties could potentially be used to carry out fault-tolerant quantum computation. Recent intriguing numerical results indicate that the 12/5 FQH state realized in GaAs could be described by the particle-hole conjugate of an RR state. However, numerically constructing the RR states for large systems, which is necessary for their characterization and for the demonstration of the exotic properties of their excitations, is computationally prohibitive. In this work, we use the parton framework to construct states that lie in the same phases as the particle-hole conjugates of the RR states. A nice feature of our parton states is that their wave functions can be evaluated for very large system sizes, thus, paving the way for the numerical investigation of parafermions.


*ERC Grant Agreement No. 678862, Villum Foundation, NSF CAREER (DMR-1753240), JQI-PFC-UMD and Sloan Research Fellowship. Some numerical calculations were performed using the DiagHam package, for which we are grateful to its authors.
11:39AM M56.00003: Bosonic Integer and Fractional Quantum Hall effect in an interacting lattice model  GAURAV KUMAR GUPTA (Presenter), Technion - Israel Institute of Technology, KRISHNAMURTHY H. R., Physics, Indian Institute of Science, SUBHRO BHATTACHARJEE, International Centre for Theoretical Sciences, Bengaluru — We explore the presence of bosonic integer, as well as the fractional quantum Hall effect in an interacting lattice model. Our model is defined over the bipartite honeycomb lattice with $\pi$ magnetic flux per unit cell and is populated by bosons with hardcore constraint. The bosons can hop to the nearest neighbor (simple hopping) and to the next nearest neighbor (correlated hopping). We use the Lanczos algorithm (Exact Diagonalization (ED)) to find the ground state as well as a few excited states of the system with an aim to characterize the different phases of the system. We have performed calculations for two different fillings and provide evidence for the presence of the bosonic integer quantum Hall effect (BIQHE) and the bosonic fractional quantum Hall effect (BFQHE). We also show the phase transition from the bosonic quantum Hall state to the superfluid (SF) state. We have also performed the adiabatic flux threading to confirm the presence of quantum Hall states.

11:51AM M56.00004: Parafermions in Hierarchical Fractional Quantum Hall States  LUIZ SANTOS (Presenter), Physics, Emory University — Non-Abelian quasiparticles are sought-after building blocks of fault-tolerant quantum computation. These quasiparticles can occur as extrinsic defects on interfaces and edges of two-dimensional Abelian topological phases, of which the Fractional quantum Hall (FQH) effect provides the most abundant realization. In this talk, we will discuss the properties of parafermion zero modes that arise as extrinsic non-Abelian defects in domain walls formed on interfaces of hierarchical FQH Jain states with filling fraction $p/(2mp+1)$ of the lowest Landau level, where $m$ and $p$ are positive integers. Exploring the condensation of bulk Abelian anyons, we use Abelian bosonization to construct local interactions that gap modes with opposite chirality at the interface of two Jain states with the same filling fraction. We identify a class of such local interactions that breaks charge conservation and gives rise to an interface anyon condensate supporting parafermion zero modes whose quantum dimension reflects the topological order and the hierarchy of the bulk FQH Jain state. Our results shed light on the hierarchy of non-Abelian defects in two-dimensional Abelian topological phases.
**12:03PM M56.00005: Josephson frequency of fractional charges from Shot Noise measurements**  
MAËLLE KAPFER (Presenter), Department of Physics, Columbia University, PREDEN ROULLEAU, MATTIEU SANTIN, Service de Physique de l'Etat Condense, CEA Saclay, IAN FARRER, Department of Electronic and Electrical Engineering, University of Sheffield, DAVID A RITCHIE, Cavendish Laboratory, University of Cambridge, CHRISTIAN GLATTLI, Service de Physique de l'Etat Condense, CEA Saclay — The determination of the quasiparticles charge $e^*$ is crucial to understand the Fractional Quantum Hall Effect (FQHE) phases occurring at fractional filling factors $\nu$. Among various attempts to measure $e^*$, the most reliable were based on the tiny shot noise produces by their granularity\(^1,2\). However, for complex FQHE states such as $\nu=2/5$ or $2/3$, noise measurements may give unexpected charges depending on experimental conditions\(^3,4\). Here, we present a novel fractional charge measurement based on the Josephson frequency $f_j = e^* V / h$ which manifests as singularities in the Photo-Assisted Shot Noise (PASN) when $f_j$ matches the microwave irradiation frequency $f$. Measurements are done on a QPC realized on high mobility GaAs/AlGaAs heterojunctions. Cross-correlated and auto-correlated current fluctuations are recorded to provide the shot noise. The Josephson frequency gives $e^* = e/5$ for $\nu=2/5$, while for $\nu=1/3$ $f_j$ gives $e^* = e/3$ even at low temperature.


**12:15PM M56.00006: Absence of diffusion on the edge**  
LUCA DELACRETAZ (Presenter), PAOLO GLORIOSO, University of Chicago — The edge of a FQH droplet supports gapless excitations that are protected by a U(1) anomaly. At small but finite temperature, diffusive spreading is expected to occur around the chiral ballistic front. We show that this chiral diffusive fixed point is never stable. Hydrodynamic long-time tails give large corrections to dissipative transport on the edge, leading to a breakdown of diffusion. We comment on the connection to a possible lack of thermalization in the $\nu u=5/2$ state.
Consequences of Chern bands in twisted bilayer graphene

SHUBHAYU CHATTERJEE (Presenter), NICK BULTINCK, MICHAEL ZALETEL, University of California, Berkeley — In magic angle twisted bilayer graphene (TBG), alignment of hexagonal Boron Nitride (h-BN) substrate with one or both graphene monolayers can lead to nearly flat Chern bands labeled by valley and spin indices. At odd-fillings, we discuss how interaction effects in topologically non-trivial bands lead to a ferromagnetic Chern insulator with an anomalous Hall conductance that has been recently observed [1,2]. At the even filling of 2 of 4 conduction bands, we argue that charged skyrmions (allowed by Chern bands) offer a natural explanation of the magnetoresistance [1]. Finally, we discuss how the Chern character of the bands also places strong constraints on superconductivity in TBG.


*SC acknowledges support from the ERC synergy grant UQUAM via E. Altman. MZ and NB were supported by the DOE, office of Basic Energy Sciences under contract no. DEAC02-05-CH11231.

Microscopic theory for the nematic fractional quantum Hall effect

BO YANG (Presenter), Nanyang Tech Univ — We analyse various properties of the nematic fractional quantum Hall effect (FQHE) in the thermodynamic limit, and present necessary conditions required of the microscopic Hamiltonians for the nematic FQHE to be robust. Analytical expressions of the degenerate ground state manifold, ground state energies, and gapless Goldstone modes are given in compact forms with the input interaction and the corresponding ground state structure factors. We relate the long wavelength limit of the neutral excitations (serving as the nematic FQHE ground state from spontaneous symmetry breaking) to the guiding center metric deformation, and show explicitly the family of trial wavefunctions for the Goldstone modes with spatially varying nematic order. We show for short range interactions, the dynamics of the nematic FQH is completely determined by the long wavelength part of the ground state structure factor. This is the only part that requires numerical studies in the future work, which is potentially more tractable than the conventional numerical approaches.
Quantum-confined electrons in one dimension (1D) constitute a Luttinger liquid, which features charge spin separation and other intriguing properties distinctly different from the Fermi liquid. Single walled carbon nanotubes (SWNTs) provide the ideal platform to explore such Luttinger liquid physics due to strong lateral quantum confinement and the presence of nanotubes of different species. But in many 1D materials including semiconducting SWNTs, the deviation from linear dispersion can greatly alter the electron behaviors. In order to describe the high-energy electron behaviors in 1D materials with nonlinear band structures, novel theoretical approaches have been employed to replace the linear dispersion with a generic one, which is known as the nonlinear Luttinger liquid theory. Here we probe the nonlinear Luttinger liquid physics in semiconducting SWNTs by combining electronic transport and infrared nano-imaging methods. The electron behaviors in semiconducting SWNTs are well captured by the nonlinear Luttinger liquid theory and are in strong contrast to the linear Luttinger liquid as in metallic SWNTs. Our findings provide novel insight into 1D systems beyond the conventional linear Luttinger liquid paradigm.
It is notoriously hard to study theoretically interacting quantum systems outside the Luttinger-liquid regime, particularly when considering higher-energy excitations in finite 1D systems. Recent theoretical work has focused on extending this theory to include such regimes [1,2], where it is predicted that, for higher-order excitations, length-dependent 'replica' parabolic dispersions with higher momenta or negative effective mass should be observed. Our work focuses on the experimental detection and quantification of these higher-order modes. We measure momentum-resolved tunnelling of electrons to and from an array of 1D wires to a 2D electron system formed within a GaAs heterostructure, and map their dispersion both in the equilibrium and nonequilibrium regimes [3,4]. We present recent experimental data obtained for a variety of wire lengths where both first- and second-order replica modes can be observed. We also observe these features even when multiple subbands are occupied, beyond the regime of the models.


*EPSRC [EP/J01690X/1 and EP/J016888/1]
1:15PM M56.00011: Competing phases and critical phenomena in three coupled spinless Luttinger liquids*

SARBAJAYA KUNDU (Presenter), Physics, University of Sherbrooke, Sherbrooke, Quebec, VIKRAM TRIPATHI, Theoretical Physics, Tata Institute of Fundamental Research, Mumbai, India — Coupled one-dimensional systems of interacting fermions appear in diverse contexts, and bosonization, along with a scaling treatment, is the usual method for studying low-energy properties of such systems. If three or more fermionic species are present, the scaling procedure generically introduces off-diagonal corrections to the stiffness matrix in the quadratic part of the bosonized Hamiltonian, requiring both rescaling as well as large rotations of the fields. In this talk, I will discuss phase competition in a system of three coupled spinless Luttinger liquids, using bosonization, along with a renormalization group analysis which takes into account these rotations, generating a coupling between different interaction channels even at the tree-level order in the coupling constants. I will further discuss the different instabilities in the particle-particle and particle-hole channels, the nature of the phase transitions, and the conditions under which valley symmetry breaking and intervalley orders may appear. These results may be directly relevant for systems with multiple small Fermi pockets (like graphite intercalates and bismuth) subject to quantizing magnetic fields, and cylindrical nanotubes at high fields.

*DST India (Swarnajayanti grant No. DST/SJF/PSA-0212012-13)

1:27PM M56.00012: Confinement Tuning of Non Magnetic Fractional Quantized Conductance*

SANJEEV KUMAR (Presenter), MICHAEL PEPPER, University College London, DAVID A RITCHIE, Cambridge University, IAN FARRER, University of Sheffield — There has been considerable interest in the possibility of fractional quantization of conductance in the absence of a magnetic field [1]. In the absence of spin-orbit coupling, appropriate systems have been modelled as 2D lattice site with a flat potential. In this work, we have investigated electron transport of a weakly confined quasi-1D quantum wire formed in a GaAs/AlGaAs heterostructure. The conductance measured almost on the verge of the 2D transition, resulted in conductance plateaux (in units of $e^2/h$) dependent on confinement conditions. Thus flat plateau can be observed with both even and odd denominators such as 1/6, 1/2 and 2/5. On the application of a fixed in-plane magnetic field of 10T, additional plateaux at 2/5 and 2/7 appeared as a function of increasing asymmetry in confinement potential. We suggest that the Coulomb interactions between electrons create correlated motion and formation of a zigzag array of electrons with a consequent emergence of fractional behavior [2,3].

References:

*The work was funded by the EPSRC, UK and SK is grateful to the UKRI for a Future Leaders Fellowship.
1:39PM M56.00013: Super van Hove singularities in graphene-like materials*  
BAOKAI WANG (Presenter), Northeastern University, BAHADUR SINGH, SZU-NUS Collaborative Center, ShenZhen University, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern University — We discuss the crossover from weak to strong correlations in Dirac materials by analyzing the excitonic insulator (EI) transition in a paradigmatic family of ‘slow’ graphenes. We consider the exciton modes at Q = (0, 0) and (π, 0), and show that pristine graphene is free of an excitonic instability. When the band structure is compressed, a gap opens first in a Q = (π, 0) EI phase before a Q = (0, 0) EI phase is triggered when the bands are further compressed. The gap in the Q = (π, 0) phase dominates over that in the the Q = (0, 0) phase throughout the band compression process. Interestingly, we find the presence of high order van Hove singularities in both the EI phases driven by the interaction-induced changes in the band structure. Our study suggests that two-dimensional slow graphenes could provide a novel platform for exploring the physics of EI phases and high order van Hove singularities.


*Work supported in part by the U.S.D.O.E.

1:51PM M56.00014: Topological Orders and Phase Transitions in Hofstadter-Chern Bands  
JIAN WANG (Presenter), LUIZ SANTOS, Emory University — The quantum Hall effect provides a realization of topological phases of matter in the presence of an external magnetic field. In conventional semiconductors, the achieved magnetic flux per unit cell is orders of magnitude smaller than the magnetic flux quantum h/e, giving rise to degenerate Landau levels enabling strong electronic correlations. Motivated by the realization of two-dimensional moiré superlattices with unit cell of few to hundreds of nanometers in linear size, we discuss a lattice composite fermion theory that accounts for topological states in the opposite regime where the magnetic flux per unit cell is of the order of the magnetic flux quantum, which gives rise to Hofstadter-Chern bands that can be partially filled by electrons. Through analytical and numerical methods, we uncover classes of candidate topological states beyond the Landau level regime, which are characterized by strong coupling of electronic states with the lattice. We explore this setting to establish the existence of topological phase transitions mediated by modulations of the lattice potential. Our study, therefore, identifies new topological orders and how to manipulate them in two-dimensional Hofstadter-Chern lattices.

Wednesday, March 4, 2020 11:15 AM - 2:03 PM

Session M57 DMP: Correlated Phases in Moire bilayers and Monolayer graphene  
Mile High Ballroom 3A - Matthew Yankowitz, Columbia University - Tag(s): Focus
Tunneling Spectroscopy of Superconducting States in Magic-Angle Twisted Bilayer Graphene

JEONG MIN PARK (Presenter), YUAN CAO, DANIEL RODAN-LEGRAIN, Massachusetts Institute of Technology MIT, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology MIT — The discovery of correlated insulating states and unconventional superconductivity in the twisted bilayer graphene (TBG) systems has instigated numerous follow-up experiments and theories in the past year. However, the origin of the superconducting states, including the nature of the correlated insulating states, parent metallic states, pairing mechanism, size of the superconducting gap, etc. still remain greatly unknown. Recent scanning tunneling spectroscopy experiments have analyzed the local density of states in the insulating states, revealing the splitting of the van Hove singularities near half-filling and the breaking of rotational symmetry. Here, we develop highly tunable magic-angle TBG systems with various gate geometries that allow several different tunneling transport regimes within each device. The results of our tunneling spectroscopy experiments on the superconducting states are presented.

Nature of superconductivity in highly-homogeneous twisted bilayer graphene

YU SAITO (Presenter), JINGYUAN GE, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ANDREA YOUNG, University of California, Santa Barbara — Twisted bilayer graphene with a twist angle of around 1.1 degree hosts superconducting, ferromagnetic and insulating states at partial band filling, all of which are associated with the formation of a nearly-flat electronic band. The experimental difficulty of this system is to fabricate highly angle-homogeneous samples, a necessary prerequisite for exploring the intrinsic properties. In this talk, I will report the results of transport measurements in several homogeneous twisted bilayer graphene at or near the flat band condition. We find that superconductivity near negative half-filling robustly appears regardless of the existence of a resistive state while the optimal critical temperature is very sensitive to the twist angle and is maximized around 1.1 degree.
11:39AM M57.00003: Proximity induced Josephson effect in twisted bilayer graphene near the magic angle

YIRAN ZHANG (Presenter), Department of Physics, California Institute of Technology, ROBERT POLSKI, HARPREEET SINGH ARORA, Watson Laboratory of Applied Physics, California Institute of Technology, YOUNGJOON CHOI, Department of Physics, California Institute of Technology, HECHEN REN, Watson Laboratory of Applied Physics, California Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, STEVAN NADJ-PERGE, Watson Laboratory of Applied Physics, California Institute of Technology — Twisted bilayer graphene (TBG) near the magic angle (~1.1°) has been established to be a highly tunable platform that hosts superconducting, ferromagnetic and correlated insulating states associated with the formation of flat bands. Though numerous models have been proposed to explain basic physics of flat bands and correlations in this system, many questions related the precise origin of insulating and superconducting states are still elusive. Here we report on the observation of the Josephson effect in correlated states of TBG near the magic angle. The detailed measurements of critical current as a function of gate voltage, temperature and magnetic field provide novel insights into the interplay between superconductivity and insulating states in this correlated system.

*This work has been partly supported by NSF CAREER program (DMR-1753306), DOE BES DE-SC0019166 and Gist-Caltech memorandum of understanding. S. N-P also acknowledges support from the IQIM (NSF funded physics frontiers center).

11:51AM M57.00004: On the electronic phases of magically twisted bilayer graphene

CHUAN CHEN (Presenter), ANTONIO HELIO CASTRO NETO, VITOR MANUEL PEREIRA, Natl Univ of Singapore — We explore in detail the electronic phases of a system consisting of three non-collinear arrays of coupled quantum wires, each rotated 120 degrees with respect to the next. A perturbative renormalization-group analysis reveals that multiple correlated states can be stabilized: a smectic or d \( \pm \) id superconductor, a charge density wave insulator, a two-dimensional Fermi liquid, and a 2D Luttinger liquid (also known as smectic metal or sliding Luttinger liquid). The model provides an effective description of electronic interactions in small-angle twisted bilayer graphene and we discuss its implications in relation to the recent observation of correlated and superconducting ground states near commensurate densities, as well as the “strange metal” behaviour at finite temperatures as a natural outcome of the 2D Luttinger liquid phase.

*This work was supported by the National Research Foundation of Singapore under its Medium-Sized Centre Programme.
12:03PM M57.00005: Interacting domain-wall network model in twisted bilayer graphene

YANG-ZHI CHOU (Presenter), Physics, University of Maryland College Park — The interacting domain-wall network systems, which are naturally realized in the twisted bilayer graphene (TBLG) at sub-degree twist angles, are discussed in this talk. Motivated by the superconductor-insulator transition in the TBLG at the magic angle, a simplified model that is composed of a collection of crossed one-dimensional quantum wires whose intersections form a superlattice. At each superlattice point, we place a locally superconducting puddle which can exchange Cooper pairs with the quantum wires. We show that for a range of repulsive intrawire interactions, the system is superconducting at `generic' incommensurate fillings, with the superconductivity being `interrupted' by an insulating phase at commensurate fillings. We further show that the gapped insulating states at commensurate fillings give way to gapless states upon application of Zeeman fields. These features are consistent with experimental observations in magic-angle TBLG despite the distinct microscopic details. We also discuss novel phases driven by the interplay of small velocity and network structure.

Ref: PhysRevB100 115128 (2019)

12:15PM M57.00006: Prominent Cooper Pairing Away From the Fermi Level and its Spectroscopic Signature in Twisted Bilayer Graphene

ALEX APERIS (Presenter), FABIAN SCHRODI, PETER OPPENEER, Uppsala University — We investigate phonon-mediated Cooper pairing in flat electronic band systems by solving the full-bandwidth multiband Eliashberg equations for superconductivity in magic angle twisted bilayer graphene using a realistic tight-binding model [1]. We find that Cooper pairing away from the Fermi level [2] contributes decisively to superconductivity by enhancing the critical temperature and ensures a robust finite superfluid density. We show that this pairing yields particle-hole asymmetric superconducting domes in the temperature--gating phase diagram and gives rise to distinct spectroscopic signatures in the superconducting state. We predict several such features in tunneling and angle resolved photoemission spectra for future experiments.

References:
12:27PM M57.00007: Quantum simulation of the Hubbard model in a moiré superlattice
[Invited] KIN FAI MAK (Presenter), Cornell University — The Hubbard model, first formulated by physicist John Hubbard in the 1960s, is a simple theoretical model of interacting quantum particles in a lattice. The model is thought to capture the essential physics of high-temperature superconductors, magnetic insulators, and other complex emergent quantum many-body ground states. Although the Hubbard model is greatly simplified as a representation of most real materials, it has nevertheless proved difficult to solve accurately except in the one-dimensional case. Physical realizations of the Hubbard model in two or three dimensions, which can act as quantum simulators, therefore have a vital role to play in solving the strong-correlation puzzle. In this talk, I will discuss a recent experimental realization of the two-dimensional triangular lattice Hubbard model in angle-aligned WSe$_2$/WS$_2$ bilayers, which form moiré superlattices because of the difference in lattice constant between the two 2D materials. We obtain a quantum phase diagram of the two-dimensional triangular lattice Hubbard model near the half filling by probing both the charge and magnetic order of the system. Implications for future studies will also be discussed.

1:03PM M57.00008: Imaging Viscous Flow of the Dirac Fluid in Graphene Using a Quantum Spin Magnetometer* MARK JEN-HAO KU, TONY ZHOU (Presenter), Harvard University, QING LI, MIT, YOUNG J. SHIN, JING SHI, CLAIRE BURCH, HUILIANG ZHANG, FRANCESCO CASOLA, YONGLONG XIE, ANDREW PIERCE, Harvard University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, PHILIP KIM, AMIR YACOBY, RONALD L WALSWORTH, Harvard University — The electron-hole plasma in charge-neutral graphene, known as the Dirac fluid, is predicted to realize a quantum critical system whose transport features a universal hydrodynamic description, even at room temperature. In this work$^{[1]}$, we directly image viscous Dirac fluid flow at room temperature via measurement of the associated stray magnetic field. Nanoscale magnetic imaging$^{[2,3]}$ is performed using quantum spin magnetometers realized with NV centers in diamond. Our measurement reveals a parabolic Poiseuille profile for electron flow in a graphene channel near the charge neutrality point, establishing the viscous transport of the Dirac fluid. Measurement of viscosity indicates that a nearly-ideal electron fluid presides in graphene at room temperature. Our results pave the way to study hydrodynamic transport in quantum critical fluids relevant to strongly-correlated electrons in superconductors.


*see Ref [1] for funding ack.
1:15PM M57.00009: Mott insulation and superconductivity in the cluster Hubbard model for magic-angle twisted bilayer graphene* SHIN-MING HUANG (Presenter), Natl Sun Yat Sen Univ, YI-PING HUANG, Condensed Matter Theory Group, Paul Scherrer Institute, TING-KUO LEE, Natl Sun Yat Sen Univ — We investigate the strongly correlated electronic system in magic-angle twisted bilayer graphene. Owing to the extended figure of Wannier orbitals, we study the two-orbital cluster Hubbard model with spin-valley fourfold degeneracy, focusing around half filling of valence bands below the neutrality point. The theory shows relatively impotent long-ranged hoppings after renormalization and predicts multiple Mott insulator phases at fractional filling, not only for integer charges per moire site. From second-order perturbation, spin-valley fluctuations give rise to the pairing attraction, exhibiting superconducting domes adjacent to Mott insulator phases. The cluster interaction generates high entanglement among clusters, implying plenty possibilities of nontrivial states.

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Y.-P.H receives funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No. 701647.

1:27PM M57.00010: Chiral symmetry breaking induced gap and flat band in a correlated graphene CHANGHUA BAO (Presenter), HONGYUN ZHANG, LAIPENG LUO, SHAOHUA ZHOU, QIAN LI, WEI YAO, SHUYUN ZHOU, Tsinghua University — The low-energy excitations of graphene are relativistic massless Dirac fermions with opposite chiralities at K and K' valleys. Breaking the chiral symmetry could lead to gap opening (in analogy to mass generation in quantum electrodynamics) and other intriguing phenomena. Despite many theoretical predictions, so far experimental realization of chiral symmetry breaking (CSB) in a real honeycomb lattice has been missing. Here I will present our recent experimental work on graphene with large CSB induced gap. In addition, a flat band is observed near the Fermi energy, opening up new opportunity for investigating correlated physics and interaction driven superconductivity.
1:39PM M57.00011: Phonon-mediated superconductivity in graphene and hexagonal boron nitride*  
EVEN THINGSTAD (Presenter), AKASHDEEP KAMRA, JUSTIN WELLS, ASLE SUDBO, Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology (NTNU) — Insight into why superconductivity in pristine and doped monolayer graphene seems strongly suppressed has been central for the recent years' various creative approaches to realize superconductivity in graphene and graphene-like systems. We provide further insight by studying superconductivity in doped monolayer graphene based on intrinsic phonon modes and solving the gap equation using a detailed model for the effective attraction based on electron tight binding and phonon force constant models. The various system parameters can be tuned at will, and our results show that the Coulomb interaction induces non-uniform gap textures along the Fermi surface and plays a main role in suppressing superconductivity at realistic dopings. We also perform similar calculations in the gapped hexagonal boron nitride (h-BN), which has direct onset of a large density of states. Somewhat counter-intuitively, however, the dimensionless electron-phonon coupling strength cannot capitalize on this for small charge dopings.

*We acknowledge financial support from the Research Council of Norway Grant No. 262633 "QuSpin" and Grant No. 250985, "Fundamentals of Low-dissipative Topological Matter".

1:51PM M57.00012: Ultrafast dynamics of electron-phonon coupling in correlated graphene revealed by time- and angle-resolved photoemission spectroscopy*  
HONGYUN ZHANG (Presenter), CHANGHUA BAO, SHAOHUA ZHOU, LAIPENG LUO, QIAN LI, SHUYUN ZHOU, Tsinghua University — Electron-phonon coupling plays important roles in many intriguing physics, including superconductivity, charge and spin density waves. Graphene is a model material with novel electronic properties and provide an ideal platform to study electron-phonon interactions. Despite many researches on non-equilibrium graphene electron system, the direct observation of momentum-resolved electron-phonon coupling dynamics is still missing. Here, by using time- and angle-resolved photoemission spectroscopy, we directly observe multiple electron-phonon coupling and ultrafast dynamics in correlated graphene. In addition, we observe significant suppression of decay rate induced by self-energy effects, which provide important information for controlling and understanding many-body interactions in graphene.

*State Key Laboratory of Low Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing 100084, P.R. China. 
Collaborative Innovation Center of Quantum Matter, Beijing, P.R. China.
M57.00013: Gate tunable exciton superfluid and topological phases in van der Waals heterobilayer* QIZHONG ZHU (Presenter), South China Normal University, WEI-YUAN TU, The University of Hong Kong, QINGJUN TONG, Hunan University, HUAZHENG SUN, YONG WANG, Nankai University, WANG YAO, The University of Hong Kong — Van der Waals heterostructures of 2D materials provide a powerful approach toward engineering various quantum phases of matter. In one work, we show that heterobilayers of 2D valley semiconductors can be tuned through interlayer bias between an exciton superfluid, a quantum anomalous Hall insulator, and a QSH insulator. The tunability between these distinct phases results from the competition of Coulomb interaction with the interlayer quantum tunneling that has a chiral form in valley semiconductors. In another work, we realize electrically tunable QSH insulator with large gap in van der Waals heterobilayer of monolayer transition metal dichalcogenide and hexagonal boron arsenide (BAs), in particular the WSe$_2$/BAs heterobilayer. Our findings point to exciting opportunities for harnessing both protected topological edge channels and bulk superfluidity in an electrically configurable platform.


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Wednesday, March 4, 2020 11:15 AM - 1:03 PM

Session M58 DCP: Plyler Prize, Jankunas Award Mile High Ballroom 3B

11:15AM M58.00001: Understanding Electron Correlation via Computational Quantum Chemistry JOONHO LEE (Presenter), MARTIN P HEAD-GORDON, University of California, Berkeley — Computational quantum chemistry has become a valuable tool to understand complicated physics arising from the correlated motion of electrons in molecules and materials. In quantum chemistry, we categorize electron correlation mainly into two classes: weak and strong correlation. Weakly correlated electrons can be efficiently handled by perturbation theory (PT). On the other hand, such PT methods completely break down for systems with strong correlation, which then usually requires far more computationally demanding approaches. My thesis addresses multiple aspects of the challenges posed by these two classes of correlation. In this talk, I will present three representative examples from my thesis. First, I will discuss the development of a PT method that can distinguish weak and strong correlation [1]. Secondly, I will present a Kohn-Sham density functional theory approach that can handle some strongly correlated systems by breaking time-reversal symmetry [2]. Lastly, I will discuss the development of a method that can efficiently treat strong spin correlation between electrons and its application to a single molecular magnet [3].


JOHN SOUS (Presenter), Columbia University — Striking emergent phenomena crucial to understanding the dynamical behavior of complex many-body molecular systems manifest thanks to coupling to vibrational excitations, including vibrationally stabilized Rydberg molecules and vibration-mediated binding of electron pairs in superconductors. Here, I show that the Peierls coupling, describing the modulation of electron motion due to vibrations, stabilizes light yet strongly bound bipolarons that survive strong Coulomb repulsion. I show that these properties result from the specific form of the vibration-mediated interaction, which is of 'pair-hopping' instead of regular density-density type. Furthermore, I provide evidence suggestive of a regime of bipolaronic phases stable against phase separation. These light bipolarons could well undergo Bose-Einstein condensation at high temperatures, opening a door to a new mechanism for high-temperature superconductivity. This may help resolve open questions regarding superconductivity in vibrationally coupled systems.

12:03PM M58.00003: Quantum control of cold molecular collisions using Stark-induced adiabatic Raman passage*  

WILLIAM PERREAULT (Presenter), Stanford Univ — One of the most fundamental goals in chemical physics is to understand the interaction forces that bind matter together at the quantum level. Molecular scattering experiments are the foremost tool with which to interrogate these forces, but the amount of detailed information that can be extracted from these experiments is limited by how precisely the input and output quantum states are defined. This talk will present the progress made by our group towards completely quantum state controlled scattering experiments. We first developed the Stark-induced adiabatic Raman passage technique to prepare specific internal molecular quantum states in simple molecules, and then used this technique to study the rotationally inelastic scattering of state-prepared molecules at very low collision energies. Under these conditions, nearly complete control over the quantum states was achieved, allowing us to experimentally derive insight into the dynamics of molecular scattering. This work shows the power of complete control over the input quantum states and complete measurement of the output quantum states to understand the molecular-scale world experimentally.

*This work has been supported by the U.S. Army Research Office.
Quantum Chemistry in the Continuum [Invited] ANNA KRYLOV (Presenter), Univ of Southern California — Owing to the progress in many-body theories and computer hardware, quantum chemistry tools are now routinely used in chemistry and physics, providing both high-quality quantitative data (often rivaling experimental measurements) and invaluable qualitative insights (crucial for interpretation of experimental observations). Despite its success in treating a broad range of electronic structures, ranging from ground-state closed-shell molecules to excited states and strongly correlated systems, quantum chemistry is still lagging behind when electronically metastable states (i.e, resonances embedded in the ionization continuum) are concerned. This lecture will provide an overview of the progress in extending quantum chemistry into the continuum. The main emphasis will be on exploring the ideas of non-Hermitian quantum mechanics within the framework of coupled-cluster and equation-of-motion coupled-cluster theory.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M59 DMP: Antiferromagnetic Kagome metals Mile High Ballroom 3C -

11:15AM M59.00001: Tuning magnetic properties of a Weyl semimetal with low current density QIUYUAN WANG (Presenter), YI ZENG, KAI YUAN, XING CHENG, YU YE, Peking Univ — Recently, Co$_3$Sn$_2$S$_2$ was proved to be a magnetic Weyl semimetal, which may serve as an ideal platform to realize chiral magnetic effects and quantum anomalous Hall effect. In a perfect quantum anomalous Hall state, theoretical works have predicted that Co$_3$Sn$_2$S$_2$ has a larger domain-wall moving velocity and a smaller field threshold to drive domain-wall motion than conventional metals. This feature is highly attractive for energy-efficient and high-performance spintronic devices, such as magnetic domain-wall racetrack memories. Here we report experimental results of current modulation of the magnetic properties of Co$_3$Sn$_2$S$_2$, and observed a lower current density threshold than conventional metals.
11:27AM M59.00002: Multipole control of large electric and magnetic responses in Weyl antiferromagnets* [Invited] SATORU NAKATSUJI (Presenter), Department of Physics, University of Tokyo — Antiferromagnets have attracted recent interest for designing next generation high-density and ultrafast spintronics devices because they produce no stray fields and have much faster dynamics. Here we present novel functionality found in chiral antiferromagnets with vanishingly small magnetization, namely, topological Weyl magnets that can be easily controlled by magnetic field, produce large responses, and thus could be useful for applications. In particular, we discuss frustrated antiferromagnets, Mn3X (X =Sn and Ge) as the examples of a magnetic Weyl semimetal or Weyl magnet [1,2,3]. We show that the cluster multipole order on the kagome lattice of Mn moments can be easily controlled and allows the system to exhibit a variety of new functions at room temperature that have never been seen in antiferromagnetic metals. These include the large anomalous Hall and Nernst effects [1,2,4], large magnetic optical Kerr effect [5] and a novel type of spin Hall effect (magnetic spin Hall effect) [6]. Finally, we show that they should be significantly useful for designing antiferromagnetic spintronics [7], and energy harvesting technology for magnets [8]. This presentation is based on the collaboration with T Tomita, T Higo, M Ikhlas, Y Otani, M Kimata, K Kondo, K Kuroda, T Kondo, S Shin, P Goswami, H Chen, A MacDonald, R Arita, M Suzuki, T Koretsune.


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**12:03PM M59.00003: Magnetic structure of Weyl semi-metal candidate Mn$_3$Sn**

YOUZHE CHEN (Presenter), JONATHAN GAUDET, GUY G MARCUS, SAYAK DASGUPTA, Johns Hopkins University, MUHAMMAD IKHLAS, TAISHI CHEN, TAKAIRO TOMITA, Univ of Tokyo-Kashiwanoa, JIAO LIN, Spallation Neutron Source, Oak Ridge National Laboratory, WANGCHUN CHEN, YANG ZHAO, NIST Center of Neutron Research, National Institute of Standards and Technology, MATTHEW STONE, Spallation Neutron Source, Oak Ridge National Laboratory, SATORU NAKATSUJI, Univ of Tokyo-Kashiwana, OLEG TCHERNYSHYOV, COLLIN LESLIE BROHOLM, Johns Hopkins University — The interplay between frustrated magnetism and itinerant electrons can give rise to topological non-trivial properties such as anomalous Hall and Nernest effects in Mn$_3$Sn. Density functional thoery shows Weyl points close to Fermi energy are responsible for anomalous transport properties and can be controled by magnetism via spin-orbit coupling.

In this talk, I will present our neutron diffraction results at various temperatures and magnetic fields to understand the magnetic structure of Mn$_3$Sn in different magnetic phases. With vertical magnet and polarized neutron beam, we are able to clear the ambiguity in previous works and establish the exact k=0 anti-chiral spin structure at room temperature. For the incommensurate phase, the relation between ordering vectors and temperature was investigated and a refined mangetic structure at 250K will be presentated. At the end of this talk, the orgin of the incommensurabilities will be discussed with a proposed Hamiltonian.

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331.

**12:15PM M59.00004: Magnetic Phase Diagram of Non-Collinear Antiferromagnetic Weyl Metal Mn$_{3-x}$Sn$_{1-x}$**

MUHAMMAD IKHLAS (Presenter), TAKAIRO TOMITA, ISSP, The University of Tokyo, SATORU NAKATSUJI, Department of Physics, The University of Tokyo — The non-collinear antiferromagnet Mn$_3$Sn shows large spontaneous time-reversal odd responses [1-4] in the inverse triangular spin structure state, which are considered to be signatures of Weyl nodes near the Fermi energy [5]. Mn$_3$Sn single crystals are known to be stable in the presence of excess manganese atoms. Depending on the composition, three distinct magnetic phases can be realized as a function of temperature, namely the high temperature triangular spin structure phase ($\mathbf{q} = 0$), the intermediate-temperature helical phase ($\mathbf{q} \neq 0$), and the low-temperature cluster spin glass phase [7]. Here we present our study on the compositional dependence of Mn$_{3-x}$Sn$_{1-x}$ and discuss the systematic evolution of the three magnetic phases in Mn$_3$Sn based on transport and magnetic properties.

12:27PM M59.00005: Observation of zero bias anomaly in noncolinear antiferromagnet/heavy metal heterostructures  
JOYNARAYAN MUKHERJEE (Presenter), KARTHIK RAMAN, TIFR Centre for Interdisciplinary Sciences — Noncolinear antiferromagnets (NC-AFMs) show exotic transport phenomena such as anomalous and topological Hall effect due to their non-vanishing Berry curvature\(^1\). Although many reports have focused on the transport properties of NC-AFMs, we have explored the differential conductance spectroscopy to probe the electronic structure of heterostructured device comprising of NC-AFM, Mn\(_3\)Pt, in proximity to heavy metal(Ta). Mn\(_3\)Pt/Ta and Ta/Mn\(_3\)Pt/Ta heterostructures were grown by co-sputtering on STO (100) substrate. We observe a strong zero bias conductance peak (ZBCP), only in the Mn\(_3\)Pt/Ta structure, below 10 K with the peak amplitude increasing with cool down and saturating at 4 K, with a magnitude of 4 times the conductance in the flat regime at high bias. Additionally, we observe sister peaks on both sides of the ZBCP twice in magnitude of conductance in the flat regime. Similar phenomena are reported in Dirac semimetal/superconductor heterostructure\(^2\) attributed to the superconducting nature of the device. Our study therefore, highlights that such ZBCP may be observed even in non-superconducting devices and may be driven by interface effects in these topologically nontrivial materials.


12:39PM M59.00006: A new stress dilatometer, and measurement of the thermal expansion under uniaxial stress of Mn\(_3\)Sn  
KENT SHIRER (Presenter), Max Planck Institute for Chemical Physics of Solids, MUHAMMAD IKHLAS, Institute for Solid State Physics, the University of Tokyo, PO-YA YANG, ANDREW MACKENZIE, CLIFFORD W. HICKS, Max Planck Institute for Chemical Physics of Solids, SATORU NAKATSUJI, Institute for Solid State Physics, the University of Tokyo — We present new a new device for measuring the thermal expansion of materials under tunable uniaxial stress. We have performed first measurements on Mn\(_3\)Sn - a room temperature antiferromagnet (AFM) that exhibits a spontaneous Hall effect\([1]\). Measurement of thermal expansion provides thermodynamic data about the nature of phase transitions, and uniaxial stress provides a powerful tuning method that does not introduce disorder. Mn\(_3\)Sn exhibits an anomaly in its thermal expansion near \(\sim270\) K, associated with a first order change in the magnetic structure. We show that this transition temperature is suppressed under uniaxial compression along the c-axis. These results show the efficacy of our stress-dilatometer as well as provide new, thermodynamic insight into the response to applied stress of Mn\(_3\)Sn.

Magnetic and topological properties of Kagome metal YMn$_6$Sn$_6$

NIRMAL GHIMIRE (Presenter), Department of Physics and Astronomy, George Mason University, LEKhanath POudel, REbecca DALLy, NIST Center for Neutron Research, National Institute of Standards and Technology, NISHChal THAPA MAGAR, NICHOLAS BISHOP, Department of Physics and Astronomy, George Mason University, MICHAEL MCguire, Materials Science and Technology Division, Oak Ridge National Laboratory, J SAMUEL JIANG, Materials Science Division, Argonne National Laboratory, IGoR MAZIN, Department of Physics and Astronomy, George Mason University, JOhn MITCHELL, Materials Science Division, Argonne National Laboratory, JEFFREY LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology — The Kagome lattice has historically been known for frustration-driven novel phenomena, such as spin-liquid phases. Recent experiments have indicated that 3D kagome magnets provide a natural platform to study the effect of the interplay between magnetism and electronic topology. For example, Weyl fermions and a non-collinear spin texture are observed in Mn$_3$Sn, heavy Dirac bands are reported in frustrated ferromagnet Fe$_3$Sn$_2$, and flat bands and Dirac cones are realized in antiferromagnetic FeSn. Here we present our recent findings of the complex nature of the magnetism and topological features in the electronic structure of a ternary kagome magnet, YMn$_6$Sn$_6$. This compound orders with a commensurate antiferromagnetic helical structure below 340 K, which on cooling shows an incommensurate double helical structure. Both wave vectors are temperature dependent with the difference in $q$ between the two helices gradually decreasing with decreasing temperature but remaining in the ground state. Electronic band structure calculations show the presence of a Dirac point near the Fermi energy, and a linear magnetoresistance is observed at low temperature when a magnetic field is applied along c-axis.
1:03PM M59.00008: Neutron diffraction results on the in-field magnetic structure of Y\text{Mn}_6\text{Sn}_6  
REBECCA DALLY (Presenter), LEKHANATH POUDEL, NIST Center for Neutron Research, National Institute of Standards and Technology, NISHCHAL THAPA MAGAR, Department of Physics and Astronomy, George Mason University, MARKUS BLEUEL, NIST Center for Neutron Research, National Institute of Standards and Technology, J SAMUEL JIANG, Materials Science Division, Argonne National Laboratory, MICHAEL MCGUIRE, Materials Science Division, Oak Ridge National Laboratory, JOHN MITCHELL, Materials Science Division, Argonne National Laboratory, JEFFREY LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology, NIRMAL GHIMIRE, Department of Physics and Astronomy, George Mason University — A current focus of condensed matter physics is to find materials where magnetism can tune topological properties or vice versa. Research has focused on the study of non-centrosymmetric compounds with Dzyaloshinskii-Moriya interactions, but recent studies suggest that magnetic frustration is another route to search for topological properties. Our measurements indicate that Y\text{Mn}_6\text{Sn}_6 is a promising candidate to explore the interplay of magnetic and topological properties. It is a centrosymmetric, antiferromagnetic (AF) metal with layered kagome networks of magnetic Mn atoms. The ground state magnetic structure is helical and competing ferromagnetic and AF interlayer exchange is the source of frustration in the system. The structure is far from standard though, as two, long-range, incommensurate wavevectors persist throughout a large region of the $B$-$T$ phase space. We will focus on neutron diffraction data that track the evolution of these two wavevectors as a function of magnetic field, which clearly elucidates the nature of the multiple field-induced transitions seen in AC susceptibility. Additionally, the topological Hall resistivity undergoes changes as a function of field that can be connected to those in the magnetic structure, signifying a strong interplay between the two.

1:15PM M59.00009: Transport evidence of Chern gapped Dirac fermions in the kagome magnet TbMn6Sn6  
XITONG XU (Presenter), WENLONG MA, HUIBIN ZOU, SHUANG JIA, Peking Univ — The kagome magnet TbMn6Sn6 is a new member of correlated topological metals, featuring Chern gapped Dirac fermions from the spinless Haldane model. Here we report combined electric and thermal transport study of TbMn6Sn6. Quantum oscillations are observed both in magnetoresistance and magneto-thermopower. The derived Fermi length, the cyclotron mass and their angle-dependence confirm the picture of 2D Dirac dispersion in this hard magnet. Besides, we observe complex Fermi surfaces arising from interlayer interactions, which probably consist of 2D networks and 3D sheets. We also found a phase reversal in the thermal conductivity oscillations, which may be related to competition between electronic contribution and electron-phonon interaction in thermal conductivity. Our observations provide crucial information for theoretical modelling this quantum material.
HISASHI INOUE (Presenter), Tohoku University, MINYONG HAN, LINDA YE, TAKEHITO SUZUKI, JOSEPH G CHECKELSKY, Massachusetts Institute of Technology — Kagome metals are metals with the crystal structures of the kagome lattice, the two-dimensional structure with atoms arranged in corner-sharing triangles, and other two-dimensional layers. The hexagonal arrangement and the lattice symmetry produce Dirac fermions in its band structure [1]. FeSn is an antiferromagnetic version of kagome metal where magnetic element Fe populates the kagome lattice. Taking advantage of magnetic interactions, FeSn is a promising platform to control the properties of Dirac fermions by the magnetic degree of freedom in electronic devices. Here we report the first realization of high quality epitaxial FeSn thin films [2]. Using optimized growth schemes, and electrical and magnetic torque measurements, we observed that the thin films show residual resistivity ratio between 300 K and 2 K up to 24, and support an antiferromagnetic ordering temperature 353 K comparable to the bulk one. This opens a route toward electronic and spintronics device applications of magnetic Dirac fermions.


*This work is supported by the Gordon and Betty Moore Foundation, ARO, STC Center for Integrated Quantum Materials, NSF, and the Tsinghua Education Foundation.
Magnetic Imaging of Antiferromagnetic Domain Walls in Magnetic Topological Materials*

PAUL SASS (Presenter), WENBO GE, WEIDA WU, Department of Physics and Astronomy, Rutgers University, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, DIMUTHU OBEYSEKERA, JUNJIE YANG, Department of Physics, New Jersey Institute of Technology — The study and control of domains and domain walls (DW) in topological materials is crucial to understanding and utilizing their exotic phenomena, such as axion insulator and quantum anomalous Hall states\textsuperscript{1-3}. Domains of alternating sign in these materials cancel out these states and thus it is imperative to understand how these antiferromagnetic (AFM) domains form and can be controlled. Despite many efforts, it has been challenging to directly visualize AFM domains or DWs with nanoscale resolution in general, especially in magnetic field. Here, we report the magnetic imaging of domains and DWs in several uniaxial AFMs, the topological insulator MnBi\textsubscript{2}Te\textsubscript{4} family\textsuperscript{4} and the topological semimetal EuMnBi\textsubscript{2}\textsuperscript{5}, using cryogenic magnetic force microscopy (MFM)\textsuperscript{6}. Our MFM results reveal higher magnetic susceptibility or net moments inside the DWs than in domains. DWs in these AFMs form randomly with strong thermal and magnetic field dependences.

\textsuperscript{1} Otrokov, M. M. \textit{et al.} \textit{PRL}. \textbf{122}, 107202 (2019).

*This work is supported by DOE BES under award DE-SC0018153.
1:51PM M59.00012: Topological surfaces states of MnBi$_2$Te$_4$ at finite temperatures and at domain walls KEVIN GARRITY (Presenter), SUGATA CHOWDHURY, FRANCESCA TAVAZZA, National Institute of Standards and Technology — MnBi$_2$Te$_4$ has recently been the subject of intensive study, due to the prediction of axion insulator, Weyl semimetal, and quantum anomalous Hall insulator phases, depending on the structure and magnetic ordering. Experimental results have confirmed some aspects of this picture, but several experiments have seen zero-gap topological surfaces states at low temperature, in conflict with expectations. In this work, we develop a first-principles-based tight-binding model that allows for arbitrary control of the local spin direction and spin-orbit coupling, enabling us to accurately treat large unit-cells. Using this model, we examine the behavior of the topological surface state as a function of temperature, finding a gap closure only above the Neel temperature. In addition, we examine the effect of magnetic domains on the electronic structure, finding that the domain wall zero-gap states extend over many unit-cells and can mimic the high temperature topological surface state when many domains are averaged over, potentially reconciling theoretical results with experiments.

2:03PM M59.00013: Mobius Insulator and Higher-Order Topology in MnBi$_{2n}$Te$_{3n+1}$* RUIXING ZHANG (Presenter), FENGCHENG WU, University of Maryland, College Park — We propose MnBi$_{2n}$Te$_{3n+1}$ as a magnetically tunable platform for realizing various symmetry-protected higher-order topology. Its canted antiferromagnetic phase can host exotic topological surface states with a Mobius twist that are protected by nonsymmorphic symmetry. Moreover, opposite surfaces hosting Mobius fermions are connected by one-dimensional chiral hinge modes, which offers the first material candidate of a higher-order topological Mobius insulator. We uncover a general mechanism to feasibly induce this exotic physics by applying a small in-plane magnetic field to the antiferromagnetic topological insulating phase of MnBi$_{2n}$Te$_{3n+1}$, as well as other proposed axion insulators. For other magnetic configurations, two classes of inversion-protected higher-order topological phases are ubiquitous in this system, which both manifest gapped surfaces and gapless chiral hinge modes. We systematically discuss their classification, microscopic mechanisms, and experimental signatures. Remarkably, the magnetic-field-induced transition between distinct chiral hinge mode configurations provides an effective “topological magnetic switch”.

*This work is supported by the Laboratory for Physical Sciences and Microsoft. R.X.Z acknowledges a JQI postdoctoral fellowship.
11:15AM M60.00001: Majorana multipole response of topological superconductors [Invited]
MASATOSHI SATO (Presenter), Kyoto Univ — Crystalline symmetry enriches topological phases of matter. For instance, Dirac semimetals with crystalline symmetry are one of the promising ways to realize a variety of topological superconductivity. In contrast to elementary Majorana particles, emergent Majorana fermions (MFs) in topological crystalline superconductors may have electromagnetic multipoles. We developed a general theory of magnetic multipoles for surface helical MFs on time-reversal-invariant superconductors. The results show that the multipole response is governed by crystal symmetry, and that a one-to-one correspondence exists between the symmetry of Cooper pairs and the representation of magnetic multipoles under crystal symmetry. The latter property provides a way to identify nonconventional pairing symmetry via the magnetic response of surface MFs. We also find that most helical MFs exhibit a magnetic-dipole response, but those on superconductors with spin-3/2 electrons may display a magnetic-octupole response in leading order, which uniquely characterizes high-spin superconductors. Detection of such an octupole response provides direct evidence of high-spin superconductivity, such as in half-Heusler superconductors.

11:51AM M60.00002: Anomalous normal fluid response in helical spin-triplet superconductor UTe2*
SEOKJIN BAE (Presenter), HYUNSOO KIM, University of Maryland, College Park, SHENG RAN, National Institute of Standards and Technology, YUN SUK EO, I-LIN LIU, WESLEY T FUHRMAN, JOHNPIERRE PAGLIONE, University of Maryland, College Park, NICHOLAS BUTCH, National Institute of Standards and Technology, STEVEN ANLAGE, University of Maryland, College Park — We report evidence for a helical spin-triplet pairing state of UTe2 with significant surface normal fluid response. The microwave surface impedance of UTe2 crystals was measured and converted to complex conductivity. The anomalous residual normal fluid conductivity (real part) in the zero temperature limit supports the presence of a significant normal fluid response in the ground state. The superfluid conductivity (imaginary part) follows the low temperature behavior predicted for the helical spin-triplet state. The temperature dependence of the superfluid conductivity also reveals a low impurity scattering rate and low frequency-to-energy-gap ratio, implying that the observed normal fluid response is not due to an extrinsic origin. Candidate mechanisms such as a surface Majorana normal fluid, which are predicted for the helical spin-triplet superconductor, are discussed.
[Ref] arXiv:1909.09032

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Microscopic evidence for chiral superconductivity in a heavy fermion superconductor UTe$_2$*  

LIN JIAO (Presenter), SEAN HOWARD, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois Urbana-Champaign, SHENG RAN, NIST Center for Neutron Research, National Institute of Standards and Technology, ZHENYU WANG, JORGE OLIVARES RODRIGUEZ, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois Urbana-Champaign, MANFRED W SIGRIST, Institute for Theoretical Physics, ETH Zurich, ZIQIANG WANG, Department of Physics, Boston College, NICHOLAS BUTCH, NIST Center for Neutron Research, National Institute of Standards and Technology, VIDYA MADHAVAN, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois Urbana-Champaign — Spin-triplet superconductivity is a condensate of electron pairs with spin-1 and an odd parity pair wavefunction. A particularly interesting manifestation of triplet pairing is a chiral p-wave state which is topologically non-trivial and a natural platform for realizing Majorana edge modes. Triplet pairing is however rare in solid state systems and so far, no unambiguous identification has been made in any bulk compound. Since pairing is most naturally mediated by ferromagnetic spin fluctuations, uranium based heavy fermion systems containing f-electron elements that can harbor both strong correlations and magnetism are considered ideal candidate spin-triplet superconductors. In this talk I will present scanning tunneling microscopy (STM) studies of the newly discovered heavy fermion superconductor, UTe$_2$ with a $T_{SC}$ of 1.6 K. We find signatures of coexisting Kondo effect and superconductivity which show competing spatial modulations within one unit-cell. Most strikingly, STM spectroscopy at step edges show signatures of chiral edge states, indicating UTe$_2$ is a 3D chiral superconductor.

*We gratefully acknowledge support from U.S. Department of Energy under Award Number DE-SC0014335.

Effects of uniaxial pressure in Uranium-based superconductors*  

SEAN THOMAS (Presenter), FREDERICO BENEDETTO SANTOS, TOMOYA ASABA, ERIC BAUER, JOE D THOMPSON, PRISCILA ROSA, FILIP RONNING, Los Alamos National Laboratory — Uranium-based superconductors have been proposed to host a number of exotic superconducting states. In some p- and d-wave superconductors, uniaxial stress is expected to split the superconducting transition temperature between the two components of the order parameter. The anisotropic dependence of this splitting can provide hints about the underlying nature of the superconductivity in these materials. Here, we probe several Uranium-based superconductors using in-situ tuning of uniaxial stress and discuss the implications of the results on the allowed pairing mechanisms.

*Work at Los Alamos was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering.
12:27PM M60.00005: Majorana fermions in narrow zigzag honeycomb nanoribbons*  
RENA BENTO RIBEIRO CAMPOS, Physics Department, Federal Fluminense University, JORGE HUAMANI CORREA, Physics Department, Brasilia Federal University, ANTONIO CARLOS SERIDONIO, Physics Department, Paulista State University (Unesp), MARCOS FIGUEIRA (Presenter), Physics Department, Federal Fluminense University — In this work, we study the generation of Majorana fermions in narrow zigzag honeycomb nanoribbons (ZHNR) deposited over an 's' superconductor. We study the system using an effective minimal model that consists of the first nearest neighbor hopping, Rashba spin-orbit interaction, triplet superconducting pairing between the magnetic moments of the ZHNR edges and an external exchange magnetic field [1].

We present results of the band structure, density of states and conductance for the infinite case as well as the energy spectrum as a function of the chemical potential for the finite one. In the infinite case, the band structure exhibits several topological phase transitions associated with spin-up or spin-down Majorana fermions. The results for the finite ZHNR show an energy spectrum with zero-energy modes at the chemical potential, which are the signature of Majorana fermions. A striking result of the work is that the nanoribbon spins polarize the Majorana fermions, generating regions of chemical potential where there are only spin-up or spin-down zero-energy modes. The results show that the system could develop Majorana half-metallic behavior.


*We thank Brazilian agencies CAPES and CNPq to support this work.

12:39PM M60.00006: Atomic limit and inversion-symmetry indicators for topological superconductors  
ANASTASIIA SKURATIVSKA (Presenter), TITUS NEUPERT, MARK H FISCHER, University of Zurich — Symmetry indicators have proven to be extremely helpful in identifying topologically non-trivial crystalline insulators using symmetry-group representations of their Bloch states. An extension of this approach to superconducting systems requires defining an appropriate atomic limit for Bogoliubov-de-Gennes Hamiltonians. Here, we introduce such a notion of atomic limit and derive a \( \mathbb{Z}_2^d \)-valued symmetry indicator for inversion-symmetric superconductors of \( d \) dimensions. This indicator allows for a refined topological classification including higher-order phases for systems in the superconducting symmetry classes D and DIII. We further elucidate the bulk-boundary correspondence of these phases using Dirac surface theories. Requiring only the normal-state band structure and the superconducting order-parameter symmetry as an input, this indicator is well suited for a search of topological superconductors using first-principles calculations.
12:51PM M60.00007: Unconventional Superconductivity in spin-3/2 fermions  JULIA LINK  (Presenter), Physics, Simon Fraser University, IGOR BOETTCHER, Joint Quantum Institute, University of Maryland, IGOR HERBUT, Physics, Simon Fraser University — We study unconventional superconductivity in spin-orbit-coupled three-dimensional electronic systems without inversion symmetry, featuring gapless fermions with the Hamiltonian given by $H = p \cdot J$, where $J$ are the generators of total angular momentum of 3/2. These systems have a Fermi points with a fixed ratio of the Fermi velocities. A favorable short-range interaction can lead to a d-wave superconductivity which is described by a complex tensor order parameter. We investigate the structure of the corresponding Ginzburg-Landau free energy and demonstrate that already at the quartic level the superconducting state of the system is uniquely determined. For a chemical potential right at the Fermi point, the ground state of the system is given by an uniaxial nematic state. In the case of a finite chemical potential, we find that the cyclic state is favored as a ground state. The cyclic state breaks time-reversal symmetry maximally, has no average magnetization, and exhibits robust small Bogoliubov Fermi surfaces in the excitation spectrum of the quasiparticles.

1:03PM M60.00008: Chemical doping effect on a topological superconductor candidate*  KAYA KOBAYASHI (Presenter), TAKESHI TAKAHASHI, HARALD JESCHKE, JUN AKIMITSU, Okayama Univ — Au$_2$Pb crystallizing in a cubic Laves phase exhibits a bulk Dirac cone in the vicinity of the Gamma point. The material also shows superconductivity, but not in the cubic phase because the material goes through several structural transitions at low temperatures. On the other hand, one of the oldest alloy superconductors Au$_2$Bi possesses the same crystal structure as the cubic Laves phase. There is no detailed report for the latter compound apart from the superconducting transition temperature (Tc) at 1.8 K. We will report the enhancement of Tc by Bi substitution in Au$_2$Pb associated with the suppression of structural transitions.

*This work is supported by Grants-in-Aid for Scientific Research (Grant No. 18K03540, 19H01852).
Observation of half-quantum flux in topological superconductor β-Bi$_2$Pd

YUFAN LI (Presenter), XIAOYING XU, Johns Hopkins University, M.-H. LEE, M.-W CHU, Center for Condensed Matter Sciences and Center of Atomic Initiative for New Materials, National Taiwan University, CHIA-LING CHIEN, Johns Hopkins University — Magnetic flux quantization is one of the defining characteristics of a superconductor. We report the observation of half-integer magnetic flux quantization in mesoscopic rings of superconducting β-Bi$_2$Pd thin films [1]. The half-quantum fluxoid manifests itself as a π-phase shift in the quantum oscillations of the superconducting critical temperature. The superconducting ring energetically prefers half flux quanta with fractional quantum numbers of 1/2, 3/2, 5/2, etc., instead of usual integer numbers of 0, 1, 2, etc. This result is consistent with β-Bi$_2$Pd having a spin-triplet pairing symmetry, which may be expected from β-Bi$_2$Pd as a topological superconductor [2,3]. Our findings usher in new venues for studying topological superconductivity, and new designs of flux qubit for quantum computing, which may operate without external magnetic fields.


Spin-triplet Superconductivity Evidenced by Half-Integer Quantum Flux in a Non-centrosymmetric Superconductor

XIAOYING XU (Presenter), YUFAN LI, CHIA-LING CHIEN, Johns Hopkins University — Spin-triplet superconductors, rare and challenging to identify, play central roles in Majorana fermions and quantum computing. It has been proposed that superconductors with broken inversion symmetry may host spin-triplet Cooper pairs. Unique features of half-quantum fluxoid in flux quantization is one of the few methods that can identify spin-triplet superconductors [1]. We fabricated thin films of non-centrosymmetric a-BiPd by sputtering and patterned them into sub-µm-sized rings. Measurements of the Little-Parks oscillations in magnetoresistance show half-quantum fluxoid ($n + ½)\Phi_0$, a key signature of spin-triplet pairing, where flux quantum $\Phi_0 = hc/2e$ and $n$ is an integer. Our extensive measurements support mixing pairing states of spin-singlet and spin-triplet Cooper pairs in α-BiPd.

*This work was supported by the U.S. Department of Energy (DOE), Basic Energy Science award no. DESC0009390. X.X. was supported in part by SHINES, an EFRC funded by U.S. DOE Basic Energy Science award no. SC0012670.
The co-existence of spatial and non-spatial symmetries together with appropriate commutation/anticommutation relations between them can give rise to static higher-order topological phases, which host gapless boundary modes of co-dimension higher than one. Alternatively, space-time symmetries in a Floquet system can also lead to anomalous Floquet boundary modes of higher co-dimensions, with different commutation/anticommutation relations with respect to non-spatial symmetries. In my talk I will review how these dynamical analogs of the static HOTI's emerge, and also show how a coherently excited phonon mode can be used to support non-trivial Floquet higher-order topological phases.

**Wednesday, March 4, 2020 11:15 AM - 2:15 PM**

**Session M61 DMP DCMP DCOMP: Fe-Based Superconductors - Mostly FeSe & FeTe** Mile High Ballroom 4B - Leonardo Civale, Los Alamos Natl Lab - Tag(s): Focus
Ultrafast dynamics in single-layer FeSe/SrTiO$_3$, (Li$_{0.84}$Fe$_{0.16}$)OHFe$_{0.98}$Se, and Sr$_3$Ir$_2$O$_7$: revealing coupling between different degrees of freedom

JIMIN ZHAO (Presenter), Chinese Academy of Sciences — We have demonstrated ultrafast dynamics evidence of high-$T_c$ superconductivity in single-layer FeSe/SrTiO$_3$, with clear identification of the SC $T_c$, SC gap, and electron-phonon coupling (EPC) constant $\lambda$. In addition, we also observe the quasiparticle dynamics and coherent phonons in the intercalated novel superconductor of (Li$_{0.84}$Fe$_{0.16}$)OHFe$_{0.98}$Se. Furthermore, the EPC strength is compared among the single-layer FeSe/SrTiO$_3$, bulk FeSe, KFe$_2$Se$_2$, (Li$_{0.84}$Fe$_{0.16}$)OHFe$_{0.98}$Se, Fe$_{1.01}$Se$_{0.2}$Te$_{0.8}$, Fe$_{1.05}$Se$_{0.2}$Te$_{0.8}$, and many other reported iron-based superconductors, we find that the EPC strength has a positive correlation with SC $T_c$ among almost all types of iron-based superconductors, thus bridging the bulk and monolayer system, as well as FeAs- and FeSe-based superconductors. We also investigated the $A_{1g}$ coherent phonon in strong correlated iridate Sr$_3$Ir$_2$O$_7$, finding the strongest pseudospin-lattice coupling (PLC) known so far. We discover that PLC is the dominating interaction in low temperature, which leads to phonon anomaly and negative thermal expansion.

Our results demonstrate promising venues for ultrafast optical investigation of the quantum properties of oxide interfaces, bulk high $T_c$ superconductors, and transition metal oxides. It is non-contact, single-layer sensitive, and gap-perceptive, being capable of detecting ultrafast lifetime, EPC strength, and coherent bosons. Hence it provides important clues to understanding the SC mechanism and couplings between different degrees of freedom.


[2] Q. Wu, Jimin Zhao* et al., Ultrafast Quasiparticle Dynamics and Electron-Phonon Coupling in (Li$_{0.84}$Fe$_{0.16}$)OHFe$_{0.98}$Se, arXiv:1910.09859 (2019).

**11:51AM M61.00002: Frustrated spin order in FeSe**  
ANDREAS BAUM (Presenter), Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, HARRISON N RUIZ, Stanford University, NENAD LAZAREVIĆ, Institute of Physics Belgrade, YAO WANG, Harvard University, THOMAS U BOEHM, RAMEZ HOSSEINIAN AHANGHARNEJHAD, Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, THOMAS WOLF, Karlsruhe Institute of Technology, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford University, RUDOLF HACKL, Walther Meissner Institute, Bavarian Academy of Sciences and Humanities — Magnetism in the structurally simplest iron based superconductor, FeSe, poses a challenge. Unlike in the related iron pnictide compounds, no magnetic order was found down to lowest temperatures in FeSe. However, recent theoretical and experimental studies point towards frustration quenching long range order. Here we demonstrate that inelastic light scattering can distinguish between itinerant and localized magnetism. We find the Raman response from FeSe to be more similar to localized systems such as cuprates. Together with simulations of a spin-1 Heisenberg model this furnishes evidence that FeSe hosts an almost fully frustrated system of essentially localized moments.

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**12:03PM M61.00003: Angle Resolved Photoemission Measurements of Metastable Single Crystals of Tetragonal CoSe**  
CHRISTOPHER PARZYCK (Presenter), Cornell University, XIUQUAN ZHOU, Argonne National Laboratory, BRANDON WILFONG, EFRAIN RODRIGUEZ, University of Maryland, KYLE M SHEN, Cornell University — Using topochemical deintercalation methods, single crystals of the tetragonal phase of Cobalt Selenide, isostructural to the iron based superconductor FeSe, have recently been synthesized$^{1,2}$. Here, we present synchrotron angle resolved photoemission (ARPES) measurements of these metastable crystals and compare to recent ARPES measurements of MBE synthesized thin films$^{3}$ as well as density functional theory calculations$^{4}$. We discuss similarities and differences between bulk tetragonal CoSe and FeSe in terms of correlation and renormalization effects on the band structure and the effects of dimensionality.

There are profound connections between dynamical magnetism and unconventional superconductivity in Fe-based superconductors. Recently, new aspects associated with their multi-band, multi-orbital nature and the resulting orbital physics came to prominence in iron the chalcogenide family. While early neutron scattering experiments already presented indication of an orbital-selective electron localization and ferro-orbital order in the FeTe parent material [1,2], an orbital-selective Cooper pairing was recently discovered in the FeSe end member by STM [3]. Here, we present polarized neutron scattering studies of magnetic dynamics in FeTe parent material and FeTe$_{0.45}$Se$_{0.55}$ optimally doped superconductor, where we analyze the wave vector dependence of the magnetic form factor in order to understand the orbital state of magnetic electrons. Our results indicate an unusual, energy- and temperature-dependent orbital composition of dynamical magnetism revealed by polarized neutron spectroscopy.


*Work at BNL is supported by the Office of Basic Energy Sciences, U.S. Department of Energy, under contract no. DE-SC0012704
Quantum Monte Carlo calculations of dynamic spin excitations in FeSe

SEHER KARAKUZU (Presenter), Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6164, USA, JONATHAN PELLICIARI, NSLS-II, Brookhaven National Laboratory, Upton, NY, 11973, USA and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, RICCARDO COMIN, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, STEVEN JOHNSTON, Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996, USA and Joint Institute of Advanced Materials at The University of Tennessee, Ktn, THOMAS MAIER, Center for Nanophase Materials Sciences,Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6164, USA and Computational Sciences and Engineering Division, Oak Ridge Nat — The rich physics of bulk and monolayer FeSe has been widely studied in the condensed matter physics community. The pairing mechanism giving rise to the enhanced superconductivity of the monolayer is mainly attributed to spin fluctuations. Here we discuss unbiased dynamical cluster approximation (DCA) quantum Monte Carlo calculations to understand the physics of these compounds. Specifically, we calculate the dynamic spin susceptibility of a two-orbital Hubbard model with parameters tuned to describe both bulk and monolayer FeSe and use the maximum entropy method to perform the analytic continuation to real frequencies. We compare the DCA results with neutron scattering data for bulk FeSe as well as resonant inelastic x-ray spectroscopy (RIXS) data for the monolayer compound.

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

Resistivity, magnetotransport and superconductivity across the nematic quantum critical point in the iron chalcogenides

NIGEL HUSSEY (Presenter), High Field Magnet Laboratory and Radboud Univ., Nijmegen, The Netherlands — Selected by Focus Topic Organizer Leonardo Civale

Effects of Strong Correlations in the Lattice Dynamics of Iron-based Superconductors

GHANASHYAM KHANAL (Presenter), KRISTJAN HAULE, Rutgers University, New Brunswick — Strong electron-electron interaction leads to a plethora of complex physical mechanisms in many materials which includes, magnetism, spin fluctuation and high $T_c$ superconductivity. A Combination of Density Functional Theory (DFT) and Embedded Dynamical Mean-Field Theory (EDMFT) has been extremely successful for electronic structure calculations of these strongly correlated systems. We use this method on 11-type and 111-type family of iron-based superconductors (FeSC) to show that correlations play an important role to determine the vibrational properties of real systems. In this work, we present an very good agreement with the experiment to calculated values of internal parameters, phonon density of states and the phonon frequencies at high symmetry points.

*The authors acknowledge the funding from NSF DMR-1709229.
**1:27PM M61.00008: Thickness dependence of band structure of FeSe**  
JIA SHI (Presenter), Department of Physics, University of Science and Technology Beijing, DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida, QIANG GU, Department of Physics, University of Science and Technology Beijing — Thin film FeSe attracts a great deal of attention thanks to its unusually high-temperature ($T_c$) superconducting properties. We report results of our density functional theory based calculations of the electronic structures of FeSe consisting of 1 to 5 layers. For the case of monolayer, there is a gap of about 0.5 eV at Γ, the Brillouin zone center. We did not find significant difference between the band structures of higher layered FeSe, rather the characteristics slowly converge to that of bulk FeSe, in which the occupied bands cross the Fermi level overlapping with the conducting bands. We discuss the details of the electronic structure and comparison of the Fermi surfaces and phonon spectra of the thin films to shed light on the high $T_c$ behavior of monolayer FeSe.

*This work is supported in part by China Scholarship Council (J.S), the National Natural Science Foundation of China grant No. 11874038 (Q.G.) and by U.S. Department of Energy Grant DE-FG02-07ER46354 (D.L. and T.S.R.)*

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**1:39PM M61.00009: Chemical pressure effect of electron-doped FeSe films**  
NAOKI SHIKAMA (Presenter), YUKI SAKISHITA, FUYUKI NABESHIMA, ATSUTAKA MAEDA, Dept. of Basic Science, Univ. of Tokyo — The superconducting transition temperature ($T_c$) of FeSe increases from 9 K in bulk to 40-45 K with electron doping. To search for higher $T_c$, it is interesting to study the chemical pressure effect for the electron-doped FeSe. We fabricated the electric double layer transistor configuration of FeSe$_{1-x}$S$_x$ and FeSe$_{1-y}$Te$_y$ films for wide range of $x$ and $y$, and measured transport properties under finite gate voltage. Increasing S and Te content decreases $T_c$ of electron-doped FeSe$_{1-x}$S$_x$ and FeSe$_{1-y}$Te$_y$ in a similar manner. This $T_c$ behavior of electron-doped samples is very different from that of non-doped samples [1]. On the other hand, this behavior agrees well with that of the intercalated FeSe$_{1-x}$S$_x$ and FeSe$_{1-y}$Te$_y$, whose $T_c$ is also around 40 K. Our results suggest that the mechanism of superconductivity is different between 25 K class non-doped case and 40 K class doped case.


*This work was supported by JSPS KAKENHI Grant Number 18H04212 and 19K14651 and The Murata Science Foundation.*
MBE preparation and in-situ characterization of FeTe thin films

VANDA MOTA PEREIRA (Presenter), CHI-NAN WU, CHENG-EN LIU, SHENG-CHIEH LIAO, CHUN-FU CHANG, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, CHANG-YANG KUO, National Synchrotron Radiation Research Center, Hsinchu, Taiwan, CEVRIYE KOZ, ULRICH SCHWARZ, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, HONG-JI LIN, CHIEN-TE CHEN, National Synchrotron Radiation Research Center, Hsinchu, Taiwan, LIU TJENG, SIMONE G ALTENDORF, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — Within the family of Fe based superconductors, Fe chalcogenides have received particular attention due to their simple crystal structure. Fe\textsubscript{1+y}Te, which is not superconducting, has been studied extensively in bulk form and, more recently, some efforts have been made regarding the synthesis of thin films, resorting to pulsed laser deposition and molecular beam epitaxy (MBE). Here we report the results of Fe\textsubscript{1+y}Te thin films grown by means of MBE under Te-limited growth conditions. We found that epitaxial layer-by-layer growth is possible for a wide range of excess Fe values, wider than expected from what is known from studies on the bulk material. Using x-ray magnetic circular dichroism spectroscopy at the Fe $L\textsubscript{2,3}$ and Te $M\textsubscript{4,5}$ edges, we observed that films with high excess Fe contain ferromagnetic clusters while films with lower excess Fe remain nonmagnetic. Moreover, x-ray absorption spectroscopy showed that it is possible to obtain films with very similar electronic structure as that of a high-quality bulk single crystal Fe\textsubscript{1.14}Te. Our results suggest that MBE with Te-limited growth may provide an opportunity to synthesize FeTe films with smaller amounts of excess Fe as to come closer to a possible superconducting phase.

Influence of iron vacancies on the transport properties of (Fe-Ni)Te\textsubscript{0.65}Se\textsubscript{0.35} crystals

MARTA CIEPLAK (Presenter), IRYNA ZAYTSEVA, KATARZYNA KOSYL, WOJCIECH PASZKOWICZ, DARIUSZ J GAWRYLUK, Institute of Physics, Polish Academy of Sciences — The role of iron vacancies in the improvement of superconductivity is studied in Fe\textsubscript{1−y}Ni\textsubscript{y}Te\textsubscript{0.65}Se\textsubscript{0.35} single crystals, with $y$ in the range from 0 to 0.08, grown by Bridgman’s method using different crystallization rates. As shown previously [1], slow crystallization leads to crystals with single tetragonal phase, but with superconducting properties inferior to crystals obtained by fast crystallization, which contain nanometer size iron deficient regions. Using matrix formalism for multicarrier systems we extract carrier concentrations and their mobilities from the low-temperature Hall effect data for crystals with $y>$0.03, in which superconductivity is suppressed. The evolution of the majority carriers with increasing $y$ is similar for all crystals, from holes for $y<$0.06 to electrons for $y>$0.06, indicating electron doping by Ni substitution. However, at low T the T-dependence of the majority and minority carrier concentrations and their mobilities differ significantly in crystals with and without iron vacancies. These differences lead to the conclusion that inhomogeneity induced by iron vacancies enhances electron doping, what most likely contributes to the enhancement of superconducting fluctuations. Ref.: [1] D. J. Gawryluk, et al., Supercond. Sci. Technol. 24, 065011 (2011).
The Observation of Majorana Zero Mode and Conductance Plateau in an Iron-based Superconductor

HONGJUN GAO (Presenter), Institute of Physics and University of Chinese Academy of Sciences Chinese Academy of Science — Majorana zero-modes (MZMs) are spatially-localized zero-energy fractional quasiparticles with non-Abelian braiding statistics that hold great promise for topological quantum computing. Recently, by using scanning tunneling microscopy/spectroscopy (STM/STS), a new breakthrough of Majorana zero mode (MZM) was achieved in a single material platform of high-$T_c$ iron-based superconductors, FeTe$_{0.55}$Se$_{0.45}$, which combined advantages of simple material, high-$T_c$, and large ratio of $\Delta / E_F$ [1]. A detail STM/STS study of a FeTe$_{0.55}$Se$_{0.45}$ single crystal, also revealed the mechanism of two distinct classes of vortices present in this system, which directly tied with the presence or absence of zero-bias peak [2]. To further investigated the MZM, it is still needed to find a “smoking-gun” type of evidence for the existence of MZM, and a quantized conductance plateau is widely believed to be one of them.

Here we report an observation of the Majorana conductance plateau in vortices on the iron superconductor FeTe$_{0.55}$Se$_{0.45}$ surface by using STM/STS [3]. We found that both extrinsic instrumental convoluted broadening and intrinsic quasiparticle poisoning can reduce the conductance plateau value. When extrinsic instrumental broadening is removed by deconvolution, the plateau is found to nearly reach a $2e^2/h$ quantized value. The direct observation of a conductance plateau on a single zero-mode in a vortex strongly supports the existence and protection of MZMs in this iron-based superconductor, which can serve as a single-material platform for Majorana braiding at relatively high temperature.
In an effort to spatially resolve excited state properties of nanomaterials with sub-nm resolution, our group has developed an excited state imaging technique known as single-molecule absorption scanning tunneling microscopy (SMA-STM). This technique allows us to probe changes in tunneling associated with laser excitation, creating an image that maps the excited state electronic structure of nanomaterials. We have applied this technique widely to study excited state properties of quantum dots (QDs) and carbon nanotubes (CNTs) and will discuss results surrounding the interaction of optically excited QDs with CNTs. Our results show a distant-dependent transverse polarization of CNTs in the presence of an excited QD, while semiquantitative tight-binding calculations performed on an analogous system allow us to model the observed interaction. We will also discuss our preliminary work with traditional STM on carbon nanothreads and their variants, which aims to characterize the ground state electronic properties of these carbon materials. Initial results show highly variable band gaps of aggregate structures likely due to varied ordering and defects, while techniques allowing for investigation of individual threads will ultimately position us for excited state characterization.

Controlling transport in single molecules remains a major challenge, in part due to the difficulties of predicting the electronic structure of a molecule when supported in a metallic nanostructure. Here we discuss the possibility of using molecular dipole moments as built-in electric fields in single molecules to shift the energy level alignment and therefore tailor quantum transport. On the basis of advanced statistical analysis of experimental data from a set of model molecules, we are able to differentiate even rather small differences in the conductance, which enables us to investigate whether built-in electric fields are a useful approach to tailor the interfacial electronic structure in single molecule junctions.
**12:15PM M62.00004: Giant Thermopower in Quasi-One-Dimensional LaAlO$_3$/SrTiO$_3$ Quantum Wires**

PUQING JIANG (Presenter), YUHE TANG, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, JUNG-WOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — SrTiO$_3$-based heterointerfaces possess new effects ranging from superconductivity to magnetism. In particular, the two-dimensional (2D) LaAlO$_3$/SrTiO$_3$ interface was previously shown to have highly enhanced and oscillating thermopower when back-gated close to the insulating state [1]. Here we investigated the electrical and thermoelectric transport properties of quasi-one-dimensional (1D) LaAlO$_3$/SrTiO$_3$ quantum wires [2] at a low temperature of 80 mK. We find significantly enhanced and oscillating thermopower for the quantum wires, with values that are comparable to reports for 2D LaAlO$_3$/SrTiO$_3$ [1]. The Mott relation, which governs the diffusive thermopower of non-interacting electrons, works surprisingly well despite the highly ballistic nature of electron transport and evidence of electron-electron interaction in these quantum wires. Our results suggest that the highly enhanced thermopower in 2D SrTiO$_3$-based systems may originate from naturally formed quasi-1D channels at the heterointerfaces.


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**12:27PM M62.00005: Effects of writing parameters on electron transport in sketched single-electron transistors**

PHILIP SHENK (Presenter), Univ of Pittsburgh, JOHN MAIER, Department of Physics, University of Notre Dame, YANG HU, Univ of Pittsburgh, HYUNGWOO LEE, JUNG-WOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — Fabrication of single-electron transistors (SETs) and other mesoscopic devices typically requires elaborate nanofabrication techniques. We approach this challenge using a reversible conductive-AFM lithography technique that can locally control the conductivity of the LaAlO$_3$/SrTiO$_3$ interface. We characterize the properties of “sketched” nanostructures as a function of experimentally controllable variables such as writing parameters, back-gate voltage, temperature and magnetic field. Here we focus on the SketchSET geometry [1] which shows discrete addition energies that we can track as a function of source-drain bias and magnetic field. Our findings yield insights into intrinsic interactions between electrons confined within the SET islands.


12:39PM M62.00006: Controlling Nonlinear Thermoelectricity of a Quantum Dot by Quantum Interference* NOBUHIKO TANIGUCHI (Presenter), Physics Div., Univ of Tsukuba — We theoretically study how one can control and enhance nanoscale nonlinear thermoelectricity by regulating quantum interference. We take the configuration of a quantum-dot interferometer (a quantum dot embedded in the ring geometry), which can also represent a model of a single-molecule junction. One can adjust quantum coherence by modifying direct conducting channels between the leads (Fano's effect). Within the linear response theory, such Fano resonances have been suggested to enhance drastically the thermoelectric figure of merit, which reaches an order-of-unity value even for a non-thermoelectric material. We revisit the idea by examining the efficiency and the output power in the nonlinear response regime. Based on the microscopic model and nonequilibrium Green function techniques, we can incorporate the strong correlation on the dot and charge-blocking effect. We show how the presence of direct conducting channels can greatly enhance nonlinear thermoelectric performance, even when the resonance width is much larger than temperature.

*The author gratefully acknowledges financial support from JSPS KAKENHI Grant No.~19K03682.

12:51PM M62.00007: Bell-state correlation in electric currents through lead electrodes connected to a quantum dot* RUI SAKANO (Presenter), Institute for solid state physics, University of Tokyo, AKIRA OGURI, Physics, Osaka city university, MIKIO ETO, Physics, Keio university — We study quantum entanglement that is excited in currents through lead electrodes connected to a quantum dot. To assess the emerging entanglement among the lead electrode, we use Bell's inequality with cross-correlations of current fluctuations [1]. The correlations of the current fluctuations are calculated by using the Anderson impurity model and Green's function in the Keldysh formalism. Electron-hole pairs are induced between two electric leads. We show that quantum entanglement can be formed in the current even if there is no effective Coulomb interactions in the quantum dot. Namely, we investigate current that is induced by sequential tunneling or free quasiparticles scattering in the Kondo regime. Specifically, we find that application of bias-voltages among the lead electrode generate electron-hole, electron-electron, and hole-hole pairs are excited among the lead electrodes. These pairs can violate Bell's inequality


*This work was partially supported by the JST CREST Grant No. JPMJCR1876, Japan, and the Japan Society for the Promotion of Science KAKENHI Grant No. JP18K03495.
1:03PM M62.00008: Coherent Refraction Across Atomically-Precise Molecular Graphene Junctions  MORGAN BRUBAKER (Presenter), YI-TING CHEN, BEATRIZ SARAH YANKELEVICH, ALISON DAY, HARI C. MANOHARAN, Stanford Univ — The construction of functional nanoscopic devices requires an in-depth understanding of electronic transport across interfaces. Electrons in graphene exhibit lightlike behavior due to their massless dispersion relation near the Dirac points; this suggests the ability to construct nanostructures that control electrons analogously to how optical devices such as lenses control light, provided that transport at the interface is understood. Molecular graphene, assembled with atomic manipulation of individual molecules in a low-temperature, ultra-high-vacuum scanning tunneling microscope so as to confine itinerant two-dimensional electrons to a honeycomb lattice, serves as a new tunable form of graphene that features atomically-precise edges and is thus ideal for probing interface transport. We report experiments that use quasiparticle interference measurements to probe the behavior of Dirac electrons incident upon junctions between molecular graphene and a nearly-free two-dimensional electron gas, and between differently-doped regions of molecular graphene. Our results indicate that Dirac electrons are refracted coherently across the junction, analogous to light bending across an interface between two media with mismatched indices of refraction.

1:15PM M62.00009: Persistent Coulomb Blockade Across the Metal-Insulator Transition in Nanoparticle Solids  DAVIS UNRUH (Presenter), CHASE HANSEN, University of California, Davis, ALBERTO CAMJAYI, JOEL BOBADILLA, University of Buenos Aires, MARCELO J ROZENBERG, CNRS, GERGELY T ZIMANYI, University of California, Davis — Nanoparticle (NP) solids in opto-electronic and photovoltaic applications have disadvantageously low carrier mobilities. The mobility is suppressed by the disorder driving the NP solids insulators. A Filling-Controlled (FC) Coulomb blockade further suppresses transport at integer fillings. Transport at non-integer fillings can be improved by driving NP solids across a Disorder-Controlled Metal-Insulator Transition (DC-MIT) into their Metallic Phase by enhancing the kinetic energy to overcome the disorder and thus delocalizing the electron wavefunctions. However, the evolution of the FC-Coulomb blockade at integer fillings across the DC-MIT has not been analyzed yet, leaving the question open whether the FC-Coulomb blockade dissolves or persists in some form as the electron wavefunctions delocalize when the DC-MIT is crossed. The work reported here explores this question of how the FC-Coulomb blockade evolves across the DC-MIT by analyzing transport in the Insulating Phase by our Hierarchical Nanoparticle Transport Simulator, and in the Metallic Phase by Dynamical Mean-Field Theory. Remarkably, the FC-Coulomb blockade is found to persist across the DC-MIT.
1:27PM M62.00010: Theoretical Design of Topological Heteronanotubes*  CHEN HU  (Presenter), VINCENT MICHAUD-RIOUX, McGill Univ, WANG YAO, University of Hong Kong, HONG GUO, McGill Univ — We propose and investigate the idea of topological heteronanotubes (THTs) for realizing a one-dimensional (1D) topological material platform that can pave the way to low-power carbon nanoelectronics at room temperature. We predict that the coaxial double-wall heteronanotube, a carbon nanotube (CNT) inside a boron nitride nanotube (BNNT), can act as a THT. Dissipationless topological conducting pathways on the THT are protected by a valley-dependent topological invariance that originates from local topological phase transitions of the CNT modulated by the CNT-BNNT interaction. Spiral THTs, where topological current flows spirally around the tube, function as nanoscale solenoids to induce remarkable magnetic fields due to the dense moire nanopatterning.

*This work is financially supported by Natural Science and Engineering Research Council (NSERC) of Canada, and the Fonds de recherche du Québec - Nature et technologies (FRQNT) of the Province of Quebec (H.G.). We thank Compute Canada and the High Performance Computing Center of McGill University for substantial computational support.

1:39PM M62.00011: Towards quantum criticality in Al/InAs Kondo systems*  PRAVEEN SRIRAM  (Presenter), CONNIE HSUEH, Department of Applied Physics, Stanford University, ASBJORN DRACHMANN, Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, CANDICE THOMAS, GEOFFREY C. GARDNER, Microsoft Quantum at Station Q Purdue, TIANTIAN WANG, Department of Physics and Astronomy and Station Q Purdue, Purdue University, SERGEI GRONIN, MICHAEL MANFRA, Microsoft Quantum at Station Q Purdue, CHARLES MARCUS, Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, DAVID GOLDHABER-GORDON, Department of Physics, Stanford University — Hybrid metal-semiconductor two-dimensional systems are an attractive platform for exploring correlated electron-electron interactions. Flexible nanopatterning allows design of structures to emulate particular Hamiltonians with electrostatically tunable parameters. Pierre et al. recently demonstrated a quantum phase transition based on a charge Kondo effect[1]. Based in a GaAs heterostructure, the metal was an annealed ohmic contact, requiring much effort to obtain a highly-transparent interface even for a few-micron metal island. InAs may offer significant advantages: pinning of the surface Fermi level in the conduction band allows for direct electrical contact to metals. For example, in-situ epitaxy of aluminum on InAs has resulted in pristine interfaces, leveraged to probe topological superconductivity[2]. Small metallic islands with large charging energies may allow building on earlier charge Kondo work without requiring as low electron temperatures. I will present our initial efforts towards realizing charge Kondo devices on InAs 2DEGs tuned into the quantum Hall regime, with edge states controlled by lithographically defined QPCs.


*Supported by US DoE, contract DE-AC02-76SF00515
M62.00012: Kondo resonance assistant thermoelectric transport through strongly correlated quantum dot* YONGXI CHENG (Presenter), Beijing Computational Science Res Ctr, JIANHUA WEI, Renmin University of China, HONG-GANG LUO, Lanzhou University, HAI-QING LIN, Beijing Computational Science Res Ctr — We theoretically study the thermoelectric transport properties of a strongly correlated quantum dot system in the presence of Kondo effect, on the basis of accurate numerical evaluations. The thermocurrent versus gate voltage shows a distinct sawtooth line-shape at high temperature. In particular, the sign of current changes from positive (hole charge) to negative (particle charge) in the electron number N = 1 region due to Coulomb blockade effect. However, at low temperature, where Kondo effect takes place, the thermocurrent charge polarity reverses, together with also a significantly enhanced magnitude. As anticipated, the current sign can be analyzed by the occupation difference between particle and hole. Moreover, one could further define the characteristic turnover temperature, at which the influences of Coulomb blockade and Kondo resonance are in effective balance. When magnetic field is applied, a spin-polarized thermocurrent could be obtained, which could be tested in future experiments.

References:

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M62.00013: Ballistic p–n junctions in three-dimensional Dirac semimetal Cd₃As₂ nanowires

MINKYUNG JUNG (Presenter), DGIST Research Institute, DGIST, JANICE BAYOGAN, SUNG JIN AN, JUNGPIL SEO, Department of Emerging Materials, DGIST — We demonstrate a ballistic p–n junction in a three-dimensional Dirac semimetal (DSM) Cd₃As₂ nanowire with two recessed bottom gates. The device exhibits four different conductance regimes with gate voltages, confirming that device forms p–n junction. The conductance in the p–n junction regime decreases drastically when a magnetic field is applied perpendicular to the nanowire, which is due to the suppression of Klein tunneling. In this regime, the device shows quantum dot behavior. On the other hand, clear conductance plateaus are observed in the n–n regime likely owing to 1-D subbands of carriers at high magnetic fields. In other devices, we also observe Fabry-Perot interference in the p–n junctions, indicating that our devices are in the ballistic regime. Our experiment shows that the ambipolar tunability of DSM nanowires can enable the realization of quantum devices based on electron optics.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M63 DMP DCMP FIAP: Defects in Oxides and Chalcogenides Mile
High Ballroom 4D - Cyrus Dreyer, State Univ of NY - Stony Brook - Tag(s): Focus
Chalcogenide phase change materials can exist in multiple structural states at room temperature. There is a large difference in the electrical and optical properties between the structural states of these materials. Importantly the phase transition time can be just picoseconds [1], and this makes these materials ideal for both optical and electrical data storage[2]. Indeed, they have recently been commercialised in Intel’s Optane memory[3].

The most common data storage materials exist along a pseudo-binary compositional line between Sb$_2$Te$_3$ and GeTe. These materials tend to have a small electronic band gap and consequently strongly absorb visible light. This means that it is challenging to use these common PCMs for many visible photonics applications.

We will discuss how phase change materials can be used in visible photonics. We will discuss the plasmonic property of the common phase change materials and also introduce a new phase change material with an electronic band gap of 2 eV[4]. We will discuss the prospect of using electrical fields to control phase changes in these materials. We believe these results will open new opportunities to design programmable photonics devices that operate at visible wavelengths.


*We are grateful for funding from A* Star (Project: NSLM, Grant #: A18A7B0058) and the Singapore Ministry of Education (Project: Electric-field induced transitions in chalcogenide monolayers and superlattices, Grant #: MOE2017-T2-1-161).
11:51AM M63.00002: Electron mobility in crystalline and amorphous metal-oxide semiconductors

IGOR EVANGELISTA (Presenter), ANDERSON JANOTTI, Department of Materials Science and Engineering, University of Delaware — Charge carrier mobility in amorphous semiconductors is significantly reduced when compared to the crystalline phase. For instance, room-temperature electron mobility in crystalline silicon is 1400 cm$^2$/V.s, while that for amorphous silicon is only ~0.1 cm$^2$/V.s. Amorphous metal-oxide semiconductors are unique in this respect, as they display relatively high electron mobilities when compared to their crystalline counterpart. Here we investigate the microscopic origin of this intriguing effect. Using first-principles molecular dynamics to generate amorphous configurations and electronic structure calculations of prototype metal oxides, we investigate why metal-oxide semiconductors display relatively high electron mobilities even in an amorphous phase. We analyze their band structure, the effects of volume, the change in the absolute band edge positions, and provide a detailed comparison between amorphous silicon and Ga$_2$O$_3$, paying special attention to the presence of band tail states and the change in band gaps.

12:03PM M63.00003: Amorphous Oxide Semiconductors: role of disorder and composition in defect formation, carrier generation, and transport properties

JULIA MEDVEDEVA (Presenter), Missouri Univ of Sci & Tech — Unlike Si-based semiconductors, amorphous oxide semiconductors (AOSs) exhibit optical, electrical, thermal, and mechanical properties that are comparable or even superior to those possessed by their crystalline counterparts. Although amorphous materials lack grain boundaries and periodicity, the electron transport is more complex than in the crystalline phases: strong local distortions in the metal-oxygen polyhedra and intricate structural morphology in AOSs affect carrier mobility via composition, defects, thermal vibrations, nano-crystallinity, and lattice strain. Moreover, given many degrees of freedom in amorphous materials, defects in AOSs have the structural, thermal, and electronic characteristics that differ fundamentally from those in the crystalline transparent conducting oxides.

In this talk, complex deposition-structure-property relationships in several prototype AOSs are discussed. The results of systematic computationally-intensive ab-initio Molecular Dynamics followed by comprehensive structural analysis and accurate density-functional calculations, are integrated with experimental measurements to understand the origins of complex behavior in the disordered materials and to derive versatile design principles for next-generation transparent amorphous semiconductors.
Amorphous oxide semiconductors (AOS) possess many unique properties, including high carrier mobility (>>a-Si:H) and optical transparency, making them attractive materials for a wide range of optoelectronic applications. Unlike Si-based semiconductors or silica glasses, AOS exhibit strong distortions in local polyhedral structure due to weaker Metal-Oxygen bonds that are ionic in nature. These distortions have been shown to cause strong electron localization near the valence and conduction band edges and deep inside the band gap when oxygen content, known to dope the oxide materials n-type, is varied. Moreover, due to the large number of degrees of freedom in AOS, thermal or photo activation may switch bond configurations out of shallow states into deep bound states or vice versa, making a static characterization inadequate for AOS. In this work, ab-initio molecular dynamics simulations are combined with accurate density-functional calculations to study time- and temperature-dependent characteristics of defects with different formation energies and degree of localization in amorphous InOx. The microscopic understanding of the structural dynamics highlights the complex nature of AOS and helps explain the observed non-equilibrium conductivity in the materials under illumination.

Recent discoveries of amorphous and quasi-amorphous phases in SrTiO₃ (a-STO) open up a wide range of possible applications in electronic devices that prohibit utilization of crystalline STO (c-STO) due to fundamental or technological barriers. While oxygen vacancies are known to play key role in the electronic properties of c-STO, the results may not be applicable to a-STO. Upon amorphization, changes in the local structure and morphology may affect the formation energy of oxygen defects and their diffusion. In addition, a reduction of the material's density may lead to voids and other structural defects, important for material's behavior. All the above calls for a comprehensive study of the microscopic origins of the observed electronic and optical properties in a-STO.

Here we employ ab-initio molecular dynamics liquid-quench simulations and accurate density-functional calculations to understand how the local and medium-range structural characteristics change upon amorphization in STO. Specifically, we analyze the Ti-O and Sr-O coordination, polyhedra sharing, and morphology as a function of density, quench rates, and oxygen deficiency in a-STO and determine the role of the structural changes in the resulting electronic and optical properties of this disordered material.
12:39PM M63.00006: Hydrogen doping of crystalline/amorphous In$_2$O$_3$ interface: the structure and electronic properties. KAPIL SHARMA (Presenter), JULIA MEDVEDEVA, Missouri Univ of Sci & Tech — Hydrogen doped In$_2$O$_3$ has grabbed attention of scientific community due to its high carrier mobility, high carrier concentration, and transparency in near-IR region, with values exceeding those in commercial ITO. While H-doped crystalline In$_2$O$_3$ has been studied, the results may not be applicable to amorphous In-based oxides, employed in state-of-the-art display technologies. The lack of periodicity, the strong local and medium-range distortions in the Metal-Oxygen (M-O) polyhedra, and the increased number of degrees of freedom in amorphous materials are likely to affect the formation of M-OH and M-H bonds as well as their thermal stability. Hence, the resulting properties of hydrogenated amorphous oxide semiconductors may differ from those in the crystalline counterpart.

In this work, amorphous/crystalline In$_2$O$_3$ Interface with >100 initial locations of H radical is investigated using ab-initio molecular dynamics and density functional calculations. The relaxed structures and their electronic properties are analyzed based on the calculated total energy, interatomic distances, effective coordination numbers, local distortions, and charge density distribution before and after H-doping. In addition, the effect of H on the interface morphology and crystallization are investigated.

12:51PM M63.00007: Thermoelectric properties of Pb$_{2-x}$Y$_x$Ru$_2$O$_{7-z}$ pyrochlore SEPIDEH AKHBARIFAR (Presenter), WERNER LUTZE, IAN L PEGG, Catholic Univ of America — Thermoelectric materials convert heat to electrical energy and are considered for various applications such as refrigeration or in power generations. Thermoelectric properties are characterized by a figure of merit ($ZT$), $ZT=\frac{S^2\sigma T}{k}-1$. $ZT$ is a function of the Seebeck coefficient or Thermopower ($S$), electrical conductivity ($\sigma$), temperature ($T$) and thermal conductivity ($k$). This work aims to study the respective properties of lead ruthenate (Pb$_2$Ru$_2$O$_{6.5}$) doped with yttrium oxide in the temperature range of 25 to 300°C. Lead ruthenate has a defect pyrochlore crystal structure and has metal-like electrical conductivity. Y$_2$Ru$_2$O$_7$ is an insulator. Molar fractions of Pb have been substituted by yttrium, i.e., Pb$_{2-x}$Y$_x$Ru$_2$O$_{7-z}$ with $x$ varied between 0 and 1. The compounds were prepared by solid-state synthesis and characterized by XRF, X-ray diffraction, and SEM/EDX for composition, structure, phase content, morphology and crystal size. Micron-sized powders were pressed into pellets to measure the thermoelectric properties. The results will be discussed, particularly the transition from conductive to insulating and its effect of $ZT$. 
1:03PM M63.00008: Role of defects in photocatalytic water splitting: Monodoped vs codoped SrTiO\textsubscript{3} * MANISH KUMAR (Presenter), SASWATA BHATTACHARYA, Indian Inst of Tech-New Delhi — SrTiO\textsubscript{3} can be utilized as a photocatalyst for water splitting owing to its suitable band edge positions, thermal stability and low cost. However, it could not harness the visible light due to its wide band gap (3.25 eV). Doping is one of the prominent solutions to tailor the band gap and inducing the visible light response and thus, enhancing the photocatalytic activity. We address the role of monodoping of a metal (Mn) and a non-metal (N), as well as their codoping in SrTiO\textsubscript{3} for photocatalytic water splitting using state of the art density functional theory and \textit{ab initio} atomistic thermodynamics. N\textsubscript{O} reduces the band gap, but introduces the deep trap states that degrade the photocatalytic efficiency. Mn\textsubscript{Sr} could not reduce the band gap of SrTiO\textsubscript{3}. Mn\textsubscript{Ti} could reduce the band gap, but it lowers down the conduction band edge and hence, lowers the reduction power. Our results reveal that the Mn\textsubscript{Sr}N\textsubscript{O} (codoping of Mn at Sr and N at O in SrTiO\textsubscript{3}) is the promising candidate as a photocatalyst for water splitting as it induces the visible light response as well as passivates the deep level states and its band edge positions straddle the redox potential of water.

* M.K. acknowledges CSIR, India, for the fellowship [grant no. 09/086(1292)/2017-EMR-I]. We acknowledge the HPC facility at IIT Delhi.

1:15PM M63.00009: Rutile GeO\textsubscript{2}: an ultra-wide-band-gap semiconductor with ambipolar doping SIEUN CHAE (Presenter), KELSEY A. MENGLE, Univ of Michigan - Ann Arbor, HANJONG PAIK, Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM), Cornell University, JIHING LEE, JOHN HERON, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — Ultra-wide-band-gap (UWBG) semiconductors have tremendous potential to advance electronic devices as device performance improves superlinearly with increasing gap. Ambipolar doping, however, has been a major challenge for UWBG materials as dopant ionization energy and charge compensation generally increase with increasing gap. Using hybrid density functional theory, we demonstrate rutile germanium oxide (r-GeO\textsubscript{2}) to be an alternative UWBG (4.68 eV) material that can be ambipolarly doped. We identify Sb\textsubscript{Ge}, As\textsubscript{Ge}, and F\textsubscript{O} as possible donors with low ionization energies and propose growth conditions to avoid charge compensation by native acceptor-type defects. Acceptors such as Al\textsubscript{Ge} have relatively large ionization energies (0.45 eV) due to the formation of localized hole polarons. Yet, we find that the co-incorporation of Al\textsubscript{Ge} with H\textsubscript{i} can increase the solubility limit of Al and enable hole conduction in the impurity band. We also calculate electron (153.6 cm\textsuperscript{2}V\textsuperscript{-1}s\textsuperscript{-1}) and hole mobilities (4.7 cm\textsuperscript{2}V\textsuperscript{-1}s\textsuperscript{-1}) of r-GeO\textsubscript{2} at 300 K, suggesting r-GeO\textsubscript{2} has outstanding electronic properties that can compete with the state-of-the-art UWBG semiconductors such as β-Ga\textsubscript{2}O\textsubscript{3}. We will also discuss on our recent experimental progress on thin-film growth and electrical characterization of r-GeO\textsubscript{2}.
**1:27PM M63.00010: Quasiparticle Properties of Sulfur Doped SrTiO3**

GABE LOPEZ-CANDALES (Presenter), PEIHONG ZHANG, Physics, University at Buffalo — Strontium Titinate (SrTiO3) is a potential candidate for photocatalytic water-splitting application due to a favorable conduction band edge position with respect to the hydrogen reduction potential level [1]. Despite having an ideal conduction band placement, the large band gap (3.25 eV (indirect) and 3.75 eV (direct)) [1] limits its photocatalytic and photovoltaic applicability. The distorted chalcogenide-perovskite counterpart (SrTiS3), on the other hand, is predicted to have a significantly lower band gap (0.9 eV) [2]. In this work, we report GW quasiparticle calculations of the electronic properties of sulfur doped of SrTiO3 using a recently developed accelerated GW approach [4] that allows efficient GW calculations for large system. Our results elucidate a complex relationship between atomic and electronic structure, predicting a notable trade-off between band gap and structural stability.


*This work is supported in part by the NSF (Grant Nos. DMR-1506669 and DMR-1626967).

**1:39PM M63.00011: Defect physics in rare-earth doped wide band-gap materials**

KHANG HOANG (Presenter), North Dakota State Univ — Rare-earth (RE) doped wide band-gap materials are of great interest for optoelectronic and spintronic applications. The determination of defect energy levels associated with RE-related defect centers has been challenging, however, both in experimental and theoretical/computational studies. Yet such knowledge is crucial to understanding luminescence or persistent luminescence in the materials. In this talk, we present a hybrid density-functional study of the interaction between RE dopants (Er, Eu, Dy, etc.) and host materials (GaN and SrAl2O4), including intrinsic point defects and other impurities that may be present in the host materials. In light of our results, we identify possible luminescent RE-related centers and elucidate luminescence (or persistent luminescence) mechanisms in the RE-doped materials and develop guidelines for defect engineering to design materials with improved performance.
Tuning the Transport Properties of Artificial Synapses: A DFT-Supported Experimental Approach*  DIP DAS (Presenter), ARABINDA BARMAN, Department of Physics, Shiv Nadar University, India., PRANAB KUMAR SARKAR, Dept of Applied Science and Humanities, Assam University, India., RENE HUBNER, Electron Microscopy Laboratory, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstrasse, Dresden, Germany, DINAKAR KANJILAL, Ion beam facilites, Inter-University Accelerator Centre, New Delhi, India, PRIYA JOHARI, ALOKE KANJILAL, Department of Physics, Shiv Nadar University, India. — Defect engineering is an essential aspect of resistive switching (RS) memories. This work illustrates cationic dopant (Ni) controlled RS characteristics in the thin film of anatase titanium dioxide (A-TiO₂). A significant increase in ON/OFF ratio to 10^3 with a gradual change in resistance state is accomplished and such RS characteristics are highly expedient for neuromorphic computing applications. Detailed investigations by transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS) as well as density functional theory (DFT)-based first-principles calculations establish the role of Ni in memristive operation. In particular, TEM results show an evolution of two different Ni-concentration regions within the films that help to reduce the host Ti-site from its +4 valence state, as obtained from Ti-2p XPS analysis. This claim is further verified by DFT calculations, showing a change in the charge density near the Ni-site form the Bader charge analysis and electron localisation function (ELF) plots. Moreover, the role of those two Ni-concentration regions in regulating transport properties of the Au/ Ni:A-TiO₂ /Pt devices similar to the biological synapse is discussed.

*Funding acknowledgement: DST (project no. DST/EMR/2014/000971) and SNU, India.

Hot-electron mediated ion diffusion in semiconductors for ion-beam nanostructuring*  CHENG-WEI LEE (Presenter), ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Ion-beam-based techniques are widely utilized to synthesize, modify, and characterize semiconductors at the nanoscale. Interactions of the beam with the target are fundamentally interesting, as they trigger multi-length- and time-scale processes that need to be quantitatively understood to achieve nanoscale precision. Here we demonstrate for magnesium oxide¹ that, in a beam energy regime in which electronic effects are usually neglected, a proton beam efficiently excites oxygen-vacancy-related electrons and changes the charge state of the F-center. We quantify the beam-energy-dependent electronic excitation and the emerging ion dynamics using first-principles techniques. We further bridge time scales from ultrafast electron dynamics directly after impact to ion diffusion over migration barriers in semiconductors and discover a diffusion mechanism that is mediated by hot electrons. Our quantitative simulations predict that this mechanism strongly depends on the projectile-ion velocity, suggesting the possibility of using it for precise sample manipulation via nanoscale diffusion enhancement in semiconductors with a deep, neutral, intrinsic defect.


*SNL-UIUC collaboration (DOE SNL 1736375)
ONR (N00014-18-1-2605)
11:15AM M64.00001: Neutron diffraction and inelastic neutron scattering in the magnetodielectric regime of Ce$_2$O$_3$*  ALEXANDRA COTE (Presenter), ASTHA SETHI, University of Illinois at Urbana-Champaign, TARAS KOLODIAZHNYI, National Institute of Materials Science, JEFFREY LYNN, National Institute of Standards and Technology, S. LANCE COOPER, GREG MACDOUGALL, University of Illinois at Urbana-Champaign — The metastable material Ce$_2$O$_3$ has drawn recent attention due to reports of a giant magnetodielectric response of unknown origin, below a putative antiferromagnetic transition at $T_N=6.2K$. In the same temperature region, Raman spectroscopy has revealed the emergence of vibronic modes, which represent a relatively uncommon mixing of phonon and crystal field excitations.

Following up on these observations, we have performed a series of both neutron diffraction and inelastic scattering measurements on powders of Ce$_2$O$_3$. Our diffraction data allow us to comment on both the nature of the magnetically ordered state at low temperatures, and the variation in atomic structure as the material is varied through $T_N$. Our inelastic measurements focus on the temperature dependence of crystal field and phonon excitations at the energies of reported vibronic modes. I will present these data in the context of existing literature, and give our conclusions about the nature of the AF ground state and spin-lattice coupling in this material.

*This work was sponsored by the National Science Foundation, under Grant No. DMR-1455264-CAR.
11:27AM M64.00002: Local polarization in oxygen-deficient LaMnO$_3$ induced by charge localization in the Jahn-Teller distorted structure  
CHIARA RICCA, ULRICH ASCHAUER  
(Presenter), University of Bern — The functional properties of transition metal oxides result from a complex interplay between magnetism, polarization, strain, and stoichiometry. Here, we show that for materials with a cooperative Jahn-Teller distortion, such as LaMnO$_3$ (LMO), the orbital order can also couple to the defect chemistry and induce novel material properties. At low temperatures, LMO is an A-type antiferromagnet with a distorted orthorhombic perovskite structure. It is insulating due to the Jahn-Teller distortion that splits the $e_g$ orbitals of the high-spin Mn$^{3+}$ ions, leading to alternating long, short, and intermediate Mn-O bond lengths. Our DFT+$U$ calculations show that, as a result of these peculiarities, the charge localization in LMO upon oxygen vacancy ($V_O$) formation is different compared to other manganites, like SrMnO$_3$, where the two extra electrons reduce the Mn sites adjacent to the vacancy. In LMO, relaxations around the $V_O$ depend on which type of Mn-O bond is broken, affecting the $d$-orbital energies and leading to an asymmetric and hence polar localization of the excess electrons with respect to the vacancy. Furthermore, we show how isostatic and epitaxial strain can be used to affect the Mn-O bond lengths and orbital order and consequently the charge localization and polarity.

11:39AM M64.00003: Geometrical frustration and piezoelectric response in oxide ferroics*  
VALERI PETKOV (Presenter), Physics, Central Michigan Univ — Despite years of investigation, the exact structural origin of the increased piezoelectric response of oxide ferroics is still unclear. We will present results from resonant high-energy x-ray diffraction experiments on exemplary sodium-potassium niobate ferroics. In particular, we will show that their increased piezoelectric response is due to a geometrical frustration in the underlying perovskite lattice induced by local fluctuations in the tilt pattern of the constituent niobium-oxygen octahedra, and not to a crystal-crystal phase transition or distinct nanodomains. The fluctuations peak when the sodium to potassium ratio approaches one, leading to softening of the perovskite lattice and easing of polarization rotation under electric field. Based on the experimental findings and model calculations, we will also show that the fluctuations are driven by the mismatch between the radii of sodium and potassium atoms, and the increased piezoelectric response of sodium-potassium niobates indeed scales with the variance in the distribution of these radii about their average value. The relevance of our work to the ongoing search for oxide ferroics with improved functionality will be briefly discussed.

*This work was supported by DOE-BES grant DE-SC0006877.
11:51AM M64.00004: Magnetic Field Dependent Local Structure of Charge-Ordered AMnO₃ Perovskites* SIZHAN LIU, New Jersey Inst of Tech, MILINDA ABEYKOON, Brookhaven National Laboratory, TREVOR TYSON (Presenter), New Jersey Inst of Tech — Complex oxide perovskites exhibit closely lying structural phases at low temperatures. External parameters including pressure and magnetic field can be used to stabilize distinctly different structural phases. In this project, we utilize pair distribution function measurements to determine the changes in the local structure in AMnO₃ perovskites when going from the charge-ordered insulating phased to the metallic phase at fixed temperature when applying an external magnetic field. The structure on a range of length scales will be explored. The results will be compared to the corresponding temperature dependence of the structure.

*This work is supported by NSF Grant No. DMR-1809931.

12:03PM M64.00005: Infrared nano-spectroscopy of ferroelastic domain walls in hybrid improper ferroelectric Ca₃Ti₂O₇ KEVIN SMITH (Presenter), Chemistry, University of Tennessee, Knoxville, ELIZABETH NOWADNICK, Material Science and Engineering, University of California, Merced, SHIYU FAN, Physics, University of Tennessee, Knoxville, OMAR KHATIB, Physics and Chemistry, University of Colorado, Boulder, SEONG JOON LIM, BIN GAO, Physics and Astronomy, Rutgers University, NATHAN HARMS, SABINE NEAL, JUSTIN KIRKLAND, Chemistry, University of Tennessee, Knoxville, MICHAEL MARTIN, Advanced Light Source Division, Lawrence Berkeley National Lab, CHOONG-JAE WON, Laboratory for Pohang Emergent Materials, Pohang Accelerator Laboratory and Max Planck POSTECH Center for Complex Phase Materials, Pohang University of Science and Technology, MARKUS B. RASCHKE, Physics and Chemistry, University of Colorado, Boulder, SANG-WOOK CHEONG, Physics and Astronomy, Rutgers University, CRAIG FENNIE, School of Applied and Engineering Physics, Cornell University, G CARR, National Synchrotron Light Source II, Brookhaven National Lab, HANS BECHTEL, Advanced Light Source Division, Lawrence Berkeley National Lab, JANICE L MUSFELDT, Chemistry, University of Tennessee, Knoxville — Ferroic materials are well known to exhibit heterogeneity in the form of domain walls. Understanding the properties of these boundaries is crucial for controlling functionality with external stimuli and for realizing their potential for ultra-low power memory and logic devices as well as novel computing architectures. In this work, we employ synchrotron-based near-field infrared nano-spectroscopy to reveal the vibrational properties of ferroelastic (90° ferroelectric) domain walls in the hybrid improper ferroelectric Ca₃Ti₂O₇. By locally mapping the Ti-O stretching and Ti-O-Ti bending modes, we reveal how structural order parameters rotate across a wall. Thus, we link observed near-field amplitude changes to underlying structural modulations and test ferroelectric switching models against real space measurements of local structure. This initiative opens the door to broadband infrared nano-imaging of heterogeneity in ferroics.
Coupled structural distortions, domains, and control of phase competition in polar SmBaMn$_2$O$_6$ ELIZABETH NOWADNICK (Presenter), University of California, Merced, JIANGANG HE, Northwestern University, CRAIG J FENNIE, Cornell University — Complex oxides display highly tunable ground states, where small perturbations to the crystal structure can stabilize distinct electronic and magnetic phases. We use group theoretic methods and density functional theory calculations to analyze the polar crystal structure of A-site ordered SmBaMn$_2$O$_6$, which hosts a charge- and orbitally-ordered antiferromagnetic ground state. We show that a set of couplings between structural distortions are key for establishing the structural, electronic, and magnetic ground states and also establishes a hybrid improper ferroelectric mechanism in this material. We analyze the domain structure and show how the coupled degrees of freedom in SmBaMn$_2$O$_6$ leads to a network of coupled domains and domain wall vortices. Finally, we explore how competing electronic and magnetic phases may stabilize, for example at structural domain walls and in epitaxially strained thin films. This work provides new understanding of the complex physics realized across multiple length scales in SmBaMn$_2$O$_6$ and demonstrates a framework for the systematic exploration of correlated and structurally complex materials.
The search for new quantum materials with novel properties is often focused on materials containing transition-metal or rare-earth elements. The presence of the atomic-like $d$ or $f$ orbitals provides a fruitful playground to generate novel phenomena and understanding the behavior of those $d$ and $f$ electrons is essential for designing and tuning new materials. Therefore, identifying the $d$ or $f$ orbitals that actively participate in the formation of the ground state is crucial. So far, these orbitals have mostly been deduced from optical, X-ray and neutron spectroscopies in which spectra must be analyzed using theory or modelling. This, however, is also a challenge in itself, since ab-initio calculations hit their limits due to the many-body nature of the problem.

Here we developed a new experimental method that circumvents the need for involved analysis and instead provides the information as measured. With this technique, we can make a direct image of the active orbital and determine what the atomic-like object looks like in a real solid. The method, s-core-level non-resonant inelastic X-ray scattering (s-NIXS), relies on high momentum transfer in the inelastic scattering process, which is necessary for dipole-forbidden terms to gain spectral weight. To demonstrate the strength of the technique, we imaged the text-book example, $x^2-y^2/3x^2-r^2$ hole orbital of the Ni$^{2+}$ ion in NiO single crystal [1]. We will present the basic principles of s-NIXS and its experimental implementation. We will also show how we can apply this technique to unveil the active orbitals in complex oxides as well as to determine the orbital character in highly metallic systems such as elemental Cr, Fe, and Ni.

1:03PM M64.00008: Interplay of orbital selectivity and local environment in correlated materials: the case of metal-insulator transition in CaFeO$_3$  
GHEORGHE PASCUT (Presenter), MANSiD Research Center, Stefan Cel Mare University (USV), JENNIFER COULTER, 1 John A. Paulson School of Engineering and Applied Sciences, Harvard University, PREMALA CHANDRA, KARIN M RABE, KRISTJAN HAULE, Dept. of Physics and Astronomy, Rutgers University, New Brunswick — Density Functional Theory (DFT) with Embedded Dynamical Mean Field Theory (eDMFT) is a very successful method in describing novel electronic states of matter where (I) Mott and metallic orbitals coexist (orbital-selective Mott state) (II) Mott, metallic and semi-metallic orbitals coexist (site-orbital-selective Mott state) and (III) Mott and band orbitals coexist (band-Mott state). Recently, forces for structural relaxations within the DFT+eDMFT have been developed, and the predictive power of the method for electronic-structural interplay at finite temperatures was demonstrated on correlated materials that have novel states with orbital and site selectivity, such as NdNiO$_3$, LaMnO$_3$, BiMnO$_3$, TM$_2$Mo$_3$O$_8$ (TM=Mn, Fe). Through the use of this method, we apply DFT+eDMFT to study the electronic-structural interplay at finite temperature, in order to describe the interplay between Mott, band and metallic-like orbitals and the local environment (characterized by the bond length and bond angle) in CaFeO$_3$, as it goes through the metal to insulator transition.

1:15PM M64.00009: Atomic-scale insight into lattice and electronic modulation induced by the substitution of bismuth in iron garnet with enhanced magneto-optical effect*  
KUN XU (Presenter), Tsinghua University, LUO ZHANG, Beijing Normal University, H. W. ZHANG, University of Electronic Science and Technology of China, JING ZHU, Tsinghua University — In this study, Bismuth substituted lutetium iron garnet prepared by liquid epitaxial method shows large Faraday rotation up to 1.64 degree/µm at 633nm at room temperature, whose structure variation and element distribution in atomic scale have been directly interpreted by using analytical scanning transmission microscopy (STEM). The substituted Bismuth located in dodecahedral site of lutetium iron garnet can induced the change of lattice and furtherly will lead to the distortion of octahedral Fe sites, but magnetic order is not modified, which is all verified by using energy loss spectrum (EELS). Combined with density function theory (DFT) calculation, distorted octahedral magnetic sublattice contributes to the reduced crystal field splitting energy and orbital degeneracy.


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JOHN SLIMAK (Presenter), ASTHA SETHI, University of Illinois at Urbana-Champaign, TARAS KOLODIAZHNYI, National Institute for Materials Science, Japan, S. LANCE COOPER, University of Illinois at Urbana-Champaign — The energetic overlap of phonons and low-lying crystal electric field (CEF) excitations in rare-earth sesquioxides is conducive to strong electron-phonon coupling and dramatic magnetostructural phenomena. For example, our previous temperature and magnetic field dependent Raman scattering studies on a member of this series, A-type Pr2O3, revealed significant phonon softening and a level repulsion between electronic and phononic levels. To explore these results further, we present a pressure-dependent Raman scattering study of Pr2O3 aimed at tuning the coupling between electron and phonon levels to modify the low temperature phase behavior. We observe that the degeneracy of the lowest lying CEF doublet is lifted under the application of pressure below 60 K and that the energy splitting increases linearly with increasing pressure or magnetic field. These results are indicative of a pressure-induced Structural Distortion that appears to be instigated by pressure-dependent electron phonon coupling. We discuss the possible effects of pressure on the magnetostructural properties of Pr2O3.

*Work supported by the National Science Foundation under Grant No. NSF DMR 1800982.

STEVEN HARTMAN (Presenter), Institute of Materials Science and Engineering, Washington University, St. Louis, AYANA GHOSH, Materials Science and Engineering, University of Connecticut, ROHAN MISHRA, Institute of Materials Science and Engineering, Washington University, St. Louis, CHRISTOPHER STANEK, BLAS PEDRO UBERUAGA, GHANSHYAM PILANIA, Materials Science and Technology Division, Los Alamos National Lab — Perovskite compounds—with a generic formula of ABX3— represent a versatile class of materials exhibiting tremendous synthetic flexibility and technological applications. Going beyond “single” perovskites, two or more species can occupy each sublattice. While origins and design rules of cation ordering in perovskites are well known, anion ordering in heteroanionic perovskites remains a largely uncharted territory. This talk will share insights from a first principles analysis of anion-ordered AB(O0.5S0.5)3 oxysulfide chemistries, studied in all possible anion configurations, with A=Ca,Sr,Ba and B=Ti,Zr,Hf. We find that the stable local ordering is always an all-cis arrangement (i.e., a fac-type ordering) in each BO3S3 octahedron, stabilized by a combination of electronic, strain and electrostatic interactions. We further study the relative stability of this ordering as a function of A and B site chemistries and probe its effect on the electronic structure. Most remarkably, we show that the ground state anion ordering breaks inversion symmetry to create a family of polar oxysulfides with polarization >30 µC/cm², exhibiting a significant promise for electronic applications.

*We acknowledge support from Laboratory Directed Research and Development (LDRD) program (Project# 20190043DR).
1:51PM M64.00012: Symmetry analysis of anion order, cation-vacancy order, and octahedral tilting in oxyfluoride double perovskites*  RICHARD SABALLOS (Presenter), JAMES RONDINELLI, Northwestern University — In simple homoanionic double perovskites, the possible phase space based on octahedral tilting and cation ordering has been established and is useful in resolving known structures as well as performing computational studies to determine viable phase transitions [1][2]. However, a similar study incorporating octahedral tilting and ordering in heteroanionic materials has yet to be carried out. Initial work in oxynitrides has determined that by coupling octahedral tilting and anion ordering, it is possible to further lower the phase symmetries of materials [3]. This coupling can also be used to break inversion symmetry, leading to improvement in dielectric responses and ferroelectricity. Here we use the P4/nmm phase of [J]KNaNbOF₅ as a prototype structure to explore how independently and in combination anion ordering, A-site vacancy ordering, and octahedral tilting lead to variations in symmetries [4]. We apply materials physics principles to understand commonalities among the structure space and perform electronic structure calculation to ascertain the microscopic origins.


*NSF's MRSEC program (DMR-1720139) at NU.

2:03PM M64.00013: Understanding the Appearance of Local and Long-Range Anion Order in Heteroanionic Layered Perovskites*  JAYE HARADA (Presenter), JAMES RONDINELLI, Northwestern University — The prediction of the appearance, or lack thereof, of anion ordering in mixed-anion and heteroanionic materials is an important, yet unsolved problem. This issue has a significant impact on the prediction of properties in these materials, especially properties whose appearance is reliant on long-range noncentrosymmetry, such as ferroelectricity, piezoelectricity and nonlinear optical phenomena such as second harmonic generation. We examine this issue in Ruddlesden-Popper oxyfluorides where both anion ordered and disordered structures exist, such as Sr₂FeO₃F and Sr₂ScO₃F, and fluoride preferentially occupies the apical anion site of the 2D perovskite layers. We use density functional theory calculations to understand and attempt to quantify the contributions of the B-site cation size, covalency, and magnetism to the configurational entropy or the appearance of local and long-range ordered anions.

*This work is supported by the National Science Foundation Grant No. DMR 1720139 and 1454688.

Wednesday, March 4, 2020 11:15 AM - 1:51 PM

Session M65 DCMP: 2D Materials: Graphene and Transition Metal Dichalcogenides  Mile High Ballroom 4F - Sergio de la Barrera, Massachusetts Institute of Technology MIT
**11:15AM M65.00001: Observation of flat bands and singularity collapse in back-gated semiconductor artificial graphene**  
LINGJIE DU, Physics, Nanjing University, ZIYU LIU (Presenter), Columbia University, LOREN PFEIFFER, Princeton University, MICHAEL MANFRA, Purdue University, ARON PINCZUK, Columbia University — Electronic flat bands are key predicted features in tunable artificial graphene (AG) near M points in the Brillouin zone. Such dispersionless electron flat bands could support unconventional superconducting states. Here, we report the first direct observation of flat bands in semiconductor AG transistors where the electron density is tuned by applied voltage. Doublets observed in low temperature photoluminescence (PL) display a density dependence that is linked to the van-Hove singularity doublet near M points. We find that the doublets in PL persist for a large range of electron densities, suggesting a pinning of the Fermi energy in a flat band. Interestingly, as the temperature is lowered to below 10K, the lineshape of the doublet in PL spectra shows a dramatic temperature dependence in which the higher energy peak quickly collapses. This unexpected temperature dependence suggests possible formation of electron liquid states near the flat band at low temperature.

*Supported by NSF grant DMR-1306976 and DOE grant DE-SC0010695.

YEONGROK JIN (Presenter), JAEKWANG LEE, Pusan Natl Univ — The flexoelectricity, electrical polarization induced by a strain gradient, is one of the very exotic physical phenomena because it can induce the huge piezoelectricity even in centrosymmetric materials. Here, combining density functional theory calculation and mathematical analysis, we find that the corrugation generates the great out-of-plane polarization mediated by the flexoelectric effect even in centrosymmetric two-dimensional materials. The flexoelectricity in 2D materials is highly sensitive to the corrugation strength and tunable by adjusting the curvature at the nm scale. The correlation between curvature, flexoelectricity and resulting out of plane polarization will be discussed and associated underlying mechanisms will be introduced in detail.
11:39AM M65.00003: Electronically Engineered Nanoporous Graphene*  PETER JACOBSE (Presenter), RYAN MCCURDY, DANIEL RIZZO, JINGWEI JIANG, PAUL L BUTLER, GREGORY VEBER, STEVEN LOUIE, FELIX FISCHER, MICHAEL F CROMMIE, University of California, Berkeley — Recent advances in the synthesis of graphene nanoribbons using on-surface bottom-up techniques have enabled fabrication of not only atomically well-defined one-dimensional structures, but also two-dimensional structures such as nanoporous graphenes. These are particularly interesting for applications due to their sieve-like topology. Here we present a new methodology for creating covalently connected, fully conjugated two-dimensional graphene structures through the utilization of cyclopentadiene (CP) moieties. CP elements exhibit a propensity to initiate fusion between nanoribbons and result in a two-dimensional structure with well-defined interface topology. The resulting new material is analyzed using scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), and bond-resolved scanning tunneling microscopy (BRSTM). We observe emergent interface-localized electronic states that hybridize to yield a dispersive two-dimensional band of states at an energy inside the bandgap of an isolated GNR.

*Dutch Research Council
National Science Foundation
Office of Naval Research
Department of Energy, BES

11:51AM M65.00004: Band structure engineering of 2D materials using 1D superlattice*  YUTAO LI (Presenter), SCOTT A DIETRICH, CARLOS FORSYTHE, SHAOWEN CHEN, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, JAMES C HONE, CORY DEAN, Columbia University — Atomically thin 2D materials such as graphene provide promising new platforms to realize synthetic band structures by superlattice (SL) patterning. We exploit our recently developed technique of dielectric superlattices to pattern graphene with a 1D superlattice potential with periodicity as low as 47nm. We observe strong anisotropy in electrical transport features along directions parallel versus perpendicular to the SL basis vector. The main and mini Dirac points, induced by the SL potential, may be “flattened” at certain strengths of SL modulation, leading to an alternating sequence of resistance maxima and minima in the direction parallel to the SL basis vector. Our results establish a multitude of possibilities of band structure engineering on a 2D material under a 1D superlattice potential with possible applications in ballistic electron optics, van der Waal FETs, and plasmonics.

*Office of Naval Research (ONR)
**12:03PM M65.00005: Periodic strain-induced magnetization in graphene over NbSe₂**

ANTONIO MANESCO (Presenter), Kavli Institute of Nanoscience, Delft University of Technology, JOSE L. LADO, Department of Applied Physics, Aalto University, EDUARDO RIBEIRO, GABRIELLE WEBER, DURVAL RODRIGUES JR., University of Sao Paulo — Electronic correlations are known to dramatically impact the electronic properties of graphene in the presence of real or artificial gauge fields, as a consequence of the strongly enhanced density of states. Paradigmatic examples of this include the magnetically-ordered quantum Hall state in monolayer graphene, and the correlated and superconducting phases in twisted graphene multilayers. Motivated by recent experiments, here we explore the emergence of a periodic-modulated magnetization caused by epitaxial-induced strain in graphene stemming from a NbSe₂ substrate. In particular, we show the emergence of a magnetic state induced by the elastic substrate-induced pseudo gauge field, its interplay with the superconducting state of NbSe₂, and the potential tunability of the correlated state by means of external electric and magnetic fields. Our results put forward a hybrid graphene/NbSe₂ heterostructure with tunable correlations, providing a powerful platform to explore correlated physics in hybrid van der Waals materials.

*The work of ALRM was supported by São Paulo Research Foundation Grants No. 2016/10167-8 and 2019/07082-9. DRJ is a CNPq researcher.

**12:15PM M65.00006: Strain tunable magnetotransport study of ABC trilayer graphene/h-BN moiré superlattices**

CHUANKUN LIU (Presenter), RYUICHI TSUCHIKAWA, JAMESON G BERG, VIKRAM V DESHPANDE, University of Utah — The number of atomic layers changes the electronic band structure of graphene dramatically. While monolayer graphene hosts linear bands with massless fermions, trilayer ABC-stacked graphene exhibits a very flat quartic band at the K point and is a particularly suitable platform for strongly correlated physics. When ABC trilayer graphene is aligned with the h-BN layer, the addition of the moiré superlattice can create narrow minibands, and low energy bands can become flat and isolated near charge neutrality. Mott insulating states and unconventional superconductivity have been observed in ABC-TLG/h-BN heterostructures. Perpendicular electric field and strain are important ways to tune these bands. In our work, we have fabricated ABC-TLG/h-BN aligned heterostructures with dual graphite gates, on flexible substrates to apply both perpendicular electric field and intralayer strain onto the device. We study the responses of low energy bands by performing magnetotransport measurements at low temperatures.
12:27PM M65.00007: Interaction-driven broken symmetry states in moiré vdWs heterostructure*  ZHIREN ZHENG (Presenter), THAO H DINH, Massachusetts Institute of Technology MIT, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, SUYANG XU, Harvard university, NUH GEDIK, QIONG MA, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology MIT — The freedom of stacking different layers of 2D van der Waals (vdW) materials with an arbitrary twist angle opens up tremendous opportunities in studying emergent properties that are not accessible in the natural crystal form. In particular, the recently discovered magic-angle twisted bilayer graphene shows that the twist angle and moiré potential can substantially enhance electron correlations for spontaneously broken symmetry states and turn semi-metallic graphene into insulator, superconductor, and quantum anomalous Hall insulator at will. With the right system and careful design, interaction-driven broken symmetry states can have many other manifestations that are not only fundamentally intriguing but also invaluable to new device applications. Here, we report on our design and experimental exploration of a multiferroic system based on moiré vdW heterostructures. Our study will open the door to a new class of 2D multiferroics, which has a potential implementation in many important applications, such as memristive devices for neuromorphic computing.

*The work was partially supported as part of the Center for the Advancement of Topological Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

12:39PM M65.00008: Optical study of electric field tunable 2D semiconductor moiré superlattices  LIZHONG LI (Presenter), YANHAO TANG, KIN FAI MAK, JIE SHAN, Cornell University — Moiré superlattices based on graphene or transition metal dichalcogenide (TMD) heterostructures provide an interesting platform to explore emerging quantum phases in the strong correlation regime. The large electron mass in monolayer TMDs and the lack of magic angle requirement make TMD moiré heterostructures a particularly robust platform for studying problems in strong electron correlation physics[1]. For instance, it has been recently shown that WSe2/WS2 moiré superlattices can simulate the physics of the triangular lattice Hubbard model [2]. Whereas electrostatic doping can continuously tune the filling factor of the system, a vertical displacement field could also effectively tune the relative band alignment of the heterostructure and other important parameters of this strongly correlated system. In this talk, I will discuss our recent optical study on electric field tunable TMD moiré superlattices and the search for novel quantum phases of matter.

12:51PM M65.00009: Charge transfer in transition metal dichalcogenide superlattices and moiré quantum chemistry  YANG ZHANG (Presenter), NOAH YUAN, LIANG FU, Massachusetts Institute of Technology MIT — We theoretically investigate the band structure and interaction effects in moiré superlattices of transition metal dichalcogenides and find the Mott and charge-transfer insulating phases around half filling. The charge transfer length of a charge-transfer insulator can be several nanometers, and the magnetic susceptibility of the Mott insulator is also worked out as a probe for the antiferromagnetic ground state. This highly tunable system provides an ideal platform to simulate diatomic solids under strong interactions.

1:03PM M65.00010: Stokes spectroscopy applied to monolayer MoS$_2$ photoluminescence at room temperature; different helicities observed for A-exciton and A-trion  EHSAN ZOLGHADR (Presenter), SOURAV GARG, PATRICK KUNG, Univ of Alabama - Tuscaloosa, NEWTON MARTINS BARBOSA NETO, Universidade Federal do Para, PAULO T ARAUJO, Univ of Alabama - Tuscaloosa — Strong electron-electron and/or electron-hole Coulomb interactions play important roles in optical transitions in monolayer semiconducting transition metal dichalcogenides (TMDCs). These optical transitions reflect the behaviors of excitons and/or trions. Here, we present our investigation of room temperature Stokes spectroscopy applied to the photoluminescence emitted by a large-area MoS$_2$ monolayer grown by CVD technique standing on a SiO$_2$ substrate. Stokes spectroscopy allows for simultaneous measurement of any helicity, which is advantageous compared to the traditional helicity-resolved photoluminescence measurement. Our results show that the PL emission presents significant amount of circularly polarized light when non-resonantly excited with linearly polarized light at 532 nm. Analyzing the Stokes spectra leads to a deconvolution in which the A-exciton and A-trion peaks have opposite helicities. While the exact valley polarization dynamics and selection rule mechanisms that leads to the optical properties still need to be clarified, this study opens the door for a better understanding of the room temperature exciton and trion physics on monolayer MoS$_2$, an ideal candidate for industrial atomically thin opto-electronic devices such as solar cells and photodetectors.
1:15PM M65.00011: Studying Transition Metal Dichalcogenide Superlattices with nano-ARPES  
CONRAD STANSBURY (Presenter), IQBAL UTAMA, University of California, Berkeley, CLAUDIA FATUZZO, Materials Science Department, Lawrence Berkeley National Lab, CHRIS JOZWIAK, AARON BOSTWICK, Advanced Light Source, Lawrence Berkeley National Lab, JOSÉ AVILA, Synchrotron SOLEIL, ELI ROTENBERG, Advanced Light Source, Lawrence Berkeley National Lab, FENG WANG, ALESSANDRA LANZARA, University of California, Berkeley — Two-dimensional layered materials, especially monolayer transition metal dichalcogenides, have demonstrated lasting impact as a platform for combining and tuning electronic and optical behaviors on the nanoscale. The realization that moiré superlattices in these systems provide tunable control over correlations has sparked renewed interest through analogy to the family of high-temperature superconductors and in light of new phenomena such as moiré excitons. As a complement to modeling, a bottom-up understanding of these phenomena and interlayer hybridization motivates direct measurements of the electronic structures of the host materials. Nano-ARPES enables these experiments on clean, mechanically-exfoliated heterostructures where the impact of substrate and superlattice interaction on the electrons can be fully explored. In this talk, I show how this technique can address basic questions of electronic and structural order in a few model systems: heterobilayer interfaces, and in the interface of TMD monolayers with a substrate. Among the rich phenomena present at the interface, we will focus especially on the presence or absence of hybridization effects in short and long wavelength superlattices.

1:27PM M65.00012: Tip-enhanced nano-imaging of 2D alloy with gradual concentration profile  
HANA HRIM (Presenter), SHARAD AMBARDAR, DMITRI V VORONINE, Univ of South Florida — Systematic optical studies of 2D MoₓW₁₋ₓS₂ alloys, with 0.05≤x≤0.45 grown by chemical vapor deposition (CVD) on Si/SiO₂ were carried out using Raman and photoluminescence (PL) spectroscopy using 532 nm laser. Atomic force microscopy (AFM) imaging showed the correlation with the optical images. We demonstrate nano-optical imaging using tip-enhanced photoluminescence (TEPL) as a function of the composition x for obtaining the higher spatial resolution beyond the diffraction limit. Quantum plasmonic quenching of the TEPL signals was observed for larger x revealing the tunneling electron injection. In order to overcome the problem of excitation efficiency we used a 405 nm laser for TEPL which showed efficient excitation of different x components. Tip-enhanced Raman spectroscopy (TERS) confirms the alloy composition at the nanoscale.
1:39PM M65.00013: Clean 2D superconductivity in a bulk van der Waals superlattice

ARAVIND DEVARAKONDA (Presenter), Department of Physics, Massachusetts Institute of Technology MIT, HISASHI INOUE, Frontier Research Institute of Interdisciplinary Sciences, Tohoku University, SHIANG FANG, Department of Physics and Astronomy, Rutgers University, CIGDEM OZSOY KESKINBORA, Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, TAKEHITO SUZUKI, Department of Physics, Massachusetts Institute of Technology MIT, MARKUS KRIENER, Center for Emergent Matter Science (CEMS), RIKEN, LIANG FU, Department of Physics, Massachusetts Institute of Technology MIT, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University, DAVID CHARLES BELL, Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, JOSEPH G CHECKELSKY, Department of Physics, Massachusetts Institute of Technology MIT — Recent interest in bulk van der Waals systems has been driven by the search for exotic physics in thin flakes exfoliated from bulk crystals and, more broadly, the desire to add novel functionalities to those available in the van der Waals heterostructure toolkit. This top down approach has proved successful in unveiling novel phenomena, the $MX_2$ transition metal dichalcogenides being one such case where both flakes and heterostructures have been used to uncover and design exotic ground states, respectively. However, such devices have intrinsic limitations that can impede powerful experimental probes or prevent the realization of exotic physics in the first place due to disorder introduced through the fabrication process. Here, we report experimental evidence for a possible solution in the form of a bulk single crystal, van der Waals superlattice that simultaneously exhibits high cleanliness and two-dimensional superconductivity.

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Office of Naval Research - N00014-17-12883
U.S. Department of Energy - DE-SC0019300
Gordon and Betty Moore Foundation - GBMF3848

M65.00014: Algorithm on the absolute formation energy of edges in transition metal dichalcogenides

CHUEN KEUNG SIN (Presenter), JUNYI ZHU, Physics, The Chinese University of Hong Kong — Equilibrium shapes are the keys to fully understand the growth dynamics of quasi 2D structures, such as transition metal dichalcogenides. However, the intrinsic complexity of the quasi 2D nature near the edge makes it challenging to formulate successful algorithm with good accuracies. As a result, the theoretical investigations on the growth thermodynamics and kinetics are limited. To solve the fundamental problem, we proposed a new calculation scheme to calculate the formation energy of edges in monolayer MoS$_2$. With the help of electron counting model, we found the proper passivation scheme of pseudo hydrogen on the edge of ribbons and wedges and obtained semiconducting nature with excellent accuracies.

*The research is supported by HKRGC, GRF with the funding number of 14307219.

Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M66 DCMP: Fractons: from symmetry and fractionalisation to dynamics and realisations

Four Seasons 1 - Rahul Nandkishore, University of Colorado, Boulder -
11:15AM M66.00001: Fracton topological order via quantum elasticity duality* [Invited] LEO RADZIHOVSKY (Presenter), MICHAEL PRETKO, MICHAEL A HERMELE, Department of Physics, University of Colorado, Boulder — I will discuss a recent discovery that elasticity theory of a two-dimensional quantum crystal is dual to a fracton tensor and to a coupled-vector gauge theories, thereby providing a concrete realization of the “fracton order” phenomenon. The disclinations and dislocations respectively map onto charges and dipoles of these gauge theories. The fractionalized mobility of fractons matches the constrained dynamics of lattice topological defects. These dualities lead to predictions fractonic phases, and phase transitions to their descendants, that are duals of the commensurate crystal, supersolid, smectic, and hexatic liquid crystals. Extensions of this duality to generalized elasticity theories provide a route to discovery of new fractonic models and their potential experimental realizations.


*Simons Investigator Award from the Simons Foundation

11:51AM M66.00002: Foliated Fracton Order [Invited] XIE CHEN (Presenter), Caltech — The quantum information study of quantum codes and quantum memory has led to the discovery of a new class of exactly solvable fracton models. The fracton models are similar to the better understood topological models in that they also support fractional excitations and have stable ground state degeneracy. But it is also clear that the fracton models exist beyond the realm of conventional topological order due to their extensive ground state degeneracy and the restricted motion of their fractional excitations. In this talk, I will present a new framework, which we call the “foliated fracton order”, to capture the nontrivial nature of the order in a large class of fracton models. Such a framework not only clarifies the connection between various different models, but also points to the direction of search for interesting new features.

12:27PM M66.00003: Fractons: The Road to Reality [Invited] MICHAEL PRETKO (Presenter), University of Colorado, Boulder — In this talk, I will give an overview of progress towards connecting the field of fractons with experiments. I will begin with a brief introduction to fractons, describing some of the models and phenomenology encountered in the field. I will then describe some advances in proposed spin models realizing fracton behavior, along with some experimental diagnostics which are useful for detecting fractons. Finally, I will discuss several new platforms for realizing fracton physics, such as hole-doped antiferromagnets and electric circuits.
Coulomb spin liquids are well studied spin liquid states exhibiting emergent electromagnetism, having a coarse-grained description corresponding to Maxwell’s laws. It has recently been appreciated that even more exotic scenarios are possible, realizing generalizations of electromagnetism with rank-2 electric and magnetic fields. These are of particular interest since the emergent charges of the rank-2 electromagnetism can be fractons, with fundamentally constrained mobility.

In this talk I will describe an approach to finding simple, bilinear models, for classical spins which realize rank-2 Coulomb phases at low temperature [1,2]. Such models provide access to rank-2 Coulomb phase physics in a setting amenable to efficient numerical study and also suggest directions to look for rank-2 Coulomb phases in experiment.

Remarkably, we find that a traceless, vector-charged, rank-2 Coulomb phase can be generated by perturbing a simple Heisenberg model on the pyrochlore lattice with breathing anisotropy and weak Dzyalozhinskii-Moriya interactions [2]. This enables us to identify Yb-based breathing pyrochlores as potential candidate systems and to make explicit predictions for how the rank-2 Coulomb phase would manifest itself in experiment.

Ergodicity-breaking arising from Hilbert space fragmentation in dipole-conserving Hamiltonians* [Invited] FRANK POLLMANN (Presenter), PABLO SALA DE TORRES-SOLANOT, TIBOR RAKOVSZKY, RUBEN VERRESEN, MICHAEL KNAP, Department of Physics, Technical University of Munich — We show that the combination of charge and dipole conservation---characteristic of fracton systems---leads to an extensive fragmentation of the Hilbert space, which in turn can lead to a breakdown of thermalization. As a concrete example, we investigate the out-of-equilibrium dynamics of one-dimensional spin-1 models that conserve charge (total Sz) and its associated dipole moment. First, we consider a minimal model including only three-site terms and find that the infinite temperature auto-correlation saturates to a finite value. The absence of thermalization is identified as a consequence of the strong fragmentation of the Hilbert space into exponentially many invariant subspaces in the local Sz basis, arising from the interplay of dipole conservation and local interactions. Second, we extend the model by including four-site terms and find that this perturbation leads to a weak fragmentation: the system still has exponentially many invariant subspaces, but they are no longer sufficient to avoid thermalization for typical initial states. More generally, for any finite range of interactions, the system still exhibits non-thermal eigenstates appearing throughout the entire spectrum.

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Wednesday, March 4, 2020 11:15 AM - 2:15 PM

Session M67 DCMP: DCMP Prize Session Four Seasons 2-3 - Andrei Rutgers

Oliver E. Buckley Condensed Matter Physics Prize talk [Invited] PABLO JARILLO-HERRERO (Presenter), Massachusetts Institute of Technology MIT — In this talk I will review the discovery of correlated insulator states and superconductivity in magic-angle twisted bilayer graphene, as well as some of the recent developments in the field.
**11:51AM M67.00002: What have we learned from Dynamical Mean Field Theory and what lies ahead?**  
[Invited]  
ANTOINE GEORGES (Presenter), Collège de France, Paris and Flatiron Institute, New York  
— Dynamical Mean-Field Theory (DMFT) provides both an original perspective on the physics of strongly correlated electron materials and an efficient computational framework to understand and predict their properties. In this talk, I will review the main ideas at the heart of the DMFT construction and physical perspective. Through select examples, I will outline how the efforts of a whole community over almost three decades have managed to develop the theory to such a point that it can successfully be applied to a real material, taking into account its structure and chemical composition. I will also outline how the theory is being extended and generalized in many fruitful directions.

*I acknowledge the support of the European Research Council (ERC-319286-QMAC) and the Simons Foundation.

**12:27PM M67.00003: Towards a Theory of Strongly Correlated Materials the Dynamical Mean Field Theory Road**  
[Invited]  
GABRIEL KOTLIAR (Presenter), Condensed Matter Physics, Brookhaven National Laboratory  
— Strongly correlated electron materials pose great conceptual and computational challenges. Dynamical Mean Field Theory (DMFT) has enabled a community of scientists to achieve great progress in this area. We will review some basic ideas underlying this approach, such as the reduction of the full many body problem into a quantum impurity model satisfying a self consistency condition. We will then provide some examples from materials containing elements from different regions of the periodic table, ranging from 3d's(*) to 5f's(**) of how DMFT ideas and implementations in combination with electronic structure methods have enabled predictions in materials which were not tractable by other methods, work under way to overcome its limitations(*) and point towards great challenges ahead.

*  
(*) work supported by the NSF DMR-1733071  
(**) work supported by DOE BES E-FG02-99ER45761  
(*)This work was supported by the Computational Materials Sciences Program funded by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
There has been great interest in the development of composite optical materials and metamaterials for applications in modern optical technology. Materials with a strongly nonlinear response are required for many applications, and especially in photonics for processes such as all-optical switching. It is of particular interest to design composite structures that enhance the value of the third-order optical susceptibility $\chi^{(3)}$. Under ideal conditions, this composite $\chi^{(3)}$ can exceed the $\chi^{(3)}$ values of the constituents of the composite [1]. This enhancement of the nonlinear response can be understood as a consequence of the judicious use of local field effects [2]. Enhanced nonlinear response of composite materials and structures has been demonstrated for a variety of materials [3-7]. Recent work has shown an additional means of enhancing the nonlinear optical response by making use of a material that possesses a vanishingly small electric permittivity at the wavelength of interest. Such materials are known as epsilon-near-zero (ENZ) materials [8], and they have been observed to display extremely large values of the $\chi^{(3)}$ response [9]. These materials, on their own or when incorporated into metasurfaces [10], hold great promise for high-speed, all-optical switching applications and operate with minimal power requirements.


We first review the recent developments and novel applications for space-time-frequency metasurfaces. Then we outline hybrid, plasmonic-photonic meta-structures for quantum information systems and discuss a new approach for high-speed quantum photonics operating at THz rates. The use of plasmonics to optimize light-matter coupling and speed-up quantum processes so that they outpace quantum decoherence and losses will be also discussed.
11:15AM M68.00001: Three-dimensional imaging of force-generating molecular networks inside of cells using cryo-electron tomography [invited] MATTHEW SWULIUS (Presenter), Pennsylvania State University — Dynamic networks of cytoskeletal polymers commonly take part in generating fundamental cellular forces. In order to understand the mechanical role of these cytoskeletal networks in development and disease, multimodal information across multiple dimensions and scales need to be integrated. In this presentation, I will briefly overview the protein components that make and regulate these cytoskeletal networks, and talk about how my lab is using live-cell imaging and cryo-electron tomography to study these molecules in the context of neuronal outgrowth.

11:51AM M68.00002: Opening a new window into the cell with super-resolution imaging and in situ cryo-electron tomography* [invited] STEPHEN CARTER, California Institute of Technology, CHERI HAMPTON, ROBERT LANGLOIS, Columbia University, ROBERTO MELERO, Centro Nacional de Biotecnología, ZACHARY FARINO, MICHAEL CALDERON, Univ of Pittsburgh, WEN LI, Columbia University, CALLEN WALLACE, Univ of Pittsburgh, ROBERT GRASSUCCI, Columbia University, WILLIAM RICE, New York Structural Biology Center, MEIR ARIDOR, KENNETH FISH, Univ of Pittsburgh, DEBORAH FASS, SHARON WOLF, Weizmann Institute, SIMON WATKINS, Univ of Pittsburgh, JOSE MARIA CARAZO, Centro Nacional de Biotecnología, GRANT JENSEN, California Institute of Technology, JOACHIM FRANK, Columbia University, ZACHARY FREYBERG (Presenter), Univ of Pittsburgh — Super-resolution light and electron microscopy have revolutionized our ability to visualize cell machinery. We use live-cell super-resolution imaging including stimulated emission depletion (STED) microscopy together with highly inclined thin illumination (HiLo) and high-speed three-dimensional widefield imaging to visualize organelle dynamics in real time. We have integrated these approaches with in situ cryo-electron tomography (cryo-ET), and cryo-correlative light and electron microscopy (cryo-CLEM) to visualize the endoplasmic reticulum (ER) and its relationships with other intracellular organelles in near-native states. The combination of these methods has revealed a novel ER-derived compartment that is mobile, vesicular, and associated with mammalian 80S cytoplasmic ribosomes. Moreover, with cryo-focused-ion-beam (FIB) milling and cryo-ET, we show that these vesicles exist as discrete structures separate from the intact reticular ER architecture. We call these organelles Ribosome-Associated Vesicles (RAVs). Detailed characterization of the RAVs revealed that these structures are conserved across multiple cell types and species using both conventional transmission electron microscopy (TEM) and cryo-ET.

12:27PM M68.00003: Automatic analysis of cryo-electron tomography using computer vision and machine learning* [Invited] XIANGRUI ZENG, XU MIN (Presenter), Carnegie Mellon Univ — Cryo-electron tomography (cryo-ET) is an emerging technology for the 3D visualization of structural organizations and interactions of subcellular components at near-native state and submolecular resolution. Tomograms captured by cryo-ET contain heterogeneous structures representing the complex and dynamic subcellular environment. Since the structures are not purified or fluorescently labeled, the spatial organization and interaction between both the known and unknown structures can be studied in their native environment. The rapid advances of cryo-electron tomography (cryo-ET) have generated abundant 3D cellular imaging data. However, the systematic localization, identification, segmentation, and structural recovery of the subcellular components require efficient and accurate large-scale image analysis methods. We developed and adapted a suite of computer vision and machine learning methods for such analysis.

*This work was supported in part by U.S. National Institutes of Health (NIH) grant P41 GM103712. XZ was supported by a fellowship from Carnegie Mellon University's Center for Machine Learning and Health.

1:03PM M68.00004: Visualizing mitochondrial division machinery in situ [Invited] DANIELLE GROTJAHN (Presenter), Department of Integrative Structural and Computational Biology, The Scripps Research Institute — Mitochondria are dynamic organelles that serve a variety of metabolic roles for eukaryotic cells, including ATP generation and cell signaling. Unlike other organelles, mitochondria cannot be produced “de novo”, and instead rely on a tightly regulated division process called “fission”, which functions as a quality control mechanism to maintain a healthy population of mitochondria. However, several cellular stress pathways promote hyperactivation of the mitochondrial fission pathway that fragment the mitochondrial network and induce cell death (apoptosis). Despite increasing evidence that mitochondrial fragmentation is a hallmark feature of many neurodegenerative diseases, the molecular mechanisms that contribute to the mitochondrial fission process remain poorly defined. We recently developed a three-dimensional imaging approach using a combination of cryo-focused ion beam milling and cryo-electron tomography to visualize snapshots of mitochondrial constriction events in mammalian cells. Our three-dimensional reconstructions represent the highest resolution structures of the ultrastructural interactions between mitochondria and other subcellular components to date, enabling unprecedented analysis of these associations. Further analyses reveal that the endoplasmic reticulum and the cytoskeleton preferentially associate with mitochondrial membrane constrictions. Interestingly, we also observe the presence of a previously unidentified filamentous structure in association with dividing mitochondria, which we propose is a member of the septin family of intermediate cytoskeletal filaments. By mapping out the precise interactions of these components relative to mitochondrial membranes, our work describes the complete ultrastructural architecture of the mitochondrial fission machinery required for membrane constriction, and establishes cellular tomography as a valuable approach for studying snapshots of mitochondrial dynamics in situ.

1:39PM M68.00005: Anthony Fitzpatrick Invited Talk [Invited] —
Wednesday, March 4, 2020 11:15 AM - 12:03 PM

Session M70 DCMP FED DCOMP: Physics Outreach, Education and Society 208 - Jessica Thomas, American Physical Society - Tag(s): Education, Outreach, Undergrad Friendly

11:15AM M70.00001: Design and implementation of professional development workshops that support women in STEM in Tanzania*  JILL WENDEROTT (Presenter), Materials Science and Engineering, Northwestern University, JOYCE ELISADIKI, Physics, University of Dodoma — Women, particularly at the graduate and professional levels, are underrepresented worldwide in STEM fields. Empowering younger women at the secondary- and undergraduate-level to pursue STEM as a career path, as well as providing organizational tools for women in STEM once at the university level, can help to improve their retention and long-term representation in STEM fields. To meet the aim of encouraging women in STEM globally, the women supporting women in the sciences (WS2) program was developed as between Northwestern University graduate Society of Women Engineers (NU GradSWE) and graduate women in STEM from several Tanzanian universities. The first objective of the WS2 program was to build professional development workshops for women in STEM in Tanzania focused on (1) career development and (2) organizing as women in STEM. To this end, two workshops were created collaboratively via virtual meetings between NU GradSWE and Tanzanian volunteers. The workshop content was then taught online to prospective facilitators from Tanzania, with the hope to pilot the workshops in Tanzania in early 2020. This talk will discuss the stages of professional development workshop creation, as well as anticipated outcomes and long-term goals of the program.

*NSF DMR-1720139
InclusionNU Fund

11:27AM M70.00002: A Free Renewable Energy-based Physics Day Camp for Middle School Girls*  ROBERTO RAMOS (Presenter), University of the Sciences — On its seventh year, the Physics Wonder Girls Program¹ provided a free, novel renewable energy physics-based immersion experience to two cohorts of middle school girls selected from a pool of high-performing students in the Philadelphia-New Jersey area. The girls came from diverse communities, including underserved school districts. Girls were introduced to the theme of renewable energy, took a crash course on circuits using solar cell kits, and then built and raced solar cars, and solar boats on a portable pool. They compared the efficiencies of silicon cells versus organic solar cells, built solar cells based on dyes from raspberry and blackberry fruit, and used a thermal imager to audit heat leaks. They explored wind power using model turbines, digital anemometers, and a commercial turbine. They met women physicists engineers from the local food industry, toured a local food company and presented demonstrations to a community of friends and teachers.

¹Web: https://sites.google.com/usciences.edu/physicswondergirlscamp/

*R.C. Ramos acknowledges support from Constellation - an Exelon company, and Puratos Corporation
Scientists in Public Service: Running for office as a STEM candidate

SHAUGHNESSY NAUGHTON (Presenter), 314 Action — The Washington Post declared 2018 the “Year of the Scientist Running for Office.” But despite scientifically and technologically complex challenges facing elected officials, public service is still a rare path for scientists. This session seeks to demystify the ways that scientists at all levels can engage in the democratic process, from casting a ballot to being on the ballot themselves. Participants will learn what it is like to run for office and to better understand the unique barriers to entering into politics as scientists. They will engage with scientists who have first-hand experience running for office, and leave with concrete ideas about getting involved in the 2020 elections.

314 Action is the scientific community’s premier organization in electoral politics—recruiting and training scientists to run for office, uniting the community in support of STEM based candidates and working to challenge and hold accountable politicians who base policy on ideology rather than evidence.

Through its nonpartisan trainings, 314 Action has trained 1,500 scientists to run for office since 2017.

In 2018 a record number of scientists were elected to office: nine new and seven incumbent STEM Members of the 116th Congress and 35 STEM members to state legislatures across the country.

Making a basic mathematics course compulsory for everyone studying science at pre-college and college level

PRITAM MANDAL (Presenter), Durgapur Women's College — From a study based on personal teaching experiences and one-to-one and in-group interaction with a large number of students (9th to 12th Grade and UG levels) and teachers across India, we found that science students not having mathematics in their subject combination, suffer from physics-phobia.

In pre-college programs (at 11th and 12th grades) when students are first exposed to “real” science curriculum (with Physics, Chemistry, Mathematics, Biology and Computer Science), many students in India do not take up mathematics, having the option to rule out mathematics as they aspire to be medical doctors or biologists. Students are moulded into the mindset that to study biology or medical science in future, mathematics is useless. These students take admission into 11th grade with a pre-installed idea that mathematics would be an extra burden on their pathways to become biologists or doctors.

As a consequence these non-maths students severely suffer in physics classes and start viewing physics as a dry, calculation-based abstract subject, missing out the true beauty and essence of physics.

We suggest a compulsory basic mathematics course for everyone studying science at the 11th-12th grade as well in UG level in India to build better citizens of science.

Wednesday, March 4, 2020 11:15 AM - 11:15 AM
M71.00002: A Novel Focused Electrohydrodynamic Printing Method

MATTHEW STROHMAYER (Presenter), ATUL DHALL, PUJHITHA RAMESH, NATALYA TOKRONOVA, CARL VENTRICE, SUNY Polytechnic Institute — The main advantages of additive manufacturing include limited waste and the ability to build complicated structures. Recently, a cost-effective, versatile method of high-resolution printing called electrohydrodynamic (EHD) printing has been introduced. This method allows for spatial resolution in the hundreds of nanometers. This process works similarly to a typical ink jetting system, except instead of the ink/polymer being pushed out of a tip, it is pulled out by an applied electric field allowing for the resultant droplet to be much smaller than the needle diameter. EHD systems are typically used in a drop-on-demand mode. Although operating in a continuous spray mode will increase throughput, its resolution is limited because of electrostatic repulsion between the drops. To overcome this limitation, we have incorporated an Einzel lens into the system to focus the droplets. To validate this approach, simulations were performed to test for different parameters, including droplet size changes and lens optimization. These parameters were then used to build a real system. This printhead system was then characterized for how well it performed. This includes comparisons of line widths of different focusing voltages.

M71.00003: 3D printed Liquid Crystal Elastomer mechanical devices*

DEVESH MISTRY (Presenter), NICHOLAS TRAUGUTT, ROSS VOLPE, SABINA ULA, CHRISTOPHER YAKACKI, University of Colorado, Denver — 3D printing allows the creation of macro-sized Liquid Crystal Elastomer (LCE) devices.[1,2] Here we show 3 cm-scale 3D printed mechanical LCE devices. The 1st project is a dynamically crystallizing LCE spinal fusion cage designed to treat degenerative disc disease (DDD). Compared to existing devices, our device conforms to the vertebral endplates and provides a large surface area and minimizes stress concentrations – thus minimizing the chance of conditions such as subsidence and adjacent level disease.

The 2nd project explores the structure property relationships of anisotropic dissipative LCE devices. Using these materials and techniques we demonstrate a prototype total disc replacement device that offers same functionality as the natural intervertebral disc.

The third project demonstrates highly dissipative and rate dependent LCE lattice structures created via digital light processing (DLP) printing. Compared to DIW, DLP printing allows us to create complex overhanging geometries with micron-resolution. The high rate dependency of our LCE resin means our devices provide effective shock absorbance over range of impact speeds.


*Lindemann Fellowship, Army Research Office (125786)
M71.00004: Effect of Post-Processing on Thermo-Mechanical Properties of a 3D-Printed UV-Curable Polymer  
KATHERYN HUSMANN (Presenter), BRANDON MCREYNOLDS, STEPHAN COMEAU, JOHN MCCOY, New Mexico Tech, ALEXANDRIA N. MARCHI, Los Alamos National Laboratories — The effect of UV and thermal processing on the properties of a UV-curable polymer fabricated with 3D printing was studied. The polymers studied were proprietary methacrylate based resins (Formlabs) and samples were printed directly in test geometries. Uniaxial compression tests at room temperature were performed for Young's modulus, Poisson's ratio, and yield stress. Thermal tests using a Differential Scanning Calorimeter (DSC) described the glass transition temperature range, physical aging and (additional) high-temperature reactions of the samples. Post-processing consisted of either additional UV exposure time or high temperature "soak" time (or both). These indicated that post-processing has a pronounced effect on the mechanical and thermal properties. Both aspects of post-processing (UV and high-T soaks) increase the yield stress, the modulus and the glass transition. Combining high-T soaks with additional UV exposure is particularly effective.

* Los Alamos National Laboratories

M71.00005: Competition between Phase Separating and UV Curing Kinetics during Photopolymerization-Induced Phase Separation in Confined Resin Films  
ANNA SMALLWOOD (Presenter), OLIVIA T. SHERMAN, CHANG RYU, Chemistry and Chemical Biology, Rensselaer Polytechnic Institute — Polymerization-induced phase separation is the segregation of agents in a multicomponent mixture triggered by polymerization to convert low molecular weight (MW) monomers into high MW polymers or networks. Several factors control the nature and structure of polymerization-induced phase separation, including blend composition, molecular weight of the phase separation agent, and polymerization kinetics of the monomers. When properly controlled, these factors can dictate a specific morphology of the resulting structure, allowing for tuning of characteristics of the resulting network. This study seeks to investigate these factors during photopolymerization-induced phase separation. Real-time turbidity to measure UV light transmittance through a blend sample of predetermined thickness will be employed as the main tool to monitor the phase separation process during UV irradiation. UV LED intensity and wavelength, resin reactivity, and end functionality of polymer additives will be studied to investigate the effect of each on the phase separation process and resulting network morphology within the confined space of UV-curable resin films. Scanning electron microscopy and other microscopy tools will be used for the study of morphology for the photopolymerization-induced phase separation.
**M71.00006: Triplet Triplet Annihilation Polymerization for High Resolution 3D Printing**

DAVID LIMBERG (Presenter), JI-HWAN KANG, RYAN HAYWARD, Univ of Mass - Amherst — Two-photon polymerization (TPP) offers by far the highest spatial resolution (< 1 μm) of current 3D printing methods, but suffers from limited volumetric write speeds compared to conventional stereolithography and requires the use of pulsed laser sources. Here, we demonstrate a new method of high-resolution 3D printing using triplet-triplet-annihilation (TTA) that achieves sub-micron resolution while maintaining high throughput and requiring only a light emitting diode (LED) source with an intensity six orders of magnitude lower than typically required for TPP. We demonstrate a robust 3D printing mechanism capable of printing a diverse array of materials with high resolution, low surface roughness, and high write speeds, without requiring high-intensity pulsed laser illumination.

*ARO grant W911NF-19-1-0348

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**M71.00007: Digital Printers and Image Quality**

SURESH AHUJA (Presenter), xerox corporation — Photoreceptor is a central device in digital printers. The outer layer, Charge Transport Layer made up of polycarbonate and Charge Transport Molecule is prone to abrasion by stresses of developing system or cleaning system when it is repeatedly used in printing process. The abrasion of the photoreceptor causes deterioration of electrical properties such as lowering sensitivity or lower charging and results in irregular image such as lower image density and image stain. Single and multiple coating were made with filled and unfilled binder polymers and their modulus and hardness were measured by nano-indenter. The effect of the nanoparticles on composite modulus is dependent on many variables particularly on the morphology of the polymer matrix as well as the interaction between the filler and matrix. The state of dispersion depends on balance of repulsive and attractive forces. on the particles.. Charge Transport Molecule reduced modulus and hardness thus increasing photoreceptor wear rate. Nano-filler silica in the polymer either polycarbonate or polyester increased modulus and hardness with higher photoreceptor life.

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**M71.00008: Immersion Precipitation 3D Printing (ip3DP)**

RAHUL KARYAPPA (Presenter), MICHINAO HASHIMOTO, Singapore University of Technology and Design — We present a novel method of 3D printing to fabricate micro-to-nanoporous 3D models in one-step, which we termed immersion precipitation 3D printing (ip3DP). Methods to impart porosity to 3D printed objects have been limited to date. Addition of sacrificial materials to printing materials, followed by their removal, are the established approaches, but such approaches require post-processing to impart porosity. Solvent-cast 3D printing (SC3DP), which is direct 3D printing of polymer inks with in situ evaporation of solvents, has allowed fabricating 3D porous structures with stringent requirements of rheological properties of the printing ink (e.g., high viscosity and high vapor pressure). We developed an alternative approach to print polymeric inks directly in a bath of a nonsolvent and solidified them in situ via immersion precipitation. The porosity of the 3D printed objects was readily controlled by the concentrations of polymers and additives, and the types of solvents. This work is the first demonstration of three-dimensionally controlled immersion precipitation based on digitally controlled depositions of polymer solutions. Wide selection of printable materials, and the ability to tailor their morphologies and properties, make ip3DP a versatile method of 3D printing.
M71.00009: 3D Printing with Waste High-Density Polyethylene  
ANIKET GUDADHE, NIRMALYA BACHHAR, Polym Sci Engg, Natl Chem Lab, ANIL KUMAR, PREM ANDRADE, Ansys, GURUSWAMY KUMARASWAMY (Presenter), Indian Inst of Tech-Bombay — HDPE has widely been considered to be impossible to 3D print using fused filament fabrication (FFF). When HDPE is FFF printed, the printed object warps significantly and debonds off the print substrate. Therefore, it is difficult to preserve registry as the polymer filament is laid down layer by layer during FFF. We demonstrate a strategy for FFF of waste-derived HDPE. There are two aspects to our approach. (i) We formulate the HDPE by blending with dimethyl dibenzylidene sorbitol (DMDBS), that forms a nanofibrillar network in the HDPE melt as it cools and (≈ 10%) linear low density polyethylene (LLDPE). (ii) We use a thin “brim” around the printed object that helps it adhere to the print substrate using common paper glue. This dramatically reduces warpage, allowing FFF of HDPE objects with complex geometries. FEM simulations indicate that our approach decreases the stresses that develop due to crystallization induced shrinkage during cooling. Given the volume of HDPE that finds its way to the waste stream, our results have important implications for extending the use life of HDPE.

*Dept of Sci. and Tech.

M71.00010: Printing Resolution and Depth-Of-Cure Study For Stereolithography 3D Printing Resins  
KEITH DAVID DENIVO (Presenter), ANNA SMALLWOOD, CHANG RYU, Rensselaer Polytechnic Institute — Stereolithography (SLA) is a method of 3D printing of polymer resins using photoinitiated polymerization. Polymer thermosets with crosslinked networks are being formed in SLA. We have studied how the characteristics of SLA photocurable resins affect the 3D printing resolution and mechanical properties. Characteristics include the viscosity and the depth dependent UV polymerization kinetics. Real time FTIR with attenuated total reflectance sample stage was used to thoroughly study the UV penetration depth effects on the photopolymerization kinetics in terms of the rate of polymerization, on-set time for photopolymerization and monomer conversion. Three types of commercially available SLA resins are compared for the printing resolution and depth-of-cure characteristics. Additional tuning of depth-of-cure characteristics has been performed by mixing additional photoinitiator or inhibitor for the investigation of 3d printing resolution studies. Controlled post UV-curing is also performed to further manipulate their mechanical properties with an aim to elucidate how the network structure in SLA samples affect the stress-strain behavior of thermosets under tensile elongation. The layer curing process and morphology has been also investigated by DSC and microscopy techniques.
M71.00011: Geometrical and Mechanical Characterization of Interlayer Bonding Quality in Fused Filament Fabrication* LICHEN FANG, YISHU YAN, OJASWI AGARWAL, Johns Hopkins University, JONATHAN SEPPALA, National Institute of Standards and Technology, KEVIN J. HEMKER, SUNG KANG (Presenter), Johns Hopkins University — To obtain a fundamental understanding of the large variation of mechanical properties and geometry of printed parts prepared by fused filament fabrication (FFF), we focused on the interlayer bonding region of polycarbonate samples prepared by FFF and performed 3D geometrical characterizations using micro-CT followed by uniaxial tensile tests. The results showed significant property variations depending on printing conditions. Specifically, the layer height impacted bonding area. In addition, there was an almost linear relation between bonding zone area and fracture strength. However, when nozzle temperature increased, the strength showed a rising trend first then reached plateau. Interestingly, we also found a trend of Young's modulus reduction with higher layer height, which could be explained by finite element simulations based on scanned sample geometries, indicating the bonding zone geometry change is the main reason of modulus variation. We envision that our findings can guide the selection of printing parameter as well as provide benchmark data for future simulation models.

*We acknowledge the support of the National Science Foundation (DMREF- 1628974) and the start-up fund from the Whiting School of Engineering at Johns Hopkins University.

M71.00012: Study of the end-to-end probability distributions of low-molecular weight, aqueous polyethylene oxide solutions using experimental DEER measurements and molecular dynamics simulations* NICK SHERCK, THOMAS WEBBER (Presenter), DENNIS ROBINSON BROWN, Chemical Engineering, University of California, Santa Barbara, TIMOTHY KELLER, Chemistry and Biochemistry, University of California, Santa Barbara, JACOB MONROE, Chemical Engineering, University of California, Santa Barbara, MIKAYLA BARRY, Materials, University of California, Santa Barbara, RACHEL A SEGALMAN, GLENN H FREDRICKSON, SCOTT SHELL, Chemical Engineering, University of California, Santa Barbara, SONGI HAN, Chemistry and Biochemistry, University of California, Santa Barbara — Low molecular weight, dilute, aqueous polyethylene oxide (PEO) chain end-to-end distance ($R_{ee}$) probability distributions, $P(r)$, were measured experimentally and calculated from simulation, filling a fundamental gap in the existing literature for one of the most widely used water soluble polymers. The distributions were measured by Double Electron Electron Resonance (DEER) spectroscopy, resolving the full $P(r)$ distribution within the technique's range of validity (~2-9 nm). The DEER technique uses small spin probes conjugated to the polymer ends. The probes in simulation are observed to hydrophobically aggregate below the range accessible to DEER (<1.5 nm), with the perturbation to the distributions dropping off rapidly with molecular weight. The distributions and their average $R_{ee}$ indicate aqueous PEO is a semi-flexible polymer in good solvent. The average $R_{ee}$ exhibits excluded volume scaling with molecular weight above the Kuhn length (~0.96 nm), which is quantitatively consistent with scattering data from high molecular weight (>10kDa) PEO.

*This work was supported as part of the Center for Materials for Water and Energy Systems (M-WET), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0019272
M71.00013: PEO-Sn Nanofibers* MATAZ ALCOUTLABI (Presenter), MAXIMILIANO AGUILAR ALONSO, MOHAMMED UDDIN, BRYAN HOKE, FRANCISCO DESANTIAGO, ELAMIN IBRAHIM, JUAN HUITRON, MIRCEA CHIPARA, University of Texas Rio Grande Valley — Polyethylene oxide (PEO) nanofibers loaded by various concentrations of Sn have been obtained by force spinning. Homogeneous solutions of PEO in deionized water, with concentrations ranging between 8 and 12 % wt. PEO have been prepared. Various amounts on Sn nanoparticles have been added to these solutions. The as-obtained mixtures were homogenized by stirring 4 h, at room temperature and 1,000 rotations per minute and then subjected to the force spinning, at room temperature, and various spinning rates ranging between 1,000 and 9,000 rotations per minute. The structure and morphology of mates of PEO based nanofibers loaded by various amounts of Sn nanoparticles and of the corresponding thick films were investigated by Raman, FTIR, X-Ray, and UV-Vis spectroscopy. The effect of the concentration of the nanofiller on the position of Raman and FTIR lines was analyzed in detail and related to the elastic features of these nanocomposites. The differences between mats and macroscopic samples (thick films) are discussed in detail. Additional X-Ray data focused on the crystal structure including crystallites sizes and orientations are reported.

*Authors acknowledge the Department of Defense W911NF-15–1–0063 and the NSF DMR-1523577 grants.

M71.00014: Unraveling the Morphological Evolutions during Solvent Vapor Annealing for Organic Solar Cells Using in situ Resonant Soft X-Ray Scattering WENKAI ZHONG (Presenter), ISVAR CORDOVA, YUFENG JIANG, CHENG WANG, Lawrence Berkeley National Laboratory, FENG LIU, Shanghai jiaotong University, THOMAS RUSSELL, Lawrence Berkeley National Laboratory — Solvent vapor annealing (SVA) is one of the most effective pre-electrode deposition techniques, which has been applied in many efficient organic solar cells. In current research, we used a customized in situ multimodal system to reveal the dynamics of phase separation inside the bulk-heterojunction thin films during SVA via resonant soft x-ray scattering (RSoXS). Solvent-vapor-induced molecular crystallization is of importance to provide the driving force of the domain generation and evolution processes. However, with the introduction of solvent vapor for a long time, coarsening of the film appeared at the film surface, which led to the deteriorating of the device performances. These results indicated that in situ RSoXS is a quite useful technique to bridge the gap to understand the relationship of film growth mechanisms and device efficiency.
M71.00015: The Effect of Electrostatic Interactions on the Interfacial Adsorption and Covalent Reaction of Coiled Coil Bundles  
MATTHEW LANGENSTEIN (Presenter), DARRIN JOHN POCHAN, Univ of Delaware, JEFFERY G SAVEN, Chemistry, University of Pennsylvania, CHRISTOPHER J. KLOXIN, Univ of Delaware — Coiled coil bundles (CCBs), known as bundlemers, are a series of computationally designed peptides that self-assemble in water into monodisperse nanoparticles with tunable surface chemistry. We have shown CCB viability as molecular building blocks by producing predesigned 2D lattices, nanocages, and nanotubes through tailoring their surface chemistry and solution assembly conditions. Recently, we have used CCBs as macromonomers to create stiff extremely high aspect ratio supramolecular polymers through covalent chemistry between CCB ends. As the CCB library continues to grow, it’s important to develop processing methods to grow new nanostructures out of these versatile building blocks. By first templating a surface through the directed self-assembly of CCBs onto a flat planar substrate, it should be possible to grow CCB nanoforests of highly aligned nanorods with tunable surface chemistry and packing structure. Ongoing work on the formation of the template layer has shown a dependence between deposition kinetics and electrostatic interactions between CCBs. This presentation will overview the impact of pH, ionic strength, and CCB surface charge on deposition kinetics as well as show the stages of CCB deposition through a combination of AFM, QCM-D, and reflectivity measurements.

M71.00016: Development and use of a new model for the Worm Like Chain  
ANGELO SETARO (Presenter), PATRICK UNDERHILL, Rensselaer Polytechnic Institute — The behavior of polymers is determined in large part by their flexibility. Nestled between the rigid and flexible limits are semiflexible polymers, whose behavior is distinct from either of the aforementioned regimes. Whereas the rigid limit is defined by bending energetics and the flexible limit is defined by conformational entropy, the behavior of semiflexible polymers is typified by the interplay of both phenomena. This makes their behavior incredibly rich, but also incredibly difficult to model. At present, models exist to study polymers at very fine (e.g. Kratky-Porod) and very coarse (e.g. Marko-Siggia) length scales. Though efforts have been made to decrease the gap between these two modeling approaches, these still exists a length scale over which no good model currently exists. To address this modeling limitation, we utilize a different approach to develop a model for the Worm Like Chain that reproduces some of the essential behavior of the Kratky-Porod model, while being coarse grained enough to allow for study of semiflexible polymers on longer timescales and under non-equilibrium conditions.
M71.00017: Enrichment and Distribution of Pb\(^{2+}\) Ions in Zwitterionic Poly(cysteine methacrylate) Brushes at the Solid-Liquid Interface  QIMING HE (Presenter), University of Chicago, YINJUN QIAO, Tsinghua University, WEI CHEN, Argonne National Laboratory, MATTHEW TIRRELL, University of Chicago — We prepared cysteine-based (PCysMA) polyzwitterionic brushes, and surface zeta potential investigations on pH-responsiveness of these PCysMA brushes confirm their zwitterionic character at intermediate pH range, while at pH values either below pH 3.50 or above pH 8.59, they exhibit polyelectrolyte character. Under acid (pH < 3.50) or base (pH > 8.59) conditions, they possess either cationic or anionic character, respectively. In the zwitterionic region, these PCysMA brushes show positive surface zeta potential in the presence of Pb(CH\(_3\)COO)\(_2\) solutions of various concentrations. The results are in line with microscopic investigations using anomalous X-ray reflectivity (AXRR) carried out along the absorption edge of Pb\(^{2+}\) ions. By varying the photon energies around the absorption L\(_3\) edge of lead (13037 eV), the Pb\(^{2+}\) concentration normal to the silicon substrates, as a function of depth inside PCysMA brushes, could be revealed at the nanoscale. Both zeta potential and AXRR measurements confirm the enrichment of Pb\(^{2+}\) ions inside PCysMA brushes, indicating the potential of PCysMA to be used as a water purification material.

M71.00018: Oligomeric Cellulose Based Block Copolymer  XIN ZHANG (Presenter), FENG JIANG, ROBERT BRIBER, HOWARD WANG, University of Maryland, College Park — Novel water soluble block copolymer based on oligomeric cellulose and PEG was produced by coupling reaction. The oligomeric cellulose was produced by phosphoric acid assisted hydrolysis with PDI of 1.04 and a degree of polymerization of 7 (DP7). The DP7-b-PEG-b-DP7 triblock copolymer showed tunable PEG crystallization behavior by changing the molecular weight ratio between PEG and cellulose. At Mw ratio of 1:2:1, the PEG crystallization is fully suppressed. The morphologies of DP7-b-PEG-b-DP7 triblock copolymer solutions and film are also presented. The synthesis route can be extended to non-PEG based polymers.
M71.00019: Resistive Pulse Sensing of Phytoglycogen Nanoparticle Translocation: Examining Structure and Brownian motion* WILLIAM R LENART (Presenter), MICHAEL HORE, Macromolecular Science and Engineering, Case Western Reserve University — Dendrimers are an important platform for a variety of applications such as cosmetics, lubricants, and drug delivery. Understanding the relationship between structure, mobility, and mechanical properties is crucial for designing new systems for these applications. In particular, examining the transport of nanoparticles (NPs) through nanopores and nanochannels by translocation may enable high-throughput analysis of these properties. These measurements track ionic current through the nanochannel, which is blocked when a particle occludes the channel. Here, we studied experimentally the translocation of phytoglycogen NPs through single solid-state SiNx nanochannels with diameters between 40 and 100 nm, and lengths of 100 nm. Using Poisson-Nernst-Planck calculations, we quantitatively predicted the magnitude of the current blockade of phytoglycogen NPs by including a “hardness parameter” term to describe the degree to which the NPs occlude the nanochannel, and found good agreement with neutron scattering measurements. The NPs diffused through the nanochannels under pure three-dimensional Brownian motion, and diffusion coefficients were measured in quantitative agreement with dynamic light scattering.

*This work was supported by the NSF Polymers program (DMR-1651002).

M71.00020: A photo-responsive protein-polymer bioconjugate for control of a model protein JUSTIN HORN (Presenter), CHEN CHEN, ALLIE OBERMEYER, Columbia University — Stimuli-responsive bioconjugates have been investigated as a means of controlling protein behavior through conjugation of a responsive polymer to a protein. These bioconjugates have been used in many applications including purification and recovery of proteins, biosensing, and control over protein oligomer formation. We have prepared stimuli-responsive bioconjugates to provide spatiotemporal control over enzymatic activity through a covalently linked photo-responsive copolymer. Photo-responsiveness was conferred through an azobenzene-containing monomer which undergoes a light-induced cis-trans isomerization. Controlled radical polymerization was used to create a panel of polymers of varying size and azobenzene monomer content which was assayed for its ability to allow photo-control using a model protein, alkaline phosphatase (phoA). Site-specific bioconjugation of these photo-responsive polymers was achieved through introduction of a cysteine residue to wild-type phoA which reacted with the maleimide-functionalized responsive polymer. In addition to screening the influence of polymer size and composition, several conjugation sites on the protein were tested to probe the effect of distance to the active site on photo-responsivity.
M71.00021: Secondary structure drives self-assembly in weakly segregated globular protein-rod block copolymers*  HELEN YAO (Presenter), Massachusetts Institute of Technology MIT, KAI SHENG, The Scripps Research Institute, JIALING SUN, SHUPENG YAN, YINGQIN HOU, HUA LU, Peking University, BRADLEY OLSEN, Massachusetts Institute of Technology MIT — Protein-polymer bioconjugates combine protein functionality with polymer material properties and block copolymer self-assembly. The effect of polymer block secondary structure and chirality on solution-state self-assembly was studied using bioconjugates with a globular protein block (enhanced green fluorescent protein, or eGFP) and a poly(amino acid) (PAA) block with varying chirality. Block copolymers were synthesized by NCA polymerization, followed by native chemical ligation to eGFP. Homochiral $L$- and $D$- type PAAs formed $\alpha$-helices, while an achiral random copolymer of $L$- and $D$- type monomers was structureless. All bioconjugates with an $\alpha$-helical block self-assembled into lamellae with similar phase diagrams regardless of chirality type. However, bioconjugates with an achiral block remained disordered at all concentrations and temperatures measured. This was due to a non-repulsive interaction between the flexible achiral PAA and eGFP. Thus, incorporation of secondary structure into the polymer block can increase the effective segregation strength between blocks and drive self-assembly even with weak to no repulsion between blocks.

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M71.00022: Computationally designed coiled coil peptide bundle chains with positive charges: Self-assembly and click conjugation  YAO TANG (Presenter), Univ of Delaware, RUI GUO, JEFFERY G SAVEN, University of Pennsylvania, CHRISTOPHER J. KLOXIN, DARRIN JOHN POCHAN, Univ of Delaware — Computational design has been employed to predict peptide primary structure that will intermolecularly assemble into different net positively charged coiled coils nanostructures. Stable, robust, tetrahedral anti-parallel peptide bundles with net charges varying from 0 to +32 are self-assembled from the computationally designed 29-amino-acid peptides. In this research, +4 charged peptides are synthesized via solid phase peptide synthesis (SPPS) and modified with cysteine or maleimide on the N-termini of single peptides. Those two modified peptides are respectively self-assembled into 4 x 2nm cylindrical peptide bundles through non-covalent interactions and conjugated via Thiol-Michael ‘click’ react to form coiled coil bundle chains with extreme rigidity. The size and morphology of coiled coil bundle chains self-assembled under various temperatures, pH and solvent conditions are investigated by techniques such as Transmission electron microscopy (TEM) and circular dichroism (CD) spectroscopy. The self-assembled peptide bundles can be further used as building blocks to construct new 1-D nanomaterials. The effect of salt and pH on the solution behavior of the positively charged coiled coil chains will be also discussed.
M71.00023: Self-Assembly of Protein-based Block Copolymers – A Minimal Coarse-grained Model* AKASH ARORA (Presenter), HELEN YAO, BRADLEY OLSEN, Massachusetts Institute of Technology MIT — Protein-based block copolymers self-assemble into various nanostructures that are instrumental in developing next-generation biocatalysts and biosensors. Phase behavior of such block copolymers depends upon several parameters: temperature, blocks volume fractions, conjugate concentration in solution, protein shape and charge density, and multiple binary interaction parameters. In this work, a highly coarse-grained dumbbell model is developed in which protein is represented as a hard sphere linked to a soft sphere denoting a flexible polymer coil. Molecular dynamics simulations are performed with both implicit and explicit solvent. It is observed that such a simple model, incorporating primarily the various binary interactions, forms all the different morphologies that are observed experimentally. Interestingly, the model also predicts a lyotropic re-entrant order-disorder transition that is peculiar to protein-based block copolymers compared to coil-coil block copolymers. Integral-equation state theories are used to compute the solvent-mediated interactions to understand the origin of re-entrant transition. This work sheds light on the key factors governing the phase behavior of protein-based block copolymer solutions.

*This work is supported by the Department of Energy (DOE).

M71.00024: Tuning stoichiometry and physical interactions of peptide rigid rods through ‘click’ chemistry of computationally designed coiled coil* YI SHI (Presenter), Materials Science and Engineering, University of Delaware, RUI GUO, JACQUELYN BLUM, JEFFERY G SAVEN, University of Pennsylvania, CHRISTOPHER J. KLOXIN, DARRIN JOHN POCHAN, Materials Science and Engineering, University of Delaware — With computational design, peptide sequences can be customized to form specific solution self-assembly structures and to promote interactions that favor formation of unique structures such as nanotubes, needles, 2D plates. A recent publication of our collaborative group has shown that peptide rigid rods of various lengths can be formed from conjugation of N-terminal modified, anti-parallel, tetrameric coiled coil bundles by thiol-Michael reaction. Lyotropic liquid crystal behavior was observed and strong mechanical properties were expected from these peptide rods. In this work, further investigation into fine-tuning liquid crystal behavior of peptide rods and improving ‘click’ chemistry stoichiometry were carried out with computationally designed sequences. Highly charged coiled coil sequences were designed to showcase a tunable liquid crystal behavior through changing solution conditions and parallel coiled coil were designed to have inherent 1:1 stoichiometry at each end of bundle for long rods formation. Coiled coil design and preliminary results will be discussed.

*Department of Energy: DOE DE-SC0019355
M71.00025: In Situ SANS on Gelatinization of Polysaccharides  HOWARD WANG (Presenter), XIN ZHANG, FENG JIANG, ROBERT BRIBER, University of Maryland, College Park — It is desirable to understand, design and control the pathway of food preparation and consumption for the benefit of human health. Gelatinization occurs when starch/water mixtures are heated and native crystalline structures melt. The transport and distribution of water among polysaccharide molecules play a key role in the process of gelatinization. We have carried out in situ small angle neutron scattering measurements on rice grains in various aqueous solutions. Data imply the role of porosity and capillarity in the initial water uptake and the subsequent gelatinization kinetics. The interfacial tension between water and polysaccharides would alter the gelatinization process.

M71.00026: Directed Self-Assembly of Fluorine-Containing High-χ Block Copolymers using Top Coat and Electric Field  SEONGJUN JO (Presenter), SEUNGBAE JEON, TAESUK JUN, DU YEOL RYU, Yonsei University — Directed self-assembly (DSA) of block copolymers (BCPs) have been attractive for “bottom-up” approach lithographical applications. BCPs can form nanoscale structures spontaneously in long-range alignment with small feature down to 5 nm. In this study, we report a newly designed fluorine containing BCPs (polystyrene-b-poly(2,2,2-trifluoroethyl acrylate)) which the Flory-Huggins interaction parameter (χ) was above 0.2. Film experiments were demonstrated on a neutralized substrate where a sub-10 nm perpendicular lamellar morphology was observed with simple thermal annealing using the top coat strategies. The neutral conditions of the top coats for the BCP top surface was tuned by the same monomer of the BCP and the orientation was confirmed by AFM and GISAXS. Electric field was applied for the DSA, observing a long-range alignments without neither chemoepitaxy nor graphoepitaxy.

M71.00027: SCFT Study on Topological Defects of Symmetric Block Copolymers*  TIANYI HU (Presenter), WEI-HUA LI, State Key Laboratory of Molecular Engineering of Polymers, Department of Macromolecular Science, Fudan Univ, Shanghai, China — Block copolymers, as typical soft material, have a long relaxation time and are highly susceptible to thermal fluctuations, and thus their self-assembly is often accompanied by the occurrence of a variety of defects. At present, most research focuses on some simple defects in AB diblock copolymer melts, and there are few studies on the influence of block copolymer architectures on defect stability. Herein, the stability of various defects in (AB)_n linear and A_n B_n star block copolymer systems is investigated by self-consistent field theory (SCFT) and string method. We calculate the excess free energy of different defects and barriers of defect-removal in different symmetric block copolymers with the same effective segregation. The comparison of excess free energy between different defects indicate that the creation of a defect with more disconnections cost higher free energy. Moreover, our results demonstrate that (i) whether for linear or star block copolymer systems, the relationship between n and the excess free energy of a defect of the block copolymer is not monotonic and (ii) the same defect has different minimum free-energy path in different block copolymer systems.

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**M71.00028: Emergence of multi-stranded helices by the self-assembly of a new AB-type multiblock copolymer under cylindrical confinement**

LIXUN ZHANG (Presenter), Department of Macromolecular Science, State Key Laboratory of Molecular Engineering of Polymers, Fudan University, Fudan Univ, Shanghai, China — Novel nanostructures can emerge from the self-assembly of block copolymers under geometrical confinements due to the modification to the competition between interfacial energy and stretching energy. In particular, it is very appealing that helical structures can be formed by achiral AB deblock copolymers under cylindrical confinement. However, helical structures with strands more than two are rarely discovered. In previous works, most of block copolymers are hexagonal cylinder-forming in bulk. Herein, we consider a new AB-type multiblock copolymer, whose bulk cylindrical phase can be regulated by the architecture from hexagonal lattice to tetragonal one or even a graphene-like lattice. Our self-consistent field theory calculations suggest that this copolymer under cylindrical confinement can form helical structures with strands varying between 1 and 6. Our work provides a facile way for the fabrication of helical structures with a large number of strands.

*This work was supported by the National Natural Science Foundation of China (NSFC) (Grants No. 21774025)*

**M71.00029: Gyroidal Thin Films from Block Copolymer Self-Assembly as Structural Directing Templates for Fabrication of Mesostructured Crystalline Inorganic Materials**

FEI YU (Presenter), QI ZHANG, ULRICH WIESNER, Cornell University — Amphiphilic block copolymers swelled by carbon precursors self-assemble into bicontinuous gyroid mesophases (space group 214) compressed along <110> on Si wafers upon quenching after solvent vapor annealing. After pyrolysis in inert atmosphere, the resulting textured, mesoporous, and gyroidal carbon thin films are backfilled with amorphous Si (a-Si). The poor tolerance of carbon toward high temperature in air and the high melting points of inorganic materials present a seemingly insurmountable challenge in preparing crystalline mesostructured Si in the carbon templates. The stability of the carbon templates is significantly enhanced, however, when employing nanosecond transient laser heating. Melting and recrystallization of Si (a-Si melting point ~1250 °C) during this ultrafast, highly non-equilibrium process allow conformal template backfilling so that the templates' mesostructural order is inherited by the crystalized Si, which otherwise has little access to mesoscale ordering. Non-equilibrium transient laser technology in conjunction with block copolymer self-assembly in thin films opens up opportunities in fabricating materials for applications in catalysis, photonics, and beyond.

*Funding from the National Science Foundation (DMR-1707836) is appreciated.*
M71.00030: Unusual Phase Behavior by Blending Star-Shaped Block Copolymer and Linear Block Copolymer* YEOSEONG SEO (Presenter), SEONGHYEON AHN, SO YEONG PARK, JAEYONG LEE, Department of Chemical Engineering, Pohang Univ of Sci & Tech, WEI-HUA LI, Department of Macromolecular Science, Fudan University, JINKON KIM, Department of Chemical Engineering, Pohang Univ of Sci & Tech — Generally the block copolymer shows the arrangement of hexagonal patterns cylinder when volume fraction of one block is larger than that of the other. However, since all processes in the semiconductor business are geared to the rectilinear structure, it is needed to rework with time and money to apply block copolymer to the semiconductor business. Therefore, creating different structure from that of general block copolymer like square array structure or asymmetric lamellae has great significance in lithography applications. Here, we synthesized star-shaped poly polystyrene-block-poly(4-thydroxystyrene) (PS-b-PHS) and linear polystyrene-block-poly(2-vinyl pyridine) (PS-b-P2VP) and blended them in various proportions to observe the structures. Because the molecular weight of the PS on the core of star polymer is much smaller than that of the PS in linear polymer, the spacing between cylinders is limited and the large configurational entropy is formed, which leads block copolymer to have different structure.

*This work was supported by the National Creative Research Initiative Program, the National Research Foundation of Korea (2013R1A3A2042196)

M71.00031: WITHDRAWN ABSTRACT —

M71.00032: High $\chi$-low $N$ fluorine-based block copolymers for sub-10 nm lithography CIAN CUMMINS (Presenter), DANIELE MANTIONE, FEDERICO CRUCIANI, Laboratoire de Chimie des Polymères Organiques, University of Bordeaux, VIRGINIE PONSINET, Centre de Recherche Paul Pascal, University of Bordeaux, GUILLAUME FLEURY, GEORGES HADZIOANNOU, Laboratoire de Chimie des Polymères Organiques, University of Bordeaux — We will discuss the attractive properties of high $\chi$-low $N$ fluoro based BCPs and illustrate their utility for next-generation nanolithography. The synthesis, physical characterization and thin film self-assembly of a series of lamellar and cylindrical fluorine based BCPs will be described. Total BCP molecular weights ranging from 39 kg mol$^{-1}$ to 7 kg mol$^{-1}$ were synthesized using reversible-addition-fragmentation chain-transfer (RAFT) polymerization. Tailoring the fluorine containing blocks here resulted in a similar surface free energy to the well-studied polymethylmethacrylate (~ 41 mN/m) based BCPs thereby making orientational control in thin films more attractive. Solvo-thermal vapor annealing and thermal annealing of films were evaluated with a view to standardised industry methods. Period sizes ranged from 48 nm down to 14 nm with observed feature sizes as small as 7 nm. We also demonstrate the integration feasibility of our new fluorine based BCPs using sequential infiltration synthesis to form alumina nanowire hardmasks. The favorable BCP characteristics detailed here provide a versatile material option to the current library of available BCPs for nanolithography.
M71.00033: Development of Shape-Tunable Monodisperse Block Copolymer Particles through Particle Restructuring by Solvent Vapor Annealing  JAE MAN SHIN, EUN JI KIM (Presenter), YOUNG JUN LEE, MINGOO KIM, KANG HEE KU, JUNHYUK LEE, YONGJOO KIM, HONGSEOK YUN, KAIIST, KIN LIAO, Khalifa University, CRAIG J HAWKER, UCSB, BUMJOON KIM, KAIST — Uniformity and controllability of size, shape, and internal structure of block copolymer (BCP) particle are important to determine their functionality. Here, we introduce the particle restructuring by solvent engineering (PRSE) strategy to transform the size-controlled, monodisperse BCP spheres into non-spherical BCP particles with well-defined internal structure. PRSE process starts with generating monodisperse BCP spheres in a wide range of particle size using membrane emulsification. Then, successful shape transformation into non-spherical prolate and oblate was demonstrated while maintaining the monodispersity of particle size. PRSE can be applied generally to various functional BCPs including polystyrene-\textit{block}-poly(1,4-butadiene) (PS-\textit{b}-PB), polystyrene-\textit{block}-polydimethylsiloxane (PS-\textit{b}-PDMS), and polystyrene-\textit{block}-poly(4-vinylpyridine) (PS-\textit{b}-P4VP). Therefore, it allows an effective control of aspect ratio (AR) of the particles over a wide range, which was supported by theoretical calculation describing particle elongation. Further investigation on transformation kinetics during the PRSE showed that the morphological transformation was driven by reorientation of BCP domains, and it was strongly associated with overall molecular weight of the BCP and the annealing time.

M71.00034: Assessing the Capabilities of the Sharp-Interface Gradient-Based Theoretical Framework for the Simulation of Free-Surface Block Copolymers  DANIIL BOCHKOV (Presenter), FREDERIC GIBOU, University of California, Santa Barbara — Recently a sharp-interface gradient-based theoretical framework for the simulation of free-surface block copolymers within the Self-Consistent Field Theory was proposed [1,2]. In this talk, we present the results for the simulation of step edges in polymer thin films using this method. First, in the case of relatively low values of the polymer-air surface tension the results are compared to those obtained using the conventional approach based on adding `air molecules" to the system and discuss the differences in morphologies produced by the two methods. Then, we analyze the morphologies of step edges and construct phase diagrams in the case of high (more realistic) surface tensions, which are not easily accessible by the conventional approach.


M71.00035: Self-Assembly in Large Molecular Weight Block Copolymers for Dual Metal Nanodot Patterning and Optical Applications  ELEANOR MULLEN (Presenter), Trinity Coll —

Block copolymers (BCPs) have the potential to revolutionise the manufacturing of nanotechnology primarily due to their ability to self-assemble into spatially ordered nanodomains, resulting in nanoscale patterning. High molecular weight co-polymers poly(styrene-b-2-vinylpyridine) (PS-b-P2VP) and polystyrene-b-polyethylene oxide (PS-b-PEO) are used to form self-assembled patterns that act as a polymer template. This polymer template is infiltrated with the inorganic materials gold (Au) and silver (Ag). Polymer template removal leaves behind inorganic metal nanodots that exhibits surface plasmonic (SP) resonance effects that are particularly applicable for optical applications. The shape and chemical composition of metallic nanodots can be controlled by UV ozone or plasma etching removal of the polymer. It is found that dual metal nanodot arrays of Au and Ag can be used to suppress silicon reflectivity. Micelles of Au and Ag exhibit plasmonic resonance in the 400-600nm range that can be determined by the Au/Ag ratio. The transmission spectra for single metal nanodot arrays show SP dips at 430± 25nm for Au and 550 ±25nm for Ag. The resulting nanodot size, patterning and metal composition provides a low cost means of producing optical filters of tuneable plasmonic resonance effects.

M71.00036: Morphological Changes in Block Copolymer Thin Films Driven by Complex Coacervation*  HURSH SUREKA (Presenter), BRADLEY OLSEN, Massachusetts Institute of Technology MIT — Block copolymer thin films have been proposed as a method for immobilizing target molecules on a nanostructured scaffold. The use of a charged-neutral block copolymer (BC) enables the incorporation of oppositely charged molecules into thin films of the material. However, incorporation of oppositely charged macromolecules can trigger a phase change via coacervation. In this work, the effect of polyanion strength on the structure of BC self-assembly in thin films is examined. Complexation with the strong synthetic model polyanion, polystyrene sulfonate, leads to precipitation, while complexation with the weak synthetic model polyanion, poly(acrylic acid), leads to micellization. This difference in phenomena is likely driven by the ability of the weaker polyanion to charge modulate. The weakest polyanion tested was a model protein, amylase, which showed a rich set of phase behavior dependent on the blending ratio between the protein and the BC. The protein’s charge density is significantly lower than that of the synthetic polymers, which leads to weaker interactions between the protein and the BC by comparison. As a result, the structure of the BC is less disrupted by the protein than by the synthetic polymers at moderate loading (up to ~30 wt%).

*Supported by DTRA (HDTRA1-16-1-0038).
M71.00037: Self-assembly of Block Copolymers with Ionic Liquid Crystals in Thin Films

CHUQING YUAN (Presenter), Department of Chemical and Biomolecular Engineering, University of Houston, PRADIP BHOWMIK, Department of Chemistry, University of Nevada, Las Vegas, ALAMGIR KARIM, Department of Chemical and Biomolecular Engineering, University of Houston — Block copolymers (BCPs) self-assembly leads to plenty of promising applications in the area of electronics and energy storage. Thus, improving the ordering of BCP is crucial to optimize its performance in different applications. Adding ionic liquids (ILs) to BCPs has been reported a facile method to realize fast ordering because of its plasticization effect and wetting characteristics tunability. With similar chemical structure to ILs, ionic liquid crystals (ILCs) are liquid-crystalline salts also consisting of cations and anions. Differently, liquid-crystalline nature and thermotropic transition provide ILC with more fascinating features than IL when it is added to BCP. However, BCP/ILC system has not been well studied as BCP/IL system does. In this study, the effect of ILC additives on the self-assembly of BCP, PS-b-PMMA, under different annealing conditions has been investigated by using atomic force microscopy (AFM), grazing-incidence small-angle X-ray scattering (GISAXS), and time-of-flight secondary ion mass spectrometry (ToF-SIMS). We observed a drastic change of ILC selective swelling behavior during its thermotropic transition. Moreover, it can be highlighted that ILC enhances the ordering in BCP without enlarging the domain size after the zone annealing.

*NSF-DMR 1905996

M71.00038: Influence of Charge Sequence on the Adsorption of Polydispersed and Monodispersed Polyelectrolytes onto Monodispersed Polyelectrolyte Brush

VAIDYANATHAN SETHURAMAN (Presenter), KEVIN D DORFMAN, University of Minnesota — We use coarse-grained molecular dynamics to elucidate the role of charge sequence on the adsorption efficacy of oppositely charged free monodispersed and polydispersed polyelectrolytes on to a polyelectrolyte brush. We consider four different model systems wherein the free and the brush polyelectrolytes can have either brush or alternating charge sequence. Our model treats the polyelectrolytes in a bath of implicit solvent, excess salt and explicit counterions. For monodisperse systems, the adsorption efficiency is highest when both the free and the brush polyelectrolytes possess a block charge sequence, and it is lowest when both the free and the brush polyelectrolytes possess an alternating charge sequence. By computing the free energy, internal energy and entropy of adsorption using umbrella sampling methods, we find that the origin of the differences in adsorption efficiency for different charge sequences in monodispersed systems is enthalpic. Additionally, equilibrium conformations for different charge sequences reinforce the results obtained from energetic calculations. We also show the changes in adsorption efficacy as a result of polydispersity in the free polyelectrolytes.

*Materials Science Research and Engineering Center under Award No. DMR-1420013.
M71.00039: X-ray scattering characterization of polystyrene chains tagged with a single quaternary ammonium group per chain.* SANGWOO LEE (Presenter), Chemical and Biological Engineering, Rensselaer Polytechnic Institute, SUNGMIN PARK, CHULSUNG BAE, Chemistry and Chemical Biology; and Chemical and Biological Engineering, Rensselaer Polytechnic Institute, LIWEN CHEN, Chemical and Biological Engineering, Rensselaer Polytechnic Institute — Polymers containing a moderate amount of covalently bound ionic groups are widely used as membrane materials for electrochemical energy conversion devices such as fuel cells and electrolyzers. The performance of these ion-containing polymers largely depends on the microstructures, especially the structures of ion aggregates. To investigate the effects of the local chemical environment of ionic groups to the ionic aggregate and chain structures, we synthesized and characterized polystyrene chains containing a single quaternary ammonium group at the end of chains, in the middle of the chains, and right next to the secondary-butyl initiator motif using amino-functionalized diphenylethylene monomer. X-ray scattering characterization reveals three structural features of these model polystyrene chains. First, the domain spacing between ion aggregates changes with the location of the ionic groups in chains. Second, ionic groups stretch the polystyrene chains. Third, all polystyrene chains even without an ionic group display strong upturn curves in the small-angle domain, and the features of the upturn curves vary with the location of ionic groups in chains and processing pathways.

*Department of Energy, Energy Efficiency and Renewable Energy

M71.00040: Transport through ionic layers in sulfonated telechelic polyethylenes* BENJAMIN PAREN (Presenter), University of Pennsylvania, MANUEL HAEUSSLER, PATRICK RATHENOW, STEFAN MECKING, University of Konstanz, KAREN WINEY, University of Pennsylvania — We present a set of sulfonated telechelic polyethylene ionomers that demonstrate ion transport of metal cations within ionic aggregates in a crystalline polymer matrix. These precise ionomers consist of 23 or 48 backbone carbons with sulfonic acid end groups that are fully neutralized by a counterion, Li⁺ or Na⁺. Depending on spacer length and counterion, these telechelics exhibit multiple order-order transitions at T<Tₘ and order-disorder transitions at T~Tₘ, with melting points up to 300°C, as evident in both differential scanning calorimetry and X-ray scattering. At room temperature, the most common morphology is well-defined nanoscale ionic layers with a crystalline polymer backbone. The temperature-dependent ionic conductivity is characterized using electrical impedance spectroscopy. While ion transport appears decoupled from the polymer backbone at T<Tₘ under certain conditions, the conductivity remains quite low.

*NSF DMR 1506726, NSF PIRE 1545884, VIEST at Penn
M71.00041: Current-induced morphological changes in block copolymer electrolytes
WHITNEY LOO (Presenter), MICHAEL GALLUZZO, University of California, Berkeley, CHENHUI ZHU, Advanced Light Source, Lawrence Berkeley National Lab, NITASH BALSARA, University of California, Berkeley — Block copolymers are attractive electrolyte materials for lithium metal batteries due to their ability to microphase separate into distinct ion-conducting and mechanically-reinforcing domains on the nanometer-length-scale. Although the formation of current-induced gradient crystals has been previously shown when the material was heated above the glass transition temperature, $T_g$, of the mechanically-reinforcing block, it has been previously assumed that these equilibrium morphologies remain intact throughout polarization under the $T_g$, e.g. at 90 °C. In-situ small angle X-ray scattering (SAXS) experiments were used to probe morphology and electrochemical impedance spectroscopy (EIS) was used to quantify the bulk resistance of the electrolyte throughout cycles of cell polarization and subsequent cell relaxation of lithium-lithium symmetric cells as a function of polarization voltage. The electrolyte is comprised of a polystyrene–$b$-poly(ethylene oxide), PS-b-PEO, copolymer mixed with a lithium salt that forms hexagonally packed PS cylinders in a matrix of salt-containing PEO in the absence of current. We hypothesize that the formation of salt-concentration gradients within the electrolyte from the cell polarization drive the changes seen in morphology and resistance.

M71.00042: Polymer Electrolytes with Abundant Hydrogen Bonding Sites
RUIYANG WANG (Presenter), MOON JEONG PARK, Pohang Univ of Sci & Tech — Coulombic and/or dipolar interactions of polymers with embedded salts offer ion conduction across the polymer chains. Such polymers can be used in a wide range of electrochemical devices such as lithium batteries, fuel cells, and ionic actuators. Key challenges in developing practically viable devices based on polymer electrolytes are high conductivity, mechanical strength, and electrochemical stability. In this study, new polymer electrolytes possessing abundant hydrogen bonding sites for simultaneous achievement of high conductivity and improved mechanical properties. Owing to the high dielectric constant of such polymers, enhanced degree of ion dissociation and high ionic conductivity were obtained. In particular, with added inorganic salts, the hydrogen bonding sites in polymer structure effectively stabilize anion, thereby retarding the anion diffusion. This is connected to improved cation transference number of the resultant polymer electrolytes.
M71.00043: The Effect of Host Incompatibility and Polarity Contrast on Ion Transport in Ternary Polymer-Polymer-Salt Blend Electrolytes  BILL WHEATLE (Presenter), ERICK F. FUENTES, NATHANIEL A LYND, VENKATRAGHAVAN GANESAN, University of Texas at Austin — Conventional lithium-ion battery electrolytes are typically formed by blending high polarity and high mobility small-molecule components. These electrolytes tend to have ionic conductivities higher than those formed from either component alone. This is hypothesized to arise from a molecular-level synergy between miscible components. In short, molecular simulations have suggested that lithium ion solvation is dominated by the high polarity component. The solvated ions are then able to diffuse through a medium dominated by the high mobility component.

We hypothesize that similar effects can be seen in miscible polymeric blend electrolytes (PBEs) containing a high polarity and high mobility component. We have previously shown that increasing host polarity both improves solvation strength and slows dynamics. We thus investigate the role of changing the polarity of the nominally high polarity polymer on ionic conduction. Further, we study the influence of PBE miscibility on transport by varying the bare interaction parameter between polymer hosts. As hypothesized, we find that ionic conduction can be improved with increased miscibility and at intermediate levels of polarity contrast. We preliminarily investigate the effect of host molecular weight contrast on ionic transport.

M71.00044: Ion Transport in Ether-Based Polymer Electrolytes  YOUNGWOO CHOO (Presenter), Lawrence Berkeley National Laboratory, RACHEL SNYDER, BROOKS ABEL, Cornell University, NEEL SHAH, Lawrence Berkeley National Laboratory, GEOFFREY COATES, Cornell University, NITASH BALSARA, Lawrence Berkeley National Laboratory — Polymer electrolytes, typically poly(ethylene oxide) (PEO) mixed with a lithium salt, have emerged as promising solid electrolytes for lithium ion batteries. However, polymer electrolytes still exhibit lower conductivities than commercial liquid electrolytes. We report a novel ether-based polymer, poly(diethylene oxide-alt-oxymethylene), (P(2EO-MO)), which was synthesized via cationic ring-opening polymerization of the cyclic acetal monomer, 1,3,6-trioxocane. The polymer electrolytes, which are mixtures of P(2EO-MO) and various concentrations of lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) salt, were characterized by electrochemical methods. P(2EO-MO)/LiTFSI exhibits lower ionic conductivity than PEO/LiTFSI due to increasing glass transition temperatures in the presence of lithium salts. However, the steady-state transference number of P(2EO-MO)/LiTFSI is significantly higher than that of PEO/LiTFSI at most salt concentrations. We investigate the thermodynamic factor and steady-state current of P(2EO-MO)/LiTFSI as a function of salt concentration and compare the results to PEO/LiTFSI. This work suggests that the overall efficacy of ion transport in P(2EO-MO) is greater than that in PEO, and P(2EO-MO) is a favorable electrolyte for lithium ion batteries.

*JCESR (DOE-BES)
M71.00045: Entropic transport of interacting Brownian particles in a channel with reflecting boundaries*  NARENDER KHATRI (Presenter), P. S. BURADA, Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur - 721302, India — The entropic transport of overdamped biased Brownian particles in a symmetric channel is investigated numerically considering both the no-flow and the reflection boundary conditions at the channel boundaries. The constrained dynamics yields a scaling parameter f, which is a ratio of the work done to the particles to available thermal energy. The distinct transport features are observed with reflection boundary conditions, for example, the nonlinear mobility exhibits a nonmonotonic behavior as a function of the scaling parameter f, and the effective diffusion coefficient exhibits a rapidly increasing behavior at higher f, which are not observed with no-flow boundary conditions. We show that the transport properties can be significantly influenced by the nature of reflection, i.e., elastic or inelastic. In doing so, we identify that both the nonlinear mobility and the effective diffusion coefficient can be enhanced with inelastic reflection boundary conditions. In addition, by including the short range interaction force between the Brownian particles, the mobility decreases, and the effective diffusion coefficient increases for the optimal values of f.

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M71.00046: Shear-induced Counterion Redistribution of a Single Polyelectrolyte*  KAIKAI ZHENG, KUO CHEN, JIANG ZHAO (Presenter), Institute of Chemistry, Chinese Academy of Sciences — The counterion distribution of a model polyelectrolyte, sodium polystyrene sulfonate (NaPSS), as a function of shear rate is investigated at single molecular level. The fluorescence resonance energy transfer (FRET) between the fluorescence donor attached at the charged PSS- chain and the positively charged acceptor as the counterion probes shows the increase of average counterion-chain distance, indicating the expansion of counterion cloud by shear. Such a process is further verified by the emission spectra of the pH-responsive fluorophore labeled at PSS- chain end, showing the local pH value is shifted to higher values by shear. The shear-induced counterion release or counterion cloud expansion is attributed to alternation of the electric filed distribution inside the solution and the overlap of electric fields of multiple PSS- chains in the process of creating inhomogeneity in concentration inside the PSS- solution by shear.

*Project supported by the National Natural Science Foundation of China (21833012).
**M71.00047: Through-plane Structural Analysis of Engineered Nafion Surfaces**

NATALIE LINNELL SCHWAB (Presenter), Materials Science and Engineering, University of Maryland, College Park, YUANCHAO LI, TRUNG VAN NGUYEN, Chemical and Petroleum Engineering, University of Kansas, ROBERT BRIBER, Materials Science and Engineering, University of Maryland, College Park, JOSEPH A. DURA, Center for Neutron Research, National Institute of Standards and Technology — The thin-film structures of Nafion, a model perfluorinated ionomer, impact practical advances in proton-exchange membrane fuel cells (PEMFCs). Engineered Nafion surfaces were developed by Dowd et al. to reversibly and permanently alter the surface composition and wettability of Nafion [a]. Using neutron reflectometry (NR), we probe the through-plane structure of surface-treated Nafion thin-films with sub-Ångstrom resolution. Humidity-related layers of phase-separated lamellae were observed in Nafion thin-films at Au, Pt, and SiO$_2$ interfaces by Dura et al. and DeCaluwe et al. [b,c].

We develop and apply titanium nitride (TiN) substrates to minimize the neutron scattering contrast to similar Nafion-TiN interface structures, thus optimizing the sensitivity of NR to the thickness, roughness, and scattering-length density (SLD) of the engineered Nafion surfaces. The engineered Nafion thin-films are assessed in dry (0% RH) and wet (92% RH) conditions in H$_2$O and D$_2$O vapor to independently determine water content and polymer density, before and after surface modification. Additionally, we evaluate the formation structures at the Nafion-TiN interface.


*This work was supported by NIST cooperative agreement 70NANB17H301.

**M71.00048: Single-ion polymers based on ion-conducting crystalline phases**

JAEMIN MIN (Presenter), MOON JEONG PARK, Pohang Univ of Sci & Tech — Recently, single-ion conducting polymers have extensively been studied as future polymer electrolytes owing to the minimized device polarization at a given dc voltage. In this study, we investigate single-ion conducting polymers containing zwitterions. Based on computational calculations, design and synthesis of zwitterion were carried out to modulate intermolecular interactions in single-ion polymers via controlling dipolar orientation of ionic moieties. With balanced Coulombic and dipolar interactions, well-defined ionic crystals were formed within the ionic phases. Particularly, nanoconfinements given by the use of acid-tethred block copolymer matrix were a key to induce the crystallization of ionic moieties. Hierarchical self-assembly of the zwitterion-containing single-ion polymers was further characterized with a focus on the structure-transport relationship.
M71.00049: On the Transference Numbers and Inverse Haven Ratios of Ionic Liquids and Polymeric Ionic Liquids
ZIDAN ZHANG (Presenter), BILL WHEATLE, University of Texas at Austin, JAKUB KRAJNIAK, KU Leuven, JORDAN R KEITH, VENKATRAGHAVAN GANESAN, University of Texas at Austin — In this study, we used atomistic computer simulations within a non-equilibrium molecular dynamics framework to probe the transference number and inverse Haven ratio of ionic liquids and polymerized ionic liquids. In contrast to the conventional expectations, we find that the transference number is a constant at approximately 0.5 and independent of the degree of polymerization (DP). The inverse Haven ratio increases first with increasing DP and then decreases at larger DP. We demonstrate that such results arise as a consequence of the strong cation-cation correlated motions. Together, such findings challenge the premise underlying the pursuit of single ion conductors as a means towards enhanced transference numbers.

M71.00050: Comparing Ion Conductivity and Transference Number of Single-ion and Salt-doped Block Copolymer Electrolytes*
KUAN-HSUAN SHEN (Presenter), LISA HALL, Ohio State Univ - Columbus — Nanostructured block copolymer electrolytes with both ion conductive and mechanically robust microphases are strong candidates for solid battery electrolytes. However, their performance is limited by their low cation transference number (fractional contribution of the cation to the overall conductivity). Experimental work has showed a potential route of increasing transference number by tethering anions to the polymer backbone of the conducting segment of block copolymers. Due to the synthetic challenges of such materials, the design space has yet to be well explored. It is unclear how to optimize their conductivity and under what conditions these single-ion block copolymer electrolytes can more efficiently conduct lithium ion than the salt-doped materials. In this work, we perform coarse-grained molecular dynamics simulations with an applied electric field to calculate ion conductivity and transference number in both single-ion and salt-doped block copolymers. We aim to show how the choices of molecular weight, ion loading, and anion type impact ion transport to guide design of new materials.

*This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award DE-SC0014209.
M71.00051: Enhanced ion transport in block polymer electrolytes through the manipulation of salt and monomer segment distributions  PRIYANKA KETKAR (Presenter), MELODY A MORRIS, SEUNG HYUN SUNG, Chemical and Biomolecular Engineering, University of Delaware, JOSEPH A. DURA, NIST Center for Neutron Research, National Institute of Standards and Technology, RYAN NIEUWENGAAL, Materials Science and Engineering Division, National Institute of Standards and Technology, THOMAS EPPS, Chemical and Biomolecular Engineering, University of Delaware — Solid block polymer (BP) electrolytes for lithium-ion batteries can address safety and performance concerns present in conventional liquid-state electrolytes, but the ion transport in BPs requires significant improvement to meet the demands of current and future battery applications. Transport properties in nanostructured BP electrolytes can be enhanced through the modification of salt and monomer segment distributions within the ion-conducting domain. We explored two methods to tune these distributions: the synthesis of polystyrene-block-poly(oligo-oxyethylene methacrylate) (PS-b-POEM) BPs with gradient or random copolymer regions at the chemical junction between the PS and POEM blocks (i.e., tapered block polymers) and the blending of POEM homopolymers of different molecular weights into PS-b-POEM BPs. For both methods, we connected the structural characteristics, such as the salt and monomer segment distributions, determined by X-ray and neutron reflectivity, to the segmental and ion dynamics measured through differential scanning calorimetry, $^7$Li solid-state NMR, and AC impedance spectroscopy. These results elucidated design parameters in the synthesis and fabrication of BP electrolytes that can increase ionic conductivity.

M71.00052: Investigation of proton conductivity in polymer nanocomposite films  SANKET KADULKAR (Presenter), VIKRAM LAKHANPAL, DELIA MILLIRON, THOMAS TRUSKETT, VENKATRAGHAVAN GANESAN, University of Texas at Austin — Proton-conducting membranes and solid electrolytes are critical components in many electrochemical devices, and the performance of such devices is often limited by proton transport. In this work, we study proton conductivity in polymer nanocomposite films. We experimentally observe multifold increase in proton conductivity in a composite of poly(ethylene oxide) (PEO) and cerium oxide (CeO$_2$) nanocrystals, in comparison to their individual counterparts. Employing kinetic Monte Carlo simulations, we model proton transport in such systems. Our results reveal the significance of percolation and connectivity of filler/polymer interface in such systems, with further scope for improving conductivity by tuning the morphology of nanocrystals. We also study the overall proton conductivity at different nanocrystal compositions, predicting an optimum composition for maximum proton conductivity.

*Support for this research was provided by the National Science Foundation through the Center for Dynamics and Control of Materials: an NSF MRSEC under Cooperative Agreement No. DMR-1720595.
M71.00053: The effects of processing method on conductivity and dielectric relaxations in PVDF blended with a zwitterionic copolymer* ANDREW CLARK (Presenter), MIRIAM SALCEDO, NELAKA DILSHAN GOVINNA, SAM LOUNDER, AYSE ASATEKIN, PEGGY CEBE, Tufts Univ — The conductivity and relaxation dynamics of poly(vinylidene fluoride) (PVDF) blended with a random copolymer of methyl methacrylate and sulfobetaine-2-vinylpyridine (PMMA-r-SB2VP) were investigated. Films were prepared using two processing methods, compression molding and doctor blading from solution. Scanning electron microscopy revealed morphological differences between the films, with the doctor bladed films demonstrating a porous microstructure, while FTIR revealed the presence of different crystallographic phases for the films. Dielectric relaxation in the temperature range from 30 °C to 140 °C showed several relaxations in compression molded films due to the motion of dipoles in the PVDF crystal phase, segmental relaxations of PMMA, as well as a unique relaxation seen only in the blends. Blends demonstrated higher conductivity then the neat PVDF and copolymer. Doctor bladed films showed a large decrease in the dielectric constant and conductivity as well as different relaxation behavior compared to the compression molded films. These differences suggest that influence of the different processing techniques on the molecular environment plays a significant role on the dielectric properties of these PVDF zwitterionic copolymer blends.

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M71.00054: Gyroid Morphologies in Single-Ion Conducting Polymers and the Consequences for Ion Conductivity JINSEOK PARK (Presenter), University of Pennsylvania, ANNE STAIGER, CHRISTINA RANK, STEFAN MECKING, University of Konstanz, KAREN WINEY, University of Pennsylvania — The morphology of self-assembled ionic aggregates influences the ion transport in single-ion conducting polymers. Recently, our group reported that polymers with sulfosuccinate units containing sulfonate groups with their counterions (Li⁺, Na⁺, and Cs⁺) and precisely separated by 23 methylene units form ordered ionic aggregate morphologies (layered, gyroid, and hexagonal). In these ionomers, the gyroid morphology exhibits higher ion conductivity than layered and hexagonal ionic aggregates morphologies, demonstrating the importance of bicontinuous ion-containing channels for enhanced ion conductivity. These gyroid morphologies were reported at relatively high temperatures (120°C - 130°C) that are coincident with the melting point of the crystalline polyethylene unit. To produce the gyroid phase in a lower temperature range, polymers with shorter polyethylene units are being explored and results will be discussed using a phase diagram with volume fraction of sulfosuccinate units ($f_{polar}$) and temperature, similar to conventional block copolymer phase diagrams. This study endeavors to provide design strategies for single-ion conducting polymers with controlled ionic aggregate morphologies and enhanced ion conducting properties.
M71.00055: Understanding the interactions of polyols with hexafluoroisopropanol containing polynorbornene biobutanol membranes using QCM-D*  SIYUAN LI (Presenter), Univ of Akron, BRYAN VOGT, Chemical Engineering, Pennsylvania State University — Polymer membranes offer a low-cost path to separate bio-products. However, interactions of the membrane with components in the fermentation broth can alter its performance. Here we describe how ppm levels of polyl surfactant designed to inhibit foaming of the broth can dramatically swell and plasticizing the polynorbornene copolymers in the bio-butanol separation. *in-situ* quartz crystal microbalance with dissipation (QCM-D) enable the quantification of both the swelling and rheological properties. We examined the molecular-weight-dependent sorption behavior of 10ppm of polyethylene glycol (PEG) and polypropylene glycol (PPG) for a series of copolymer membranes that all contain 50 mol% hexafluoroisopropanol norbornene and 50 mol% alkyl (methyl to decyl) norbornene. Changing the alkyl side length only modestly impacts the swelling behavior, which is consistent with hydrogen bonding between hydroxy groups driving the sorption. It shows that PPG, not PEG, is the primary cause for the enhanced swelling. Increasing molecular weight of the PPG leads to increased swelling (entropic effect) but also slower the sorption rate (size effect). These results illustrate that details about components added to the broth can dramatically affect the membrane properties.

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M71.00056: Self-assembly of Linear Block Copolymers and Bottlebrush Block Copolymers in Thin Films*  MINGQIU HU (Presenter), Univ of Mass - Amherst, DARREN SMITH, Department of Chemistry, University at Buffalo, DUK MAN YU, Univ of Mass - Amherst, XINDI LI, JAVID RZAYEV, Department of Chemistry, University at Buffalo, THOMAS RUSSELL, Univ of Mass - Amherst — Semiconductor device fabrication has been developing rapidly in recent years. It's been harder to keep up with Moore's law since top-down photolithography is approaching the diffraction limit. Self-assembly of block copolymers is a promising solution for its highly reproducible self-assembly, great diversity of morphology, good etching contrast, economic efficiency and recipes compatible for industrialization. Well-aligned self-assembled patterns with sub-10 nm feature size and good etching contrast in thin films have been achieved in recent years. However, poor solubility, microdomain orientation and high energy barrier for defect annihilation remain from their application. We developed a series of linear block copolymers and bottlebrush block copolymers containing ketal groups as side chains for low-χ to high-χ conversion in the solid state. Self-assembled lamellar and cylindrical morphologies, with a 5.4 nm full pitch have been obtained in the bulk and 9.4 nm full pitch in thin films, which is among the smallest domains obtained so far.

*This work was supported by the Air Force Office of Scientific Research under contract 16RT1602.
**M71.00057: Macrorheology and particle tracking to study tracer transport, viscoelasticity and network structure of mucin and mucin-like biopolymer solutions**  JOSHUA TAMAYO (Presenter), ARVIND GOPINATH, University of California, Merced — Passive microrheology using single-particle and multi-particle techniques can be used to assess the local transport, mechanical properties and network structure of biopolymer laden biological fluids. Using single particle tracking (SPT) and multiple particle tracking (MPT) passive microrheology, we probe the dynamics of tracer particles ranging from 0.1 to 10 microns in size in mucin-like Carboxy Methylcellulose (CMC) solutions and in re-constituted mucin solutions. Tracking and linking algorithms implemented in MATLAB and Python reconstruct 2-dimensional trajectories from sequential list of particle coordinates. Corrected data is used to calculate the distributions of displacements and velocities, ensemble averaged mean square displacement, and particle velocity autocorrelations from which we extract diffusion coefficients of the particles and tracer-size dependent viscoelastic properties of the medium. Passive microrheology combined with macrorheology studies and confocal derived connectivity and morphology measurements provide a base state to understand the dynamics of living active materials such Candida albicans biofilms.

**M71.00058: Rheological Scaling of Imidazolium-Based Polyelectrolyte in Ionic Liquid Semidilute Solutions**  ATSUSHI MATSUMOTO (Presenter), AMY QING SHEN, Okinawa Inst of Sci & Tech — Polymerized ionic liquids (PILs) are a special type of polyelectrolytes with ionic liquid moieties covalently attached to a polymer backbone. Existing studies show that electrostatic interactions play a dominant role in determining the viscoelastic properties of ordinary polyelectrolytes. Recently, we found that the charge underscreening effect, in which the screening length increases with increasing the ion concentration, resulted in expanding PIL chains at high ion concentrations in the dilute regime. In this study, we investigate the effect of charge underscreening on the rheological properties of PILs in the semidilute unentangled regime by using a model system consisting of a PIL (PC$_4$–TFSI) in a mixture of an ionic liquid (BmimTFSI) and a non-ionic solvent (DMF). We observe: i) both specific viscosity $\eta_{sp}$ and relaxation time $\lambda$ are initially constants at low ion concentrations $c_s$ and then decrease with increasing $c_s$ at an intermediate $c_s$. ii) both $\eta_{sp}$ and $\lambda$ increase with increasing $c_s$. This result indicates that the charge underscreening effect is still dominant in the semidilute unentangled regime. We capture the observed trend by proposing and validating a modified scaling law accounting for the dependence of correlation length on $c_s$. 
M71.00059: Rheological Properties of Bare and Grafted Nanoparticle Polymer Networks*  
YI FENG (Presenter), PINAR AKCORA, Stevens Inst of Tech — This study investigates the rheological properties of crosslinked poly(methyl methacrylate) (PMMA) composites with bare and grafted nanoparticle constituents. We will present the influence of crosslinking density and particle loading on linear rheological properties of PMMA networks. These results will be compared with the PMMA-grafted particles in crosslinked PMMA matrices. Effects of including the short linear chains into crosslinked composites of bare and grafted nanoparticles will be discussed. Topological constraints of crosslinked matrix will be compared to the crosslinked grafted nanoparticles to understand the addition of free chains and entanglements in these two different system networks.

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M71.00060: Effect of topological constraints in semidilute polymer solutions under planar extensional flow*  
CHARLES YOUNG, CHARLES SING (Presenter), University of Illinois at Urbana-Champaign — Polymer solution dynamics and rheology are relevant to a wide range of processing methods. Developing an understanding of the polymer conformational dynamics and the emergent material properties is challenging because of the interplay of hydrodynamic interactions (HI), excluded volume, and topological constraints driven by concentration and polymer architecture. This is particularly true in extensional flow, which strongly deforms the polymers from their equilibrium conformations. Using a new technique for rapid Brownian dynamics (BD) simulation which we call the iterative conformational averaging (CA) method, we investigate the dynamics and rheology of linear, comb, and ring polymer solutions at concentrations increasing from the dilute limit into the semidilute regime. We apply step strain rate planar extensional flow and quantify the dynamics in startup, at steady state, and after flow cessation via conformational distributions and the polymer contribution to extensional viscosity. We show that flow enhances intermolecular HI and topological interactions, resulting in transient intermolecular entanglements. We investigate the effect of these constraints on polymer stretching and the transient solution stress.

*We acknowledge support from NSF grant CBET-1803757.
M71.00061: The effects of the structure of a confinement on the ejection rate of a polymer chain from a nanopore*  CHUNG BIN PARK (Presenter), BONG JUNE SUNG, Sogang Univ — Conformations of DNA inside the phage are crucial to the ejection dynamics of the DNA. The equilibrium conformation of DNA inside the viral capsid is determined by the shape of the capsid (confinement): a concentric spool DNA and a folded twist DNA are considered equilibrium conformations in a spherical capsid and an elongated capsid, respectively. Because there are a variety of viral capsids in nature, the correlation between the capsid shape and the ejection dynamics should be a topic of interest. In this study, we investigate the effects of the capsid shape on the conformation of a polymer and its ejection rate by performing Langevin Dynamics simulations. We employed two different types of capsid: 1) sphere and 2) cube capsids. We find that a polymer chain ejects out of the capsid faster in case of the sphere than the cube capsid and that the ejection rate becomes faster by up to 35% as the rigidity of the polymer increases. The segments of the polymer near the wall of the capsid travel faster than other segments, regardless of the capsid shape. However, a larger fraction of the monomers are distributed near the wall in case of the sphere capsid than the cube capsid.

*This work was supported by the Samsung Science and Technology Foundation under Project Number SSTF-BA1502-07.

M71.00062: Interfacial Dynamics Governs the Mechanical Properties of Nanoconfined Glassy Polymers  WENJIE XIA (Presenter), North Dakota State Univ — Understanding the mechanical properties of nanoconfined glassy polymers is essential in design of nanostructured soft materials. Here, we investigate the mechanical properties of free-standing polymer thin films by employing an atomistically informed coarse-grained (CG) modeling approach. By examining three representative CG polymer models, i.e., polystyrene (PS), poly(methyl methacrylate) (PMMA), and poly(1-ethylcyclopentyl methacrylate) (PECPMA), we show that the elastic moduli of nanoscale thin films are substantially reduced with decreasing film thickness compared to their bulk values at their glassy state. Specifically, the PS and PMMA films exhibit similar size-dependent elastic responses and their film moduli are reduced compared to bulk values at a thickness of less than 40 nm, whereas, for PECPMA, the length scale where elastic modulus deviates from the bulk value is much larger. The local molecular stiffness within the films assessed by Debye-Waller factor further reveals a gradient a softer interfacial layer having a size of only a few nanometers. Based on our simulations, a bilayer composite model is employed to predict the elastic moduli of thin films, which uncovers the size scaling relationship that universally holds for all three polymers.
M71.00063: Surface and bulk dynamics of compressed polystyrene films: A β-NMR study
DEREK FUJIMOTO (Presenter), University of British Columbia, OWEN BRAZIL, Trinity College Dublin, ARIS CHATZICHRISTOS, MARTIN H DEHN, VICTORIA L. KARNER, ROBERT F KIEFL, PHILIP C. P. LEVY, RYAN M. L. MCFADDEN, University of British Columbia, IAIN MCKENZIE, GERALD MORRIS, MARTIN H DEHN, MONIKA K STACHURA, TRIUMF, JOHN TICKNOR, W ANDREW MACFARLANE, University of British Columbia, GRAHAM CROSS, Trinity College Dublin — Glasses gradually densify as they relax towards equilibrium, and in doing so, their spectral density of molecular fluctuations is modified. In polystyrene (PS), only a few percent increase in density is equivalent to the passage of millions of years. To access this regime, we have plastically deformed a PS thin film with nanoimprint lithography, resulting in permanent compactification without rejuvenation. We present depth-resolved $^8\text{Li}^+$ β-NMR measurements in PS films and discuss the dynamical effects of the mechanical processing. β-NMR is a technique sensitive to nanosecond molecular dynamics through the spin-lattice relaxation of a short-lived radioisotope. Because the isotope is implanted as a low-energy ion beam, the depth is controllable with nanometer-scale resolution. This has allowed β-NMR to directly probe the dynamics in glassy polymer thin films near both the free and buried interfaces.


M71.00064: Reduction of Dielectric Signal of the Interfacial Segmental Dynamics in Polymer Nanocomposites*
IVAN POPOV (Presenter), Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, BOBBY CARROLL, Department of Physics, University of Tennessee, Knoxville, Tennessee 37996, USA, VERA BOCHAROVA, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, ANNE-CAROLINE GENIX, Laboratoire Charles Coulomb, Université de Montpellier, CNRS, F-34095, France, SHIWANG CHENG, Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan 48824, USA, AIRAT KHAMZIN, Kazan Federal University, Institute of Physics, 420008, Kremlevskaya str.18, Kazan, Tatarstan, Russia, ALEXANDER KISLIUK, ALEXEI SOKOLOV, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — In this study we focus on polymer nanocomposites (PNCs) with dispersed silica core nanoparticles. We examine the dielectric strength and relaxation behavior of segmental dynamics in the interfacial polymer layer surrounding silica nanoparticles. The presented analysis reveals the significant drop in the dielectric strength, and its anomalous temperature dependence in polymer layer adsorbed to nanoparticles. We ascribe the observed effect to the restricted amplitude of segmental relaxation in the interfacial/adsorbed layer. The theoretical model explaining the unusual temperature dependence of dielectric strength is presented. Our results provide new view on discussion of dynamics in interfacial layer in PNC that may be applied to the thin polymer films as well: Not only characteristic time scale, but also amplitude of structural relaxation can be strongly affected by the presence of an interface.

*Work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
**M71.00065: The Influence of Polymer and Ion Solvation on Counter-ion Cloud Formation and Charge Fluctuations in Highly Charged Polyelectrolytes**  
**JACK DOUGLAS (Presenter), National Institute of Standards and Technology, ALEXANDROS CHREMOS, Eunice Kennedy Shriver National Institute of Child Health and Human Development, National Institutes of Health** — We investigate the influence of solvent affinity to counter-ions and to the polyelectrolyte (PE) backbone on the charge distribution about highly charged flexible polymer chains based on coarse-grained molecular dynamics simulations that include both explicit counter-ions and solvent. Based on this framework, we find that the competitive solvation of ions and PE chains leads to an extended “cloud” of counterions about the polymers that cannot be understood without modeling the solvent explicitly. The counter-ion cloud is highly dynamic and fluctuations of the charge can be expected to great influence the polarizability of PEs in solution. After reviewing recent findings on the influence of molecular topology and interactions on the average size of the counter-ion cloud, we estimated the PE potential of the mean interaction to determine the influence of the counterion-cloud and charge fluctuation effects on inter-PE interactions. Consistent with the Kirkwood-Schumaker theory, we find evidence that charge fluctuations gives rise to a long range attractive interaction having a $1/r^2$ asymptotic decay at large interpolymer separation distances $r$ in the case of strongly hydrating counterions and a PE backbone that is not strongly hydrating, a model of relevance to many synthetic PEs.

**M71.00066: Reflection band-gap for a transversely stretched composite cholesteric elastomer**  
**GUILLERMO REYES (Presenter), ADRIAN REYES, Univ Nacl Autonoma de Mexico** — We have studied the conduction of electromagnetic waves, impinging normally in a composite cholesteric elastomer slab, doped with metallic inclusions, aleatory distributed in the structure. We performed a theoretical and numerical model, that allow us to obtain the reflection and transmission spectra, when the system is under the action of mechanical forces in transverse direction respect to cholesteric axis. We have found that by stretching transversely the elastomer slab after the critical value of stretching in which the helical structure gets unwind, it transform from a discriminatory circular filter to a polarization independent device. Intervals of conversion from right to left circularly polarized waves in the reflection spectra, are alternated with regions of resembling transmission of both circularly polarized waves. The spectra of the pure cholesteric elastomer can be modulated specially nearby the metallic resonance where the transmittances are greatly damped and reflection is considerably increased.
M71.00067: Structure Instability in Particle Filled Elastomeric Polymer Composite Under Tensile Stress  LANFANG LI (Presenter), Emulsion Polymer Institute, Lehigh Univ, WEI GUO, Oriental Yuhong North American LLC, ZHIYU JIANG, CHONG SHEN, Physics Department and Emulsion Polymers Institute, Lehigh Univ, WILLIE LAU, Oriental Yuhong North American LLC, H DANIEL OU-YANG, Physics Department and Emulsion Polymers Institute, Lehigh Univ — The buckling instability and crease development in elastomeric soft material under compression has been experimentally and theoretically studied over the past decades[1]. The structural instability of such material under tensile stress, however, has not been well understood. In this work, we present the structure instability of a polymer particle composite under tensile stress. It is observed that periodic undulation in sample surface develops as the tensile stress increases, manifested as linear ridges and valleys on the sample surface perpendicular to the direction of tension. The undulation is reversible at small strains. There is a memory effect in the undulation location at repeated strain applications. At large enough strain, the material eventually fractures from crack developed at one of the valley regions from the undulation structure.

References

M71.00068: Thermo-electro-mechanical and Rheological Properties of Rubber Composites Filled with \(sp^2\)-Hybridized Different Carbon Fillers*  EMIL FERNANDO (Presenter), THUSITHA ETAMPAWALA, LALEEN KARUNANAYAKE, Department of Polymer Science, University of Sri Jayewardenepura, Sri Lanka, DHARANI ABYESINGHE, AMANDA EKANAYAKE, NARAYANA SIRIMUTHU, Department of Chemistry, University of Sri Jayewardenepura, Sri Lanka, A R KUMARASINHGE, Department of Physics, University of Sri Jayewardenepura, Sri Lanka, DILHARA EDIRISINGHE, Department of Rubber Technology and Development, Rubber Research Institute, Sri Lanka — Rubber composites (RC) with enhanced thermo-electric properties are widely used in applications such as in flexible electrodes and solid tyres. In this work, the effect of carbon black (CB), multiwall carbon nano tubes (MWCNT) and natural graphite on thermal, electrical, mechanical and rheological properties of RC was studied. In all these fillers, carbon mainly has \(sp^2\) hybridization. When the MWCNT loading was increased from 5 to 60 phr, the electrical conductivity of RC increased by four orders of magnitude. At 60 phr MWCNT loading showed five orders of magnitude higher electrical conductivity than CB added sample. The graphite loaded RCs were nonconductive. Hardness, elastic modulus, tensile and tearing strengths increased gradually with the increase of filler loadings. The variation of modulus of graphite-loaded samples was subtle. Interestingly addition of graphite showed higher elongation at break than that of pristine rubber. Viscoelastic characteristics showed that MWCNT added samples have least time and graphite added samples have highest time for curing compared to CB loaded samples. Although carbon-based fillers responsible for a significant improvement in their overall properties type of filler controls the extent to which the property changed.

*AHEAD/RIC/SJP/SCI/NCRG
Aqueous pigment dispersions: The thermodynamics of hierarchical aggregation*  
ANDREW J MULDERIG (Presenter), KABIR RISHI, GREG BEAUCAGE, Univ of Cincinnati
— Many industrially important materials aggregate to form nanoscale mass-fractal structures. Unlike sintered aggregates such as fumed silica, aqueous pigment-based inks often consist of weakly bound nanoparticles stabilized by a surfactant that can break apart and re-form balancing mixing energy and the reduction in surface energy with aggregation. Rapid thermal motion of small elemental crystallites lead to dense primary particle clusters with slower thermal motion that aggregate into ramified mass fractals. It is proposed that the hierarchical structure relies on subtle and competitive equilibria between different hierarchical structural levels. In the context of the removal of a subunit from a cluster, the thermodynamics of nanoparticle hierarchical equilibria was explored on surfactant-stabilized pigment dispersions using the Vogtt Theory. Reversible nanoparticle aggregation could be described solely from the degree of aggregation and the volume fraction. In this case, the hierarchical thermodynamics at each of three structural levels is dominated by solubility of the nonionic dispersing surfactant that decreases with temperature (LCST).


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A model nanocomposite designed to understand the interfacial behavior in a novel thermally stiffening nanocomposite*  
CHEN GONG (Presenter), Materials Science and Engineering, Rensselaer Polytechnic Institute, KRISTINA NGUYEN, Biomedical Engineering, Rensselaer Polytechnic Institute, PINAR AKCORA, Chemical and Materials Engineering, Stevens Institute of Technology, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — A novel polymer-adsorbed silica-reinforced nanocomposite with a heterogeneous structure was recently shown to have thermal-stiffening behavior. Although the macroscopic properties of this nanocomposite were characterized via rheological experiments, the structure and dynamics at the matrix-nanofiller interface remain to be investigated. In the current study, we use a simplified 2D system to mimic the complex 3D structure of the nanocomposite. The simplified sandwich structure consists of a flat silica substrate, a thin layer of adsorbed high glass transition temperature polymer (PMMA, P2VP, and PC), and a final layer of PEO. Modulated Differential Scanning Calorimetry (MDSC) and Thermogravimetric Analysis (TGA) experiments indicated that the conformation and the relaxation in the confined environment surrounded by the hydroxyl group-rich silica surface and flexible PEO chains were significantly altered. Besides, by carefully changing the thickness, annealing condition, and molecular weight, different trends were observed which corresponds to different possible mechanisms. The results are of great help in understanding the previous real nanocomposite results and they also provide some strategies to design nanocomposites with desired properties.

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M71.00071: Compatibility/incompatibility in surface-modified, aggregated, precipitated silica nanocomposites*  LAHARI PALLERLA (Presenter), KABIR RISHI, GREG BEAUCAGE, Univ of Cincinnati — Industrially relevant products often display a complex multi-level hierarchical, nano-to macro-scale structure. Control over this complex multi-hierarchical structure can be achieved through manipulation of filler-polymer compatibility/incompatibility such as by varying the silanol surface density, by chemically-tailoring the surface, and by grafting low molecular weight polymers. These modifications control dispersion and the associated emergent multi-hierarchy. Kinetic dispersion in reinforced elastomers has been likened to thermal dispersion leading to a pseudo-thermodynamic model.[1,2] The dispersion of modified fillers is quantified using this approach. These interactions can be classified as weak and strong depending on the presence of correlations. Interactions and dispersion are modeled using a random-phase or a modified Born-Green approach. Surface alteration was linked to the emergence of a multi-hierarchy. From the mesh size and packing of an emergent network, the state of dispersion and the interaction potential for coarse-grain simulations were determined.


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M71.00072: New Insights into Hierarchical Structures in Polymer Nanocomposites: A Dissipative Particle Dynamics (DPD) Simulation Study*  ASHISH GOGIA, Univ of Dayton, KABIR RISHI, ALEX M MCGLASSON, GREG BEAUCAGE, University of Cincinnati, VIKRAM KUPPA (Presenter), Univ of Dayton — Polymeric systems such as natural rubber used in car and truck tires require the addition of suitable additives for the enhancement of numerous properties, including reinforcement and durability. The behavior of such fillers, (carbon black, silica, and metal oxides and some combination thereof), and their influence on nanocomposite effectiveness, depends on the filler structure, the interaction between filler-polymer matrix as well as the processing history. To understand this problem, we perform Dissipative Particle Dynamics (DPD) simulation of these blends, varying polymer-polymer, filler-filler, and polymer-filler interaction energy. We will discuss the effects of interaction strength, the scaling of polymer chains, and methods to quantify the filler percolation threshold and mesh size as a function of filler concentration. The simulation results are also validated against small angle x-ray scattering data. Additionally, the effect of such agglomerates on the structural and dynamical properties of the nanocomposites, measured via the radial distribution, mean square displacement, and autocorrelation function are also explored.

*Funding from the National Science Foundation via awards NSF CMMI-1635865 and NSF CMMI-1636036 is gratefully acknowledged.
M71.00073: Localizing Genesis in Polydomain Liquid Crystal Elastomers  

HAYDEN FOWLER (Presenter), BRIAN R DONOVAN, JOSELLE MCCracken, FRANCISCO LOPEZ JIMENEZ, TIMOTHY J WHITE, University of Colorado, Boulder — Programming the local orientation of liquid crystal elastomers (LCEs) is a differentiated approach to prepare monolithic material compositions with localized deformation. Our prior efforts prepared LCEs with surface-enforced spatial variations in orientation to localize deformation when the LCEs were subjected to directional load. However, because these surface alignment methods included regions of planar orientation, the deformation of these programmed LCEs is inherently directional. The absence of macroscopic orientation in polydomain LCEs results in uniform, nonlinear deformation in all axes (omnidirectional soft elasticity). Here, we exploit the distinct mechanical response of polydomain LCEs prepared with isotropic or nematic genesis. By localizing the polydomain genesis via masked photopolymerizations conducted at different temperatures, we detail the preparation of main-chain, polydomain LCEs that are homogeneous in composition but exhibit spatially localized programmability in their mechanical response that is uniform in all directions.

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M71.00074: Optical reconfiguration of the blue phase in liquid crystalline elastomers  

KYLE SCHLAFMANN (Presenter), TIMOTHY J WHITE, University of Colorado, Boulder — Liquid crystalline elastomers (LCEs) have been a topic of significant interest, largely motivated by their compelling performance as material actuators. Here, we detail distinctive optical reconfiguration of solid LCE compositions based on the cubic blue phases. These phases are retained in the LCE composition and exhibit selective reflection attributable to a periodic lattice superstructure. Strain-induced tuning of the selective reflection is detailed, associated with dimensional changes to lattice parameters. These materials exhibit mechanical properties that diverge from those observed within cholesteric LCEs. The influence of preparation conditions on the retention of the blue phase as well as processing conditions to increase platelet size will be discussed.
M71.00075: Predicting Stress-Strain Behavior of Thermoplastic Elastomer by Theoretical Calculation and Deep Learning*

TAKESHI AOYAGI (Presenter), CD-FMat, National Institute of Advanced Industrial Science and Technology (AIST) — Thermoplastic elastomer (TPE) is a typical industrial product where the microphase separation of block copolymer is utilized. This elastic behavior is one of the examples where the phase separated structure affects the physical properties. However, it is not simple to find the relation between complicate phase separated structure and stress-strain behavior. To tackle the problem, we applied coarse-grained simulation and deep learning technique. Stress-strain curve of various phase separated structures of ABA type triblock copolymers, where A blocks and B blocks form glassy domain and rubbery domain respectively, are investigated by the collaborative simulation of self-consistent field theory and coarse-grained molecular dynamics. Furthermore, we applied deep learning approach to make regression between the phase separated structure and stress-strain (S-S) behavior obtained by the computational simulation. The prediction of S-S behavior using trained deep learning network showed reasonably good results, and was very fast comparing to the computationally intensive simulation.

*This work was supported by JSPS Grant-in-Aid for Scientific Research on Innovative Areas “Discrete Geometric Analysis for Materials Design”: Grant Number 17H06464

M71.00076: BigSMILES: A Digitalization Scheme for Data-Driven Macromolecules Research*

TZYY-SHYANG LIN (Presenter), BRADLEY OLSEN, Massachusetts Institute of Technology MIT — In polymer research, a major hurdle preventing the adoption of data-driven approaches to modeling is the lack of a general digitalization scheme for polymeric systems. To address this issue, a digitalization scheme is proposed that consists of two components: first, a structurally based line notation that specifies how different repeating units interconnect to form polymers, and second, a data format that quantitatively specifies the distributional properties associated with the structure presented in the first part. The new line notation, BigSMILES, built on top of the popular line notation SMILES, encodes the chemical structures of polymeric fragments with “stochastic objects” that specify the constituent repeating units and the permissible set of connectivity patterns between them. Along with the accompanying data standard, BigSMILES provides a compact, machine-friendly yet versatile route to digitally encode and report polymeric materials. It is hoped that the proposed scheme can be easily utilized by both material scientist and modelling experts to enable rapid development of data-driven polymers research.

*This work was funded by the Center for the Chemistry of Molecularly Optimized Networks, a National Science Foundation (NSF) Center for Chemical Innovation (CHE-1832256).
**M71.00077: Achieving Atomic Scale Resolution of Metastable Polymers in Solution using Machine Learning**  
THOMAS OWEIDA (Presenter), North Carolina State University, HO SHIN KIM, Pacific Northwest National Laboratory, JOHNNY DONALD, YAROSLAVA YINGLING, North Carolina State University — Single-stranded DNA (ssDNA) is a metastable biopolymer that plays an important role in biological processes and has shown promise for applications in medicine and DNA nanotechnology. Understanding the structure of ssDNA in solution can provide a framework on how to control and manipulate the self-assembly and structure of ssDNA-based materials. Typically, experimental methods such as Small Angle X-ray Scattering (SAXS) are used to resolve conformational distributions of ssDNA; however, the low resolution does not provide enough information on structural details. We have developed a new method that utilizes molecular dynamic (MD) simulations in conjunction with machine learning (ML) that can obtain converged structures of metastable polymers. This study specifically performs MD simulations on ssDNA and evaluates the conformational landscape with respect to SAXS. ML methods are first used to obtain a comprehensive collection of possible ssDNA structures through simulation and subsequently used to optimize which group of individual chains closely match experimental SAXS curves. Ultimately, this process lets us break down the ensemble average embedded in SAXS and find the most probable group of metastable conformations in solution with structures defined at the atomic scale.

**M71.00078: Structural Prediction and Inverse Design by a Strongly Correlated Neural Network**  
JIANFENG LI, Fudan University, JEFF CHEN (Presenter), University of Waterloo — Macromolecules contain molecular units as the coding information for their correlated structures in physical dimensions. The relationship between these two features is governed by the interaction energies of the involved molecular units and their encoded sequences. We present a neural network algorithm that treats molecular units themselves as neural networks, which has the flexibility to allow each unit to respond to its own environment and to influence others in the system. Through a deep neural network and a self-consistent procedure, molecular units in the network establish a strong correlation to produce the desirable features in the physical world. The proposed framework is applied to the HP model. Both the forward problem of predicting folded structures from given sequences and the inverse problem of predicting required sequences for a given structure are examined.
**M71.00079: High-throughput study of mechanical properties of organic stable glasses by nanoindentation**  SARAH WOLF (Presenter), SAGE FULCO, AIXI ZHANG, YI JIN, SHIVAJEE GOVIND, HAOQIANG ZHAO, PATRICK WALSH, KEVIN TURNER, ZAHRA FAKHRAAI, University of Pennsylvania —

Glasses with enhanced stability over ordinary glasses have been formed by the process of Physical Vapor Deposition using a sufficiently slow deposition rate and appropriate temperatures. These stable glasses have been shown to exhibit higher density, lower enthalpy, and better kinetic stability over ordinary glasses, and are typically optically birefringent. These properties depend on the temperature at which the substrate is held during deposition, with temperatures near \(.85T_g\) (glass transition temperature) producing the most stable glasses. Given such exceptional properties, it is of interest to further investigate how the properties of stable glasses vary with deposition temperature and compare to those of ordinary glasses. In particular, the mechanical properties of these glasses remain relatively under-investigated. Nanoindentation is a useful technique for determination of mechanical properties, though it can present a problem of surface detection in cases of soft surfaces. Correcting for this, and using a temperature gradient sample for high-throughput acquisition of data, mechanical properties are obtained for several organic glass-formers in order to explore the relationship between chemical structure, deposition temperature, and mechanical properties of stable glasses.

**M71.00080: Photovoltaic and Electrical Properties of Diketopyrrolopyrrole Based Organic Semiconductors**  MAJHARUL HOQUE (Presenter), ANDREW LEVINE, SAUL BLAIN, JOSEPH HAMMER, VISHAL NARANG, ADAM BRAUNSCHWEIG, MILAN BEGLIARBEKOV, The Graduate Center, City University of New York —

Methylated-diketopyrrolopyrrole (MeDPP) is a small molecule, air-stable organic semiconductor with relatively high mobility, which is capable of undergoing excitonic singlet fission. Here we study the electrical transport and optical properties of MeDPP-based field effect transistors and photovoltaic devices. Using the magnetic field dependence of photocurrent in MeDPP solar cells we present strong evidence of efficient harvesting of charge carriers from triplet excitons. These results suggest that MeDPP is a promising candidate for high efficiency, air stable photovoltaic devices.

*NSF CREST IDEALS*
M71.00081: Low-temperature carrier transport of purely organic radicals embedded in double tunnel junctions* TUHIN BASU (Presenter), RYOMA HAYAKAWA, International Center for Materials Nanoarchiteconics (WPI-MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan, MIKHAIL KABDULOV, THOMAS HUHN, Department of Chemistry, University of Konstanz, 78457 Konstanz, Germany, NAHO TSUNETOMO, KAZUHIRO MARUMOTO, Division of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan, YUTAKA WAKAYAMA, International Center for Materials Nanoarchiteconics (WPI-MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan — Purely organic radicals hold promise for molecular spintronics because the molecules have weak spin-orbit coupling and the feature is expected to achieve long spin relaxation time [1]. In this work, we evaluated the carrier transport through stable oligo(p-phenylene ethynylene)-based radical molecules (TEMPO-OPE) at cryogenic temperature (<20 K). A striking point of our device is that molecules are embedded in insulating layer of a metal–oxide–silicon (MOS) structure, where the structure acts as a double-tunnel junction [2]. Obvious stepwise currents were observed in the current-voltage measurements. Furthermore, the peak positions in differential conductance curves were consistent with the molecular orbitals of the TEMPO-OPE. These results clarify that the molecules still keep their radical characters even in solid-state devices. Our proposed device therefore paves the way to realize new molecular spintronics devices with further prospect of the integration into current silicon device.


*Japan Society for the Promotion of Science (JSPS), National Institute for Materials Science (NIMS)

M71.00082: Glass Transition Temperature from the Chemical Structure of Conjugated Polymers* RENXUAN XIE (Presenter), ENRIQUE D GOMEZ, Chemical Engineering, Pennsylvania State University, University Park, RALPH COLBY, Materials Science and Engineering, Pennsylvania State University, University Park — The glass transition temperature ($T_g$) is a key property that dictates the applicability of conjugated polymers. The $T_g$ demarks the transition into a brittle glassy state, making its accurate prediction for conjugated polymers crucial for the design of soft, stretchable, or flexible electronics. In this work, only one adjustable parameter is used to build a relationship between the $T_g$ and the molecular structure of 32 semiflexible (mostly conjugated) polymers that differ drastically in aromatic backbone and alkyl side chain chemistry. An effective mobility value, $m$, is calculated using an assigned atomic mobility value within each repeat unit. The only adjustable parameter in the calculation of $m$ is the ratio of mobility between conjugated and non-conjugated atoms; the value for this ratio is supported by results from molecular dynamics simulations. We show that $m$ correlates strongly to the $T_g$, and that this simple method predicts the $T_g$ with a root-mean-square error of 13 K for alkylated conjugated polymers.

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M71.00083: Investigating vapor doping dynamics in poly(3-alkylthiophenes) using *in situ* technique

MARK DITUSA (Presenter), GARRETT GROCKE, TENGZHOU MA, SHRAYESH PATEL, University of Chicago — For conjugated polymers to be utilized in future organic electronic technology, their conductivity must be able to be controlled. Molecular doping has been used for this purpose, but details of this process are not well understood. Here, we report on a study of vapor doped poly(3-alkylthiophenes), a conjugated-polymer system that has been widely characterized. We use traditional dopant 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane and its less fluorinated cousins, along with poly(3-alkylthiophenes) with varying sidechain length, to probe how HOMO-LUMO overlap and spacing of the polymer affects the dynamics of the vapor doping process. These results are enhanced with characterization of the materials energetically and structurally at various time-points throughout the doping process. Spectroscopies such as UV-Vis, FTIR, and Raman give insight to the efficiency and mechanism of doping. This study shows how these techniques can be leveraged to probe how variables such as polymer structure, strength of dopant, and processing affect the final properties of molecularly-doped conjugated polymers.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. (DGE-1746045).

M71.00084: Mechanism of charge transfer and separation in polymer/nonfullerene acceptor organic solar cells

NOZOMI OHTA (Presenter), Japan Women's Univ-Facul Sci, KOICHI YAMASHITA, Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, AZUSA MURAOKA, Japan Women's Univ-Facul Sci — Recently, in the research fields on the organic solar cells (OSCs), it has been reported that it succeeded in synthesizing polymer/nonfullerene acceptor OSCs, and showed the power conversion efficiency (PCE) higher than polymer/fullerene type. Also, it was reported that nonfullerene acceptors were successfully fluorinated and showed higher PCE than non-fluorinated nonfullerene types. In this study, from the viewpoint of electronic structure, absorption spectrum, and HOMO–LUMO gap, we consider the mechanism of charge transfer and separation in polymer/nonfullerene acceptor OSCs, using time dependent density functional theory method.

We compared the absorption spectra and HOMO–LUMO gap of the PTB7/ITIC complex with those of the fullerene PTB7/PC_{71}BM complex, with those of the non-fluorinated nonfullerene PTB7/IT-4F complex. It turns out that nonfullerene type has an absorption band in the longer wavelength region compared to the fullerene type. Moreover, fluorination causes the absorption band to be slightly red shifted. In the nonfullerene type, Voc is reduced, but the PCE is increased. Therefore, the improvement in PCE is due to the Jsc improvement due to the increase in light absorption of nonfullerene acceptor.
**M71.00085: Towards the prediction and design of low-glass transition Donor-Acceptor semiconducting polymers**

SONG ZHANG (Presenter), Polymer Science and Engineering, Univ of Southern Mississippi, AMIRHADI ALESADI, Civil and Environmental Engineering, north dakota state university, SIMON RONDEAU-GAGNE, department of chemistry and biochemistry, University of Windsor, WENJIE XIA, Civil and Environmental Engineering, north dakota state university, XIAODAN GU, Polymer Science and Engineering, Univ of Southern Mississippi — Past efforts on conjugated polymers, especially donor-acceptor (D-A) type polymers have mainly focused on the understanding of their structure-optoelectronic property relationship. However, the designing rule for fabricating soft and deformable semiconducting polymers is largely neglected. Here, we report a predictive linear model to quantitatively connect the glass transition behavior of D-A polymers to the flexibility of polymer chains, which is further verified through molecular dynamics simulation. The thermomechanical performance was characterized through pseudo-free-standing tensile test, thin film DMA and verified by AC-chip calorimetry. X-ray scattering and solution neutron scattering were applied to investigate the thin film morphology and polymer chain rigidity for further proof. This model shows its guidance role in molecular engineering of a low-glass transition pristine polymer with high mechanical deformability (~ 100%).

*We thank the financial support from U.S. Department of Energy, Office of Science, Office of Basic Energy Science under award number of DE-SC0019361

**M71.00086: Tuning side chains to affect phase behavior and charge mobilities of PCPDTBT donor-acceptor conjugated polymers**

JAMES SUTJANTO (Presenter), ENRIQUE D GOMEZ, Chemical Engineering, Pennsylvania State University — Elucidating the critical components of molecular design would accelerate the implementation of conjugated polymers for electronic and energy applications. Using a donor-acceptor alternating copolymer based on a polycyclopentadithiophene benzothiadiazole backbone (PCPDTBT), we modify side chains to perturb phase behavior and charge mobilities in organic field-effect transistors. We use both branched and linear side chains of varying length and observe changes in glass transition temperatures, melting temperatures and liquid crystalline clearing temperatures using a combination of calorimetry, rheology, and X-ray scattering. Fabricating and testing field-effect transistors with PCPDTBT as the active layer yield field-effect mobilities that depend on the side chain substituent. Optimizing side chain composition and architecture is likely crucial to achieve remarkable charge mobilities of 10 cm^2/Vs that is observed with devices based on PCPDTBT.

*Financial support from The National Science Foundation under Award DMREF-1921854 and The National Science Foundation Graduate Research Fellowship Program under Award DGE-1255832 are acknowledged.
M71.00087: The Impact of Illumination on the Photoluminescence and Depth Profile of MEH-PPV/dPS Thin Films  JOSHUA MONCADA (Presenter), University of Tennessee, TANGUY TERLIER, RAFAEL VERDUZCO, Rice University, MARK DADMUN, University of Tennessee — This study focuses on the changes in photoluminescence and film structure due to white light exposure during annealing of conjugated polymer blend thin films. Previous studies in our group have shown that annealing similar polymer blend thin films above the T_g of the polymers in a dark or illuminated environment alters the film structure. These structural changes should influence the photoluminescence (PL) activity observed for the film. The present work aims to investigate the correlation between light exposure, film morphology and photoluminescence for four film compositions, 5, 20, 35, and 50% MEH-PPV. The PL of the films are measured using Raman microscopy, which showed differences in PL activity depending on illumination during annealing at 125 °C. Samples that are exposed to light during annealing exhibited lower PL. Time-of-Flight Secondary Ion Mass Spectroscopy provides the depth profile of the films that enables the correlation of the film’s morphology and depth profile to the observed PL.

M71.00088: Controlling the Backbone Flexibility of Conjugated Polymer to Achieve Superior Backbone Tensile Alignment  LUKE GALUSKA (Presenter), Polymer Science and Engineering, Univ of Southern Mississippi, WILLIAM MCNUTT, Chemistry, Purdue University, ZHIYUAN QIAN, SONG ZHANG, SUJATA DHAKAL, ZHIQIANG CAO, Polymer Science and Engineering, Univ of Southern Mississippi, JIANGUO MEI, Chemistry, Purdue University, XIAODAN GU, Polymer Science and Engineering, Univ of Southern Mississippi — Recent reports have shown increased interest in the capacity of conjugation-break spacers (CBS) to soften relatively rod-like conjugated polymers (CP) while maintaining charge mobility. Here, we provide a holistic approach to understand the thermomechanical influence of CBS length on an n-type NDI-based conjugated polymer, denoted by PNDI-Cx. CBS lengths are varied from C0 (fully conjugated) to C7 with the CBS engineered into each repeat unit for systematic evaluation. Solution small angle neutron scattering and melt shear rheology were employed to provide the first quantitative evidence of CBS influence over CP chain rigidity and entanglement molecular weight (M_e), demonstrating an increase in chain flexibility, as well as a M_e independent of CBS length. Thermomechanical property, including: modulus, glass transition temperature, and melting temperature were all shown to decrease with increasing CBS length, while a high ductility was observed for PNDI-C4 which we attribute to a large number of entanglements. Furthermore, a high degree of backbone alignment was observed upon strain through GIXD, polarized UV-vis, and AFM. We will also discuss coalignment in a blend system of PNDI-C0 (tie-chain) in a ductile PNDI-C4 (matrix) to yield enhanced charge mobilities.
M71.00089: Photoabsorption of acceptor molecules in non-fullerene type organic thin film solar cells  SUMIRE IKEYAMA (Presenter), NOZOMI OHTA, Japan Women’s Univ-Facul Sci, KOICHI YAMASHITA, Kyoto University, Elements Strategy Initiative for Catalysts and Batteries, AZUSA MURAOKA, Japan Women’s Univ-Facul Sci — The π-conjugated system is important as a semiconductor material in organic electronics such as organic light emitting diodes, field effect transistors, and organic solar cells (OSCs). Organic semiconductors can adjust the energy levels of HOMO and LUMO, so it is also possible to adjust the relative energy between the molecular orbital of the organic semiconductor and the Fermi level of the metal electrode. Therefore, selective insertion/transport of holes/electrons is essential to the realization of organic devices. Recently, it has been reported that the bulk heterojunction OSCs, which contain fluorinated naphtho[1,2-c:5,6-c’]bis[1,2,5]thiadiazole-based non-fullerene acceptors has a better photovoltaic performance. In this study, we theoretically investigate the effects of fluorine atoms on the properties and photovoltaic performance from the perspective of molecular structure, HOMO-LUMO energy gap, and absorption spectrum. FNTz-Teh-FA was found to have a lower LUMO energy. Therefore, by fluorine substitution, it is expected that $J_{SC}$ will be increased, and charge separation will be enhanced. These results provide the key to develop new organic semiconductors with the application of donor-acceptor type donors and non-fullerene acceptor materials in OSCs.

M71.00090: Controlling mixed Li/electronic conduction in conjugated polymeric ionic liquids through the addition of ionic and electronic dopants  DONGWOOK LEE, DAKOTA RAWLINGS (Presenter), University of California, Santa Barbara, IOAN-BOGDAN MAGDAU, California Institute of Technology, ELAYNE THOMAS, University of California, Santa Barbara, THOMAS MILLER, California Institute of Technology, RAM SESHADRI, RACHEL A SEGALMAN, University of California, Santa Barbara — Conjugated polymeric ionic liquids (conjugated PILs) may be useful in electrochemical applications, owing to their potential for simultaneous ionic and electronic conductivity. The addition of ionic and electronic dopants is essential to control the mixed conductivity, although the doping design rules remain largely unknown. Here, we investigate the roles of LiBF$_4$ as an ionic dopant and NOBF$_4$ as an electronic dopant on the overall mixed conduction of a model conjugated PIL, P3HT(Im$^+$)BF$_4^-$. The thiophene backbone is selected to allow hole conduction while the ionic (Im$^+$)BF$_4^-$ sidechain solvates mobile ions. The addition of either the ionic dopant LiBF$_4$ or the electronic dopant NOBF$_4$ leads to a simultaneous increase in the mixed conductivity. Improvements in ionic conduction by LiBF$_4$ and NOBF$_4$ can be interpreted as a result of plasticization and increased mobile ion density respectively. The enhanced electronic conductivity is thought to proceed from oxidative or Lewis acid doping of the polymer backbone by NOBF$_4$ or LiBF$_4$ respectively. Molecular dynamics simulation will reveal the role of LiBF$_4$ to enhanced electronic conductivity. This study offers a new insight on the impact of ionic and electronic dopants on mixed conduction and future optimization of conjugated PILs.
M71.00092: Effect of pH on the phase behavior of multiple proteins in oppositely charged weak polyelectrolyte solution  RITUPARNA SAMANTA (Presenter), VENKATRAGHAVAN GANESAN, University of Texas at Austin — We discuss the effect of pH on the phase behavior of weakly dissociating proteins in the presence of oppositely charged polyelectrolytes. We have used a hybrid methodology of coarse-grained single chain mean field simulation with constant pH method in a semi-grand canonical framework to include the fluctuating charge of the proteins and polyelectrolytes. Using the characteristics of the resulting phase behavior pertaining to multiple proteins and several polyelectrolytes, we compare the results due to charge regulation and equivalent fixed charge distribution on proteins.

M71.00093: Effect of divalent ions on mixtures of like-charged polyelectrolytes  CARLOS LOPEZ (Presenter), Physical Chemistry, RWTH Aachen — We study the rheology of mixtures of carboxymethyl cellulose and polyacrylate, two anionic polyelectrolytes in the presence of monovalent and divalent ions of the alkaline earth group. $\text{M}^{2+}$ are shown to promote interactions between the two systems, the nature of which depends on the specific interactions between the carboxyate groups and the metal cations. Addition of NaPA to $\text{M}^{2+}$CMC in salt-free solution leads to a non-monotonic dependence of the viscosity, entanglement modulus and longest relaxation time of the mixtures, presumably arising from an interplay of single chain collapse due to electrostatic screening and network strengthening resulting from associative interactions.

M71.00094: Interpolymer Hydrogen Bonding in the Presence of a Low-Molecular Competitor  ALIAKSEI ALIAKSEYEU (Presenter), VIKTOR SELIN, Materials Science and Engineering, Texas A&M University, JOHN F ANKNER, Spallation Neutron Source, Oak Ridge National Laboratory, SVETLANA SUKHISHVILI, Materials Science and Engineering, Texas A&M University — We examine the effect of dimethyl sulfoxide (DMSO) on binding enthalpy, strength of association between hydrogen-bonding polymers (poly(methacrylic) acid, PMAA), and polyvinylpyrrolidone, PVP) and their deposition within layer-by-layer (LbL) films, In solution, isothermal titration calorimetry (ITC) showed that the addition of DMSO to aqueous solutions resulted in a switching in enthalpy of binding from endothermic to exothermic. In good agreement with the ITC data, the growth mode of PVP/PMAA LbL films changed from linear to exponential with an increase in DMSO content. Neutron reflectometry (NR) studies showed that while LbL films constructed from DMSO-free solutions were stratified, significant layer intermixing occurred in the films constructed from polymer solutions with high DMSO content. This study demonstrates a facile means to control binding of polymer components and structure of assembled films in hydrogen-bonded systems.
ALEXANDER E. MARRAS (Presenter), JEFFREY VIEREGG, MATTHEW TIRRELL, Pritzker School of Molecular Engineering, University of Chicago — Polyelectrolyte complex micelles (PCMs) are widely used in the delivery of hydrophilic payloads. As oppositely charged polyelectrolytes assemble, counterions are liberated, however, when counterion concentrations are sufficiently high they prevent, or disrupt, polyelectrolyte complexation. Measuring complex stability versus salt provides a metric for the strength of ion pairing between polymers. PCM attributes are also strongly dependent on the size and chemical structure of each polymer block. Neutral blocks drive nanoscale phase separation while charged blocks control micelle core size and stability. An understanding of physical property behavior controlled by block size, chemistry, and salt conditions is crucial when designing for use in dynamic or biological environments and provide a greater understanding of the physics of polyelectrolyte assembly. In this work, we use small angle x-ray scattering, light scattering, and electron microscopy to determine scaling behaviors of micelle shape, size, and stability for many commonly used polyelectrolytes.

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CONNOR BILCHAK (Presenter), Department of Chemistry, University of Pennsylvania, SHAWN MAGUIRE, THERESA TSAGGARIS, SAMUEL WELBORN, JOHN CORSI, ERIC DETSI, Department of Materials Science and Engineering, University of Pennsylvania, JAMIE FORD, Nanoscale Characterization Facility, Singh Center for Nanotechnology, University of Pennsylvania, JAMES PRESSLY, Department of Materials Science and Engineering, University of Pennsylvania, ZAHRA FAKHRAAI, Department of Chemistry, University of Pennsylvania, RUSSELL COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania — Most research on polymer composites has focused on the addition of discrete nanofiller to a polymer matrix to enhance properties. However many applications would benefit from a percolated network of the organic or inorganic phase, such as ion conductivity. This work focuses on the development of bicontinuous materials created by infiltrating polymer into nanoporous gold (NPG) thin films. The optical properties of the NPG, characterized via ellipsometry, are reminiscent to those of gold nanorods exhibiting a plasmon peak, which is controllable through the ligament size. Polymer films of amorphous Poly(Styrene) and Poly(2-Vinyl Pyridine) which have different affinities for the gold scaffold, are infiltrated into the NPG through thermal annealing, which provides further control over the optical response. A range of chain molecular weights are studied to probe the relation between chain radius of gyration and average NPG pore size and its effect on film properties. The polymer chains in the confined pores exhibit a slowdown in segmental dynamics measured through the glass transition temperature. The broad tunability of these hybrids represents a unique template for designing functional network composite structures from flexible electronics to fuel cell membranes.

*NSF PIRE #1545884
**M71.00097: Morphological Effects on Ionic Conductivity in Solid Polymer Nanocomposite Electrolytes**

SHAWN MAGUIRE (Presenter), Materials Science & Engineering, University of Pennsylvania, ANDREEA-MARIA PANA, Chemical and Biomolecular Engineering, University of Pennsylvania, HYUN-SU LEE, Materials Science & Engineering, University of Pennsylvania, PATRICE RANNOU, MANUEL MARÉCHAL, UMR5819-SyMMES (CNRS/CEA/UGA), French National Centre for Scientific Research (CNRS), KOHJI OHNO, Polymer Chemistry, Kyoto University, RUSSELL COMPOSTO, Materials Science & Engineering, University of Pennsylvania — Perfluorosulfonic acid (PFSA) polymers, such as the benchmark Nafion®, are consistently used as proton exchange membranes (PEMs) in fuel cells and batteries. However, PFSA polymers’ high price, environmental safety issues and reduced lifetime have motivated the search for adequate alternatives. This work investigates two systems: a neat sulfonated polystyrene random copolymer (PS-S\_x) and a blend of PS-Sx mixed with sulfonated PS grafted iron oxide nanoparticles (PS-S\_x NP). Random copolymer films were characterized with electrochemical impedance spectroscopy (EIS). Conductivity values were determined for PS-S\_x with sulfonation levels ranging from 0.7mol% to 47.9mol% as a function of relative humidity (RH, 30%, 60%, 90%) at 40°C. The highest sulfonation level of PS showed a conductivity value of 0.04 S/cm at 90% RH, half that of Nafion®. The conductivity of the binary composite is investigated as a function of film morphology (i.e. discrete or percolated NP domains) and characterized through small-angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). These morphologies aim to provide increased mechanical strength and ionic conductivity compared to pure PS-S\_x systems, and offer insights into ion mobility through percolated domains.

*NSF PIRE - 1545884

**M71.00098: Spectroscopic Investigations of PEO Based Polymers and Nanofibers**

MIRCEA CHIPARA (Presenter), MOHAMMED UDDIN, OMOSOLA ORIRETAN, ELAMIN IBRAHIM, KAREN LOZANO, CARLOS DELGADO, DORINA CHIPARA, University of Texas Rio Grande Valley — Polyethylene oxide (PEO) is a special polymer, soluble in both water and some organic solvents (such as chloroform). Fullerenes are not soluble in water but are soluble in chloroform. These features have been exploited in the study of the effect of solvent and nanofiller nature on the morphology and crystalline structure of PEO. Both “bulk” samples and mats of PEO nanofibers obtained by force spinning from solutions of PEO in water or chloroform have been investigated by spectroscopic techniques (Raman, UV-VIS, X-Ray diffraction). X-Ray investigations were focused on the crystallites’ size, the unit crystal parameters, and potential stress effects as revealed by the dependence of the X-Ray line position and width on the spinning rate, PEO concentration in the solvent, and Sn load. Additional information regarding crystalline phases and the mechanical stresses/strains in PEO polymers and mats of nanofibers have been obtained by Raman spectroscopy, using as excitation both a green (583 nm) and a red (785 nm) laser. The dependence of the position of Raman lines on spinning rate and nanofiller concentrations investigated in detail.

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**M71.00099: Deformation Mechanisms of Polyolefin Hard-Elastic Films during Uniaxial Stretching**

YUANFEI LIN (Presenter), South China Univ of Tech, LIANGBIN LI, University of Science and Technology of China — Polyolefin hard-elastic films composed of highly oriented lamellar stacks can serve as one ideal sample to study the intrinsic deformation mechanisms of lamellar stacks, the basic structural and deformation unit in semi-crystalline polymers. With the quick development of synchrotron radiation X-ray scattering techniques, we were able to track the structural evolutions of hard-elastic polyolefin films during uniaxial stretching with the aid of a home-made tensile device. The effects of strain, strain rate and temperature on the nonlinear mechanical behavior and structural evolution of oriented lamellar stacks were systematically studied. And the different dominant deformation mechanisms, including microphase separation within interlamellar amorphous, microbuckling behaviors, crystal slipping and melting-recrystallization, dominate in different external tensile fields. The roadmap of microstructural evolutions of oriented lamellar stacks was constructed in temperature-strain space, which might aid to guiding the real processing of high-performance polymer films.

**References:**

Polymer 2019, 178, 121579.
Polymer 2018, 148, 79-92
Polymer 2018, 154, 48-54.

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**M71.00100: The Rheology of Crystallizing Polymers: Towards a Universal Description**

KALMAN MIGLER (Presenter), DEBRA AUDUS, National Institute of Standards and Technology — A longstanding goal in polymer rheology is to develop a physical picture that relates the growth of mechanical moduli during polymer crystallization to that of structure. We have recently shown that the rheology is dominated by the formation and growth of the spherulitic superstructures. Here, we aim to develop a universal description of the process by exploring the roles of temperature, surface and bulk nucleation densities, and gap thickness. We study the model system of isotactic polypropylene (iPP) through simultaneous mechanical rheology and optical microscopy, with augmentation by deterministic reconstruction and stochastic simulations. We collapse the variable space by considering two scaled parameters; one related to bulk nucleation density and the other to surface.
M71.00101: Suppression of crystallization in thin films of cellulose acetates and its effect on gas transport characteristics*  HAIQING LIN (Presenter), State Univ of NY - Buffalo — This study elucidates the discrepancy in gas permeability between bulk films and asymmetric membranes of semi-crystalline cellulose acetates (CAs) from perspectives of thickness-confinement and crystallization suppression. CAs are the workhorse membrane materials for industrial CO₂/CH₄ separation. Bulk films of CAs often exhibit CO₂ permeability values of 1.8-6.6 Barrers at 35 °C, which correspond to permeance values of 36-132 GPU for asymmetric membranes with assumed selective layers of 50 nm. However, commercial CA membranes can have CO₂ permeance values as high as 200 GPU with a CO₂/CH₄ selectivity comparable to the bulk polymers. We hypothesize that as the CA films become thinner, the thickness confinement inhibits crystallization and thus increases gas permeability while retaining gas selectivity. To validate this hypothesis, freestanding cellulose diacetate (CDA) films with thicknesses ranging from 218 nm to 20 µm were prepared, and their crystallinity was determined using Differential Scanning Calorimetry and Wide-angle X-ray Diffraction. Crystallinity can be suppressed by the decrease in the film thickness. Gas solubility and permeability can be satisfactorily correlated with the crystallinity using the empirical equations available in the literature.

*NSF

M71.00102: Prefreezing of Different Folding States of Linear Polyethylene on Graphite
OLEKSANDR DOLYNCHUK (Presenter), ANN-KRISTIN FLIEGER, THOMAS THURN-ALBRECHT, Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg — Prefreezing is the interface induced crystallization of a melt on a solid substrate. In contrast to heterogeneous nucleation, prefreezing is an equilibrium phenomenon that refers to the reversible and abrupt formation of a crystalline layer at a temperature $T_{\text{max}}$ above the bulk melting point $T_m$. Recent experimental results evidenced that thin films of oligomeric linear polyethylene prefrozen on graphite have a complex structure consisting of a thin layer of extended chain (EC) crystals directly at the graphite and folded chain (FC) crystals on top of this layer. Temperature dependent AFM experiments showed that EC crystals prefreeze at a higher $T_{\text{max}}$ than that of FC crystals: $T_{\text{max,EC}} > T_{\text{max,FC}}$. To explain this behavior, we extend the recently developed phenomenological theory of prefreezing to the case when a melt can crystallize in phases of different thermal stability with melting temperatures $T_{m1} > T_{m2}$. Our analytical results indicate that while the more stable crystal phase prefreezes at a higher temperature $T_{\text{max}1}$, prefreezing of the less stable phase is thermodynamically preferred at lower temperatures, $T_{\text{max}2} < T_{\text{max}1}$. This behavior is in contrast to bulk crystallization, where crystallization of the less stable FC crystals is often kinetically preferred.
M71.00103: Epitaxial Crystallization of PE Atop Graphene by Vapor Deposition  YUCHENG WANG (Presenter), RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — Epitaxial crystallization of polymers is a fascinating phenomenon that drives crystal structures under lattice matching conditions as a result of the interfacial interactions between specific pairs of a polymer and an underlayer material. However, fundamental investigations of epitaxial crystallization are impeded by the difficulties in preparing uniform ultrathin polymer layers and fine tuning of the film thickness, especially for polymers with low solvent solubility or fast crystallization kinetics such as polyethylene (PE). In this study, exploiting a physical vapor deposition technique, an additive bottom-up approach that is attracting more interest in processing polymers, we demonstrate the ability to achieve better film quality and control of layer thicknesses. By applying the flexible control of substrate temperature and deposition time to the model system of PE epitaxial growth atop graphene substrates, we determine how temperature and film thickness influence crystal structure and lamellar orientation. Characterization include grazing incidence x-ray diffraction (GIXD), TEM and AFM.

M71.00104: Chiral Recognition of Poly(Lactic Acid) Stereocomplex*  TOSHIKAZU MIYOSHI (Presenter), WEI CHEN, Univ of Akron — Chiral recognition is a very important concept for structural formation of stereocomplex (SC) of right and left handed helices. A well known system is Poly(Lactic acid) SC. Recently, re-investigation of X-ray fiber diffraction proposed that there is no chiral recognition in PLA SC. In this work, solid-state NMR spectroscopy can be used to study both chain-packing and folding structure of PLA SC by $^{13}$C isotope labeling and Double quantum (DQ) spectroscopy. $^{13}$C CPMAS NMR spectra supported by isotope labeling technique provides stoichiometry of L:D in the SC phase in varied mixing ratio in the blends. DQ spectroscopy provides detailed packing structure as well as chain-folding structure. Uniqueness of intermolecular packing (chiral recognition) in SC will be highlighted.

*NSF DMR Polymers 1708999

M71.00105: Chain-Level Structure of Semi-crystalline Polymer in Thermodynamically Stable Crystal and Quenched Glass*  YI ZHANG (Presenter), FAN JIN, TOSHIKAZU MIYOSHI, Univ of Akron — Crystallization of long polymer chains changes random coil state to folded structure in thin crystal lamellae. In this work, we will study chain-level structure of $^{13}$C CH$_3$ labeled Poly (Lactic Acid) with diverse molecular weights in thermodynamically stable a crystal and quenched glass by using Solid-state NMR spectroscopy. Molecular weight effect on folding event and crystallization will be discussed.

*NSF DMR Polymers 1708999
**M71.00106: Nanoindentation of nanocomposites**  SURESH AHUJA (Presenter), materials, xerox corporation — The spray coatings were dried and the dried coatings were subjected to nano-indentation using a nano-indenter made by Hysitron. Contact area was calibrated by using silica and polycarbonate of known modulus and hardness. This work on nano-indentation of polycarbonate containing nano-particles of silica shows that there is an increase in modulus and hardness up to a certain concentration threshold in concentration. As the level of silica increases beyond a threshold level, aggregates form which results in weakening of the structure. Polymer silica interface is found to be weak as silica is non-interacting promoting interfacial slip at silica-matrix junctions. At critical stress level for silica-polymer interfacial slip is reached and filler-matrix debonding (sliding) is activated resulting in a decrease in the composite's stiffness. Departure from the analytical composite models is analyzed in terms of interface adhesion between nanofiller and polymer matrix. Results on polycarbonates are compared with those of nanocomposites of polyesters where the effect of composite hardness and modulus depended on dispersion of nano-filler in polycarbonate or polyester. Experimental results are compared against analytical models.

**M71.00107: Physical Aging in Anhydride-Cured DGEBA Epoxy**  CATHERINE GROVES (Presenter), JAMIE M KROPKA, Sandia National Laboratories, JOHN MCCOY, New Mexico Tech — In amorphous polymers, there is a temperature \( T_g \) reached upon cooling at which the thermal energy is insufficient to allow for molecular rearrangements on the time scale of the temperature change. At this point, the material becomes kinetically trapped in a glassy, non-equilibrium state characterized by excess free volume and enthalpy. Physical aging occurs as a material is held below \( T_g \) and begins to relax towards equilibrium. This relaxation can change the properties of the material and is important to understand when considering the long-term reliability in applications. In this work, the physical aging of an anhydride (Aradur 917, Huntsman) cured DGEBA resin (EPON 828, Hexion) was investigated. Four sets of samples were held between 8°C and 35°C below \( T_g \) (132°C) for 0 to 4000 hours. The properties of these samples were tested through uniaxial compression and differential scanning calorimetry to observe the changes in yield stress and heat capacity.

*Sandia National Laboratories is a multimission laboratory managed and operated by NTESS, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525.
M71.00108: Accelerated aging of an epoxy glass under elevated temperatures and compressive stresses* NOAH WHITE (Presenter), STEPHAN COMEAU, GABE ARECHEDERRA, JOHN MCCOY, New Mexico Tech, JAMIE M KROPKA, Sandia National Laboratories — The aging of the diglycidyl ether of bisphenol-A (DGEBA) cured with diethanolamine was studied both in its "neat" state and filled (at 50 vol%) with glass microballoons (D32-4500, 3M). Cylindrical test samples were compressed uniaxially and the stress-strain curves were analyzed for materials properties (principally the maximum, or yield, stress). Samples were oven-aged at five sub-Tg temperatures for extended times before testing at their aging temperatures and a range of strain rates. As the glass densifies during aging, the yield stress increases. The effect of applying uniaxial stress to the samples during aging is also studied. The samples are held at ~70% of the yield stress over periods of time (up to 24 hrs.), unloaded and then reloaded through yield. The recovery strain and yield stress are found. The yield stress is found to increase and the recovery strain to decrease as aging time increases. The rate of increase of the yield stress is compared to the oven-aged tests.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

M71.00109: Metallization of Chiral and Grooved Polymers at Nanoscale ANTHONY GRAY (Presenter), KYRA FULEIHAN, BENJAMIN SCHUTSKY, CHRISTOPHER LA FOND, MEGHAN EVANS, PETR V SHIBAEV, Physics and Engineering Physics, Fordham University — Different types of polymers with chiral or grooved pattern on the surface were covered (decorated) with metal nanoparticles (silver, gold, nickel, etc.) or thin metal films (silver) in order to create surfaces with increased light reflection and to study possible plasmonic effects arising from ordered arrangement of nanoparticles and metal films. Decorated surfaces were inspected under the microscope and studied by atomic force microscopy (AFM). It was shown that for chiral surfaces the nanoparticles tend to arrange themselves along the spirals not only on the surfaces of original chiral polymers with focal conic domains but also on their replicas made from different polymers. Changes in light scattering and transmission were attributed to the presence of metal inclusions on the surface and are discussed in detail.
M71.00110: Apparent effect of crosslinker concentration on structure and dynamics of polymeric microgels* KIRIL STRELETZKY (Presenter), SAMANTHA C TIETJEN, Cleveland State University, SAMANTHA R HUDSON, Hiram College — The effect of the amount of crosslinker on the structure and dynamics of polysaccharide microgels synthesized in a surfactant solution was studied below and above volume phase transition. When the relative amount of crosslinker was varied by a factor of a hundred, three apparent behavioral regimes emerged from static and dynamic light scattering measurements. At low crosslinker concentrations, microgel behavior was found to be consistent with homogenously crosslinked microgels that displayed uniform reversible deswelling above the transition temperature. These microgels became more diffusive with temperature increase. At high crosslinker concentrations, microgels showed an unusual temperature dependence and signs of inhomogeneous crosslinking. In this regime, microgels grew in size and became less diffusive with increase in temperature. At intermediate crosslinker concentrations, microgels didn't show significant dependence of their size on temperature except for a reproducible jump in size at the transition temperature. The apparent regimes are likely due to nonuniform crosslinker distribution in the polymer microgel, which leads to nonuniform density of microgel particles, especially at large concentrations of the crosslinker.

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M71.00111: Guided Design of Composite Graphene-Polymer Foams: From Graphene Stabilized Emulsion to Electrically Conductive Foams* ZILU WANG, YUAN TIAN (Presenter), HEYI LIANG, ANDREY DOBRYNIN, Polymer Science, The University of Akron, DOUGLAS ADAMSON, Chemistry, University of Connecticut — The surface activity of graphene enabled synthesis of composite polymer/graphene foams showing a strong coupling between electrical and mechanical foam properties. To develop a general framework for computationally driven design of composite polymer/graphene foams we use large scale coarse-grained molecular dynamics simulations. In particular, we study the affinity of the 2D elastic graphene-like sheets (G-sheets) to the interface between two immiscible solvents. The established envelop of interaction parameters was used to model emulsion polymerization resulting in polymeric foams which cells are coated with elastic G-sheets (G-shells). Upon uniaxial deformation or under foam swelling conditions, the percolating network of the G-sheets coating foam cells breaks down. This break down is manifested as an increase of the foam's electrical resistance. The disruption of the graphene networks occurs through crack formation of the G-shells covering the surfaces of the polymeric foam cells. The results of the computer simulations are compared with corresponding experimental studies of the graphene stabilized emulsions and of mechanical and electrical properties of composite graphene/polymer foams.

*NSF DMR-1535412
M71.00112: Designing Polymer Nanocomposites for Membrane Gas Separation: an Integrated Experimental and Modeling Approach*  HAIQING LIN (Presenter), State Univ of NY - Buffalo — Membrane technology is an energy-efficient approach for pre-combustion CO₂ capture and H₂ purification. Conventional membranes are based on rigid polymers with strong size sieving ability, such as poly[2,2'-(m-phenylene)-5,5'-bisbenzimidazole] (PBI) that provides high H₂/CO₂ diffusion selectivity. In this study, we demonstrate enhanced H₂ sorption and diffusion in PBI films with embedded palladium (Pd) nanoparticles, which have strong affinity towards H₂. Pd nanoparticles with uniform diameters of 6 - 8 nm are prepared via a hot-injection colloidal synthesis. The loading of Pd nanoparticles in PBI increases H₂ sorption by almost 1,000 times, and at high Pd loadings, the Pd nanoparticles may form fast channels allowing the H₂ molecules to jump from one particle to another and thus increasing the effective H₂ diffusivity. For example, adding 70 wt.% Pd in PBI increases H₂ permeability from 25 to 70 Barrers, and H₂/CO₂ selectivity from 13 to 29 at 150 °C. Such performance is above the Robeson's upper bound for H₂/CO₂ separation, demonstrating the potential of these new materials for industrial H₂/CO₂ separation. The gas transport in these PBI-Pd nanocomposites is being modeled using computational fluid dynamics (CFD) to elucidate the mechanisms for the facilitated H₂ transport.

*DOE

M71.00113: Fabrication of Carbonized Block Copolymer Particles for Cathode Catalyst of Proton Exchange Membrane Fuel Cell  YOUNG JUN LEE (Presenter), JUHYUK CHOI, HYUNJOO LEE, BUMJOON KIM, KAIST — A porous carbon particle attracted great attention as supporting material for electrocatalyst due to its high conductivity and large surface area. Herein, we demonstrate a robust strategy to carbonize block copolymer (BCP) particles with maintained their size and morphology using etchable BCP (i.e., polystyrene-block-polydimethylsiloxane (PS-b-PDMS)). Key of generating porous carbon material is to introduce cross-linking, which can enhance the thermal stability of linear BCP during carbonization. We produced monodisperse cylinder-forming BCP particles using membrane emulsification, followed by cross-linking and carbonization. We confirmed that its morphology and size distribution is well maintained after carbonization. Moreover, we demonstrate carbonized BCP (cBCP) particles as a supporting material of electrocatalyst with depositing low amount (1 wt%) of platinum (Pt) catalyst on the cBCP particles (Pt@cBCP). Pt@cBCP showed 3.6 times-higher mass activity than commercial Pt/C catalyst in oxygen reduction reaction (ORR). Moreover, we confirmed the advantages of the porous structure by comparing them with a nonporous carbon sphere.
M71.00114: Effects of Heterogeneous Segmental Friction on the Decoupling of Segmental and Chain Dynamics  
WALTER YOUNG (Presenter), Polymer Science & Engineering, University of Massachusetts Amherst, JOESPHER P. SAEZ, Chemical Engineering, University of Massachusetts Amherst, THOMAS D. KUMLIN, Chemistry, University of Massachusetts Amherst, REIKA KATSUMATA, Polymer Science & Engineering, University of Massachusetts Amherst — Segmental and chain dynamics often deviate from Rouse model predictions due to dynamic heterogeneity introduced by interfaces or temperature reduction. However, the effect of heterogeneous segmental friction on such multi-scale dynamics of polymers remains poorly understood. This work aims to elucidate a possible mechanism for the decoupling of segmental and entire chain motion by systematically altering segmental friction in statistical copolymers. A model statistical copolymer of styrene and 2-vinyl pyridine (2VP) is loaded with amine functionalized silsesquioxane nanoparticles. These nanoparticles form hydrogen bonds with 2VP, while not interacting strongly with styrene monomers. Thus, the heterogeneous polymer architecture leads to heterogeneous segment-nanoparticle friction. Segmental relaxation is studied by differential scanning calorimetry, while the chain relaxation is studied by rheology. These measurements suggest that segmental and entire chain dynamics are slowed due to increasing copolymer-nanoparticle friction by increasing nanoparticle loading and/or increasing the 2VP content of the polymer. The relationship between segmental and entire chain dynamics of these copolymer/nanoparticle composites will be discussed in this presentation.

M71.00115: Effect of Softness of Polymer Grafted Nanoparticles on the Co-assembly Behavior in 3D Confined Nanoparticle/Block Copolymer Hybrid System  
MENG XU (Presenter), HONGSEOK YUN, KANG HEE KU, BUMJOON KIM, KAIST — Controlling the spatial alignment of inorganic nanoparticles (NPs) within polymer matrix is of great importance due to its great potential for building novel hybrid materials. Herein, we demonstrate the precise spatial distribution tuning of softness-controlled polystyrene-grafted Au NPs (Au@PS) within polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) particles. The softness of Au NPs was controlled by changing the ratio of the PS ligand length to the inorganic core size. The hybrid particles produced via solvent-evaporative emulsions led to the formation of spherical PS-b-P4VP particles with radially-stacked lamellar morphology, while the spatial distributions of Au@PS NPs showed strong dependence on the softness of Au@PS NPs within PS-b-P4VP particles. Au@PS showing the characteristics of hard spheres were excluded from the block copolymer domains and formed well-ordered hexagonal packing on the particle surface. In stark contrast, Au@PS with the characteristics of soft spheres hierarchically stacked within the inner favorable domains and showed stronger selectivity to the domains which close to the center of onion particles. Finally, the phenomena will be explained by considering the entropic interactions between the BCP chains and PS ligands on Au surface.
**M71.00116: Interconnected Nanoporous Polysulfone Membranes by Microphase Separation of Randomly End-linked Copolymer Networks**  
JAECHUL JU (Presenter), RYAN HAYWARD, Univ of Mass - Amherst — Co-continuous nanostructures have been widely studied in blends, block copolymers, interpenetrating networks (IPN), and other polymer architectures. In contrast to block copolymers where equilibrium self-assembly yields ordered co-continuous phases over only small regions of composition (~5 vol. %), microphase separation in randomly end-linked copolymer networks (RECNs) has been shown to provide a kinetically insensitive route to co-continuous nanostructures and interconnected nanoporous materials across broad ranges of composition. Previously, interconnected nanoporous polystyrene (PS) materials were realized by selective etching of polylactic acid (PLA) in co-continuous PS/PLA RECNs. However, the resulting nanoporous PS structures have proven too brittle to be applied as membranes. To overcome this, we extend the concept to an engineering polymer, polysulfone (PSU), and generate co-continuous PSU/PLA RECNs and interconnected nanoporous PSU. We demonstrate that co-continuous PSU/PLA displays better mechanical properties than co-continuous PS/PLA, and that the resulting interconnected nanoporous PSU structures offer potential for applications as nanoporous templates and membranes.

*Department of Energy (DOE), DE-SC0016208

**M71.00117: Brush Structure of Polymer Grafted SiO₂ Nanoparticles Measured with Neutron Scattering**  
YUAN WEI (Presenter), MICHAEL HORE, Case Western Reserve University — Polymer chains are grafted to nanoparticles (NPs) surfaces for a variety of purposes, including altering their solubility and dispersion within a polymer matrix. Here, we have grafted either poly(methyl acrylate) (PMA) or poly(N-isopropylacrylamide) to $d \approx 10$ nm SiO₂ nanoparticles, and measured the structure of the brush with small-angle neutron scattering (SANS). For moderate grafting densities ($\sigma \approx 0.3 \text{ nm}^{-2}$), high molecular weight polymers adopt two primary conformations. Polymer chains near the NP core are stretched in the concentrated polymer brush region (CPB). Farther away from the core, polymer chains are less confined and the conformation becomes more ideal in the semi-dilute polymer brush region (SDPB). To highlight scattering from these two regions, we took advantage of selective deuteration and contrast matching. SANS measurements are analyzed using the “core-chain-chain” form factor that we recently developed. We compare and contrast the conformation of poly(methyl acrylate) in a good solvent to that of PNIPAM in both D₂O and ethanol-d₆, in which PNIPAM has LCST and UCST behavior, respectively.

*This work was supported by the NSF Polymers program (DMR-1651002).
M71.00118: Quantum metamaterials from block copolymers: synthetic pathways to and emergent properties of superconducting gyroids from triblock terpolymer nanocomposites

PETER BEAUCAGE (Presenter), Materials Science & Engineering, Cornell University — The last three decades have established block copolymer self-assembly as a scalable route to complex morphologies with exquisite control over the resulting mesostructures. The incorporation of inorganic nanoparticles into these materials has produced record-setting solar cells, batteries, and other devices. However, most of these applications make little use of the crystallographically ordered and highly topologically complex nature of the resulting domains. This unique strength of block copolymers has been shown in simulations to result in emergent properties including negative refractive indices in the visible and circularly polarized light propagation. The primary barrier to realization of these properties has been a lack of synthetic approaches to produce electronic-grade materials, such as superconductors, using block copolymer self-assembly. Using thermal treatments of PI-b-PS-b-PEO triblock terpolymer-niobium oxide nanocomposites, we develop synthetic routes to niobium carbonitride superconductors whose transition temperature varies with morphology and confinement, a first example of the plethora of emergent phenomena we expect from this exciting new class of quantum metamaterials.

*PAB thanks the NIST-NRC postdoctoral fellowship and the NSF GRFP (DGE-1650442) for support.

M71.00119: Deformation-Structure Correlations in Glassy Polymer-Grafted Nanoparticle Assemblies

ALLEN SCHANTZ, Air Force Research Lab - WPAFB, FLORIAN KÄFER, Cornell University, JINHO HYON, Rice University, JASON STREIT, Air Force Research Lab - WPAFB, CHRISTOPHER OBER, Cornell University, EDWIN THOMAS, Rice University, LAWRENCE DRUMM, RICHARD ARTHUR VAIA (Presenter), Air Force Research Lab - WPAFB — Composites made from polymer-grafted nanoparticles (PGNs) with entangled canopies can avoid the nanoparticle aggregation common in polymer-nanoparticle blends, and have allowed mechanically robust designs for structural, separation, electronic, and optical applications. Recent studies have elucidated the relationship between PGN architecture (graft density $\Sigma$, graft degree of polymerization $N$, and nanoparticle core radius $r_0$) and the retention of mechanical strength and polymer-like plasticity (i.e. crazing) below $T_g$. In parallel, the ARGET-ATRP emulsion-polymerization method has expanded the available composition and quantity of PGNs. Herein, we discuss the correlations between the structure of PGN assemblies derived from ARGET-ATRP and their elasticity, plasticity, and failure mechanisms, with a focus on elucidating the impact of secondary interactions within and between canopies, and the impact of core shape and composition.
M71.00120: Controlling Morphology of Self Assembling Nanocrystalline Reinforcing Domains by Grafting Density Design*  
AARUSHI SRIVASTAVA, JOHN MEYERHOFER, YIHONG ZHAO, Univ of Akron, SUSANA TEIXEIRA, National Institute of Standards and Technology, LI JIA, MARK FOSTER, WENHAN ZHAO (Presenter), Univ of Akron — Thermoplastic elastomers (TPEs) attain good mechanical performance by virtue of hard, reinforcing domains resulting from microphase separation of two immiscible, covalently connected parts of the chains. The use of monodisperse hard segments with a strong tendency to self-assemble into β-sheet secondary structures via cooperative multiple hydrogen bonds has received attention as a strategy for forming reinforcing domains. The β-alanine trimer grafted polyisobutylene (βA_3-g-PIB) studied here are TPEs. The β-sheet crystals provide physical crosslinks and reinforcement, and the PIB chains provide elasticity. In molecular designs f-PIB-g-βA_3 and p-PIB-g-βA_3 the chain tethering density on the surfaces of the β-sheet crystals was varied to change the long dimension of the reinforcing domains. Small Angle X-ray Scattering (SAXS) and Small Angle Neutron Scattering (SANS) measurements reveal that indeed when the chain tethering at the crystal surface is more crowded the domain dimension in the direction of β sheet stacking is reduced from over 200 nm to less than 10 nm, so all three domain dimensions are truly “nano”. SANS of samples swollen with deuterated cyclohexane show that portions of the backbone near the grafting points are stretched

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M71.00121: Influence of Graft Chain Properties on Polymer Grafted Nanocomposites*  
ANDREW EHLERS (Presenter), Materials Science and Engineering, Rensselaer Polytechnic Institute, PINAR AKCORA, Chemical Engineering and Materials Science, Stevens Institute of Technology, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — The viscoelastic behavior of polymer grafted nanocomposites (PGNs) with significantly different glass transition temperatures (T_g) between the graft and matrix polymers is investigated with molecular dynamics simulations. The effect of the dynamic coupling of the grafted and matrix polymer chains is studied by molecular dynamics simulations. These types of PGNs have been shown to have reversible and repeatable stiffening behavior upon heating (Senses, E.; Isherwood, A.; Akcora, P. ACS Appl. Mater. Interfaces 2015, 7, 14682). This unique thermal stiffening behavior was attributed to the dynamic coupling of the high-T_g adsorbed chains and low-T_g matrix chains. The PGN studied in the current work consists of a nanoparticle with grafted high-T_g polymer chains in a low T_g polymer matrix. The influence of the matrix density on viscoelastic properties is investigated to identify the mechanism of the observed stiffening in these types of PGNs. The influence of the graft properties (density and length) is also investigated to identify the mechanism of the aforementioned stiffening behavior.

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M71.00122: Development of a CVD assisted PLD system for growing atomic monolayers
SINJAN MAJUMDER (Presenter), DAVID MARK CORNELISON, KARTIK GHOSH, Missouri State Univ —
The fundamental step for development of semiconductors involves stacking of layers of thin films of materials with desired properties on a particular substrate. PLD is a technique employed for growing thin films using laser ablation of a target material. CVD is an alternate method used to deposit solid materials from a gaseous phase. However, combining these two techniques can enhance plume, gas and laser interaction to facilitate the growth of novel materials with new properties. Conformity and purity play pivotal roles in the thin film growth process. While working under Ultra-high vaccum can eliminate impurities, on the other hand, proper screening and thermal activation of the plasma of ablated materials ensures a smooth registration of the film with the substrate. In order to control the ratio of CVD to PLD action, we use an optical chopper. We also aim at studying the effect of substrate, temperature and carrier gas on the resulting film. For analysis and characterization of the developed film, we employ standard techniques like SEM, XRD, Raman spectroscopy, fluorescence and profilometry. For initial proof of concept, we demonstrate growing a metal nitride.

M71.00123: Nonlinear Elasticity and Swelling of Comb and Bottlebrush Networks*
MICHAEL JACOBS (Presenter), HEYI LIANG, Polymer Science, University of Akron, ERFAN DASHTIMOGHADAM, BENJAMIN MORGAN, SERGEI SHEIKO, Chemistry, University of North Carolina, ANDREY DOBRYNIN, Polymer Science, University of Akron — We use a combination of analytical calculations, coarse-grained molecular dynamics simulations and experiments to elucidate the effect of branched architecture on swelling of comb-like and bottlebrush networks. The equilibrium swelling ratio of such networks is shown to be larger than that of conventional linear chain networks as a result of two effects: architectural disentanglement of network strands and amplification of polymer-solvent interactions by side chains. For networks of brush-like strands with poly(dimethyl siloxane) side chains in toluene, we achieve a swelling ratio of $Q = 30$, which is larger than that of linear chain networks with the same strand length. All of the studied systems, including linear chain, comb, and bottlebrush networks, follow a universal scaling relation, $G(Q) \sim Q^{-\delta}$, between the shear modulus $G(Q)$ and swelling ratio $Q$ with scaling exponents $\delta = 2.6\pm0.08$ (simulations) and $\delta = 2.6\pm0.12$ (experiments). These values agree with the theoretically predicted exponent $\delta = 8/3$, confirming dominant contribution of three body interactions to the osmotic pressure which drives network swelling.

*The authors acknowledge funding from the National Science Foundation DMR-1921923.
Gelation of DGEBA epoxy in the presence of a tertiary amine for temperatures above and below the ceiling temperature

JOHN MCCOY (Presenter), CATHERINE T. HOUSE, New Mexico Tech, JAMIE M KROPKA, Sandia National Labs — DGEBA epoxy is reacted with the curative diethanolamine (DEA). DEA has a single secondary amine that reacts rapidly with epoxide forming a non-crosslinked adduct in about 30 minutes under normal, 70°C, cure conditions. The subsequent crosslinking reaction is much slower, taking 24 hrs. at 70°C to near completion for the standard DGEBA/DEA mix. Cures at elevated temperature (above ~80°C) display a slowing of the overall rate of reaction in a "ceiling temperature" effect which results from a series of reactions associated with the zwitterion driven addition reaction. Here we measure the gel point across a wide range of temperature. At low temperatures, a simple bubble viscometer is used, while traditional rheology is employed for high temperature tests. We find that the extent of cure at gelation is 42±3% for all cases. We show that our measurements are in good agreement with predictions of Carothers and Flory-Stockmayer Theories of gelation.

The effect of water sorption, high temperature aging, and cooling rate on the calorimetric signature of the aging of an epoxy glass

STEPHAN COMEAU (Presenter), BRANDON MCREYNOLDS, TAYLOR LE, JOHN MCCOY, New Mexico Tech, JAMIE M KROPKA, Sandia National Laboratories — Stephan Comeau, Brandon McReynolds, Taylor Le, John D. McCoy, Jamie M. Kropka 2
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2) Sandia National Laboratories

The cure of DGEBA with diethanolamine results in an epoxy that is susceptible to complex aging signatures. Aging at room temperature (about 50°C below Tg) and ambient humidity results in three distinct features: a pre-Tg peak starting 30°C below Tg, a broad post-Tg Shoulder from Tg (75°C) to 175°C, and a decrease in Cp between 175°C and 200°C (chemical aging). Unlike the other features the high-T decrease in Cp persists after the first heat. Extended isothermal holds at 200°C remove the high-T decrease in Cp and slightly increase the Tg (indicating additional cure). Water soaked samples and samples stored in sub ambient conditions, show an evolving pre-Tg peak and an evolving post Tg-shoulder. The pre-Tg peak also occurs in Samples rapidly cooled (10°C/min) from above Tg and then aged.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
M71.00126: Introducing imide-based functional groups for enhanced self-healing properties of polyurethane*  HEE JEONG PARK (Presenter), Dankook University, SUNG WOO HONG, Korea Institute of Industrial Technology, DONG HYUN LEE, Dankook University — A functional polyurethane with imide moiety (PUI) is synthesized and the self-healing properties are compared with conventional polyurethane (PU). As the imide-based molecules with either mono-hydroxyl or di-hydroxyl groups are added to the mixtures of reactants including polyols and cross-linkers, the imide groups are successfully incorporated to the polyurethane chains. Therefore, while the mono-hydroxyl imide-based molecules give only interacting sites to PU chains, the di-hydroxyl imide-based molecules provide both interacting sites and chemical crosslinks. Interestingly, despite a small amount of the imide moiety in polyurethane, it is observed that the self-healing properties are drastically enhanced as compared to those of PU. Especially, PUI based on imide derivative with di-hydroxyl groups exhibits more excellent self-healing performances compared with that with mono-hydroxyl groups because of the unique intermolecular networks of reversible interactions and chemical crosslinks.

*This research was supported by Gyeonggi Regional Research Center (GRRC) program (GRRC DANKOOK 2016-B02 / GRRC DANKOOK 2017-B01), Korea Institute for Advancement of Technology (KIAT) grant funded by the Korea Government (MOTIE)(P0002007, The Competency Development Program for Industry Specialist).

M71.00127: Relationship of Local Strain-Field and shape of Crack-tip in the Dynamic Crack of Filled Elastomers  THANH-TAM MAI (Presenter), KENJI URAYAMA, Kyoto Institute of Technology — The correlation between the crack-tip shape and local strain-field in the dynamic crack with both subsonic ($V < C_s$) and supersonic ($V < C_s$) motion of filled elastomers is investigated, where $V$ and $C_s$ are crack-growth rates and shear wave speed. The shape of the crack-tip is characterized by the deviation from the parabolic shape ($\delta$) and the opening displacement (CTOD). The strain-field around the crack-tip is calculated by the two-dimensional digital image correlation technique (DIC) on the basis of the speckle images captured by a high-speed camera. The vertical strain field ($e_{yy}$) near the crack-tip can be characterized by the relation $e_{yy} \sim (1/r)^{\alpha}$, known as a crack-tip singularity. We discuss the correlation between the features of the local strain field ($\alpha$ and strain field distribution) and those of the crack-tip shape ($\delta$ and CTOD).
M71.00128: From quantum mechanics to viscoelasticity: A multiscale modeling and characterization of radical initiated modification of polyolefin in molten state  WEIZHONG ZOU (Presenter), Massachusetts Institute of Technology, AMBER TUPPER, Cooper-Standard Automotive Inc., NATHAN REBELLO, WONTAE JOO, DUMINDA S. RANASINGHE, TZYY-SHYANG LIN, Massachusetts Institute of Technology, GENDING JI, Cooper-Standard Automotive Inc., SARAH KHANNICHE, BRADLEY OLSEN, WILLIAM H. GREEN, Massachusetts Institute of Technology, KRISH GOPALAN, CHRISTOPHER COUCH, Cooper-Standard Automotive Inc. — Multiscale approaches for peroxide-initiated grafting of vinyl silane monomers to polyolefins have been investigated with the intention of the development of a mechanistic model for the synthesis of functional copolymers by melt phase processing. A comprehensive mechanistic view of the complex radical mediated reactions is achieved by determining the reaction kinetics through both quantum theory and model compound study. Our results clearly show that the overall mechanism is dominated by grafting single monomer of vinyl silane to hydrocarbon substrates, rather than forming localized or homopolymer grafts, and this occurs at the expense of polymer crosslinking due to the termination of radicals via combination. A fundamental kinetic model is therefore established to depict the general chemistry involving all the critical reactions in modification of molten polymer and their relationships to processing conditions. Combined Fourier transformation infrared spectroscopy with gel permeation chromatography, the further implement of this kinetic model to our recently-developed topology-based viscoelastic model allows, for the first time, to estimate both the yield of graft content and the change of rheological properties during the synthesis of polyolefin graft copolymer in molten state.

M71.00129: Electro-mechanical transduction of ionoelastomer junctions* MATTHEW MCBRIDE (Presenter), HYEONG JUN KIM, Univ of Mass - Amherst, BAOHONG CHEN, ZHIGANG SUO, Harvard Univesity, RYAN HAYWARD, Univ of Mass - Amherst — Ionoelastomers are an emerging class of ion conducting materials wherein one of the ionic moieties of an ionic liquid pair is covalently attached to a polymer backbone, leading to solid-state electrolytes that selectively conduct ions of one charge. Herein, two oppositely charged ionoelastomers were prepared based on 1-ethyl-3-methyl imidazolium (3-sulfopropyl) acrylate (ES) and (1–(2–acryloyloxy–ethyl)–3–buthyl–imidazolium bis(trifluoromethane) sulfonimides (AT). At the interface of ES/AT, an ‘ionic double layer’ (IDL) is formed due to diffusion of mobile ions away from the interfacial region, resulting in a build-up of excess fixed charges with a capacitance of ~ 1 mF/cm$^2$. Thanks to the highly elastic properties of ILEs, along with stretchable electrodes based on embedded carbon nanotubes or graphene, ILE diodes can be repeatedly deformed to large strains (~ 100%) without failure. Remarkably, we have found that uniaxial stretching of an ILE diode produces a spike in the open circuit voltage, or correspondingly a current when the system is connected to an electrical load. This effect can be used for strain sensing or energy harvesting, especially for ambient mechanical energy sources with relatively low frequency and large strain.

*Funding from NSF through grant DMR-1609972
M71.00130: Comparison of the mesh size for semi-dilute worm-like micelles obtained through rheology, neutron scattering, cryo-TEM, and theory.  

HANQIU JIANG (Presenter), The China Spallation Neutron Source (CSNS), Institute of High Energy Physics, KABIR RISHI, GREG BEAUCAGE, KARSTEN VOGTT, Univ of Cincinnati — Worm-like micelles (WLMs) are amphiphilic structures that display viscoelastic properties due to entanglement of robust thread or hair-like morphology. In the semi-dilute regime, the properties of wormlike micelle solutions are no longer governed by the features of individual micelles but rather by the emergent inter-micellar structure reflected in a transient network characterize by the mesh size. A new approach was developed to obtain the mesh size information from small-angle neutron scattering (SANS) data. This observed mesh size was compared with those obtained through rheology, cryo-TEM and by theory. The different physical origins of these values are discussed. The corresponding osmotic pressure was also calculated based on the mesh size from SANS at various salt concentrations and temperatures. It was used to predict concentration and thermal critical points which correspond with observed phase separation. Reasonable agreement was found for the dynamic, structural, and theoretical mesh size, sufficient to support structural interpretations of rheological data which form a basis for theoretical predictions of the complex rheology displayed by WLM systems.

*Procter & Gamble Company

M71.00131: Nonlinear shear flow experiments suggest no missing physics in slip-link models of entangled polymer melts  

DIEGO BECERRA, ANDRES CORDOBA, Chemical Engineering, Universidad de Concepcion, JAY SCHIEBER (Presenter), Illinois Institute of Technology — The idea that the dynamics of concentrated, high-molecular weight polymers are largely governed by entanglements is now widely accepted and typically interpreted through the tube model. However, recent work has shown that tube models can not predict the maximum strain, of polymer melts under start-up of shear flow at high Rouse-Weissenberg numbers. Based on these observations it has been suggested that there are physics missing in the tube theory. Here, we show that the slip-link model can predict all the features observed in start-up of shear experiments for melts and solutions of various chemistries (PS, PI, PBD, SBR) and for various numbers of entanglements. Specifically we use the the open-source GPU implementation of the clustered fixed slip-link model, and perform simulations for the startup of shear flow for melts with 14 and 30 entanglements. We find that the maximum strain depends weakly on the number of entanglements and that it does not necessarily follow a single power law, in agreement with data. Moreover, a master curve is obtained for the shear stress normalized by its peak value vs. strain normalized by its value at the maximum stress, also in agreement with experiments.

*Funded by FONDECYT grant 11170056
**M71.00132: Electrical Properties of Hafnium Dioxide**  
CHRISTOPHER ROBLEDO (Presenter), KARTIK GHOSH, SANCHALI DAS, ZACHARY LEUTY, Missouri State Univ — Since the discovery of graphene in 2004, there has been a renewed interest in 2D materials—which have the potential to increase efficiency and speed, and decrease cost, size, and power consumption within electronic devices. Current insulating material, such as silicon dioxide, limits our ability to comply with Moore's Law—which predicts that the number of transistors within an integrated circuit doubles about every 2 years. To scale devices even further, hafnium dioxide (hafnia) has shown to be a suitable replacement in the gate oxide insulating layer in complementary metal oxide semiconductor devices due to its comprehensive performance. Atomic Layer Deposition of hafnia was grown and annealed at various temperatures between 1-2 hours and its electrical characteristics were examined. Results show that with an annealing temperature of 700°C for 1 hour, the crystallinity of the bulk material improved significantly compared to lower temperatures regardless of the annealing time. Results also show that the capacitance remains nearly constant with increasing voltage frequency. Also, the dielectric loss remains the lowest in the same sample. However, the decrease in impedance shows no significant improvement among other samples annealed at different temperatures.

**M71.00133: Biaxial Stretching of Nearly Critical Gels with Extremely Sparse Network Structures**  
TAKUMA AOYAMA (Presenter), NAOTO YAMADA, KENJI URAYAMA, Kyoto Inst of Tech — Nearly critical gels, which are obtained slightly beyond the gel point, have very low modulus due to their extremely sparse network structures. The nonlinear elasticity of such sparse polymer networks is intriguing, but their very low modulus has prevented the characterization of the large deformation behavior. The present study investigates the biaxial stress-strain behavior of nearly critical gels by means of a custom-built tensile tester optimized for soft gels. The biaxial data show that the cross-effect of strains becomes smaller as the gels approach the gelation point, and that the effect vanishes in the nearly critical gels.

**M71.00134: Capturing change in microstructure of physically assembled gels as a function of temperature and strain using in-situ RheoSAXS technique**  
ROSA MARIA BADANI PRADO (Presenter), SATISH MISHRA, Mississippi State Univ, WESLEY ROTH BURGHAHRT, Northwestern University, SANTANU KUNDU, Mississippi State Univ — The mechanical properties of physically assembled gels depend on their microstructure. During large deformation, gel microstructure changes leading to a change in their mechanical properties. Here, we have considered two gels that consist of 10% and 20%(w/w) of poly(styrene)-poly(isoprene)-poly(styrene) [PS-PI-PS] in mineral oil, a midblock selective solvent. At room temperature, collapsed PS-blocks form aggregates, which are bridged by the PI-chains resulting in a three-dimensional gel. We capture the microstructural transformation as a function of temperature in a RheoSAXS setup. The scattering data capturing the change in gel microstructure subjected to oscillatory shear-strain was collected in the 1-2 plane. Strain amplitude values of 10, 100, and 300% were applied on the gels, therefore we have been able to collect data both at small and large strain amplitude. At high strain amplitude, an elliptical two-dimensional scattering pattern has been observed indicating structural orientation along the applied strain direction. To quantify such orientation, we have estimated the anisotropic factor as a function of strain from these patterns.
M71.00135: The Geometric State of a Solid-Solid Interface  THOMAS PILVELAIT (Presenter), School of Engineering and Applied Sciences, Harvard University, SAM DILLAVOU, Physics, Harvard University, SHMUEL RUBINSTEIN, School of Engineering and Applied Sciences, Harvard University — The evolution of a static frictional interface is surprisingly elaborate. It is well known that the frictional strength of a solid-solid interface changes with normal load, but it also evolves in another way: slowly over time, in a process known as ‘aging.’ The effects of aging and a change in normal load on an interface are traditionally seen as unimportant, if they are assumed to exist at all. In a glass-silicone rubber interface, we hold the real area of contact constant over time and demonstrate the existence of differences between these two types of evolution as well as their dependence on contact geometry. This suggests that a frictional interface cannot be fully described by the real area of contact, or any such instantaneous variable, as different configurations of the same interface could all have the same total real area of contact. As the real area of contact is often used as a proxy for frictional strength, these results have important implications for contemporary models of friction, such as the widely used Rate and State Laws.

M71.00136: Surface Micro Replicas of Self-Assembled Chiral Polymers and Grooves  KYRA FULEIHAN (Presenter), CHRISTOPHER LA FOND, PETR V SHIBAEV, ANTHONY GRAY, BENJAMIN SCHUTSKY, MEGHAN EVANS, Fordham University — Transparent polymer replicas of different surface patterns appearing on chiral surfaces and gratings are created and studied at nanoscale by atomic force microscopy (AFM), infra-red (IR) spectroscopy and optical methods. Replicated polymers were represented by chiral cholesteric glassy materials with focal conic domains [1] and isotropic networks with grooved surfaces. Polymer replicas were successfully prepared from different types of glassy polymers by direct deposition from either solution or melt, creating novel opportunities for designing novel nanostructures. Different methods of replica preparation employed and optimal strategies leading to the most effective transfer of chiral surface patterns and grooves were developed and discussed. Studies of light scattering and reflection from polymer replicas were conducted in order to evaluate their suitability for subsequent metallization and design of optical metamaterials.

[1] Surface reconstruction of chiral glassy oligomers under the action of volatile organic compounds (VOCs)
P Shibaev, D Carrozzi, L Vigilia, A Panariti, GA Schwartz
Liquid Crystals 46 (1), 102-107
M71.00137: Interactions and Competitive Adsorption at Solid/Liquid Interface

NITYANSHU KUMAR (Presenter), SUKHMANJOT KAUR, Univ of Akron, RAJAT KUMAR, Biomedical Engineering, Stony Brook University, SARANSHU SINGLA, MICHAEL C WILSON, SELEMON BEKELE, MESFIN TSIGE, ALI N DHINOJWALA, Univ of Akron — Broadness in vibrational spectrum is usually associated with heterogeneity of surrounding environment. At solid/liquid interface, surface-sensitive sum-frequency generation spectroscopy (SFG) has shown wide distributions of frequency shifts of sapphire surface hydroxyl groups with several liquids in contact. Even though the shifts were associated with the interfacial interactions, the origin of variation and a physical picture of interfacial interactions are elusive in experiments. To better understand the interfacial interactions, we perform molecular dynamics (MD) simulations of liquid molecules (acetone, chloroform, and dimethylformamide) in contact with sapphire. The energy distribution profiles from MD correlate well with the experimental SFG spectra, highlighting the ability to interpret spectroscopic features with the physical insights gained from MD simulations. Further, we use MD simulations to gain insights into the preferential adsorption of acetone from acetone-chloroform binary mixtures on sapphire. The current study paves the way for the theoretical understanding of adsorption, which can benefit the development of new technologies in adhesion, coatings, and medicine.

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M71.00138: Nanoparticles as Universal Adhesives

RYAN SAYKO (Presenter), University of Akron, ZHEN CAO, MIT, HEYI LIANG, ANDREY DOBRYNIN, University of Akron — Nanoparticles are shown to be able to act as effective adhesives capable of binding two soft materials together. We performed coarse-grained molecular dynamics simulations to study contact mechanics of hard and soft nanoparticles at the interfaces between two elastic surfaces. Our simulations have shown that a nanoparticle at the interface between two elastic substrates could be in a bridging or Pickering state. The degree of penetration of a nanoparticle into a substrate is shown to be determined by nanoparticle size, strength of nanoparticle-substrate interactions and nanoparticle and substrate elastic properties. Using the Weighted Histogram Analysis Method, we calculated the potential of mean force for separation of two substrates which interface was reinforced by deformable nanoparticles. These simulations show that interface reinforcement is a function of nanoparticle size and elastic modulus. In particular we have shown that the softest nanoparticles are most effective in interface reinforcement demonstrating about eight times increase in the work of adhesion.
M71.00139: Does Flexoelectricity Drive Triboelectricity?*  CHRISTOPHER MIZZI (Presenter), ALEX Y.W. LIN, LAURENCE D. MARKS, Northwestern University — Since the first reports of friction-induced static electricity in 600 B.C., the phenomenon of triboelectricity has fascinated, and perplexed, generations of scientists. While much progress has been made in the ensuing centuries regarding the nature and identification of charged species transferred during tribocharging, a universal thermodynamic driver for charge transfer has not been found. We identify flexoelectric potential differences induced by inhomogeneous strains at nanoscale asperities as the thermodynamic driver for tribocharge separation [PRL 123, 116103 (2019)]. Using single asperity elastic contact models, we show that nanoscale flexoelectric potential differences of 1–10 V or larger arise during indentation and pull-off. Importantly, we also demonstrate our model agrees with several experimental observations including bipolar charging during stick slip, inhomogeneous tribocharge patterns, charging between similar materials, and surface charge density measurements.

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M71.00140: Unravelling the Behaviour of Brush Block Nanocomposites at Ultrahigh Strain Rates*  SRAVYA NUGURI (Presenter), ANURAAG GANGINERI PADMANABAN, JAE-HWANG LEE, JAMES J WATKINS, Univ of Mass - Amherst — Poly(tert-butyl acrylate)-block-polyethylene oxide (PtBA-b-PEO) brush block (BB) copolymers offer rapid self-assembly kinetics and ready access to long-range order. Taking advantage of cooperative self-assembly using hydrogen bonding additives, we incorporate phenol formaldehyde (Resol) resins into the PEO block to create a crosslinked network, and thus enable formation of alternating soft (PtBA) and hard (Resol crosslinked) multi-layered films. We then explore ultrahigh strain rate behaviour (>10^6 s^{-1}) of these BB nanocomposites films using Laser Induced Projectile Impact Test (LIPIT). Rigid spherical alumina particles of 15-25 µm in diameter are accelerated towards these composites with velocities ranging from 50 to 450 m/s and the corresponding impact and residual flight paths are captured by ultrafast stroboscopic imaging with exposure times of less than 1 ps. We analyse the change in kinetic energies, the deformation depth as measured by profilometry, and scanning electron microscopy images to interpret real-time deformation propagation across the BB nanocomposite.

*This work is supported by the Army Research Lab.
M71.00141: Guided Design of Strain-Adaptive Polymer Networks*  HEYI LIANG (Presenter), ANDREY DOBRYNIN, Univ of Akron, MOHAMMAD VATANKHAH-VARNOSFADERANI, ANDREW N. KEITH, SERGEI SHEIKO, Department of Chemistry, University of North Carolina at Chapel Hill — Mimicking the mechanical behavior of biological tissues is crucial for medical implants and wearable electronic devices. Many biological tissues are supersoft at small deformations (Young's Modulus $E_0<10$ kPa) and stiffens as deformation increases. This combination of softness and nonlinear elasticity cannot be duplicated by synthetic elastomers composed of linear polymers. Graft polymers (combs or bottlebrushes), consisting of linear backbones with grafted side chains, endow polymeric materials with diluted backbone entanglements and backbones pre-stretching due to steric repulsions between side chains. These distinct features pave the way for the design of supersoft materials with controllable nonlinear elasticity. Such materials can be prepared by chemical crosslinking of graft polymers or by self-assembly of linear-bottlebrush-linear triblock copolymers. We have developed a design strategy to encode the nonlinear mechanical response of soft materials through the architecture of graft polymer networks by changing the strand length, side chain length, side chains grafting density and block lengths. Materials replicas of jellyfish, artery and skin tissues based on poly(dimethylsiloxane) bottlebrushes were synthesized to verify the design approach.

*NSF DMR-1535412, DMR-1921923

M71.00142: A Comparative Study of Hydrogen Bond Organization between Hyperbranched Polymers and Dendrimers Based on bis-MPA*  BEIBEI CHEN (Presenter), SAMANTHA DAYMON, MALIHA N. SYED, Univ of Southern Mississippi, OLUWAPELUMI KAREEM, MCKENNA REDDING, Tulane University, BRIAN OLSON, Univ of Southern Mississippi, SCOTT M GRAYSON, Tulane University, SERGEI NAZARENKO, Univ of Southern Mississippi — Physical properties hyperbranched polymers (HBPs) based on 2,2-bis(hydroxymethyl) propionic acid (bis-MPA), which have been widely studied, are largely determined by the hydrogen bonds (H-bonds). However, similar studies have not yet been extended to bis-MPA based dendrimers which require considerable synthetic efforts. In this study, hydrogen bond organization and interrelated structural order formation of a bis-MPA based second-generation dendrimer (D2) were investigated in comparison with its HBP analogue (HBP2). WAXS spectra of both polymers showed similar structural ordering originated from clustering of multiple hydroxyl groups mediated via H-bonds. MD simulations well predicted the WAXS spectra and revealed ‘chain-like’ clusters of different lengths from single H-bond associations to clusters containing tens of hydroxyls. D2 showed higher propensity of forming long clusters than HBP2 indicating terminal hydroxyls are more capable of forming long associations than linear ones. Meanwhile, an additional narrow peak which superimposed on the amorphous halo was only observed on the WAXS spectra of HBP2. The origin of this narrow peak was assigned to a pseudo-hexagonal mesophase formed by linear chain segments.

*This work was supported by National Science Foundation.
M71.00143: Unusual Protein Adsorption Phenomena on Ultrathin Homopolymer Films
YUTO KOGA (Presenter), Cornell University, YASHASVI BAJAJ, DANIEL SALATTO, ZHIXING HUANG, Stony Brook University, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory, DMYTRO NYKYPANCHUK, Brookhaven National Laboratory, MAYA ENDOH, TAD KOGA, Stony Brook University — Recently, we designed a new anti-fouling polymer nanolayer of a few nanometer-thick composed of non-charged homopolymer chains physically adsorbed onto a solid [1]. Interestingly, the anti-fouling property of this polymer nanolayer emerged regardless of the degree of hydrophilicity of the polymers against a model protein (bovine serum albumin (BSA). However, it was observed that 50 nm-thick spin-cast thin films composed of the same homopolymers showed BSA adsorption. To shed light on the anti-fouling/fouling switching between the nanolayer and thin film, BSA adsorption was studied on a series of ultrathin films of different thicknesses (2-200 nm in thickness) using polystyrene, poly(2-vinyl pyridine), polybutadiene, poly(methyl methacrylate), and polypropylene. Additionally, we examined the adsorption behavior of another protein, Fibrinogen, to see generality/differences in the anti-fouling/fouling switching. To quantify the protein adsorption, photon counting spectrofluorometry along with the fluorescence-labeled proteins was utilized. We will discuss the universal anti-fouling/fouling switching as a function of film thickness regardless of the polymer and protein choice.

M71.00144: Unravelling the mechanism behind adhesion failure events at the polymer-solid interfaces
ZHIXING HUANG (Presenter), DANIEL SALATTO, JUSTIN CHEUNG, MAYA ENDOH, TAD KOGA, State Univ of NY - Stony Brook — Polymer thin films on solid substrates play a crucial role in nanocomposite materials as well as protective industrial coatings. In particular, polymethylpentene (PMP) has been reported to have a wide array of very promising properties such as high heat tolerance (melting point of 220°C) and resistance to a variety of both inorganic and organic chemicals and materials. In this presentation, we chose PMP thin films on a weakly attractive silicon substrates as a rational model to understand the mechanism of adhesion failure at the solid interface. We will discuss the critical role of a physically adsorbed polymer layer (“adsorbed nanolayer“) at the polymer-substrate interface in the adhesion failure event.
M71.00145: Phase behavior of disk-coil block copolymers under cylindrical confinement: Curvature-induced structural frustrations*  MIN YOUNG HA (Presenter), Seoul Natl Univ, YONGJOO KIM, Korea Advanced Institute of Science and Technology, WON BO LEE, Seoul Natl Univ — We explore the self-assembly of disk-coil block copolymers (BCPs) confined within a cylinder using molecular dynamics simulations. We obtained concentric lamellar structures with a different number of alternating disk-rich and coil-rich bilayers as a function of the cylinder diameter and coil length. Our study focuses on the curvature-induced structural behavior in the disk-rich domain after self-assembly, investigated by local density distribution $P(r)$ and orientational distribution $G(r, \theta)$. In the inner layers of the cylinder-confined system, both $P(r)$ and $G(r, \theta)$ show characteristic asymmetry within a bilayer, directly contrasted to its bulk and slab-confined counterparts. We successfully attribute the curvature-induced structural behavior of disks to (1) packing frustration of disks, and (2) asymmetric stretching of coils to regions with different curvatures of a bilayer. Our results are important to understand the self-assembly of BCPs containing rigid motif in confinement, such as the self-assembly of bacteriochlorophyll confined by lipid layer to form a chlorosome, the photosynthetic antennae complex found in nature.

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M71.00146: Disordered Assemblies of Rubber Bands as a Model of Polymer Rings  NICOLAS GARCIA (Presenter), Institut Laue-Langevin, 71 Avenue des Martyrs, 38042 Grenoble, France, LEOPOLDO R GOMEZ, Department of Physics, UNS - IFISUR - CONICET, Bahía Blanca, Argentina, THORSTEN POESCHEL, MSS, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — A comprehensive understanding of the packing structure of dense assemblies of semiflexible rings is not only fundamental for the dynamical description of polymer rings but also key to understand biopackaging, such as observed in the circular DNA of viruses or genome folding.

In this work, we use X-ray tomography to study disordered packings of rubber bands in a cylindrical container as a simple model of semiflexible polymer rings. Using advanced computational tools, we study the geometrical and topological features of disordered packings of rubber bands at a single ring-level. The degree of entanglement in the structures is quantified through minimal surfaces and generalized Voronoi tessellations. We found that assemblies of short bands assume a liquid-like disordered structure, with short-range orientational order, revealing a minor influence of the container. In the case of longer bands, the confinement causes folded configurations, and the bands interpenetrate and entangle. Most of the systems are found to display a threading network that percolates the system. Surprisingly, for long bands whose diameter doubles the diameter of the container, we observe that all bands interpenetrate each other in a complex fully-entangled structure.
M71.00147: Multiple arms star polymer translocation from a cylindrical cavity subject to a pulling force  MESAY TILAHUN ABEBE, YERGOU TATEK (Presenter), Addis Ababa Univ — A Langevin dynamics computer simulation is used to investigate the dynamics of star polymer translocation from a cylindrical cavity (tube), which is connected to a plane wall having a circular nanopore along the tube axis. Star polymers of different masses and number of arms or functionalities are considered in the present study. The translocation is carried out by applying an external pulling force which is exerted only on the end monomer of one arm. For a strong pulling force regime and for a given functionality, the translocation time exhibits a power law dependence on the polymer mass where the exponent is found to be close to 2. We have also found that the translocation dynamics of chains of constant mass but varying functionality is significantly affected by the pore radius. For wider pores, the translocation time decreases continuously as the number of arms increases, while in the case of smaller pores, the average exit time shows a non-monotonic behavior with a minimum around a critical functionality $f_c$. In addition, the translocation dynamics was also investigated in terms of tube length and tube aspect ratio.

M71.00148: The Cononsolvency Effects: A Coarse Grained Simulation Study  JING ZONG (Presenter), DONG MENG, Mississippi State Univ — One puzzling phenomenon about polymer conformations in a mixture of solvents is the cononsolvency effect -- polymers in a good solvent undergo reentrant coil-to-globule-to-coil transition upon addition of a good cosolvent. Recent studies have suggested the generic nature of the cononsolvency effect independent of chemically specific details of the polymer and solvents. In this study, we first reinforce such claim by showing that a coarse-grained soft model frequently used in studying polymers is able to reproduce the reentrant transition at the single-chain level, provided that solvents are treated explicitly. In our Monte Carlo simulations, the coil-to-globule-to-coil transition occurs as the chemical potential of polymers in solution decreases upon increasing the cosolvent fraction, ruling out increasingly worse solvent quality as the cause of collapse. To further our microscopic understanding, we apply the soft model to studying conformational responses of surface-grafted polymers under the cononsolvency effect. By analyzing the inter-polymer density correlations, we illustrate the highly correlated nature of polymer clustering mediated by the cosolvents. Conformational responses of high grafting density brushes will also be discussed in the context of smart sensor surfaces.
M71.00149: Detection of Hip Infections Using an Injectable Hydrogel Based Synovial Fluid pH Sensor*  SACHINDRA KIRIDENA (Presenter), UTHPALA WIJAYARATNA, MD. ARIFUZZAMAN, JEFFREY N. ANKER, Clemson University — A hydrogel-based sensor was developed which could be attached to prosthetic hips prior to implantation, to measure pH in the joint fluid in order to detect, monitor, and study infection. A common complication of hip surgeries are post-surgery infections. Delayed diagnosis would lead to reduced function, increased morbidity and may require more complex surgeries. Therefore, early detection of infections is important for successful management of hip infections. In order to detect infection biomarkers, the joint is aspirated and the synovial fluid is analyzed. However, joint aspiration performed by a radiologist under fluoroscopy or ultrasound guidance is painful and is impractical for routine screening or serial monitoring during treatment. The developed synovial fluid sensor provides a method of early detection and monitoring of hip infections using plain radiography. The sensor is made of a pH responsive polyacrylic acid-based hydrogel and the response was determined from the radiograph by measuring the position of a radio-dense tantalum bead embedded in the hydrogel. Thus, the developed sensor could be used as a potential X-ray imaging functional chemical sensor.

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M71.00150: WITHDRAWN ABSTRACT —

M71.00151: Shape-Switchable Block Copolymer Particles Exhibiting Light-Responsive Surfactants  KANG HEE KU, MIT, JUNHYUK LEE, YOUNG JUN LEE (Presenter), BUMJOON KIM, KAIST — Particles capable of changing their shape in response to external light irradiation may serve as promising bio-inspired, smart materials for clinical and biomedical applications due to their remarkable spatial/temporal resolution. Herein, we report polystyrene-block-poly(2-vinylpyridine) (PS-b-P2VP) block copolymer (BCP) particles exhibiting shape and morphological transition induced by light irradiation. Key of forming light-dependent BCP particles is to design surfactants containing light-active groups (i.e., nitrobenzyl ester and coumarin ester), which can light-dependently modulate interfacial activity. With irradiating light, a sphere with onion-like inner morphology changes to prolate or oblate ellipsoids with axially stacked nanostructures. In addition, wavelength-selective shape transformation of BCP particles is achieved by a mixture of two light-active surfactants, which respond to the light with different wavelengths (i.e., 254 and 420 nm). Moreover, we demonstrate the color- and shape-changing particles in response to the light, which can be achieved by the use of light-emitting, photo-responsive surfactants. Finally, we integrate shape-switchable BCP particles into a hydrogel film to demonstrate the modulation of the particle shape in sub-micrometer resolution.
M71.00152: Configurational contribution to the Soret effect of a protein ligand system*  
JUTTA LUETTMER-STRATHMANN (Presenter), Physics and Chemistry, University of Akron — Many of the biological functions of proteins are closely associated with their ability to bind ligands. Since binding state and conformation of a protein affect its response to a temperature gradient, they may be probed with thermophoresis. In recent years, thermophoretic techniques to investigate biomolecular interactions, quantify ligand binding, and probe conformational changes have become established. To develop a better understanding of the mechanisms underlying the thermophoretic behavior of proteins and ligands, we employ a simple, off-lattice model for a protein and ligand in explicit solvent. To investigate the partitioning of the particles in a temperature gradient, we perform Wang-Landau type simulations in a divided simulation box and construct the density of states over a two-dimensional state space. This method gives us access to the entropy and energy of the divided system and allows us to estimate the configurational contribution to the Soret coefficient. For dilute solutions of hydrophobic proteins, we find that a hard-sphere solvent model captures important aspects of protein-ligand interactions and allows us to relate the binding energy to the change in Soret coefficient upon ligand binding.

*Research Center Juelich and the University of Halle (DFG - SFB TRR 102)

M71.00153: Packing density, homogeneity, and regularity: quantitative correlations between topology and thermoresponsive morphology of PNIPAM-co-PAA microgel coatings*  
CAMDEN CUTRIGHT (Presenter), North Carolina State University, ZACH BROTHERTON, Chemical Engineering, University of Texas- Austin, JAKE HARRIS, LANDON ALEXANDER, KAIHANG SHI, SAAD KHAN, JAN GENZER, STEFANO MENEGATTI, North Carolina State University — We investigated the formation of monolayers of microgel particles comprising poly[(N-isopropylacrylamide)-co-(acrylic acid)] on solid substrates, their surface morphology, and stimuli-responsiveness. Crosslinked microgels with different composition were produced showing a range of response in swelling with temperature and pH. Microgels were deposited on silicon wafers primed with a bilayer of poly(octadecene-alt-maleic anhydride) and polyethyleneimine. The characterization of the microgel-coated wafers led to the identification of three metrics describing microgel arrangement: density (ρ); heterogeneity (H), which correlates strongly with ρ and depends on deposition temperature and pH; and packing efficiency (PE), which portrays the regularity of microgel arrangement and exhibits no correlation with ρ nor H. The values of ρ, H, and PE calculated for in silico models of microgel coatings confirmed that these three metrics portray distinct characteristics of surface topology. Finally, laser profilometry showed that microgel coatings respond to thermal stimuli with sensible variations in surface roughness; which correlate strongly with ρ and H, and to a lesser extent with PE.

*National Science Foundation GRFP fellowship # 2017220114.
M71.00154: Magnetically Induced Self–Healing in Iron Oxide–Poly(ethylene oxide) Nanocomposites

DONOVAN WEIBLEN (Presenter), SARAH DALAKOS, Materials Science and Engineering, Rensselaer Polytechnic Institute, CHARLOTTE TEUNISSE, Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, VANESSA R SWEPSON, Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, GRACE L GIONTA, Chemical and Biological Engineering, Rensselaer Polytechnic Institute, DENIZ RENDE, Center for Materials, Devices, and Integrated Systems, Rensselaer Polytechnic Institute, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Current research aims to quantify self-healing capabilities of iron oxide (Fe₃O₄) nanoparticle (NP) infused poly(ethylene oxide) (PEO). Iron oxide NPs of varying surface chemistries (bare, aminopropyl triethoxysilane coated, and polyethylene glycol α–, ω–diphosphate coated) are used to prepare nanocomposites of varying concentrations less than 1% by weight. Each sample, in the form of a cylindrical disc, is indented using a LECO M400 Microindenter at five different locations between the center and edge. The indentation site is examined before and after being placed in an alternate magnetic field (AMF) to induce healing. The micrographs of each indent were collected with an Olympus PMEG microscope at the same imaging parameters. Healing efficiency is quantified using visual and software-based image analysis, identifying the percentage of healing as a function nanoparticle concentration and surface chemistry. Multiple methods of software-based image analysis were developed to perform this analysis. Nanoindentation experiments were also carried out to evaluate impact of surface coating and concentration on mechanical properties and viscoelastic behavior of these nanocomposites.

*This material is based upon work supported by NSF Grant 1825254.

M71.00155: Tuning Diblock Copolymer Morphologies by Stimuli-Responsive Supramolecular Interactions

XIANGYU ZHANG (Presenter), JING ZONG, DONG MENG, Mississippi State Univ — Ability to tune the microstructures formed by block copolymers via easy-to-use physical approaches offers additional handles to the materials for practical applications. One common approach is through adding homopolymers, which induces morphological changes due to preferential partitioning of homopolymers into specific micro-domains. Recently, supramolecular forces that are chemistry-specific and stimuli-responsive have been exploited to enable stimuli-switchable morphologies. To offer microscopic insights into this process, here we present a simulation study of diblock copolymers blended with homopolymers that are associative to one of the blocks through supramolecular forces. By manipulating the manner of associations, we investigate structural changes induced by supramolecular complexations, and to elucidate the differences from the counterpart van der Waals (VDW) force-driven systems. It is found that the homopolymer-receiving microdomain exhibits non-monotonic size changes accompanied by cluster formation as preferential partitioning occurs. Dynamics analysis suggests that both morphologies and supramolecular binding kinetics exert significant influence on the diffusion of homopolymers across the microdomains, implicative of the extent of “responsiveness” of such materials.
**M71.00156: Water Dynamics and Poly(N-isopropyl acrylamide) Co-nonsolvency in Water-Methanol Solutions at Variable Temperature and Pressure**

BART-JAN NIEBUUR, Physics Department, Technical University of Munich, WIEBKE LOHSTROH, Heinz Maier-Leibnitz Zentrum (MLZ), TU Munich, CHIA-HSIN KO, Physics Department, Technical University of Munich, MARIE-SOUSAI APPAVOU, Jülich Centre for Neutron Science at MLZ, TU Munich, ALFONS SCHULTE (Presenter), Physics Department, Univ of Central Florida, CHRISTINE PAPADAKIS, Physics Department, Technical University of Munich — The phase behavior of 25 % poly(N-isopropyl acrylamide) (PNIPAM) in a 80:20 v/v water methanol mixture is investigated by quasi-elastic neutron scattering (QENS) and Raman spectroscopy at variable temperature and pressure with focus on the co-nonsolvency effect. The susceptibility spectra span the frequency range from 2 GHz to 2 THz at momentum transfers between 0.2 to 1.7 Å⁻¹ and reveal the relaxation peak of the hydration water near 10 GHz, in addition to the known processes of bulk water. The solvent phase is enriched with methanol at high pressure, implying that water is preferentially adsorbed at the chains. The exchange of methanol with water takes place mainly at the hydrophilic Amide groups of PNIPAM. The hydrophobic hydration of alkyl groups in the side chain and the backbone of the polymer in the presence of methanol is reduced at ambient and high pressure. In the two-phase region the preferential adsorption of water at the chains is diminished.

**M71.00157: Phase behavior and self-assembly of liquid-crystalline block copolymers in nematic solvents**

CHANGYEON LEE (Presenter), University of Pennsylvania, DENNIS NDAYA, REUBEN BOSIRE, RAJESWARI M. KASI, University of Connecticut, CHINEDUM OSUJI, University of Pennsylvania — Block copolymers (BCP) are an attractive class of materials that can be utilized for active/stimuli-responsive/adaptive materials. The performance of BCPs in various target applications largely relies on their controlled, long-range assembly with high fidelity. In this context, liquid-crystalline BCP (LC BCP) is a compelling material platform because of its ability to control the directional and positional arrangement by leveraging the nature of the LC block. While ranging successful examples have been showcased using LC BCPs in recent years, one may envision that incorporating LC BCPs into other material systems can be the next step forward to open up new possibilities for formulating multi-functional materials. However, neither the fundamental studies on these blend systems nor their useful functionality has been rarely reported thus far. Here, we present the phase behavior and self-assembly of LC BCPs in the blends with other LC materials such as labile mesogens and lamellae-forming block molecules. We demonstrate that LC BCPs are co-assembled with other LC materials with preserving or shifting their original phases as a function of the composition. It is also demonstrated that the blended LC materials can be aligned uniaxially under the magnetic-field.
M71.00158: Toward molecular modeling of ductility and drawablity of semi-crystalline polymers*  

MASOUD RAZAVI (Presenter), SHIQING WANG, Univ of Akron — We contrast the mechanical responses of different crystallizable polymers such as PLA, PET, PA and PS in their respective amorphous and semicrystalline states using uniaxial extension and compression at varying temperatures below and above $T_g$. Coherent phenomenology will be presented in terms of the stress response to ongoing deformation, stress relaxation behavior from both preyield and postyield, creep and real-time POM images, aiming to develop a detailed understanding of the mechanical/structural interactions between amorphous and crystalline regions. Through these experiments, we expect to gain more insights regarding the molecular mechanisms for ductility ($T < T_g$)/drawability ($T > T_g$) and effective strategies to avoid brittleness/non-drawability.

*This work is supported by NSF (DMR-1905870) and ACS PRF# 60897-ND7.

M71.00159: Probing the Impact of Polymer Hydrophobicity on Solution and Hydrated Surface Conformation*  

AUDRA DESTEFANO (Presenter), SALLY JIAO, Chemical Engineering, University of California, Santa Barbara, MIKAYLA BARRY, SEGOLENE ANTOINE, Materials, University of California, Santa Barbara, TIMOTHY KELLER, Chemistry, University of California, Santa Barbara, SCOTT SHELL, Chemical Engineering, University of California, Santa Barbara, SONGI HAN, Chemistry, University of California, Santa Barbara, RACHEL A SEGALMAN, Chemical Engineering, University of California, Santa Barbara — Sequence controlled polypeptoids provide a valueable platform for systematic study of molecular level changes in polymer patterning and chemistry; however limitations in our understanding of sequence effects on polymer conformation and challenges in modeling polypeptoids persist. In this work, distributions of end-to-end distances calculated with molecular dynamics (MD) simulations are compared to those obtained experimentally via Double Electron Electron Resonance (DEER) spectroscopy. This pulsed electron paramagnetic resonance technique determines a distribution of distances between spin labels placed at each end of a polymer chain, providing insight on sequence-conformation relationships and validation of existing simulation force fields. Together, MD and DEER provide a methodology for understanding the impact of polymer sequence and chemistry on polymer conformation as well as confidence in MD prediction of other properties, such as local hydration dynamics at polymer surfaces.

*This work was supported as part of the Center for Materials for Water and Energy Systems (M-WET), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0019272.
M71.00160: Unfolding of Polymer Thin Films on Liquid Surfaces*  R. KONANE BAY (Presenter), Polymer Science and Engineering, University of Massachusetts Amherst, KLARA ZARYBNICKA, JOSEF JANCAR, Brno University of Technology, ALFRED J CROSBY, Polymer Science and Engineering, University of Massachusetts Amherst — Ultrathin polymer films are difficult to handle. Liquid support layers are often used to ease the manipulation of these films. However, removing the film from the liquid support leads to the fluid draining from the interface, and without the liquid, the polymer interface adheres to itself, forming a crumpled film. The polymer thin film will remain crumpled or tear due to the adhesion forces being higher than the strength of the film. Here, we report a processing method to allow for reversible folding and unfolding of ultrathin polymer films from liquid surfaces. We explain the folding and unfolding mechanism through tuning the surface interactions at the polymer-liquid interface. We demonstrate the ability to fold and unfold several types of polymer thin films on different liquid surfaces.

*NSF DMR 1608614, Czech Grant Agency No. 15-18495S

M71.00161: Polymers in confinement: Free energy scaling and folding transitions*  MARK TAYLOR (Presenter), ANTONIA SIKON, TROY PRUNTY, Dept. of Physics, Hiram College — Geometric confinement of a polymer chain results in loss of conformational entropy. For an athermal polymer the associated free energy increase is expected to exhibit power law scaling with an exponent that depends on confinement dimensionality. For a chain that can fold into a compact native state, confinement primarily reduces the number of possible unfolded states, thereby providing entropic stabilization of the folded state and allowing for the possibility of confinement driven folding [1]. Here we investigate these confinement effects for flexible hard-sphere (HS) and square-well (SW) sphere chains (where the latter exhibit all-or-none folding characteristic of many small proteins [2]). We use a Wang-Landau simulation approach to construct the partition function for a polymer confined within a hard-wall slit, a cylindrical pore, and both a cylindrical and spherical cavity. Scaling analysis of the HS-chains shows significant finite size effects. For the confined SW-chain, isothermal reduction of the confinement dimension can induce folding, unfolding, or crystallite restructuring. Scaling results and phase diagrams will be presented. [1] Taylor, Macromolecules 50, 6967 (2017); [2] Taylor, Paul, and Binder, J. Chem. Phys. 145, 174903 (2016).

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M71.00162: Tunable Assembling of Soft Polymer Janus Nanoparticle at Liquid Interface*
YUFENG JIANG (Presenter), University of California, Berkeley, RAMZI CHAKROUN, ANDRÉ GRÖSCHEL, Physical Chemistry and Center for Nanointegration (CENIDE), University of Duisburg Essen, THOMAS RUSSELL, Polymer Science and Engineering, University of Massachusetts Amherst — We present a study on the assembly of polymeric Janus nanoparticles (pJNPs) at the toluene/water interface. The soft spherical polymeric Janus nanoparticles pJNPs, made by cross-linking polystyrene-block-polybutadiene-block-poly(methyl methacrylate) (PS-PB-PMMA), show a high interfacial activity where the preferential affinity of the PMMA to the aqueous phase causes a spreading of the PMMA block at the interface, even though neither component is soluble in water. The Janus character is later tailored by substituting the PMMA domain to poly-tert-butylmethacrylate (PtBMA) or poly(methacrylic acid)(PMAA) to probe the influence of Janus balance (solvophilic-to-solvophobic balance) to areal density of assemblies of JNPs at the liquid interface and the response of the assemblies to a compression. We investigated the influence of structural asymmetry of JNPs on the assembly, packing, stability and responsiveness of pJNP assemblies by varying the PS-to-PB-to-PMMA ratio. We demonstrate the potential of structure one liquid structure in another by using JNPs complex with salt at liquid interface to obtain bi-continuous liquids.

*This work was supported by the Army Research Office under contract W911NF-17-1-0003.

M71.00163: Mussel inspired polymers for flexible electronics applications*
ELENI PAPANANOU (Presenter), University of California, Santa Barbara, REIKA KATSUMATA, polymer science and engineering, university of massachusetts amherst, RUBAYN GOH, University of California, Santa Barbara, FENG LIU, MINGQI LI, PETER TREFONAS, Electronic Materials, Dupont, RACHEL A SEGALMAN, University of California, Santa Barbara — Electroless plating of solid metals from a solution onto a catalytically active surface has been widely used in the printed circuit board industry for production of wiring layers and inter-layer (via) connections. Smooth substrate surfaces, like polyimide (PI) for flexible electronics applications, are particularly challenging as the electrolessly plated metal tends not to adhere to the surface. It is therefore desirable to develop new chemistries that can be used for adhesion promotion between the polyimide substrate and the deposited copper. Herein, we introduce a mussel-inspired universal adhesive moiety, dopamine, as a side group to a water soluble polymer backbone and demonstrate its application as an adhesion promotion layer for electroless plating of flexible substrates. When the polymer is deposited on a substrate surface, the DOPA moiety reacts with the substrate and adheres to it while the polymer chain extends and folds to generate a smoother outer surface through minimizing the surface energy, creating a smooth and uniform coat of deposited copper.

*Dupont Electronic Materials University Partnership Initiative
M71.00164: Study of a passive enhancement architecture for FRET-enabled molecular communication.*  MATTHEW HAWKINS (Presenter), HEMALI P RATHNAYAKE, JOSEPH M STAROBIN, Univ of NC - Greensboro — Nanomachine technology has advanced by improving complexity and function yet, their future value relies upon superior control and communication; this requires reliable and highly efficient networks. Data transfer techniques of global networks are not scalable for nanomachines, and thus a different approach is needed. Non-radiative energy transfer offers high efficiency, localized, and rapid signal transfer: Förster Resonant Energy Transfer is one of such promising paradigms. Application of light-induced FRET, by combining donor/acceptor pairs with a nanostructure architecture, creates nanosecond signaling data transfer to highly specified locations. Developed through novel, arene-based, donor/acceptor moieties - integrated into a thin-film device designed for signal enhancement - a theoretical and experimental approach has been developed and implemented for tuning scattered excitation energy for increased absorption by the donor for higher energy transfer to the acceptor. This architecture results in increased energy transfer and overall higher output of acceptor emission passively increasing the signaling performance and feasibility of application to molecular communication.

*SENIC (ECCS-1542174), JSNN, and the Office of Research, University of North Carolina at Greensboro.

M71.00165: Charge density gradients of polyelectrolyte thin films generated by diffusion and reaction in the vapor phase  YEONGUN KO (Presenter), JAN GENZER, North Carolina State University — We present fabrication and characterization of charge density gradients on polymeric thin films. Tertiary amines in poly(2-dimethylaminoethyl methacrylate) (PDMAEMA) thin films were quaternized with methyl iodide (MI) through vapor phase diffusion and reaction. The quaternized PDMAEMA (qPDMAEMA), a strong polyelectrolyte, bears permanent charges. The degree of quaternization (DQ) was characterized by FT-IR spectra as well as a refractive index from ellipsometry at elevated temperature to minimize moisture uptake. The resulting films have position-dependent gradients of charge density. The gradient location on the sample depends on process time and concentration of MI. We discovered that the diffusion of MI through air is the rate-limiting step for the entire process. The vapor phase reaction allows for creating charge density gradients in both grafted PDMAEMA brushes and non-grafted PDMAEMA films. In addition, we also evaluated the coefficient of thermal expansion (CTE) and thermo-optic coefficient (TOC) as a function of DQ and showed their linear relationship.
M71.00166: Spontaneous degrafting of weak and strong polycationic brushes in aqueous buffer solutions  JAN GENZER (Presenter), YEONGUN KO, North Carolina State University, YUANCHAO LI, Sun Yat-Sen University — Polymers grafted to substrates have usually been considered to be stable because of the covalent bonds that anchor the macromolecules to the substrate. Several recent reports have reported on degrafting polymers from substrates under specific conditions. We have conducted a systematic study of degrafting polycationic brushes with different degrees of quaternization (DQ), molecular weight, grafting density, which have been incubated in buffer solutions (pH 4, 7.4, and 9) with the same ionic strength (0.05 M). We also explored the effect of the bonding environment at the anchoring point of the polymer graft on the overall stability of polymer assemblies on the substrate. The major findings in this study are: 1) Degrafting of polycationic grafts from flat silica substrate increases with increasing DQ of the polymer, 2) Polymer degrafting likely occurs both in the initiator ester group and the silane head-group at the silicon substrate, 3) The degrafting kinetics can be described by time-dependent rate constant modeled by stretched exponential function.

M71.00167: Structure of Irreversibly Adsorbed Star Polymer Layers*  GIZEM KIREVIYASI (Presenter), Department of Chemistry, Bogazici University, DAVID UHRIG, KUNLUN HONG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, BULENT AKGUN, Department of Chemistry, Bogazici University — Viscosity, glass-transition temperature, and diffusivity of polymer chains in thin films deviate from bulk values due to the presence of adsorbed polymer chains on the substrate. The structure of irreversibly adsorbed layers (IALs) formed by linear chains has been extensively investigated and found to be composed of two layers: high density inner layer in which chains are flattened and bulk-like density outer layer in which chains adopted more tail and loop conformations. However, the role of chain branching on the structure of adsorbed layer is not clear.

Well-defined linear polystyrene (PS), 4-arm and 8-arm star PS chains with the same total molecular weight, and 8-arm star PS with different molecular weights are used to elucidate the effect of polymer architecture on the structure of IAL by ellipsometry, X-ray reflectivity (XR) and atomic force microscopy measurements. Our results indicated that the normalized layer thickness increases as the number of arms increases and arm length decreases on both SiOₓ and Si-H surfaces. Adsorbed star polymers formed thicker layers on Si-H surfaces compared to SiOₓ surfaces. Adsorbed layer thickness is found to be a function of initial film thickness up to 100 nm.

*This project is funded by TUBITAK 215Z334 and TUBA-GEHIP.
M71.00168: Visualization of interface effect on the molecular morphology in block copolymer thin films by SVSEM tomography  AMANDA SUAREZ (Presenter), XUEYAN FENG, EDWIN THOMAS, Rice University — Applications of block copolymer thin films include their use in lithography, photonics and biomedical devices, and is in large part, due to their internal nanostructures. Thin films are particularly sensitive to surface confinement effects, which on one hand enriches the molecular assembly while on the other hand can produce distortions of the structure from thermodynamically stable symmetries. Here, we study polystyrene-b-poly(2-vinylpyridine) thin films with different microdomain morphologies (double gyroid, lamella, disordered network). By applying Slice-and-View scanning electron microscopy (SVSEM) tomography, the domain structures, distortions, and defects within the polymer films can be measured over large areas/volumes and the influence of the field of the interface (substrate/film and film/air) on the molecular assembly morphologies examined.

M71.00169: Universal cohesive law governing interaction between nanoparticles in hairy nanoparticle assemblies*  NITIN HANSOGE (Presenter), AGAM GUPTA, SINAN KETEN, Northwestern University — Polymer-grafted nanoparticle assemblies have significant advantages over traditional nanocomposites as they overcome the dispersion issues, attain high structural order and allow accurate tailoring of mechanical properties. Modeling these assemblies using atomistic or even coarse-grained molecular dynamics simulations is quite challenging due to spatiotemporal limitations. To overcome this challenge, in this work, we develop a universal cohesive law that governs the interaction between nanoparticles in these assemblies. This effective interatomic potential is based on the strain energy density between two nanoparticles modeled as plates. We find that the potential consists of empirical constants dependent on polymer fragility, molecular weight and grafting density. Using these design parameters, we were able to collapse all the strain energy curves into a universal curve governing the interaction between nanoparticles. By eliminating the need to explicitly model polymer beads, we can simulate micron scale systems of these hairy nanoparticle assemblies without the loss of underlying physics.

*ONR Director of Research Early Career Award (PECASE, award #N00014163175)
**M71.00170: Recyclable Bio-based Thermoset Furan-Epoxy Networks via Diels-Alder Crosslinks**

LUC LE (Presenter), KARL JACOB, KYRIAKI KALAITZIDOU, Georgia Inst of Tech — Strong and lightweight thermoset polymeric can be used for many structural applications. However, thermoset materials may cause significant environmental problems since many of such materials cannot be recycled and have to be stored in landfills. Thus, thermoset that can be recycled, or even renewed will have a substantial impact on reducing the adverse environmental impact of such materials. Renewable polymer composite is a promising path for reducing environmental pollution while improving the sustainability of such materials for the long future. By introducing the thermo-reversible covalent bonds in the molecular network, the thermoset material can be reprocessed upon a suitable thermal trigger. One of the most effective reversible covalent bonds is the Diels Alder (DA) bond between furan and maleimide because of its relatively fast kinetics and mild reaction conditions. In this work, the reversible DA networks were prepared from bio-based furan grafting on epoxy and maleimides crosslinkers of different structures. The kinetics and thermodynamics properties of the dynamic network were studied following the evolution of structure formation and dissociation.

*Renewable Bioproducts Institute at Georgia Tech

**M71.00171: SOFT MATTER PHYSICS —**

**M71.00172: Ordering kinetics and steady state in Active Nematic with quenched disorder**

SAMEER KUMAR (Presenter), SHARDHA MISHRA, Indian Institute of Technology (BHU) —

A finite disorder in an active liquid crystal has a significant effect on the ordering dynamics and the steady-state. System of self-propelled apolar particles with nematic interaction is one of the way to understand the defect topology and their dynamics in an active liquid crystal and hence, the ordering kinetics in the system. We construct a two-dimensional monolayer of self-propelled apolar particles with the quenched inhomogeneous field. We write hydrodynamic equations of motion for the hydrodynamics fields, viz. density $\rho$ and orientation $Q$ in a coarse-grained description with the addition of finite quenched disorder. We found that, although the presence of disorder in the system slows down the ordering dynamics, static and dynamic scaling properties remains the same. Our study will motivate experimentalists to verify results and may find applications in living and artificial systems in the presence of inhomogeneous quenched disorder.

*SK and SM would like to thank DST-SERB India for their financial support. SK and SM would like to thank Prof. S. Ramaswamy for his useful suggestion.
M71.00173: Multicellular Magnetotactic Bacteria under an Applied Magnetic Field Form Active Crystals  ALEJANDRA ROSSELLI (Presenter), ALEXANDER PETROFF, BENJAMIN ROQUE, Clark University — Multicellular Magnetotactic Bacteria (MMB) of the species Magnetoglobus multicellularis live in spherical colonies composed of 10-50 individual bacteria. These bacteria are the known known obligately multicellular bacteria. The colony swims as a single unit parallel to the Earth’s magnetic field. When a magnetic field is oriented normal to a glass surface, aggregates accumulate into a monolayer on the glass surface. As the magnitude of magnetic field increases, the density of the colonies increases. At a critical field strength, the mean free path of the colonies shrinks to the radius of a single colony. The colonies display a crystalline packing. Unlike previous examples of active crystals (e.g., with colloids and fast swimming bacteria), these bacteria spontaneously detach and reincorporate into the structure at rates dependent on the strength of the applied field. As a result, active crystals composed of MMB display numerous vacancies. We describe the dynamics is this new state of active matter and compare them to active crystals and active super-critical fluids.

M71.00174: Polar flock with bond disorder*  JAY SINGH (Presenter), Indian Institute of Technology (BHU), SUDIPTA PATTANAYAK, Physics, A.S.N.B.C.B.S Kolkata, SHRADHA MISHRA, Indian Institute of Technology (BHU) — Understanding the collective behaviour of self-propelled particles (SPP’s) is an active area of research. Although collection of SPP’s are made of similar particles. But each individual can differ due to their much details of biological complexity. We focus on difference in interaction ability with neighbours. Hence in this study we introduced a collection of SPP’s interecting through a short range Vicsek type alignment interaction, but strength of alignment is different for different particle and obtained from random distribution. Equalibrium analog of one model is XY-model with bond disorder. we find that presence of such bond disorder, long range ordering (L.R.O) remains unchanged as for clean system. Also ordering kinetics remain uneffected but large disorder.

*I would like to thank MHRD (Govt. of India) and iit bhu for their financial support in this work.
**M71.00175: Measuring Force Fluctuations and Diffusion in Active Baths**

**HUNTER SEYFORTH** (Presenter), **WYLIE AHMED**, **MAURICIO GOMEZ**, California State University, Fullerton — Actively driven systems such as suspensions of active colloids, bacteria, and enzymes have been observed to enhance diffusion at the microscopic scale. Active suspensions also exhibit anomalous mechanical properties that are not observed in typical equilibrium fluids. To investigate the interplay between enhanced diffusion and fluid response we measure fluctuations of forces, motion, and viscosity in active baths composed of actively swimming bacteria. To do so, we use two approaches: (1) Differential Dynamic Microscopy, to analyze motion in the form of image intensity fluctuations to quantify decorrelations of the active suspension. (2) Optical tweezers, to trap suspended colloids and measure the force fluctuation spectrum due to non-equilibrium fluctuations of the active bath. We quantify the space-time correlations and calculate the energy dissipated by non-equilibrium processes to extract information about the system.

*California State University, Fullerton*

**M71.00176: role of annulus confinement on 2D active nematic behaviour**

**ZAHRA ZAREI** (Presenter), **MICHAEL M NORTON**, **CHAITANYA JOSHI**, **MICHAEL HAGAN**, **SETH FRADEN**, Brandeis Univ — Defects play an important role in active-matter systems. They are nucleated because of the bend instability and in steady state are continuously created and annihilated. In this study we investigate a 2D active nematic confined in an annulus, which exhibits a rich dynamical behavior of the plus and minus half defects. The confinement effectively transforms the turbulent dynamics of the active nematic into coherent flow. We measure the positional-orientational distribution of defects in different confinements. We define three different states for the defects based on their positions and orientations, and calculate their transition rates.

*MRSEC*

**M71.00177: Physical Basis for Coordination among Bacterial Cells in a Proto-Multicellular Colony**

**BENJAMIN ROQUE** (Presenter), **ALEXANDER PETROFF**, **ALEJANDRA ROSSELLI**, Clark University — Multi-cellular Magnetotactic Bacteria are the only known obligately multi-cellular bacteria. Cells live within a colony composed of 10-50 cells. Each cell precipitates a magnetic crystal. The average magnetic moment of the colony aligns with the Earth’s magnetic field. The outer surface of each cell is covered in about 30 flagella. Colonies move as a single unit as individual cells in the colony rotate their flagella. It is not understood how cells in a colony align their magnetosomes, how this order is maintained during division, or how cells coordinate their flagella to exert a force parallel to their average magnetic moment. Here, we propose a physical mechanism to show this coordination may arise without direct cell-cell communication. We use published data to show that the organization of the cells in a colony is consistent with a Fibonacci packing. Next, we show that coupling chemotaxis to magnetotaxis allows cells to exert a net force parallel to the average magnetic moment of the colony. These results give insight into the evolution of complex life by showing that cells in a protomulticellular organism may coordinate their behaviors through purely physical mechanisms before the evolution of shared chemical signaling pathways.
M71.00178: Near-surface Motion of Bacteria in Polymer Solutions

DING CAO (Presenter), Chinese Univ of Hong Kong — Many bacteria live on solid-liquid interface and they are surrounded by polymers that naturally exist or excreted by themselves. Polymers may facilitate the formation of biofilm by protecting bacteria from external stress. In addition, the interactions between swimming bacteria, polymer and surface are crucial for dynamic processes of bacteria such as surface attachment and dispersal. Here we will present our preliminary work on how polymers may affect the single cell motion pattern near solid surfaces and assist the spreading of bacterial colony.

*This work was supported by the Research Grants Council of Hong Kong SAR (RGC numbers 2130439, 2130493 and 2130613), and from the National Natural Science Foundation of China (NSFC 21473152).

M71.00179: Evolutionary game theory of sticky motile bacteria

GURDIP UPPAL, DERVIS VURAL (Presenter), University of Notre Dame — Bacteria typically reside in heterogeneous environments with varying nutrition and toxin profiles. Motile cells can gain an advantage over non-motile cells by migrating to more favorable environments. Since motility is energetically costly, cells must optimize their swimming speed and behavior to maximize their fitness. Here we look at how cheating strategies might evolve where slow or non-motile microbes exploit faster ones by sticking together and "hitching a ride." We theoretically and computationally study the effects of sticking on the evolution of run speed in a controlled chemostat environment. We find stickiness allows slow cheaters to dominate only at intermediate distance between nutrition sources. In contrast, for long run durations slow microbes do gain a small advantage from sticking, but only get so far before falling behind; and for short run durations it is best for no one to swim.

M71.00180: Failure propagation in multicellular tissues as mediated by advective flow

GURDIP UPPAL, GOKHAN BAHCECIIOGLU, PINAR ZORLUTUNA, DERVIS VURAL (Presenter), University of Notre Dame — Aging is not just due to the death of cells but due to systemic failures due to the accumulation of malfunctions in a network of interdependent components. Here we experimentally and theoretically study how failure propagates in a synthetic multicellular tissue, as mediated by cooperative factors transported by diffusion as well as advective flow. We first experimentally show that fluid flow induces a reduced death rate upstream. Based on this observation, we then develop a model where cells secrete cooperative factors that enhance their survival which diffuse, decay, and advect in space according to the laws of fluid dynamics. From this model, we derive further predictions for the conditions for which a propagating front of failure should form, and its velocity.

*We Acknowledge National Science Foundation grant CBET-1805157
M71.00181: Aggregation Dynamics of Active Spinning Superparamagnetic Particles in Dense Passive Media  JOSHUA STEIMEL (Presenter), Univ of the Pacific, JUAN ARAGONES, Universidad Autonoma de Madrid, DANIEL MADERA, SAGE MORELAND, Univ of the Pacific, ALFREDO ALEXANDER-KATZ, MIT — Active matter systems exhibit emergent non-equilibrium dynamical phenomenon which is driven by the activity-induced effective interactions between active particles or units. Here we study aggregation dynamics of many active spinning superparamagnetic particles, spinners, embedded in a dense complex 2D colloidal monolayer of passive particles. Utilizing coarse grained Lattice-Boltzmann simulations and experiments we observed that the aggregation of dynamics of active spinning particles resemble classical 2D Cahn-Hilliard coarsening. The spinners will aggregate and display Cahn-Hilliard coarsening when the passive monolayer is dense enough so that it behaves elastically and when the spinner activity exceeds a minimum activity threshold. For the concentrations investigated here the cluster size scaling is independent of the number of active units. We also observe a critical cluster size which maximizes spinner aggregation by minimizing viscous drag through the dense passive monolayer while maximizing the stress applied on the passive medium. In simulations, we can create ternary mixtures of co-rotating, counter-rotating, and passive particles. The aggregation behavior of such mixtures show distinct aggregates of co and counter-rotating spinners.

M71.00182: Confinement effect on active turbulent dynamics*  YUHAO WANG (Presenter), Chinese Univ of Hong Kong — Dense bacterial suspensions organize into mesoscale active turbulent vortices when confined in quasi-2D or 3D chambers. The spatial and temporal length scale of the turbulent vortices is dependent not only on the active fluid itself but also on the rheological properties of the confinement interface. Moreover, the turbulent vortices transform into a single spiral vortex state when the confinement size reaches the turbulent correlation length. Here we discuss the confinement interface and dimension effects on active turbulent dynamics and hence the macroscale behavior. This study is aiming to provide physical insights for designing environments of controllable collective motion and active assembly.

*This work was supported by the Research Grants Council of Hong Kong SAR (RGC numbers 2130439, 2130493, and 2130613), and from the National Natural Science Foundation of China (NSFC 21473152).
M71.00183: Statistical mechanical sum rules for active colloids at surfaces - a touch of equilibrium*  RENÉ WITTMANN (Presenter), HHU Düsseldorf, FRANK SMALLENBURG, Univ. Paris-Sud, Univ. Paris-Saclay, JOSEPH BRADER, Université de Fribourg — We study the mechanical properties of active particles in the presence of curved walls by computer simulation of Active Brownian Particles (ABPs), Active Ornstein-Uhlenbeck Particles (AOUPs) and a passive system with effective interactions. The effective theory admits analytic results for pressure, surface tension and adsorption of an active ideal gas at a two-dimensional circular wall. It further predicts that an equilibrium sum rule also holds for active fluids, which we confirm numerically for both ABPs and AOUPs in the limit of small curvature.

More precisely, we find within each model that the slope of the pressure as a function of the curvature equals the surface tension and adsorption (up to an effective temperature scale) on a planar wall. Intriguingly, the explicit value of these coefficients is model-dependent, which can be explained by the different velocity distributions.

We also discuss the influence of interactions and find that the effect of curvature on the wall pressure is reduced when increasing the density. Within numerical accuracy, the equality of the slope of the pressure and the planar surface tension appears to hold at finite density.


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M71.00184: Capillary Forces on a Janus Sphere Straddling a Liquid-Gas Interface*  SHENGFENG CHENG (Presenter), YANFEI TANG, Virginia Tech — Particles with a patterned surface can exhibit interesting packing and self-assembly behavior. One class of such particles is Janus particles whose surfaces are divided into two halves with distinct physical properties. We compute the capillary forces on a Janus sphere, one side of which is solvophobic while the other is solvophilic, straddling a liquid-gas interface via molecular dynamics simulations. In equilibrium, the liquid-gas interface is flat in the horizontal plane and intersects with the equator of the Janus sphere, with its solvophilic side immersed in the liquid. When the Janus sphere is pulled or pushed out of its equilibrium position along the vertical direction, a capillary rise or fall occurs but the contact line is first pinned at the equator. The contact line only starts to slide when the apparent contact angle becomes equal to the acute (obtuse) contact angle on the solvophilic (solvophobic) side for the Janus sphere pulled upward (pushed downward). An analytical model is developed to explain the observation. The capillary force on a Janus sphere oriented upside-down with the solvophobic side submerged in the liquid is also computed with simulations and possible metastable configurations are found.

*Supported by a research grant from the 4-VA Consortium.
**M71.00185: Achieving highly ordered nanoparticle structures in polymer solution without chemical grafting**  
SOL MI OH (Presenter), SO YOUN Y KIM, Ulsan Natl Inst of Sci & Tech —  
Nanoparticle arrays with highly ordered structures have drawn great attention based on their potentials to improve the physical properties compared to the randomly oriented structures. However, it is often difficult to disperse nanoparticles in order in a neat polymer matrix keeping the liquid-like processability, thus requiring complicated and time expensive laborious procedures. In this work, we report that nanoparticles can be highly ordered by simply dispersing them in poly(ethylene glycol) derivative solution. Without chemical grafting, the strong hydrogen bonding between nanoparticles and the PEG complex could retain the superstructures in the liquid-phase with excess amount of water. The systematic investigation is carried out by varying molecular weight/concentration of polymers/nanoparticles and temperature with small-angle X-ray scattering and oscillatory rheometry experiments.

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**M71.00186: Sticky diffusion: How to achieve complex motion with random sticky feet ?**  
SOPHIE MARBACH (Presenter), Courant Institute of Mathematical Sciences, JEANA(AOJIE) ZHENG, DAVID J PINE, NYU, Center for Soft Matter Research, MIRANDA HOLMES-CERFON, Courant Institute of Mathematical Sciences —  
Beating equilibrium diffusion is a paradigm challenge that biological or artificial systems of small particles have to face to achieve complex functions. Some cells (like leucocytes) use ligand-receptor contacts (sticky feet) to crawl and roll along vessels. Sticky DNA (another type of sticky feet) is coated on colloids to design programmable interactions and long-range assembly features. The dynamics of such sticky motion are complex as sticky events (attaching/detaching) often occur on very short time scales that affect the overall motion of the particle on much longer time scales, and makes predictions challenging. Here we present analytical predictions in several cases (with different geometries of sticky feet). We rationalize what parameters control diffusion and how they can be compared to existing systems. We investigate furthermore how complex motion like rolling may be favored compared to lateral motion.
M71.00187: Droplets of Colloidal Ferromagnetic Nanoplates*  MIN SHUAI, XI CHEN, CHEOL PARK (Presenter), JOSEPH E MACLENNAN, MATTHEW A. GLASER, NOEL ANTHONY CLARK, University of Colorado, Boulder — Disk-shaped, ferromagnetic barium hexaferrite nanoplates in isotropic solvents exhibit a first-order transition from a paramagnetic isotropic (I) phase to a ferromagnetic nematic (N_F) phase for sufficiently high volume fractions [Nat Comm, 7: 10394, 2016]. In samples prepared at a volume fraction within the I – N_F coexistence range, it is possible to create metastable dispersions of oblate spheroidal N_F droplets in an isotropic background. Magnetostatic interactions strongly favor tangential alignment of the N_F magnetization field and the corresponding nematic director field along lines of latitude. However, such a circumferential director configuration requires the formation of a +1 disclination line along the symmetry axis of the droplet, with a correspondingly large elastic free energy cost. The formation of a disclination line is avoided through the escape of the polar director field into the third dimension, giving rise to spontaneously chiral droplets whose handedness is determined by the sign of twist of the magnetization. Coalescence of droplets leads to highly complex morphologies that depend on the polar and chiral structure of the constituent droplets.

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M71.00188: Elucidation of Structural Information of Colloidal Assemblies from Binary Particles using Scattering Techniques*  ANVAY PATIL (Presenter), SARANSHU SINGLA, Polymer Science, The University of Akron, ZIYING HU, Chemistry, Northwestern University, JING-JIN SONG, Materials Science & Engineering, University of California San Diego, MARKUS BLEUEL, Center for Neutron Research, National Institute of Standards and Technology, NATHAN C. GIANNESCHI, Chemistry, Northwestern University, SUNIL K SINHA, Physics, University of California San Diego, ALI N DHINOJWALA, Polymer Science, The University of Akron — Self-assembly plays an important role in materials and life sciences, for example, in production of structural colors in various taxa, folding and assembly of proteins in living cells, and creation of metamaterials by self-assembly of complex nanostructures. Previously we have reported a simple one-pot emulsion-based process to form photonic colloidal assemblies called supraballs. In this work, we have measured the small angle neutron scattering from supraball assemblies constructed using binary mixtures of melanin and silica particles. The neutron scattering results can be used to determine the various partial structure factors of the nanoparticles, which is important in understanding scattering of visible light. Designing tunable structural colors is of interest for many applications including cosmetics, paints, and food colorings.

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M71.00189: Dynamical processes of interstitial diffusion in a two-dimensional colloidal crystal
SUNGCHEOL KIM, Watson Research Center, IBM Research, LICHAO YU, Google, ALEXANDROS PERTSINIDIS, Sloan-Kettering Cancer Institute, XINSHENG LING (Presenter), Brown University — We report the first study of the dynamical processes of interstitials in a 2D colloidal crystal. The diffusion constants of both mono- and di-interstitials are measured, and found to be significantly larger than those of vacancies. Di-interstitials are clearly slower than mono-interstitials. We found that, by plotting the accumulative positions of 5- and 7-fold disclinations relative to the center-of-mass position of the defect, a 6-fold symmetric pattern emerges for mono-interstitials. This is indicative of an equilibrium behavior that satisfies local detailed balance that the lattice remains elastic and can be thermally excited between lattice configurations reversibly. However, for di-interstitials the 6-fold symmetry is not observed in the same time window, the local lattice distortions are too severe to recover quickly. This observation suggests a possible route to creating local melting of a lattice (similarly one can create local melting by creating di-vacancies). This work opens up a new avenue for microscopic studies of the dynamics of melting in colloidal model systems.

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M71.00190: Glass Transition in PEO-C$_{60}$ Nanocomposites
OMOSOLA ORIRETAN, DORINA CHIPARA, MOHAMMED UDDIN, DANNA CAPITANACHI AVILA, KAREN LOZANO, MIRCEA CHIPARA (Presenter), University of Texas Rio Grande Valley — Nanocomposites of polyethylene oxide (PEO) loaded by various amounts of fullerenes have been prepared by dissolving PEO into a given solvent and homogenizing the PEO-solvent solution by stirring. Fullerenes nanoparticles have been added to the PEO solution, then the mixture was stirred for about 1 h at 1,000 rotations per minute followed by a 30 minutes high power sonication. The homogenized mixture/solution was poured on microscope slides and the solvent was removed in an oven at 90 °C, for 12 hours. The complete removal of the solvent was confirmed by TGA. Two solvents: deionized water and chloroform were used. The nanofiller is not soluble in water but is soluble in chloroform, opening thus the door towards a refined understanding of the differences between a nanocomposite and a molecular dispersion. The as-obtained nanocomposites were investigated by using a TA Instruments Q 50 DSC at various heating and cooling cycles with rates ranging between 5 °C/min to 30 °C/min. The research is focused on the effect of the heating/cooling rates, solvent type, and concentration of fullerenes on the glass transition temperature of PEO-C$_{60}$ nanocomposites.

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M71.00191: Hierarchically Organized Chiral Supraparticles of Twisted Gold-Cysteine Sheets

PRASHANT KUMAR (Presenter), YUEFEI WANG, WENFENG JIANG, NICHOLAS KOTOV, Univ of Michigan - Ann Arbor — The structural complexity of composite biomaterials and mineralized particles arises from hierarchical ordering of inorganic building blocks over multiple scales. While empirical observations of complex structures from nanoparticles are abundant, assembly mechanisms leading to their geometrical complexity are still puzzling especially for non-uniformly sized components. Here, we report the assembly of hierarchically organized particles (HOPs) with twisted spikes and other morphologies from polydispersed Au-Cys nanoplatelets. Complexity of HOPs is comparable to biological counterparts as enumerated by graph theory methods. Their intricate hierarchical organization emerges from competing electrostatic and elastic restrictions that render assembly pathways primarily dependent on nanoparticle symmetry rather than size. Upon varying the enantiomeric excess and synthesis temperature, a large family of colloids with complex architectures and unusual chiroptical and chemical properties are explored.

M71.00192: Terahertz time-domain spectroscopic study on an oxide glass with entropic elasticity

JEONGHYUK KIM (Presenter), TATSUYA MORI, Division of Materials Science, University of Tsukuba, SEIJI INABA, Research Center, AGC Incorporated, TAKANARI KASHIWAGI, Division of Materials Science, University of Tsukuba, YASUHIRO FUJII, Department of Physical Sciences, Ritsumeikan University, SUGURU KITANI, HITOSHI KAWAJI, Materials and Structures Laboratory, Tokyo Institute of Technology, AKITOSHI KOREEDA, Department of Physical Sciences, Ritsumeikan University, SOO HAN OH, JAE-HYEON KO, Department of Physics, Hallym University, SEIJI KOJIMA, Division of Materials Science, University of Tsukuba — For disordered systems, universal excitation called boson peak appears in the terahertz range. In addition, for polymeric glasses, fractal dynamics, so-called fracton, is expected to appear above boson peak frequency as a result of self-similarity of monomer unit. In this study, we performed terahertz time-domain spectroscopy on an oxide glass with entropic elasticity: mixed alkali metal metaphosphate glass with the chemical composition Li$_{0.25}$Na$_{0.25}$K$_{0.25}$Cs$_{0.25}$PO$_3$, to detect the boson peak and fracton. Obtained spectra are compared with results of low-frequency Raman scattering and low-temperature specific heat measurement.

M71.00193: Proton Conductivity in Protic Ionic Liquids (PILs)

AMANDA YOUNG-GONZALES (Presenter), ALEXEI SOKOLOV, SHENG ZHAO, University of Tennessee, Knoxville — Protic ionic liquids (PILs) have attracted significant attention due to their promising properties and potential use in various applications. Recent studies revealed strong decoupling of proton conductivity from structure relaxation in a mixture of lidocaine with phosphoric acid, $^1$ in which the proton conductivity of this mixture even exceeds that of phosphoric acid at the same viscosity. In this study, we selected bases that exhibit similar properties to lidocaine to facilitate the formation of hydrogen bonded networks to promote high proton diffusivity. Using broadband dielectric spectroscopy (BDS), the conductivity relaxation of several different mixtures with phosphoric acid can be compared and used to determine the best structures for increased conductivity.

**M71.00194: Self-limiting electrospray deposition on polymer masks**  
LIN LEI (Presenter), ARIELLE MARIE GAMBOA, CHRISTIANNA KUZNETSOVA, SUNSHINE LITTLECREEK, JINGREN WANG, QINGZE ZOU, JEFFREY ZAHN, JONATHAN SINGER, Rutgers University, New Brunswick — Electrospray deposition (ESD) can produce monodisperse generations of droplets down to hundreds of nanometers in diameter by applying high voltage to liquids flowing through capillaries. This deposition method has been combined with insulated stencil masks for fabricating micro patterns by spraying nanoparticles, polymers, or biomaterials. To optimize the fabrication process for micro coatings, a self-limiting electrospray deposition (SLED) method has recently been developed. Here we combine SLED with a pre-existing polymer film to study the fundamental behavior of this process in a bilayer geometry. SLED has been observed when insulating materials are sprayed onto conductive substrates. A thickness-limited film will occur when charge accumulates and repels the arrival of additional charged droplets. In this study, polystyrene (PS) and Parylene C thin films of varying thicknesses are utilized as insulated spraying substrates. Polyvinypyrrolidone (PVP), a thermoplastic polymer is sprayed to investigate the SLED behavior on the pre-deposited insulating films. Moreover, to examine the effects of in-plane confinement on the spray, a microhole array patterned onto the PS thin film by focused laser spike (FLaSk) dewetting was sprayed with PVP in the SLED mode.

**M71.00195: Contact singularity between curved dielectric surfaces**  
HUADA LIAN (Presenter), JIAN QIN, Stanford Univ — The induced polarization charges density on two dielectric surfaces in proximity appear to diverge as separation decrease. This diverging charge density cannot be resolved by the conventional numerical methods or series expansions because the surface charges demand ever-increasing spatial resolution that becomes intractable in the near-contact regime. We analyze the asymptotic behavior of this contact singularity by adopting the 'lubrication' approximation, and demonstrate explicitly the singular dependence on the gap distance and the curvature of two approaching surfaces. The result agrees with the known logarithmic singularity for conducting surfaces and, for dielectric surfaces, provides a means for isolating the singularity and calculating the cohesive energy for ensembles of dielectric particles in close contact.
M71.00196: Programmable Multistable Mechanisms for Locomotion* MOHAMED ZANATY (Presenter), Harvard University, PATRICK FLÜCKIGER, ILAN VARDI, SIMON HENEIN, EPFL — We characterized the stability behavior of a multistable mechanism and applied the results to create a new locomotion mechanism based on serially connected bistable beams. The beams of our mechanisms have axial loads that can tune their stiffness and thereby modify the number and location of the stable states. This mechanism is an instance of programmable multistable mechanisms introduced in our previous work.

Using analytical modeling, numerical simulation, and experimental measurements, we demonstrated how the transition sequence between the stable states depends on the beams' axial loads. We exploited this property to produce locomotion with a highly simplified control system. We applied our concept to construct a skating robot, where velocity can be tuned by varying beam stiffness.

*M. Z. acknowledges the financial support provided by the Swiss National Science Foundation under grant number P2ELP2_184497

M71.00197: Jamming in a bubble raft: order, disorder and glassy behavior* KLEBERT FEITOSA (Presenter), CHRISTOPHER EATON, ANDREW JOYCE, BRIAN C SEYMOUR, CHRISTINE O'DEA, Dept. of Physics and Astronomy, James Madison University — Soap bubbles floating at an air-liquid interface form stable aggregates resulting from capillary attraction between bubbles. Under external forcing the aggregates unjam and experience plastic events. By using bubble shape deformations as a proxy for the stress, we correlate bubble rearrangements with the stress field as the raft is subject to uniaxial oscillatory compression between parallel plates. We find that most rearrangement events occur immediately after a turning point in the cycle when the stress field changes direction and is most heterogeneous. We also compute metrics from tessellations of polygonal regions set by idealized contact points as well as particle bond orientations and analyze their statistics at different stages of the cycle.

*This research was funded by 4-VA, a collaborative partnership for advancing the Commonwealth of Virginia.
M71.00198: Systematic control of anisotropy and percolation in patchy particle gels  JAKE SONG (Presenter), Massachusetts Institute of Technology MIT, BRIAN LYNCH, MEHEDI RIZVI, North Carolina State University, JAN ILAVSKY, Argonne National Laboratory, DAVID MANKUS, Massachusetts Institute of Technology MIT, JOSEPH TRACY, North Carolina State University, NIELS HOLTEN-ANDERSEN, GARETH H MCKINLEY, Massachusetts Institute of Technology MIT — Patchy particle interactions enable the design of so-called ‘equilibrium gels’, a system where arrest is achieved without an underlying phase separation, resulting in structurally equilibrated gels which do not undergo coarsening-induced aging. We show that nanoparticle-incorporated supramolecular hydrogels - consisting of reversibly polymer-grafted metallic nanoparticles which are cross-linked with end-functionalized polymers – exhibit behaviour consistent with systems undergoing equilibrium arrest. We show that the interaction patchiness of this system can be controlled through the ratio of polymeric linkers to nanoparticles, thus resulting in a canonical system with tunable self-assembly, local structural anisotropy, and mechanical percolation thresholds. Moreover, we show that the addition of metal ions as a second competitive reversible cross-linking species results in the stabilization of locally anisotropic nanoparticle structures, thus resulting in a globally anisotropic structure and a dramatic reduction in the mechanical percolation threshold of the nanoparticle network in the hydrogel. These findings allow the systematic design of stable particle gels with tunable morphology and rigidity.

M71.00199: Effect of chain architecture on self-diffusion in a model associative network.* IRINA MAHMAD RASID (Presenter), NIELS HOLTEN-ANDERSEN, BRADLEY OLSEN, Massachusetts Institute of Technology MIT — Associative networks are ubiquitous both in natural and synthetic materials, and self-diffusion within these networks dictates many of their desirable properties such as self-healing and stress relaxation. Self-diffusion studies of various associative networks have shown that over length scales of several times the radius of gyration, the dynamics of the network lead to the observation of an apparent super-diffusive regime prior to transitioning to the Fickian regime at larger length scales. In this work, the effect of chain architecture was investigated by comparing the self-diffusion of a random copolymer with one where the stickers are clustered at the end of the chain. Since the chemical composition of the model associative networks is kept constant, this approach allows for a more direct comparison of the role of chain architecture. The insights gained from this study will improve our understanding of the effect of sticker distribution on the transport properties of natural and synthetic associative networks and how it could impact the macroscopic properties that rely on these processes.

*Institute for Soldier Nanotechnologies (ISN)
-Office of Naval Research (ONR)
-Center for Materials Science and Engineering (CMSE)
-National Science Foundation (NSF)
M71.00200: Chiral Elastic Waveguide  OSWALDO ADAPTA (Presenter), ADRIAN REYES, National Autonomous University of Mexico — In this work, we investigate the propagation of elastic transverse and longitudinal waves in a helical medium through a cylindrical waveguide. By solving the Navier-Cauchy equations together with the constitutive equations for a helical medium. By assuming quasi-planar waves, we reduce our system to a set of ordinary differential equations. We have obtained the band structure of the system and the propagation parameters by imposing the corresponding boundary conditions for vacuum outside the waveguide. We also calculate the corresponding strain and stress distributions within the waveguide. We discuss our result and address our conclusions.

M71.00201: Binary Clay – Graphene Oxide Liquid Crystals*  BARBARA PACAKOVA (Presenter), Dept. of Physics, NTNU Trondheim, ROMULO TENORIO, Comissão Nacional de Energia Nuclear - (CNEN) and Centro Regional de Ciências Nucleares - (CRCN), Brazil, MARIAN MATEJDES, Bayerisches Polymer Institut und Lehrstuhl für Anorganische Chemie 1, Universität Bayreuth, Bayreuth, Germany, YVES MEHEUST, Geosciences Rennes, Université Rennes 1, Rennes, France, PAULO BRITO, Dept. of Physics, NTNU Trondheim, JOSEF BREU, Bayerisches Polymer Institut und Lehrstuhl für Anorganische Chemie 1, Universität Bayreuth, Bayreuth, Germany, JON OTTO FOSSUM, Dept. of Physics, NTNU Trondheim — Colloidal suspensions (CS) of electrically charged nanosheets (NSTs) form liquid crystalline phases in polar solvents, such as graphene oxide\(^1\) or clays\(^2,3\). Self organization of NSTs due to competing van der Waals attraction and electrostatic repulsion forces can form several coexisting phases such as isotropic (I), nematic (N) or lamellar (L). Several single-component CS\(^1,2\) exhibit transition from I to N liquid crystalline phase; moreover, existence of L phase for CS of electrically charged NSTs has been observed recently\(^4\).

In contrary, complexity of binary CS (BCS) of charged NSTs can result in multi-phase systems. This study is focused on BCS of negatively charged synthetic clay\(^5\) and graphene oxide, serving as promising precursor for fabrication of clay-graphene oxide mixed ionic-electronic conductors. Results obtained using X-ray diffraction (SAXS, WAXS) and imaging (optical, MRI) techniques will be discussed, emphasizing formation of N and mixed-domain states.


*Research Council of Norway, Nano2021 project no. 250619.
M71.00202: Chiral Composite Networks for Sensing Volatile Organic Compounds Towards Liquid Crystal Nose (LC-nose).  MEGHAN EVANS (Presenter), BENJAMIN SCHUTSKY, ANTHONY GRAY, KYRA FULEIHAN, CHRISTOPHER LA FOND, PETR V SHIBAEV, Fordham University — Composite chiral networks were prepared by co-polymerization of cholesteric siloxane monomers with low molar mass monomers bearing hydrogen bonding, polar and non-polar side groups (acrylic acid, vinylpyridine, benzyl acrylate, and aliphatic acids). Polymerization was conducted between two plastic plates at elevated temperatures when compounds formed chiral liquid crystalline state. After polymerization thin polymer films were formed, the upper plastic film was peeled off and the surface of polymer composite was exposed to a particular VOC. The response of polymer films to VOCs (spectral shift of the selective reflection band) was studied by spectroscopic methods and morphological surface changes were studied by atomic force microscopy (AFM). It was shown that by varying the composition of materials it is possible to change their sensitivity to polar and non-polar VOCs. The mechanism of this sensitivity was also studied by modeling both gas diffusion inside the polymer and polymer optical properties. The selectivity of the whole system can be further improved by comparing relative spectral and color changes of a few polymer films simultaneously. Thus, the prototype of LC-nose based on polymer networks could be created.

M71.00203: Environmentally Sensitive Optical Fibers and Waveguides Based on Hydrogen-Bonding Compounds  BENJAMIN SCHUTSKY (Presenter), ANTHONY GRAY, KYRA FULEIHAN, CHRISTOPHER LA FOND, MEGHAN EVANS, PETR V SHIBAEV, Fordham University — Novel optical fibers and waveguides were designed and created from blends of hydrogen bonding compounds (polyvinyl alcohol, polyvinylpyridine, acrylic acid) with glassy polymers and low molar mass liquid crystals. Optical fibers display significant birefringence in their cores since the drawing procedure of the fibers lead to the higher concentration and orientation of liquid crystal inside the core of the fiber. The fibers were studied by differential scanning calorimetry and optical methods. It was shown that fibers gain additional stability if they are physically crosslinked with diacidic low molar mass compounds (sebacic acid). Optical response of the fibers (changes in propagating light intensity or additional leakage of light) to the action of volatile organic compounds (VOCs) was studied and discussed for different types of polar and non-polar VOCs. It was found that optical response depends on structural reorganization of the fibers that starts in the outer layer and then propagates towards the core in a way similar to the response of liquid crystals [1].

M71.00204: Optics of multilayered cholesteric liquid crystals with disorder: towards LC-nose.  EMAIYAH GULLATT (Presenter), PETR V SHIBAEV, OLEKSIY ROSLYAK, JOSEPH PLUMITALLO, Fordham University, UPALI APARAJITA, Borough of Manhattan Community College — Optical properties of multilayered disordered cholesteric liquid crystals (CLC) with different types of disorders were performed by employing 4x4 matrix method in order to simulate a diffusion of volatile organic compound (VOC) molecules inside the cholesteric material. A simulated CLC consisted of three layers, the central layer being unaffected by VOCs and two outer layers being subjected to diffusion of VOC molecules. The diffusion of VOCs inside the CLC was simulated by changing either the order parameter or helical pitch of the two outer layers of the CLC. The results were compared with experiments of VOC diffusion in a number of CLC systems. It was determined that the change of order parameter plays an important role in liquid CLCs and change of helical pitch mostly affects CLC polymers. The applicability of these calculations for designing artificial LC-nose [1] is discussed.

[1] Liquid crystal nose, chiral case: towards increased selectivity and low detection limits

PV Shibaev, D Carrozzi, L Vigilia, H DeWeese
Liquid Crystals, 1-9

M71.00205: Verifying XY-Model Predictions for Topological Defects in Films of Smectic Liquid Crystals*  CHEOL PARK (Presenter), ADAM GREEN, STIAN HOWARD, ERIC MINOR, JOSEPH E MACLENNAN, MATTHEW GLASER, NOEL ANTHONY CLARK, Physics and Soft Materials Research Center, University of Colorado Boulder — We describe experiments exploring the applicability of the XY model to defect-rich smectic C liquid crystal films. Topological defects in the orientation field are created by rapidly deflating a hemispherical `bubble' of a molecularly thin film, resulting in a flat film with a high density of defects. The subsequent pair-wise annihilation of these defects is captured with sub-millisecond resolution using high-speed, polarized light video microscopy. The simplest theoretical description of the orientation field, the XY model, makes specific predictions about the annihilation dynamics, predicting sub-logarithmic scaling of the number of defects present at short times and logarithmic scaling at longer times. Progress towards verifying the applicability of the XY model to these systems at early times has been stymied by experimentally difficulties in tracking the defects. Through improvements in illumination and by leveraging recent advances in machine-learning, we can now identify and track individual defects at early times, allowing us to confirm the predictions of the XY model.

*Work supported by NASA Grant No. NNX-13AQ81G and NAG No. NNX17AC74G and by the Soft Materials Research Center under NSF MRSEC Grant No. DMR-1420736.
M71.00206: Study of a cylindrical fiber cored by a double twisted chiral nematic.
FERNANDO MAGANA, GERARDO-JORGE VAZQUEZ FONSECA (Presenter), ADRIAN REYES, LAURA PALOMARES PALOMARES, Univ Nacl Autonoma de Mexico — We study a region of the space where an electromagnetic field is propagating within a waveguide consisting of a material having double helix as found in some chiral nematic materials such as blue phases. We establish the electromagnetic equation governing the dynamics of the propagating modes. We found the band structure of the mentioned modes, the profiles field amplitudes and the Poynting vector distributions versus the radius of the fiber. We discuss the composition and conditions for the modes to propagate.

M71.00207: Deformation of structurally chiral polymer stabilized networks in electrically tunable filters*
BRIAN P RADKA (Presenter), TIMOTHY J WHITE, Chemical and Biological Engineering, University of Colorado, Boulder — The cholesteric liquid crystalline phase self-organizes into a helical structure. In the planar orientation, the periodicity naturally exhibits a selective interference reflection. Dynamic optical responses observable as red-shifting tuning, blue-shifting tuning, or bandwidth broadening can be achieved under an electrical field with the inclusion of a polymer network. Our recent research activities have focused on further elucidating the fundamental electrochemical response of the ion-mediated deformation of the polymer stabilizing network in the cholesteric phase. A variety of liquid crystalline and non-liquid crystalline monomers are selected in order to determine how intermolecular forces and liquid crystalline interactions affect the performance of the material. Multiphoton fluorescent imaging is used to visualize pitch and polymer network deformation. The correlated influence of photopolymerization conditions and ionic impurities will be discussed.

*We gratefully acknowledge the financial support of the Air Force Research Laboratory via Azimuth Corporation

M71.00208: Electro-optical switching and order parameter measurements of dual-frequency nematic liquid crystals: regimes of thin and thick cells.
OLHA MELNYK (Presenter), University of Colorado, Colorado Springs, YURIY GARBOVSKIY, Central Connecticut State University, ANATOLIY GLUSHCHENKO, University of Colorado, Colorado Springs — Liquid crystals utilized in conventional display applications typically have a layer thickness of less than 10 µm. However, emerging non-display applications of liquid crystals require thicker material layer with faster response. Electro-optical performance of relatively thin liquid crystal cells is well-documented, but little is known about the properties of thicker layers. Also to address the need for the fast electro-optical switching a dual frequency liquid crystals are investigated. We are presenting the electro-optical response of dual-frequency nematic liquid crystals using a broad range of the cell thickness (2–200 µm). Two regimes of electro-optical switching of dual-frequency nematics are observed and analyzed. To uncover the origin of the observed two regimes of electro-optical switching, measurements of the orientational order parameter of dual frequency nematic liquid crystals were carried out over the same range of thicknesses. The non-monotonous dependence of the order parameter $S$ on the cell thickness obtained for relatively thin layers (< 60 µm), and is followed by a rapid monotonous decay for thicker (60-200 µm) samples. This provides a basis for understanding of two regimes of electro-optical switching of thin and thick layers of dual frequency nematics.
M71.00209: Assembly of microparticles in disclination of LCLCs confined to cylindrical capillaries. SUJIN LEE (Presenter), ELSA REICHMANIS, JUNG O PARK, MOHAN SRINIVASARAO, Georgia Inst of Tech — We investigate the assembly of microparticles in nematic lyotropic chromonic liquid crystals (LCLCs) confined to cylindrical capillaries. Two line defects with double helical configuration is observed for Sunset Yellow FCF with the homeotropic anchoring being obtained by parylene-N coating. Here, we show that disclinations in Sunset Yellow FCF can act as templates for particle dispersions. Additionally, we use magnetic micropaticles to study effect of external magnetic fields on the lclcs. The observed assemblies extend our understanding of the structure of disclinations and ability to design the architectures of soft materials.

M71.00210: Predicting the Steady Flow of a Fluid with Particles by Deep Learning* HIROTO OZAKI (Presenter), TAKESHI AOYAGI, CD-FMat, AIST — Computational Fluid Dynamics (CFD) simulation has the potential for application in material science. In these applications, a common study object is a highly viscous fluid that passes structures in the microscale. However, its computational cost is a barrier to application. Meanwhile, some recent studies successfully reduced the computational cost of CFD by utilizing machine learning and deep learning techniques [1, 2].

Using deep learning, the authors predicted the steady flow around a large number of particles and examined the effectiveness of the prediction for the study of materials development. The particle-fluid interaction is computed using the Smoothed Profile Method [3]. After learning the flow that passes the particles obtained by iterative calculation, the deep learning quickly and accurately predicted the flow of the system with unknown particle concentration and arrangement. The fluid force applied to each particle was also accurately predicted.

References

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M71.00211: Deep Convolutional Neural Network for Tomographic Reconstruction of Strain

MATTHEW CONNOLLY (Presenter), DAMIAN LAURIA, National Institute of Standards and Technology Boulder — The neutron transmission Bragg edge method has gained interest over the past decade as a technique for providing a fast, high spatial-resolution and high sample penetration mapping of strain. Since its advent, there has been a strong desire to extend the transmission Bragg edge method to provide a full 3D tomographic reconstruction of the full strain tensor. However, it has been shown that traditional tomographic reconstruction algorithms are, in general, unable to provide a unique solution as the mathematical problem of inversion of Bragg edge data is ill-posed. The major complication of strain tomography compared to traditional scalar tomography is the directional dependence of the strain tensor. Deep Convolutional Neural Networks (DCNNs) have shown success in scalar tomographic reconstruction, in particular for cases in which scalar tomography is ill-posed (e.g. when sample exposure or rotation is limited). We show that DCNNs can be extended to perform tomographic reconstruction of strain tensors based on neutron transmission Bragg edge data. We show three training strategies and a DCNN architecture with success in reconstructing 2D strain fields. Additionally, we explore the advancements necessary to make a fully generalizable model for tomographic reconstruction of strain.

M71.00212: Machine learning for detecting microscopic parameters characterizing mechanical properties of liquid crystal elastomers*

HIDEO DOI (Presenter), KAZUAKI TAKAHASHI, Research Center for Computational Design of Advanced Functional Materials, National Institute of Advanced Industrial Science and Technology (AIST), HARUKA YASUOKA, KENJI TAGASHIRA, Research Association of High-Throughput Design and Development for Advanced Functional Materials, JUNICHI FUKUDA, Faculty of Science, Kyushu University, TAKESHI AOYAGI, Research Center for Computational Design of Advanced Functional Materials, National Institute of Advanced Industrial Science and Technology (AIST) — Liquid crystal elastomers (LCE) are of great scientific and technical interest because of the potential of sensors and soft actuators. Molecular dynamics (MD) simulation is a promising means to clarify macroscopic deformation of LCE from a microscopic viewpoint, however, a detection of major parameters characterizing the deformation is difficult because there are many microscopic parameters. Therefore, a systematic analysis should be done for detecting the relation between microscopic parameters and mechanical properties. In this study, a machine learning (ML) approach is used to explore the relation between microscopic characteristics and mechanical parameters. With these models, we perform MD simulations and compute stress-strain curves. Then a regression analysis with random forest method to explain the difference of stress-strain curves is performed with 20 types of microscopic parameters. The ML results reveal the effective set of data descriptors that predict well the stress-strain curves. Therefore, ML technique has a capability to overcome the difficulty to manually explain the complex relation between microscopic parameters and macroscopic properties.

*This work was funded by New Energy and Industrial Technology Development Organization of Japan (NEDO) Grant (P16010).
**M71.00213: Predicting Soft Matter Evolution Using Machine Learning**  ZITONG ZHANG  
(Presenter), Tsinghua University, BO LI, STEVE GRANICK, Institute for Basic Science — Soft matter including colloids, polymers and granular material display behavior and self-organization that are difficult and sometimes impossible to predict due to complex interactions with the environment, which itself can change and self-organize. The traditional approach to understand these problems is to study structural evolution by theory and experiment. We are taking the different approach of machine learning. We build convolutional neural networks (CNNs) to process the large amounts of data. We are applying these new tools to direct imaging in rheo-optics, to fitness evaluation of cell growth when they pass near obstacles, and to ecological microsystems with soft matter flavor. The common element is to predict properties varying with time.

**M71.00214: Confined filaments in soft vesicles - case of sickle red blood cells**  ARABINDA BEHERA (Presenter), GAURAV KUMAR, ANIRBAN SAIN, Physics, Indian Institute Of Technology Bombay — Abnormal shapes of red blood cells (RBC) have been associated with various diseases. Diverse RBC shapes have also been intriguing for membrane biophysics. In our work, we focus on sickle-shaped RBC which form due to abnormal growth of semi-rigid Hemoglobin (HbS) fibers confined in RBC. Using the area difference elasticity (ADE) model for RBC and worm-like chain model for the confined HbS fibers, we explore shape deformations at equilibrium using Monte-Carlo simulation. We show while a single HbS fiber is not rigid enough to produce sickle-like deformation, a fiber bundle can do so. We also consider multiple disjoint filaments and find that confinement can generate multipolar RBC shapes and can even promote helical filament conformations which have not been discussed before. We show that the same model, when applied to microtubules confined in phospholipid vesicles, predicts vesicle tubulation. In addition, we reproduce tube collapse transition and tennis racket type vesicle shapes, as reported in experiments. We conclude that with a decrease in the surface area to volume ratio, and membrane rigidity, the vesicle prefers tubulation over sickling.

*We thank the University Grant Commission, India, and IRCC-IIT Bombay for financial support.

**M71.00215: AZO-modified lipids bilayer and their dynamics associated with optical stimulation.**  CINTIA MENENDEZ (Presenter), Pritzker School of Molecular Engineerin, The University of Chicago, ARASH MANAFIRAD, ANTHONY DUPRAT DINSMORE, Department of Physics, University of Massachusetts, JUAN DE PABLO, Pritzker School of Molecular Engineerin, The University of Chicago — In this work we have studied the dynamics of membranes with azo-modified lipids from molecular scales (atomistic molecular dynamics simulations) to vesicle scale (experimental work), with the aim of increasing understanding regarding steady states, elastic constants and membrane permeability. We have found that vesicles dilate and become flexible and much more permeable as a result of trans-to-cis conversion. Therefore, to the best of our knowledge, these are the first studies to look at the membrane dynamics associated with optical stimulation. In addition, the relative energies of cis and trans states were theoretically determined. Finally, it is worth to highlight that this combined studies (computational and experimental work) open new avenues regarding rational molecular design in order to tune response.

*This work was supported by the Air Force Office of Scientific Research (FA9550-12-1-0435) and the U.S. Army Research Office (W911NF-15-1-0568).
M71.00216: Enhanced diffusion of tracer microspheres in a temporally fluctuating porous structure  
RAPHAEL SARFATI (Presenter), CHRISTOPHER P CALDERON, DANIEL K SCHWARTZ, 
University of Colorado, Boulder — Transport in porous materials is at the center of a wide range of natural and industrial processes. While many studies have focused on the properties of porosity with spatial fluctuations, much less is known about the effects of temporal fluctuations in the medium's structure. We have designed a simple experimental system aimed at investigating the transport properties of a crystalline porous material made of a hexagonal lattice of 2um spheres, which are either static, or fluctuating in time about an average position (dynamic). Using complementary illumination, we can image and track both diffusive tracers (100-400nm) and lattice spheres. We compare the transport properties of the static and dynamic lattices with similar average densities and find that diffusion is significantly faster within the dynamic lattice. We hypothesize that this might be due to a combination of different effects. First, the motion of lattice spheres could reduce the hydrodynamic hindrance of the tracers, and increase diffusivity within a cavity. Second, fluctuations in pore sizes, induced by the fluctuations in distances between adjacent spheres, could permit a higher transition rate between cavities than a fixed pore size of the same mean value. We present results relating to these two effects.

M71.00217: Fibers on the surface of thermo-responsive gels induce controllable formation of helical structure  
TAO ZHANG (Presenter), VICTOR V YASHIN, ANNA BALAZS, Univ of Pittsburgh — We use computational modeling and analytical calculation to investigate the behavior of gel-fiber long thin films; we specifically show that the arrangement of fibers localization on the outer surface of the sample provides a powerful means of tailoring the overall shape of the sample, as to form helical structure with controlled chirality. We focus on thermo-responsive gels, which exhibit a lower critical solubility temperature (LCST) and thus shrink when heated above a certain temperature. The stiff fibers are attached to this gel and inhibit the nearby network from undergoing the heat-induced collapse. Away from the fibers, however, the network can readily shrink in response to the increased temperature. This competition between the constrained regions and the unconstrained regions of the heated gel regulates the structural evolution and final geometry of the sample. Our simulations use the gel lattice spring model (gLSM) to determine how the temperature, arrangement and number of the fibers control the bending and twisting of thin ribbons. Our comprehensive 3D analytical calculation incorporates elasticity, differential geometry, and variational principles.
M71.00218: Curved Geometries from Planar Director Fields: Solving the Two-Dimensional Inverse Problem*  ITAY GRINIASTY (Presenter), Laboratory of Atomic and Solid State Physics, Cornell University, EFI EFRATI, HILLEL AHARONI, Weizmann Institute of Science — Thin nematic elastomers, composite hydrogels, and plant tissues are among many systems that display uniform anisotropic deformation upon external actuation. In these materials, the spatial orientation variation of a local director field induces intricate global shape changes. Despite extensive efforts, until recently there was no general solution to the inverse design problem: How to design a director field that deforms exactly into a desired surface geometry upon actuation, or whether such a field exists. In this work, we phrase this inverse problem as a hyperbolic system of differential equations. We prove that the inverse problem is locally integrable, provide an algorithm for its integration, and derive bounds on global solutions. We classify the set of director fields that deform into a given surface, thus paving the way to finding optimized fields.

*E. E. thanks the Alon fellowship and the Ernst and Kaethe Ascher Foundation. I.G. is grateful to the Azrieli Foundation for the award of an Azrieli Fellowship. This work was supported by ISF Grant No.1479/16 and Minerva Grant No.712273. H. A. was supported by NSF Grant No. DMR-1262047.

M71.00219: Elastic-Viscoplastic transition in a modified Soft Glassy Rheology model*  JUN DONG PARK (Presenter), Kumoh Inst of Tech — The elastic-viscoplastic transition of glassy materials is studied with a modified Soft Glassy Rheology (SGR) model that is newly suggested for more accurate description of rheological behavior of glassy materials. The modified SGR model incorporates sophisticated features of glassy materials, such as collective dynamics. The modified SGR model demonstrates different elastic-viscoplastic transitions depending on conditions such as methods of glassy dynamics description, flow conditions, and shear history. The rheological transition of SGR model under startup shear is interpreted in terms of local strain distribution change that represents physical state change. Based on the findings, we interrogate how various features of glassy dynamics affect the elastic-viscoplastic transition in glassy materials and discuss effective ways to describe glassy materials. Our results provide some clue to understand the physical origin of the elastic-viscoplastic transition in glassy materials.

*This work was supported by the National Research Foundation(NRF) of Korea grant funded by Korean government (Ministry of Science and ICT) (2019R1G1A1100555).
M71.00220: Bifurcated yielding response of aging fibrillar networks  
RYAN POLING-SKUTVIK (Presenter), CHINEDUM OSUJI, University of Pennsylvania — Yielding in disordered materials occurs with a remarkably broad variety of characteristics and remains a poorly understood phenomenon. Here, we investigate the yielding and aging behavior of disordered fibrillar networks of cellulose nanofibrils (CNF), micron-sized semiflexible fibers with aspect ratios >100. At high concentrations, CNF form dense physical networks that support finite stresses and in which terminal relaxations are suppressed. We observe a strong decrease in the yield strain of the networks with increasing volume fraction ($\gamma_y \sim \phi^{-2}$). Further, we observe a strong aging response of the system after an initial yielding event. Subsequent yielding occurs at a time $t_y$ that depends sensitively on the magnitude of applied stress and the aging time $t_w$ between initial yielding and reapplication of stress. The yield time diverges at finite waiting times for small stresses and asymptotes towards a finite yield time at large stresses, with bifurcation around a critical stress that is similar to the yield stress of the system. The waiting time at which the yield time diverges increases with applied stress below the critical stress, indicating that the bifurcation is rooted in the rate of thermally driven network restructuring relative to stress-driven de-structuring.

M71.00221: Yielding of FCC crystals at zero deformation rate: evidence for hidden transition  
PASWA NATH (Presenter), TIFR Centre for Interdisciplinary Sciences — Despite much effort, no theory, consistent with all rigorous thermodynamic constraints, has been derived that can predict the yield point of a real solid. An exact result states that the free energy of any material, made up of entities interacting with short ranged forces, cannot depend on the shape of the boundary. This implies that crystalline solids are guaranteed to yield at infinitesimal stresses when deformed at vanishing rates. Here we present our work on yielding of an ideal FCC solid in the strictly zero strain rate limit. In this limit, the yield point vanishes for infinitely large systems. Earlier, we showed, for an ideal 2d triangular crystal that the yielding phenomena is a dynamic consequence of a hidden first order phase transition. Our calculations of the free energy of such solids also show that the solid phase is always metastable at any finite temperature and infinitesimal deformation. Our prediction for the dynamical yield points agree with MD simulations for a wide range of deformation rates. We describe, here, our extension of this previous work to the initially defect-free FCC crystal. We discuss about commensuration, finite-size effects and consequences of systematically introduced disorders as random interactions of varying strength in such solids.
**M71.00222: Interfacial Thermodynamics of Surfactants at Elevated Pressure**  
ZACHARY HINTON (Presenter), NICOLAS ALVAREZ, Department of Chemical and Biological Engineering, Drexel University — While surfactant use under elevated pressures is not a novel field, experimental measurements of surfactants in extreme environments is lacking in the literature. Thermodynamically, pressure impacts the concentration of surfactants at a pressurized interface, thus affecting the interfacial tension. The relationship between the concentration, pressure, and interfacial tension for a given surfactant has not been measured sufficiently for nearly any surfactant. In this work we use a novel high pressure microtensiometer to probe surfactant transport and equilibrium thermodynamics at the water-CO$_2$ vapor interface. We show that surfactant isotherms are highly dependent on pressure illustrating that key thermodynamic and kinetic parameters are strong functions of pressure. Furthermore, we show that surfactant performance is significantly decreased at elevated pressures. We outline the importance of experimental measurements of surfactant behavior on predicting high pressure performance of a variety of surfactant chemistries.

**M71.00223: Role of solvent identity in impact-activated solidification of dense suspensions**  
LIANG ZHAO (Presenter), MICHAEL VAN DER NAALD, GRAYSON JACKSON, HEINRICH M. JAEGGER, University of Chicago — Applied stress can drive flowing suspensions of solid particles in a Newtonian liquid into a shear-jammed solid state. Beyond steady state rheology, recent work demonstrated that high-speed ultrasound imaging could be used to visualize transient flow fields generated by impact and track the propagation of “jamming fronts” in optically opaque cornstarch suspensions [1][2]. We here use this ultrasound imaging technique to reconstruct the flow fields caused by impact of dense suspensions containing silica nanoparticles in polymeric liquids. We find that the solvent molecular weight plays an important role in mediating frictional contacts between particles required for shear jamming. [1] E. Han, I. R. Peters and H. M. Jaeger. High-speed ultrasound imaging in dense suspensions reveals impact-activated solidification due to dynamic shear jamming. *Nat Commun*, 7:12243, 2016.  
**M71.00224: Colloidal Assembly at Curved Liquid-Liquid Interface**  
ZICHEN LING (Presenter), Chemical Engineering, Wayne State University, NAMITA SHOKEEN, Physics and Astronomy, Wayne State University, YINGXI ELAINE ZHU, Chemical Engineering, Wayne State University, ASHIS MUKHOPADHYAY, Physics and Astronomy, Wayne State University — Colloidal particles can readily assemble into crystalline structure under confinement. When confined on a flat surface, spherical particles can pack efficiently with an arrangement of hexagons. However, the regular hexagonal packing configuration could be disrupted on a curved surface with resulting formation of defects. In this study, we investigated the self-assembled crystallography of fluorescence labeled polystyrene (PS) microspheres at lutidine-water interfaces, where liquid-liquid separation occurs as increasing the temperature to exceed the critical solution temperature of the mixture around 27-28 °C. We determined the assembled packing microstructure of PS microspheres at the liquid-liquid interface of varied curvature by direct confocal microscopic particle tracking. We observed disordered-to-crystalline structural transition in self-assembled PS colloidal monolayer at curved liquid-liquid interfaces when a critical curvature is exceeded.

**M71.00225: Unique assembly structures of amphiphilic Janus particles in ionic liquid solutions**  
AYUNA TSYRENOVA, MUHAMMAD FAROOQ, JARED ANDERSON, SHAN JIANG (Presenter), Iowa State University — Janus particles assemble into remarkable superstructures due to different chemistry on the two sides of a single particle. The directional interactions present new structures and the ensuing physics are essential to the formation of intriguing clusters, chains and crystals. Our recent experiments demonstrate unique assemblies of Janus particles in ionic liquid solutions that have never been observed before. Despite extensive studies focused on purified Janus particles, their self-organization in the presence of surface-active molecules has not been systematically studied. The intriguing orientation correlation and crystal structures formed in this multicomponent system cannot be explained by the current theory. Our central hypothesis is that the association of surface active molecules with Janus spheres, especially the boundary on the particle surface dividing the two sides, can effectively modulate the interactions among Janus particles and alter their assembly behaviors. The results provide critical information regarding new phenomena observed through experimentation and offer guidance for future applications of Janus particles.

JESSICA BICKEL (Presenter), KIRIL STRELETZKY, Cleveland State University — Researchers at Cleveland State University's Department of Physics and Department of Chemical & Biomedical Engineering collaboratively study the unique properties and applications of soft matter materials. Together, we are in our third year of an NSF-sponsored Research Experiences for Undergraduates (REU) site on Synthesis, Assembly and Characterization of Soft Matter Systems. The objective of our site is to involve undergraduate physics and engineering majors in meaningful interdisciplinary research projects within soft matter science and engineering. A primary focus of our site is to encourage students to continue in STEM fields as either graduate students or workforce members. CSU’s focus on Engaged Learning has cultivated a strong culture of support for undergraduate research, and REU participants benefit from this culture. Students receive one-on-one mentoring from experienced faculty and participate in a variety of professional development opportunities. This poster will give an overview of the student research accomplishments over the last three years. It will also discuss the benefits of the experience to both students and faculty mentors.

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M71.00227: Introducing Mutations in an artificial self-replication system*  

HENG NI, FENG ZHOU (Presenter), RUOJIE SHA, NADRIAN C SEEMAN, PAUL M CHAIKIN, New York Univ NYU — We have started a study of Darwinian evolution using an artificial self-replication system of DNA origami dimer rafts. By introducing a small error (3 bases) in the sticky-ends recognition strands, there is a small chance for the system to mutate templating a different dimer raft which can replicate itself effectively starting a new species. The mutation rate is small, but the mutated nanostructure shares the same replication ability as the original dimers. Although the original dimers are dominant at the beginning of self-replication, after many replication cycles we should have an equal mixture of mutated and original dimers. In addition, we can modify the mutated structures with the capability of growing faster, then after many replication cycles, the mutated species will take over the system. We can use the functionality of the different species to affect this takeover. Mutation and population domination by the fittest species would amount to natural selection in this artificial system.

*This research has been primarily supported by DOE DE-SC0007991 and DE-SC0000989.
M71.00228: Flow-induced fracture in freestanding wet colloidal pillars*  JUSTIN BEROZ
(Presenter), ALVIN T.L. TAN, KENNETH N KAMRIN, JOHN HART, Massachusetts Institute of Technology
MIT — Self-assembly of colloidal particles is an attractive means to create materials with engineered properties by controlling the hierarchy of particle composition, size, ordering and macroscopic form. We recently demonstrated a direct-write method [1] that enables self-assembly of colloidal particles from liquid suspension into centimeter-scale freestanding crystalline structures by utilizing a combination of evaporation-driven liquid flow and capillary attraction. However, in a subset of the structures we constructed, cracks formed during drying, throughout the height and at the free end. We detail our observations and explain how the Darcy flow of liquid through the structure drives fracture, despite the structure being compressed by a uniform capillary pressure at its surface. We derive a criterion for the presence and spacing between cracks, based on an energy scaling argument, that compares favorably with our experiments. This work ultimately provides a guideline for constructing crack-free 3D colloidal structures, which can potentially achieve complex freeform macroscale geometries.

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M71.00229: Block copolymer assemblies under 3D confinement: from spherical boundary to continuous network template  XUEYAN FENG (Presenter), WENPENG SHAN, Rice University, ABBY JUHL, Air Force Research Laboratory, INBAL WEISBORD, TAMAR SEGAL-PERETZ, Technion, EDWIN THOMAS, Rice University — Depending on the interplay between polymer chain stretching and interfacial energy of the intermaterial dividing surface (IMDS), different self-assembled block copolymer nanostructures can be achieved. Directed self assembly in 2D employing confinement via walls, posts and various surface treatments can improve long range order and induce new microdomain patterns. By applying templates with spatially varying 3D geometric boundary conditions, block copolymers have the possibility to form a host of new morphologies and complex, hierarchical block polymer/template 3D ordered composites. The self-assembly behaviors of a bulk phase lamella-forming polystyrene-b-polydimethylsiloxane diblock copolymer within different 3D confinement boundary conditions are presented. The 3D confinement varies from that of within a simple sphere to occupation of the connected void space of a complex 3D network template. By taking advantage of Slice-and-View scanning electron microscope tomography, large volume 3D information of the polymer/template assemblies can be produced at high resolution. The domain morphology, IMDS curvature, polymer chain stretching, and morphological defects are discussed.
M71.00230: Hydrodynamically-driven assembly of nanoparticles in an anisotropic media
STIVEN VILLADA GIL, Universidad Nacional de Colombia sede Medellín, Politécnico Colombiano Jaime Isaza Cadavid, VIVIANA PALACIO-BETANCUR (Presenter), Institute for Molecular Engineering, University of Chicago, JULIO C. ARMAS-PÉREZ, División de Ciencias e Ingenierías, Campus León, Universidad de Guanajuato, JUAN P. HERNÁNDEZ-ORTIZ, Departamento de Materiales y Minerales, Universidad Nacional de Colombia sede Medellín, JUAN DE PABLO, Institute for Molecular Engineering, University of Chicago.

Argonne National Laboratory —
Nanoparticle (NP) self-assembly in liquid crystals (LCs) depends on the elasticity of the material to form arrays with crystalline symmetry. These arrays can be tuned via the anchoring of the NP, and the orientation of the director field, effectively using the defects around the NP as sites for assembly. Additionally, confinement and hydrodynamic fields can also be used to control the assembly. Scenarios often consider one, two, or three NPs under various flow regimes and in moderate confinement. The simulations presented here use the Stark-Lubensky formalism, where the Landau-de Gennes free energy functional is coupled with the momentum balance through a Poisson-bracket formulation. To describe NP-LC suspensions, a transient three-dimensional Galerkin finite element framework was implemented to achieve a numerical solution. We show that, independent of NP anchoring, defects are displaced in the up-stream direction, ultimately forming a hedgehog defect. The assembly mechanism for a pair of NPs is modified in the large Ericksen regime, where the NPs show an unexpected non-monotonic tendency to aggregate. The modifications to the defect structure and the free energy landscape open a new avenue to the directed assembly of NPs immersed in LC under conditions far from equilibrium.

M71.00231: Knitting Patterns of Pentasil Chains reveal MFI-MEL Heterostructures in Two-Dimensional Zeolite Nanosheets
PRASHANT KUMAR (Presenter), NEEL RANGNEKAR, HAO XU, EVGENII FETISOV, J. ILJA SIEPMANN, TRAIAN DUMITRICA, University of Minnesota, MICHAEL TSAPATSIS, John Hopkins University, K. ANDRE MKHOYAN, University of Minnesota —
The zeolite MFI is a widely used catalyst and adsorbent, which also holds promise as a thin film membrane for the separation of hydrocarbon isomers and other difficult to separate mixtures. The discovery of nm-thick 2-dimensional (2D) MFI nanosheets has enabled methods for thin film zeolite fabrication that open new horizons for membrane science and engineering. However, the crystal structure of 2D-MFI nanosheets and its relationship to separation performance remain elusive. Using transmission electron microscopy, we find that one- to few-unit-cells wide intergrowths of the zeolite MEL exist within 2D-MFI. We identify the planar distribution of these 1-dimensional (1D) or near-1D-MEL domains, and show that a fraction of individual nanosheets have high MEL content while the majority of nanosheets are MEL-free. Atomistic simulations suggest that commensurate knitting of 1D-MEL within 2D-MFI creates more rigid and highly selective pores as compared to those in pristine MFI nanosheets and permeation experiments show an unprecedented separation factor of 60 using an industrially relevant (undiluted 1 bar xylene mixture) feed.
M71.00232: Structural and mechanical properties of nucleic acid nanotubes: A combined all-atom and coarse-grained molecular dynamics study*  SUPRIYO NASKAR (Presenter), HIMANSHU JOSHI, MOUNIKA GOSIKA, Indian Institute of Science - Dept of Physics, BANANI CHAKRABORTY, Department of Chemical Engineering, Indian Institute of Science, NADRIAN C SEEMAN, Department of Chemistry, New York University, PRABAL K MAITI, Indian Institute of Science - Dept of Physics — In this work, we introduce a computational framework to model nucleic acid nanotubes and estimate their mechanical properties using various levels of theory. Using atomistic molecular dynamics (MD) simulations, we report the enhancement of the structural and mechanical stability of DNA nanotube (DNT) by changing the salt concentrations. The calculated persistence length \( L_p \) of the DNTs is \( \sim 1-2 \) μm which is an order of magnitude higher than that of a single dsDNA. DNTs have stretch modulus \( \gamma \) value in the range of \( \sim 6-8 \) nN. We find that, with the gradual increment of salt concentration, an increase in \( L_p \) and \( \gamma \) which reaffirms the structural and mechanical stability of the DNT at higher salt concentrations. We also model DNT using two widely used coarse-grain (CG) models – namely Martini and oxDNA. We compare and contrast the all-atom MD and experimental results with the results obtained using these CG models. We also propose a model of hexagonal nanotubes made of dsRNA connected by double crossover at different positions. The calculated \( \gamma \) and \( L_p \) of the in silico modeled RNTs are in the same range of values as in the case of DNTs. Using helicoidal parameters of individual base pairs, we explain the relative flexibility and rigidity of the RNTs having different sequences.

*CSIR IISc

M71.00233: Role of Chirality in Self-Assembly of Amino Acid Tryptophan on Au (111)  YONGCHAN JEONG (Presenter), JUNGPIL SEO, Daegu Gyeongbuk Institute of Science and Technology — Proteins only use single L-enantiomer of amino acids owing to the homochirality in a living system. Interestingly, a small amount of tryptophan (Trp), which is one of the essential amino acids, is required in the proteins. We studied the self-assembly of Trp on Au (111) using scanning tunneling microscopy and density functional theory. When single Trp enantiomers were deposited on Au (111), we confirmed 1D chain structures. The deposition of racemic mixture of two opposite Trp enantiomers also built chain structures, but these structures differed from those formed by single Trp enantiomers. In the self-assembly of two opposite Trp enantiomers, the absence of the single Trp enantiomers-formed chain structures is because the heterochiral configurations were more favorable energetically than the homochiral ones. In the heterochiral chain structures, an enantiomer obstructed the access between amino and carboxyl groups in the opposite enantiomers, resulting in the hindrance of formation of peptide bonding between the opposite enantiomers. From these results, we can estimate that proteins utilize a small amount of Trp to avoid the disturbance of peptide bonding formation. In addition, our study also will contribute to the understanding for origin of homochirality in a living system.
M71.00234: Biomimetic Tunable Disordered Photonic Structures via Programmable Polymer Blend Phase-Separation  
ASRITHA NALLAPANENI, University of Akron, MARKUS BLEUEL, NIST, JAN ILAVSKY, CHENHUI ZHU, ANL, MATTHEW SHAWKEY, University of Ghent, ALAMGIR KARIM (Presenter), University of Houston — Biopolymers such as proteins undergo self-assembly resulting in complex hierarchical structures with well-defined structure and fascinating multi-functional properties. For example, disordered photonic structures in avian birds are responsible for white and blue non-iridescent colors. These structures are thought to arise from phase-separation between β-keratin and cytoplasm during cell growth and the degree of disorder determines coloration. We utilized temperature-induced phase-separation in polymer blends as an approach to attain multi-functional non-iridescent structural colors similar to nature. We further examined the dynamics of phase-separation to gain insights into the molecular self-assembly process and understand the temporal-evolution of structural and optical disorder. Our results indicate that structural disorder scales with domain-size as well as phase-separation time and a strong direct correlation between structural and optical disorder is observed. Tunable disordered photonics can also be obtained simply by tuning the molecular weight of the polymer blend components. In future photonic designs, it is important to exercise good control on structural disorder at multiple length scales in order to obtain tunable visible colors with multi-functionality.

M71.00235: Oscillatory Microdroplet Constituted Urea Biosensor Stimulated by Acoustic Waves*  
SIDDHARTH THAKUR (Presenter), Department of Chemical Engineering, Indian Inst of Tech-Guwahati, MITRADIP BHATTACHARJEE, Centre for Nanotechnology, Indian Institute of Technology Guwahati, ASHOK KUMAR DASMAHAPATRA, Department of Chemical Engineering, Indian Inst of Tech-Guwahati, DIPANKAR BANDYOPADHYAY, Centre for Nanotechnology, Indian Institute of Technology Guwahati — A proof of concept microdroplet based urea biosensor has been presented that employs a facile but robust detection technique. To substantiate, variation in electrical resistance across a 10 µL salt-laden water microdroplet placed on a glass substrate was observed when it was subjected to sinusoidal acoustic waves at its natural frequency, ~ 320 Hz. For the biosensing application, the conducting water microdroplet was loaded with a suspension of urease-linked gold/cadmium sulfide nanocomposite. Upon adding urea solution in the droplet under the influence of acoustic waves, the changing electrical resistance could be effectively correlated with the changing urea concentration. Higher reaction rate was observed owing to the presence of nanocomposites which provided enzymatic stability and higher interfacial area. Also, the confined droplet geometry resulted in formation of vortices that improved the mixing characteristics. A calibration chart was prepared across a wide range of urea concentrations that was employed for working with unknown human serum samples.

Reference  

*MeitY, MHRD, DST-FIST
M71.00236: Proton Dynamics of CsH$_2$PO$_4$ Solid Acid using $^1$H and $^{31}$P Magic Angle Spinning Nuclear Magnetic Resonance (MAS-NMR)  SE-HUN KIM (Presenter), Jeju National University — This study investigated hydrogen-bonded CsH$_2$PO$_4$ (CDP) solid acid using $^1$H and $^{31}$P high-resolution nuclear magnetic resonance (NMR). Below the superprotonic phase transition temperature, the temperature dependence of the H NMR spectra was observed with two different hydrogen-bonded networks in the CDP structure. The systematic evolution of the lineshape with temperature dependence indicates hydrogen hopping in the chemical structure of hydrogen-bonded networks in a solid acid lattice. The proton conduction under two types of hydrogen-bonds—interchain and intrachain—in CsH$_2$PO$_4$ in the chemical environments of PO$_4$ tetrahedra is discussed.

M71.00237: Distinguishing protein aggregates from contaminants in viscous mixtures with holographic video microscopy*  LAURA PHILIPS (Presenter), ANNEMARIE WINTERS, MARY ANN ODETE, FOOK C CHEONG, Spheryx, Inc — We demonstrate how holographic video microscopy detects, counts, and characterizes individual sub-visible protein aggregates ranging in diameter from 0.5 μm – 10 μm in concentrations and viscosities typical of biologic pharmaceutical formulations. Protein aggregates are distinguished from other contaminants that are found in pharmaceutical manufacturing, including silicon oil emulsion droplets, air bubbles, tungsten metal particles and breakdown products of industry standard surfactants. A study was also performed comparing the holographic signatures of protein aggregates and other contaminants in solvents of different viscosities. These results differentiates uniform spherical particles from particles composed of an irregularly shaped aggregation of proteins. Holographic characterization’s unique ability to measure refractive index provides a basis for differentiating protein aggregates from contaminants. For example, silicone oil droplets are clearly distinguished from protein aggregates on the basis of refractive index, even when they have the same size.

*Supported by the NSF, Award #1631815 7, NIH, Award #R44TR001590.
M71.00238: Gripping, Catching, and Conveying with a Soft, Toroidal Hydrostat*  SAMUEL ROOT (Presenter), GEORGE M. WHITESIDES, Harvard University — This work describes how a toroidal hydrostat can be used to perform three functions found in both living and engineered systems: gripping, catching, and conveying. We first demonstrate a gripping mechanism that uses the inversion characteristic of the toroid to encapsulate and grip onto objects under a uniform hydrostatic pressure. Using this mechanism, we demonstrate gripping forces ranging from 1-80 N, depending (in a predictable way) on the geometry and material properties of the system. We next demonstrate a catching mechanism akin to that of a chameleon's tongue: the elasticity of the membrane is used to store mechanical energy and drive a rapid acceleration to capture moving objects out of the air. Finally, we show how the toroidal topology can be exploited to construct a soft conveying mechanism that continuously inverts and passes objects through its center—serving a similar function to that of esophageal peristalsis, while eliminating the requirement of a lubricated interface. In general, we show that the use of inflatable topological structures comprising soft polymeric films is a promising approach to designing soft robotic actuators with novel, bio-inspired functionality.

*Department of Energy

M71.00239: Comparison of the Helmholtz, Gibbs, and Collective-modes methods to obtain nonaffine elastic constants*  BINGYU CUI (Presenter), EUGENE M TERENTJEV, Univ of Cambridge — We review and compare the Born-Huang and the Lemaitre-Maloney's theories that lead to analytical expressions for elastic constants, accounting for affine and nonaffine deformations in a lattice. The Born-Huang method is based on Helmholtz energy while the Lemaitre-Maloney's formalism focus on Gibbs force. Although starting from different perspectives, in the linear elastic limit, and in equilibrium, elastic material constants must be the same in all these methods. This is explicitly verified on examples of linear chains, and numerical simulation of a non-centrosymmetric crystal.

*B. C acknowledges the financial support of CSCCambridge Scholarship.
M71.00240: Hydrodynamics and rheology of a vesicle doublet suspension*  BRYAN QUAIFE, Scientific Computing, Florida State University, YUAN-NAN YOUNG (Presenter), New Jersey Inst of Tech — The dynamics of an adhesive two-dimensional vesicle doublet under various flow conditions is investigated numerically using a boundary integral method. In a quiescent flow, two nearby vesicles move slowly toward each other under the adhesive potential, pushing out fluid between them to form a vesicle doublet at equilibrium. A lubrication analysis on such draining of a thin film gives the dependencies of draining time on adhesion strength and separation distance, which are in good agreement with numerical results. In a planar extensional flow, a stable vesicle doublet forms only when two vesicles collide head-on. In a microfluid trap where the stagnation of an extensional flow is dynamically placed in the middle of a vesicle doublet through an active control loop, novel dynamics of a vesicle doublet are observed. Numerical simulations show that there exists a critical extensional flow rate above which adhesive interaction is overcome by the diverging stream, thus providing a simple method to measure the adhesion strength between two vesicles. In a planar shear flow, numerical simulations reveal that a vesicle doublet may form provided that the adhesion strength is sufficiently large at a given vesicle reduced area.

*Y.N.Y. acknowledges support from NSF-DMS 1614863 and 1412789

M71.00241: Continuum modeling of colloid-polymer mixtures in microgravity*  LAUREN BARNES (Presenter), BORIS KHUSID, LOU KONDIC, New Jersey Inst of Tech, WILLIAM V MEYER, NASA Glenn Research Center, ANAND OZA, New Jersey Inst of Tech — We present a continuum model of colloid-polymer mixtures in a microgravity environment. Such mixtures are an archetype for phase transition processes, but the variety of observed colloidal structures remain poorly understood. We construct, analyze and numerically simulate a phase-field model for structure evolution in colloid-polymer mixtures. The model consists of the Cahn-Hilliard equation, which describes phase separation processes in multicomponent mixtures, coupled with the Stokes equation for the viscous fluid flow. The results of the model will be compared against experiments performed on the International Space Station, using data available on the NASA Physical Sciences Informatics system.

*We acknowledge support from the NASA Physical Science Research Program.

M71.00242: STATISTICAL AND NONLINEAR PHYSICS —
**M71.00243: Understanding Fundamental Principles of Emergent Collective Behavior from Simple Bristlebots**  SKANDA VIVEK (Presenter), SAIRAM TANGIRALA, Georgia Gwinnett College — While it's known that simple interactions between active constituents reproduces collective phenomena such as flocking and schooling, there is a lack of comprehensive understanding of emergent collective behaviors arising from different kinds of interactions, increasingly relevant in the modern era. Take connected vehicles as an example: increasingly sophisticated sensors and software are being used to make complex decisions, and a basic understanding of how these changes in vehicular interactions in turn affects collective behaviors such as traffic is unknown. We built a model platform for studying various emergent collective behaviors in the real world, using customizable low-cost bristlebots. We find that certain intrinsic behaviors of the bristlebots such as shape and confinement significantly affect collective behaviors. Ultimately, our system provides an accessible, low-cost model to experimentally study and understand fundamental principles of collective behavior, highly relevant in the modern era.

**M71.00244: Energy Stability of Gravitationally Interacting Rods and Dumbbells**  MELITA F WILES (Presenter), JOHN LINDNER, College of Wooster — We extend classic dynamical results for two or three gravitationally interacting point masses to ideal rods and dumbbells. We derive equilibrium configurations by demanding that the vector of first derivatives of energy at constant angular momentum vanish. We investigate their stability by checking if the spectrum of the Hessian matrix of second derivatives is positive. The additional degrees of freedom allow the objects to store and exchange angular momentum and enable us to elucidate the behavior of non-spherical celestial bodies like asteroids and comet nuclei.

*Funded in part by NSF DMR-1852095

**M71.00245: A Continuous-time, Analog Approach to Boolean Satisfiability Problems**  SHUBHA RAJ KHAREL (Presenter), FERENC MOLNAR, ZOLTAN TOROCZKAI, Physics, University of Notre Dame — Recently, a continuous-time, deterministic analog solver based on ordinary differential equations was introduced, to solve Boolean satisfiability (SAT) problems, a family of discrete constraint satisfaction problems. As SAT is NP-complete, efficient algorithms would benefit solving a large number of decision type problems, both within industry and the sciences. Here we present a detailed analysis of the performance of this continuous-time solver and several variants of it, implemented on digital machines, on hard random SAT and very hard Ramsey-type coloring problems. We also present a randomization theorem connecting the entropy generation rate of the dynamics with solution time and problem hardness.

*Funding: NSF CCF-1644368 and 1640081, and by SRC-NRI Nanoelectronics Research Initiative 2698.004
M71.00246: Weighted Network Analysis of Biologically Relevant Chemical Spaces* MARIKO ITO (Presenter), TAKAAKI OHNISHI, Graduate School of Information Science and Technology, The University of Tokyo — In cheminformatics, network representations of the space of compounds have been suggested extensively. Among these, the threshold-network consists of nodes representing molecules. In this network representation, two molecules are connected by a link if the Tanimoto coefficient, a similarity measure, between them exceeds a preset threshold. However, the topology of the threshold-network is affected significantly by the preset threshold. In this study, we collected the data of biologically relevant compounds and bioactivities. We defined the weighted network where the weight of each link between the nodes equals the Tanimoto coefficient between the bioactive compounds (nodes) without using the threshold. We investigated the relationship between the strength of the link connection and the bioactivity closeness in the weighted networks. We found that compounds with significantly high or low bioactivity have a stronger connection than those in the overall network.

*This work was supported by the JSPS Grant-in-Aid for Scientific Research on Innovative Areas: JP17H06468.

M71.00247: Modeling the Response of Rayleigh-Van der Pol Oscillators to Stochastic Excitation Near the Hopf Bifurcation BINGSHEN LU (Presenter), MASOUD ASADI-ZEYDABADI, RANDALL TAGG, Physics, University of Colorado Denver — The Rayleigh-van der Pol equation for nonlinear oscillation has been a useful model for studying critical behavior near a Hopf bifurcation, including effects of external forcing and noise. Moreover, this equation has been found to be a good model of the long-term behavior of an experimental system consisting of the Wien bridge oscillator. We will describe work to study measures of noise variance, phase relations and other features of this combined model and experimental system, extended to coupling of two or more oscillators.

M71.00248: Granular Crystallization Driven by Dynamic Jamming Front KUN XUE (Presenter), JIARUI LI, Beijing Institute of Technology — Mono-dispersed particle systems under moderate vibration or continuous shearing are prone to form crystallized packing structures. Our grain scale simulations also find a collection of initially unjammed mono-dispersed particles would jammed into ordered packing structures by uniaxial compression via a rake. The crystallization degree, indicated by the local order of individual particles and the number of ordered particles, is found to be strongly influenced by the inter-particle friction. For the smooth particles, crystallization ensues the propagating jamming front regardless of the disorder degree of initial particle arrangement. A trivial friction (m = 0.01) suffices to markedly reduce the crystallization degree from above 90% to 68% thanks to the emergence of shear bands. An increased friction (m = 0.3) induces profuse shear bands, contributing to a significant reduction of crystallization degree (below 40%) which is also correlated with the initial disorder degree. As expected, the order-to-disorder transition of jammed structure induced by increasing particle friction dictates the jammed packing fraction and consequently the dynamic of jamming front. We also reveal mechanisms underlying the dynamic crystallization and its degeneration due to the elevated particle friction.
M71.00249: Self-Entanglement of a Tumbled Circular Chain  BEATRICE SOH (Presenter), Massachusetts Institute of Technology MIT, ALEXANDER KLOTZ, California State University, Long Beach, PATRICK DOYLE, Massachusetts Institute of Technology MIT — The spontaneous knotting of linear chains has been well studied, but little attention has been given to the self-entanglement of chains with more complex topologies. In this work, we perform experiments with granular chains that undergo tumbling motion to investigate the self-entanglement of circular chains, which lack the chain ends essential for forming knots. We study the entanglement probability and types of self-entanglements formed on linear and circular chains, using the well-studied self-entanglements on a linear chain to frame our understanding of self-entanglements on a circular chain. We describe a characterization method that views a self-entangled circular chain as a link of two components and use it to characterize the self-entanglements on circular chains with known topological descriptors from knot theory. By examining the formation pathway of several self-entanglements, we infer a general mechanism for the self-entanglement of circular chains.

M71.00250: Effect of mechanical coupling on the synchronization regimes of coupled optomechanical systems  XUEWEI ZHANG (Presenter), Texas A&M University, Kingsville — The objective of this work is to investigate the effect of mechanical coupling strength on the bistable synchronization regimes of two coupled optomechanical systems. Classically, the system is described by an effective Kuramoto-type model. Quantum mechanically, the system has been defined by a Hamiltonian and can be studied using semi-classical Langevin equation method. Previous research concluded that the quantum fluctuations are responsible for the appearance of the bistable synchronization regime. In this work, it is shown that, at some critical value of mechanical coupling, the synchronization can be bistable even in the absence of quantum fluctuation. Further, the numerical results of systems with detuning and thermal noise are obtained. These results collectively are used to extract a statistical measure that differentiate bistable synchronous states and unsynchronous states.

M71.00251: Instability power laws and planes from the variational principle*  JUSTIN BEROZ (Presenter), JOHN HART, JOHN W M BUSH, Massachusetts Institute of Technology MIT — Stable thermodynamic equilibrium of a physical system exists for a finite range of its physical parameters. Beyond this range, the system may transition to a dynamical one or undergo a phase change; determining the stability limit is often challenging for complex and nonlinear systems. We show that, for a broad range of physical systems, the stability limit may be formulated in terms of physical parameters that are independent with respect to an arbitrary variation of the system. Consequently, the stability limit is simply a power law if the thermodynamic potential describing the system comprises only two energy quantities; if comprised of more than two quantities, the stability limit is generally represented as a plane. Our result is shown to be valid for several solid, fluid and gas systems, and is especially useful for determining the stability limit of systems for which no analytical solution exists. As an example of the latter, we experimentally and theoretically investigate the stability limit of a liquid droplet exposed to an electric and gravitational field. The connection with statistical physics is also discussed.

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M71.00252: The conditions leading to dry lumps and dry granular jets when dispersing grains across a liquid-air interface* XIN YI ONG, CPE, U.Surrey, SPENCER E. TAYLOR, Chemistry, U.Surrey, MARCO RAMAIOLI (Presenter), UMR 782, Institut National Recherche Agronomique (INRA) — Avoiding the formation of dry lumps when dispersing powders into water is key for many industrial processes.

This study identifies experimentally the conditions leading to i) the dispersion of individual grains ii) the formation of a dry lump or iii) the formation of a dry granular jet when pouring grains onto a liquid-air interface by varying systematically grain size, density, contact angle and the grain flow rate.

Once a granular island is formed onto an interface, it can grow till reaching a maximum number of grains, above which either individual grains leave the interface or the whole island sinks. These two phenomena are governed by a different scaling law and a critical Bond number can be identified, above which grains disperse. The latter depends on two dimensionless numbers: the relative grain density and on their contact angle. Conversely, the formation of dry granular jets depends on the dimensionless kinetic energy of the grains when impacting the interface and on their contact angle.

A physical interpretation is provided to explain common practical strategies used to promote grain dispersion in industrial processes.

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M71.00253: Processing and Characterization of Ultralow-Binder-Content Particulate Composites* KIWON OH, YU QIAO (Presenter), University of California, San Diego — We developed the technique of compaction self-assembly (CSA), through which ultralow-binder-content (UBC) particulate composites were produced, with the binder content (c) in the range from 2 to 8 wt.%. In CSA, a high pressure is applied on premixed binder and granular filler, so that the material is densified and the binder is self-assembled into polymer micro-agglomerations (PMA) at critical load-carrying locations. Such a microstructure minimizes the system redundancy. The flexural strength of the UBC composite is ~25 MPa and the compressive strength is more than 50 MPa. This technology may find important applications for advanced pharmaceutical manufacturing, green cement, energy storage materials, among others.

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**M71.00254: Automated Measurement of the Profile of an Avalanching Conical Bead Pile**
BENNETT W ANDERSON (Presenter), SUSAN LEHMAN, College of Wooster — A conical bead pile subject to slow driving is used as a model system to experimentally investigate critical behavior in a granular system. The pile is composed of roughly 20,000 steel beads, 3 mm in diameter; we drive the pile by adding one bead at a time to the pile apex. We record the changes in pile mass over the course of tens of thousands of bead drops to characterize the distribution of avalanche sizes. To better understand the dynamic effect of individual avalanches, we now capture a profile image of the pile at every bead drop. By automating analysis of the images in Matlab, we can track changes in the overall height of the pile as well as variations in the angle of repose as the pile responds to each bead drop. In our previous work, we have characterized the changes in avalanche size distribution as we tune the cohesion in the system. Specifically, as cohesion is added, the size and number of the largest avalanches in the system increase. Using the new profile measurements, we investigate the effect of cohesion on the overall angle of repose as well as the variation in the angle. We find larger variations in the angle of repose as the cohesion is increased, and we correlate these variations with the mass of individual avalanches.

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**M71.00255: Onset of dynamic jamming in granular medium subject to explosion**
KUN XUE (Presenter), PANPAN HAN, Beijing Institute of Technology — The dynamic jamming of granular media consisting of glass spheres subjected to explosion is investigated experimentally via a radial heleshaw cell connected with a vertical shock tube. The evolution of velocity fields as well as the resulting strain rate fields are attained via the imaging technique, namely Particle Image Velocimetry (PIV). As the expanding internal surface accelerates outwards, a highly localized and exponentially decayed flow field is induced and becomes increasingly diffusional with an increased decay length. The end of the acceleration phase of the advancing internal surface corresponds to the transition of exponentially decayed flows to a jammed band with largely constant velocity in the wake of a circular dynamic jamming front across the thickness of which a large velocity gradient is discerned. The onset of a steady dynamic jamming commences from the transition of flow fields. Afterwards, most compression and shear deformations occur throughout the thickness of the jamming front in a highly heterogeneous manner in contrast with the deformation mode in the prior transient period. The statistical analysis of strain fields reveals a characteristic length scale which may well arise from the grain-scale heterogeneity of granular materials.
**M71.00256: Multi-functional Tw-Kagomé lattices: Tuning by pruning mechanical metamaterials** DANILO LIARTE (Presenter), Cornell University, OLAF STENULL, TOM LUBENSKY, University of Pennsylvania — We study phonon and elastic properties of randomly-diluted twisted-Kagome lattices with tunable structures that include auxetics with negative Poisson ratios. Intelligent protocols to tune the Poisson ratio of elastic networks can be used in the design of metamaterials with flexible mechanical properties. Here we introduce two periodic lattice models that access negative values of the Poisson ratio, one of which accesses the full range from -1 to +1. Besides tunable auxetic transitions, these models exhibit rich critical phenomena that include rigidity percolation (where both the bulk $B$ and shear $G$ moduli continuously vanish), jamming (where $B$ undergoes a discontinuous jump and $G$ grows continuously from zero), shear-jamming (where $G$ undergoes a discontinuous jump and $B$ grows continuously from zero), and “double jamming” (where both $B$ and $G$ undergo a discontinuous jump).

**M71.00257: Visualizing the Interfacial Jamming of Nanoparticles on a Liquid Surface**

ZACHARY FINK (Presenter), SATYAM SRIVASTAVA, Univ of Mass - Amherst, PAUL Y KIM, Lawrence Berkeley National Laboratory, ALEXANDER E RIBBE, DAVID HOAGLAND, THOMAS RUSSELL, Univ of Mass - Amherst — Two-dimensional assemblies of nanoparticles (NPs) are model systems for studying jamming and vitrification, with slowed dynamics, rate dependence, and dynamic heterogeneities. We developed a scanning electron microscopy (SEM) technique to image NP assemblies on a nonvolatile ionic liquid (IL) droplet where areal density, $\varphi$, is well-controlled. SEM precisely images the real time location of each NP on the droplet surface, allowing NP dynamics to be determined as a function of $\varphi$. The packing structure and interactions between NPs can be rigorously measured as assemblies transition from the liquid state to the glassy or jammed state. Here, monodisperse PEGylated silica NPs and gold NP tracers (100-250 nm) were cast on the surface of 1-ethyl-3-methylimidazolium ethyl sulfate IL and imaged. By measuring the mean square displacement as a function of time, NP diffusion coefficients were found and compared with phenomenological models. Assembled structures were also analyzed at each $\varphi$ by order parameters $<\psi_6>$ and $T^*$, Voronoi tessellation, and pair correlation functions. The results show that as $\varphi$ increases, NPs diffuse more slowly and their assembly transitions from a liquid-like structure to a crystalline structure.

*NSF DMR-1807255*
M71.00258: Extreme Energy-Absorbing Metamaterials Based on Liquid Crystal Elastomers*
SEUNG-YEOL JEON, ZEYU ZHU, Johns Hopkins University, CHRISTOPHER YAKACKI, University of Colorado, Denver, THAO NGUYEN, SUNG KANG (Presenter), Johns Hopkins University — Liquid crystal elastomers (LCEs) are fascinating materials for energy dissipation, due to their extreme damping behavior emerging from an internal degree of freedom of LC molecules, which is coupled to elastic deformations of polymer network. Here, we report metamaterials composed of LCE beams for extreme energy absorption. We have synthesized LCEs through a two-stage thiol-acrylate reaction to consider the effects of the alignment of LC molecules within LCE beam elements. The energy-absorbing capability of metamaterials consisting of bistable beams with differently arranged LC molecules was characterized at strain rates from $10^{-4}$/s to $10^{3}$/s and it followed a power-law relation. We observed that metamaterials based on LCE showed increase of the energy absorption at a higher strain rate. Moreover, the strain-rate dependency could be tuned by LCEs with different degree of alignment. We envision that our study can contribute to harnessing the interplay between snapping-based architectures and enhance dissipation of LCEs to enable the metamaterials with extreme energy-absorbing capabilities.

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M71.00259: Valley Hall In-Plane Edge States as Building Blocks for Elastodynamic Logic Circuits*
JIHONG MA (Presenter), Department of Civil, Environmental, and Geo- Engineering, University of Minnesota - Twin Cities, KAI SUN, Department of Physics, University of Michigan, STEFANO GONELLA, Department of Civil, Environmental, and Geo- Engineering, University of Minnesota - Twin Cities — Although waveguiding is vital in mechanical signal processing and energy harvesting, conventional techniques are prone to significant backscattering from corners or junctions. Inspired by the quantum Valley Hall effect, we create and study topologically protected in-plane waveguides that are immune to backscattering. In addition, the waveguides are exploited to realize multi-interface junctions that act as logic ports with unconventional wave-manipulation capabilities, including asymmetric transport, energy trapping and rerouting, and mechanical signal delaying. These ports can ultimately serve as the building blocks for a practically endless array of elastodynamic circuits.

*National Science Foundation (NSF grant EFRI-1741618).
M71.00260: Brownian Motions in Two Dimensions under Non-harmonic Potentials: Nonequilibrium Steady-State Dynamics  
HSIN CHANG (Presenter), CHI-LUN LEE, PIK-YIN LAI, YUNG-FU CHEN, Natl Central Univ — A Brownian gyrator features a two-dimensional random particle under a harmonic potential, while random thermal kicks are of distinct temperatures along the two axes [Filliger and Reimann, Phys. Rev. Lett. 99, 230602 (2007)]. In our current work, we replace the harmonic potential by other types of potentials, and we investigate the nonequilibrium steady states (NESS) through simulation studies. In contrast to the Brownian-gyrator case, where the average flux circulates along the probability contour, our results for the non-harmonic cases do not follow this signature. Moreover, the violation of this feature exists even near the potential energy minima, where the harmonic approximation work. For the special case with a symmetric quartic potential, we provide a simple argument for this less intuitive behavior.

M71.00261: Time-reversal-invariant scaling of light propagation in one-dimensional non-Hermitian systems*  
JOSE HERNANDEZ (Presenter), LI GE, CUNY College of Staten Island — Light propagation through a normal medium is determined not only by the real part of the refractive index but also by its imaginary part, which represents optical gain and loss. Therefore, two media with different gain and loss landscapes can have very different transmission and reflection spectra, even when their real parts of the refractive index are identical. Here we show that while this observation is true for an arbitrary one-dimensional medium with refractive index n(x) and its time-reversed partner with refractive index n*(x), there exists a universal scaling that gives identical transmittance and reflectance in these corresponding systems. Interestingly, the scaled transmittance and reflectance reduce to their standard, unscaled forms in a time-reversal-invariant system, i.e., one without gain or loss.

*This work was supported by the NSF under Grant No. DMR-1506987 and by PSC-CUNY under Award No. 61787- 49.
M71.00262: Examining Human Unipedal Quiet Stance: Temporal Correlations in the Jerk Record*  MATTHEW SEMAK (Presenter), NOAH J BLAIR, Physics and Astronomy, University of Northern Colorado, GARY HEISE, School of Sport and Exercise Science, University of Northern Colorado — We investigated the quality of smoothness during human unipedal quiet stance. Smoothness is quantified by the time rate of change of the accelerations, or jerks, associated with the motion of the foot and can be seen as being indicative of how controlled the balance process is. To become more acquainted with this as a quantity, we wanted to establish whether it can be modeled as a (stationary) stochastic process and, if so, explore its temporal scaling behavior. Specifically, our study focused on the jerk concerning the center-of-pressure (COP) for each foot. Data were collected via a force plate for individuals attempting to maintain upright posture using one leg (with eyes open). Positive tests for stochasticity allowed us to treat the time series as a stochastic process and, given this, we took the jerk to be proportional to the increment of the force realizations. Detrended fluctuation analysis (of various orders) was the primary tool used to explore scaling behavior. Results suggest that both the medial-lateral and anterior-posterior components of the jerk display persistent and antipersistent correlations which can be modeled by fractional Gaussian noise over three different temporal scaling regions.

*Colorado Space Grant Consortium/NASA

M71.00263: Morphological Properties of Shrinkage-Induced Crack Patterns*  SHIN-ICHI ITO (Presenter), The University of Tokyo, SATOSHI YUKAWA, Osaka University — We investigate morphological properties of shrinkage-induced crack patterns, which are observed such as on cooling lava and drying soil, through numerical simulations of a phase-field (PF) model. Since our PF model does not require any assumptions related to crack nucleations and numerical lattice configurations, we can investigate the pattern formations that purely depend on material/external parameters. We find that our PF model shows various types of pattern formations depending on a shrinkage rate and material constants, and in particular, the shrinkage rate provides a significantly qualitative difference in the pattern formations. Cellular patterns resulting from sequential fragmentations of straight cracks can be observed when using a slow shrinkage rate, while random network patterns resulting from connections of micro cracks that appear simultaneously can be observed when using a rapid shrinkage rate. We quantify the difference of the pattern formations statistically, and explain the origin of the difference on the basis of a simple continuum theory of a thin layer of viscoelastic material.

*This work was supported by JSPS KAKENHI Grant number 19K14671.
M71.00264: Reaction-diffusion waves interacting with fractals, spirals, and concave & soft obstacles*  
YANG YU (Presenter), CHASE A FULLER, MARGARET K. MCGUIRE, NIKLAS MANZ, JOHN LINDNER, College of Wooster — We simulate the recovery and delay of reaction-diffusion wave fronts colliding with various obstacles in narrow two-dimensional channels by numerically integrating the two-variable Tyson-Fife reduction of the three-variable Oregonator model of the chemical Belousov-Zhabotinsky reaction. We investigate the influence of obstacles on the wave front's shape and its recovery after passing around/through fractals (e.g. Hilbert curve, Peano curve, inverse Sierpinsky carpet), Archimedian spirals, and convex & concave polygons by plotting the wave front's left most point and delay versus time. We find that wave fronts behave the same when propagating through symmetric obstacles (e.g., Hilbert curve and Sierpinski carpet) at specific angles, which is in contrast to non-symmetric obstacles such as the Peano curve. At long times, wave fronts follow the same power-law recovery behavior as previously observed for convex obstacles. We also construct two types of chemical clocks, using illumination gradients with the light-sensitive reaction term or using space-dependent diffusion constants in the diffusion term.

*Sherman-Fairchild Foundation

M71.00265: Reaction-Diffusion Waves as a Black Hole Event Horizon Analogue*  
SAMUEL CAVENDER (Presenter), SAMUEL NASH, MARC E. MANHEIM, NIKLAS MANZ, College of Wooster — Hydrodynamic systems have been build to model the interaction between electromagnetic waves and black/white hole event horizons using gravity waves in water tanks as they behave analogously to electromagnetic waves traveling through space-time. We present a further scaled-down table-top size experiment using a chemical reaction-diffusion (RD) system, the Belousov-Zhabotinsky (RD) reaction. These RD waves propagate forward without any mass transport. When moving in a channel with a flow-rate gradient it is possible to achieve a situation when the medium's flow rate equals the propagation speed of the BZ wave front, creating the illusion of a stationary wave, the black/white hole horizon.

*National Science Foundation grant DMR-1852095 and The College of Wooster

M71.00266: Harvesting energy from the thermal motion of gas molecules in gravity  
TOM ZHU (Presenter), Tom Zhu — This presentation will describe how to produce energy, e.g. electricity, from the thermal motion of gas molecules under the effect of the gravity. We will describe the motion of the gas molecules in the gravity, and the consequence of such motion. We will shown the conditions for making use of the thermal motion of the gas molecules to produce electricity.
M71.00267: Transport and Dynamical Properties of Two-Dimensional One Component Plasma  
VASSILIOS FESSATIDIS (Presenter), Department of Physics & Engineering Physics, Fordham University, Bronx, New York, KARE N. PATHAK, Department of Physics, Panjab University, Chandigarh-160014, India, GIRIJA DUBEY, Department of Earth & Physical Sciences, York College-CUNY, New York & Fordham University, Bronx, New York, GODFREY GUMBS, Department of Physics & Astronomy, Hunter College-CUNY, New York — We present a new theoretical model based on Fick's law for calculating the diffusion constant for a two-dimensional (2D) one-component plasma in the presence or absence of magnetic field. Both 1/r and ln(r) potentials are employed in conjunction with various values of coupling parameters. Our model predicts diffusion constants in agreement with recent simulation results. We also present detailed comparison of our results with those obtained from other theoretical models. Additionally, we compare our transport coefficients for the 1/r and ln(r) potentials for 2D systems.

M71.00268: Two-Scale Factor Universality in O$_2$ and H$_2$*  
DERECK MORGADO (Presenter), CHRISTIAN G HAWKINS, ANA OPRISAN, College of Charleston, GURUNATH GANDIKOTA, DENIS CHATAIN, Universite Grenoble Alpes, YVES GARRABOS, Universite de Bordeaux, DANIEL A BEYSENS, Laboratoire de Physique et Mécanique des Milieux Hétérogènes — Video images are increasingly used in science, supplanting current methods such as light scattering by a statistical evaluation of the images. In this paper, it is shown that light turbidity data, a quantity due to density-induced refractive index fluctuations, can be directly obtained from image analysis. We fitted the turbidity data to a theoretical expression that allowed us to estimate the critical amplitudes of isothermal compressibility and correlation length. Images of an oxygen-filled cell and a hydrogen-filled cell were taken near their respective critical temperatures of 155 and 33 K. Images for Hydrogen were analyzed and values of isothermal compressibility and fluctuation correlation lengths obtained from turbidity fitting were compared against literature values. In order to go very close to the critical point, the fluids are placed under weightlessness using a magnetic levitation device. Our data analysis shows a large sensitivity of the fitting parameters to the refractive index value and to even minute density deviations from criticality.

*This research was supported by NASA SC Space Grant Palmetto Academy “Two-scale factor universality in O$_2$ and H$_2$”. The College of Charleston Department of Physics and Astronomy also supported this research project.
M71.00269: A Computational Study of The Villin Headpiece Subdomain HP36: The Effect of Hydration on Side Chain Dynamics in the Hydrophobic Core* TANJA KOVACEVIC (Presenter), Chemistry, University of Colorado Denver, JILLIAN OVIEDO, Biochemistry, University of Colorado Denver, LILIYA VUGMEYSTER, HAI LIN, Chemistry, University of Colorado Denver — Hydrophobic side-chain interactions are considered the major dynamic force in the folding of globular proteins and aggregation of non-globular proteins. Due to its small size, a villin headpiece subdomain HP36 is an ideal system to compute the influence of hydrophobic side-chain interaction on protein stability. Alzheimer’s has been attributed to the interactions between the hydrophobic side chains, such as phenylalanine, to drive beta-amyloid (AB) aggregation. Molecular modeling is used to gain insight into how protein-protein interactions and flexibility of the hydrophobic core are altered with the hydration level of HP36. The calculated free energy profiles will be used to estimate the rate constant for ring flipping and determine the effects of relative solvation on transition frequencies, lifetimes, and populations of the residues. These results can have implications on the hydrophobic residue interactions that drives the aggregation of AB plaques in patients with Alzheimer’s.

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M71.00270: Theoretical modelling of stock price dynamics in stock markets using a phynance approach.* LEONARD MUSHUNJE (Presenter), Applied Mathematics and Statistics, Midlands State University — This paper presented time to time price dynamics associated with stock assets within stock markets. Our conjecture was that, stock prices are stochastic and time variant and as such they do attain and posses different values from time to time. We aimed to model the old way phenomenon of stock price dynamics using a distinct model from the physics field. We used the two-forms of Schrodinger equation and identified the one which best describes the dynamic nature of stocks. Our results suggested that, stock price dynamics can well be modelled and presented using the time independent Schrödinger equation (SE) with traceable stock price changes. This supported our conjecture as stock prices are traditionally known to be stochastic in nature and normally they are non-stationary. Additionally, we objectified to suggest another unique way of solving the Schrödinger equation contextualized into our case. We derived the solution using Frobenious method and the method of undetermined factors borrowed from ordinary differential equations. Fortunately, all the chosen methods proved to work well and to provide significant solutions. We therefore concluded that stock prices are non-stationary and recommend the wider use of such physics models.

*I have no funding yet.
M71.00271: Market crashes as second-order phase transitions*  JACK SARKISSIAN (Presenter), Algostox Trading — We study the behavior of ensemble features of financial markets during crash periods to see if they exhibit the behavior typical for second-order phase transitions. We find that during market crashes the order parameter (defined as the ensemble-average correlation) sharply increases and fluctuations (defined as ensemble volatility) exhibit a spike. In addition, the hysteresis effect is observed for correlations and drawdown (market drop) and a similar effect exists for trading volume and drawdown. These facts point that during crashes the markets not only resemble, but undergo a second-order phase transition. Market phases can be identified on a trading volume vs drawdown diagram as regions with high and low order parameter. While market dynamics has a self-coordinated nature, the two inputs on phase diagram are measurable directly from the markets.

*None

M71.00272: Policies for allocation of information in task-oriented groups: elitism and egalitarianism outperform welfarism  SANDRO MARTINELLI REIA, Instituto de Física de São Carlos, Universidade Estadual de São Paulo, PAULO FREITAS GOMES (Presenter), Universidade Federal de Goiás, JOSÉ FERNANDO FONTANARI, Instituto de Física de São Carlos, Universidade Estadual de São Paulo — Communication is probably the most controllable factor that are known to impact on the problem-solving capability of task-forces. In the case connections are costly, it is needed a better policy to allocate them to the individuals. We use an agent-based model to study how distinct allocation policies affect the performance of a group of agents whose task is to find the global maxima of NK fitness landscapes. The larger the influence neighborhood of an agent, more information it receives. We find that the elitist policy in which agents with above-average fitness have their influence neighborhoods amplified is optimal for smooth landscapes, provided the group size is not too small. For rugged landscapes, however, the elitist policy can perform very poorly for certain group sizes. In addition, we find that the egalitarian policy, in which the size of the influence neighborhood is the same for all agents, is optimal for both smooth and rugged landscapes in the case of small groups. The welfarist policy, in which the actions of the elitist policy are reversed, is always suboptimal, i.e., depending on the group size it is outperformed by either the elitist or the egalitarian policies.

M71.00273: Digital sustainability: A high dimensional ML problem  DEEDER AURONGZEB (Presenter), Johns Hopkins University — The Brundtland report states sustainability as : “development that meets the needs of the present without compromising the ability of future generations to meet their own needs” (World Commission on Environment and Development 1987, p. 37). However, due to serious asymmetry of knowledge and technology around the world with digital (know how) based economy, a high dimensional definition is needed before we can begin to address this issue. We show that digital sustainability is a sparse high dimensional problem with independent features. We use framework by Friedman, J.H. Data Mining and Knowledge Discovery (1997) 1: 55., to minimize digital sustainability problem and suggest a ML framework.
M71.00274: Themodynamical aspects of self-similar relaxation evolution of dense star clusters  
YUTA ITO (Presenter), The Graduate Center, City University of New York — Occurrence of negative heat capacity has been predicted and reported for various systems of particles and objects. Examples are granular gases, plasmas, atomic- and molecular- clusters, self-gravitating systems (black holes, stars, star clusters), ... The Antonov's pioneering work assumed an isothermal sphere (a self-gravitating system described by Maxwellian distribution function of particles at constant temperature) enclosed by an adiabatic wall. The work showed no maximum entropy state can be achieved for the sphere beyond a certain large-density contrast between the center and edge. Without the wall, the system expands and particles flow from the dense core to the ambient. Due to the negative heat capacity and conservation of energy/particle, the core heats up and shrinks while the ambient gets sparse and elongates. Such toy model has helped astrophysicists/astronomers to understand the structures of dense star clusters (e.g. globular cluster). More sophisticated models have predicted the clusters can evolve in a self-similar fashion at the late stage of relaxation evolution. The present work discusses the thermodynamical aspects of the self-similar-evolution model compared to classical models, such as the isothermal sphere, polytropic sphere and King model.

M71.00275: Steady-state thermodynamics: reservoir independence*  
LEONARDO CALAZANS (Presenter), RONALD DICKMAN, Univ Fed de Minas Gerais — For stochastic lattice models in spatially uniform nonequilibrium steady states, a thermodynamic temperature T and chemical potential μ can be defined via coexistence with heat and particle reservoirs. Here we ask whether the values so obtained depend on the nature of the exchange between system and reservoir. For example, a stochastic particle reservoir is usually taken to insert or remove a single particle in each exchange, but one may also consider a reservoir that inserts or removes a pair of particles in each event. In equilibrium, equivalence of pair and single-particle reservoirs is guaranteed by the canonical form of the probability distribution on configuration space. We examine whether this equivalence persists in nonequilibrium steady states.
*CAPES and CNPq from Brazil

M71.00276: Graphlet Degree correlations reveal evidence of partial spatial embedding in complex networks*  
JOSHUA PARKER (Presenter), RAJEEV AGRAWAL, U.S. Army Engineer Research and Development Center — By virtue of most complex networks being comprised of real world objects or entities that can be assigned a location, the interactions that drive edge formation and network growth are affected by the spatial arrangement of the network's nodes. This means that most networks can be considered "partially embedded" in space, and the degree to which the network is embedded is determined by network growth rules. We utilize recent advances in network alignment techniques based on "Graphlet Degree Similarity" (GDS) to quantify how topological quantities change due to varying levels of spatial embedding in simulated complex networks. We demonstrate that the graphlet degree cross correlation matrix can be used to quantify the level of spatial embedding, and discuss how similar measures can be used to investigate the spatial hierarchy of complex networks.
*Funding provided by the Engineer Research and Development Center, which is a division of the US Army Corps of Engineers
M71.00277: Non-equilibrium statistical physics of systems with finite heat baths*  DAVID WOLPERT (Presenter), Santa Fe Inst, JAN KORBEL, Complexity Science Hub Vienna — In this presentation I analyze the thermodynamics of a system connected to a single, finite heat bath. I concentrate on the case where the work reservoir can only change the Hamiltonian of the system, not the Hamiltonian of the bath, nor the interaction Hamiltonian coupling the system to the bath. In order to apply the tools of conventional stochastic thermodynamics, I assume that the system is coupled to a second, infinite heat reservoir, in addition to the finite heat bath. I prove that in this scenario the entropy production rate of the joint system—finite—bath is lower-bounded by the rate of change of the mutual information between the system and the finite bath. This means that while it is possible to use a semi-static process to simultaneously extract the no-nequlibrium free energy of the system considered by itself, together with the non-equilibrium free energy of the finite bath considered by itself, it is impossible to at the same time extract the free energy stored in the mutual information of those two systems.

*This work was supported by the Santa Fe Institute, and by Grant No. CHE-1648973 from the NSF.

M71.00278: Maximizing free energy gain*  ARTEMY KOLCHINSKY (Presenter), Santa Fe Inst, IMAN MARVIAN, Duke, CAN GOKLER, ZI-WEN LIU, PETER SHOR, OLES SHTANKO, KEVIN THOMPSON, MIT, DAVID WOLPERT, Santa Fe Inst, SETH LLOYD, MIT — Maximizing the amount of free energy that a system extracts from its environment is important for a wide variety of physical, biological and technological processes, from energy harvesting processes such as photosynthesis to energy storage systems such as fuels and batteries. We extend recent results from non-equilibrium thermodynamics to derive closed-form expressions for the maximum amount of free energy that a system can extract from its environment over the course of a fixed process. We also analyze how our bounds on extractable free energy vary with the initial distribution of the states of the system. Simple equations allow us to compare the amount of free energy that can be extracted under the optimal initial distribution with that for a sub-optimal initial distribution. We show that the problem of finding that optimal initial distribution is convex and solvable via gradient descent. We demonstrate our results by analyzing how the amount of extractable free energy varies with the initial distribution of a simple Szilard engine.

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M71.00279: FLUID DYNAMICS —

M71.00280: WITHDRAWN ABSTRACT —
**M71.00281: Drop breakup in yield stress fluids**  
JUAN REIMONDO (Presenter), Texas Tech Univ, JOSEFA GUERRERO MILLAN, Augusta University, YA-WEN CHANG, Texas Tech Univ — We study the production of droplets inside yield stress fluids (YSFs) using an extrusion-based 3D printer device. Microgel-based YSFs have recently gained traction in 3D printing applications due to their ability to be molded when stresses are applied, followed by immediate solidification to hold shapes when stresses are removed. The capillary breakup of an immiscible Newtonian fluid inside a YSF can be eliminated completely when the yield stress of the YSF is sufficiently high. This contrasts with simple liquids, where the dispersed phase of co-flowing streams always breaks into spherical droplets. There is, however, and intermediate regime where the evolution of capillary breakup and shape relaxation of drops is arrested, resulting in droplets of non-spherical shapes. By carefully tuning the flow and shear parameters, we demonstrate precision control of dispersed drop shapes through simple physical parameters in ‘co-flowing’ streams of a Newtonian fluid and a surrounding YSF.

**M71.00282: Interfacial thermodynamics of spherical liquid nanodroplets: Molecular understanding of surface tension via hydrogen bond network**  
QHWAN KIM (Presenter), WONHO JHE, Seoul National University — Surface tension plays a important role in nucleation of atmospheric liquid droplets. Especially, understanding of interfacial thermodynamics of the 1 nm scale nucleus is essential for characterization of nucleation such as the activation energy barrier. Despite theoretical and experimental studies performed for decades, determination of surface tension of the nanodroplet is still a topic of ongoing controversies. Here, we investigate surface tension of spherical nanodroplets by both molecular dynamics and density functional theory, and find that surface tension decreases appreciably below 1 nm diameter, whose analytic expression is derived from the Tolman's equation. In particular, analysis of the free energy of nanodroplets shows that the change of surface tension originates from the configurational energy of molecules, which is evidenced by the disrupted hydrogen bond network of nanodroplet. Our results may further illuminate the molecular mechanisms of the interface-related phenomena associated with molecular fluctuations such as ice nucleation or biomolecule adsorption where the macroscopic thermodynamic quantities are ill-defined.

*This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea Government (MSIP) (No. 2016R1A3B1908660).
M71.00283: Hydrodynamic Analog for Spontaneous Emission Radiation  JUSTIN EDWARDS (Presenter), YU CHE HO, LUIS GRAVE DE PERALTA, Texas Tech Univ — It has been shown that a drop of fluid can be made to bounce on a vertically oscillating bath of fluid. These droplets, known as “walkers”, couple to the waves they generate and are propelled forward. When a variation of depth in the fluid bath is introduced it creates a difference in potential; droplets crossing the barrier must do so on a transmitted exponentially decaying wave. We have created a system which spontaneously generates walker droplets to simulate particles leaving a potential well. Previous studies of walker droplets have used forcing amplitudes just below the Faraday instability threshold to study the drop’s path about the fluid bath. In this system we use a forcing amplitude well above the threshold in order to generate walker droplets autonomously. The droplets then tunnel across a potential barrier to a damped region where the fluid is below the instability threshold. The formation of these droplets and their resulting kinetic energy is related to the amplitude and frequency of the driving oscillation. We present a statistical study of droplet emission from a potential well. The system could provide an analog to radioactivity in which particles spontaneously tunnel across a potential barrier, showing promise for future analysis.

M71.00284: Ejection of individual microparticles from an electrified meniscus*  JUSTIN BEROZ (Presenter), KAIHAO ZHANG, HENRY MERROW, JOHN W M BUSH, JOHN HART, Massachusetts Institute of Technology MIT — On-demand production of 2D and 3D parts with complex geometries and/or high value material requirements is significant to many industries, and a broad goal of additive manufacturing. State-of-the-art methods for metal, ceramic, and advanced engineering materials typically utilize powder feedstocks, and the dimensional resolution of parts is limited to several particle diameters or larger, which limits precision applications. To address this challenge, we present a method to direct-write individual microparticles onto substrates using an electrohydrodynamic process. A liquid droplet, confined at an orifice and containing microparticles on its surface, is electrified, resulting in the dynamic ejection of individual microparticles from the droplet’s apex. We experimentally detail the electrohydrodynamic process of particle ejection and the parameter regime for which particles print individually. Scaling for ejection speed, liquid entrainment on the particle and satellite droplet formation are also discussed.

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M71.00285: Observing phase separation of temperature-responsive colloids under shear*
JOHN BRADY (Presenter), RYAN J. MCGORTY, Univ of San Diego — We use colloidal microgel particles, PNIPAM and PNIPMAM, in a colloid-polymer system to study phase separation. We synthesize particles of various sizes and characterize their temperature-tunable size with differential dynamic microscopy. When these colloidal particles are mixed with a depletant we observe fluid-fluid phase separation as well as gelation. The process of phase separation is observed using a custom-built light-sheet microscope. With a two-color fluorescent labeling scheme we can track single colloidal particles as well as the phases that emerge as an originally-mixed sample phase separates. Furthermore, we observe our samples under shear in both a custom-built cylindrical shear cell with our light-sheet microscope and in a commercial rheometer using brightfield microscopy. Studying the behavior of multiphase systems like our colloid-polymer samples strengthens our understanding of non-equilibrium thermodynamics while providing novel routes for structuring complex fluids.

*American Chemical Society Petroleum Research Fund (#57326-UNI10) and a Research Corporation Cottrell Scholar award

M71.00286: Bravais lattice structures settling in viscous media: scaling of terminal velocity with porosity*
SEBASTIAN BÜRGER, Univ Leipzig, RAHUL CHAJWA (Presenter), Fluid Dynamics and Turbulence, International Centre for Theoretical Sciences TIFR, Survey no. 151, Bengaluru 560089, GANGA SRINIVASA PRASATH, Harvard School of Engineering and Applied Sciences, 29 Oxford Street, Cambridge, MA 02138, USA, RAMA GOVINDARAJAN, Fluid Dynamics and Turbulence, International Centre for Theoretical Sciences TIFR, Survey no. 151, Bengaluru 560089 — The settling velocity of porous objects in Stokes flow depends on their geometry. Complex geometries of such objects occur in nature and technology, such as marine snow, particles in pulmonary drug delivery, chemical catalysts and pollen grains. To model the fundamental building blocks of porous geometries, we conduct experiments on sedimentation of various Bravais lattice unit-cell structures at low Reynolds numbers (\( \sim 10^{-4} \)), where each structure consists of equally sized spheres connected by thin rods. For each of these structures, porosity becomes a function of the lattice parameter. We show that the sedimentation behaviour of all Bravais lattices can be collapsed when the settling velocity is scaled using the number of particles in the lattice. A ball-and-stick model using Stokesian hydrodynamic kernel for spheres and slender-body theory for connecting rods, captures the settling behaviour accurately. We perform PIV measurements of flow inside these structures to understand the dependence of permeability on porosity and also the validity of our theoretical model. Our experiments and calculations pave the way for understanding sedimentation of systems closer to reality by introducing disorder in the lattice.

*Sebastian Bürger thankfully acknowledges the DAAD RISE stipend.
M71.00287: Wave damping of a sloshing wave by an interacting turbulent vortex flow*  
CLAUDIO FALCON (Presenter), Univ de Chile, FRANCISCO REYES, Universidad de Santiago, VICENTE TORREJÓN, Univ de Chile — We report on the enhancement of the hydrodynamic damping of gravity waves at the surface of a fluid layer as they interact with a turbulent vortex flow in a sloshing experiment. Gravity surface waves are excited by oscillating horizontally a square container holding our working fluid (water). At the bottom of the container, 4 impellers in a quadrupole configuration generate a vortex array at high Reynolds number, which interact with the wave. We measure the surface fluctuations using different optical non-intrusive methods and the local velocity of the flow. In our experimental range, we show that as we increase the angular velocity of the impellers, the gravity wave amplitude decreases without changing the oscillation frequency nor generating transverse modes. This wave dissipation enhancement is contrasted with the increase of the turbulent velocity fluctuations from PIV measurements. To rationalize the damping enhancement a periodically forced shallow water model including viscous terms is presented, which is used to calculate the sloshing wave resonance curve as a function of the turbulent fluctuations. From these measurements we compute the dependence of the shallow water viscous friction coefficient

*ICM Millenium Nucleus of Soft Smart Mechanical Metamaterials

M71.00288: WITHDRAWN ABSTRACT —

M71.00289: A mathematical model of mitochondrial calcium-phosphate dissolution as a mechanism for persistent post-CSD vasoconstriction*  
SHIXIN XU, Duke Kunshan University, JOSHUA CHANG (Presenter), CARSON C CHOW, National Institutes of Health - NIH, HUAXIONG HUANG, York University — Cortical spreading depolarization (CSD) is the propagation of a relatively slow wave in cortical brain tissue that is linked to a number of pathological conditions such as stroke and migraine. Most of the existing literature investigates the dynamics of short term phenomena such as the depolarization and repolarization of membrane potentials or large ion shifts. Here, we focus on the clinically-relevant hour-long state of neurovascular malfunction in the wake of CSDs. This dysfunctional state involves widespread vasoconstriction and a general disruption of neurovascular coupling. We demonstrate, using a mathematical model, that dissolution of calcium that has aggregated within the mitochondria of vascular smooth muscle cells can drive an hour-long disruption. We determine the rate of calcium clearance as well as the dynamical implications on overall blood flow. Based on reaction stoichiometry, we quantify a possible impact of calcium phosphate dissolution on the maintenance of F0F1-ATP synthase activity.

*This research was supported in part by NSERC, the Fields Institute, and the Intramural Research Program of the NIH, NIDDK.
M71.00290: Light-Driven Ballistic Nanoparticle Swimmers*  EUNGYU LEE, TENGFEI LUO (Presenter), University of Notre Dame — Directed high-speed motion of nanoscale objects in fluids can have a wide range of applications. However, directed movement and high speed in the nanoscale are rarely compatible. Light is a convenient source that can drive nano objects to move by applying optical pushing forces due to momentum conservation when photons are scattered off the objects. In theory, optical forces from a planewave can also be “negative” that pull objects against the light propagation direction in a homogeneous medium if some unique optical configurations of the objects can be realized, but this is yet to be demonstrated. Nevertheless, these optical forces are too weak to enable fast-moving swimmers in fluids. Here, we report ballistic plasmonic Au nanoparticle (NP) swimmers with unprecedented speeds (~397,000 mm s\(^{-1}\)) realized by both optical pushing and pulling forces from a single Gaussian laser beam. The Au NP excited by the laser at the surface plasmon resonance (SPR) peak interact with the NP both thermally and optically, leading unique conditions for ballistic movements and “negative” optical forces.

*This work is supported by National Science Foundation (1706039) and the Center for the Advancement of Science in Space (GA-2018-268).

M71.00291: Enhancing propulsion efficiency of biomimetic elastic propulsor using hybrid actuation*  ERSAN DEMIRER, FIKAYO OSHINOWO (Presenter), ALEXANDER ALEXEEV, Georgia Institute of Technology — Bio-inspired propulsion of a robotic swimmer can be achieved by periodic actuation of an elastic caudal fin. We use three-dimensional computer simulations to probe how the hydrodynamic performance of a caudal fin can be enhanced by combining two distinct types of fin actuation. The fin is represented by an elastic rectangular plate that is actuated at the base to perform sinusoidal oscillations. The actuation frequency is set to match the fundamental frequency of the plate yielding the maximum bending amplitude. In addition to this plunging actuation, the plate is actuated by a distributed bending moment with the magnitude that periodically changes in time with the same frequency as the fin base. We introduced a phase difference between the base and the internal actuation and investigate the resultant hydrodynamic thrust and efficiency. We compared the hybrid fin actuation to the base actuation and to the internal actuation to identify the parameter space in which the synergetic effects of the two action mechanisms are the most beneficial for swimmer propulsion.

*This work is supported by NSF CBET 1705739
M71.00292: Scattering of a fast-swimming bacterium off of a surface: Methods  SCHUYLER MCDONOUGH (Presenter), BENJAMIN ROQUE, ALEXANDER PETROFF, Physics, Clark University — Thiovulum majus is the fastest known bacteria. In its natural habitat, near the penetration depth of oxygen in salt marsh sediment, these bacteria create fluid flows that pull nutrient-rich water through the pore space. As cells navigate the pore space in which they live, they frequently collide with grains of sand. To better understand the ecology of these microbes, we investigate the dynamics of a collision of a T. majus with a solid surface. This presentation focuses on the experimental techniques needed to perform these measurements. These bacteria cannot be grown in pure culture. We first describe how we enrich T. majus from mud, collected from a Massachusetts salt marsh. Next, we analyze the motion of these cells in a microfluidic device. This device confines the motion of cells to two dimensions. We present techniques that allow us to track several thousand collisions between fast swimming cells and the chamber walls. We show that there are two types of collisions. If a cell approaches the wall at a glancing angle, it initially turns to swim parallel to the wall and then returns to the fluid. In the case of head-on collision, the cell becomes hydrodynamically bound to the surface.

M71.00293: WITHDRAWN ABSTRACT  —

M71.00294: Distinguishing Complex Locomotory Patterns in C. elegans*  SUSANNAH ZHANG (Presenter), Physics and Astronomy Department, University of Georgia, JENNY MAGNES, Physics and Astronomy Department, Vassar College, HAROLD HASTINGS, Physics Department, Bard College at Simon's Rock, KATHLEEN SUSMAN, Department of Biology, Vassar College, MIRANDA R HULSEY-VINCENT, Physics and Astronomy Department, Vassar College — Caenorhabditis elegans, more commonly known as C. elegans, are transparent nematodes approximately 1 mm long that inhabit soil in temperate environments. C. elegans have 302 neurons that are similar in form and function to that of humans. This similarity and the small number of neurons has spiked the interest of neurological and biological communities. With over 70 phenotypes, it is possible to quantitatively distinguish many C. elegans phenotypes according to different locomotory patterns. Time-Dependent Diffraction by oversampling provides information about the locomotion in the form of a single time-series; nevertheless, visually the different locomotion types are indistinguishable. We investigate the locomotion of two types of C. elegans, Wildtype (N2) and Roller (OH7547), using Recurrence Plots (RP) to analyze the complex dynamics collected. This method of analysis allows us to keep all of the dynamics of motion since every point in the diffraction pattern is a superposition of light rays diffracted from each point on the worm. Through the RPs, we dive deeper into the difference between locomotory patterns to be able to separate these two types of C. elegans.

*Lucy Maynard Salmon Research Fund
**M71.00295: Comparison between direct experimental measures of surface excess concentration in surfactant solutions with estimates based on the Gibbs Adsorption Isotherm**

ERNESTO HERNÁNDEZ-ZAPATA (Presenter), Recursos de la Tierra, Universidad Autónoma Metropolitana, LUCIANO MARTÍNEZ-BALBUENA, Departamento de Física, Universidad de Sonora, ARACELI ARTEAGA-JIMÉNEZ, Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada, Instituto Politécnico Nacional, CÉSAR MÁRQUEZ-BELTRÁN, Instituto de Física, Benemérita Universidad Autónoma de Puebla — Recently, Menger et al [J. Am. Chem. Soc. 131 (30): 10380 (2009)] have suggested that the Gibbs Isotherm Method (GIM) is not the best way to estimate surfactant surface excess concentration from surface-tension measurements at the air-water interface. Important experimental techniques, such as Neutron Reflectivity and the radiotracer method, have arisen in recent years helping to clarify the controversy. This is because they are able to measure the surface excess concentration without the use of the GIM. We review the best available surface-tension data for some ionic and nonionic surfactants, and apply the GIM to them in order to directly compare with Neutron Reflectivity and radiotracer data [Adv. Coll. Int. Sci. 247: 178 (2017)]. As the thermodynamic theory behind the GIM predicts the agreement is good for concentrations smaller than the CMC, both for ionic and nonionic surfactants. In the case of nonionic surfactants, we found also a good agreement for concentrations larger than the CMC.

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**M71.00296: Solvent diffusivity and viscosity in graphene oxide membrane for water-ethanol separation**

GOBIN ACHARYA (Presenter), PETER HOFFMANN, Wayne State Univ — Graphene oxide (GO) membranes were recently suggested for applications in separation of ethanol from water using a vapor permeation method. Understanding microscopic diffusivity of water and ethanol in graphene oxide membranes is important for separations applications. It is also important to study the anisotropy of water and ethanol diffusivity between the direction perpendicular to the plane and in-plane direction. We used quasielastic neutron scattering (QENS) to measure the temperature dependence of the diffusivity of water and ethanol, and its anisotropy by the utilization of Q-dependence of QENS signals obtained from BASIS at Oak Ridge National Lab. We will also discuss how dynamic measurements from QENS can be correlated with atomic force microscopy measurements of the temperature dependence of viscosity in water/ethanol confined in GO.

*We thank Wayne State University for funding and ORNL for providing access to BASIS through a user proposal.*

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**M71.00297: BIOLOGICAL PHYSICS**
M71.00298: Estimating the posture of coiled and overlapping worms using a neural network  
AVELINO JAVER, JENS RITTSCHER, University of Oxford, ANDRE BROWN (Presenter), Imperial College London — The first step in studying postural dynamics is typically animal tracking. A range of deep learning approaches have proven effective for human posture tracking and several groups have adapted these methods to laboratory animals. These methods typically detect key points on the body and they work particularly well for jointed animals where there are clear landmarks. For tracking the nematode worm *C. elegans*, some challenges remain. We generated a manually annotated data set with tens of thousands of frames including coiled and overlapping worms to train a neural network to find equidistant points along the worm midlines. During training we rely on simple image synthesis augmentations and use priors that incorporate the worm morphology into the loss function. We show that the new algorithm performs well with challenging backgrounds, for coiled worms, and for multiple overlapping worms. We apply the network to mating, a behaviour that necessarily involves overlapping worms.

M71.00299: Piezoelectric based sensor development to measure sound intensity in aquatic environments.*  
ELIJAH WATERS (Presenter), Physics and Astronomy, Georgia Southern University, SILVIU C. SARARU, MIHAELA T. UDRISTIOIU, Sciences, University of Craiova, VINOTH SITTARAMANE, Biology, Georgia Southern University, DRAGOS AMARIE, Physics and Astronomy, Georgia Southern University — When aquatic animals are presented with unfamiliar environments they tend to alter their behavior. To gain insight on such behavioral actions and changes there is a need for a submersible sensor designed to measure sound intensity given by the specimen. Our device builds around the property of a piezoelectric element that gives off an electrical signal when undergoing mechanical stress. This small signal is then boosted by means of a pre-amplifier connected to the piezo element within the device's housing. In experimentation, the device is placed in a position that allows for exposure of the piezo element surface into the aquatic environment. A clear gel containing the animal's food or prey within is applied on the surface. In an attempt to get food, or attack, the animal will strike, thus apply a force on the piezo. This provides the mechanical stress needed to gain the electrical signal that is recorded into a digital audio workstation (DAW) as audio. DAW is used to analyze the audio in decibels over time. Software is used to process the data as sound intensity produced by the specimen and quantify the striking intensity. Being able to measure these changes in behavioral habits we would be able to study embryonic learning.

*Office of Research, Georgia Southern University
M71.00300: Epigenetic regulation enhances stability of somatic differentiation state*
TIANCHI CHEN (Presenter), MUHAMMAD ALI AL-RADHAWI, EDUARDO SONTAG, Northeastern University — Stem cell treatments, such as those affecting the states of the network of pluripotency genes, are expected to play a central role in future personalized medicine. The genetic regulatory network consisting of the Oct4, Nanog, and TET transcription factors (TF's) is understood to control cell fate, specifically the transitions between somatic and pluripotent states. In the classical view, the steady states of a dynamical system modeling the genes, mRNAs, and proteins in this network are identified with the above two types of states. In this work, we investigate the role of epigenetic regulation in further stabilizing the two states. Specifically, we present a mathematical model that combines TF's and DNA methylation, which is one of the most important forms of epigenetic regulation. Our starting point is a mechanistic model formulated in the language of chemical reaction networks that describe promoter binding together with transcription/translation. We conclude that the effective rate of DNA methylation increases stability (relative size of the basin of attraction) of the somatic cell state, while increasing DNA demethylation rate, which is controlled by Nanog-guided TET protein, increases stability of the pluripotent state.

*NSF 1716623

M71.00301: Characterizing the spread of the effect of mutations on the protein-protein interaction network
ANUSH DEVADHASAN (Presenter), ITALO FARIA DO VALLE, Northeastern University, ISTVAN KOVACS, Physics, Northwestern University, ALBERT L BARABASI, Northeastern University — Networks can serve as a powerful tool for dissecting phenomena in complex biological systems. Of particular interest in biology is the effect of mutations on the resulting phenotype. Although numerous prior studies address this for specific cases, a generalized mechanistic theory of the phenotypic effect of mutation-induced perturbations does not exist. Here we identify patterns and principles characterizing the spread of the effect of mutations on the protein-protein interaction (PPI) network. Specifically, we propose network-based laws to identify differentially expressed genes (DEGs) following loss-of-function (LOF) mutation by studying the interplay between the topology of the PPI network and its response following node removal. We utilize cell line gene expression data following LOF mutation to evaluate network measures involving the DEGs and the knocked-out gene (KOG). We find that for 26/53 genes the DEGs form a statistically significant connected subgraph in a PPI network comprised of interactions curated from literature. Furthermore, we find that DEGs are significantly proximal to the KOG in 10/53 cases. This work contributes fundamental systems-level observations which may be exploited for the development of a predictive framework for general use in biological research.
M71.00302: Human Gene Expression and the Protein-Protein Interaction Network: Identification of Potential Disease Module Association to Differential Gene Expression for Patient-to-Drug Matching  AYDIN WELLS (Presenter), Northeastern University, DEISY MORSELLI GYSI, Center for Complex Network Research, ALBERT L BARABASI, Northeastern University — The relationship between human gene expression (GE) and precision medicine applications is central in understanding how patients are affected by and how to better treat a disease. Even though it is of extreme importance, this knowledge is still absent from almost any disease analysis resulting in misdiagnosis and mistreatment based on symptomatic and physical observation criteria devoid of high throughput sequencing technologies. By detecting disease modules in the protein-protein interaction (PPI) network, along with the identification of patient differential GE sets (DGE), we can suggest effective individual treatment options. Here, we collect public RNA sequencing data for a diverse population and arrange unique GE patient profiles. DGEs are computed using machine learning techniques and are identified within the PPI network, where disease modules can be pinpointed. Those modules can be used for disease classification specific to expression levels and cohort phenotype. By elucidating these interactions using network approaches with an individual patient's features, human diseases can be identified not by peripheral approaches, but by a personal genetic diagnosis; essentially redefining disease diagnostics from a “one size fits all” philosophy, to a “one size fits you” reality.

M71.00303: Effects of Stochasticity in Biological Oscillators  CHAITRA AGRAHAR (Presenter), Physics, UIC, MICHAEL RUST, University of Chicago — Many processes need to occur periodically for proper functioning of the cell, despite fluctuations in its environment. A cell must remain robust against irrelevant fluctuations, while simultaneously responding to relevant cues. We study how network topologies optimize the trade-off between maintaining robust oscillations and biosynthetic expenditure.

Many studies concur that motifs with positive and negative feedback are most robust to variations in the deterministic limit [1, 2], and in the stochastic regime [3, 4]. However, there is no mechanistic understanding for predicting the performance of different topologies.

Our findings suggest that deterministic amplitude, along with the distribution of angular velocities along the phase-space orbit of dynamical variables can lead to a mechanistic understanding of this trade-off. Regulation mechanisms and tuning of interaction strengths play a pivotal role in this optimization.

**M71.00304: Multivalent Binding of Patterned Polymers**  
EMIKO ZUMBRO (Presenter), ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology MIT — Using inspiration from biology, we can leverage multivalent binding to enhance weak, monovalent binding between molecules. Synthetic glycopolymers have been shown to successfully bind to viruses and toxic proteins. This binding indicates that multivalent polymers are a promising tool for inhibiting target attachment to and subsequent infection of cells. Previous work from our group focused on how structural features of uniform binding site polymers create high affinity and specificity to a single target. In contrast, real synthetic polymers might find it desirable to have multiple binding moieties along the chain. Multiple binding site types allow polymers to target multiple species creating broad-spectrum binding or allow for tracking or imaging in addition to targeted binding. Heterogeneity in binding site patterns can also be a byproduct of chemical synthesis methods. We use a reactive-binding, Brownian dynamics simulation and machine learning to examine how patterning of heterogeneous binding sites along a polymer chain controls binding of a multivalent polymer. Our results provide direction for the rational design of multivalent binders.

*The authors were supported by the Department of Defense through the National Defense Science & Engineering Graduate Fellowship Program.*

**M71.00305: Using structural adaptations in plants for desalination**  
ADAM WOOD (Presenter), RAGHAV GARG, KYLE JUSTUS, TZAHI COHEN-KARNI, ALAN RUSSELL, PHILIP R LEDUC, Carnegie Mellon Univ — Biologically-inspired abiotic systems are becoming a central pillar in how we respond to critical grand challenges that accompany exponential population growth, uncontrolled climate change and the reality that 96.5% of the water on the planet is saltwater. One fascinating biologic adaptation to saltwater is the growth of mangrove trees in brackish swamps and along the coasts. Through salt exclusion, the mangrove maintains a near freshwater flow from roots to leaves for survival. One abiotic approach to water desalination is capacitive deionization (CDI), which uses electrostatic force to adsorb ions from a feed stream to a pair of charged electrodes. In this work, we use one-step carbonization of mangrove roots with developed aerenchyma tissue to enable highly-permeable, freestanding flow-through (FT) CDI electrodes. We demonstrate the use of the intact carbonized mangrove roots as electrodes in a FT-CDI system. We also show that the structure of carbonized aerenchyma from mangrove roots reduces the resistance to water flow through the electrodes by 65-fold relative to carbonized plant structure lacking this biological adaptation (woody biomass). These findings have implications in a range of fields including desalination, bioinspired materials, and plant-structure functionality.
M71.00306: Correlative Atomic Force Microscopy and Photo-Activated Localization Microscopy of Nano-cellulose Fibrils from Tunicate and Poplar*  LIN KANG (Presenter), CONGZHOU WANG, Nanoscience and Nanoengineering, South Dakota School of Mines & Technology, SHI-YOU DING, Department of Plant Biology, Michigan State University, STEVE SMITH, Nanoscience and Nanoengineering, South Dakota School of Mines & Technology — The molecular structure of cellulose in its native nano-fibril form is difficult to characterize and consequently still not well understood. We report simultaneous Atomic Force Microscopy (AFM) and Photo-Activated Localization Microscopy (PALM) of cellulose nano-fibrils (CNFs) from Tunicate and Poplar. PeakForce Quantitative Nanomechanical Mapping (PFQNM) is employed to characterize sample stiffness and modulus mapping. To complement the AFM measurements, the nano-fibrils were exposed to recombinant family 3 Carbohydrate Binding Modules (CBM3) specifically binding to the hydrophobic surface of crystalline CNF. The CBM3 was also tagged with a photoactivatable fluorescent protein PA-mCherry to allow super resolution imaging by PALM. We compare the distribution of CBM binding sites to the nano-fibril topography to draw conclusions about the degree of crystallinity of the elemental CNF and the distribution of amorphous areas within the CNF and at morphological kinks, which show a non-Gaussian distribution related to the crystallographic planes of cellulose.

*Funded by the National Science Foundation (DMR 1206908 BMAT).

M71.00307: The SWCNT-DNA hybrid for imaging and vector delivery applications A. Adesina, S. Pourianejad, T. Ignatova Nanoscience Department, University of North Carolina at Greensboro, Greensboro, NC, USA* ADEYINKA ADESINA (Presenter), Univ of NC - Greensboro — Single Wall Carbon Nanotubes (SWCNTs), being quasi-one-dimensional materials, are extensively investigated for intracellular imaging and bio-sensing applications since discovery of the hybridization of ssDNA molecules to SWCNTs. When functionalized, SWCNT can be introduced within the cell and co-localized with the sub-cellular organelles. SWCNTs exhibit resonance Raman scattering, with sharp, high intensity Raman peaks quite different from that of the hybrid or the cell itself. Raman signal of SWCNTs is chirality specific hence it can be used for nanotube identification and to assess their aggregation in cell environment. The long-term intracellular studies of SWCNTs within neural stem cells have been conducted using micro-Raman spectroscopy indicating the viability of SWCNTs as an efficient tracking agent. Additionally, we investigated the affinity of the ssDNA for SWCNT in presence of complementary strand. Here, the results on the equilibrium and dynamic study of DNA displacement from the nanotube surface, temperature dependence, Manning-Oosawa counterion condensation, and pH variation will be presented.

*Joint School of Nanoscience and Nanoengineering, SENIC and NNCl, supported by National Science Foundation ECCS-1542174); to the UNC Inter-institutional Planning Grant A20-0089-001
M71.00308: Investigating Zika Virus RNA Conformational Switching using Molecular Dynamics* NAOMI BRANDT (Presenter), RNA Institute, University at Albany (SUNY), SIMI KAUR, Chemistry Department, University at Albany (SUNY), ALAN CHEN, Chemistry Department, RNA Institute, University at Albany (SUNY) — Previous attempts at modeling RNA folding for relatively large systems have demonstrated limited sampling of conformation space due to the presence of kinetic traps. In this work, we used a novel method of molecular dynamics simulations, a 2D replica exchange protocol in which RNA replicas cycle through both temperature variations and base-pairing restraint strength using experimentally determined base-pairing patterns. This method refines the energy landscape, biasing the structure to preserve only the most stable conformations at low temperatures.

Using this approach, we designed all-atom models of sections of the 3’ untranslated region of Zika Virus RNA in order to predict pseudoknot formation between the 3’ dumbbell region and other nearby structures. The dumbbell is theorized to be a driving mechanism that allows switching between the translation and replication phases of the RNA lifecycle. From our simulations, we were able to infer the kinetic and structural favorability of proposed pseudoknots, and investigate potential intermediaries required to trigger switching.

*This work was supported by NIH Grant 1R35GM13346901.

M71.00309: Restraint-Biased 2D Molecular Dynamics Simulations SIMRANPREET KAUR (Presenter), PARISA EBRAHIMI, Chemistry, SUNY Albany, NAOMI BRANDT, RNA Institute, SUNY Albany, ALAN CHEN, Chemistry and RNA Institute, SUNY Albany — Although recent experimental and computational advances have strived to understand RNA structure-function relationships, the roles of many RNAs are dependent upon a complex network of motifs, including hairpins, internal loops, pseudoknots and long-range contacts, that are not easily captured by these methods. Ab-initio modeling using all atom molecular dynamics simulations is limited by the available energy functions and the required sampling of an extensive conformational space. We have developed a hybrid replica exchange method that incorporates secondary structure information from experiments in the form of piecewise linear-harmonic distance restraints (bias forces) to efficiently fold RNA in 3D detail. This sharpens the free energy landscape by reducing the number of conformations that satisfy an optimum 3D fold. Replica exchange conducted in both temperature and position space, where replicas with variable bias forces and temperatures run in parallel and periodically swap, also allows molecules to overcome kinetic barriers surrounding local minima. A range of possible structures are uncovered from higher temperatures, but only the most stable conformations are retained at lower temperatures.
M71.00310: Flow Analysis and UniverScope: complementary techniques to monitor spheroid growth* SHANJIDA KHAN (Presenter), Drew University — The Bioimaging & Optofluidics laboratory has developed an encapsulation technique that allows to produce multicellular spheroids as model tissue at a very high throughput and controlled manner. To monitor the growth of spheroids, we use two complementary techniques. The first one relies on an image-free analysis of the light absorbed by the spheroids; the second one consists of building a microscope that allows parallelized imaging of spheroids in physiological conditions. These two methods are aimed at measuring the spheroid radius as a function of time and at gaining insight into the fate of cells within the spheroids.


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M71.00311: Expanding Without Exploding: Measuring and Modeling the Biomechanics of Pollen Hydration KARI MILLER, ANDERS CARLSSON (Presenter), ELIZABETH HASWELL, Washington University, St. Louis — To carry male gametes to female plants, pollen grains must undergo desiccation. They subsequently rehydrate before extending a tube to fertilize the egg cell. Hydration involves dramatic changes in both the turgor pressure and cell wall properties of the pollen. Little is known about the mechanics of hydration, especially the mechanisms that allow the pollen grain to tolerate the large forces that occur. Here we combine mathematical modeling with experimental data to clarify the role of a membrane-bound tension-sensitive ion channel (MSL8) during hydration. This channel is known to be essential for pollen survival during hydration, but its exact role is not known. New data presented here reveal that MSL8 contributes to rapid stabilization of the pollen grain volume during hydration. In the absence of MSL8, the pollen grain continues to expand indefinitely, often leading to overexpansion and bursting. We develop a mathematical model of rehydration dynamics embodying the interplay between turgor pressure, cell wall mechanics, membrane mechanics, and tension-sensitive channels. This model finds, consistent with the data, that the absence of tension-sensitive channels causes continued expansion of the cell.
M71.00312: Interaction of Electromagnetic Radiation with DNA  DAVID ORTEGA (Presenter), SAMINA MASOOD, University of Houston, Clear Lake — Cells are known to be affected significantly due to constant exposure to electromagnetic radiation. DNA can be damaged with electromagnetic waves in a variety of ways. Cellular multiplication plays an important role in the survival of life. This multiplication involves a chain of DNA replication going through several steps including auto-repair mechanisms to protect DNA from damages. These repair mechanisms range from specific "locate and repair" systems to "damage tolerance" repairs. With many damage events per cell per day the errors that do make it through the repair process are seen as mutations to the genetic code and may be expressed as changes in morphology. Applying an appropriately modified Jaynes-Cummings model with an extra potential we re-investigate the DNA replication considering the entangled states of the nucleotide. Interaction of DNA with radiation is studied as an interaction of matter with electromagnetic waves. This approach is used to measure the probability of changes in morphology due to the interaction of DNA with radiation.

M71.00313: Polymerization Characteristics of Different Microtubules’ Interaction with Tau Protein and Taxol*  JANE BRESLIN (Presenter), IBUKUNOLUWA AKINTOLA, MITRA SHOJANIA FEIZABADI, Seton Hall Univ — We previously reported that the interaction of one of the microtubule-associated protein (MAP), tau protein, is significantly different on two different types of microtubules; brain microtubules versus human breast cancer microtubules in vitro. These two types of microtubules are distinct from one another due to structural differences that exist in beta-tubulin isotype distributions. In addition, microtubules are known as one of the best targets for anti-cancer drugs such as Taxol. It is known that the direct interaction of Taxol with tubulin or microtubules changes the polymerization specifications of them. Due to the existence of Tau protein in brain cells and some breast cancer cells, it is important to study how the presence of both Tau protein and Taxol may affect the polymerization specifications of these two structurally different microtubules. In this study, we explain the outcomes of our experiments in identifying the distinct polymerization properties of Tau protein and Taxol interacting with different beta-tubulin isotypes in these two types of microtubules.

*We acknowledge the funding from Clare Boothe Luce for Jane Breslin.
M71.00314: A Nano-Technology Approach to Screen the Charge of Molecular Motors

RAMIZ ALEJILAT (Presenter), ALEXIS DUFFY, MITRA SHOJANIA FEIZABADI, Seton Hall Univ — A better understanding of the nature of the electrostatic interactions between molecular motors and microtubules requires a thorough examination of, not only the charge of microtubules, but molecular motors as well. Several reported studies have been conducted to screen and evaluate the charge of microtubules in vitro. However, our knowledge about the electric charge of molecular motors is still limited to the evaluation of the association rate they express in conjunction with microtubules.

With the goal of screening and evaluating the charge that molecular motors carry, we have designed a nanotechnology-based method. In this approach, the charge of motors can be screened in vitro by monitoring their behavior inside a uniform electric field. This novel in vitro approach minimizes the cellular factors that can potentially interfere with evaluating the charge of motors, leading to a better capability of evaluating the charge of these bio-motors in a more exclusive framework.

*We acknowledge the funding from Clare Boothe Luce for Alexis Duffy.

M71.00315: Optical Imaging of Magnetic Particle Rotation in High Viscosity Fluids

RIVER GASSEN (Presenter), DENNIS THOMPKINS, GUY HAGEN, KATHRIN SPENDIER, BioFrontiers, UCCS — The purpose of this experiment is to study the oscillation and rotation of nanoparticles in fluids of different viscosities. The investigations have practical applications to the medical field, specifically drug delivery through high viscosity fluids like mucus. Magnetic barium hexaferrite (BaFe12O19) and iron oxide (Fe3O4) particles were suspended in distilled water or various glycerol concentrations. The mixtures had a concentration of 2.50mg/ml for the BaFe12O19 and 1.00mg/ml for Fe3O4. Magnetic particles were exposed to oscillating or rotating magnetic fields and imaged with an optical microscope. Time-varying magnetic fields ranging from 10Hz to 180Hz are created by pairs of home-made wire coils that insert into the microscope. Magnetic field amplitudes can be varied from 0-12 mT. The resulting measured frequency of the particle oscillation or rotation equaled the drive frequency when the drive frequency was less than half the frame rate. For high viscosity fluids, higher magnetic field strength was necessary for particle motion. Further investigation will need to be done to determine how the viscosity, particle size, and drive frequency impact the movement of the particles, going from oscillating at the driving frequency to no particle motion.

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**M71.00316: The Dynamics of Human Society Evolution**
RAM POUDEL (Presenter), Tribhuvan University, JON MCGOWAN, University of Massachusetts Amherst — Human society is an open system that evolves by coupling with various known and unknown (energy) fluxes. How do these dynamics precisely unfold? Energetics may provide further insights. We expand on Navier-Stokes’ approach to study non-equilibrium dynamics in a field that evolves with time. Based on the ‘social field theory’, an induction of the classical field theories, we define social force, social energy and Hamiltonian of an individual in a society. The equations for the evolution of an individual and society are sketched based on the time-dependent Hamiltonian that includes power dynamics. In this paper, we will demonstrate that Lotka-Volterra type equations can be derived from the Hamiltonian equation in the social field.
Keywords: evolution; energetics; social field theory; capital; capabilities.

*We did not seek any funding for this research. RP acknowledges a sabbatical granted by the Institute of Engineering, Tribhuvan University.*

**M71.00317: Ecological mechanisms of direct and indirect bacteriotherapies in generalized Lotka-Volterra systems**
ERIC JONES (Presenter), JEAN M CARLSON, University of California, Santa Barbara — Over the last two decades, an association between microbiome composition and some human diseases has been unambiguously established. The correlation between gut microbe composition and these diseases has prompted medical interest into bacteriotherapies, which seek to modify the gut microbiome composition in the hopes of treating the correlated disease. In this work we use generalized Lotka-Volterra (gLV) models to probe the ecological mechanisms through which these bacteriotherapies function. We first describe direct bacteriotherapies, which drive a microbiome to a target state via an instantaneous influx of foreign microbes (e.g. probiotics or fecal microbiota transplantation). Then, we present a novel control framework for indirect bacteriotherapies, which drive a microbiome to a target state by deliberately modifying its environment (e.g. diet, acidity, or nutrients). These dual control methods for gLV systems, interpreted as bacteriotherapies, could eventually inform personalized medicine for the microbiome.

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M71.00318: Competing for Resources: on the Emergence of Property Rights  CLELIA DE MULATIER (Presenter), University of Pennsylvania, CRISTINA PINNERI, Max Planck Institute for Intelligent SystemsMax Planck Institute for Intelligent Systems, Tübingen, Germany, MATTEO MARSILI, International Centre for Theoretical Physics — A game theory approach to the evolution of animal conflicts has shown that choosing an initial asymmetric feature, such as first come first served, to settle a contest is evolutionarily stable, as it avoids the costs of animal fights. In this context, we investigate the optimal strategies of a population of non-aggressive agents competing for multiple resources. Resources provide different payoffs and can only be exploited by one agent at a time. If an agent tries a resource that turns out to be occupied, it then looks for another resource, which has a cost. We show theoretically and numerically that this system admits two types of Nash equilibria. In an under-crowded system, resources are equally shared between agents; our reinforcement learning simulations find multiple optimal solutions, where agents each exploit different sets of resources but all earn the same average payoff. The average strategy of these agents matches with the theoretical mean-field solution. Over-crowded systems are instead conducive to the emergence of inequality; some agents can earn more than the others by establishing themselves as property owner of a medium-payoff resource. In the reinforcement learning simulations, such lucky agents emerge naturally from their random learning experience.

M71.00319: A model to explain the propagation of small dysfunctional mitochondrial DNAs in budding yeast  CHRISTOPHER NUNN (Presenter), SIDHARTHA GOYAL, Univ of Toronto — Mitochondrial DNA (mtDNA) in budding yeast is unstable, resulting in a high rate of spontaneous respiratory-deficient mutants [1]. These respiratory-deficient mutants (called petites) can, however, grow on fermentable media. A petite cell often contains small, incomplete mtDNA fragments, that replicate and pass on from generation to generation with no known function in the cell. These selfish mtDNAs often do better than wild type mtDNA and outcompete (suppress) them if they are present together in a cell [2]. The features that allow these selfish mtDNAs to outcompete wild type mtDNA, as well as the potential for mechanisms that select against selfish mtDNAs remains to be fully characterized. To address these questions we have characterized a set of spontaneous petite mitochondrial genomes, and developed a model to explain what features of their structure inform their suppressivity when mixed with wild type mtDNA.

M71.00320: Information costs in the control of protein synthesis  REBECCA ROUSSEAU (Presenter), Physics, California Institute of Technology, WILLIAM S BIALEK, Physics, Princeton University — Efficient protein synthesis depends on the availability of charged tRNA molecules. With 61 different codons, shifting the balance among the tRNA abundances can lead to large changes in the protein synthesis rate. Previous theoretical work has asked about the optimization of these abundances, and there is some evidence that regulatory mechanisms bring cells close to this optimum, on average. We formulate the tradeoff between the precision of control and the efficiency of synthesis, asking for the maximum entropy distribution of tRNA abundances that is consistent with a desired mean rate of protein synthesis. Our analysis, using data from *E. coli*, indicates that reasonable synthesis rates are consistent only with rather low entropies, so that the cell's regulatory mechanisms must encode a large amount of information about the “correct” tRNA abundances.

M71.00321: Contours information and the perception of various visual illusions*  EE HOU YONG (Presenter), Nanyang Technological University — The simplicity principle states that the human visual system prefers the simplest interpretation. However, the conventional coding models could not resolve a contradiction between the global minimum principle and the local minimum principle. By quantitatively evaluating information content along the contours under our framework, it is shown that the most plausible interpretation of a stimulus (the one correctly predicted by local minimum principle) possesses the lowest information globally, hence resolves the contradiction. This model could also explain the perception of various visual illusions including Kanizsa illusions, Ehrenstein illusions and Rubin's vase via estimating the lower bound of the spread parameter of the von Mises distribution governing human visual expectation. This provides new insight into the celebrated simplicity principle and could serve as a fundamental explanation of the perception of illusory boundaries and the bi-stability of perceptual grouping.

*Research for this project was made possible by a Start-Up Grant No. M4081583 from Nanyang Technological University, Singapore.
M71.00322: The robust bioinformatic analysis of the protein sequences with phase behavior
ALEKSANDRA ELZBIETA BADACZEWSKA-DAWID (Presenter), DAVIT POTOYAN, Iowa State University — Liquid-liquid phase separation (LLPS) of many proteins is critical in the biological function of membrane-less organelles. Reversible nature of biomolecular PS in cells suggests that phases of proteins and nucleic acids are like to be tightly regulated. Post-translational modifications and single-residue mutations have been shown to lead to the dissolution of biomolecular droplets or phase transition into aggregated forms. Based on the wealth of experimental data, it reasonable to expect that the PS of proteins is highly sequence-specific. To reveal common motifs of protein sequences that promote PS, we have carried out large-scale statistical analysis of phase separating protein deposited in the LLPSDB database. For each motif, the most significant interactions have been identified (e.g. charge, hydropathy, polarity, pi-stacking). The bioinformatic analysis provides us with crucial knowledge about sequence conservation, secondary structure preferences, aggregation tendency, post-translational modification prediction, and binding affinity. The long-term goal of our research is the creation of a publically accessible database that would be used by both experimentalists for designing controlled mutations and for computationally-oriented scientists for developing new modeling tools.

M71.00323: Reentrant Liquid Condensation of Ribonucleoprotein–RNA Complexes
MURALIKRISHNA RAJU (Presenter), RABIA LAGHMACH, DAVIT POTOYAN, Iowa State University — Intracellular Ribonucleoprotein (RNP) granules are membrane-less liquid condensates that dynamically form, dissolve, and mature into a gel-like state in response to a changing cellular environment. RNP condensation is largely governed by attractive inter-chain interactions mediated by low-complexity domains. Using an archetypal disordered RNP, fused in sarcoma (FUS), here we employ atomistic simulations to study how RNA, a primary component of RNP granules, can modulate the phase behavior of RNPs by controlling both droplet assembly and dissolution. Electrostatic interactions are found to be the primary driving force behind condensate formation. Monotonically increasing RNA concentration initially leads to droplet assembly via complex coacervation and subsequently triggers an RNP charge inversion, which promotes disassembly. We construct phase diagrams based on Droplet density and Shannon entropy calculations, wherein three distinct regimes can be identified based on RNA and peptide concentrations. Increasing salt concentration is found to inhibit the formation of liquid condensates and narrow the coexistence region. The internal organization and dynamics of the condensates are investigated as a function of RNA/peptide concentrations, RNA chain length and salt concentration.
M71.00324: Liquid-liquid phase separation driven compartmentalization of reactive nucleoplasm  RABIA LAGHMACH (Presenter), MURALIKRISHNA RAJU, DAVIT POTOYAN, Iowa State University — Organization and regulation of intracellular biochemistry are achieved by compartmentalizing biomolecules through the liquid-liquid phase separation process (LLPS) and its associated chemical reactions into membrane-bound and membrane-less organelles. The LLPS of proteins/RNA within the nucleus plays a crucial role in the gene regulation of eukaryotic cells. Here, we present a reaction-diffusion model of transcription which connects the phase separation of proteins-RNA mixture inside nucleoplasm with transcriptional and catalytic reactions. Our model shows the existence of a variety of complex protein-RNA patterns that arise from the competition between different mechanisms including LLPS, biomolecular interactions, and biochemical reactions. The protein-RNA pattern formation is strongly dependent on the interplay of time-scales for diffusion, transcription, and translation. Under appropriate kinetic regimes, we can dramatically accelerate or slow down the phase-separation process, thereby leading to arrested phases.

M71.00325: Liquid-liquid phase separation driven compartmentalization of reactive nucleoplasm  RABIA LAGHMACH (Presenter), MURALIKRISHNA RAJU, DAVIT POTOYAN, Iowa State University — Organization and regulation of intracellular biochemistry are achieved by compartmentalizing biomolecules through the liquid-liquid phase separation process (LLPS) and its associated chemical reactions into membrane-bound and membrane-less organelles. The LLPS of proteins/RNA within the nucleus plays a crucial role in the gene regulation of eukaryotic cells. Here, we present a reaction-diffusion model of transcription which connects the phase separation of proteins-RNA mixture inside nucleoplasm with transcriptional and catalytic reactions. Our model shows the existence of a variety of complex protein-RNA patterns that arise from the competition between different mechanisms including LLPS, biomolecular interactions, and biochemical reactions. The protein-RNA pattern formation is strongly dependent on the interplay of time-scales for diffusion, transcription, and translation. Under appropriate kinetic regimes, we can dramatically accelerate or slow down the phase-separation process, thereby leading to arrested phases.

M71.00326: Complex Coacervate Core Micelles for Protein Delivery  RACHEL KAPELNER (Presenter), ALLIE OBERMEYER, Columbia University — Proteins are an increasingly important class of therapeutics. There are, however, several challenges in the development and production of protein based therapeutics. These include relative temperature sensitivity and propensity to aggregate at therapeutically relevant concentrations, both of which contribute to the their relatively short shelf-life and short circulation times. Previous work has developed protein delivery platforms that increase circulation time while maintaining protein activity, but suffer several shortcomings such as low-levels of protein loading and controlled release. To address these limitations, we have investigated the use of block-polyelectrolytes to form complex coacervate core micelles (C3Ms) to be used as a protein delivery vehicle. While C3Ms allow for controlled protein loading and release, they also have the potential to improve protein stability at therapeutically relevant concentrations and increased temperatures. In this work, we identified protein and polymer design parameters that govern complex coacervation of model proteins to form C3Ms that remain phase separated under physiological conditions and study how incorporation of proteins in C3Ms influences protein stability and delivery to cells.
M71.00327: The role of epigenetics and microenvironment in breast cancer evolution

J. ROBERTO ROMERO-ARIAS (Presenter), Mathematics and Mechanics, Institute for Research in Applied Mathematics and Systems, UNAM, GUILLERMO RAMÍREZ-SANTIAGO, CALOS GONZÁLEZ-CASTRO, Institute of Mathematics, UNAM Juriquilla — Cancer is a disease driven by aberrant signaling pathways that control and maintain the malignant phenotype. Among the different aspects that drive these aberrant behavior are epigenetic changes that favor the uncontrolled growth and longer survival of malignant cells. These molecular changes affect microenvironment and cellular function subjecting cells to stress due to the lack of sufficient nutrients (glucose) and oxygen. On the other hand, estrogens have been found to play a major role in promoting the proliferation of both normal and neoplastic cells and they are believed to stimulate the occurrence of neoplastic mutations. Here, we incorporate these biological processes into a quantitative model to understand how microenvironmental conditions affect genetic dynamics and phenotypic diversity. Our results suggest that the evolution of malignancy and heterogeneity in a tumor arise and can be controlled by local epigenetic changes. This yields support to the believe that controlling local microenvironmental aspects might prevent the further development of a tumor.

M71.00328: Geometry and mechanics of a model epithelium with irregular cells and a clonal inclusion

DIEGO A CONTRERAS, VINCENT HAKIM (Presenter), FRANCIS CORSON, Ecole Normale Superieure — An important role in the modeling of epithelial tissue mechanics has been played by vertex models, with cells idealized as polygons, and tricellular junctions as vertices joined by straight interfaces. Numerical simulations of these models in the presence of cell divisions display geometrically irregular cells, similar to those of epithelia, even when cell properties are homogeneous. Yet existing theoretical analyses are mostly confined to the mechanics of regular hexagonal lattices. We develop an analytical description of geometrically disordered vertex models. We first quantify, in numerical simulations, geometrical properties such as the distributions of cell areas and perimeters, and mechanical properties such as the tissue bulk and shear moduli, with different sources of disorder, e.g. different division rules or simply relaxation in the presence of noise. We then develop a simple mean-field description that accounts for these properties. Finally, we apply our analytical description to a simple case of interest in different biological contexts: a clonal group of cells with material properties that differ from the surrounding tissue and that may also grow at a different rate. We compare our results with data obtained on epidermis differentiation in flies.

*ANR-14-CE11-0010
**M71.00329: Chemotaxis of Tumor Spheroids in 3D Extracellular Matrices**

YOUNG JOON SUH (Presenter), YU LING HUANG, Cornell University, JEFFREY SEGALL, Albert Einstein College of Medicine, MINGMING WU, Cornell University — Cytokine-mediated tumor migration (chemotaxis) plays a crucial role in cancer metastasis. Previous studies have explored the chemotactic behavior of single cells embedded within 3D extracellular matrices (ECM). However, due to the vastly different nature of single cells and tumors, a single cell 3D model cannot recapitulate the in vivo tumor invasion behavior. In this talk, we will present a 3D tumor spheroid model for tumor chemotaxis studies. Breast tumor spheroids using MDA-MB-231 cells were engineered and embedded within a collagen matrix. Tumor spheroid dynamics were imaged and analyzed when subjected to well-defined cytokine (Epidermal growth factor, hEGF) gradients provided by a microfluidic platform. Differential behavior of single tumor cell and spheroid chemotaxis will be discussed.

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**M71.00330: On the mechanical principles of biofilm formation**

JING YAN, QIUTING ZHANG, JAPINDER NIJJER (Presenter), Molecular Cellular and Developmental Biology, Yale University — Bacteria, once thought to be solitary and asocial, can grow in large, dynamic, multi-cellular communities known as biofilms, which consist of bacteria embedded in an extracellular matrix. However, the manner in which these three-dimensional, surface-adhered communities are built in space and time still remains to be shown. Using the human pathogen *Vibrio Cholerae* as model biofilm former, we examine the growth of biofilms from single founder cells to mature three-dimensional colonies. We find that biofilms grow from disordered, two-dimensional layers into three-dimensional structures with long-range order consisting of vertically aligned cores and horizontally aligned periphery. Using agent-based modelling, we find that verticalization occurs due to mechanical instabilities at the cell-scale and we quantitatively test these predictions by varying the cell lengths, surface roughness and osmotic conditions.

**M71.00331: WITHDRAWN ABSTRACT**

**M71.00332: Probing tissue mechanical properties in Drosophila embryos using magnetic tweezers**

AN PHAM (Presenter), Department of Physics and Soft Matter Center, Duke University, DANIEL P KIEHART, Department of Biology, Duke University, CHRISTOPH F. SCHMIDT, Department of Physics and Soft Matter Center, Duke University — The amnioserosa is a single-cell-deep epithelial cell sheet that contracts during dorsal closure in Drosophila melanogaster embryos. Displacement can be easily observed by microscopy and strains can be inferred from UV laser ablation experiments. The material properties of the amnioserosa and surrounding cell layers, however, remain elusive, which challenges a complete understanding of the driving forces in developing tissues. We have constructed an experiment to quantify mechanical properties of the amnioserosa cells during dorsal closure using magnetic tweezers. Complex shear moduli of the tissues are directly measured by exerting calibrated magnetic forces and observing displacements of bound magnetic beads.
M71.00333: Interpretation of Phase Boundary Fluctuation Spectra in Biological Membranes with Nanoscale Organization*  
SAHITHYA IYER (Presenter), Indian Institute of Science, ARCHIT NEGI, Department of Physics, Indian Institute of Technology, Bombay, ANAND SRIVASTAVA, Indian Institute of Science — In this work, we use a computationally less expensive and more automated Support Vector Machine algorithm to detect simple and complex interfaces in atomistic and coarse-grained molecular simulation trajectories of phase separating lipid bilayer systems. We find that the power spectral density of the interfacial height fluctuations and in turn line tension of the systems depends on the order parameter used to identify the intrinsic interface. To highlight the effect of length scale used to identify the interface on the fluctuation spectra, we perform a convolution of the boundaries identified at molecular resolution with a 2D Gaussian function of variance equal to the experimental resolution limit. The region of fluctuation spectra that scales according to capillary wave theory formalism relies on the complexity of the interfacial geometry, which may not always be detected at experimental resolutions. We propose that the different $q$-regimes in the fluctuation spectra can be used to characterize mode dependent interfacial tensions to understand the interfaces beyond the linear line tension calculations.

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M71.00334: External Forces generated by the Attachment between embryonic Tissue and Egg Shell affect Gastrulation in Insects  
STEFAN MUENSTER (Presenter), Max-Planck-Institute of Molecular Cell Biology and Genetics, ALEXANDER MIETKE, Max-Planck-Institute for Physics of Complex Systems, AKANKSHA JAIN, PAVEL TOMANCAK, STEPHAN GRILL, Max-Planck-Institute of Molecular Cell Biology and Genetics — Gastrulation is a critical step during the development of multicellular organisms in which a single-layered tissue converts into the multi-layered germband. This shape change is characterized by tissue folding and large-scale tissue flow. The myosin-dependent forces that underlie this process have been increasingly investigated; however, thus far, a possible interaction between the moving tissue and the rigid shell surrounding the embryo has been neglected. Here, we present our quantitative findings on the physical mechanisms governing gastrulation in the red flour beetle, Tribolium castaneum. We investigated the forces expected within the tissue given the myosin distribution observed by multi-view light-sheet microscopy and discovered that an additional external force must be counteracting this tissue-intrinsic contractility. We then identified that a specific part of the tissue tightly adheres to the outer rigid shell. This attachment is mediated by a specific integrin whose knock-down leads to a complete loss of the counter-force. Moreover, in the fruit fly Drosophila melanogaster, knock-down of another integrin leads to a severe twist of the germband, suggesting that the integrin-mediated interaction between tissue and vitelline envelope may be conserved in insects.
M71.00335: Size and shape control dynamics in an early diverging animal* PRANAV VYAS (Presenter), MANU PRAKASH, Bioengineering, Stanford University — Animals have traditionally been characterized as clonal cell populations with complex tissue architectures which have specific developmental programs that guide the morphogenesis of organs and in turn whole animals. On the other hand, very early diverging metazoans display simple tissue architecture with a lesser division of labour that allows high plasticity and scalability. High plasticity in such tissues allows dynamic shape changes at time scales of ~five minutes and a scalable tissue architecture allows size variation of over two orders of magnitude. For such tissues, size and shape are deeply interdependent due to physical constraints. Using high throughput long term scanning microscopy, we collect datasets on shape and size variation in lab culture conditions and quantify their temporal trajectories. Using perturbations to these 'natural' trajectories, we decouple size and shape parameters to decipher the principles that the system uses to exercise control over growth. Utilizing large datasets and growth-based models, our study provides abstract principles that would have governed size and shape control in very primitive `animal-like' multicellular clusters.

*SGF, SIGF (Fellowships), HHMI, CZI Biohub (Lab)

M71.00336: Single-Chain Variable Fragment Bearing Silica Nanoparticle Evaluation in HER2+ Over Expressing Tumor Tissues Using Optical Super-Resolution Microscopy* JOSHUA HINCKLEY (Presenter), NIRMALYA BAG, JACOB ERSTLING, ULRICH WIESNER, Cornell University — Active targeting of therapeutics or imaging probes to cancer cells is the primary pharmacological strategy in cancer therapy and diagnostics. Recent years have witnessed a boom in nanotechnologies, such as antibody-functionalized nanoparticles, in cancer theranostics which provide unique advantages over standard treatments. However, nanomedicine has is currently suffering from a lack of characterization and quantitative methods that provide understanding of the complex interactions in tumor tissues. The challenge in making quantitative methods for large samples usually lies in cost and availability of equipment. However, optical microscopy is a well-established and relatively low-cost alternative which is equipped, due to various super-resolution techniques, with the capability to study objects smaller than 100 nm. Here we demonstrate the use of coordinate base colocalization and nearest neighbor distance analysis with optical super-resolution microscopy to determine the quality of nanomedicine targeting using HER2 overexpressing tumor tissues.

*This study was funded by MedImmune and grants from the National Institutes of Health (U54 CA199081-01 to M.S.B. and U.W.) and Sloan Kettering Institute (Core Grant P30 CA008748CCSG).
M71.00337: Exploring the Dynamics of Biological Macromolecules at Angstrom Scale

ZAHRA ALAVI, CALVIN FOSS (Presenter), Loyola Marymount Univ — This research project plans to study Guanylate Kinase (GK) using nano-rheological techniques. These biological macromolecules will be immersed in solutions with different solvents in order to observe how the conformational dynamics of the molecules change.

An oscillatory force will be applied by attaching enzymes to a gold-coated surface and to gold nanoparticles. An additional gold-coated surface will be placed on top of the setup in order to create a parallel plate capacitor configuration. An oscillatory voltage will then be applied across the capacitor to drive the gold nanoparticles and exert a force on the enzymes. The setup will detect the ensemble averaged movement of the enzymes at the Angstrom scale in order to measure the conformational dynamics.

The specific goals of this research project include the following: creating a one-of-a-kind experimental setup which will be useful for a plethora of other experiments in the future, deforming enzymes and recording their levels of deformation, changing what enzymes and solvents are used, and comparing data from the experiments. The results of the enzymes’ viscoelastic behavior which will be useful for further research in the fields of Biophysics, Biology, and Chemistry.

M71.00338: Effect of Carbon Nanotubes on The Propagation of Neural Signals*

AHMED ELRASHIDY (Presenter), GARY PENNINGTON, JOHN LEVENTIS, Towson Univ —

Studies have shown that carbon nanotubes scaffolds promote the growth of neurons along the nanotube axis and also enhance neural signaling. In addition carbon nanotubes have been successfully incorporated into cells as transmembrane channels and as bridges connecting with the intracellular and intercellular microtubule scaffolds which function as cellular transportation highways. Based on laboratory experiments in the literature, it is clear that carbon nanotubes will play an ever increasing role in neurological research acting to enhance properties or to serve in a sensing capacity.

To investigate the effects of nanotubes on neuron properties, we report finite element based simulations of voltage pulse propagation along neural membranes in the presence of incorporated carbon nanotubes. Results will be used to help determine the origin of neural enhancement in neuron-nanotube complexes and to look for mechanisms by which a nanotube proximal to a neuron may act as a sensor allowing imaging of neural signals.

* We acknowledge support from the Jess and Mildred Fisher College of Sciences and Mathematics at Towson University.
M71.00339: Dynamical Model of Cytokines in Rheumatoid Arthritis in the Presence of Additive Noise  TIMOTHY DUREN (Presenter), MASoud ASADI-ZEYDABADI, RANDAll TAGG, University of Colorado, Denver, COLIn O’DONNELL, CHRISTOPHER COLLORA, KEVIN DEANE, University of Colorado Anschutz Medical Campus — A dynamical model from Baker et. al* is used to explore the possibility of predicting onset of Rheumatoid Arthritis. The model is based on nonlinear interaction of pro-inflammatory and anti-inflammatory cytokines. In the model, a parameter measures the effect of the pro-inflammatory cytokine concentration on further growth of pro-inflammatory cytokines. As this parameter increases, a healthy state jumps to a disease state through a fold bifurcation. By adding noise to the model, we observe precursor flickering and large-scale fluctuations that might appear clinically as early clues to incipient onset. *M. Baker, S. Denman-Johnson, and M. R. Owen, “Mathematical modelling of cytokine-mediated inflammation in rheumatoid arthritis” Mathematical Medicine and Biology (2013) 30, 311–337


M71.00341: A synthetic transcriptional counter*  TIANCHI CHEN (Presenter), MUHAMMAD ALI AL-RADHAWI, Bioengineering, Northeastern University, CHRISTOPHER VOIGT, Biological Engineering, MIT, EDUARDO SONTAG, Bioengineering, Northeastern University — Elementary sequential logic circuits have been proposed in synthetic biology. The long-term goal is to obtain more complex circuits, capable of finite-automaton computation, in analogy to central processing units in digital computers. We design here a single bit counter, i.e. a parity checker, that can be implemented with current technology by a genetic circuit. When excited by a sequence of N sufficiently separated pulses of an external input (which might be a chemical inducer or a physical signal such as light at a specific frequency), the network will produce an output to indicate whether the number N of pulses seen so far is even or odd. Our circuit is the key component of a distributed-computation m-bit counter, in which a count modulo 2^m of the observed number N of pulses is stored and displayed. The m-bit counter can be in principle assembled from a set of m single-bit counters, together with additional gates that implement "carry" operations. In this design, communication among cells could be biologically implemented by diffusing chemicals (for example, quorum-sensing molecules).

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SRC SB-2837
M71.00342: Dose-rate effects in the radiation induced mutation of Drosophila*  TAKAHIRO WADA (Presenter), TOMONORI OHNISHI, Kansai Univ, YUICHIRO MANABE, MASAKO BANDO, Osaka Univ. — We proposed a mathematical model to study the biological effects of radiation which we call WAM model. (1) An important feature of the model is that it can describe the dose-rate dependence of the effects of radiation. We succeeded in reproducing the existing data of dose/dose-rate dependence of mutation frequencies of 5 species including animals and plants. (2) We hope to develop the model to describe the whole process from mutation to cancer generation.

In 1926, Herman Muller conducted the famous experiments of the radiation-induced mutation in Drosophila, which shows a linear increase with the total dose. Later, Purdom and McSheehy irradiated Drosophila with much lower dose rate to find out if there is a dose-rate dependence in the mutation frequency. (3) Here, we reexamine their data with WAM model and found that the data is reproduced well with our model. We will discuss the possible dose-rate dependence of the radiation-induced mutation frequency in Drosophila.

References

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M71.00343: Understanding Base Pairing Interactions in Aqueous Environment*  RONGPENG LI (Presenter), CHI H MAK, Univ of Southern California — Base pairing plays a pivotal role in DNA functions. But while the complementarity between Watson-Crick matched bases is conventionally believed to arise from the different number of hydrogen bonds in G|C pairs versus A|T, the energetics of these hydrogen bonds are heavily renormalized by the aqueous solvent. We computationally extracted the solvent components of the free energy, entropy and enthalpy for canonical and some wobble and stacked base pairs. For all of them, the solvent's contribution to the base pairing free energy appears to be exclusively destabilizing. While the direct hydrogen bonding interactions in the G|C pair is much stronger than A|T, the thermodynamic resistance produced by the solvent also pushes back more forcefully against G|C pair formation compared to A|T, generating a difference in thermodynamic stability of only ~1 kcal/mol between them. We have profiled the density of water molecules in the solvent adjacent to the bases and observed a decrease in the solvent's entropy as a result of a "freezing" transition where waters are recruited into the gap between the bases to compensate for the unsatisfied hydrogen bonds between them.

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M71.00344: **Stochastic Lattice Model of the RAD51 Nucleoprotein Filament Formation on Single-Stranded DNA**

MARY SUTTON, Univ of Northern Iowa, COLLEEN CALDWELL, MARIA SPIES, Biochemistry, University of Iowa, ALI TABEI (Presenter), Univ of Northern Iowa — Homologous recombination (HR) is one of the most enigmatic processes in DNA metabolism and is a fundamental driver of evolution. Its central step involves the search for homology between two DNA molecules and the subsequent exchange of the DNA strands. We use a Monte Carlo model to study the statistics and dynamics of the recombinase filament nucleation, extension, and disassembly. We use our developed computational toolbox for analyzing single-molecule data to build a predictive model to test different binding hypotheses.

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University of Iowa FUTURE in Biomedicine Program

M71.00345: *In silico* studies of “DNA Flossing” through a Double-Nanopore system

ANIKET BHATTACHARYA (Presenter), SWARNADEEP SETH, Univ of Central Florida — We carry out *in silico* study of “DNA Flossing” (X. Liu et al., bioRxiv: http://dx.doi.org/10.1101/77817) in a model Double Nanopore Device, where the DNA conformations oscillates back and forth from one nanocavity to the other while translocating through a double nanopore when the linear segment between the nanopores gets scanned. We simulate the conditions for efficient multiple scans as well as the reduction of the variance in measurement of genomic length from these scans. In particular, we vary the dimensions of the cavities, the distance between the nanopores, and nature of the feedback forces to optimize the measurement of genomic lengths through flossing mechanism.

M71.00346: Loss of CTCF loops on human interphase chromosome organization

DAVIN JEONG (Presenter), GUANG SHI, DAVE THIRUMALAI, University of Texas at Austin — Chromatin looping, mediated by CTCFs, is a widespread principle in chromatin folding. Despite many studies that elucidate the importance of the insulator protein CTCF and cohesin complex in regulating genome folding, how chromatin loops determine the overall genome organization is unclear. We created a Chromosome Copolymer Model (CCM) to investigate the impact of CTCF loop loss on human interphase chromatin organization. We show that chromatin folding associated with loop domains is extended with a decrease in the number of CTCF loops. Surprisingly, the degree of epigenetic compartmentalization increases. In contrast, local topological associating domain (TAD) is only affected by removal of adjacent CTCF loop. Furthermore, deletion of some CTCF loops causes abnormal contacts between certain insulated loci with adjacent TADs merging, while others do not, indicating that CTCF loop is required to form a subset of TADs. The TADs whose formations are mainly driven by underlying epigenetic states have minimal dependence on CTCF loops. Moreover, our results employing complete CTCF depletion are in good agreement with experiments, supporting that cohesin is necessary for the formation of CTCF loops.
M71.00347: Role of Liquid-Liquid Phase Separation in Organization and Regulation of Chromatin MURALIKRISHNA RAJU (Presenter), ALEKSANDRA ELZBIETA BADACZEWSKA-DAWID, DAVIT POTOYAN, Iowa State University — Genomic DNA is densely compacted in the nucleus of eukaryotic cells into chromatin. However, mechanisms that regulate the assembly and compaction of the genome remain unclear. Here we employ atomistic simulations to study how histone tail-driven interactions drive liquid-liquid phase separation (LLPS) of archetypal DNA-histone mixtures, resulting in formation of mesoscale condensates. The role of histones H1, H2a, H2b, H3 and H4 are individually explored under a range of physiological salt concentrations. Histone H1 is found to play a critical role in chromatin organization by promoting LLPS, denser compaction and slower dynamics within the condensates. Electrostatic interactions are found to be the primary driving force behind condensate formation and consequently histone acetylation is found to inhibit LLPS. We construct phase diagrams based on Droplet density and Shannon entropy calculations, wherein distinct regimes can be identified based on histone concentrations. The spatial organization and dynamics of the droplets are investigated as a function of histone concentrations, DNA chain length and salt concentration.

M71.00348: Nuclear chromatin patterns: modeling dynamics of intra-chromatin interactions and its impact on structure organization RABIA LAGHMACH (Presenter), Iowa State University, MICHELE DI PIERRO, Center for Theoretical Biological Physics, Rice University, DAVIT POTOYAN, Iowa State University — The description of chromatin organization and its dynamics, at a large scale, are functionally important factors in the genome regulation function. Growing evidence suggests that chromatin within the nucleus has a liquid-like behavior mediated by phase separation into micro-droplets with distinct transcriptional states. The formation and spatial arrangement of chromatin droplets within the nucleus depending on their transcriptional states either active (euchromatin) or inactive (constitutive and facultative heterochromatin) genes are important features of the nuclear architecture. Understating mechanisms that control the dynamics and spatiotemporal regulation of droplets formation is a possible way to elucidate the relationship between nuclear architecture and gene regulation. Here, we introduce a mesoscale liquid model of nucleus (MELON) that incorporates dynamic of interactions between A-B-C chromatin compartments of the nucleus, as well as the affinity between constitutive heterochromatin and Lamina at the nuclear envelope and nucleus deformation. Using MELON framework, we show that phase separation together with surface tension effects and nuclear shape deformation is sufficient for recapitulating large-scale morphology and dynamics of chromatin along the life cycle of cells.
M71.00349: United we stand, divided we fall: Response to antibiotics in a bacterial swarm* 
HARSHITHA SHANKAR KOTIAN (Presenter), HITHYSINI K. N., AMITH ZAFAL ABDULLA, VARSHA SINGH, MANOJ M VARMA, Indian Institute of Science — Bacterial swarms consist of millions of bacterial cells collectively colonizing a nutrient rich agar plate. *Pseudomonas aeruginosa* is a bacterial species in which swarming is modulated by the interplay of surfactant driven fluid flow and chemotactic motility of individual cells, leading to the formation of a sparse branched pattern over the agar plate. The branches of the swarm do not intersect due to repulsive forces from the surfactant gradients. However, when an antibiotic drop is added near one of the growing branches, its growth gets arrested and the neighbouring branches intersect to join this branch. This is quite non-intuitive as the bacterial cells move towards the branch exposed to antibiotic as opposed to escaping the area to protect themselves. Moreover, this behaviour requires a complex signalling mechanism as the bacterial cells cannot directly sense the antibiotic as they lack the receptors specific to the antibiotic (gentamicin). We present experimental data and a mathematical model to unravel the mechanism behind this behaviour. Our findings reveal that stress on the bacterial community drives them into collaborating with each other to demonstrate collective resistance and avoidance of antibiotic toxicity.

*This study was funded by DST-ICPS programme.

M71.00350: Delay embedding of low-dimensional attractors of local field potentials from optogenetic data* 
XANDRE CLEMENTSMITH (Presenter), SORinel OPRISAN, College of Charleston, TAMAS TOMPA, ANTONIETA LAVIN, Medical University of South Carolina — We investigated the effect of acute cocaine injection in conjunction with dopamine (DA) receptor antagonists on the medial prefrontal cortex (mPFC). In his study we used D1-like receptors antagonist SCH 23390 or D2-like receptors antagonists sulpiride. The goal of the study was to determine the changes in the gamma oscillations and their relationship to short term neuroadaptation that may mediate addiction. In this study we used 17 mice and recorded optogenetically evoked local field potentials (LFPs) in vivo. The optical stimulus was a brief 10 ms laser light pulse. Data preprocessing involved computing a Euclidian distance-based dendrogram to separate the 100 trials for each animal in disjoint clusters. The classifier is not perfect as it gives a minimum 20% overlap between the control data and DA receptor antagonists trials. We used the delay-embedding method to reconstruct neural activity attractor. The lag time was determined both using the correlation time and the mutual information methods.

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M71.00351: System identification in the brain: inferring ARMA dynamics from sensory data
 TIBERIU TESILEANU (Presenter), CCB, Flatiron Institute, SAMANEH NASIRI, Emory University, ANIRVAN M SENGUPTA, Rutgers University, DMITRI CHKLOVSKII, CCB, Flatiron Institute — Sensory information reaches the brain as a stream with non-trivial correlations across time. In a generative model, these correlations can be seen as the result of a dynamical system acting on a white noise source signal. Learning the parameters describing this system enables a variety of applications, from detecting changes in the input dynamics to inferring dynamical rules in the environment.

Here we present biologically plausible neural networks for performing system identification from time series data. The starting point is the mutual information between the past and the future, which in the case of one-dimensional Gaussian signals is equal to a kind of cepstral norm. By searching for the autoregressive moving-average (ARMA) filter that minimizes this mutual information, we develop algorithms that learn an inverse model to the dynamical system generating the data. Employing update rules based on Givens rotations we ensure that our algorithms work online, an essential ingredient to maintain biological plausibility. We also look for implementations that rely on local learning rules, such that synaptic updates only require information that is available to them from pre- and post- synaptic activity.

M71.00352: Dynamics of multi-domain bio-macromolecules by neutron scattering  LAURA-ROXANA STINGACIU (Presenter), Oak Ridge National Lab, RALF BIEHL, ANDREAS STADLER, JCNS, Juelich Research Center — Conformational ensembles of synthetic polymers and intrinsic disorder in proteins are both aspects of the varying degree of order and disorder that are crucial for the properties of macromolecules. Neutron scattering techniques, in particular small angle scattering and neutron spin echo, have an important contributions to understand conformation and dynamics of macromolecules with regards to polymer physics. The possibility for altering and defining accessible conformational spaces through localized or intermediate and long-range interactions of segments along a polypeptide chain are limited by chain stiffness and local hydrodynamic friction. Our research aims for a deeper understanding of this challenging topic. We will present the dynamics of several bimolecular species based on results of neutron scattering and the comparison with secondary and segmental relaxations, Rouse and reptation dynamics in polymers, with emphasis on the significant difference between dynamics of random coil of synthetic polymers and the dynamics of globular proteins.
M71.00353: Decoupling Effect between Dynamics of Proteins and their Hydration Water at Elevated Temperature  
LIRONG ZHENG (Presenter), ZHUO LIU, LIANG HONG, Shanghai Jiao Tong Univ — Water, as a life solvent, is primary to the energy transfer, biomacromolecules assembly, biological reaction and so on. Particularly, the dynamical transition at ~200 K in proteins, which hydration water is essential for, leads the state of proteins from rigid, nonfunctional state to flexible, functional state. So far, a large number of studies have suggested that the dynamical transition at ~200 K is coupled to the activation of translational motion of the hydration water on the protein's surface, i.e., the dynamics of proteins and that of their hydration water are coupled. However, by performing elastic neutron scattering experiments of atomic dynamics of proteins with different secondary structures under various instrumental resolutions, we surprisingly find that the dynamics of proteins and that of their hydration water molecules show a resolution-independent and a resolution-dependent behavior at elevated temperature, respectively. These results suggest that there actually exists the decoupling effect between dynamics of proteins and that of their hydration water at elevated temperature, and gives a new comprehension in protein dynamical transition.

M71.00354: A new heteropolymer theory to describe conformation of Intrinsically Disordered Proteins  
JONATHAN HUIHUI (Presenter), TAYLOR FIRMAN, KINGSHUK GHOSH, Univ of Denver — Intrinsically Disordered Proteins (IDPs) perform many vital functions and yet have no native structure. This is in contrary to the commonly held notion that protein sequence determines the unique folded structure that in turn dictates the function of the protein. IDPs exhibit an ensemble of conformation, instead of a unique folded structure, making them amenable to tools of polymer statistical physics. Presently, homopolymer theories are commonly used in order to describe the conformation of IDPs. However, IDPs consist of amino acids of different chemical properties, including positive and negative charges. We present a novel heteropolymer theory to describe the sequence specific conformational ensemble of IDPs. Our theory provides rich ensemble average distance maps that are more informative about conformation than coarse-grain measures like radius of gyration or scaling exponents. We will showcase application of this novel analytical theory – benchmarked against all-atom simulations – to multiple naturally occurring IDPs. We highlight how biology can achieve variability with the ability to induce drastic conformational changes by making concise changes in the sequence — termed as hot spots -- such as post-translational modifications (PTMs), often used as a regulator.
M71.00355: Into the Vast Unknown: Structure-Function Relationships in Uncharacterized Bacteriophage Proteins*  KRISTA FREEMAN (Presenter), SAEED BINSABAAN, ANDREW VANDERMARK, GRAHAM HATFULL, Univ of Pittsburgh — With an estimated global population of $10^{31}$ particles, bacteriophages (viruses that infect bacterial hosts) are Earth's most abundant biological entities. Billions of years of evolution have granted phages unparalleled genetic diversity and given rise to a vast collection of genes. We have sequenced and analyzed the genomes of over 3,000 phages and sorted their hundreds of thousands of encoded proteins into phamilies. The functions of over 70% of these protein phamilies are unknown, with a complete dearth of functionally informative sequence-based homology for guidance. We hypothesize that these hypothetical phage proteins represent an unexplored reservoir of genetic, functional, and possibly structural novelty. To address this, we have developed a research pipeline to structurally and functionally characterize subsets of phage-encoded proteins. We have successfully advanced a number of proteins through various stages of this pipeline, which combines bioinformatics, molecular biology, biochemistry and biophysical approaches. This presentation will address our progress on elucidating structure-function relationships in these bacteriophage proteins.

*This work was supported by National Institutes of Health grant GM131729 and by Howard Hughes Medical Institute grant GT12053.

M71.00356: The Impact of Deep Eutectic Solvent on the Structural Stability of Myoglobin*  LINH PHAM (Presenter), JOSE L BANUELOS, SUPRIYO RAY, University of Texas, El Paso, JENNIFER KIST, GARY BAKER, Department of Chemistry, University of Missouri- Columbia — The stability of Myoglobin (Mb) in hydrated Deep Eutectic Solvent (DES) is investigated as a function of temperature and DES concentration. Determining the effect of DES on protein structure can lead to understanding the properties of DES, and allow their use to expand to cost-effective, and simple synthesis applications. Mb in 2 DESs: 35% wt glyceline-water and 5% wt reline-water and the resulting structure were compared to Mb in water. Small Angle X-ray Scattering results show that Mb's tertiary structure remains relatively unchanged in both DESs until the temperature reaches 80°C (for glyceline) and 70°C (for reline) at which globular structure of Mb starts to gradually unfold. However, in water, Mb's tertiary structure unfolds slowly and linearly with temperature until reaching a major transition at 80°C. In addition, circular dichroism spectroscopy measurements show that Mb loses substantially more secondary structures with increased temperature in DES mixtures than in water solvent, yet DES allows better recovery of Mb secondary structure.

*This work was supported by Office of the Provost, Campus Office of Undergraduates Research Initiatives (COURI) under the Summer Undergraduate Research Program Assistantship (SURPASS) of the University of Texas at El Paso.
M71.00357: Adaptive Sampling of Markov-state models with MD Simulations to assess the rates of biologically relevant processes*  JOHN OSSYRA (Presenter), University of Tennessee, Knoxville, ADA SEDOVA, JEREMY SMITH, Oak Ridge National Laboratory — It is a challenge for classical molecular dynamics to directly simulate the time and length scales of biologically relevant processes. Incomplete sampling makes the calculation of macroscopic observables such as rates for major state transitions difficult to estimate correctly. A number of techniques bias the energy landscape to accelerate processes that are difficult to reach with direct simulation. However the altered landscape introduces artifacts that obscure rate estimates. Here we show how adaptive-sampling workflows that iteratively redirect swarms of trajectories can enhance the sampling of the slowest kinetic processes. Markov-state models are then adaptively refined with continual updates from these parallel swarms resulting in unbiased, well-sampled estimates of kinetic rates. We demonstrate how this method can be applied to provide long-timescale kinetics for atomistic simulations of protein-protein interactions.

*This work was supported from a Laboratory Directed Research and Development award from the US Department of Energy.

M71.00358: Data-Driven Modeling of Discrete Synchronization in Firefly Swarms  RAPHAEL SARFATI, JULIE HAYES, ORIT PELEG (Presenter), University of Colorado Boulder — Fireflies are a landmark example of synchronization in nature. During mating season, males of synchronous firefly species flash in unison within swarms containing tens of thousands of individuals. This magnificent display inspired numerous mathematical models that aim to explain how global synchronous patterns emerge from local interaction rules. However, experimental data to validate these models has been rarely reported. To address this gap, we obtained quantitative measurements of the spatiotemporal flashing pattern of synchronous firefly swarms. Using the North American synchronous firefly species *Photinus carolinus* as a model system, we recorded the flashing patterns of the fireflies in their natural habitat as well as within light controlled environments, and for the first time, we were able to perform a 3D reconstruction of the synchronous flashing positions of thousands of individuals. This talk will focus on analysis of the spatiotemporal patterns observed in our experiments and connecting it to mathematical models that account for the species specific discontinuous flash pattern, short range spatial correlations, and spatial mixing due to movement of individuals within the swarm.
M71.00359: A Quest for a Science of Social Dynamics* RAM POUDEL (Presenter), Tribhuvan University — Humans are social beings. Social interactions inform the state of an individual in society. We proposed a new social field theory in order to define the state in terms of Hamiltonian of an individual. In a multi-dimensional social field, social interactions are conceived in terms of the energetic exchanges of various fluxes including information. Such exchanges govern the change of states of an individual. The transport equations of change for an individual and ensemble of individuals include source terms and power dynamics. For an ensemble of individuals, the equation takes a form of an implicit Fokker-Planck equation. A target of this paper is to formulate the “equations of motion for social systems” Wolfgang Weidlich has long sought for. Lotka-Volterra equations can be derived from the proposed equations of motion for the social field.

*We did not seek any funding for this research. RP acknowledges a sabbatical granted by the Institute of Engineering, Tribhuvan University.

M71.00360: Physics of the Brain. Treatment of Neurological Diseases via the Brain Waves, Using the Multi-photon Pulsed-operated Fiber Lasers in the Ultraviolet Range of Frequencies.* V. ALEXANDER STEFAN (Presenter), Institute for Advanced Physics Studies, Stefan University — The novel study of the brain waves (BW)[1] in connection to neurological diseases is proposed. It is based on the pulsed-operated (amplitude modulation) multi-photon (frequency modulation) fiber-laser interaction with the brain neuro-topion (the neurological disease area).[2] The repetition frequency, Ω, (5-100 pulses per second) matches the frequency of a particular brain wave, Ω_{BW}. The tunable fiber laser frequencies, Δω (multi photon operation), are in the ultraviolet frequency range, thus enabling monitoring of the electrical charge dynamics in the neuro-topion of a particular disease within the 10s of milliseconds.


*Supported by, The American Society for Laser Neuroscience (Stefan University).
M71.00361: Dynamics of timescales on complex lattices  GECIA BRAVO-HERMSDORFF, AHMED EL HADY (Presenter), Princeton University — A popular idea in biology is that the intrinsic timescale of an individual “unit” plays a crucial role in the information processed by the system as whole. For example, it has been proposed that the intrinsic timescales of single neurons in different brain areas are related to functional differences between these areas. However, disentangling between intrinsic and collective timescales remains a highly nontrivial task, and could benefit by drawing intuition from simple physical toy models. To this end, we consider the prototypical model of collective temporal behavior: kinetic Ising models, where identical units are connected with a given topology, and neighboring units stochastically interact with one another. We analyze how the behavior of such models is altered when considering many aspects relevant to their computational implementation, namely, finite temporal resolution, topological connectivity, and finite system size. Not coincidentally, these considerations have biological analogues. For example, the clock speed of processor is functionally similar to an “inverse refractory period” of a neuron. While locality of interactions can be exploited for parallel simulation of physical systems, the diversity of topologies in biological systems is key to their expressive power.

M71.00362: Development of control in brain networks over temporal and spatial scales using graph models LINDSAY M. SMITH (Presenter), HARANG JU, DANIELLE BASSETT, University of Pennsylvania — Regions of the human brain vary in their capacity to control whole brain activity, in large part due to their location in the underlying structural network of interconnections crisscrossing the cortex. Recent work suggests that this capacity for control differs across spatial and temporal scales of the brain’s dynamics and can be formally probed using the Laplacian eigenspectrum of the brain’s structural network. Yet how such spatiotemporal control might differ from one human to another, potentially supporting and explaining differences in cognitive function, remains unclear. Here, we address this question by measuring several summary statistics of spatiotemporal control from human brain network architecture, as reflected in diffusion tensor imaging data acquired from 882 youth between the ages of 8 years and 22 years. We found that distinct features of network topology are correlated with a region’s capacity to enact distinct control strategies, and we investigate these relationships as a function of discrete timescales, from markedly slow modes of dynamics to relatively swift modes of dynamics. Our results provide insight into how local variation in connectivity gives rise to distinct processes of global control as a function of timescales over modes of activity.
M71.00363: Kinesin Model for Brownian Dynamics Simulations of Stepping Efficiency

MATT MURROW (Presenter), Physics & Astronomy, Vanderbilt University, JUTTA LUETTMER-STRATHMANN, Physics and Chemistry, University of Akron — The motor protein kinesin plays an integral role in cell function, transporting, for example, cargo from the center to the periphery of a cell. Kinesin molecules have been shown experimentally to walk along microtubules in a hand-over-hand stepping motion, carrying their cargo eight nanometers per step. However, details of the stepping process are still under investigation. Kinesins are difficult to study with atomistic simulations due to the size of the proteins and the long time-scales involved. In this work we develop a 3D model of kinesin stepping on a rigid microtubule substrate that can be simulated efficiently with Brownian dynamics simulations. The interactions governing the motor protein conformations and the interactions between kinesin sites and the microtubule sites are designed to reproduce important aspects of the biological system. We perform simulations spanning many kinesin steps to investigate the stepping efficiency of the motor protein for different neck linkers. We find that neck linkers close to the wild-type length yield a stepping efficiency of about 90%, in agreement with experimental data. In addition, we find that increasing the neck-linker length leads to a decrease in efficiency, as has also been observed in experiments.

M71.00364: Correlating synaptic vesicle motion to cytoskeletal structure of the presynapse and axon.

BRIA STORR (Presenter), Univ of Alabama - Birmingham, MICHAEL W GRAMLICH, Physics Department, Auburn University — Two neurons communicate via release of neurotransmitter from a presynapse of one neuron to a post-synapse of another. This neurotransmitter is carried from the inside of the presynapse to the membrane of the presynapse using a presynaptic vesicle. The transport mechanics of presynaptic vesicles thus influences presynaptic communication. Presynaptic vesicles undergo many types of motion, but it is still unclear how their motion corresponds to the overall structure of the synapse. High resolution fluorescence microscopy has recently been shown to be an effective tool to understand vesicle motion. We take advantage of recent three-dimensional microscopy experiments and develop a three-dimensional computational analysis method of single vesicle motion in live cells. We use the computational method to classify types of motion, then distinguish different types of motion relative to the known structure of the synapse observed. We show that this approach can distinguish types of vesicles motion relative to the synapse. This method also allows us to take a closer look at the vesicles when the motion is directed.
M71.00365: A micromechanical model for interactions of curvature sensing septin filaments with membrane  WENZHENG SHI, KEVIN S CANNON, AMY S GLADFELTER, EHSSAN NAZOCKDAST (Presenter), Univ of NC - Chapel Hill — Cells reconfigure their shape in micron-scale in response to internal and external forces. Septins are filament-forming GTP-binding proteins that can sense curvature in micron-scale by preferentially accumulating in membrane regions with high curvature. Yet, the underlying mechanisms by which a nanoscopic septin hetero-octamer senses curvature in micron-scale remains unclear. We combine biophysical modeling and experiments and propose a micromechanical model for interactions of septin filaments with membranes. We propose that the rate of attachment of septins filaments to membranes is controlled by a combination of membrane's thermal and stored elastic energy, while the rate of detachment is controlled by the bending energy of the curved membrane-bound septin filaments. Moreover, our model predicts a qualitative change in septins curvature sensing as they assemble into micron-scale filaments in larger concentrations. We verify these predictions experimentally, by measuring the attachment/detachment kinetics under different bulk concentrations of septins on beads of different radii, covered with lipid bilayer.

M71.00366: One-dimensional contact process with both temporal and spatial disorder  XUECHENG YE (Presenter), THOMAS VOJTA, Missouri Univ of Sci & Tech — We investigate the non-equilibrium phase transition in the contact process under the influence of both temporal and spatial disorder using large-scale Monte-Carlo simulations. Spatial disorder alone is known to lead to an exotic infinite-randomness critical point [1]. More recently, it was shown that temporal disorders also produces unconventional critical behavior dubbed infinite-noise critical behavior [2]. We perform a series of simulations adding weak temporal disorder to a spatially disordered space and vice versa. We find that the critical behavior remains unchanged by these perturbation, in agreement with the generalized Harris criteria [3]. We then focus on the case where both temporal and spatial disorder are strong.


M71.00367: Modeling Swimming Microorganisms using Macroscopic Experiments*  MACKENZIE CONKLING, JACOB PFALLER, BRUCE RODENBORN (Presenter), Centre College — The swimming of microorganisms is typically analyzed using biological experiments or numerical simulations because the Reynolds number is much less than one. Our research group uses model macroscopic experiments with typical length scales of ~ 10 cm, but match the low Reynolds number of microorganisms by using a highly viscous silicone oil. The fluid has a viscosity that is $10^5$ larger than water but with approximately the same density. We can therefore build laboratory scale robotic swimmers and model microorganisms that are typically ~10 μm. We can also explore fundamental theories such as our project to build a laboratory scale three-link swimmer to test theoretical predictions (Purcell 1977, Hatton et al. 2013).

*Centre College Faculty Development Fund
M71.00368: Single molecule force spectroscopy to determine specific receptor densities on live cancer cells under varying conditions*  RAMESH CHANDRA TRIPATHI (Presenter), PETER HOFFMANN, Wayne State Univ — We have used atomic force microscopy to study the single-molecule interaction between the ligand and receptors in live cancer cells under different conditions. We particularly focused on discoidin domain receptors (DDR), an important player in cancer metastasis. DDRs are receptors that dimerize in response to collagen and initiate a signaling chain within the cell. To mimic the cancer environment, we constructed gel substrates of varying stiffness and collagen concentration. The goal of the research is to determine receptor levels, dynamics and interactions as a function of cell type and environment. Using an improved AFM analysis method, we were able to determine not only binding probability and kinetic parameters, but also ligand densities. We will present preliminary results from this research.

*We acknowledge the Richard Barber foundation and Wayne State University for funding for this research.

M71.00369: CHEMICAL PHYSICS —

M71.00370: Photoprotective properties of a eumelanin building block: Ultrafast excited state relaxation dynamics in 5,6-dihydroxyindole  SARITA SHRESTHA (Presenter), University of Georgia — Skin plays the significant role in protection of body from ultraviolet radiation. The protection is primarily done by a type of pigment called eumelanin. Eumelanin chromophores absorb the energy of the radiation, and through internal conversion, dissipate them quickly in the form of heat. The process takes place in femtosecond time scales. A bottom-up approach is used to study the photophysics of eumelanin which focuses on individual building blocks to gather the overall information of the complex system. Time-Resolved Photoelectron Spectroscopy (TRPES) is implemented to understand the underlying excited state relaxation mechanism in 5,6-dihydroxyindole. This method allows to see the associated dynamics in terms of photoelectron kinetic energy.

M71.00371: Fabrication of CFO@C Core/Shell Nanoparticles by Pulsed Laser Ablation  JOY ROY (Presenter), KARTIK GHOSH, Missouri State Univ — A considerable research work is going on worldwide among the therapeutic scientific communities to use magnetic nanoparticles (NPs) for drug delivery system. Challenges to use those NPs for such in vivo applications successfully, are-biocompatibility and functionality of those NPs and control over the complex drug release system. In this project, we synthesized carbon coated cobalt ferrite (CFO) core shell nanoparticles (CSNPs) by ablating a solution of toluene and cobalt ferrite NPs with varying number of pulsed laser shots. The structure of the CSNPs was further investigated through X-ray diffraction, UV-VIS, Raman spectra and also with the high-resolution transmission electron microscopy (TEM). The XRD analysis shows that the inner structure of CFO is intact after the laser shots. Raman spectra confirms that with increasing laser shots the G band peak for Carbon becomes more prominent which infers to the crystallinity of carbon. Preliminary TEM line scan data concludes that laser ablation technique is quite efficient to manufacture carbon coated magnetic metal oxide CSNPs.

M71.00372: WITHDRAWN ABSTRACT —
M71.00373:Kinetic compensation effect due to the variation in the concentration of an additive

NAYELI ZUNIGA-HANSEN (Presenter), Louisiana State University, Baton Rouge, LEO SILBERT, Central New Mexico Community College, MARIA CALBI, University of Denver — As part of a systematic study on the kinetic compensation effect, we use kinetic Monte Carlo simulations to study the effects of the change in the concentration of a chemical species in the Arrhenius parameters - effective activation energy $E_a$, and preexponential factor $\nu$ - during the thermal desorption of a binary mixture of interacting and non-interacting adsorbates from two dimensional ordered and disordered surfaces. A chemical additive, such as a catalyst, can have an effect in the overall rate at which a process occurs. In this study we quantify the transient variations in the Arrhenius parameters when the concentration of one of the chemical species in the mixture, which is treated as an additive, is varied. The purpose is to observe if a compensation effect and/or isokinetic relation occur when this 'experimental parameter' is altered. We expect our results to help advance the understanding of the microscopic origins of compensation effects in our system of study but also in other fields where these effects have been reported.

M71.00374: Probing structure-property relationships of BODIPY dimers on the efficiency for symmetry breaking charge transfer

LAURA ESTERGREEN (Presenter), Univ of Southern California, SEAN ROBERTS, University of Texas at Austin, MIKE KELLOGG, AUSTIN R MENCKE, Univ of Southern California, NADIA KOROVINA, National Renewable Energy Laboratory, MARK E THOMPSON, STEPHEN EDMUND BRADFORTH, Univ of Southern California — Symmetry breaking charge transfer (SBCT) is the process in which a pair of identical chromophores are coupled such that post excitation an exciton (electron-hole pair) can dissociate between the two chromophores. The product is an uncoupled, spatially separated electron and hole pair, reducing the probability of recombination. The resulting uncoupled charges from SBCT are beneficial for photoelectrochemical and photovoltaic applications. BODIPY dimers have been shown to undergo SBCT in femto-to-pico-second timescales\(^1\). The dipyrrinato dimer analogues have also been studied and shown to undergo SBCT where they are ligated via the nitrogen termini through a zinc (II) center\(^2\). Herein the BODIPY and dipyrrinato dimers are analyzed to understand the effect of different bridging methods and increased substituents on the efficiency of SBCT. Efficiency in the context of this analysis is the rate of formation and longevity of the SBCT state. We find that direct linkage where torsion is not sterically hindered results in the fastest SBCT formation and that orthogonally fixed geometries result in the slowest decay times of the SBCT state.


*Department of Energy
M71.00375: Stimulated Raman spectroscopy for characterizing two-dimensional crystals
HWANSOO JEON (Presenter), SUNMIN RYU, Pohang Univ of Sci & Tech — Two-dimensional dielectric materials such as hexagonal BN and mica give very weak signals in conventional spontaneous Raman scattering using visible excitation lasers. In this work, we report a micro-spectroscopy setup for stimulated Raman scattering (SRS), which gives a substantial increase in overall sensitivity. Pump and Stokes beams with temporal width of a few ps were prepared by spectrally slicing 200 fs pulses from an optical parametric oscillator. The pulse slicer acting as a narrow band-pass filter consisted of a grating (1200 grooves/mm), a cylindrical lens, a mirror, and a mechanical slit that were arranged in the 4f-configuration. Whereas the Stokes pulses were fixed at 1040 nm with a bandwidth of 0.7 nm, the pump pulses were varied from 734 nm to 998 nm for the Raman shift in the range of 400 ~ 4000 cm⁻¹. The pump beam intensity-modulated by interaction with the Stokes beam in thin hexagonal BN crystals was detected with a photodiode connected to a lock-in amplifier. The sensitivity of the SRS setup and its spatial resolution in raster-scan imaging will be presented.

M71.00376: WITHDRAWN ABSTRACT

M71.00377: Visualization of orbital free models of Kinetic Energy density in solids
BRIELLE TILSON (Presenter), ANTONIO CANCIO, Ball State University — The metaGGA functional for describing the exchange-correlation (XC) energy in density functional theory (DFT) is conventionally constructed as a functional dependent on the density, density gradient, and kinetic energy density (KED). The addition of the KED makes metaGGA's a more accurate functional than ones that use the density and its gradient alone but also more computationally expensive for some applications such as ab initio molecular dynamics simulations. The calculation of the XC energy in meta-GGAs can be made less expensive by replacing the explicit orbital dependence in the KED with expressions involving only the particle density and its gradient and Laplacian. We test the validity of recent deorbitalization strategies in the literature by visualizing their predictions for the KED and related quantities, and comparing these to exact calculations. For an effective test, we perform these calculations on ionic, semiconductor, simple metal, and transition metal solids to see how well the KED for these different binding topologies can be represented by a single metaGGA model in terms of the scaled gradient and Laplacian of the density. The calculations of exact KED and electron density are done with the ABINIT DFT plane-wave pseudopotential code.
M71.00378: Bayesian Calibration assisted by Markov Chain Monte Carlo in DFT+U for Iron Compounds

ALDO H ROMERO, DAVID S. MEBANE, PEDRAM TAVADZE, REESE BOUCHER

(Presenter), West Virginia Univ — Density Functional Theory (DFT) revolutionized condensed matter physics by mapping the electron problem solved by the Schrodinger's Equation to a series of mean field electron independent equations. In DFT, the most crucial approximation is from the exchange correlation functional. Although many have attempted the development of accurate functionals, they all fail to reproduce the behavior of strongly correlated materials when kinetic energy is as large as the Coulomb interaction. To solve this problem, local exchange correlation functionals are corrected by a Hubbard term. This is DFT+U which depends on two extra parameters, U (on-site coulomb interaction) and J (on-site exchange interaction). These parameters are usually fitted from experimental values or obtained by using density functional perturbation theory. Either way the quality of the parameter values can only be assessed by comparing to experimental data. In this work, we use uncertainty quantification methods to study the dependence of different experimental observables where we evaluate the relevance of errors by utilizing Bayesian Calibration facilitated by Markov Chain Monte Carlo simulation with a number of strongly correlated materials.

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M71.00379: Accurate effective potential for density amplitude and the corresponding Kohn-Sham exchange-correlation potential calculated from approximate wavefunctions

ASHISH KUMAR (Presenter), Physics, Indian Insitute of Technology Kanpur, U.P., Indian, 208016, RABEET SINGH, Physical sciences, National Institute of Science Education and. Research, Jatni, Odisha-752050., MANOJ K HARBOLA, Physics, Indian Insitute of Technology Kanpur, U.P., Indian, 208016 — It is well known that direct inversion of an accurate but approximate density leads to KS exchange-correlation potential which has spuriously large deviations from the exact one. On the other hand, a different approach which employs wavefunction directly to obtain KS exchange-correlation potential is found to lead to potentials close to the exact one. This approach utilises the Levy-Perdew-Sahni expression for the effective potential used in the equation for the square root of the density.

We present why the Kohn-Sham exchange-correlation potential obtained by using an approximate wavefunction in the Levy-Perdew-Sahni expression for effective potential is accurate while the direct inversion of density associated with the same wavefunction may lead to pathological features in it. By analysing the Levy-Perdew-Sahni equation, we show that quantities like effective and exchange-correlation potentials, calculated from approximate wavefunctions are free from spurious features and close to the corresponding exact ones. The study also suggests possibility of a new approach for the calculation of accurate densities from approximate wavefunctions. These densities are closer to the exact ones than those obtained from the wavefunction directly.
M71.00380: Mechanical and electronic properties of mechanically-bent monolayer transition metal dichalcogenides (MX$_2$) in the ground state using SCAN density functional*  

NIRAJ NEPAL (Presenter), Temple Univ, LI-PING YU, University of Maine, QIMIN YAN, ADRIENN RUZSINSZKY, Temple Univ — As an alternative to graphene, transition metal dichalcogenides (TMD) have gained a lot of interest as promising candidates for future flexible nano-electronics due to the mechanical and electronic properties related to their high flexibility [1]. Though the TMD thin layers have a promising future, traditional methods of tuning the band gap such as doping with impurities or contact engineering suffer strong Fermi-level pinning or even damage the materials. However, due to the high bending and in-plane stiffness, thin monolayer MoS$_2$ can be bend mechanically to tune the bandgap as well as reducing Fermi level pinning to some extent [2]. In this work [3], we extend the study to exploring the other TMD monolayers corresponding to transition metals from groups IV to X in the periodic table in the ground state, using the recently developed meta-GGA SCAN.


*Center for Complex Materials from First Principles (CCM), an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under Award No. DE-SC0012575.

M71.00381: A simple self-interaction correction to the RPA+ correlation energy*  

SHIQI RUAN (Presenter), Temple Univ, TIM GOULD, Griffith University, ADRIENN RUZSINSZKY, Temple Univ — The exchange energy of the Random Phase Approximation is exact for a many-body ground state, but the correlation energy is often overestimated. The error comes from the poor description of the short-range correlation. The RPA+ approximation [1] largely reduces this error for atoms, for the jellium surface and for the uniform electron gas by adding a local or semi-local correction. While the RPA+ is accurate for the total energies of atoms, it fails for single-electron systems like stretched H$^{2+}$, and systems where spin-polarization plays a significant role such as ionization energies, electron affinities, and atomization energies. In this work, we have introduced a simple correction to the RPA+ correlation energy to make the new gRPA+ [2] approximation exact for single-electron systems. We are assessing this computationally feasible approximation beyond RPA for various molecular test sets and we analyze the impact of self-interaction correction.


*Work was supported by National Science Foundation under Grant No. DMR-1553022.
**M71.00382: Quasiparticle energies of the uniform electron gas**

PRADEEP BHETWAL (Presenter), ANDREW PONENTO, ALEXANDER TRACKMAN, JOHN P. PERDEW, Temple Univ —

The uniform electron gas (UEG) model is the simplest model of a metal, a large volume of electrons subject to a uniform background of positive charge. Existing parametrizations of the UEG correlation energy allow us to perform calculations in Kohn-Sham density functional theory (KS-DFT). While the Kohn-Sham and generalized Kohn-Sham orbital energy eigenvalues are not single-particle excitation energies [1,2], how well do they predict the occupied bandwidth of the uniform electron gas or of alkali metals like Na? In this work, we aim to answer this question using the local spin density approximation (LSDA), the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE GGA), and the PBE0 hybrid functional (with 25% of Hartree-Fock exchange). We benchmark our DFT values against the results of higher-level theories and experiment.


*Supported by NSF DMR-1607868

**M71.00383: Pressure-induced New Oxidation States**

GUOCHUN YANG (Presenter), Department of Physics, Northeast Normal University —

The formalism of the oxidation state of atoms in compounds is a key concept in chemistry. Finding novel compounds containing elements with unusually high oxidation states allows a deeper understanding of chemical behavior of elements. On the other hand, high oxidation state compounds usually bring new types of bonds with interesting physical and chemical properties. Thus, the preparation of compounds with unusual oxidation states becomes an attractive topic in chemistry and condensed-matter physics. Gold (Au) is a well-known fascinating element, but still hides interesting surprises to be discovered, especially for oxidation state. Here, we propose that high pressure becomes a controllable method for preparing high negative oxidation state of Au through its reaction with lithium. Au acts as a 6p-element in dense lithium aurides. Moreover, we identify two hitherto unknown stoichiometric compounds, AuF4 and AuF6, exhibiting typical molecular crystal character, in which Au demonstrates +4 and +6 oxidation states. On other hand, we also achieve several compounds with unusual stoichiometry such as IrF₈, IF₈, and BaF₅.

*I acknowledge the funding supports from the Natural Science Foundation of China under No. 21573037 and 21873017.*
ABHISHEK AGGARWAL (Presenter), Department of Physics, Indian Institute of Science, SAIENTAN BAG, Institute of Nanotechnology, Karlsruhe Institute of Technology, RAVINDRA VENKATRAMANI, Department of Chemical Sciences, Tata Institute of Fundamental Research, MANISH JAIN, PRABAL K MAITI, Department of Physics, Indian Institute of Science — Double-stranded DNA (dsDNA) and dsRNA hold great promises in molecular electronics. We characterize the charge transport properties of dsRNA for different sequences and compare them with similar sequences of dsDNA in two extreme charge transport regimes - incoherent charge hopping regime and coherent electron transport regime. We find that the relative conductance of A-form dsRNA and B-form dsDNA depends on the mechanism of charge transport. This is attributed to various structural differences in dsDNA and dsRNA. We also study the effect of stretching and propose a method to detect conformational changes using electrical measurements. Despite the twist-stretch coupling of dsRNA and dsDNA being different under external force, dsRNA shows similar structural polymorphism to dsDNA under different pulling protocols. Our atomistic MD simulations show that overstretching dsRNA along the 3’ ends (OS3) leads to the emergence of S-RNA whereas overstretching along the 5’ ends (OS5) leads to melting of dsRNA. Using the dsRNA morphology from pulling MD simulations, we use a multiscale method involving ab initio DFT calculations and Kinetic Monte Carlo (KMC) simulations to estimate the conductance of dsRNA and find that the conformational changes drastically affect its conductance.

M71.00385: Tuning the adsorption properties of transition metal dichalcogenides (TMD) monolayer by bending* SANTOSH NEUPANE (Presenter), NIRAJI NEPAL, ADRIENN RUZSINSZKY, Temple Univ — Due to their exceptional catalytic performance, there has been a growing interest in understanding the adsorption properties of transition metal dichalcogenide (TMD) monolayers. Previous studies focused on tuning the adsorption energies and distances in these 2D materials using mechanical strain as well as doping with impurities. Besides that, 2D materials are highly flexible. Moreover, some recent works [1,2] have shown the importance of mechanical bending for tuning various mechanical and electronic properties of TMD monolayers. Using first-principles calculations, we report the effect of mechanical bending on the adsorption properties of the monolayers using a single hydrogen atom as the adsorbate.


Work is supported as part of the Center for Complex Materials from First Principles (CCM), an Energy Frontier Research Center supported by the U.S. Department of Energy (DOE), Basic Energy Sciences (BES), under Award No. DE-SC0012575.

M71.00386: WITHDRAWN ABSTRACT —
M71.00387: WITHDRAWN ABSTRACT —
M71.00388: Modelling the electronic kinetic energy density and Pauli potential by orbital free density functional theory.  BISHAL THAPA (Presenter), ANTONIO CANCIO, Ball State University —

In Kohn Sham density functional theory, the kinetic energy (KE) functional is described by fictitious Kohn-Sham (KS) orbitals. This causes a computational bottleneck for large systems that require many KS orbitals. Much recent research is going into Orbital-Free Density Functional Theory (OFDFT), which models the Kinetic Energy as a functional of density and other ingredients that are derived from density directly, avoiding the need for orbitals. There are reasonable OFDFT models for Kinetic Energy at the meta-GGA level, such the Perdew-Constantin model [1], that properly treat the nonnegativity constraint for the Pauli contribution to the KED, which describes the correction to the von-Weizsäcker KED, which describes the KE of a single electron pair. However, an issue arises of Pauli potentials that are not physically reasonable and difficult to find convergent solutions for. Our goal is to construct meta-GGA level models with potentials which vary smoothly. We test them against calculations of the exact Kohn-Sham KE density and potential for atoms, with atomic densities constructed from the fhi98pp code. As another design goal we will try to incorporate the calculation of linear response.


M71.00389: Stable Structures and NMR Analysis of (Na)$n$ with pore size in hard carbon by DFT calculations  AYANE SUZAKI (Presenter), AZUSA MURAOKA, Japan Women's Univ-Facul Sci, KOICHI YAMASHITA, Kyoto University, Elements Strategy Initiative for Catalysts and Batteries — The lithium ion batteries (LIB) which are a typical secondary batteries, is widely used as an energy storage system by having high voltage, good charge and discharge cycles. However, due to problems with the resources and costs of lithium in LIB, there is a growing interest in resource-rich sodium-ion batteries (NIB) with equivalent electrode potential. In recent years, a NIB using a Na metal oxide as the positive electrode and hard carbon (HC) as the negative electrode has attracted attention in particular. To develop a NIB with high capacity, high efficiency, long life, and acceptable safety, it is essential to elucidate the state of the sodium ion and the mechanism of charge and discharge on the electrode. The states of sodium electrochemically inserted in HC samples have been experimentally reported using solid 23Na NMR. In this study, in order to study the correlation of NMR shift of Na clusters (n = 1-8) with pore size in HC and structure, DFT calculations are performed at B3LYP/6-31G(d) level using the Gaussian 16. From NMR analysis it can be seen that the value of chemical shielding shifts significantly depending on the strength of bonding between Na atoms and the size of clusters.
M71.00390: Investigation the nature of CO2 binding to borophene $\chi_3$  FARIDEH ZERGANI (Presenter), Kashan University — Global warming following the release of greenhouse gases, especially CO2, is one of the important areas of research to adsorption of CO2 to remove it from the environment. But the CO2 binding to the surfaces is weak, and scientists want to correct this defect. Here we used borophene $\chi_3$ as a novel 2D material with the hole density ($\eta=1/4$) and investigated the nature of CO2 binding to its surface. DFT calculations and plane-wave basis set with the ultrasoft pseudopotentials were used in the quantum espresso. The GGA approximation with PBE functional was applied for the electron exchange-correlation energy. The VDW interactions were taken into account using the DFT-D2 method. The binding site for CO2 was determined and the adsorption energy and electronic properties of the $\chi_3$-CO2 were analyzed. The calculated binding energy (~0.2eV) and distance of CO2 to the surface (~3.5Å) indicated weak adsorption. The charge density differences calculation shows the charge depletion between the boron sheet and CO2. The Bader charges analysis shows that the CO2 tends to capture electrons from boron atoms during the adsorption. Therefore, because of the electron deficiency of the surface, the CO2 physisorbed. Therefore, to achieve stronger adsorption, the surface modifications were needed.

M71.00391: Theoretical study of charge and discharge process and NMR in Na ion battery anode material Sn  KEI KUDO, AZUSA MURAOKA (Presenter), Japan Women’s Univ-Facul Sci, MASANORI KANEKO, KOICHI YAMASHITA, Kyoto University, Elements Strategy Initiative for Catalysts and Batteries — Sn can be used as an anode material for secondary battery Na ion batteries because it can work with Na with a composition ratio of up to $\text{Na}_{15}\text{Sn}_4$ by alloying with Na. For practical application, it was reported from both experiments and calculations that there were multiple plateaus in the charging curve of Na-Sn system based on the structural change in the sodiation/desodiation process of Na-Sn system. In this study, we investigated the detailed mechanism of charge and discharge processes in Sn anodes by theoretically clarifying the structural changes, charge and discharge curves, and $^{23}\text{Na}$ NMR chemical shift properties of the anode material Sn in Na ion batteries. We used VASP-5.3.2 to optimize the structure of Na-Sn systems with different composition ratios during the charge/discharge process, and calculated their formation energy. The boundary composition ratio was clarified from the charging curve obtained by estimating the change in potential with respect to the Na/Sn composition ratio. We calculated chemical shift tensors for Na-Sn system, Na and NaCl by GIPAW method. As a result of theoretical calculation of the $^{23}\text{Na}$ chemical shift, it was possible to obtain a number of shielding effect values corresponding to the number of independent Na sites in each Na-Sn composition.
M71.00392: Alternative diffusion Monte Carlo methods for fermions*  
OTO KOHULAK, Department of Physics, University of Ostrava, MATUS DUBECKY (Presenter), Advanced Technologies Research Institute, Slovak University of Technology in Bratislava — Current continuum diffusion Monte Carlo methods for fermions are limited by the sign-problem, or, fixed-node approximation, computationally inefficient in cases that require far more than single determinant to reliably describe leading correlations. We devise and critically examine some alternative approaches that enable maintaining Fermi statistics within continuum DMC simulations.

*We acknowledge financial support by the Czech Science Foundation (18-24321Y), and Slovak Research and Development Agency (APVV-18-0161).

M71.00393: Self-Interaction correction using Fermi-Lowdin orbitals: Methodology and Parallelization*  
LUIS BASURTO (Presenter), YOH YAMAMOTO, CARLOS DIAZ, TUNNA BARUAH, RAJENDRA ZOPE, Physics, University of Texas at El Paso — Density functional theory is a popular electronic structure method that can handle comparatively much larger systems than quantum chemical methods. However, density functional approximations suffer from self-interaction errors which limits its reliability for certain properties. The Perdew-Zunger (PZ) self-interaction correction (SIC) method removes self-interaction on an orbital by orbital basis and is computationally expensive. Recent implementation of Fermi-Lowdin orbital based SIC (FLOSIC) is a promising method that removes many computational complexities of PZ-SIC. We present some details of the FLOSIC methodology and present parallelization strategies using MPI+MPI and recent shared memory features of MPI-3 to make efficient use of large supercomputers. Using this implementation, we achieved parallel efficiency above 80% for 3360 processors. Applications of the FLOSIC method using the FLOSIC code on water clusters and carbon fullerenes will be presented.

*US DOE under grants DE-SC0018331 and DE-SC0006818
M71.00394: Synthesis of carbon nanodots from caramelized glucose solutions  HARSH UPPALA (Presenter), DAVID SIDEBOTTOM, Creighton University — Carbon nanodots are a class of zero-dimensional carbon-based nanoparticles that have been used increasingly in the fields of bioimaging, drug delivery, and optronics. Despite their popularity, carbon nanodots remain difficult to isolate when synthesized by a bottom-up approach, especially through the thermal treatment of carbohydrate solutions due to the presence of many molecular byproducts which result from the Maillard reaction [1].

We investigated multiple possible methods of purification of glucose solutions [2]. Glucose solutions were heated at 120 °C for a period of 48 hours to produce carbon nanodots. We found that dialysis combined with solid phase extraction preserved the photoluminescent properties of dissolved carbon nanodots, while eliminating measurable traces of other chemical byproducts, as measured by Fourier-Transform IR spectroscopy, Carbon-NMR, and Hydrogen-NMR.


M71.00395: Synthesis and Characterization of Barium Titanate and Carbon-based core-shell nanoparticles  MOUDIP NANDI (Presenter), KARTIK GHOSH, CHRISTOPHER ROBLEDO, Missouri State Univ — Core-shell nanoparticles (CSNP) have diverse applications such as biology and electronic field of studies. Among so many oxide nanoparticles, Barium Titanate nanoparticles are of current interest due to their good electronic and ferroelectric properties.

There are some studies based on the synthesis and characterization of oxide-oxide and oxide-sulfide based core-shell nanoparticles. Here we are trying to synthesize and characterize oxide-carbide based core-shell nanoparticles, where the core is made of Barium Titanate and the shell is made of Carbon. There are various synthesis approaches like hydrothermal synthesis, sol-gel method, emulsion polymerization etc to produce core-shell nanoparticles, here we have synthesized these core-shell nanoparticles with a unique method. The shell is made of Carbon which is a biocompatible element and it can be used as a connector between organic and inorganic materials. Shell made of carbon shows interesting optical properties and they can be useful for biosensing and optoelectronic applications. We used different methods like XRD, RAMAN, SEM, and TEM to characterize and analyze these CSNP. Some of the findings will be discussed here.
M71.00396: A Gd@C$_{82}$-based single electron transistor device with ferroelectric-like switching behavior  FENGQI SONG (Presenter), KANGKANG ZHANG, Nanjing Univ — Ferroelectricity arises from permanent dipole and has led to technology innovation in memory devices. However, maintaining ferroelectricity at nanoscale is challenging, greatly limits its application in nanoscale devices. Here we report the gate-controlled switching between two sets of single-electron characteristic stability diagrams in the electrical transport of a Gd@C$_{82}$-based single molecular device. It is operated in a hysteresis-like loop with a coercive gate field of up to 0.5 V/nm. The theoretical calculations attribute the two diagrams to the energy levels of two trapping states of the Gd atom in the C$_{82}$ cage, which possess two different permanent electrical dipole configurations. The switching thus originates from the electrical field driven dipole flipping and demonstrate the ferroelectricity at the single molecule level.

M71.00397: Evolution of plasmonic response of individual size-selected Au clusters from nanoscale to atomic-scale  FENGQI SONG (Presenter), SIQI LU, Nanjing Univ — We have studied the evolution of plasmonic response of individual size-selected Au clusters by scanning transmission electron microscopy-electron energy loss spectrum (STEM-EELS) from nanoscale to atomic scale. The clusters are prepared and selected by magnetron sputtering time-of-flight cluster source to get an atomic number precision. To distinguish surface and bulk plasmon mode, we put the electron beam at the edge or center of clusters, where we can get a pure surface mode or a mixture of surface and bulk mode. Both surface and bulk mode exist when the gold clusters are large enough. However when the atom numbers decrease to 887, the bulk mode disappears abruptly while the surface mode still appears. The surface mode excitation probability of a single incident electron shows a square relationship versus atom numbers from 70000 to 300, but deviates from it when the atom number reaches 175. What's more, a new peak higher than surface mode appears when the gold clusters are smaller than Au$_{500}$. After a slight redshift from Au$_{70000}$ to Au$_{887}$, an obvious blue-shift happens in the range Au$_{887}$ to Au$_{300}$, showing a combined influence between quantum size effect and classical size effect of electron mean free path.
Infrared Spectroscopy Investigation of Ammonium Sulfate at Low Temperatures

LUCAS EHINGER (Presenter), Seattle Univ, KRISHNA KHAREL, OZGE GUNAYDIN-SEN, Lamar University, AMAL B AL-WAHISH, University of Washington — We present a comprehensive study of ammonium sulfate between 30 and 300K using Fourier transform infrared (FTIR) spectroscopy, differential scanning calorimetry (DSC) and neutron powder diffraction (NPD) to investigate the paraelectric to ferroelectric phase transition. Heat capacity measurements taken with DSC show a clear anomaly at the phase transition (223 K). This phase transition in ammonium sulfate is associated with temperature dependent hydrogen bonding and presents an interesting and challenging research area.¹ We characterize the hydrogen bonds at different-temperatures and compare our NPD at room temperature with previously reported results². We then analyze FTIR spectral features of the sample and demonstrate their temperature dependent displacement.


Activation of CO₂ at chromia-nanocluster-modified rutile and anatase TiO₂

MICHAEL NOLAN, Tyndall National Institute, MARCO FRONZI (Presenter), IRCRE, Xi'an Jiaotong University — Converting CO₂ to fuels is required to enable the production of sustainable fuels and to contribute to alleviating CO₂ emissions. In considering the conversion of CO₂, the initial step of adsorption and activation by the catalyst is crucial. In addressing this difficult problem, we have examined how nanoclusters of reducible metal oxides supported on TiO₂ can promote CO₂ activation. In this paper we present density functional theory (DFT) simulations of CO₂ activation on heterostructures composed of clean or hydroxylated extended rutile and anatase TiO₂ surfaces modified with chromia nanoclusters. Our results highlight that a metal oxide support modified with reducible metal oxide nanoclusters can activate CO₂, thus helping to overcome difficulties associated with the difficult first step in CO₂ conversion.
M71.00400: Logarithmic Expansion of Swellable Organosilica Material*  
BRIAN P CORBIN, JOHN LINDNER (Presenter), PAUL A BONVALLET, College of Wooster — Swellable organically modified silica (SOMS) is a matrix of crosslinked polysilsesquioxanes that undergoes rapid reversible swelling upon contact with organic solvents. This material has applications in environmental remediation, catalysis, and personal care products. We demonstrate that SOMS exhibits a logarithmic stress-strain relationship when it swells. Using a two-piston force sensor, we measured the swelling force exerted by various samples of SOMS when treated with acetone. As the mass of SOMS inside the force-measurement apparatus increases, the force generated by the swelling also increases, up to a maximum value of approximately 180 N at 650 mg of SOMS. However, the rate-of-change of the force generated by SOMS decreases at larger masses, implying that SOMS is dynamic rather than static. A data collapse of two different SOMS samples (Osorb® and Cyclasorb®) shows that the underlying behavior of SOMS is uniform across sample types.

*Research supported by NSF DMR-1852095

M71.00401: Carrier Injection Mechanisms in Diketopyrrolopyrrole Organic Semiconductors  
SHAWN KILPATRICK (Presenter), VISHAL NARANG, ANDREW LEVINE, MAJHARUL HOQUE, ADAM BRAUNSCHWEIG, MILAN BEGLIARBEKOV, NanoScience, CUNY Advanced Science Research Center — Organic semiconductors based on diketopyrrolopyrrole (DPP) are a new class of small molecule semiconductors which are air-stable, possess relatively high mobilities, and have been recently shown to undergo excitonic singlet fission. Realizing high quality (Ohmic) contacts to DPP is essential for the fabrication of high quality devices. In this work we use a combination of scanning Kelvin probe microscopy and electrical transport measurements to spatially map the work function in several DPP-based semiconductors and study the carrier injection mechanism in thermally evaporated DPP films.

M71.00402: Novel phase transitions as bridges for broken ergodicity in confined colloidal prisms*  
PRAJWAL BANGALORE PRAKASH (Presenter), FERNANDO A ESCOBEDO, Cornell University — We used Monte Carlo simulations to study the assembly behavior of square and hexagonal prisms under quasi-2D confinement separations, within a hard-wall slit. Our results for hexagonal prisms revealed two types of first order phase transitions at increasing concentration: 1) solid-solid transition (6-fold → 4-fold symmetry solid) occurring through lattice symmetry breaking, and 2) solid to dense-liquid (disorder) to solid. The predicted dense-liquid has a density intermediate to those of the two solid phases and high translational/orientational mobility. We showed that similar phase behavior can be expected for other n-gonal prisms (n > 6). For square prisms, we observed a solid-solid phase transition where a square lattice spacing rearrangement gives rise to a polycrystalline phase with multiple locally ordered domains. These unusual phase transitions are attributed to the broken ergodicity associated with a dynamically disconnected rotational phase space accessible to the particles. As an experimentally viable strategy to dynamically bridge those rotational states observed for hard-slit phase behavior, we also investigated and validated a soft-repulsive wall model.

*Partial funding support from NSF awards CBET-1907369 and 1402117
M71.00403: Non-Adiabatic Molecular Dynamics of Molecules in the Presence of Strong Light-Matter Interactions*  YU ZHANG (Presenter), TAMMIE NELSON, SERGEI TRETIAK, Theoretical Division, Los Alamos National Laboratory — The mixing between the light and matter characters modifies the photophysical and photochemical properties. In this work, a theoretical model and an efficient numerical method for studying the dynamics of molecules strongly interacting with quantum light are developed based on non-adiabatic excited-state molecular dynamics. The methodology was employed to study the cis-trans photoisomerization of a realistic molecule in a cavity. Numerical simulations demonstrate that the photochemical reactions can be controlled by tuning the properties of the cavity. In the calculated example, the isomerization is suppressed when polaritonic states develop a local minimum on the lower polaritonic state. Moreover, the observed reduction of isomerization is tunable via the photon energy and light-molecule coupling strength. But the fluctuation in transition dipole screens the effect of light-matter, which makes it harder to tune the photochemical properties via the coupling strength.

*The work at Los Alamos National Laboratory (LANL) was supported by the LANL Directed Research and Development Funds. This research used resources provided by the LANL Institutional Computing (IC) Program. LANL is operated by Triad National Security, LLC, for the NNSA of the U.S. DOE (Contract No. 89233218NCA000001).

M71.00404: Strong plasmon-molecule coupling at the nanoscale revealed by first-principles modeling*  TUOMAS ROSSI (Presenter), PAUL ERHART, TIMUR SHEGAI, Department of Physics, Chalmers University of Technology, TOMASZ ANTOSIEWICZ, Faculty of Physics, University of Warsaw — Strong light-matter interactions in both the single-emitter and collective strong coupling regimes attract significant interest due to emerging applications in quantum optics as well as opportunities for modifying material-related properties. Exploration of these phenomena is theoretically challenging, as polaritons exist at the intersection between quantum optics, solid state physics, and quantum chemistry. In this presentation, we shed light on nanoscale polaritons in small strongly-coupled plasmon-molecule systems by using time-dependent density-functional theory (TDDFT) [1]. By analyzing the electron-hole transitions involved in the excitation process, we dissect the symmetric and antisymmetric polaritonic modes caused by strong coupling between plasmon and molecular excitation, resulting in Rabi oscillations in time domain. Our results indicate that cavity quantum electrodynamics description holds down to resonators of a few cubic nanometers in size. In a broader perspective, first-principles methods enable parameter-free in-depth studies of polaritonic systems for emerging applications.


*EU Horizon 2020 research and innovation programme, Marie Sklodowska-Curie grant No 838996
High-order harmonics generated from a quasi-one-dimensional hexagonal solid*  
GUOPING ZHANG (Presenter), Y. H. BAI, Indiana State University — High harmonic generation has attracted enormous attentions. Here we report a completely new kind of harmonics in a quasi-one-dimensional and hexagonal barium titanium sulfide: Under circularly polarized laser excitation, harmonics are generated only at first, fifth, seventh and eleventh orders. These magic harmonics appear only with circularly polarized light, not with linearly polarized light. Neither cubic nor tetragonal cells have magic harmonics even with circularly polarized light. Through a careful group-theory analysis, we find that two subgroups of symmetry operations unique to the hexagonal symmetry cancel out third and ninth harmonics. This feature presents a rare opportunity to develop HHG into a crystal-structure characterization tool for phase transitions between hexagonal and nonhexagonal structures.

Refs.

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M71.00406: Deciphering photoacidity by following electronic charge distribution changes along the photoacid Förster cycle with picosecond nitrogen K-edge x-ray absorption spectroscopy

SEBASTIAN ECKERT, MARC-OLIVER WINGHART, CARLO KLEINE, JAN LUDWIG, MARIA EKIMOVA, Max Born Inst, AMBAR BANERJEE, Department of Physics, Stockholm University, JESSICA HARICH, Institute for Nanostructure and Solid State Physics, University of Hamburg, ROLF MITZNER, Institute for Methods and Instrumentation for Synchrotron Radiation Research, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, DANIEL AMINOV, EHUD PINES, Department of Chemistry, Ben Gurion University of the Negev, NILS HUSE, Institute for Nanostructure and Solid State Physics, University of Hamburg, PHILIPPE WERNET, Department of Physics and Astronomy, Uppsala University, MICHAEL ODELIUS, Department of Physics, Stockholm University, ERIK T. J. NIBBERING (Presenter), Max Born Inst — Photoacids are molecular systems that show a strong increase in acidity in the first electronic excited state. The underlying mechanisms for photoacidity and photobasicity have until now remained unsolved. We use picosecond N K-edge x-ray absorption spectroscopy to determine how the transient electronic-structure changes and hydrogen-bond dynamics determine the acidity of a prototypical photoacid, 8-aminopyrene-1,3,6-trisulfonate (APTS), in aqueous solution. We follow in time the characteristic spectroscopic signatures of N-H σ* and N-lone pair interactions of the proton donating functional amine group as well as aromatic pyrene π* anti-bonding orbitals of APTS along the different stages in the Förster photocycle. With our flatjet system for x-ray absorption spectroscopy in transmission and with the picosecond x-ray pulses at BESSY II (in multibunch mode), we elucidate how UV excitation converts the photoacid into the conjugate photobase form on a time scale of 150 ps, followed by electronic excited state fluorescence decay on nanosecond time scales. With these results we demonstrate that a systematic electronic-structural approach to the ultrafast dynamics of photoacids in aqueous solution can be established.
M71.00407: Microscopic study of proton kinetic energy anomaly for confined water*

MOHAMMAD MOID (Presenter), Indian Institute of Science - Dept of Physics, YACOV FINKELSTEIN, Nuclear Research Center-Negev, Beer-Sheva, RAYMOND MOREH, Department of Physics, Ben-Gurion University of the Negev, Beer-Sheva, PRABAL K MAITI, Indian Institute of Science - Dept of Physics — Several anomalies, related to structural and dynamical transition, have been reported for water at different thermodynamic conditions and environments. Of particular interest, the reported anomalies of the proton mean kinetic energy, Ke(H), in nanoconfined water, as measured by deep inelastic neutron scattering (DINS), are a longstanding problem related to proton dynamics in hydrogen-bonded systems. We used classical MD method to deduce Ke(H) by calculating the proton vibrational density of states, H-VDOS, for the case of water inside single wall carbon nanotubes (SWCNT) of varying diameters. The mean vibrational density of states (VDOS) of protons in water nanoconfined inside single wall carbon nanotubes (SWCNTs) is calculated as a function of temperature and SWCNT diameter, D\text{CNT}. The calculated VDOS are utilized for deducing the mean kinetic energy of the water protons, Ke(H), by treating each phonon state as a quantum harmonic oscillator. The calculation depicts a strong confinement effect as reflected in the drop of the value of Ke(H) at 5K for D\text{CNT} < ~12Å, while absent for larger diameters. The results also reveal a very significant blue and red shifts of the stretching and bending modes respectively compared to those in bulk ice, in agreement with experiment.

*CSIR, IISc

M71.00408: Evidence of topologically non-trivial phase trough unusual Shubnikov-de Haas oscillations*

JOÃO VITOR IGNÁCIO COSTA (Presenter), Sao Carlos Institute of Physics at the University of Sao Paulo, DENIS CANDIDO, Department of Physics and Astronomy and Optical Science and Technology Center, University of Iowa, SIGURDUR INGI ERLINGSSON, School of Science and Engineering, Reykjavik University, CARLOS EGUES, Sao Carlos Institute of Physics at the University of Sao Paulo — Topological features in bulk related phenomena are still an uncharted territory as opposed to edge and surface effects, making Shubnikov-de Haas (SdH) oscillations an interesting phenomenon to explore in topological systems. Here we investigate the bulk magneto-oscillations in connection with topological bands of 2D systems. We describe our systems by the BHZ model [1] and use a convenient trace formula [2] to describe the density of states of broadened Landau levels within a phenomenological Drude-like transport description. Our preliminary results show unusual beatings in the SdH oscillations for the topological regime, which are absent in the trivial regime. These can be traced back to the coexistence of both electron- and hole-like carriers, present in the “Mexican hat” band structures. This suggests SdH oscillations as a possible bulk probe for the non-trivial band topology of 2D systems.


*This work was supported by the Reykjavik University Research Fund, CNPq, CAPES, FAPESP Grant No. 2016/08468-0.
M71.00409: Stacking-type dependence of topological phase transitions in a superlattice of topological and normal insulators*  
GUN SANG JEON (Presenter), Department of Physics, EWHA Woman's Univ — We consider a superlattice of topological and normal insulating layers. It is known that topological phase transitions occurs with the variation of the interlayer hopping when two-dimensional quantum spin Hall insulator is hybridized with the normal insulators in the AA-type stacking. We examine how the nature of topological phase transition changes depending on the stacking type. The resulting phase diagram exhibits rich phases such as semimetal and topological ones. The properties of the edge states are also investigated in the sample of finite width. Finally we discuss the topological features of alternately stacked layers of topological and normal insulators.

*This work was supported by the National Research Foundation of Korea through Grant No. NRF-2018R1D1A1B07048749.

M71.00410: The physical basis of using MRI to detect cancer  
DONALD CHANG (Presenter), Hong Kong University of Science and Technology — Nowadays, the most effective way of detecting cancer in a patient is using MRI (Magnetic Resonance Imaging). This technique is based on the measurement of hydrogen nuclear spin signal of water molecules inside the body. During the development of the MRI technique, it needed to overcome two major difficulties: (1) How to produce a contrast between water molecules inside the cell and the extra-cellular water? (2) How to differentiate the water signals contributed by cancer cells from those contributed by normal cells? These difficulties were resolved mainly through the discovery that the relaxation times of water protons inside the cells are very different from those of the extra-cellular water. Furthermore, the relaxation times of water molecules in normal cells are found to be significantly different from those in the cancerous cells. In this presentation, I will give a concise review of the evidence for these discoveries. Finally, I will discuss the possible physical basis that may account for the relaxation time difference between different cells.

M71.00411: Influence of self-heating on noise of SiGe heterojunction bipolar transistors at cryogenic temperatures  
NACHIKET NAIK (Presenter), AUSTIN MINNICH, Caltech — Cryogenic low noise transistor amplifiers (LNA) at microwave frequencies have long been of interest for radio astronomy and more recently for quantum computers. While high electron mobility transistors have been the primary device of choice for these applications, SiGe HBTs are increasingly competitive due to increases in cutoff frequency and their relatively high yield. However, an understanding of the influence of self-heating on noise at cryogenic temperatures is lacking. In this work, we report noise measurements on SiGe HBT LNAs from 4 – 50 K. The influence of self-heating on the temperature of electrons at the base-emitter junction is evaluated by comparing measurements in vacuum with those in liquid Helium baths. Our work helps to identify a path for SiGe HBTs to achieve noise figures competitive with those of HEMTs.
M71.00412: Transfer of Linear and Angular Momentum from Evanescent Fields of an Optical Fiber to Isotropic and Anisotropic Dipolar Spheres.* DUSTIN SAVELLI (Presenter), Ohio State Univ - Columbus, ARIEL XIE, CODY LEARY, Physics, College of Wooster — We calculate the force and torque on a transparent isotropic dipolar sphere due to the higher-order evanescent field modes propagating outside a few-mode optical fiber immersed in water. After applying these results to find the orbital trajectory and spin dynamics of an isotropic sphere, we then use perturbation theory to calculate the orbital trajectory of a weakly anisotropic sphere.

*We would like to thank the National Science Foundation for their NSF grant #1852095

M71.00413: Capacitive Compactness and Surface Charge Density Variation in Pluronic (F-127) Micelles using Small-Angle X-ray Scattering TAHMIDA IQBAL (Presenter), JOSE L BANUELOS, Physics, University of Texas at El Paso — The spatial extent of a charged colloid or an electrode is usually characterized by its Debye length which is independent of important physical features including colloidal charge and electrostatic ion correlations. To describe the colloidal stability of electrified nanoparticles more accurately we need tools to study the structure of the electrical double layer. Colloidal particles can be used in diverse technological applications involving colloidal stability of charged solutions, or storage capacity of electrical energy in batteries or supercapacitors. Capacitive compactness is a novel description of the diffuse electrical double layer extension in terms of an effective capacitor and has ability to consider important physical characteristics of the solute. We have chosen Pluronic F-127 in this work because it is a temperature responsive triblock copolymer with well-known adsorption and colloidal properties. In this work, we studied the surface charge density of Pluronic F-127 micelles at different concentration and pH to understand how interparticle interactions relate to capacitive compactness. Small-angle x-ray scattering results were used to analyze the micelle-micelle structure factor and relate it to pH dependent changes in the capacitive compactness.

M71.00414: WITHDRAWN ABSTRACT
M71.00415: Nano Spray-Dried Block Copolymer Nanoparticles and Their Transformation into Hybrid and Inorganic Nanoparticles  INBAL WEISBORD (Presenter), NETA SHOMRAT, Chemical Engineering, Technion - Israel Institute of Technology, HEN MOSHE, ALEJANDRO SOSNIK, Materials Science and Engineering, Technion - Israel Institute of Technology, TAMAR SEGAL-PERETZ, Chemical Engineering, Technion - Israel Institute of Technology — Block copolymers (BCPs) self-assemble into highly ordered structures with periodicities of 5-50 nm. When BCP self-assembly is confined in macro and nano spheres various morphologies can be achieved by tailoring BCP chemical composition, solvent, and process parameters, making them attractive materials for applications like drug delivery and catalysis. So far, BCP NPs were mainly fabricated through emulsion-based methods. However, there is need to develop novel, potentially scalable, BCP NP fabrication methods which will enable new NP morphologies. We present a new route for BCP NP fabrication through BCP confinement in sprayed nanodroplets using Nano Spray-Drying (NSD). PS-b-PMMA and PS-b-PVP were NSD from toluene and chloroform. SEM and TEM were used to study the effects of BCP chemistry, solvent, and NSD process parameters on BCP NP morphology. Following NSD, BCP NPs were suspended in non-solvents and solvent annealed with chloroform to tune internal NP morphology. Finally, hybrid organic-inorganic particles were created through Sequential Infiltration Synthesis (SIS), a method that enables growth of metal-oxides within polymers. Using SIS, alumina and zinc-oxide were selectively grown in BCP polar domains, transforming the BCP NP into hybrid or BCP-templated inorganic NPs.

M71.00416: Fabrication of low dimensional oxide thin films using cuprates as sacrificial layers  YAO-WEN CHANG (Presenter), JHIH-BANG YI, CHUN-CHIEN CHIU, YU-CHEN LIU, JAN-CHI YANG, Department of Physics, National Cheng Kung University — The characteristics and functionalities of complex oxide caught a lot of attention recently. For oxide perovskite thin film, an available modulation is to form heterostructure. Applying different perovskite allows strain manipulating and other effects that would change the characteristic which form a unique system. Unfortunately, not all kinds of complex oxide are acceptable to heterostructure. To give a wider range of combination for oxides, freestanding membrane was developed. La$_{0.7}$Sr$_{0.3}$MnO$_3$ and Sr$_3$Al$_2$O$_6$ are the two commonly used buffer layer. By etching the buffer layer, the thin film that deposit after the buffer layer can be separated from the substrate. In this work, we used YBa$_2$Cu$_3$O$_{7-x}$ as a buffer layer, this method takes less time etching but maintain a fine freestanding membrane for later procedure. Furthermore, the process allows us to separate materials like La$_{0.7}$Sr$_{0.3}$MnO$_3$ with acid etchant because of the time etching YBa$_2$Cu$_3$O$_{7-x}$ takes a few minutes while etching La$_{0.7}$Sr$_{0.3}$MnO$_3$ takes a few hours. Our goal is to develop a universal freestanding method that could applied to all kind of materials which could give access to more combination of complex oxide thin films.

Wednesday, March 4, 2020 12:15 PM - 1:45 PM

Session N01 APS: Planned Giving Luncheon (12:15pm - 1:45pm) 204
12:15PM N01.00001: Planned Giving Luncheon (12:15pm - 1:45pm) — Discover opportunities for creative gift arrangements that offer immediate tax benefits for you, and long-term benefits for the science community. Join the APS Development Office for a conversation facilitated by:

David Morrison, Partner; Prosperion Financial Advisors
and
Brian B. Schwartz, Ph.D., Professor of Physics; Brooklyn College and The Graduate Center of CUNY

Light refreshments and handouts will be provided. This session is free to members of APS and their guests. You do not need to be registered for the March Meeting to attend.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P00 APS: Kavli Foundation Special Symposium: Frontiers of Computation: Machine Learning and Quantum Computing

2:30PM P00.00001: Vignettes of machine learning in the natural sciences [Invited] PATRICK F RILEY (Presenter), Google Accelerated Science, Google, LLC — The promise of machine learning to aid in scientific discovery is now a frequent topic in journals and conferences. For the last 5 years, the Google Accelerated Science team has been partnering with scientists in a variety of natural science fields to make this promise a reality. I’ll sample a few of our achievements with examples in scientific computing and molecular design while also highlighting the current and future challenges in the effective use of machine learning in the sciences.

3:06PM P00.00002: Machine Learning and the Complexity of Quantum Simulation [Invited] ROGER MELKO (Presenter), University of Waterloo — Computational approaches to condensed matter have long influenced the theoretical development of quantum many-body physics. For example, quantum Monte Carlo (QMC) ties our understanding of the computational efficiency of simulating quantum systems to the sign structure of the Hamiltonian. The Density Matrix Renormalization Group motivated the modern field of Tensor Networks (TNs), which relate computational efficiency to the entanglement entropy of a wavefunction. This trend now continues with the rapidly-developing field of machine learning, which has introduced a host of new strategies and architectures for the simulation and data-driven reconstruction of quantum many-body systems. Over the last three years, progress has been made in framing various machine learning approaches within the context of traditional methods such as QMC or TNs; however, it has also become apparent that some aspects differ substantially. In this talk I will provide an overview of the landscape of machine learning strategies in simulating quantum systems. I will speculate on how our theoretical framework of quantum many-body physics can influence the development of new machine learning strategies, and vice versa.
In recent years, machine learning methods such as "deep learning" have proven enormously successful for tasks such as image classification, voice recognition, and more. Despite their effectiveness for big-data classification problems, these methods have had limited success for time series prediction, especially for complex systems like those we see in weather, solar activity, and even brain dynamics. In this talk, I will discuss how a Reservoir Computer (RC) - a special kind of artificial neural network that offers a "universal" dynamical system - can draw on its own internal complex dynamics in order to forecast systems like the weather, far beyond the time horizon of other methods. Like many other machine learning architectures, the RC provides a knowledge-free approach because it builds forecasts purely from past measurements without any specific knowledge of the system dynamics. By building a new approach that judiciously combines the knowledge-free prediction of the RC with a knowledge-based model, we demonstrate a further, dramatic, improvement in forecasting complex systems. This hybrid approach can given us new insights into the weaknesses of our knowledge-based models and also reveal limitations in our machine learning system, guiding improvements in both knowledge-free and knowledge-based prediction techniques.

Decades of efforts in improving computing power and experimental instrumentation were driven by our desire to better understand the complex problem of quantum emergence. However, increasing volume and variety of data made available to us today present new challenges. I will discuss how these challenges can be embraced and turned into opportunities by employing machine learning. It is important to note that the scientific questions in the field of electronic quantum matter require fundamentally new approaches to data science for two reasons: (1) quantum mechanical imaging of electronic behavior is probabilistic, (2) inference from data should be subject to fundamental laws governing microscopic interactions. Hence machine learning quantum emergence requires collective wisdom of data science and condensed matter physics. I will review rapidly developing efforts by the community in using machine learning to solve problems and gain new insight. I will then present my group's results on the machine-learning-based analysis of complex experimental data on quantum matter.

*I acknowledge support by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-SC0018946, DOE and the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875).
4:54PM P00.00005: Quantum computing: Current status and future prospects [Invited]  JOHN PRESKILL (Presenter), Caltech — Noisy Intermediate-Scale Quantum (NISQ) technology is now becoming available for the first time. Quantum computers with of order 100 qubits may be able to perform tasks which surpass the capabilities of today's classical digital computers, but noise in quantum gates will limit the size of quantum circuits that can be executed reliably. NISQ devices will be useful tools for exploring many-body quantum physics, and may have other useful applications, but the 100-qubit quantum computer will not change the world right away --- we should regard it as a significant step toward the more powerful quantum technologies of the future. Quantum technologists should continue to strive for more accurate quantum gates and, eventually, fully fault-tolerant quantum computing.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P01 DAMOP: Precision measurements for fundamental physics, interferometry, and trapped ions 103 - Norman Yao, University of California, Berkeley

2:30PM P01.00001: JILA’s search for the electron’s electric dipole moment: a novel approach to searches for new physics  TANYA ROUSSY (Presenter), WILLIAM B CAIRNCROSS, DANIEL A PALKEN, BENJAMIN M BRUBAKER, DANIEL N GRESH, JILA and The University of Colorado, Boulder, MATTHEW GRAU, Institute for Quantum Electronics, ETH Zurich, KEVIN COSSEL, National Institute of Standards and Technology, KIA BOON NG, YUVAL SHAGAM, YAN ZHOU, JILA and The University of Colorado, Boulder, VICTOR FLAMBAUM, University of New South Wales, JUN YE, ERIC A. CORNELL, JILA and The University of Colorado, Boulder — We are probing TeV-scale physics with a unique tabletop experiment which combines trapped molecular ions, rotating bias fields, orientation-resolved detection, and over a dozen lasers to both measure the electron's electric dipole moment and constrain potential dark matter candidates. In this talk I will introduce the essence of our measurement as well as our methods for constraining both dark matter and parity-violating physics.
Towards a More Sensitive Measurement of the Atomic Electric Dipole Moment of Radium-225

Permanent atomic electric dipole moments (EDMs) violate parity (P) and time reversal (T), and, assuming CPT symmetry, combined charge-conjugation and parity transformation (CP). Observable EDMs are enhanced in large-Z atoms with octupole-deformed, or pear-shaped, nuclei. Radium-225 has a significantly larger octupole deformation than nuclei used in other EDM experiments. In the Ra EDM experiment, radium atoms are vaporized, slowed, trapped, and transported to a science chamber between two high voltage electrodes. The first measurements of the upper limit of the EDM of Radium-225 were carried out in 2014 and 2015. For the second generation of measurements (2019—2020), upgrades to the atom detection method and applied electric field magnitude will improve our measurement sensitivity by up to two orders of magnitude. Additionally, we validated plans for a better longitudinal atom slower by experimentally verifying critical theorized branching ratios. The new slower is expected to provide an order of magnitude improvement in measurement sensitivity.

*Work funded by MSU and US DOE Office of Science, Office of Physics, DOE Oak Ridge Institute for Science and Education, and DOE National Nuclear Security Administration under contracts DE-AC02-06CH11357, DE-SC0014664, and NSSC DE-NA0003180.

Modeling a dual-Sagnac interferometer for rotation sensing

A recent experiment performed in the group of Cass Sackett, implemented a dual Sagnac interferometer for rotation sensing using a Bose-Einstein condensate confined in an harmonic potential. The condensate is first split into two pieces using standing-wave Bragg lasers and then allowed to fly apart until the two pieces come to a stop. These two pieces are then split again along a perpendicular direction creating two pairs of condensates moving around a circle in opposite directions. They re-overlap after one trip around the circle at which point they are split a third time and the number of stationary atoms is measured. We have simulated this experiment using a model based on the Lagrangian Variational Method where the condensate pieces are represented by Gaussian clouds. We have mapped out the region of validity of this model by direct numerical simulation using the 3D Gross-Pitaevskii equation. In addition to performing simulations under experimental conditions where the number of atoms was N=10⁴, we also simulated the interferometer operation for larger condensates where atom-atom interactions must be accounted for.


*This work was supported by the US National Science Foundation grant no. PHY-1707776.
3:06PM P01.00004: Mechanism for producing smooth flow by stirring a racetrack BEC*
MARK EDWARDS (Presenter), DANIEL FOGARTY, Georgia Southern University, CHARLES CLARK, National Institute of Standards and Technology — We studied the production of smooth flow in a Bose-Einstein-condensed (BEC) gas in a racetrack atom-circuit potential. The BEC is confined into a thin horizontal sheet by laser light. The racetrack potential is a channel having two straight channels connected by circular endcaps. The system is assumed to follow the Gross-Pitaevskii model. Flow is produced by stirring the BEC with a rectangular barrier. We have studied in-depth how flow is produced by this stirring. As the barrier strength increases, a backflow develops in the barrier region producing a vortex/anti-vortex pair. The outside vortex circulates like the stir. Above a critical barrier height, the vortices swap places. This generates two disturbances: (1) the vortex/antivortex pair moves off in the anti-stir direction and (2) a compression wave moving the other way. This repeats until the flow produced overtakes the barrier speed. Each new unit of flow creates another pair of disturbances. These disturbances convert the localized circulation of the vortices into macroscopic flow around the racetrack. The flow oscillates around this value until the barrier falls below the critical value determining the final flow.

*This work was supported in part by the US National Science Foundation grant no. PHY-1707776.

3:18PM P01.00005: Phase-sensitive amplification and SU(1,1) interferometry via multimode four-wave mixing*
ERIN KNUTSON (Presenter), J. SAM CROSS, SARA WYLLIE, RYAN T GLASSER, Tulane Univ — We demonstrate a useful phase dependence in a multi-pump four-wave mixing configuration. We find that, for certain phase values, the intensity noise of an output mode is lower than that of its phase-insensitive counterpart. This lower-noise amplification has been demonstrated previously in atomic four wave mixing, but only with the use of significantly more complex experimental configurations, e.g. dual homodyne detection or cascaded vapor cells. Additionally, our method naturally results in four beams that can be quantum correlated with one another.
These findings have obvious applications in the simplification of quantum optical experiments that involve the generation or amplification of more than two correlated modes. Additionally, we describe how this result may be employed in a “touchless” or interaction-free SU(1,1) interferometry scheme, wherein a phase measurement may be made remotely on a pair of modes without introducing loss or destroying any squeezing between them.

*We acknowledge support from the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1154145, and from the Louisiana State Board of Regents.
3:30PM P01.00006: Search for non-Newtonian gravity with optically-levitated microspheres*
CHARLES P BLAKEMORE, ALEXANDER FIEGUTH (Presenter), AKIO KAWASAKI, DENZAL MARTIN, NADAV PRIEL, ALEXANDER D RIDER, GIORGIO GRATTA, Stanford Univ — The universal law of gravity has undergone stringent tests for a long time over a significant range of length scale, from an atomic scale to a planetary scale. Of particular interest is the short distance regime, where modifications to Newtonian gravity may arise from axion-like particles and extra dimensions. We have constructed an ultra-sensitive force sensor based on optically-levitated microspheres with a force sensitivity of $\sim 10^{-17}$ N/\(\sqrt{\text{Hz}}\) for the purpose of investigating non-Newtonian forces in the 1-100 \(\mu\text{m}\) range. Microspheres interact with a variable-density attractor mass made by alternating silicon and gold segments with periodicity of $\sim 50$ \(\mu\text{m}\). The attractor can be located as close as a few \(\mu\text{m}\) to a microsphere. We report on the characterization of this system, its sensitivity, and preliminary results. Further technological developments to reduce background are investigated to provide orders of magnitude improvement in the sensitivity, going beyond current constraints on non-Newtonian interactions.

*This work was supported, in part, by NSF grants PHY1502156 and PHY1802952, ONR grant N00014-18-1-2409, and the Heising-Simons Foundation.

3:42PM P01.00007: Ultrasensitive torque detection and ultrafast rotation with an optically levitated nanoparticle*
JONGHOON AHN (Presenter), ZHUJING XU, JAEHOON BANG, PENG JU, XINGYU GAO, TONGCANG LI, Purdue Univ — Torque sensors have enabled great accomplishments in physics including the discovery of Coulomb's law and Cavendish's first determination of the gravitational constant, and is widely used for studies such as small-scale magnetism and the Casimir effect. Here, we develop an ultrasensitive torque sensor with an optically levitated nanoparticle in vacuum and experimentally demonstrate a torque sensitivity of \((4.2 \pm 1.2) \times 10^{-27}\) Nm / \(\sqrt{\text{Hz}}\) at room temperature [1] without the need of complex nanofabrication or cryogenic cooling. With the optically levitated particles, we are also able to achieve a record high mechanical rotation exceeding 5 GHz [1,2]. Our calculations suggest our torque sensor will allow detection of vacuum friction near a surface under realistic conditions.


*We are grateful to supports from the Office of Naval Research under grant No. N00014-18-1-2371, the NSF under grant No. PHY-1555035, and the DARPA NLM program.
Towards mass sensing using cavity optomechanics readout

EWA REJ (Presenter), MERT YUKSEL, WARREN FON, MATTHEW MATHENY, MICHAEL ROUKES, California Institute of Technology — The minute size of nanoelectromechanical systems (NEMS), combined with their large quality factors, has provided a large class of sensors capable of measuring the properties of single molecules. In particular, NEMS have allowed the mass of individual adsorbed molecules, such as protein complexes, to be measured. I will present results showing NEMS based mass spectrometry of individual proteins and explain how the mass resolution is governed by the phase noise of the system, with contributions from the resonator itself, readout circuitry and thermomechanical noise. I will outline our new approach based on a superconducting cavity optomechanics readout scheme for improved sensor performance. The transduction by cavity optomechanics is expected to greatly reduce system phase noise as readout-self heating is minimal. This will directly yield improved resolution in detecting the spatial mass distribution of individual analytes.

Searching for scalar dark matter with compact mechanical resonators*

JACK MANLEY (Presenter), RUSSELL STUMP, University of Delaware, DALZIEL WILSON, University of Arizona, DANIEL GRIN, Haverford College, SWATI SINGH, University of Delaware — We discuss the viability of laboratory-scale mechanical resonators as detectors for ultralight scalar dark matter. The signal we investigate is an atomic strain due to modulation of the fine structure constant and the lepton mass at the Compton frequency of dark matter particles. The resulting stress can drive an elastic body with breathing modes, producing displacements that are accessible with opto- or electromechanical readout techniques. To address the unknown mass of dark matter particles (which determines their Compton frequency), we consider various resonator designs operating at kHz to MHz frequencies, corresponding to $10^{-12}$-$10^{-5}$ eV particle mass. Current resonant-mass gravitational wave detectors that have been repurposed as dark matter detectors weigh ~$10^3$ kg. We find that a large unexplored parameter space can be accessed with ultra-high-Q, cryogenically-cooled, cm-scale mechanical resonators possessing ~$10^7$ times smaller mass[1].


*This work was supported by the National Science Foundation grant PHY-1912480.
4:18PM P01.00010: Realization of a second-generation scheme for dissipative entanglement of hyperfine beryllium-ion qubits* DANIEL COLE (Presenter), STEPHEN D ERICKSON, Time & Frequency Division, National Institute of Standards and Technology Boulder, KARL HORN, Department of Physics, Universität Kassel, FLORENTIN REITER, Institute for Quantum Electronics, ETH Zürich, PANYU HOU, JENNY WU, Time & Frequency Division, National Institute of Standards and Technology Boulder, CHRISTIANE KOCH, Department of Physics, Freie Universität Berlin, ANDREW C WILSON, DIETRICH LEIBFRIED, Time & Frequency Division, National Institute of Standards and Technology Boulder — The generation of entanglement using engineered dissipation has recently attracted attention because this approach can be competitive in fidelity and robustness against noise when compared with methods of entanglement generation based on controlled unitary evolution, and can enable optical pumping directly into entangled resource states for quantum protocols [1]. In a dissipative entanglement generation scheme, population is trapped in a target entangled state through evolution according to dissipative dynamics that have the target state as a steady state. We will discuss the generation of entangled states of hyperfine beryllium-ion qubits using engineered dissipation. In particular, we will present experimental realization of a ‘second generation’ scheme for dissipative production of an entangled singlet state that offers an improvement in speed and fidelity, along with reduced experimental complexity [2]. This scheme involves engineering suitable spin-motion couplings in the Hamiltonian, which are then combined with dissipation in the form of pumping to and decay from an electronic excited state.


*NIST Quantum Information Program
IARPA LogiQ Program

4:30PM P01.00011: Surface-science studies of electric-field noise from ion-trap electrodes DUSTIN HITE (Presenter), KYLE MCKAY, PHILIP KENT, DAVID PAPPAS, National Institute of Standards and Technology Boulder — Heating of the motional modes of ions in a rf Paul trap is a major obstacle to trapped-ion quantum information processing (QIP). It is caused by electric-field noise from the surface of the trap electrodes, which couples to the ions’ net charge. A better understanding of the physical origin of this surface noise will help to mitigate this heating in trapped-ion QIP applications. To aid in tackling this problem, our group has constructed a one-of-a-kind trapped-ion surface probe, where the ion is used to measure noise from the surfaces of nearby samples positioned into close proximity. This novel surface probe is operated in situ with traditional surface science tools, namely SPM, XPS, and SPA-LEED, where the sample is transferred from instrument to instrument in vacuum. Various treatments to the sample surfaces will elucidate possible origins of the noise. For example, in situ cleaning of the trap electrodes by Ar-ion bombardment reduces this noise by 1 – 2 orders of magnitude. In this talk, I will describe the composition and surface-potential landscape of typical as-fabricated and treated ion-trap electrodes and show results where we have demonstrated the efficacy to use trapped ions as a probe to nearby surfaces.
Towards Improved Quantum Simulations and Sensing via Parametric Amplification  
MATTHEW AFFOLTER (Presenter), ELENA JORDAN, KEVIN A. GILMORE, SHAUN BURD, JOHN JACOB BOLLINGER, NIST - Boulder — Improving spin coherence is a fundamental challenge in quantum simulations and sensing experiments on trapped ions. Here we discuss preliminary experiments attempting to enhance spin-motion coupling in large ion crystals via parametric amplification without a reduction in the spin coherence. These experiments are performed on 2D crystal arrays of over a hundred Be\(^+\) ions confined in a Penning trap. This device has been used to perform quantum simulations and sense displacements of the ion crystal that are small compared to the ground state zero-point fluctuations\(^1\). By modulating the trapping potential at twice the center-of-mass mode frequency, we squeeze the motional mode, which can enhance spin-motion coupling while maintaining the spin coherence. This should enable higher fidelity simulations and improve our sensitivity to small displacements.
\(^1\)K. A. Gilmore et al. PRL 118, 263602 (2017).

Quantum measurement and many-body dynamics for the Dicke model  
YUNJIN CHOI (Presenter), SHANE KELLY, SHAN-WEN TSAI, University of California, Riverside — The Dicke model (DM) is a well-suited system for exploring enhanced metrology and quantum information processing. An entangled spin-boson cat-state in the DM is obtained when the spin and boson degrees of freedom interact in the strong coupling limit. This entangled spin-boson cat-state is a metrological resource to the spin cat-state in terms of the spin degrees of freedom. However, it is difficult to experimentally explore features of coherence of the entangled spin-boson cat state, and it is hard to control and measure the boson and spin degrees of freedom simultaneously. Treating the spin subsystem as the main system of interest, we consider the bosonic degrees of freedom as an environment that can be controlled and probed to some extent. We investigate a measurement process on the bosonic system to extract partial information about the spin system. The degree to which the spin system is affected by such a measurement can be controlled by the coupling strength between the spin and boson systems. We also discuss the measurement context on the bosonic system to preserve or retrieve coherence of the spin subsystem.
Study of the mechanical loss of amorphous mirror coatings for gravitational wave detectors using two level system model

JUN JIANG (Presenter), ALEC MISHKIN, University of Florida, KIRAN PRASAI, RICCARDO BASSIRI, MARTIN M. FEJER, Stanford University, HAI-PING CHENG, University of Florida — For future generation of laser interferometer gravitational-wave observatory (LIGO), thermal noise from amorphous mirror coatings will be a limiting noise source in the most-sensitive frequency band (about 150 Hz). In our previous studies, two level system (TLS) model was used to study the mechanical loss of the pure and doped amorphous SiO$_2$, Ta$_2$O$_5$ coatings. With reverse Monte Carlo (RMC) method, we generate amorphous models for both as-deposited and heat treated samples based on measurements of grazing-incidence pair distribution function (GI-PDF). In this work, we further refine the RMC models of 50% ZrO$_2$ doped Ta$_2$O$_5$ with first-principles atomic structure relaxation and improve the previous TLS model by correctly taking into account two relaxation times associated with one asymmetrical TLS transition. From the mechanical loss calculation based on these models, we find that annealing will partially eliminate voids (or pores) larger than 200 Å$^3$ and smaller than 100 Å$^3$ making the atomic structures more uniform, which is correlated with high mechanical loss at low temperature.

This work is supported by the NSF through grants PHY-1707870 and PHY-1404110.

Atomic Tritium Production and Trapping for Neutrino Mass Measurement in Project 8

ALEC LINDMAN (Presenter), Johannes-Gutenberg Univ — Project 8 is a phased experiment using tritium β decay to investigate the absolute neutrino mass. Good energy precision, high statistics, and well-controlled systematics are required to reach an electron antineutrino mass limit of ≤ 40 meV. Our technique, Cyclotron Radiation Emission Spectroscopy (CRES), has achieved eV-scale resolution at 17.8 keV, near the tritium endpoint. Project 8 was the first to observe the fW-scale radiation from individual electrons. The event rate in CRES scales with volume; we will instrument our fiducial volume with a spatially-resolving antenna array, eliminating pileup. Project 8 will be the first laboratory neutrino mass experiment to use atomic tritium (T). Decay of a T$_2$ molecule excites rovibrational states that smear the observed energy by 1 eV. The decay of T, however, has an energy smearing of ≤ 0.1 eV. Our baseline calls for trapping 30 mK atomic tritium in a 2-T-deep, 10+-m$^3$ superconducting magnetic bottle. I will discuss our approach to this large-volume atomic CRES experiment, focusing on production and handling techniques for recombination-prone tritium atoms.

This work is supported by the US DOE Office of Nuclear Physics, the US NSF, the PRISMA+ Cluster of Excellence at the University of Mainz, and internal investments at all institutions.
2:30PM P02.00001: Pressure-temperature-magnetic field phase diagram of the molecule-based multiferroic (CH$_3)_2$NH$_2$]Mn(HCOO)$_3$ AMANDA CLUNE (Presenter), NATHAN HARMS, KENNETH R O’NEAL, KEVIN ARTHUR SMITH, KENDALL HUGHEY, Chemistry, University of Tennessee, Knoxville, DIMUTHU OBEYSEKERA, JUNJIE YANG, Physics, Central Michigan University, JOHN HADDOCK, NARESH S DALAL, Chemistry and Biochemistry, Florida State University, ZHENXIAN LIU, Civil and Environmental Engineering, The George Washington University, JANICE LYNN MUSFELDT, Chemistry, University of Tennessee, Knoxville — We employ high pressure susceptibility and vibration spectroscopy to reveal the properties of (CH$_3)_2$NH$_2$]Mn(HCOO)$_3$. Combining with prior high field work, we unveil the $P$-$T$-$H$ phase diagram of this molecule-based multiferroic. Specifically, we focus on the behavior of the formate bending mode across the order-disorder temperature to expose the role of the formate ligand in the framework stability and symmetry.

2:42PM P02.00002: A new pulse-magnetic field diamond anvil cell* DANIEL JACKSON (Presenter), MUN K. CHAN, Pulse Field Facility, National High Magnetic Field Laboratory, Los Alamos National Laboratory — Measurements in extreme conditions provide valuable insight into material properties. Combining high magnetic field, high pressure, and cryogenics allows for smooth tuning of parameters in a 3-dimensional phase space. The highest magnetic fields are generated using pulse-field magnets and provide more than twice the maximum field compared to direct-current magnets, 100 T vs 45 T. However, pulse fields invariably generate eddy currents in any conductive parts. A diamond anvil cell (DAC) was designed with slits to reduce eddy current loop area. The DAC was machined out of titanium, a poor thermal conductor, and was machined using a tabletop 5-axis CNC. I will present preliminary results from measurements in pulse field at high pressure, and details of the design of the cell.

*DEJ aknowledge support from LANL LDRD XWR500
DEJ would like to thank Jon Betts, Fedor Balikerev and Dan Sun for help with development of these capabilities.
The Role of Hydrogen Bonding in Aromatic Molecular Crystals at High Pressures*  
HANNAH SHELTON (Presenter), Physics Division, Lawrence Livermore National Laboratory,  
PRZEMYSŁAW DERA, Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa,  
SERGEY TKACHEV, GSECARS, University of Chicago, TOMMY YONG, Department of Earth Sciences, University of Hawaii at Manoa — Noncovalent interactions wield remarkable control in molecular crystals, which can alter properties such as impact sensitivity and chemical reactivity. The presence of hydrogen bonding has been shown to stabilize organic molecular crystals against pressure-dependent polymorphism and amorphization. These effects can be seen in melamine (C\textsubscript{3}H\textsubscript{6}N\textsubscript{6}; 1,3,5-triazine-2,4,6-triamine) and resorcinol (C\textsubscript{6}H\textsubscript{6}O\textsubscript{2}; 1,3-dihydroxybenzene), which are used industrially to produce laminates, adhesives, and flame retardants. Melamine is chemically and structurally similar to many energetic materials, including TATB and RDX. In the crystalline state melamine forms corrugated sheets of individual molecules linked by extensive intra- and inter-plane N-H hydrogen bonds. In comparison, resorcinol has less hydrogen bonding ability as only two hydroxyl groups form intermolecular links. At high pressure, melamine experiences a symmetry change from monoclinic to triclinic above approximately 36 GPa in helium. Conversely, resorcinol remains crystalline to only approximately 6 GPa. Examining the high-pressure intermolecular interactions in these compounds may allow their improved utilization as chemical feedstocks and analogues for related energetic compounds.

*Prepared by LLNL under Contract DE-AC52-07NA27344.

Tuning Octahedral Tilting of Ruddlesden-Popper Chalcogenide via Pressure  
SHANYUAN NIU (Presenter), FENG KE, Stanford University, BOYANG ZHAO, JAYAKANTH RAVICHANDRAN, University of Southern California, YU LIN, WENDY MAO, Stanford University — Transition metal perovskite chalcogenides (TMPCs) are currently of substantial interest as a class of emerging semiconductors for optoelectronic and photonic applications. Ruddlesden-Popper (RP) phases of perovskite chalcogenides have been predicted to be promising candidates to achieve ferroelectric semiconductors with static polar order. Hybrid improper ferroelectricity can be realized in such n=2 RP compounds with $a^-a^-c^+$ tilt system as Ba\textsubscript{3}Zr\textsubscript{2}S\textsubscript{7} via coupling of out-of-phase octahedral tilting around in-plane directions and in-phase rotation mode around the stacking direction. However, experimentally obtained Ba\textsubscript{3}Zr\textsubscript{2}S\textsubscript{7} is in a higher symmetry centrosymmetric phase with only one octahedral tilting mode. Pressure offers a unique perspective to drive such octahedral tilting and study the phase transitions. We report the high-pressure study of Ba\textsubscript{3}Zr\textsubscript{2}S\textsubscript{7} up to 50 GPa using diamond anvil cells. In-situ Raman spectroscopy and X-ray diffraction analysis are carried out to probe the structural changes. Structural transitions of Ba\textsubscript{3}Zr\textsubscript{2}S\textsubscript{7} under pressure have been observed. Efforts in stabilizing the low-symmetry phases with hybrid improper ferroelectricity will also be discussed.
High Hydrostatic Pressure (0.5–2.5 GPa) Synthesis and Properties of Bulk “nnx” Rare-Earth Nickel Oxides ($R_nNi_nO_x$)*

SARA J IRVINE (Presenter), GREGORIO PONTI, QUINN D. B. TIMMERS, ZACHARY P. KUKLINSKI, JOHN MARKERT, Department of Physics, University of Texas at Austin — We have undertaken rare-earth and alkaline-earth substitutions in known nickel oxide phases, and a search for new such phases, using a hot press. We prepared starting materials both by ambient solid-state reaction (650°C–975°C) and by using high-oxygen-pressure (150–200 bar), high-temperature ($T \approx 1000°C$) syntheses, producing either nominal-composition mixed-phase $RNiO_x$ materials, or the nearly-simple-perovskite $RNiO_3$ phases, respectively. We then subjected such parent materials [$R = Pr, Nd, (La,Y)$], as well as hole- and electron-doped varieties, to high quasi-hydrostatic pressures using a hot piston-cylinder apparatus (5–25 kbar, i.e., 0.5–2.5 GPa) at high temperatures (950°C–1050°C). The technique¹ can include oxidizers (KClO₄), or can be naturally reducing, the latter augmentable by hydrogen. We report product phases; initial syntheses have provided specimens with decreases in undesired starting phases. Our study of other nickelate phases, e.g., $R_3Ni_3O_7$ and infinite-layer $RNiO_2$, with this technique is ongoing, exploring both steric effects and hole- ($Sr^{2+}$) and electron-doping ($Ce^{4+}$) in targeted $R_nNi_nO_x$ structures.


*Support from University of Texas, College of Natural Sciences Freshman Research Initiative.

Superconductivity of platinum hydride PtH*

TAKAHIRO MATSUOKA (Presenter), JIAM, University of Tennessee, Knoxville, MASAHIRO HISHIDA, Department of Materials Science and Technology, Gifu University, KEIJI KUNO, Environmental and Renewable Energy Systems Division, Gifu University, NAOHISA HIRAO, YASUO OHISHI, Japan Synchrotron Radiation Research Institute (JASRI), SHIGEO SASAKI, Department of Electrical, Electronic and Computer Engineering, Faculty of Engineering, Gifu University, KAZUSHI TAKAHAMA, KATSUYA SHIMIZU, Center for Science and Technology under Extreme Conditions, Osaka University — Pt has a strong electron-phonon (e-p) coupling [1]. On the other hand, the 5d conduction electrons show strong spin fluctuations on the short length and time scales, which suppress the superconductivity. In PtH, hybridization between Pt 5$d$ and H 1$s$ [2] and the resulting strengthened e-p coupling and $T_c$ above 10 K have been predicted [2-5]. We report the ac magnetic susceptibility, electrical resistance, and x-ray diffraction measurements of PtH in diamond anvil cells. At 30 GPa, when PtH is in a $P6_3/mmc$ structure, PtH exhibits the superconducting transition at 7 K. The observed $T_c$ is higher than that of powdered Pt by more than three orders of magnitude. It is suggested that the noble metal hydrides possibly have higher $T_c$ than elements.


*This study was supported by JSPS KAKENHI Grant No. 25800195, Specially Promoted Research (26000006), and by a Nikki-Saneyoshi (JGC-S) Scholarship Foundation Grant for Young Researchers.
**3:42PM P02.00007: O\textsuperscript{1} earthquake-like precursors: a MaxEnt-\(\mu\)SR MgO study**  
CAROLUS BOEKEMA (Presenter), CARLOS MORANTE, MINA TAVAKOLZADEH, San Jose State University, FRIEDEMANN T FREUND, NASA, AMES — Earthquake-like precursor O\textsuperscript{1} effects [1,2] are studied by analyzing Muon-Spin-Resonance (\(\mu\)SR) MgO data using Maximum Entropy (ME). [3,4] MgO is ideal due to its presence in the Earth's crust: O\textsuperscript{1} or positive-hole formation results from a 2-stage break-up of an O anion pair under high-T or high-P conditions. [2] As T increases above room temperature (RT) a small O-ion \% is predicted to produce an O\textsuperscript{1} state.[2] ME analysis of transverse field (TF; 100 Oe) \(\mu\)SR data of a 3N-MgO single crystal show above RT a Gaussian signal at 1.36 MHz and a Lorentzian signal at 1.4 MHz. For similar oxides like MnO, TF\(\mu\)SR show only the \(\mu\)O Gaussian signal, as positive muons probe near negative O ions. [3,4] The extra 1.4-MHz MgO signal indicates the existence of extended O 2p states. [1, 2] Between 200 & 400 °C where O\textsuperscript{1} formation occurs, we find evidence of a missing (3rd \(\mu\)SR) fraction. The relation of O-valency effects and earthquake-like precursors is discussed. 1] FT Freund, Nat Hazards Earth Sys Sci 7(2007) 1. 2] FT Freund et al, Phys Chem Earth 31(2006) 389. 3] C Boekema and MC Browne, MaxEnt 2008, AIP Conf Proc #1073 p260. 4] S Lee et al, HUIC Educ, Math & Eng Tech Conf, Uo HI (2013).

*Research is supported by ISIS, NASA, SJSU & AFC.

**3:54PM P02.00008: Relaxation, Viscosity and Density Scaling of the Hydrogen-bonded System Glycerol at Pressures above 5 GPa**  
WILLIAM OLIVER (Presenter), KEVIN W LYON, Univ of Arkansas-Fayetteville — Using Tg(P) data for glycerol up to very high pressures of 6.7 GPa, we reanalyze viscosity and relaxation data taken by several groups over different temperature and pressure ranges, constraining these earlier data with our isochronous Tg(P) curve. This analysis allows new insights into the pressure dependence of fragility in such glass forming systems over pressure ranges in which the hydrogen bonded network is broken up. Attempts at thermodynamic scaling are also discussed for glycerol over this large pressure range.

*Earlier parts of this work were supported by NSF-DMR grants. More recent work was supported in part by the Honors College and the J. William Fulbright College of Arts and Sciences at the University of Arkansas.
**4:06PM P02.00009: Observation of nine-fold coordinated amorphous TiO$_2$ at high pressures**

YU SHU (Presenter), High Pressure Collaborative Access Team, X-ray Division, Argonne Natl Lab, YOSHIOKONO, Geodynamics Research Center, Ehime University, GUOYIN SHEN, High Pressure Collaborative Access Team, X-ray Division, Argonne Natl Lab, YANBIN WANG, Center for Advanced Radiation Sources, The University of Chicago, ROSTISLAV HRUBIAK, High Pressure Collaborative Access Team, X-ray Division, Argonne Natl Lab — Understanding pressure-induced structural changes in amorphous dioxides (a-AO$_2$) is of great importance in many fields of science. Here we report new experimental results of high pressure polyamorphism in amorphous TiO$_2$ (a-TiO$_2$) with the Ti-O coordination number (CN) close to 9. Our experimental data show that CN increases from 7.2 at 15.7 GPa, to 8.8 at 70.2 GPa, and finally reaches a plateau ~8.9 at pressures up to 85.7 GPa. We find that CN of both crystalline TiO$_2$ and a-TiO$_2$ follows a similar and systematic dependence on the ratio ($\gamma$) of the ionic radii of Ti and O. The $\gamma$ of a-TiO$_2$ is 0.614 at 15.7 GPa, which is similar to that of baddeleyite-type TiO$_2$ (~0.61), and increases continuously with pressure. At 70.2 GPa, $\gamma$ of a-TiO$_2$ is 0.701, which is similar to that of cotunnite-type TiO$_2$ (~0.693). It appears that the CN=9 plateau of a-TiO$_2$ correlates to the cotunnite-type and Fe$_2$P-type polymorphs, which have the same CN=9 but correspond to different $\gamma$ values. This CN-$\gamma$ relationship is applicable to other a-AO$_2$ of a-SiO$_2$ and a-GeO$_2$. All three compounds show surprisingly consistent between CN and $\gamma$, implying a unified relation between CN and $\gamma$ in a-AO$_2$. The established CN-$\gamma$ relationship may be used to predict the compression behavior of a-AO$_2$ compounds to extreme conditions.

**4:18PM P02.00010: Enhancing broadband emission in indirect bandgap lead halide perovskites by hydrostatic pressure**

SHENYU DAI (Presenter), College of Electronics & Information Engineering, Sichuan University, ZHAOJUN QIN, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, VIKTOR G. HADJIEV, Texas Center for Superconductivity, University of Houston, CHONG WANG, School of Materials Science and Engineering, Yunnan University, ZHIMING M. WANG, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, GUOYING FENG, College of Electronics & Information Engineering, Sichuan University, JIMING BAO, Department of Electrical and Computer Engineering, University of Houston — Although broadband emission caused by self-trapped excitons (STE) has been widely studied in direct bandgap perovskites, few attention has been paid to indirect bandgap perovskites. Here we report that indirect bandgap all-inorganic perovskite exhibits typical STE induced broadband emission. We use diamond anvil cell to study the response of optical properties of 2D perovskite microplates to hydrostatic pressure. The broadband emission intensity increases significantly with increasing pressure, and the peak position is largely blue-shifted by 650 meV. The mechanism of these phenomena is discussed using experimental methods and theoretical calculations. This work shows a potential method to control and utilize indirect bandgap perovskites materials in optoelectronic devices.
Molecular-Like Equilibrium Behavior of Anatase Nanoparticles in Compressed Hydrothermal Conditions

HENGZHONG ZHANG (Presenter), Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China, JINYUAN YAN, MARTIN KUNZ, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States, BIN CHEN, Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China, JILLIAN F. BANFIELD, Department of Earth and Planetary Science, University of California, Berkeley, California 94720, United States — Nanocrystals are intermediate in size between molecules and micron-scale crystallites. They usually exhibit size-dependent properties and behaviors that are closer to the latter than the former. However, in this work, we found that small titania nanoparticles present molecular-like phase equilibrium behavior under compressed hydrothermal conditions, as evidenced by the fact that both the phase contents and particle sizes of involved titania nanoparticles can increase or decrease in response to altered temperature and/or pressure applied to shift a phase equilibrium. Thermodynamic analysis showed that the phase content of a solid nanophase contributes to the free energy change of the phase equilibrium, in contrast to the textbook knowledge that the thermodynamic activity of a pure solid phase equals one and as such the phase content of a pure solid phase makes no contribution to the equilibrium. This result suggests that much more frequent and stronger collisions among nanoparticles at high-T&P conditions can enhance the energy transfer among individual nanoparticles in a fluid, making them behave collectively more like solute molecules in a solution. This finding renews our understanding of the physical-chemical properties of nanoparticles with strong interparticle interactions.

Study on refractive index, EOS and polarizability of atomic, molecular and mixed gases at high pressures up to 60 MPa

CHENGJUN LI (Presenter), Institute of Fluid Physics, China Academy of Engineering Physics — The refractive index of initially transparent gases at high pressures is very important for shock velocity measurements in shock compression experiment since the measured shock velocity has to be modified by the refractivity of the initial sample. In this work, by using optical frequency domain interferometer (OFDI), we measured the refractive index of atomic (He, Ne, Ar, Kr, Xe), molecular (H2, D2, O2, N2, CO, CH4) and mixed gases (H2-D2, H2+Ar, D2+He, He-Ar, He-Xe) up to 60 MPa. The EOS of part of above gases were measured experimentally, while others were calculated. The polarizability of different gases were derived from their refractive index and density according to Lorentz-Lorenz formula. The mixing rule below 60 MPa were verified by the experimental results of mixed gases investigated in this work.
4:54PM P02.00013: Quasi One-Dimensional Compound and Superconductivity Induced by Pressure*  JINLONG ZHU (Presenter), Southern University of Science and Technology, JUN ZHANG, hpstar, XIANCHENG WANG, CHANGQING JIN, EX5, Institute of Physics, Chinese Academy of Sciences — Ba$_3$TiTe$_5$ was synthesized at HP/HT with infinite face-sharing octahedral TiTe$_6$ chains and Te chains along the c axis, exhibiting a strong 1D characteristic structure. The calculations confirmed the 1D conductor characterization, and can be considered a starting point to explore the exotic physics induced by pressure to move the 1D conductor to a high-dimensional metal. High-pressure techniques were employed to study the emerging physics dependent on interchain hopping, such as the Umklapp scattering effect, spin/charge density wave, superconductivity and non-Fermi liquid behavior. Finally, a complete phase diagram was plotted. The superconductivity emerges at 9GPa, near which the Umklapp gap is mostly suppressed. $T_c$ is enhanced and reaches a maximum of 6K at 37 GPa, where the SDW or CDW is completely suppressed, and a non-Fermi liquid behavior appears. Our results suggest that the appearance of superconductivity is associated with the fluctuation due to the suppression of the Umklapp gap and that the enhancement of the $T_c$ is related to the fluctuation of the SDW or CDW.

*National Key R&D Program of China under grant no. 2018YFA0305700, 2017YFA0302900, and 2015CB921300; NSFC under grant no. 11474344; National Natural Science Foundation of China (Grant no. U1530402)

5:06PM P02.00014: Non-uniform thermal gradient evolution in thermally cycled ytterbium silicate-silicon environmental barrier coatings  DAVID OLSON (Presenter), JEROEN DEIJKERS, KATHLEEN QUIAMBAO, JOHN T GASKINS, ELIZABETH OPILA, HAYDN N G WADLEY, PATRICK HOPKINS, Univ of Virginia — The primary purpose of barrier coating materials is to protect underlying media from harsh temperatures and/or environmental conditions that pose to undermine the performance of a system. Thus, materials with high thermomechanical stability and low thermal conductivity are choice candidates as thermal/environmental barrier coating top coats. Systems that implement a ytterbium-disilicate have shown to be promising candidates for next generation gas turbine engines. However, a robust examination of the microscale structural and thermal effects has yet to be performed over a range of cycling conditions. Considering the multi-phase, anisotropic constituents of such systems, a robust understanding of these mechanisms is necessary. In this work, we examine the microstructural and thermal evolution in ytterbium silicate-silicon environmental barrier coatings. The coating system cannot be defined by a single thermal conductivity, as local variations in thermal conductivity arise due to these multi-phase, anisotropic systems. Understanding the evolution and distribution of the thermal gradients associated with high-temperature steam-cycling is necessary for the continued development of these materials as hot-section components in gas-turbine engines.
Understanding the structural dynamics of ultrafast laser-induced melting is important for applications ranging from laser micromachining to warm dense matter experiments. Direct experimental observations of ultrafast melting have previously not been possible because of the small time and length scales involved. However, recent advances in ultrafast-electron-diffraction (UED) techniques [1] have opened up an exciting opportunity to study the transient atomic dynamics with femtosecond temporal resolution.

Here we report on the melting dynamics studies of femtosecond-laser irradiated metallic nanofilms with UED at relativistic energies. In our experiments, we employed 400nm, 130fs (FWHM) laser pulses as the heater and 3.2MeV, 350fs (FWHM) electrons as the probe. With this pump-probe technique, we have recently resolved for the first time the transition between heterogeneous and homogeneous melting regimes in warm dense gold [2]. These results provided a direct testing to predictions from molecular-dynamics (MD) simulations and revealed the melting sensitivity to nucleation seeds. We have also applied this technique to study the melting dynamics of tungsten with externally-driven defects from radiation damage [3]. We found that radiation-damaged tungsten liquefied at a lower temperature than pristine tungsten. Combining the experimental data with MD simulations allowed us to quantify, for the first time, how the ultrafast melting process is affected by radiation damage.


*This work is supported by DOE Office of Science, Fusion Energy Science under FWP 100182, and the DOE BES Accelerator and Detector R&D program.
3:06PM P03.00002: Nuclear Quantum Effects in Two-temperature Hydrogen via Orbital-free DFT Path Integral MD*  
SAM TRICKEY (Presenter), University of Florida, DONGDONG KANG, Physics, National University of Defense Technology, KAI LUO, Geophysical Laboratory, Carnegie Institution of Washington, VALENTIN KARASIEV, Laboratory for Laser Energetics, Univ. of Rochester, KEITH RUNGE, Materials Science and Engineering, Univ. of Arizona — Among systems at extreme conditions, hydrogen is special: its small nuclear mass implicates significant nuclear quantum effects (NQEs). An increasingly important set of extreme-condition systems has electrons driven to temperature $T_e$ far from the ion temperature $T_i$. For such two-temperature hydrogen, we report path integral molecular dynamics calculations driven by state-of-the-art orbital-free DFT calculations for the electrons. When the ratio of the ionic thermal de Broglie wavelength to their mean distance is larger than about 0.35, the ionic radial distribution function is strongly affected by NQEs. Moreover, NQEs induce a substantial increase in both the ionic and electronic pressures.

*S.B.T. and K.L. were supported by U.S. Dept. of Energy grant DE-SC0002139. D.K. was supported by Science Challenge Project of China grant TZ2016001, NSFC grant 11874424, the National Key R&D Program of China grant 2017YFA0403200, and by the China Scholarship Council. V.V.K. was supported by U.S. Dept. of Energy National Nuclear Security Administration award DE-NA0003856.

3:18PM P03.00003: A new capability for large-scale linear scaling Kohn Sham DFT calculations for materials at high temperatures.*  
SEBASTIEN HAMEL (Presenter), Lawrence Livermore Natl Lab, MANDY BETHKENHAGEN, Physics, University of Rostock, JOHN PASK, Lawrence Livermore Natl Lab, PHANISH SURYANARAYANA, Georgia Tech, BABAK SADIGH, Lawrence Livermore Natl Lab — We developed a new capability for the accurate and efficient quantum simulation of material properties across an extreme range of densities, pressures and temperatures. This code, SQDFT, enables the use of full Kohn-Sham quantum molecular dynamics from the condensed matter regime, through the warm dense matter regime and into the plasma regime, well beyond the previous state-of-the-art which was restricted to temperatures below approximately 100 000 Kelvins. We demonstrate this new capability by calculating the Hugoniot curve of different materials up to millions of degrees Kelvin and Gigabar of pressure and investigating the structural and transport properties of the materials under these extreme conditions. We also present a performance study of our SQDFT code on various supercomputing platforms. SQDFT scales linearly with system size which allows us to run full Kohn-Sham QMD simulations with several thousand of atoms.

*Funding Acknowledgement: This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. We gratefully acknowledge support from the Laboratory Directed Research and Development Program.
**3:30PM P03.00004: Atom-in-jellium equations of state and melt curves in the white dwarf regime**

DAMIAN SWIFT (Presenter), THOMAS LOCKARD, SEBASTIEN HAMEL, CHRISTINE J WU, LORIN BENEDICT, PHILIP A STERNE, HEATHER WHITLEY, Lawrence Livermore Natl Lab — Atom-in-jellium calculations of the electron states, and perturbative calculations of the Einstein frequency, were used to construct equations of state (EOS) from around $10^{-5}$ to $10^{7}$ g/cm$^3$ and $10^{-4}$ to $10^{6}$ eV for elements relevant to white dwarf (WD) stars. This is the widest range reported for self-consistent electronic shell structure calculations. Elements of the same ratio of atomic weight to atomic number were predicted to asymptote to the same T = 0 isotherm. A generalized Lindemann criterion based on the amplitude of the jellium oscillations, previously used to extrapolate melt curves for metals, was found to reproduce previous thermodynamic studies of the melt curve of the one component plasma with a choice of vibration amplitude consistent with low pressure results. For elements for which low pressure melting satisfies the same amplitude criterion, such as Al, this melt model thus gives a likely estimate of the melt curve over the full range of normal electronic matter; for the other elements, it provides a useful constraint on the melt locus.

*Work performed under the auspices of the U.S. Department of Energy under contract DE-AC52-07NA27344.

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**3:42PM P03.00005: First Principles Calculations of the Equation of State of MgSiO$_3$ in the Gigabar Regime**

FELIPE GONZALEZ (Presenter), Department of Earth and Planetary Science, University of California, Berkeley, FRANCOIS SOUBIRAN, Laboratoire de geologie de Lyon, CNRS UMR 5276, Ecole Normale Superieure de Lyon, HENRY PETERSON, BURKHARD MILITZER, Department of Earth and Planetary Science, University of California, Berkeley — The equation of state (EOS) of silicates at extreme conditions is of significant interest in planetary science and high-pressure physics. Using path integral Monte Carlo (PIMC) and density functional theory molecular dynamics (DFT-MD) simulations, we study the properties of MgSiO$_3$ enstatite in the regime of warm dense matter. We generate a consistent equation of state for MgSiO$_3$ over a wide range of temperature and density conditions, ranging from $10^4$ to $10^8$ K and 0.1- to 20-fold the ambient density. An analysis of the structural and thermodynamic properties of the liquid is provided as L and K shell electrons are ionized with increasing temperature and pressure. The shock Hugoniot curve, that we derived from our EOS, is in very good agreement with the experimental data available for megabar pressures. In the gigabar regime, shock experiments are predicted to reach maximal compression. We analyze the shape of the Hugoniot curve under these conditions and demonstrated that the shock compression is controlled by the ionization of L and K shell electrons of the three nuclei.

*NSF-DOE grant DE-SC0016248, DOE-NNSA grant DE-NA0003842, and the U.C. Lab. Fees Res. Prog. grant LFR-17-449059. F.G.-C. ack. CONICYT Postdoc fellowship, grant 74160058. Comp. Resources by Blue Waters and NERSC.
3:54PM P03.00006: Ionization Potential Depression in Dense Plasmas Predicted with Ab Initio Methods  BURKHARD MILITZER (Presenter), University of California, Berkeley, MAXIMILIAN BÖHME, Helmholtz-Zentrum Dresden-Rossendorf, GERARD MASSACRIER, Ecole Normale Superieure de Lyon, JAN VORBERGER, Helmholtz-Zentrum Dresden-Rossendorf, FRANCOIS SOUBIRAN, Ecole Normale Superieure de Lyon — The degree of ionization is an important quantity that directly affects the equation of state of plasmas as well as their optical and transport properties. At high density, the electronic states are affected by the interaction with nearby particles. In energy space, bound states are pushed closer to the continuous spectrum of free-particle states. These changes are typically encapsulated in the terms of ionization potential depression (IPD). An accurate description of IPD becomes important when spectroscopic measurements are employed to determine the thermodynamic state of plasmas. In their seminal work, Stewart and Pyatt (SP) have developed an analytical model to describe the IPD. However, in Physical Review E 97 (2018) 063207, diverging trends between SP predictions and ab initio results were reported for hot, dense aluminum. Here, we report results from a comprehensive set of density functional molecular dynamics simulations that were designed to study the IPD of different materials under various thermodynamic conditions. We analyze the strengths and weaknesses of SP models and discuss possible reasons why they may become unreliable at high density.

4:06PM P03.00007: High Temperature Density Functional Theory Calculations*  PATRICK HOLLEBON (Presenter), TRAVIS SJOSTROM, Los Alamos National Laboratory — Kohn-Sham density functional theory calculations are widely used as an accurate ab-initio approach to solving the many-body problem in the warm dense matter regime, encompassing conditions approximately ranging from 0.1 to 50 times solid density and temperatures from 0.5 to 100 eV. Nonetheless computational costs can quickly become prohibitive with rising temperature due to the growing number of partially occupied states involved. This is particularly pertinent for accurate molecular dynamics simulation that require large box sizes and timescales to reach convergence. For these reasons, orbital-free methods are an attractive alternative for temperatures beyond approximately 10 eV, however the increased computational efficiency of simple kinetic energy functionals comes at the cost of physical accuracy. Here we present a hybrid approach in which the Kohn-Sham equation is solved for the low-lying states only, whilst an orbital-free method is applied to describe the remaining electrons. Our hybrid methods are used to perform equation of state calculations in the warm dense matter regime which we then benchmark against conventional Kohn-Sham calculations.

*This work has been supported by the U.S Department of Energy and Los Alamos National Laboratory LDRD.
4:18PM P03.00008: Electron-thermal contribution to the equation of state model based on two-temperature quantum molecular dynamics simulations* LIN YANG (Presenter), JOHN EMRICH KLEPEIS, PHILIP A STERNE, HEATHER D WHITLEY, Lawrence Livermore Natl Lab, SHUAI ZHANG, Laboratory for Laser Energetics, University of Rochester — We present results using two-temperature quantum molecular dynamics (QMD) simulations to identify the electron-thermal contributions to the equation of state (EOS) and make comparison with the Purgatorio-based model. The two-temperature approach treats the electron and the ion temperature independently in a QMD simulation. We applied the method to some low-Z materials (B, BN, and B$_4$C) and a high-Z transition-metal oxide at temperatures ranging from room temperature to $10^6$ K and 1 to 5 times compression in densities. Our results suggest that the electron-thermal contribution begins to dominate around $1.2 \times 10^5$ K (10 eV) and is material as well as density dependent. For each material, we identify the temperature-density regime where the electron-thermal contribution is independent of ionic configurations. We illustrate our findings by comparing electron pressure and specific heat with Purgatorio-based model.

*Work performed under the auspices of LLNL under Contract DE-AC52-07NA27344.

4:30PM P03.00009: Atom-in-jellium equations of state for high Z elements TOM LOCKARD (Presenter), LORIN BENEDICT, CHRISTINE J WU, PHILIP A STERNE, DAMIAN SWIFT, Lawrence Livermore Natl Lab — We have previously reported atom-in-jellium (AJ) predictions of the equation of state (EOS) and melt locus of low- and mid-Z elements. Here we report equivalent results for a selection of high Z elements that are also under experimental investigation at high energy density facilities. In comparison with previous EOS models for these substances, based on Thomas-Fermi theory, the shock Hugoniot exhibits structures corresponding to the ionization of successive electron shells. Proportionately, the difference from TF theory is less than was found for lower Z elements, though it can still amount to a factor ~2 in pressure as each ionization occurs. The broad trend of the Hugoniot is however closer to TF predictions than was observed at lower Z. The cold curve and ambient isochore deduced from AJ calculations is generally quite close to the corresponding TF calculation.
4:42PM P03.00010: Multiscale Simulation Method for Plasma Flows  ABDOURAHMANE DIAW  
(Presenter), JEFF HAACK, MIKE MCKERNS MCKERNS, ROBERT PAVEL, Los Alamos National Laboratory — In high-energy density flows, a number of dynamical and structural data is needed to be collected at the microscale using first principles calculations. Experimental results and their analysis, on the other hand, are determined by measurements at the macro-scale in space over long scales in time. Thus, one major disparity that is currently inhibiting progress in this area is the extrapolation of microscale information into macroscopically relevant scales. Inertial confinement fusion experiments, for example, are fundamentally multi-physics in nature; understanding the connection between experimental observables, and the underlying microphysics, is needed to fully assess capsule performance. In this work, we use uncertainty quantification driven learning algorithms coupled with directed sampling to automate the learning of a multiscale model that is valid for both atomistic processes and continuum phenomena. The multiscale framework couples a molecular dynamics with a Boltzmann kinetic model to describe mesoscale phenomena, and which is tuned by minimizing the model error. We will discuss the code written to build a valid multiscale model relevant to high-energy density experiments, and how that tool may be leveraged to facilitate the learning of plasma models.

4:54PM P03.00011: Spin-orbit coupling in first-principles optical and X-ray spectroscopy spectra under WDM conditions  NILS BROUWER, VANINA RECOULES, MARC TORRENT  
(Presenter), CEA, DAM, DIF. France — The prediction and analysis of optical and X-Ray spectra of materials under WDM conditions is of great scientific interest. The Kubo-Greenwood (KG) formula associated with the Projector Augmented-Wave (PAW) approach [1] has proven its efficiency to compute these spectra and has been implemented in a few DFT codes, including the ABINIT code [2]. One important aspect when treating optical and X-Ray spectroscopy, especially for heavier elements, is the spin-orbit coupling (SOC).

We present some improvements in the implementation of the calculation of optical and X-Ray spectra. Spinors are now treated explicitly; SOC is added in the velocity operator and is taken into account in the dipole matrix elements in the KG formula. We are now able to predict the spin-orbit splitting and the ratio of the X-ray absorption edges correctly.

We present two applications in the WDM regime. We show that the inclusion of SOC allows for the correct description of the splitting and branching ratio of the L2/L3 edge in copper. We also show that SOC has a small and visible -- but still not sufficient -- effect on the optical properties of gold. We explore other options to improve the optical spectra of gold.

**5:06PM P03.00012: Quasi-isentropic compression of strongly nonideal plasmas: correlations, degeneracy and plasma phase transitions**  
VLADIMIR E. FORTOV (Presenter), Joint Institute for High Temperatures of Russian Academy of Sciences, RADII I. IL'KAEV, Federal State Unitary Enterprise RUSSIAN FEDERAL NUCLEAR CENTER - All-Russian Research Institute of Experimental Physics, MIKHAIL I. KULISH, Institute of Problems of Chemical Physics of Russian Academy of Sciences, PAVEL R. LEVASHOV, Joint Institute for High Temperatures of Russian Academy of Sciences, VIKTOR B. MINTSEV, Institute of Problems of Chemical Physics of Russian Academy of Sciences, MIKHAIL A. MOCHALOV, Federal State Unitary Enterprise RUSSIAN FEDERAL NUCLEAR CENTER - All-Russian Research Institute of Experimental Physics, DMITRY N. NIKOLAEV, Institute of Problems of Chemical Physics of Russian Academy of Sciences, VLADIMIR V. STEGAILOV, Joint Institute for High Temperatures of Russian Academy of Sciences — A series of experiments with intense quasi-isentropic compression of the plasma D2 and He were carried out to get strongly coupled nonideal plasma. Two-stage spherical explosively driven devices were used in these experiments. Recordary high parameters of strongly coupled deuterium plasma were obtained in the experiments: pressures up to 18 TPa and density up to 14 g/cc. Helium plasma was compressed ~ 200 times up to density of 8 g/cc and pressures of P ~ 5 TPa. Remarkable features of helium and deuterium plasma behaviour at these extremely high pressures, temperatures and densities are discussed with the use of nonideal plasma models as well as of the results of computer simulation calculations using first principle approaches. The different theoretical models of plasma phase transitions are discussed in comparison with shock wave experiments. Exclusively important role of quantum degeneracy effects as well as of strong correlation effects is analysed on the basis of the experimental data obtained.

**5:18PM P03.00013: Measurement of the fs laser-induced structural modification process inside transparent materials**  
LIN ZHANG (Presenter), ZHICHENG ZHONG, HAO JIANG, SHIYUAN LIU, Huazhong University of Science & Technology — Femtosecond laser pulses can cause structural modification when focused inside transparent material, which can be used in the formation of optical waveguides, 3D micromachining and other photonic machining applications. However, the structural modification process of the material is still unclear, which often occurs in the picosecond scale.  
Here, we proposed a pump-probe based method to detect the laser-induced structural modification process inside transparent material. A fs laser pulse was acted as the pump pulse and focused inside fused silica, while a linear chirped pulse was adopted to probe the pump area. According to the mapping relationship between time and frequency of the chirped pulse, we have obtained the time dependent refractive index change process and the structural modification process in a single shot measurement. Results show that the volume and refractive index of the modified area gradually increase with time. Besides, we also observed the static structure after the experiment, and the microscopic image shows a donut-like structure was formed at the shock region, a void surrounded by a compressed shell, which is consistent with the micro-explosion theory.


**Wednesday, March 4, 2020 2:30 PM - 5:18 PM**
Multiexciton quantum interference in semiconductor nanocrystal quantum dots*  
HIROKAZU TAHARA (Presenter), MASANORI SAKAMOTO, TOSHIHARU TERANISHI, YOSHIHIKO KANEMITSU, Institute for Chemical Research, Kyoto University — Semiconductor nanocrystal quantum dots are one of the most suitable materials to examine strongly confined electron-hole pairs. It is desired to clarify their multiple carrier dynamics such as carrier multiplication and charged exciton properties. Here, we studied ultrafast multiexciton dynamics immediately after photoexcitation using quantum interference measurements [1]. The dipole oscillations containing single excitons, biexcitons, and triexcitons were observed by using the phase-locked interference detection method in transient absorption spectroscopy. We found that multiexcitons form harmonic quantum coherence, i.e., dipole oscillations with integer multiples of the exciton resonance frequency [2]. The coherent dynamics also play an important role in photogeneration processes of multiexcitons [3]. These results provide a deep understanding of multiexciton dynamics leading to advanced optoelectronic devices.


*Part of this work was supported by JSPS KAKENHI (Grant No. 18K13481 and 19H05465).

Ultrafast molecular dynamics of strongly adsorbed species on oxide surface  
MD AFJAL KHAN PATHAN (Presenter), AAKASH GUPTA, MIHAI E. VAIDA, Univ of Central Florida — In this contribution, the ultrafast dynamics of molecules strongly attached to oxide surfaces are studied using the femtosecond pump-probe mass spectrometry technique. As a model system, the molecular dynamics of CD₃I with random orientations on amorphous CeO₂ thin films is studied. The reaction dynamics is monitored through the detection of reaction intermediates and final products with time-, mass-, and kinetic-energy resolution. In contrast to the previous studies on surface-aligned CD₃I on crystalline oxide films, in the current investigation, in which CD₃I has random adsorption geometries, the CD₃⁺ and I⁺ transient signal intensities decay after the radicals are formed. The decay time constant of I⁺ (8.0 ps) coincided with the formation dynamics of a new peak at mass 254 amu corresponding to I₂⁺. The decay time constant of CD₃⁺ (2.5 ps) coincides with the formation dynamics of a new peak at 144.5 amu, corresponding to a highly energetic CD₃I⁺, which is reformed at the surface due to the increased collision between the I and CD₃ fragments, facilitated by the random adsorption geometry of the CD₃I molecules. In addition, power dependence measurements and kinetic energy-resolved mass spectra are employed to gain insights into the surface reaction dynamics.
2:54PM P06.00003: Phase-resolved 2D coherent spectra of exciton-polaritons and biexcitons in a semiconductor microcavity*  JAGANNATH PAUL (Presenter), JARED K WAHLSTRAND, Nanoscale Spectroscopy Group, National Institute of Standards and Technology, ALAN BRISTOW, Department of Physics and Astronomy, West Virginia University — Monolithic semiconductor microcavities host exciton-polaritons when the exciton modes are near cavity resonance. The light-matter interactions increase and the electronic states are modified by strong coupling. Biexcitons are still present and interact with the lower polariton branch [1]. Many-body effects, such as excitation-induced dephasing and shifts, appear clearly in phase-resolved 2D coherent spectra (2DCS) in bare quantum well systems. However, to date published 2DCS in microcavity systems have examined the amplitude of the signal without the phase information. This is in part due to the strength and complexity of the optical interaction with the macroscopic sample. Here we use an experimental method that allows for capturing phase-resolved 2DCS for numerous polarization [2]. Measurements are performed on a sample containing an InGaAs quantum well as a function of the detuning between the cavity and exciton modes. Analysis of both the polariton and biexciton modes is reported.


*National Institute of Standards and Technology (Scientific and Technical Research and Services)

3:06PM P06.00004: Ultrafast thermal response of bismuth and indium nanoparticles near their melting points*  HUI XIONG, YUELI ZHANG, HANI ELSAYED-ALI (Presenter), Old Dominion University — The thermal response of Bi and In nanoparticles on carbon film and In nanoparticles embedded in Al are studied by ultrafast electron diffraction (UED) with a temporal resolution up to ~1.5 ps. The results show that the thermal response of nanoparticles near their melting points upon excitation by the femtosecond laser pulses deviates from that by heating under equilibrium conditions. A subset of the Bi nanoparticles and the In nanoparticles embedded in Al shows crystal integrity above their bulk melting points, consistent with transient superheating. For the Bi nanoparticles, this may be attributed to faceting of some of the nanoparticles, while for the embedded In nanoparticles the In/Al interface may suppress the growth of the In surface molten layer. We also investigated the anisotropic thermal expansion of the nanoparticles by measuring the angular shift of the diffraction peaks with UED.

*This study is based on research supported by the National Science Foundation under Grant No. 1708717.
3:18PM P06.00005: PT-Symmetry in Colloidal Quantum Dot Microdisk Lasers with Engineered Notches*  QINGJI ZENG (Presenter), EVAN LAFALE, University of Utah, ZHIQUN LIN, VLADIMIR V TSUKRUK, Georgia Institute of Technology, VALY VARDENY, University of Utah — Whispering gallery mode resonators are susceptible to parasitic splitting of clockwise and counterclockwise modes due to the sensitivity of optical modes to perturbations of the circular resonator boundary. This makes them useful devices for optical sensing and allow for evanescently coupling of modes of different resonators. We have studied laser mode behavior when a notch is engineered into the boundary of circular microdisk resonator based on colloidal quantum dots. We found substantive reduction of the parasitic mode splitting and enhanced emission directionality for resonators with by tuning the size of the notch. We also investigated the effects of Parity-Time (PT) symmetry in evanescently coupled microdisk pairs with variation of the gain and loss induced by the optical pump. We demonstrate that the exceptional point behavior of these systems can be controlled by the size of the engineered notch.

*This project is supported by MURI grant (MURI FA 9550-14-1-0037) at AFOSR

3:30PM P06.00006: Photogeneration and recombination dynamics of trions and biexcitons in CsPbX$_3$ nanocrystals revealed by double-pump transient-absorption spectroscopy*  ETSUKI KOBAYAMA (Presenter), SATOSHI NAKAHARA, HIROKAZU TAHARA, TOKUHISA KAWAKI, MASAKI SARUYAMA, RYOTA SATO, TOSHIHIKO TERANISHI, YOSHIHIKO KANEMITSU, Kyoto Univ — Lead halide perovskite nanocrystals (NCs) attract much attention because of their excellent optical properties such as high photoluminescence quantum yields. However, detailed dynamical processes of excitons, trions, and biexcitons have not been understood yet [1]. Here, we investigate the photogeneration and recombination dynamics of trions and biexcitons in all-inorganic perovskite CsPbX$_3$ (X = Cl, Br, I) NCs by conducting double-pump transient-absorption spectroscopy. In this method, the population of trions and biexcitons in NCs can be controlled by changing excitation intensity and time interval of two pump pulses. We revealed that Auger recombination of biexcitons and radiative and nonradiative recombination of trions determines ionization and neutralization processes in halide perovskite NCs [2]. In addition, we examined the difference in optical gain between single- and double-pump conditions. Our findings provide essential insights for low-threshold lasing.


*Part of this work was supported by JSPS KAKENHI (Grant No. 19H05465 and 18K13481).
3:42PM P06.00007: Observation and control of a photoinduced terahertz plasmonic mode in InAs mushroom arrays* SIEKHL RUBAIAT UL HAQUE (Presenter), Physics, University Of California, San Diego, XIAOGUANG ZHAO, Mechanical Engineering, Boston university, JINGDI ZHANG, Physics, Hong Kong University of Science and Technology, STEPHEN MARCH, SETH BANK, Electrical & Computer Engineering, The University of Texas at Austin, XIN ZHANG, Mechanical Engineering, Boston university, RICHARD AVERITT, Physics, University Of California, San Diego — Optical tuning of complex materials paves the ways towards control of macroscopic properties while also providing insight into novel physics under non-equilibrium conditions. We report the observation and control of a plasmonic resonance via photoexcitation in InAs mushroom metamaterial arrays. This is accomplished using optical pump broadband THz probe spectroscopy. A dramatic blueshift of plasmon resonance occurs (from ~1 to 7 THz) with increasing photoexcitation fluence. Clear signatures of plasmon-optical phonon coupling are observed, in agreement with simulations. In this presentation, we will clarify how the mushroom geometry provides dielectric isolation, thereby enabling broad photoinduced plasmonic tunability.

*The authors acknowledge funding from the Defense Advanced Research Projects Agency (DARPA), Defense Sciences Office (DSO) under the Driven Nonequilibrium Quantum Systems (DRINQS) program, grant number D18AC00014.

3:54PM P06.00008: Mapping out transient topological states in graphene by dichroic time-resolved photoemission* MICHAEL SCHUELER (Presenter), Stanford Univ, UMBERTO DE GIOVANNINI, HANNES HUEBENER, ANGEL RUBIO, MICHAEL SENTEF, Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany, PHILIPP WERNER, University of Fribourg, THOMAS DEVEREAUX, Stanford Univ — We study the build-up of the Floquet-Chern insulator state in graphene and its implications in time- and angle-resolved photoemission (ARPES). In particular, we show that the circular dichroism in the angular distribution is directly related to the induced pseudospin texture and thus the Berry curvature of the Floquet band structure. Our conclusions are corroborated by realistic time-dependent simulation under experimentally relevant conditions. Including electron-electron and electron-phonon scattering, we reveal the crucial role of scattering mechanisms for the effective thermalization of the Floquet band structure. These calculations are combined with accurate onestep calculations, yielding an excellent description of the circular dichroism in ARPES (CD-ARPES). Albeit the system is highly excited, we show that CD-ARPES provides the unique possibility of discerning light-engineered topological properties of the effective band structure and the Floquet side bands.

*We acknowledge financial support from the Swiss National Science Foundation via NCCR MARVEL and the European Research Council via ERC-2015-AdG-694097 and ERC Consolidator Grant No. 724103, and the Alexander von Humboldt Foundation for its support with a Lynen scholarship.
**4:06PM P06.00009: Time Resolved Investigation of Coherent Surface Phonon Polaritons**

PIERRE-ADRIEN MANTE (Presenter), Lund Univ/Lund Inst of Tech — The sub-wavelength confinement and enhanced electric field created by plasmons render accessible precise sensing and strong coupling at room temperature. [1, 2] However, the high frequency and short lifetime of plasmons inhibit the full potential of this technology and substitutes with longer lifetime and that can be studied in the time domain are being sought-after. [3] Here, we propose and demonstrate an experimental approach using femtosecond pump-probe spectroscopy allowing the time-domain study of surface phonon polaritons. We first build a theoretical framework for the generation and detection of these modes that we verify experimentally. By comparing experiments and Finite Difference Time Domain simulations we highlight that dark and bright modes are simultaneously generated. Thanks to this time-domain method, we then investigate mode dependent decay and energy transfer to the environment. Our observations open the way to deeper investigations of the role of coherence in the rich polariton physics.


*Grant 2017-05150 from the Swedish Research Council (VR).*

**4:18PM P06.00010: Superconducting Higgs Mode Metamaterials**

IAN HAMMOCK (Presenter), KELSON KAJ, SHEIKH RUBAIAT UL HAQUE, Physics, University of California, San Diego, CHUNXU CHEN, XIAOGUANG ZHAO, Mechanical Engineering, Boston University, KEVIN A CREMIN, GUFENG ZHANG, JACOB S SCHALCH, Physics, University of California, San Diego, JINGDI ZHANG, Physics, The Hong Kong University of Science and Technology, XIN ZHANG, Mechanical Engineering, Boston University, RICHARD AVERITT, Physics, University of California, San Diego — In this work, we investigate the possibility of using metamaterials to couple to the Higgs amplitude mode in an optimally doped thin film cuprate superconductor, YBa$_2$Cu$_3$O$_{7-d}$ (YBCO). To coherently drive the condensate amplitude, we employ table top high-field terahertz radiation coupled with field enhancement metamaterials (that also serve as a bandpass filter). We utilize a metamaterial “tape” design that allows us to adhere the subwavelength resonators to the YBCO film without the need for photolithography. We will describe the design of the metamaterial tapes and present our preliminary experimental results using these tapes to access non-equilibrium order parameter dynamics in superconductors.

*The authors acknowledge funding from the DARPA DSO under the Driven Nonequilibrium Quantum Systems (DRINQS) program, grant number D18AC00014*
4:30PM P06.00011: Plasmonic nano-focused spectroscopy and imaging: from few-fs dynamics to a new regime of nonlinear nano-optics  
YIJIAN CAI (Presenter), TAO JIANG, University of Colorado, Boulder, VASILY KRAVTSOV, ITMO University, MARKUS B. RASCHKE, University of Colorado, Boulder — Probing ultrafast dynamics and coherence with nm-fs spatio-temporal resolution is of crucial importance for understanding quantum coherence at the nanoscale and further advancing nonlinear optical applications. However, ultrafast nanoimaging has long been experimentally challenging. Our unique approach of combining grating coupled plasmonic nanofocusing with scanning probe techniques enables nonlinear optical imaging with nanometer spatial and femtosecond temporal resolution. We will discuss how spatial nano-confinement and near-field momenta provide new pathways for enhancing nonlinear frequency conversion where, e.g., plasmonic gradient-field effects amplify dipole-forbidden nonlinear responses. We further demonstrate non-local enhancement in four-wave mixing in graphene associated with Doppler broadening due to the broad distribution of near-field momenta. By implementing both spatio-spectral and spatio-temporal nanoimaging we can resolve the few-fs dynamics of electron coherence in graphene. We discuss the extension of these studies to other layered materials like transition metal dichalcogenides, providing insight into the heterogeneity of nanoscale electronic properties, enhanced frequency conversion, and roles of associated band structures, defects and grain boundaries.

4:42PM P06.00012: Terahertz Quasiparticle Dynamics and Control in Ca$_3$Ru$_2$O$_7$*  
KELSON KAJ (Presenter), KEVIN A CREMIN, Physics, University of California, San Diego, YU WANG, Physics, Pennsylvania State University, IAN HAMMOCK, MUSTAFA ALI, RUBAIAT HAQUE, GUFENG ZHANG, PETER KISSIN, Physics, University of California, San Diego, YAKUN YUAN, Materials Science and Engineering, Pennsylvania State University, DANIELO PUGGIONI, Materials Science and Engineering, Northwestern University, VENKATRAMAN GOPALAN, Materials Science and Engineering, Pennsylvania State University, ZHIQIANG MAO, Physics, Pennsylvania State University, JAMES RONDINELLI, Materials Science and Engineering, Northwestern University, RICHARD AVERITT, Physics, University of California, San Diego — We have investigated the terahertz electrodynamics of single crystals of the Ruddlesden-Popper ruthenate Ca$_3$Ru$_2$O$_7$ using optical-pump terahertz-probe spectroscopy. This correlated semimetal orders antiferromagnetically at $T_N = 56$ K, with the opening of a pseudogap (~2 THz) at $T_C = 48$ K. We predict that Ca$_3$Ru$_2$O$_7$ exhibits novel non-equilibrium states, with the possibility that excitation of c-axis apical oxygen phonons could result in novel phases absent from the equilibrium phase diagram. In the present study, we have investigated near-IR changes in the THz reflectivity following near-infrared excitation. We observe clear signatures of pseudogap dynamics in the spectrally resolved dynamics. In this presentation, we will present a detailed account of these dynamics along with an update of the phonon driven electrodynamic response.

*Work supported by the US Deparment of Energy (U.S. DOE), Office of Basic Energy Sciences (BES) under Grant No. DE-SC00012375.
4:54PM P06.00013: Topological light for the control of skyrmionic textures and spin waves*

MASAHIRO SATO (Presenter), Department of Physics, Ibaraki University, HIROYUKI FUJITA, Institute for Solid State Physics, University of Tokyo — Topological light is the laser whose wave front has a geometric singularity, and a typical one is the vortex beam carrying orbital angular momentum. Its several applications have been intensively studied in optics, while its potential have not been explored well in condensed-matter physics. Very recently, such structural lights have been gradually applied to find new photo-induced phenomena in solids. In the last few years, we have theoretically proposed ways of controlling magnetism with topological light [1-4]. Among them, I would like to report two proposals: a systematic way of creating ring-type spin textures such as skyrmioniums by applying high-frequency vortex beams to chiral magnets [1], and spin-wave resonance driven by terahertz vortex beams in ordered magnets [2]. These offer ways of printing the information about the beam onto magnets. [1] Fujita and MS, PRB 95, 054421 (2017). [2] Fujita, and MS, PRB 96, 060407(R) (2017). [3] Fujita and MS, Sci. Rep. 8, 15738 (2018). [4] Fujita, Tada, and MS, New. J. Phys. 21, 073010 (2019).

* M. S. was supported by Grant-in-Aid for Scientific Research on Innovative Area, “Nano Spin Conversion Science” (Grant No. 17H05174) and “Quantum Liquid Crystals” (Grant No. 19H05825) as well as JSPS KAKENHI (Grants No. 17K05513 and No. 15H02117).

5:06PM P06.00014: Low-Temperature Phases of Er$_{1-x}$Y$_x$FeO$_3$ Mapped Out by Terahertz Time-Domain Spectroscopy

NICOLAS MARQUEZ PERACA (Presenter), Department of Physics and Astronomy, Rice University, XINWEI LI, Department of Electrical and Computer Engineering, Rice University, MOTOAKI BAMBA, Department of Physics, Kyoto University, CHIEN-LUNG HUANG, Department of Physics and Astronomy, Rice University, NING YUAN, Department of Physics, Shanghai University, GARY T NOE, Department of Electrical and Computer Engineering, Rice University, EMILIA MOROSAN, Department of Physics and Astronomy, Rice University, SHIXUN CAO, Department of Physics, Shanghai University, JUNICHIRO KONO, Department of Physics and Astronomy, Rice University — When the strength of coupling between an ensemble of two-level atoms and a single mode of light becomes a significant fraction of the natural frequencies in the system, a novel regime of light-matter interaction, known as the ultrastrong coupling regime, emerges. As the coupling is further increased, a quantum phase transition, referred to as the superradiant phase transition (SRPT), is theoretically predicted to occur. To date, a SRPT in thermal equilibrium has never been realized experimentally, and even its observability is a topic of ongoing debate in the literature. However, there remains a strong possibility to observe a phase transition analogous to the SRPT in magnetically ordered systems, which would provide new insight into the underlying physics behind the original photon SRPT. In the present work, we performed an extensive study of the low-temperature phases of Er$_{1-x}$Y$_x$FeO$_3$ as a function of temperature, magnetic field and x through terahertz time-domain magneto-spectroscopy. Through comparison with our detailed calculations, we found that there is a phase transition that can be interpreted as a magnon analogue of the SRPT in an extended Dicke model and that the cooperative coupling of spins and magnons plays a key role in the experimental realization of this phenomenon.
Quantum sensing beyond the standard quantum limit with 2D arrays of trapped ions

Kevin Gilmore (Presenter), Matthew Affolter, Elena Jordan, NIST Boulder, Robert J. Lewis-Swan, Diego Barberena, Athreya Shankar, Murray J Holland, Ana Maria Rey, University of Colorado, Boulder, John Jacob Bollinger, NIST Boulder — Quantum sensing protocols using trapped-ions can enable detection of weak electric fields (<1 nV/m) by sensing displacements surpassing the Standard Quantum Limit (SQL) – the sensitivity achievable with a coherent state. We present experiments investigating the limits of electric field sensing via the excitation of the center-of-mass (COM) motion of 100s of ions in a 2D crystal. By coupling the mechanical motion of the ions to their spin states by way of an optical potential, the displacement of the ion crystal can be read out via the spin state [1].

Recently, phase stabilization of this optical potential has improved the sensitivity by an order of magnitude. Probing on resonance with the COM mode provides the maximum sensitivity to electric fields. Using a scheme that cancels the thermal and zero-point motion ideally allows for detection of displacements ~15 dB below the SQL. Currently, frequency fluctuations of the COM mode limit this sensitivity to ~5 dB below the SQL. With future improvements, we predict electric field sensitivities of ~1 nV/m. Electric fields of this size may be produced by dark matter candidates: axion and hidden photon dark matter in the neV (MHz) regime has not been experimentally explored at this level.

Spin-squeezing using optimized parametric driving

PETER GROSZKOWSKI (Presenter), Pritzker School of Molecular Engineering, University of Chicago, CATHERINE LEROUX, University of Sherbrooke, LUKE GOVIA, Raytheon BBN Technologies, AASHISH CLERK, Pritzker School of Molecular Engineering, University of Chicago — Spin-squeezed states are desirable for meteorological applications as they allow for sensing beyond the standard quantum limit. A variety of mechanisms for generating such states have been proposed theoretically, and in some cases, realized experimentally. Nevertheless, approaches that reach the Heisenberg-limited scaling (eg. 'two-axis twist') often require elaborate experimental setups, making them difficult to realize in practice, while ones that are more experimentally viable, (eg. 'one-axis-twist') have sub-optimal scaling. In this talk we consider a parametrically driven cavity, coupled to a spin ensemble. We show that a careful control of the parametric drive detuning and amplitude can let one achieve Heisenberg-limited scaling. We also discuss the impact of dissipation on performance. Our approach is general enough to be experimentally viable in a variety of systems including spin ensembles coupled to superconducting microwave cavities (e.g. [1]), but also spins that are strain-coupled to a nanomechanical resonator (e.g. [2,3]).


*This work is supported by the DARPA DRINQS program (award D18AC00015).

Detecting spin polarization in 2D MoSe2 with nitrogen vacancy centers in diamond

BO DWYER (Presenter), TROND I ANDERSEN, GIOVANNI SCURI, Harvard University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute of Materials Science, PHILIP KIM, HONGKUN PARK, MIKHAIL LUKIN, Harvard University — Since the isolation of monolayer graphene, the catalog of exfoliatable two dimensional materials has grown to include materials with a host of properties, including semiconductors, ferromagnets, and even superconductors. Of particular interest are the transition metal dichalcogenides (TMDCs), which in the monolayer limit are direct band gap semiconductors that support tightly bound excitons. Due to spin orbit coupling and a lack of inversion symmetry, spins in the two inequivalent K valleys are polarized, which has led to great interest in TMDCs for spin- and valley-tronic applications. While the spin properties of TMDCs have been studied with optical techniques, these offer limited spatial resolution and are difficult to extract quantitative values from. We report on progress towards the measurement of optically induced spin polarization in hole doped MoSe2 using nitrogen vacancy centers in diamond as nanoscale magnetic field probes. The close proximity of these sensors, coupled with available superresolution techniques, will enable nanoscale imaging and quantification of other exotic phenomena in TMDs such as the valley hall effect and imaging of Moire superlattice TMDC structures.

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3:06PM P07.00004: Observation of ac Photocurrent Vortices in Monolayer MoS$_2$ Using NV Centers* PAUL JERGER (Presenter), Pritzker School of Molecular Engineering, University of Chicago, BRIAN ZHOU, Department of Physics, Boston College, KAN-HENG LEE, MASAYA FUKAMI, FAUZIA MUJID, JIWOONG PARK, DAVID AWSCHALOM, Pritzker School of Molecular Engineering, University of Chicago — Photocurrents are central to understanding the interaction of light with matter. Although widely used, transport-based detection cannot resolve the spatial distribution of photocurrents and can suffer from low photocarrier collection efficiency. We demonstrate a contact-free method to spatially resolve photocurrents using nitrogen-vacancy (NV) centers in diamond, and discover that optical excitation of MoS$_2$ produces photocurrent vortices via the Nernst effect. We use a near-surface ensemble of NV centers to map the magnetic field profile of photocurrents in a monolayer of MoS$_2$ transferred onto the diamond surface. By synchronizing pulsed photoexcitation with NV ac magnetometry, we perform a quantum lock-in measurement to resolve time-dependent photocurrent densities as small as 20 nA/µm. Spatiotemporal measurements reveal a photocurrent rise time dependent on the sample's thermal properties. This work establishes a novel probe for optoelectronic phenomena, ideally suited to two-dimensional materials, for which making contacts is challenging and can alter the intrinsic material properties.


*This work is supported by the AFOSR, ARO, ONR, and NSF.

3:18PM P07.00005: Electric Field Sensing Using an NV Center Under Perpendicular Magnetic Field ZIWEI QIU (Presenter), ASSAF HAMO, URI VOOL, ANDREW PIERCE, RUOLAN XUE, TONY ZHOU, AMIR YACOBY, Harvard University — Nitrogen-vacancy (NV) centers in diamond can sense locally both magnetic and electric fields and hence may offer unique insight into strongly correlated matter. While NV magnetic sensing is well established, NV electric sensing is not yet widely utilized. Here we explored electric field sensing using an NV in the presence of a strong magnetic field acting perpendicular to the NV axis. We use shallow NVs (~20nm below the surface) in bulk diamonds and nanotips to explore the optimal conditions for electric field sensing. Under a perpendicular field, the original spin states mix into bright and dark states. These states hybridize with the $^{15}$N nuclear spin due to hyperfine interaction, giving rise to periodic modulations in the spin-echo signal. Surprisingly, this hyperfine coupling strength appears to be tunable by the magnitude of the perpendicular field and is linear at least up to 200G. These findings may offer a new pathway for prolonging the coherence of the nuclear spin.
3:30PM P07.00006: Diamond parabolic reflectors for nanoscale quantum sensing  BRENDAH SHIELDS (Presenter), NATASCHA HEDRICH, DOMINIK ROHNER, MARIETTA BATZER, PATRICK MALETINSKY, University of Basel — The nitrogen-vacancy (NV) center in diamond is an atomic-scale atom-like system with an electronic spin that can be initialized and detected optically, making it an exceptional system for quantum sensing of magnetic phenomena requiring high field sensitivity, fine spatial resolution, quantitative imagery [1, 2]. A particularly powerful approach is to incorporate the NV sensor in a scanning probe, allowing for nanometer spatial resolution. Key challenges for such a system are to ensure high collection efficiency and NV-sample spacing below a few 10s of nm.

We address these challenges with all-diamond parabolic scanning probes containing single NVs. The parabolic shape redirects 80% of the NV emission into a strongly collimated mode [3]. To achieve a small NV-sample spacing we truncate the probe apex such that the NV sits at the focus of the parabola for optimal collection efficiency while achieving a tip-to-sample spacing of < 50 nm. We demonstrate the performance of these scanning probes through magnetometry on antiferromagnetic, thin-film Cr$_2$O$_3$ [4].


3:42PM P07.00007: Extending the quantum coherence of a near-surface qubit by coherently driving the paramagnetic surface environment*  DOLEV BLUVSTEIN (Presenter), ZHIRAN ZHANG, CLAIRE MCLELLAN, NICOLAS RYAN WILLIAMS, ANIA JAYICH, Physics, University of California, Santa Barbara — Surfaces enable useful functionalities for quantum systems, e.g., as interfaces to sensing targets, but often result in surface-induced decoherence where unpaired electron spins are common culprits. Here we show that the coherence time of a near-surface qubit is increased by coherent radio-frequency driving of surface electron spins, where we use a diamond nitrogen-vacancy (NV) center as a model qubit [1]. This technique is complementary to other methods of suppressing decoherence and, importantly, requires no additional materials processing or control of the qubit. Further, by combining driving with the increased magnetic susceptibility of the double-quantum basis, we realize an overall fivefold sensitivity enhancement in NV magnetometry. Informed by our results, we discuss a path toward relaxation-limited coherence times for near-surface NV centers. The surface-spin driving technique presented here is broadly applicable to a wide variety of qubit platforms afflicted by surface-induced decoherence.


*NSF CAREER Grant No. DMR-1352660 and DARPA DRINQS program (Agreement No. D18AC00014)
3:54PM P07.00008: Observation of a quantum phase from classical rotation of a single spin
ALEXANDER WOOD (Presenter), LLOYD C. L. HOLLENBERG, ROBERT E SCHOLTEN, ANDY M MARTIN, School of Physics, University of Melbourne — The theory of angular momentum connects physical rotations and quantum spins together at a fundamental level. Physical rotation of a quantum system will therefore affect fundamental quantum operations, such as spin rotations in projective Hilbert space, but these effects are subtle and experimentally challenging to observe due to the fragility of quantum coherence. Here we report a measurement of a single-electron-spin phase shift arising directly from physical rotation, without transduction through magnetic fields or ancillary spins. This phase shift is observed by measuring the difference between the phase of a microwave driving field and that of a rotating two-level electron spin system, a phase difference that can accumulate nonlinearly in time. We detect the nonlinear phase using spin-echo interferometry of a single nitrogen-vacancy qubit in a diamond rotating at 200,000 rpm. Our measurements demonstrate the fundamental connections between spin, physical rotation and quantum phase, and will be applicable in schemes where the rotational degree of freedom of a quantum system is not fixed, such as spin-based rotation sensors and trapped nanoparticles containing spins.

*This work was supported by the Australian Research Council Discovery Scheme (DP150101704, DP190100949)

4:06PM P07.00009: Long-living coherences and magnetic sensing with strongly-coupled quantum spins driven by pulse trains
VIATCHESLAV DOBROVITSKI (Presenter), WALTER HAHN, QuTech, Delft University of Technology — The systems comprised of a large number of strongly coupled quantum spins, driven by trains of 180° pulses, often demonstrate long-living quantum coherences, extending far beyond the "usual" coherence decay time (e.g. Hahn echo decay time) [1-3]. This effect is generic for various spin systems in different dimensions, from 1D to ∞-D (where every spin is coupled to all others), and the appearance of the long-living coherences is associated with the accumulated effect of the spin dynamics during the pulses (such as rotation angle deviating from 180°, or finite pulse width).

In this work, we present the protocols that employ the long-living coherences for quantum-assisted sensing of ac magnetic fields. In these protocols the pulse polarity is periodically changed, thus modulating the effect of pulses, so that the resulting long-living coherence oscillates in time with the frequency depending on the ac magnetic field. We also discuss application of such protocols beyong sensing of ac magnetic fields, to other quantum-assisted metrology tasks.


*This work was supported by Dutch Research Council (NWO) and by DARPA DRINQS program.
4:18PM P07.00010: Phase-estimation optimization in GaAs quantum dots* ANGEL GUTIERREZ-RUBIO (Presenter), PETER STANO, DANIEL LOSS, RIKEN — We address the optimization of phase estimation in the context of GaAs quantum dots [1]. This allows to track the hyperfine field in real time with maximum precision, quenching the main dephasing source. We prove that the mean entropy is the ultimate figure of merit to be minimized for such a purpose, in contrast to the ubiquitous use of the variance in the literature [2,3]. In accordance, non-adaptive and feedback strategies for the tunable interaction times are devised. Whereas global optimization is out of reach, we provide with the optimal offline strategy among the class of memoryless patterns. Remarkably, it indefinitely sustains its maximum precision despite frequency fluctuations and is robust in terms of self consistency. Moreover, we devise a computationally feasible online method to improve the precision for a given non-adaptive strategy, which could be applied to the experimental realization of Kitaev's algorithm. Finally, the scaling of the achieved precision beyond the shot-noise limit is discussed.


*We acknowledge the project CREST JST (JPMJCR1675) through the Japanese Science and Technology Agency.

4:30PM P07.00011: Imaging the crossover between ohmic and hydrodynamic electron flow in graphene with a single spin magnetometer* ALEC JENKINS, SUSANNE BAUMANN, SIMON A MEYNEILL, HAOXIN ZHOU, DAIPENG YANG (Presenter), Department of Physics, University of California, Santa Barbara, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ANDREW LUCAS, Department of Physics, University of Colorado, Boulder, ANDREA YOUNG, ANIA JAYICH, Department of Physics, University of California, Santa Barbara — In conventional conductors, transport is typically dominated by electron-phonon and electron-impurity scattering, giving rise to a direct proportionality between current and electric field known as Ohm's law. In ultra-clean graphene devices where the momentum-conserving electron-electron interaction dominates, transport is expected to obey hydrodynamics in which the electrons behave like a classical fluid. By measuring the stray magnetic field created by the current flow, we directly image the crossover from ohmic to viscous flow in a high mobility graphene constriction using nitrogen-vacancy center magnetometry. At room temperature, current flow concentrates at the edges of the constriction regardless of carrier density, indicating ohmic transport. However, below 200K, we observe a crossover into the viscous flow where the current concentrates at the center of the constriction. Our imaging technique provides a direct observation of collision-dominated electron transport.

*We acknowledge support from NSF CAREER Grant No. DMR-1810544
CHARLOTTE BOETTCHER (Presenter), URI VOOL, Harvard University, JOEL WANG, Physics, MIT, GREG CALUSINE, DAVID K KIM, DANNA ROSENBERG, JONILYN YODER, MIT Lincoln Lab, AMIR YACOBY, Harvard University, WILLIAM OLIVER, Physics, MIT — High-impedance superconducting resonators are important tools for quantum information and quantum sensing, as their resilience to magnetic fields and their highly concentrated local electric fields allow for strong coupling to small defects.

We propose to use this technique to study condensed-matter systems, and particularly the properties of graphene in the quantum Hall regime. In the dispersive regime, a change in the density-of-states of graphene will affect the resonator mode, allowing for RF detection.

We will present a design of titanium nitride resonators, optimized for high electric and magnetic coupling, resilient to in-plane magnetic field up to several Tesla. In addition, we will discuss the hybrid devices combining such resonators with a graphene-hBN stack.

*This research was funded in part by the HRL Matisse program; and by the Department of Defense via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.

TIM HUGO TAMINIAU (Presenter), Delft University of Technology — Nuclear magnetic resonance (NMR) is a powerful method for determining the structure of molecules and proteins. While conventional NMR requires averaging over large ensembles, recent progress with single-spin quantum sensors has created the prospect of magnetic imaging of individual molecules and other spin systems. As an initial step towards this goal, isolated nuclear spins and spin pairs have been mapped. However, large clusters of interacting spins — such as found in molecules — result in highly complex spectra. Imaging these complex systems is an outstanding challenge due to the required high spectral resolution and efficient spatial reconstruction with sub-angstrom precision. Here we develop such atomic-scale imaging using a single nitrogen-vacancy (NV) centre as a quantum sensor, and demonstrate it on a model system of 27 coupled 13C nuclear spins in a diamond. We present a new multidimensional spectroscopy method that isolates individual nuclear spin interactions with high spectral resolution (< 80 mHz) and high accuracy (2 mHz). We show that these interactions encode the composition and interconnectivity of the cluster, and develop methods to extract the 3D structure of the cluster with sub-angstrom resolution. These results demonstrate a key capability towards magnetic imaging of individual molecules and other complex spin systems.

*We acknowledge support from the Netherlands Organisation for Scientific Research (NWO/OCW) through a Vidi grant, as part of the Frontiers of Nanoscience (NanoFront) program, and as part of the Quantum Software Consortium programme (project number 024.003.037 / 3368).
2:30PM P08.00001: Projecting NISQ-era quantum advantage with QAOA

GIAN GIACOMO GUERRESCHI (Presenter), Intel Corp - Santa Clara, JASON LARKIN, DANIEL JUSTICE, Software Engineering Institute, Carnegie Mellon University — A major milestone in quantum computing research is the demonstration of quantum supremacy, where some computation is performed by a quantum computer that is unfeasible classically. Recently, the efforts culminated in the experiment by Google's quantum teams and collaborators of sampling from random circuits. However, it is important to recognize that supremacy demonstrations based on artificial tasks bring very limited advantage for practical applications. A common problem used in benchmarking high performance computing is MaxCut, with applications in domains such as machine scheduling, image recognition, electronic circuit layout, and others. Maxcut has been used extensively, both theoretically and experimentally, to assess the performance of the hybrid Quantum Approximate Optimization Algorithm (QAOA), one of the leading candidates to demonstrate quantum advantage in the NISQ era. Here we project the performance of QAOA by considering the challenges due to its variational and stochastic nature and compare it with several among the best performing classical solvers in terms of time to solution and quality. The results demonstrate the importance of algorithm and problem selection and we discuss the performance data in the context of projecting NISQ-era quantum advantage.

2:42PM P08.00002: Small-parameter and operator series approaches for quantum approximate optimization*

STUART HADFIELD (Presenter), TAD HOGG, ELEANOR RIEFFEL, NASA Ames Research Center, Quantum AI Lab (QuAIL) — We show a calculus for analyzing algorithms based on quantum alternating operator ansatze, in particular the quantum approximate optimization algorithm (QAOA). Our framework relates cost gradient operators, derived from the cost and mixing Hamiltonians, to classical cost difference functions that reflect cost function structure. For QAOA we show an exact series expansion in the algorithm parameters and cost gradient operators. This enables analysis in different parameter regimes which yields novel insights. In the small-parameter regime, for single-layer QAOA-1 the leading-order change in solution probability is determined by cost differences; for sufficiently small parameters probability provably flows from lower to higher cost states on average (or vice versa via parameter selection). On the other hand, we derive a classical random algorithm which emulates QAOA-1 in the same small-parameter regime, i.e. outputs samples with the same probabilities up to small error. Our results apply generally under minimal cost function assumptions. For deeper QAOA-p circuits we derive analogous results in several settings. We discuss applications to performance, parameter setting, and design of more effective QAOA mixing operators.

*Supported by AFRL-ID (F4HBKC4162G001) & IARPA (IAA 145483).
Reinforcement Learning for Finding QAOA Parameters

YURI ALEXEEV (Presenter), Argonne Natl Lab, SAMI KHAIRY, Department of Electrical and Computer Engineering, Illinois Institute of Technology, RUSLAN SHAYDULIN, Clemson University, LUKASZ CINCIO, Los Alamos National Laboratory, PRASANNA BALAPRAKASH, Argonne Natl Lab — Quantum Approximate Optimization Algorithm (QAOA) is an important variational hybrid quantum-classical algorithm for approximately solving combinatorial optimization problems on NISQ devices. The quality of the solution obtained by QAOA depends on the performance of the classical optimizer used to optimize the variational parameters, but finding these optimal parameters can be hard to achieve. To address this problem, we formulate the problem of finding optimal QAOA parameters as a learning task in which the knowledge gained from solving training instances can be leveraged to find high-quality solutions for unseen test instances using two machine learning based approaches. We used reinforcement learning (RL) framework to learn a policy network to optimize QAOA circuits and a kernel density estimation (KDE) technique to learn a generative model of optimal QAOA parameters. In both approaches, the training procedure is performed on the small-sized problem instances, which can be simulated on a classical computer; yet the learned RL policy and the generative model can be used to efficiently solve larger problems. Our proposed RL and KDE based approaches reduce the optimality gap by factors up to 30 when compared to other commonly used standard optimizers.

Quantum approximate optimization of the exact-cover problem on a superconducting quantum processor

ANDREAS BENGTSSON (Presenter), PONTUS VIKSTÅL, CHRISTOPHER WARREN, Microtechnology and Nanoscience, Chalmers University of Technology, MARIKA SVENSSON, Computer Science and Engineering, Chalmers University of Technology, GÖRAN JOHANSSON, PER DELSING, GIULIA FERRINI, JONAS BYLANDER, Microtechnology and Nanoscience, Chalmers University of Technology — Superconducting qubits are one of the leading technologies for building useful quantum processors. Currently available devices, where error correction and fault tolerance is not yet possible, are usually referred to as noisy intermediate-scale quantum (NISQ) devices. Such processors hold yet great promise, for instance they might allow for running heuristic quantum algorithms solving combinatorial optimization. On small-scale quantum processors, these algorithms serve as important technology demonstrators. Here, we use the quantum approximate optimization algorithm (QAOA) to solve small instances of the NP-complete exact-cover problem. This problem has many real-world applications, such as work-shift scheduling and tail assignment for airlines. We implement the QAOA on our hardware platform consisting of two superconducting transmon qubits and one parametrically modulated coupler. We explore iteration levels of the algorithm up to two, and compare the performance of three different black-box optimizers. Our results show that the exact-cover problem can be solved by the QAOA with high success probability.
The QAOA is one of the candidates for quantum algorithms which might outperform classical approaches, while being amenable to NISQ devices. The target application for this approach is finding approximate solutions to combinatorial optimization problems. Since real world combinatorial optimization problems almost always have hard constraint, the algorithm was generalized to the Quantum Alternating Operator Ansatz. This approach consists of two alternating operators. First the phase separation operator which stems from the original cost function and second, a suitable mixing operator which explores the whole feasible subspace while conserving the hard constraints.

In this work, we present a Quantum Alternating Operator Ansatz for the problem of optimal assignment of airplanes to gates in a large airport hub. This is a hard operational planning problem with real world impact. We investigate several problem variations and their different relationships to NP-hard graph coloring problems. Our primary contribution is the development of novel mixing operators for the different problem settings and facilitate efficient QAOA implementation. For each case we analyse the quantum resource requirements and discuss the feasibility of using real-world problem input data.
3:30PM P08.00006: Probing topological defect formation in a quantum annealer  YUKI BANDO, Tokyo Institute of Technology, Nagatsuta-cho, Midori-ku, Yokohama 226-8503, Japan, FERNANDO J. GÓMEZ-RUIZ, 2. Donostia International Physics Center, E-20018 San Sebastián, Spain, MASAYUKI OHZEKI, HIROKI OSHIYAMA, NAOKAZU SHIBATA, 3. Tohoku University, Sendai 980-8579, Japan, YUKI USA, Tokyo Institute of Technology, Nagatsuta-cho, Midori-ku, Yokohama 226-8503, Japan, SEI SUZUKI, 4. Saitama Medical University, Moroyama, Saitama 350-0495, Japan, DANIEL A LIDAR, 5. University of Southern California, Los Angeles, California 90089, USA, ADOLFO DEL CAMPO (Presenter), 2. Donostia International Physics Center, E-20018 San Sebastián, Spain, HIDETOSHI NISHIMORI, Tokyo Institute of Technology, Nagatsuta-cho, Midori-ku, Yokohama 226-8503, Japan — When a quantum phase transition is crossed in finite time, the breakdown of adiabatic dynamics leads to the formation of topological defects. The average density of defects scales with the quench rate following a universal power-law predicted by the Kibble-Zurek mechanism. The later provides useful heuristics for adiabatic quantum computation. Physics beyond the Kibble-Zurek mechanism can be probed by characterizing the full counting statistics of topological defects. We argue that the distribution of the number of defects generally follows a Poisson binomial distribution with all cumulants exhibiting a universal power-law scaling with the quench rate. As an example, we report the exact kink number distribution in the transverse-field quantum Ising model. For this system, we test kink statistics in a D-Wave machine and show that the study of the kink number distribution can be used to benchmark the performance of a quantum processor.

References:
3:42PM P08.00007: Simulations of the Ising Model on a Shastry-Sutherland Lattice by Quantum Annealing* PAUL KAIRYS (Presenter), University of Tennessee, Knoxville, KELLY BOOTHBY, ISIL OZFIDAN, JACK RAYMOND, ANDREW D KING, D-Wave Systems, Inc., ARNAB BANERJEE, TRAVIS HUMBLE, Oak Ridge National Laboratory — The Ising Hamiltonian offers a versatile model for studying the microscopic behavior of several material systems. We study an Ising Hamiltonian on a geometrically-frustrated Shastry-Sutherland lattice, which has been used to explain the magnetic properties of the rare-earth tetraborides. Variants of this model can produce a complex phase diagram with emergent fractional magnetization plateaus. We present a novel embedding of the lattice into the D-Wave 2000Q processor and use forward and reverse annealing to compute the phase diagram and probe the magnetization plateaus in the classical limit of zero transverse field. Empirical results enable us to calculate the static structure factor in the different phases and critical regimes opening opportunities for direct comparisons to reciprocal-space experimental techniques. Using quantum Monte-Carlo calculations to validate our results, this work indicates that quantum annealing provides a versatile method of material simulation that can accelerate scientific discovery.

*This work is supported by the Department of Energy, Office of Science, Early Career Research Program. This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

3:54PM P08.00008: Excited-state search by quantum annealing toward quantum chemistry calculations* YUYA SEKI (Presenter), YUICHIRO MATSUZAKI, SHIRO KAWABATA, Nanoelectronics Research Institute, National Institute of Advanced Industrial Science & Technology (AIST) — We report two methods to obtain an excited state of a spin-1/2 system using quantum annealing (QA) and adiabatic quantum computation (AQC), and evaluate their performance based on the fidelity of the output states. Although QA and AQC has been developed to search ground states of Ising Hamiltonians, excited state is also required when we analyze quantum systems such as electrons in molecules. We propose two methods to obtain the excited states: methods using non-adiabatic transition and adiabatic transition. It is unclear which method is better under noisy environment. In order to compare the methods, we numerically solved the Lindblad master equation for a certain simple model, and compared their fidelity of output states. As a result, we found that the output of method using adiabatic transition was as high fidelity as the other even when the problem seemed to be difficult for the adiabatic method.

*This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO), Japan. This work was also supported by Leading Initiative for Excellent Young Researchers MEXT Japan, and is partially supported by MEXT KAKENHI (Grant No. 15H05870).
**4:06PM P08.00009: Isomer Search on the D-Wave Quantum Annealer**

*SUSAN MNISZEWSKI (Presenter), Los Alamos National Laboratory, JASON TERRY, University of Georgia, PROSPER AKROBOTU, University of Texas at Dallas, CHRISTIAN F. A. NEGRE, Los Alamos National Laboratory — Isomer search or molecule enumeration refers to the problem of finding all the isomers for a given molecule. Many classical search methods have been developed in order to tackle this problem. However, the availability of quantum computing architectures has given us the opportunity to address this problem with new (quantum) techniques. This paper describes a procedure for determining all the structural isomers of alkanes. We first formulate the problem as a quadratic unconstrained binary optimization (QUBO) problem. We use the D-Wave quantum annealer to enumerate all structural isomers of all alkanes with fewer carbon atoms (n < 10) than Decane (C10H22). The number of isomer solutions increases with the number of carbon atoms. We find that the sampling time needed to identify all solutions scales linearly with the number of carbon atoms in the alkane. We probe the problem further by employing reverse annealing as well as a perturbed QUBO Hamiltonian and find that the combination of these two methods significantly reduces the number of samples required to find all isomers.

*This research has been funded by Los Alamos National Laboratory (LANL) Laboratory Directed Research and Development (LDRD). And additionally by the National Science Foundation (NSF).*

**4:18PM P08.00010: Exploring phase transitions in a quantum dimer using a quantum annealer**

*BIBEK POKHAREL (Presenter), Univ of Southern California, KABUKI TAKADA, HIDETOSHI NISHIMORI, Tokyo Institute of Technology, DANIEL A LIDAR, Univ of Southern California — It is well known that problems with exponentially decreasing gaps can cause adiabatic quantum computation (AQC) to fail. However, this does not imply that open-system quantum annealing (QA) will also fail for these problems. We consider an archetypical problem that is classically trivial, but difficult for AQC: an Ising ladder exhibiting a first-order phase transition with an exponentially closing gap, and a second-order phase transition with a polynomially closing gap. We investigate the performance of QA at these quantum phase transitions/ gap scalings theoretically using open quantum systems theory and experimentally using the D-Wave quantum annealer.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.*
4:30PM P08.00011: Solving the Graph Isomorphism Problem on a Quantum Annealer* ZOE GONZALEZ IZQUIERDO (Presenter), ITAY HEN, Univ of Southern California, RUILIN ZHOU, Northwestern University — The Graph Isomorphism (GI) problem—the task of deciding whether two graphs are isomorphic—has garnered considerable interest both for its wide range of applications in industry and for its particular computational complexity. One possible approach is measuring certain graph invariants—quantities that remain unchanged under vertex relabeling. While a complete graph invariant that would unequivocally distinguish non-isomorphic graphs is yet unknown, the energy spectrum of the quantum Ising Hamiltonian is a possible candidate. This is the Hamiltonian implemented by commercially available quantum annealers, making quantum annealing a natural tool for solving certain hard instances of the GI problem. Following the lead of previous work, we use a D-Wave quantum annealer to distinguish between pairs of graphs with the same classical Ising spectrum by gathering statistics on the energy and other observables. We show that introducing a pause at intermediate points in the anneal yields clearly different results for graphs that had previously been undistinguishable using standard annealing schedules.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050.

4:42PM P08.00012: Optimizing annealing parameters using genetic algorithms* SAMUEL STROMSWOLD (Presenter), QuAIL, NASA Ames Research Center, FILIP WUDARSKI, USRA - Univ Space Rsch Assoc, ELEANOR RIEFFEL, QuAIL, NASA Ames Research Center — Quantum annealing is an emerging technology that has the potential to be useful for solving combinatorial optimization problems such as maximum satisfiability. Prior work showed that annealing times [1] and inclusion of pauses [2] can significantly impact the probability of obtaining exact solutions. Less is known about leveraging other parameters such as flux biases implemented on the most recent D-Wave 2000Q annealer. We seek to bridge this gap by using genetic algorithms to select parameters. We explore various statistical measures, such as stochastic for ranking settings. Evaluations are performed using the Ames Research Center annealer.


* We are grateful for support from NASA Ames Research Center, the Intelligence Advanced Research Projects Activity (IARPA), via IAA 145483, and the AFRL Information Directorate under grant F4HBKC4162G001. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of IARPA, or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Governmental purpose notwithstanding any copyright annotation thereon.
4:54PM P08.00013: Quantum annealing applied to ionic diffusion analysis  KEISHU UCHIMURA, School of Materials Science, JAIST, TOM ICHIBHA, Physical Sciences Directorate, Oakridge National Laboratory, KOUSUKE NAKANO, Condensed matter theory, SISSA, KENTA HONGO, Research Center for Advanced Computing Infrastructure, JAIST, RYO MAEZONO (Presenter), School of Information Science, JAIST — We applied the quantum annealing framework to a problem of ionic diffusions in solids. The problem has been one of the important issues both in scientific and industrial sense in the field of materials science, which originally attracted interests in the microscopic analysis of mechanical strengths but is recently getting more active in exploring better batteries because the ionic diffusions as the charge carriers affect the efficiency in the solid electrolytes. We developed a scheme to formulate the problem in terms of the mapping into a quantum spin systems described by the Ising Hamiltonian. A key quantity to describe the diffusion can be evaluated from the output of annealing simulations, which has been quite difficult to be obtained by classical counterparts.

5:06PM P08.00014: Experimentally Testing Quantum Critical Dynamics Beyond the Kibble-Zurek Mechanism*  FERNANDO GOMEZ-RUIZ (Presenter), Physics, Donostia International Physics Center, JIN MING CUI, YUN-FENG HUANG, CHUAN-FENG LI, GUANG-CAN GUO, CAS Key Laboratory of Quantum Information, University of Science and Technology of China, ADOLFO DEL CAMPO, Physics, Donostia International Physics Center — We experimentally verify the distribution of kink pairs resulting from driving a one-dimensional quantum Ising chain through the paramagnet-ferromagnet quantum phase transition, using a single trapped ion as a quantum simulator in momentum space. The number of kink pairs after the transition follows a Poisson binomial distribution, in which all cumulants scale with a universal power-law as a function of the quench time in which the transition is crossed. We experimentally verified this scaling for the first cumulants and report deviations due to noise-induced dephasing of the trapped ion. Our results establish that the universal character of the critical dynamics can be extended beyond the paradigmatic Kibble-Zurek mechanism, which accounts for the mean kink number, to characterize the full probability distribution of topological defects.

5:18PM P08.00015: Quantum Simulations of Superconducting Flux Circuits* THOMAS HALVERSON (Presenter), Information Sciences Institute, University of Southern California, LALIT GUPTA, Department of Physics, University of Southern California, MOSHE GOLDSTEIN, School of Physics and Astronomy, Tel Aviv University, ITAY HEN, Information Sciences Institute, University of Southern California — One of the main avenues being explored as of late to obtain quantum speedups by annealing is that of quantum simulations, wherein one performs measurements mid-anneal. To that aim, there is a tremendous ongoing effort to fabricate superconducting flux circuits which are non-stoquastic in their qubit representation. Because of this these circuits are thought to be “unsimulatable” by classical approaches such as quantum Monte Carlo; however, we present the results of a study which aims to simulate the circuit Hamiltonian directly by utilizing an infinite Hilbert representation that is, in fact, stoquastic. Our approach obviates the reduction to a qubit representation and produces results that we feel are more in spirit with the experiential setup.

* The research is based upon work (partially) supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050. This material is based on research sponsored by the Air Force Research laboratory under agreement number FA8750-18-1-0044.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P09 DQI: Quantum Foundations II 106 - Mark Wilde, Louisiana State University, Baton Rouge - Tag(s): Focus

2:30PM P09.00001: Objectivity In Different Quantum Reference Frames* THAO LE (Presenter), University College London, PIOTR MIRONOWICZ, PAWEL HORODECKI, International Centre for Theory of Quantum Technologies, University of Gdansk — Quantum Darwinism and its frameworks describe objectivity of quantum systems via their information in the environment. However, the observation of these environments must be done with respect to a frame of reference. Given so, is objectivity consistent across different reference frames? Here, we take the quantum reference frame structure of [1] and consider the scenario where system and environment are static particles distributed across space. In this prescription, entanglement and coherence are interchangeable frame-dependent properties, and statistical mixedness and classical correlations are equivalently interchangeable. We find that the consistency of objectivity depends on the distinguishability of states in all relevant quantum reference frames, which in turn depends on non-degenerate relative separations, sharp localisation, and sufficiently large macro-fractions.


*TPL acknowledges funding from EPSRC.
2:42PM P09.00002: The Nakano-Nishijima-Gell-Mann Formula From Galois Fields

SATOSHI TANDA (Presenter), TOMOO OHAGA, KEIJI NAKATSUGAWA, Applied Physics, Hokkaido University, TOSHIYUKI FUJII, Physics, Asahikawa Medical University, TOYOKI MATSUYAMA, Physics, Nara University of Education — If world has a finite compact space (\(I_{120}\): Poincare Dodecahedron) [1] and discrete coordinates [2,3], what happens? In this case, the problem of infinities in gravity and in the standard model might be avoided. To avoid this problem, quantum gravity theories such as the superstring theory or the loop quantum gravity are developing, but neither of those theories have been completed. We reconstruct the Nakano-Nishijima-Gell-Mann (NNG) formula by using a discrete Galois field without using continuous coordinate. When we reconstruct new theories with a Galois field, these new theories must satisfy fundamental conservation law related to unitary, Lorentz, and gauge invariance. Here, we reexamine previous model [2] using isospin \(I_z\). Consequently, instead of the NNG formula, we obtained the alternate formula \(Q = 2(n + I_z)\), where \(Q\) is charge number and \(n\) is multi-valuedness in Galois field. These results may be a starting point to develop a theory without many problems of infinity.


2:54PM P09.00003: Quantum Fields from Quantum Cellular Automata? A No-Go Theorem and a Path Forward

TODD BRUN (Presenter), LEONARD MLODINOW, Univ of Southern California — A quantum walk (QW) is a unitary analogue of a classical random walk, and a quantum cellular automaton (QCA) is a unitary analogue of a classical cellular automaton. QWs can be treated as the one-particle sector of a QCA. Since quantum walks on the body-centered cubic lattice give rise to relativistic wave equations in the long wavelength limit, it is natural to seek for QCAs that give rise to quantum field theories in a similar limit. We show that this can be done in one spatial dimension, with the QCA being naturally described in terms of creation and annihilation operators that create or destroy particle locally, evolve straightforwardly under the QCA unitary, and obey the usual anticommutation relations (ACR). However, generalizing this construction to two or more spatial dimensions fails: the requirements on the creation and annihilation operators are inconsistent with a local QCA. For a QCA to give rise to a quantum field theory in the long-wavelength limit, one must give up at least one of the desired properties. A likely choice is to give up the requirement that the creation and annihilation operators create and destroy localized states.
**3:06PM P09.00004: Quantum mechanics and the covariance of physical laws in quantum reference frames** [invited] FLAMINIA GIACOMINI (Presenter), Perimeter Inst for Theo Phys — In physics, every observation is made with respect to a frame of reference. Although reference frames are usually not considered as degrees of freedom, in all practical situations it is a physical system which constitutes a reference frame. Can a quantum system be considered as a reference frame and, if so, which description would it give of the world? In my talk, I will introduce a general method to quantise reference frame transformations, which generalises the usual reference frame transformation to a “superposition of coordinate transformations”. With this method, it is possible to describe states, measurement, and dynamical evolution in different quantum reference frames, without appealing to an external, absolute reference frame, and find that entanglement and superposition are frame-dependent features. The transformation also leads to a generalisation of the notion of covariance of dynamical physical laws, and to the possibility of defining the rest frame of a quantum system. This last feature allows us to find an operational definition of the relativistic spin of a Dirac particle, and to devise a "relativistic Stern-Gerlach experiment".

**3:42PM P09.00005: Quantum Mechanics of a Single Photon and the question of its Localizability in Space** HASSAN BABAEI (Presenter), Department of Physics, Univ of Illinois - Chicago, ALI MOSTAFAZADEH, Department of Mathematics and Physics, Koç University — We use the dynamical Maxwell equations to determine the space of state vectors of a single photon. We endow this space with a relativistically invariant positive-definite inner product to make it into a Hilbert space. We identify the Hamiltonian operator with the generator of time translations, construct momentum and helicity operators, and introduce a chirality (direction-of-time) operator. Next, we construct a position operator that has commuting components. These also commute with the helicity and chirality operators. We obtain the eigenstates of the position operator, which we identify with the localized states of the photon, and use them to determine photon's position wave function. The position wave function for the localized states has a delta-function singularity at a single point in space, but their electromagnetic fields diverge on a particular plane containing this point. This behavior turns out to be related to an implicit freedom in the choice of the position operator. Each choice for the position operator determines the plane at which the electromagnetic fields of a given localized state diverge.
**3:54PM P09.00006: Quantized Electromagnetic-Field Propagation in a General Non-Local and Non-Stationary Dispersive and Absorbing Medium**

VERNE JACOBS (Presenter), United States Naval Research Laboratory — We develop dynamical descriptions for the propagation of quantized electromagnetic fields, in the presence of environmental interactions. These descriptions are systematically and self-consistently developed in the complimentary Schrödinger and Heisenberg pictures. An open-systems (non-equilibrium) quantum-electrodynamics and quantum-statistical description is thereby provided for electromagnetic-field propagation in a general non-local and non-stationary dispersive and absorbing optical medium, including a fundamental microscopic treatment of decoherence and relaxation processes due to environmental collisional and electromagnetic interactions. Particular interest is centered on entangled states and other non-classical states of electromagnetic fields, which may be created by non-linear electromagnetic interactions and detected by the measurement of various electromagnetic-field correlation functions. Accordingly, we develop dynamical descriptions based on general forms of electromagnetic-field correlation functions involving both the electric-field and the magnetic-field components of the electromagnetic field, which are treated on an equal footing.

*Work supported by the Office of Naval Research through the Basic Research Program at The Naval Research Laboratory.

**4:06PM P09.00007: Probability arises from entropy in axiomatic information thermodynamics [Invited]**

MICHAEL WESTMORELAND (Presenter), Denison University — Axiomatic information thermodynamics (Entropy 2018, 20(4), 237) is a formal mathematical system that describes thermodynamic processes including those in which information is acquired, transformed or discarded. A central concept in the theory is the "eidostate", which is a simple array of possible states, including both thermodynamic macrostates and information records. Well-motivated axioms lead to an entropy function that describes the irreversibility of eidostate processes, and this function in turn leads to a unique probability measure for the states and records in a uniform eidostate. Does this development shed light on the kinds of reasoning available to physical agents that observe and intervene in the quantum world?

**4:42PM P09.00008: Emergence of the Born rule in quantum optics**

MORGAN WILLIAMSON (Presenter), BRIAN LA COUR, University of Texas at Austin — The Born rule provides a fundamental connection between theory and observation in quantum mechanics, yet its origin remains a mystery. We consider this problem within the context of quantum optics using only classical physics and the assumption of a quantum electrodynamic vacuum that is real rather than virtual. The connection to observation is made via classical intensity threshold detectors that are used as a simple, deterministic model of single-photon detection. By following standard experimental conventions of data analysis on discrete detection events, it can be shown that this model is capable of reproducing several observed phenomena thought to be uniquely quantum in nature.

*This work was supported by the Office of Naval Research under Grant No. N00014-14-1-2107.
Interaction-Free Energy Transfer  MORDECAI WAEGELL (Presenter), Institute for Quantum Studies, Chapman University, CYRIL ELOUARD, University of Rochester, BENJAMIN HUARD, Physics, Ecole Normale Superieure, ANDREW N JORDAN, University of Rochester — The interaction-free measurement scheme of Elitzur and Vaidman enables a probe particle to detect the presence of an object blocking one arm of a Mach-Zender (MZ) interferometer without the probe ever locally interacting with that object. THE MZ is tuned so that without the block, the dark port detector never fires. The presence of the block changes the interference pattern in the MZ, allowing the dark port to fire, in which case the block is detected while the probe traveled the unblocked arm. We consider a quantum block in the ground state of a confining potential, a superposition of inside and outside one arm of the MZ. When the dark port detector fires, the quantum block is localized inside the arm, which increases its energy. This energy is delivered by the probe even though it traveled the unblocked arm to reach the dark port, and we thus obtain interaction-free energy transfer. This effect obtains even though the coupling Hamiltonian is local.

Diffraction-based Interaction-Free Measurements*  SPENCER ROGERS (Presenter), University of Rochester, YAKIR AHARONOV, Chapman University, CYRIL ELOUARD, ANDREW N JORDAN, University of Rochester — We consider the problem of determining if a single-slit contains a bomb in its middle region using a single photon test. We notice that the quantum case allows the bomb to significantly increase the probability for the photon to reach certain detection positions, in particular the dark bands of the single-slit pattern. The bomb's presence can be inferred without exploding it when the photon lands at one of these positions. We thus find a diffractive extension to the interaction-free measurement protocol of Elitzur and Vaidman. In addition, we consider the role of time in interaction-free measurements. We find that, if the bomb is thought of as a measuring device which checks periodically if the photon is in its space, then it can only find the particle (and "explode") if its measurement rate is finite. The alternative is the Zeno limit, where the bomb acts like an infinite potential barrier. Critics of interaction-free measurement may find it interesting that the normal, non-Zeno bomb can be passed through without setting it off.

*This work was supported by the NSF grant DMR-1809343. Y.A. acknowledges support from the Israel Science Foundation (Grant 1311/14), Israeli Centers of Research Excellence Center “Circle of Light,” and the German-Israeli Project Cooperation.

Quantum mysteries for anybody: Solved  WILLIAM STUCKEY (Presenter), Physics, Elizabethtown College — In 1981, Mermin published a now famous paper titled, "Bringing home the atomic world: Quantum mysteries for anybody." Therein, he presented the 'Mermin device' that illustrates the conundrum of entanglement per the spin singlet state for the "general reader." He then challenged the "physicist reader" to explain the way the device works "in terms meaningful to a general reader struggling with the dilemma raised by the device." I will show how conservation per no preferred reference frame (NPRF) answers that challenge, but still leaves a mystery for those who seek dynamical explanation via hidden variables or 'causal influences'. Since NPRF also underwrites the postulates of special relativity, we see a common theme between relativistic and non-relativistic modern physics.
Session P15 DFD DSOFT: Drop II 210/212 - Daphne Klotsa, University of North Carolina at Chapel Hill

2:30PM P15.00001: Microfluidics platform for generation of microparticles and capsules through Electrohydrodynamics  DANISH EQBAL, VENKAT GUNDABALA (Presenter), chemical engineering, Indian Institute of Technology Bombay — In this work we present a microfluidics based implementation of electrohydrodynamics for generation microparticles and capsules. Electric fields are applied through a novel interface-crossing of the precursor single and double emulsion droplet. The particles are alginate based and the capsules have oil core with alginate shell. The particle and capsule sizes were investigated as functions of the applied electric field strength, when the droplet generation happened in the electrodripping mode. It was observed that the obtained particle/capsule sizes were much lower than non-EHD methods and the monodispersity is much better than external EHD approaches. Thus we show an efficient approach that couples EHD with microfluidics to generate uniformly sized microparticles and microcapsules.

3:06PM P15.00002: Numerical Modeling of In-Situ Curing of a Photopolymerizing and Spreading Drop with Applications in 3D-Printing*  SIDDHARTHA DAS (Presenter), VISHAL SIVASANKAR, HARNOOR SACHAR, SHAYANDEV SINHA, University of Maryland, College Park, DANIEL HINES, Laboratory for Physical Sciences — The key to understand droplet-based direct writing (DW) printing processes like Aerosol Jet Printing (AJP), Ink-jet printing, syringe printing, etc. is to quantify the behavior of ink droplets during deposition. For instance, the resolution of the print depends on minimum drop radius and also to the extent of the droplet spread (spreading radius). In this study, we investigate the spreading behavior of a polymer drop in conditions similar to that of the Aerosol Jet Printing (AJP) process. Here, the drop is undergoing simultaneous spreading and photopolymerization with timescales of \( \tau_s \) and \( \tau_p \) respectively. We conduct a comparative study of the droplet behavior for two cases, \( \tau_s \ll \tau_p \), where the spreading is much faster than polymerization and \( \tau_s \sim \tau_p \), where the spreading and polymerization have similar timescales. Droplet spreading is unaffected by the polymerization process in the former case. However, in the latter case the spreading of the droplet is hindered by the polymerization process due to a tremendous increase in viscosity. We further study this complex thermo-fluid-solutal dynamics by comparing the time dependent curing profiles for the two cases.

*NextFlex Consortium, Laboratory for Physical Sciences
3:18PM P15.00003: A Comparative Study of the Pattern Formation in the Drying Protein Droplets suspended in the De-ionized water ANUSUYA PAL (Presenter), GERMANO S IANNACCHIONE, Worcester Polytech Inst — Pattern formation in drying bio-relevant systems continues to attract major attention of the researchers because of its medical applications. Here, an extensive description of drying evolution and the final patterns are presented, highlighting the concentration dependence (from 1 to 13 wt%) on two globular proteins, lysozyme (Lys) and bovine serum albumin (BSA) prepared in de-ionized water. The drying process starts with a constant contact radius mode and shifts to a mixed-mode where both contact radius and contact angle changes. The contact angle decreases monotonically, whereas, the contact radius exhibits two regimes: an initial linear, and a later non-linear regime. Unlike linear regime, the non-linear regime is faster for Lys droplets. This results in the formation of a `mound'-like structure and a new feature, a `dimple' is observed in this structure and found to be influenced by the initial concentration. The cracks which are only seen near the edge of BSA droplets, are spread throughout Lys droplets. In particular, Lys shows a hierarchy from delaminated to spiral cracks, and the spirals obey the well-known logarithmic equations. The mean crack spacing is found to be smaller than BSA droplets, and finally, these patterns are interpreted using a mechanical shear mechanism.

3:30PM P15.00004: Flow of Emulsions with Insoluble Surfactant through Porous Media JACOB GISSINGER (Presenter), ALEXANDER Z ZINCHENKO, ROBERT H DAVIS, Chemical and Biological Engineering, University of Colorado Boulder — While our understanding of surfactants' effect on single-drop dynamics has recently been improving, the general rheology of confined and contaminated emulsions remains less characterized. In particular, complex multiscale behavior results when the drop size is larger than granular interstices. In such cases, the emulsion cannot be treated as a single phase and a droplet-resolved model is required. A pressure-driven, concentrated emulsion flowing through a packed bed of spheres is modeled using a three-dimensional boundary-integral algorithm. The emulsion is initially monodisperse and uniformly coated with surfactant, and subsequently advected using a recently-developed robust algorithm for insoluble surfactant transport, with added options for complex equations of state as well as drop breakup. The ensemble-averaged permeabilities of the drop and continuous phases are studied versus degree of contamination and capillary number, with an emphasis on the effect of surfactant on the droplet-breakup cascade. The possibility of daughter drops having a significantly different surfactant concentration, and therefore capillary number, compared to the original drops results in particularly rich local and global dynamics.
MARINA MACHADO DE OLIVEIRA, Chemical Engineering, University of Wyoming, JOSEPH R MURPHY, Physics, University of Wyoming, JOHN ACKERMAN, Chemical Engineering, University of Wyoming, WILLIAM RICE, Physics, University of Wyoming, VLADIMIR ALVARADO (Presenter), Chemical Engineering, University of Wyoming — Ice adhesion measurements for impact ice are critical for solving important aerospace challenges. Previous measurements have shown that the ice adhesion on surfaces of apparently identical materials differ significantly under similar measuring conditions. This striking observation indicates that surface properties, e.g. roughness, may significantly affect ice formation and its adhesion response. Roughness properties can regulate the water-air-substrate contact-line dynamics. In this work, we focus on water-air contact angle hysteresis on metal substrates of interest, e.g. aluminum, using a pendant-drop system over a frequency range 0.1-10 Hz. Surface roughness of metal substrates is measured using confocal microscope profilometry. To establish a quantitative correlation between roughness and contact angle hysteresis, we analyzed the spatial roughness correlation function, including its angular dependency. Contact angle hysteresis results reveal a weak dependency on frequency, but a strong function on anisotropy, spatial correlation and surface roughness. The effect depends highly on drop size, which might explain differences in ice accretion under atmospheric conditions.

*We acknowledge funding support from NASA Grant WY-80NSS17M0049

GESSE ROURE (Presenter), ROBERT H DAVIS, Department of Chemical and Biological Engineering, University of Colorado, Boulder — The method of froth flotation by small air bubbles has been traditionally used in industry to capture fine minerals and other hydrophobic particles. This method, however, has shown to not be efficient for capturing smaller particles. The present work is motivated by a new agglomeration method proposed to overcome this lack of efficiency. It consists of mixing a particle suspension and saltwater-filled droplets covered with semi-permeable oil layers. The present work investigates the two-particle dynamics of a solid particle and an expanding semi-permeable spherical drop in an external pure extensional flow field. The computational results from the numerical integration determine a collision efficiency, which describes the influence of hydrodynamic interactions and osmotic flow on particle capture. An engulfment parameter measures the relative effects of droplet growth and convective flow.
Experiments in liquid-spray physics  
GARY LAPHAM (Presenter), Mathematics, Maine Maritime Academy, JOHN MCHUGH, Mechanical Engineering, University of New Hampshire — Waves on the ocean surface interacting with solid objects create complex and visually spectacular patterns of spray. The solid object can be a breakwater, drilling rig, or a ship. Another spray-related case is the presence of large industrial tanks of liquid, and often dangerous liquids, that exist throughout the world. These tanks are becoming obsolete in great numbers. When such tanks burst it is often catastrophic. Recent experience has shown, that when such tanks burst, the resulting spray may shoot several hundreds of meters from the tank —distances that are not readily explained. These tanks often have a wall or dam (containment barrier) surrounding them in an attempt to contain a violent breach or leakage. When the tank bursts it is akin to the dam-break problem. A wall of water rushes forth and impinges on the barrier creating spray. Previous experiments (McHugh and Watt, 1998) considered the related configuration of a solitary wave impinging on a vertical wall. Present experiments discussed will include tank experiments that more closely model the bursting tank case and smaller-scale experiments that attempt to identify some of the fundamental mechanisms of spray formation.

The Cheerios Effect under a thin elastic film  
CARMEN LEE (Presenter), ABIGAIL BULLER, KARI DALNOKI-VERESS, McMaster Univ — An air bubble placed in a liquid bath will rise through the bath until it reaches the liquid-air interface. The surface tension of the interface will keep the bubble from escaping into the air, but the bubble will in turn deform the flat interface. An equilibrium is reached between the buoyant force of the bubble and the surface tension of the liquid. Furthermore, an air bubble will move along the interface to reach a minimum in potential energy, in this case, the maximum height. Two bubbles in proximity to each other will attract each other due to the surface deformation from the other bubble. This mechanism is analogous to the famous Cheerios effect. Here, we examine the effect of replacing the liquid-air interface with a thin, elastic film. By floating a thin film onto the surface of a clean water bath, we can precisely place two monodisperse air bubbles below and observe the attraction between the bubbles, while altering the interface. We examine the effect of the thin film on the equilibrium position of the bubble as well as the attractive force between the two bubbles and present a theoretical model.
4:30PM P15.00009: Stability limit of electrified droplets and bubbles* JUSTIN BEROZ
(Presenter), JOHN HART, JOHN W M BUSH, Massachusetts Institute of Technology MIT — In many physical processes, including cloud electrification, electrospray and electrocoalescence, droplets and bubbles are exposed to electric fields and may either remain whole or burst in response to electrical stresses. Determining the stability limit of a droplet exposed to an external electric field has been a century-long mathematical challenge, and the only analytical treatment to date is an approximate calculation for a free-floating droplet. In this talk, we demonstrate, experimentally and theoretically, that the stability limit of a conducting droplet exposed to an external electric field is described by a power law with broad generality that applies to the cases in which the droplet is pinned or sliding on a conducting surface or free floating. The power law is simply derivable by the variational principle, provided the physical quantities defining the instability are selected to be independent of an arbitrary variation of the system. Practically, our finding provides a simple formula that captures the parameter range of bubbles and droplets that can be supported on electrified surfaces.

*Financial support provided by grants from BAE Systems, MIT Deshpande Center, MIT Lincoln Laboratory (FA8721-05-C-0002) and NSF (CMMI-1346638 to A.J.H., CMMI- 1727565 to J.W.M.B.)

4:42PM P15.00010: Superpropulsion of liquid droplets in sharpshooter insects* ELIO CHALLITA (Presenter), RAGHAV ACHARYA, Georgia Institute of Technology, RODRIGO KRUGNER, United States Department of Agriculture, SAAD BHAMLA, Georgia Institute of Technology — Sharpshooters are plant-sucking agricultural pests that constantly discharge large quantities of discrete water-based droplet excreta while feeding on plant’s xylem. Owing to a catapult-like mechanism powered by a biological spring located at their anal stylus, sharpshooters are able to blast away discrete droplet excrements at high accelerations reaching 200 m/s². Here, we unravel the propulsion mechanism exploited by sharpshooters that enables them to optimize the droplet ejection kinematics. Unlike the take-off speed of a rigid projectile that is set by maximum speed of the launching spring, we find that the elastic liquid droplets in sharpshooters can achieve take-off velocities that are up 3X faster than the underlying spring. This ‘superpropulsion’ behavior reveals that the frequency of the insect stylus is tightly tuned to the Rayleigh frequency of droplets \( f_0 \sim R^{-3/2} \), providing insight into the physical limits on the maximum size and speed droplets in these extraordinary insects.

*NSF BIO

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P16 DQI: Multi-mode and 3D-Cavity Circuit QED Systems I Bruno Taketani, Univ Federal de Santa Catarina
SOPHIA SOSNINA (Presenter), JAMES WILLS, SIMONE D FASCIATI, SALHA JEBARI, GIULIO CAMPANARO, SHUXIANG CAO, PETER SPRING, TAKAHIRO TSUNODA, IAN YANG, PETER J LEEK, BRIAN VLASTAKIS, University of Oxford — Alternative qubit design is an active field of research in superconducting quantum systems. In particular, multi-mode quantum circuits can allow error-protected subspaces, nonlinear coupling for multi-qubit operations, and additional mechanisms for state readout or control. In this talk we introduce a simple multi-mode coaxial transmon qubit - a two-mode qubit with a dipole-like differential mode and a coaxial common mode. We discuss the qubit Hamiltonian, analyze its sensitivity to fabrication imperfections, and discuss the effects of quasi-particle tunnelling in this system. Finally, we consider extensions of the design to multi-qubit settings.

*This work was supported by the EPSRC, Oxford Quantum Circuits Ltd, and from the European Union's Horizon 2020 research and innovation programme under grant agreement MSCA-IF-EF-ST 832814.

JAMES WILLS (Presenter), SOPHIA SOSNINA, SIMONE D FASCIATI, SALHA JEBARI, GIULIO CAMPANARO, SHUXIANG CAO, PETER SPRING, TAKAHIRO TSUNODA, IAN YANG, PETER J LEEK, BRIAN VLASTAKIS, University of Oxford — We discuss experimental results on a multi-mode qubit operating within a coaxial circuit QED architecture. This device includes a two-mode coaxial transmon qubit with out-of-plane coupling to a coaxial LC resonator. We discuss the characterisation of devices using two-tone spectroscopy and coherence measurements. We observe a strong cross-Kerr coupling between the differential and common modes of the qubit, which results in a qutrit-like behavior. Finally, we investigate charge sensitivity in such a device, and discuss its potential as a novel probe of charge fluctuations in superconducting quantum systems.

*This work was supported by the EPSRC, Oxford Quantum Circuits Ltd, and from the European Union's Horizon 2020 research and innovation programme under grant agreement MSCA-IF-EF-ST 832814.
2:54PM P16.00003: Chiral cavity quantum electrodynamics in a 3D microwave lattice
coupled to a transmon qubit (Part 1)*  MARGARET PANETTA (Presenter), University of Chicago,
CLAI OWENS, California Institute of Technology, SRIVATSAN CHAKRAM, BRENDAN SAXBERG,
GABRIELLE ROBERTS, University of Chicago, RUICHAO MA, Purdue University, JONATHAN SIMON,
DAVID I SCHUSTER, University of Chicago — Recent advancements in the ability to create and
manipulate superconducting quantum systems have created an exciting opportunity to construct
from the ground up quantum materials tailored to host rich interactions. We have designed a
two-dimensional meta-material in which microwave photons inhabiting a lattice of
superconducting 3D microwave cavities interact strongly with ferrimagnets, realizing a quarter-
flux Hofstadter model for light. We perform state tomography on the lattice and demonstrate
chiral, time-reversal symmetry broken edge transport with lifetimes ~1000 times larger than the
site to site tunneling rate. This is the first photonic topological lattice platform compatible with
strong interactions. We have coupled a single transmon qubit to this lattice, enabling this
platform to study chiral cavity quantum electrodynamics. Here we discuss the design and testing
of this system and describe prospects for its application.

*This work was supported by the Chicago MRSEC, which is funded by NSF through grant DMR-
1420709; and by ARO Grant No. W911NF-15-1-0397. It was also based on work supported by the
National Science Foundation Graduate Research Fellowship under Grant Nos. DGE-1144082 and
DGE-1746045.

3:06PM P16.00004: Chiral cavity quantum electrodynamics in a 3D microwave lattice
coupled to a transmon qubit (Part 2)*  CLAI OWENS (Presenter), Applied Physics, California Institute
of Technology, MARGARET PANETTA, SRIVATSAN CHAKRAM, BRENDAN SAXBERG, GABRIELLE
ROBERTS, JONATHAN SIMON, DAVID I SCHUSTER, Physics, University of Chicago — We have
previously realized a chiral meta-material for microwave photons. We now describe our
work combining a single transmon with this topological lattice, achieving, for the first
time, a platform for chiral cavity quantum electrodynamics. We show strong coupling
between the qubit and the topological lattice. Using the qubit we prepare arbitrary
quantum states of the lattice edge modes and we can non-destructively measure their
photon occupation. Finally, we describe a path towards coupling a transmon to each site
of the lattice, enabling exploration of a Harper-Hubbard model which is anticipated to
support fractional Chern insulating many-body phases.

*This work was supported by the Chicago MRSEC, which is funded by NSF through grant
DMR-1420709; and by ARO Grant No. W911NF-15-1-0397. It was also based on work
supported by the National Science Foundation Graduate Research Fellowship under Grant
Nos. DGE-1144082 and DGE-1746045.
3:18PM P16.00005: Driving a Dark State Qubit in 3D Waveguide QED* MAXIMILIAN ZANNER (Presenter), CHRISTIAN M. F. SCHNEIDER, Univ of Innsbruck, MATHIEU L. JUAN, OSCAR GARGIULO, IQOQI, Austrian Academy of Sciences, STEFAN OLESCHKO, Univ of Innsbruck, ALEKSEI SHARAFIEV, IQOQI, Austrian Academy of Sciences, GERHARD KIRCHMAIR, Univ of Innsbruck — The collective behavior of coupled qubits in a waveguide leads to sub-radiant and superradiant states. This effect was extensively studied theoretically and experimentally over the last decade. The appearing dark states can be used to generate an effective two level system that has longer coherence times than a single qubit in the same physical configuration. We engineered a system that creates subradiant and superradiant states by using a direct dipole-dipole, as well as a waveguide-mediated interaction. We show experimentally that this two-qubit dark-state can be used as a qubit state even though it is embedded in an open system. Furthermore, we use the bright state to read out the qubit encoded in the dark state.

*FWF, ÖAW, ERC, DK ALM

3:30PM P16.00006: Universal control of superconducting cavities with weak nonlinearity* ALEC EICKBUSCH (Presenter), SALVATORE S ELDER, Yale University, PHILLIPE CAMPAGNE-IBARCQ, QUANTIC Team, INRIA Paris, ZHENGHAO DING, SHANTANU JHA, NICHOLAS FRATTINI, CHRISTA FLÜHMANN, LUIGI FRUNZIO, ROBERT SCHOELKOPF, MICHEL H. DEVORET, Yale University — In superconducting cavities, fast universal control usually requires an inherited Kerr nonlinearity on the order of a few kHz. However, in many bosonic quantum error correction codes, such nonlinearities corrupt encoded information, causing errors. Recently, we have engineered an effective quadrature coupling between a cavity and an ancillary qubit based on an arbitrarily weak native dispersive interaction through the use of large phase space displacements. In this talk, we extend the idea of using large displacements in a cavity's phase space to perform universal control of a superconducting cavity with Kerr nonlinearity on the order of 1 Hz. This control will pave the way toward more sophisticated quantum error correction protocols applied to nearly linear bosonic systems.

*Work supported by ARO and YINQE
3:42PM P16.00007: Entangling Bosonic Modes via an Engineered Exchange Interaction*

[Invited] YVONNE GAO (Presenter), Natl Univ of Singapore, BRIAN LESTER, MICHEL H. DEVORET, LUIGI FRUNZIO, LIANG JIANG, STEVEN GIRVIN, ROBERT SCHOELKOPF, Yale University — The realization of robust universal quantum computation with any platform ultimately requires both the coherent storage of quantum information and (at least) one entangling operation between individual elements. The use of continuous-variable bosonic modes as the quantum element is a promising route to preserve the coherence of quantum information against naturally-occurring errors. However, operations between bosonic modes can be challenging. In analogy to the exchange interaction between discrete-variable spin systems, the exponential-SWAP unitary can coherently transfer the states between two bosonic modes, regardless of the chosen encoding, realizing a deterministic entangling operation in a programmable fashion. Here, we develop an efficient circuit to implement this unitary and realize the operation in a three-dimensional circuit QED architecture. We demonstrate high-quality deterministic entanglement between two cavity modes with several different encodings. Our results provide a crucial primitive necessary for universal quantum computation using bosonic modes.

*Y.Y.G. was supported by an A*STAR NSS Fellowship; B.J.L. is supported by Yale QIMP Fellowship; S.M.G. by the National Science Foundation (DMR-1609326); L.J. by the Alfred P. Sloan Foundation (BR 2013-049) and the Packard Foundation (2013-39273). Facilities use was supported by the Yale Institute for Nanoscience and Quantum Engineering (YINQE), the Yale SEAS cleanroom, and the National Science Foundation (MRSECDMR1119826)

4:18PM P16.00008: The Kerr-cat qubit: efficient readout and two-qubit gates*

NICHOLAS FRATTINI (Presenter), ALEXANDER GRIMM, SHRUTI PURI, CHAN U LEI, Yale University, MAZYAR MIRRAHIMI, QUANTIC team, Inria Paris, MICHEL H. DEVORET, Yale University — Superpositions of two opposite-phase coherent states in an oscillator, so-called Schrödinger cat states, can encode a noise-biased qubit, meaning a qubit with a strong protection against one error channel. Such a protected "cat qubit" has the ability to significantly reduce the overhead associated with quantum error correction in, for instance, a surface-code-style architecture. This overhead reduction relies on the ability to perform all gates in a manner that preserves the noise bias. In this talk, we review our implementation for the Kerr-cat qubit, which is based on the interplay between two-photon driving and Kerr nonlinearity. This scheme is compatible with fast, high-fidelity single qubit gates and achieves a strong noise bias. We will report on experimental improvements, the efficiency of the quantum non-demolition (QND) readout of this qubit, and our progress towards the realization of a noise-biased CNOT gate between two such Kerr-cat qubits.

*Work supported by: ARO, NSF, and YINQE.
4:30PM P16.00009: Multiplexed photon number measurement of a cavity using the fluorescence of a coupled qubit. * ANTOINE ESSIG (Presenter), QUENTIN FICHEUX, PERONNIN THEAU, NATHANAEL PIERRE COTTET, Université Lyon, ENS de Lyon, Université Claude Bernard, CNRS, Laboratoire de Physique, F-69342 Lyon, France, RAPHAEL LESCANNE, Laboratoire Pierre Aigrain, Département de physique de l'ENS, Ecole normale supérieure, PSL Research University, Université Paris Diderot, Sorbonne Paris Cité, Sorbonne Univer, ALAIN SARLETTE, PIERRE ROUCHON, Centre Automatique et Systèmes, Mines ParisTech, PSL Research University, 60 Boulevard Saint-Michel, 75272 Paris Cedex 6, France, ZAKI LEGHTAS, Laboratoire Pierre Aigrain, Département de physique de l'ENS, Ecole normale supérieure, PSL Research University, Université Paris Diderot, Sorbonne Paris Cité, Sorbonne Univer, BENJAMIN HUARD, Université Lyon, ENS de Lyon, Université Claude Bernard, CNRS, Laboratoire de Physique, F-69342 Lyon, France — Measuring the photon number of an electromagnetic mode in a quantum nondemolition manner is instrumental to control the quantum state of a cavity, detect photon emission or measure work. In the microwave domain it can be done using the dispersive coupling between the cavity of interest and a coupled Rydberg atom or superconducting circuit. This method has been used successfully to count up to about a dozen photons, to realize Quantum Zeno dynamics experiments, or count photon number parity. Yet this technique has constraints on the measurement time. In particular it increases with the maximal number of photons. In this contribution, we present a technique that avoids this constraint by using the resonant fluorescence of a qubit coupled to the resonator of interest and a multiplexing measurement of the fluorescence field. We show an experiment where an independent quantum state tomography can be performed on the resonator to compare the result of the conventional method to this new technique.

*We thank MIT Lincoln labs that provided us a Traveling Wave Amplifier. The project was supported by the foundation Simone et Cino Del Duca.

4:42PM P16.00010: Full characterization and universal control of a superconducting 3D transmon qudit* XIAN WU (Presenter), LUIS MARTINEZ, YANIV J ROSEN, JONATHAN L. DUBOIS, Lawrence Livermore Natl Lab — While high fidelity single qubit and two-qubit gates have been realized for transmons, use of higher levels as a quantum resource has not yet been systematically studied. Coherent control of these higher energy states offers a direct route to increasing the available quantum volume of a given quantum circuit. In addition, the increasing charge dispersion present in higher level states offers a unique tool for studying charge noise. Here, we use the lowest four levels of a 3D transmon as the quantum register, qudit, which is computational equivalent to two qubits. We measure the decoherence times for each of the excited state. We also demonstrate multiplexing readout and universal control of the qudit with a single drive line.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was partially supported by the LDRD19-DR-005, the DOE ASCR quantum testbed pathfinder and ASC Beyond Moore's Law program (LLNL-ABS-795437)
4:54PM P16.00011: Advancements in 3D cavity fabrication and design for improved multimode quantum memories*  ANDREW ORIANI (Presenter), SRIVATSAN CHAKRAM, KEVIN HE, ALEXANDER ANFEROV, AKASH DIXIT, JOHN CLAI OWENS, DAVID I SCHUSTER, University of Chicago — Superconducting multimode cavities can provide a hardware efficient means for quantum information storage and processing. To increase mode density, reduce cross-talk, and increase gate fidelities, it is important to build cavities with tailored mode spacing and very long coherence times. In this talk we present advances in materials processing and design of 3D microwave resonators to increase mode lifetimes beyond that of state-of-the-art aluminum cavities. This includes moving to higher Tc superconductors and quantifying the efficacy of various surface treatment procedures in reducing dissipative loss mechanisms. In doing so we will present a pathway for developing these cavities into novel 3D multimode architectures for next-generation randomly accessible quantum memories and processors.

*This research was supported by Samsung Advanced Institute of Technology Global Research Partnership.

5:06PM P16.00012: Towards strong multi-mode coupling between a transmon and a metamaterial resonator  SAGAR INDRAJEET (Presenter), Syracuse University, HAOZHI WANG, Quantum Electromagnetics Division, University of Colorado Boulder, B.L.T. PLOURDE, Syracuse University, MATTHEW D. LAHAYE, United States Air Force Research Laboratory, Rome, NY, MATTHEW D HUTCHINGS, Syracuse University, BRUNO TAKETANI, Univ Federal de Santa Catarina, FRANK WILHELM, Saarland University — A high density of modes can be produced using metamaterial resonant structures made from arrays of lumped circuit elements, to which a flux-tunable transmon qubit can be coupled. For such a system, we have measured the coupling strength of the qubit to multiple modes by tuning the flux and observing the splitting in the transmission of each mode. In these initial measurements, the coupling strengths were larger than the individual mode linewidths, but did not exceed the inter-mode spacing. We discuss approaches to decrease the mode spacing in this system and simulate the spectrum numerically. In addition, we discuss techniques for increasing the coupling strength between these modes and the transmon qubit. For appropriate parameters, we show that it will be to possible to reach the regime where the qubit can be coupled to multiple modes simultaneously, which will have applications in analog quantum simulations and multi-mode cQED.
Within the stopband, where the density of states is zero, no travelling modes are allowed through the waveguide. However, evanescent modes, exponentially localized around the atoms' position can give rise to atom-photon bound states as theoretically predicted in Ref. [1] and experimentally observed in a photonic crystal configuration on a chip [2]. Here, we report observation of an atom-photon bound state with a transmon qubit inserted in a three-dimensional rectangular waveguide. Rectangular waveguides naturally exhibit low-frequency cut-off and the atom-photon bound states shows stronger localization compared to a photonic crystal realization [3]. We provide evidence of exponential localization of the atom-photon bound states through spectroscopic measurements, study their radiative emission and coherent interaction.


*This research was supported by the Australian Research Council Centre of Excellence for Engineered Quantum Systems (EQUS, CE170100009),

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P17 DQI: Quantum Computing with Donor Spins 203 - RUICHEN ZHAO,
National Institute of Standards and Technology Boulder - Tag(s): Focus
2:30PM P17.00001: Demonstration and benchmarking of electron and nuclear 2-qubit logic gates with implanted donors in silicon* [Invited] ANDREA MORELLO (Presenter), Univ of New South Wales — Ion-implanted $^{31}$P donors in silicon have attained 1-qubit gate fidelities >99.9% [1]. Here we present the realization of a 2-qubit CNOT gate between weakly J-coupled electron spins, deploying our proposal of using the nuclear spins to detune the individual qubit frequencies [2]. In a second experiment we realize a nuclear 2-qubit CNOT gate using a two-donor cluster where both $^{31}$P nuclei are hyperfine-coupled to the same electron. The CNOT gate is obtained by performing a CZ gate via a geometric phase imparted through a 2$\pi$ rotation of the electron, preceded and followed by $\pi/2$ gates on one of the nuclei [3]. Gate-Set Tomography benchmarks the fidelity of this universal gate set, which approaches the threshold for fault-tolerant quantum error correction.


*Funded by Australian Research Council (CE170100012), DST (AUSMURI00002) and US ARO (W911NF-17-1-0200). Sandia National Laboratories is a multi-missions laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for DOE's National Nuclear Security Administration under contract DE-NA0003525.

3:06PM P17.00002: Driven dynamics of an electron coupled to spin-3/2 nuclei in quantum dots* ARIAN VEZVAEE (Presenter), Department of Physics, Virginia Tech, GIRISH SHARMA, School of Basic Sciences, Indian Institute of Technology Mandi, SOPHIA ECONOMOU, EDWIN BARNES, Department of Physics, Virginia Tech — The problem of hyperfine interaction between a confined electron in a self-assembled quantum dot and its surrounding nuclear spin environment features interesting physics. Driving of the electron spin leads to dynamic nuclear spin polarization of the bath, and feedback effects on the electron spin can qualitatively change its dynamics. While for most systems of interest the nuclei have a spin of 3/2 or higher, in which case quadrupolar terms are present, the majority of existing theoretical treatments assume a nuclear spin-1/2 bath. In this work, we present a comprehensive theoretical framework of a driven electron spin coupled to a nuclear spin-3/2 bath based on a mean-field approach, and we use it to study the effects of higher nuclear spin on dynamic nuclear polarization.

* This research is supported by NSF (award number 1839056).
Long-time noise characteristics of an isotopically-enriched silicon nuclear spin bath

MATTHEW D GRACE (Presenter), WAYNE M WITZEL, Sandia National Laboratories —

Electron spin qubits in silicon are known to have long coherence times, especially in isotopically-enriched materials with few nuclear spins. As a variety of silicon qubit devices are explored experimentally, it is useful to have a theoretical understanding of noise characteristics as induced by nuclear spins to know when other noise sources should be suspected. We present a quantitative study of nuclear spin dynamics for moderately-sized baths over a range of timescales. We approximate the quantum dynamics by adapting the cluster-correlation expansion (CCE) technique to calculate bath “flip-flop” probabilities, improving the accuracy of simulations for longer timescales by introducing random, projective measurements throughout the time evolution as a semiclassical approximation. In this way, we are able to estimate the spectral density of noise induced by a nuclear spin bath for a wide range of frequencies and study the variation for different instances of nuclear spin samples. We present results of our modified CCE technique, comparing it to exact analytical and numerical solutions. SAND2019-12116A

*SNL is a multimission laboratory managed & operated by NTESS, LLC, a wholly-owned subsidiary of Honeywell International Inc., for the US DOE's NNSA under contract DE-NA0003525.

A silicon quantum-dot-coupled nuclear spin qubit

BAS HENSEN, WISTER WEI HUANG, CHIH-HWAN YANG, KOK WAI CHAN, JUN YONEDA (Presenter), TUOMO I TANTTU, FAY E. HUDSON, ARNE LAUCHT, University of New South Wales, KOHEI M ITOH, Keio University, THADDEUS D LADD, HRL Laboratories, ANDREA MORELLO, ANDREW STEVEN DZURAK, University of New South Wales — Single nuclear spins in the solid state have long been envisaged as a platform for quantum computing. However, establishing long-range interactions between multiple dopants or defects is challenging. Conversely, in lithographically-defined quantum dots, tunable interdot electron tunneling allows direct coupling of electron spin-based qubits in neighboring dots. Moreover, compatibility with semiconductor fabrication techniques provides a compelling route to scaling. Unfortunately, hyperfine interactions are typically too weak to address single nuclei. In this presentation, we report that for electrons in silicon metal-oxide-semiconductor quantum dots the hyperfine interaction is sufficient to initialize, read-out and control single silicon-29 nuclear spins, yielding a combination of the long coherence times of nuclear spins with the flexibility and scalability of quantum dot systems. We demonstrate that the nuclear and electron spins can be entangled and that they both retain their coherence while moving the electron between quantum dots, paving the way to long range nuclear-nuclear entanglement via electron shuttling. Our results establish nuclear spins in quantum dots as a powerful new resource for quantum processing [1].

*Funded by the Australian Research Council (CE170100012) and the US Army Research Office (W911NF-17-1-0200)
3:54PM P17.00006: Coherent electrical control of a single high-spin nucleus in silicon

MARK JOHNSON (Presenter), SERWAN ASAAD, VINCENT MOURIK, BENJAMIN JOECKER, UNSW Sydney, ANDREW BACZEWSKI, Sandia National Laboratories, HANNES ROLAND FIRGAU, MATEUSZ T MADZIK, VIVIEN SCHMITT, JARRYD PLA, FAY E. HUDSON, UNSW Sydney, KOHEI M ITOH, Keio University, JEFFREY C MCCALLUM, University of Melbourne, ANDREW STEVEN DZURAK, ARNE LAUCHT, ANDREA MORELLO, UNSW Sydney — We report the discovery of Nuclear Electric Resonance (NER) in a single 123 Sb donor, implanted in a silicon nanoelectronic device [1]. NER enables the coherent control of a high-spin nucleus through the electrical modulation of its quadrupole coupling. This effect was first proposed in the 1960s but never observed in a non-polar, non-piezoelectric material, or in a single atom. Our experiments are quantitatively matched by a microscopic theory that elucidates how an electric field distorts the bond orbital around the atom and results in a modulation of the electric field gradient at the nucleus. The observation of a large quadrupole splitting in a single 123 Sb nucleus paves the way to the realization of a quantum chaotic “kicked-top” model [2] or the encoding of quantum information in an 8-level nuclear spin qudit.


*Funded by Australian Research Council (DP180100969) and DST (AUSMURI00002). Sandia National Laboratories is a multi-missions laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for DOE's National Nuclear Security Administration under contract DE-NA0003525.
4:06PM P17.00007: Decoherence of Dipole Coupled Flip-Flop Qubits*  
JOHN TRUONG (Presenter), XUEDONG HU, State Univ of NY - Buffalo — A recent proposal for a scalable donor-based quantum computer scheme promises excellent coherence properties, fast qubit couplings and insensitivity to donor placement. The suggested system consists of two different types of qubits per donor: a flip-flop qubit consisting of the electron and nuclear spin states, and a charge qubit of the donor electron tunneling between the donor and an interface quantum dot. In this scheme, the qubits can be coupled to each other via the electric dipole interaction between their respective charge qubits. We study in detail this effective coupling, especially the effect of charge noise on two-qubit gates utilizing this coupling. We find that due to the proximity of the charge excited states to the flip-flop logical states, the presence of charge noise greatly reduces the fidelity of two-qubit operations. We calculate the qubit-noise interaction strengths, and identify leakage from the qubit Hilbert space as the main culprit of the reduced gate fidelity. We also explore different bias conditions to mitigate this decoherence channel.

*We thank support from US ARO.

4:18PM P17.00008: Full configuration interaction simulations of exchange coupled donors in silicon in an effective mass theory framework*  
BENJAMIN JOECKER (Presenter), Center for Quantum Computation and Communication Technology, University of New South Wales, ANDREW D. BACZEWSKI, Center for Computing Research, Sandia National Laboratories, JOHN K GAMBLE, Microsoft Research, JARRYD PLA, ANDREA MORELLO, Center for Quantum Computation and Communication Technology, University of New South Wales — Several proposals for multi-qubit gates with donor spin qubit in silicon rely on the exchange interaction, using either weak exchange and microwave pulses [1], or strong tunable exchange [2]. Designing the optimal devices to embody these control strategies requires accurate models of the dependence of the exchange interaction on lattice placement, orientations, and electric fields. Here, we use a full configuration interaction method within an established multivalley effective mass theory framework [3] to model the two-electron wavefunction for different donor configurations. In particular, we investigate the exchange interaction and valley population along different lattice orientations, and the tunability of exchange with external electric fields.


*Funded by the Australian Research Council (CE170100012) and the US Army Research Office (W911NF-17-1-0200). Sandia National Laboratories is a multi-missions laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for DOE's National Nuclear Security Administration under contract DE-NA0003525.
**4:30PM P17.00009: Simultaneous Comparison of Coulomb Blockade Linewidths of P Donor-based and MOS-based Si Quantum Dots**  
YANXUE HONG (Presenter), University of Maryland, College Park, ARUNA N RAMANAYAKA, MICHAEL DAVID STEWART, XIQIAO WANG, RANJIT KASHID, PRADEEP NAMBOODIRI, RICHARD SILVER, JOSHUA POMEROY, National Institute of Standards and Technology — In solid-state quantum computation, noise often presents a limitation for coherence or device integration. One indicator of the noise levels, the effective electron temperature ($T_{\text{eff}}$), must be as low as possible to enable high-fidelity coherent measurements. High $T_{\text{eff}}$ in the measurement may come from noise sources extrinsic to the device or from intrinsic noise in the device, which can be measured by the broadening of Coulomb blockade peaks. To study the extrinsic systematic noise origins and the intrinsic lattice couplings, here we report on the comparison of $T_{\text{eff}}$ on two different quantum dot systems, P donor-based and MOS-based Si quantum dots simultaneously measured using the same measurement setup on the same platform. T-dependent and bias-dependent conductance are measured in different cryogenic setups over temperatures ranging from 10 mK to 25 K. The $T_{\text{eff}}$ is extracted using a theoretical model. By initially rearranging ground configuration and noise filtering, we have successfully reduced the $T_{\text{eff}}$ in a dilution refrigerator with 10 mK base temperature to $< 0.5$ K.

**4:42PM P17.00010: Evaluating effective mass models of the phosphorous donor in silicon**

LUKE PENDO (Presenter), XUEDONG HU, State Univ of NY - Buffalo — Evaluating effective mass models of a phosphorus donor in silicon is made difficult by conflation of mathematical and physical approximations. We propose a scheme to solve a class of effective mass models with high precision. We construct donor electron states using envelope functions expanded in freely extensible basis sets equipped with tunable parameters. With these states, we compute the expectation values of both the donor's energy as well as the energy variance. We variationally optimize the parameters of these basis states to find stationary points of the energy functional, with variance of the expectation energy used to evaluate the precision of our candidate eigenstates. In this manner, we can find exact energy eigenstates of the implied Hamiltonian of an effective mass model.

To improve the physical verisimilitude of a given effective mass model, we evaluate models of the donor atom’s Coulomb potential, in particular considering the effects of a dielectric constant with dynamic response. We present a phenomenological pseudopotential for exchange and correlation effects from the donor's valence electrons. Finally, we include symmetry breaking perturbations, in particular the effect of an electric field upon the donor electron.

*Acknowledgment: We thank support by US ARO.*
4:54PM P17.00011: A two-qubit gate between phosphorus donor electrons in silicon

YU HE, SAMUEL KEITH GORMAN (Presenter), DANIEL J KEITH, LUDWIK KRANZ, JORIS GERHARD KEIZER, MICHELLE Y SIMMONS, Univ of New South Wales — Electron spin qubits formed by atoms in silicon have large orbital energies and weak spin-orbit coupling giving rise to isolated electron spin ground states with seconds long coherence times. The exchange interaction promises fast two-qubit gate operations between single-spin qubits. Until now, creating a tunable exchange interaction between two electrons bound to phosphorus atom qubits has not been possible. This reflects the challenges in knowing how far apart to place the atoms to turn on and off the exchange interaction, whilst aligning atomic circuitry for high fidelity independent read out of the spins. Here we report a ~800 ps √SWAP gate between phosphorus donor electron spin qubits in silicon with independent ~94 % fidelity single shot spin read-out. By engineering qubit placement on the atomic scale, we provide a route to the realisation and efficient characterisation of multi-qubit quantum circuits based on donor qubits in silicon.

*The research was supported by the Australian Research Council Centre of Excellence for Quantum Computation and Communication Technology (CE170100012), the US Army Research Office (W911NF-17-1-0202) and Silicon Quantum Computing Pty Ltd. This work was performed in part at the NSW node of the Australian National Fabrication Facility.

5:06PM P17.00012: Donor-bound excitons in Cl doped ZnSe quantum wells

AZIZ KARASAHIN (Presenter), University of Maryland, College Park, MARVIN MARCO JANSEN, ALEXANDER PAWLIS, Peter Grünberg Institut PGI-9, EDO WAKS, University of Maryland, College Park — Quantum information processing heavily depends on the ability to generate the high number of indistinguishable single photons and to interface them with long-lived coherent spin states. Quantum dots as emerged as promising scalable solid-state platforms by offering bright photon emissions. However, epitaxially grown quantum dots are not immune to size variations and they suffer short coherence times due to interactions with host material nuclear spin bath.

Quantum emission from electron-bound to F donor impurities in bulk ZnSe and ZnSe quantum wells are shown previously. Unlike quantum dots, these emitters show small inhomogeneous broadening\(^1\), short decay times\(^1\), and long-coherence times\(^2\). Together with the possibility of spin purification of the host material, donor impurities in such quantum wells may open the possibility to generate efficient spin-photon interfaces.

Here we investigate emission properties of donor bound excitons in Cl doped ZnSe/ZnMgSe quantum wells. Spectral properties of emitters are investigated in cryogenic temperatures. Time-resolved fluorescence experiments show that these emitters exhibit sub-nanosecond decay times. Second-order time-correlation measurements prove the single-photon emission.
Spins in semiconductor quantum dots are among the leading candidates for quantum computing. To lift spin degeneracy, a large in-plane magnetic field is applied. This has sizable effects on the confined electron, allowing the shape and orientation of the orbitals to be inferred in this way, see Camenzind et al. PRL112, 207701 (2019).

Here, we present experiments studying the effect of the strength and direction of in-plane magnetic fields on the spin structure of an electron in a gated GaAs quantum dot. We have measured an anisotropic correction of about 7% and an isotropic correction pushing the average g-factor 10-15% below the bulk value |g|=0.44. The experiment is compared to theory by Stano et al. PRB98, 195314 (2018), finding rather good agreement. The anisotropic correction is given by the Dresselhaus spin-orbit coupling, matching well using a coefficient of 10.6 eVÅ. The isotropic term is dominated by the well-known Rashba term and an additional 43-term appearing in finite B-field. These corrections are predicted to depend strongly on the thickness of the wave function in the z-direction perpendicular to the 2D gas, and may also depend on the strength of the in-plane field.

*Supported by Swiss NSF, Swiss Nanoscience Institute SNI, and European Microkelvin Platform EMP

Wednesday, March 4, 2020 2:30 PM - 4:18 PM

Session P20 DFD: Computational Fluid Dynamics 301 - Anand Oza, New Jersey Inst of Tech

2:30PM P20.00001: Multicanonical Studies of Fluid Behavior*  DAVID YEVICK (Presenter), MING TONG, University of Waterloo — We applied the multicanonical procedure to the nonlinear Schrodinger equation in order to generate the probability distribution function (pdf) of rogue wave heights in the region of extremely small probabilities. This yielded a simple parametrization of the dependence of the slope of the pdf on the nonlinearity coefficient for large amplitudes. [M. Tong and D. Yevick, Wave Motion 66, 56 (2016) We subsequently investigated the pdf of the drag generated by of a rectangular obstacle associated with random changes to either the input flow pattern or the boundary profile. Our results demonstrated that by integrating the multicanonical and lattice Boltzmann procedures, the probability of highly unlikely drag values can be determined with high accuracy. [M. Tong and D. Yevick, Physics of Fluids 30, 033605 (2018)

*The Natural Sciences and Engineering Research Council of Canada (NSERC) is acknowledged for financial support.
2:42PM P20.00002: Rotating Cylinder as a Flow Split Controller in a Rectangular T-channel: Power-Law Fluids  
ANAMIKA MAURYA (Presenter), NAVEEN TIWARI, Chemical Engineering Department, IIT Kanpur, R.P. CHHABRA, Chemical Engineering Department, IIT Ropar — The present work endeavours to understand numerically the flow characteristics of power-law fluids in a rectangular T-channel over a wide range of conditions: power-law index \(0.2 \leq n \leq 1\), the rotational velocity of the cylinder \((-5 \leq \alpha \leq 5\) at \(Re = 45\). A rotating cylinder (both in the clockwise \((\alpha > 0)\) and anticlockwise \((\alpha < 0)\)) placed at the T-junctions is used here as a flow rate controlling strategy from the channel outlets. The flow is assumed to be steady, laminar and incompressible. The detailed flow kinematics has been visualized in terms of streamline patterns, flow-split ratio (i.e., the ratio of the main branch flow rate to the side branch flow rate), hydrodynamic forces (total and its pressure component) over the cylinder surface and torque (due to the force required to maintain the cylinder rotation in the free stream of power-law fluid). The flow split ratio is seen to be significantly affected by the cylinder rotation while the stationary cylinder is found to divide the flow equally in both main and side branches. The total hydrodynamic force and its pressure coefficient are seen to be a strong function of cylinder rotation as well as the power-law index. The magnitude of the torque is seen to be independent of the direction of cylinder rotation.

2:54PM P20.00003: Scale resolving simulations of flow past a heated sphere using non-linear eddy viscosity closure  
SAGAR SAROHA, KRISHNENDU CHAKRABORTY, SAWAN SINHA (Presenter), Applied Mechanics, Indian Institute of Technology Delhi, SUNIL LAKSHMIPATHY, GexCon — The partially-averaged Navier-Stokes (PANS) method of turbulence computations has been employed in recent years to perform scale-resolving simulations of various canonical as well as flows of practical interest. While in most flows PANS shows improvements over the Reynolds-averaged Navier-Stokes (RANS) method, further scope of improvement still exists, especially in massively separated flows, wherein the linear eddy viscosity assumption is suspected to misrepresent some essential flow physics. With the motivation to address this shortcoming, we augment the PANS methodology using a non-linear (quadratic) constitutive equation. We examine the performance of this enhanced PANS methodology in flow past a heated sphere at Reynolds number of 10000. We find that the non-linear PANS methodology shows improvements over its conventional counterpart (PANS using linear eddy viscosity assumption) in terms of several hydrodynamic (drag and pressure profiles over the sphere surface, axial and transverse velocity profiles and wake structures), as well as some temperature-related flow features (mean temperature profiles around the sphere and Nusselt number). In this talk these results along with some pertinent explanations and insights will be presented.
**3:06PM P20.00004: Lattice Boltzmann Simulations of Magnetohydrodynamic Flows on a Rectangular Grid using a Central Moments Formulation**  
EMAN YAHIA (Presenter), KANNAN PREMNATH, University of Colorado, Denver — Simulations of magnetohydrodynamic (MHD) flows, especially in wall-bounded flows involving the resolution of Hartmann layers, are particularly effective with numerical techniques based on stretched grids. Lattice Boltzmann methods (LBMs) are highly parallelizable local algorithms based on collide-and-stream steps. Here, we extend a prior LBM formulation for MHD, which was constructed for square grids, to handle rectangular lattice grids. Our approach is based on augmenting the equilibria of a vector distribution function with terms involving the grid aspect ratio obtained via a Chapman-Enskog analysis in such a way that it consistently solves the magnetic induction equation. Similarly, the equilibria of another scalar distribution function representing the electrically conducting fluid motion subjected to the Lorentz force are extended with corrections terms based on the aspect ratio so that it correctly recovers its isotropy. For robust simulations, the collision steps of both the scalar and vector distribution functions are based on the relaxation of their central moments to the corresponding equilibria. Computations of various MHD flows at different Hartmann and magnetic Prandtl numbers based on our novel LB formulation demonstrates its accuracy and effectiveness.

**3:18PM P20.00005: Data-driven A priori analysis of sub-grid scale stress closures**  
AVIRAL PRAKASH (Presenter), KENNETH JANSEN, JOHN A EVANS, University of Colorado, Boulder — Better affordability of computational resources over the past decade has led to increased use of scale-resolving simulation techniques such as Large-Eddy Simulations (LES) by industries. These techniques involve the use of a model to account for the effect of small-scale unresolved turbulence structures on large scale resolved structures. The most commonly used models are often based on simplified assumptions such as gradient viscosity hypothesis and turbulence quasi-equilibrium and often fail to replicate higher-order statistics.

This talk will discuss the use of a data-driven approach i.e. neural nets for determining a functional mapping that governs the physics behind the problem. We present an A priori study conducted on the homogeneous isotropic turbulence to determine a model for modeling sub-grid scale stress tensor and compare it with common gradient-viscosity hypothesis based models. A comparison of higher-order statistics will shed light on the universality of small-scale turbulent flow structures as hypothesized by Kolmogorov 1941 theory. The importance of selecting correct input features and the design of the model form for obtaining a physically-consistent relation will also be discussed.
3:30PM P20.00006: Adaptive time-step selection in volume of fluid (VOF) simulations
ASHKAN DAVANLOU (Presenter), Siemens Digital Industries Software — In numerical simulations, Volume of Fluid (VOF) approach is a well-established method in capturing the interface and solving multiphase problems. However, choosing the appropriate time step can be a challenging task for majority of users both with commercial software as well as in house codes. Therefore, we implemented a CFL based time-step control that can target a given area such as the cells intersecting the free surface, such that the CFL limit can be imposed where it is needed. In addition, we keep the sub-steps constant. This enhancement is useful in casting, tank sloshing and marine applications.
In this presentation, we focus on a tank sloshing simulation with Simcenter STAR-CCM+ aiming to demonstrate the merits of using adaptive time-step for VOF multi step simulations. We highlight the add on value from two perspectives 1) reduction in overall computational time for a range of transient examples that are known to have non-constant timescales, 2) demonstrate an improvement in convergence compared to a constant time step set at the average of the variable timestep run.

3:42PM P20.00007: Control of Unstart Phenomenon in a Hydrogen Fuelled Scramjet model
ANCHAL VARSHNEY (Presenter), MEHUL VARSHNEY, MF BAIG, Aligarh Muslim University — The present work involves the development of a numerical methodology to model supersonic combustion using 8 species, 13-reaction chemical model. The governing equations of continuity, momentum, energy, and combustion(species conservation) have been solved using commercial code of Fluent. The methodology has been then used to model the unstart phenomenon in a scramjet engine. A control system based on the mitigation of unstart by leaking high-pressure fluid from the slots designed on the lower and sidewall of the scramjet has been studied[1]. The effect of the slot size position on control mechanism has been studied. The unstart is initiated by a) raising a solid flap downstream of the isolator b) heat release due to combustion of fuel. An automatic slot control mechanism has been suggested to control the unstart phenomenon. The effect of bleeding ratio through slots on engine performance parameters has also been explored.


3:54PM P20.00008: Experimental & CFD Analysis, Design & Optimisation of the Cooling System of a Formula Student Racecar
AYUSH MITTAL (Presenter), RWTH - Aachen, ANCHAL VARSHNEY, MEHUL VARSHNEY, Department of Mechanical Engineering, Aligarh Muslim University — FSAE cars witness a persistent problem of Engine overheating because of inefficient cooling system used. Paper emphasises on complete designing and analysis of the cooling system of FSAE Car along with the integration of Side-pods to increase residence time, heat transfer across the radiator and enhance engine cooling by natural convection. The stock radiator parameters were experimentally determined, theoretically confirmed and validated using CFD analysis. Features like fin density, heat transfer coefficient, flow rates, side-pod geometry, presence of gills, chimneys were analysed to design an optimised cooling system resulting in increased efficiency by over 150%.
Flow dynamics in an aneurysm: Effect of prolonged exercise  MEHUL VARSHNEY (Presenter), ABDULLAH Y. USMANI, Aligarh Muslim University — Present work involves the study of non-invasive treatment of unruptured Abdominal Aortic Aneurysm subjecting the patient to certain physiological level of heart. This technique was initially studied by Varshney et al. [1] Flow topology for 3-D axisymmetric and asymmetric aneurysm is studied under resting (Re=200), mild exercise (Re = 750) & moderate exercise (Re=1200) conditions. Pulsatile flow is given at inlet. Hemodynamic indicators are quantified in terms of time-averaged wall shear stress, oscillatory shear index. The trajectories of vortex-core movement (using Q-criterion) are correlated to pressure peaks attained at the wall. For symmetric aneurysm, it was seen that the resting condition manifests the aneurysmal wall to recirculating fluid for most of the cycle time. Moderate and high exercise exposes the aneurysmal wall and the distal end to high pressure, which otherwise has low intensity under mild activity Thus, mild exercise for a prolonged duration is effective in non-invasive symmetrical aneurysmal treatment. Similar study will be done for an asymmetric aneurysm.


Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P21 GERA: Semiconductors and Quantum Dots for Energy Applications 302

A Computational Survey of Semiconductors for Power Electronics
PRASHUN GORAI (Presenter), ROBERT W MCKINNEY, Colorado School of Mines, NANCY M HAEGEL, ANDRIY ZAKUTAYEV, National Renewable Energy Laboratory, VLADAN STEVANOVIC, Colorado School of Mines — Power electronics (PE) are used to control and convert electrical energy in a wide range of applications from consumer products to large-scale industrial equipment. While Si-based power devices account for the vast majority of the market, wide band gap semiconductors such as SiC, GaN, and Ga$_2$O$_3$ are starting to gain ground. However, these emerging materials face challenges due to either non-negligible defect densities, or high synthesis and processing costs, or poor thermal properties. We performed a broad computational search aimed at identifying promising materials for future power electronic devices beyond SiC, GaN, and Ga$_2$O$_3$. We consider 863 oxides, sulfides, nitrides, carbides, silicides, and borides reported in the crystallographic database and exhibit finite calculated band gaps. We utilize *ab initio* methods with models for intrinsic carrier mobility, and critical breakdown field to compute the Baliga figure of merit. We also compute the lattice thermal conductivity as a screening parameter. In addition to correctly identifying known power electronic materials, our survey has revealed a number of promising candidates exhibiting the desirable combination of high figure of merit and high lattice thermal conductivity, which we propose for further experimental investigations.
2:42 PM P21.00002: Towards efficient green emitters: Heteroepitaxial ZnGeN$_2$ on GaN by molecular beam epitaxy  MARSHALL TELLEKAMP (Presenter), CELESTE MELAMED, ANDREW NORMAN, ADELE TAMBOLI, National Renewable Energy Laboratory — GaN-based LEDs have revolutionized the lighting industry, yet phosphor converters are still required to achieve green and amber wavelengths in a white light emitter. The ‘green gap’ refers to this lack of efficient emitters from 510 nm – 610 nm. InGaN active layers theoretically can reach this range, however the increased In-content results in complications including phase separation and increased spontaneous polarization mismatch which leads to decreased radiative recombination efficiency. II-IV-N$_2$ materials are an optically relevant class of materials with direct gaps across the visible spectrum. ZnGeN$_2$ is nearly lattice matched to GaN, providing a direct route to device integration within a mature system, and can potentially enable green and amber emission at much lower lattice mismatch than InGaN. The heteroepitaxial growth of ZnGeN$_2$ on GaN by molecular beam epitaxy will be discussed, highlighting the impact of Zn desorption and interfacial surface energy on nucleation rate. Insights into growth regimes and limitations will be given, highlighting practical considerations for the characterization of potentially cation-disordered materials. Heterostructure growth represents a major step toward enabling hybrid III-N/II-IV-N$_2$ optical devices.

2:54 PM P21.00003: Combinatorial Investigation of Structural and Optical Properties of Cation-Disordered ZnGeN$_2$  CELESTE MELAMED (Presenter), REKHA SCHNEPF, Colorado School of Mines, JIE PAN, National Renewable Energy Laboratory, ALLISON MIS, Colorado School of Mines, RACHEL WOODS-ROBINSON, University of California, Berkeley, KAREN HEINSELMAN, National Renewable Energy Laboratory, JACOB CORDELL, Colorado School of Mines, JOHN PERKINS, STEPHAN LANY, National Renewable Energy Laboratory, ERIC TOBERER, Colorado School of Mines, ADELE TAMBOLI, National Renewable Energy Laboratory — In this work, we present a combinatorial study of sputtered ZnGeN$_2$ thin films with cross-cutting applications in fundamental materials science and novel device development. The II-IV-N$_2$ materials offer the possibility of groundbreaking optoelectronic properties through greater chemical and structural tunability than the III-Ns. ZnGeN$_2$ is lattice-matched to GaN and is predicted to exhibit a direct bandgap with strong absorption, but experimental studies to date report inconsistent optical properties. Additionally, minimal work has explored variation with cation composition, which has been shown to impact properties of other II-IV-N$_2$ materials. Here, we present a study of combinatorial ZnGeN$_2$ grown by RF co-sputtering. X-ray diffraction reveals phase-pure films in the expected cation-disordered wurtzite structure for cation compositions from 30% to 60% Zn/(Zn+Ge) and synthesis temperatures from 200°C to 600°C. Changes in crystallinity are explored as a function of cation composition, synthesis temperature, and in-situ and ex-situ annealing. Finally, spectroscopic ellipsometry is performed to investigate optical properties with changing synthesis conditions. This study reaffirms the potential for tunability of thin film ZnGeN$_2$ as a direct- and wide- bandgap optoelectronic material.
3:06PM P21.00004: Cathodoluminescence measurement of high bandgap CdTe-based devices  
AIDA TORABI (Presenter), CLAUDIA BECK, Texas A&M University, Central Texas, AMIT MUNSHI, CAREL REICH, WALAJABAD SAMPATH, Colorado State University, TAYLOR HARVEY, Texas A&M University, Central Texas — High band-gap CdTe-based devices are being developed as top films to be used in tandem solar cells. CdTe can be alloyed with Mg and Zn to form Cd$_x$Mg$_{1-x}$Te (CMT) or Cd$_x$Zn$_{1-x}$Te (CZT) to increase the band gap; however, doping and passivation of these films continue to be a fundamental challenge. Films exhibiting better recombination lifetimes have been demonstrated by incorporating Se in CMT and CZT to from quaternary alloys. A fundamental understanding of the film properties are needed for all these films to realize their potential as photovoltaic absorbers. Optical characterization is one method to understand and aid in the development of high band-gap CdTe films. Scanning electron mapping of the luminescence of these film gives insight into film composition, homogeneity, and crystal quality. Herein we present our study of the optical properties of these materials using cathodoluminescence(CL). Additionally, electron beam-induced current (EBIC) is measured and correlated to the optical response. Unexpected peak shift and secondary peak presence indicate potential phase segregation or trap state formation.

3:18PM P21.00005: Investigation of the photocorrosion of GaP, III-V photoanode in acid with in situ UV/vis spectroscopy*  
SAHAR PISHGAR (Presenter), Univ of Louisville, JOSHUA SPURGEON, Conn Center for Renewable Energy Research — Although III-V semiconductors are one of the most promising group of materials for high efficiency solar fuels applications, they are prone to self-corrosion in strongly acidic or alkaline solutions. In-situ Investigation of photo-corrosion process are now limited to very expensive and complicated methods that are not available in every lab. Developing methods that enable researchers to do in-situ study of photo-corrosion process could make a profound impact on this field. Herein we studied self-corrosion of GaP photoelectrodes, a promising III-V material for tandem top subcells, in acidic electrolyte via in-situ UV-Vis spectroscopy. In-situ measurement of concentration of dissolved Ga and P species that come off from the electrode to electrolyte, calculation of corrosion faradaic efficiency as a function of applied bias and time along with SEM and XPS characterization are utilized to expound the photo-corrosion process of n-GaP and p+-GaP photoelectrodes which have shown different corrosion behavior. In addition, TiO$_2$ protective layer was deposited on some samples to study the change in corrosion faradaic efficiency as a function of deposition parameters.

*Conn Center for Renewable Energy Research
3:30PM P21.00006: Influence of epitaxial anatase and rutile TiO\textsubscript{2} thin films as electron transport layers for perovskite solar cell

YEON SOO KIM (Presenter), HYE-JIN JIN, HYE RI JUNG, JIHYUN KIM, WILLIAM JO, EWHA Woman’s Univ — The effective electron transport layer (ETL) is essential for high-power conversion efficiency (PCE) of perovskite solar cell (PSC). TiO\textsubscript{2} is the most widely used material for ETL owing to proper band alignment, enough optical transmittance, and high electron mobility. There are two representative thermodynamically stable crystal phases of TiO\textsubscript{2}: anatase and rutile. However, it is still debated which phase is more effective for the ETL. To solve the concern, single-phase thin film is strongly needed. We deposited epitaxial anatase- and rutile-TiO\textsubscript{2} thin films on LaAlO\textsubscript{3} and g-sapphire substrate, respectively, using pulsed laser deposition technique. X-ray diffraction analysis shows that both films have high crystallinity. In addition, both phases of epitaxial Nb-doped TiO\textsubscript{2} films are grown in order to enhance carrier injection/extraction of ETL. The variation of chemical states of elements resulting from Nb dopants was observed by X-ray photoelectron spectra. Steady-state photoluminescence (PL) spectra and time-resolved PL reveals PSC with anatase-TiO\textsubscript{2} has more effective carrier transporting and charge separating than with rutile-TiO\textsubscript{2}. Finally, the photocurrent density-voltage (J-V) measurements were conducted for estimating PCE.

3:42PM P21.00007: First-Principles Calculation of Charge Carrier Mobility using Complex Band Structure

ANDREW V BROOKS (Presenter), YUE YU, DMITRY SKACHKOV, HAI-PING CHENG, XIAOGUANG ZHANG, University of Florida — We compute charge carrier mobilities from the complex band structure, using the Quantum Espresso suite and a previously developed method\textsuperscript{1}. Carriers with finite lifetimes due to scattering may be represented by Bloch states with complex energies. Our method determines the constant complex potential that must be added to a perfect crystal to induce the scattering effects seen in a crystal with defects, which we deduce from a series of complex band calculations. The mean scattering lifetime is computed from the imaginary part of this complex potential, and the carrier mobility is obtained from the scattering lifetime using the Boltzmann transport theory. Mobility is calculated for graphene, hybrid organic-inorganic perovskites, and 2D FeCl\textsubscript{2} half-metal system, as a function of temperature due to phonon scattering, impurity and absorbed molecules.


\*This work was supported as part of the Center for Molecular Magnetic Quantum Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0019330.
Towards Monolithically Integrated Thin Film Bypass Diodes

TIMOTHY SILVERMAN, LORELLE MANSFIELD, STEPHEN GLYNN, TIMOTHY REMO, KAREN BOWERS, BART STEEVENS, MATTHEW REESE (Presenter), National Renewable Energy Laboratory — Bypass diodes can make photovoltaic (PV) modules more resilient, for instance preventing local heating when one portion is shadowed and another is not. This is significant because hot spot formation due to partial shading can cause sudden, non-linear permanent degradation. Presently, if incorporated at all, bypass diodes must be integrated as discrete components. Thin film photovoltaics can be fabricated in a manner where by thoughtfully choosing growth and scribing order “monolithic” integration can be achieved. We will present electrical simulations of diodes placed in an edge configuration to highlight the tradeoffs of designing real-world modules considering such variables as lateral resistance, PV cells per diode, and diode leakage current. Simulations incorporate both optimal and experimentally grown thin film diode characteristics to allow the tradeoffs and areas for improvement to be better understood.


Injection-dependent non-radiative SRH recombination via interstitials and dislocations in multicrystalline Si

ANDREY SEMICHAEVSKY (Presenter), Lincoln University — This paper deals with models of NR carrier recombination in mc-Si, which limits the efficiency of photovoltaic conversion. Experimental minority lifetimes in Si show a variety of dependences on injection levels. Models of non-radiative recombination in silicon were proposed for point defects (e.g., Fe interstitials) and extended defects (e.g., dislocations). High-resolution measurements of carrier transport are technically difficult, so models are used instead to relate carrier recombination processes in mc-Si to minority carrier lifetimes. While the SRH recombination due to shallow and deep point defects may result in a lifetime dependence on concentration with a distinct maximum, the recombination via arrays of dislocations leads to a monotonically increasing lifetime with the carrier concentration.


The NSF HRD 1505377 grant was used to produce results in this presentation.
4:18PM P21.00010: Transition Metal Doped Quantum Dots for Photovoltaic Applications*
TRIEU LE (Presenter), Physics, State University of New York - Oswego, THILINI EKANAYAKA, Physics and Astronomy, University of Nebraska at Lincoln, ANNIKA NEUFELD-KREIDER, Physics, State University of New York - Oswego, ARCHIT DHINGRA, TAKASHI KOMESU, Physics and Astronomy, University of Nebraska at Lincoln, ANDREW J. YOST, Physics, Oklahoma State University, CAROLINA C. ILIE, Physics, State University of New York - Oswego — In recent years, semiconductor zinc sulfide (ZnS) quantum dots have been considerably studied for various applications such as light emitting diodes, flat panel display, UV sensor and solar cell application. We discuss herein the optical and transport properties of the transition metal doped quantum dots and optimize them for better photovoltaics. Zinc sulfide has an excellent optical and electronic performances due to its wide band gap. In addition, cobalt-nickel doped zinc sulfide brings a versatility of the band gap energy. This is corresponding to an enhancement in the photo-to-current efficiency of doped quantum dots in sensitized solar cell. In this study, we explore how the different dopants lead changes in the band gap and discuss the characteristic of these doped quantum dots. The absorption data shows that cobalt-nickel doped ZnS has the highest absorbance the visible range out of all the single and co-doped and tri-doped quantum dots which made it the best candidate for optoelectronic device fabrication.

*This research was supported by the NSF Grant Nos. NSF-ECCS 1740136 and 1508541, SRC-NCORE, Nebraska Public Power District -Nebraska Center for Energy Sciences Research at the University of Nebraska-Lincoln, NCESR grant No. 19-SE-2018, NSF - MRSEC grant No. DMR-1420645.

4:30PM P21.00011: Glucose-Derived Carbon Nanodots in Dye-Sensitized Solar Cells to Increase Efficiency*
MAX MARKUSON-DIPRINCE (Presenter), HARSH UPPALA, GRACE DIRKS, LOGAN SMITH, JOHN VOSICKY, ANDREW G BARUTH, Creighton University — Although carbon nanodot isolation remains difficult due to the presence of molecular byproducts in a bottom-up synthesis approach using thermal treatment of carbohydrate solutions, their resultant photoluminescence shows promise for down-converting UV photons. In particular, excitation at 390nm results in significant luminescence from 490–540nm, with an excitation wavelength dependence of luminescence (peak absorption occurs at 290nm). Carbonaceous nanodot solutions were derived from high-concentration glucose solutions at 120°C for a 48 hour period and then incorporated into Ruthenium-based dye-sensitized solar cell devices to enhance external quantum efficiency for high energy photons. We found that dialysis combined with solid phase extraction retained photoluminescent properties while allowing for carbon dot isolation in acetonitrile, a soaking solvent for dye-sensitization of TiO₂ nanoparticles, with minimal measurable traces of other chemical byproducts. Successful purification processes, photoluminescence, external quantum efficiency, and J-V curves of these carbon dot-modified devices will be shown to verify this low-cost, earth abundant approach to efficiency enhancement of dye-sensitized solar cells.

*NASA Nebraska Space Grant & Nebraska EPSCoR
Omaha Public Power District
4:42PM P21.00012: Nano-biohybrid Organisms: In-vivo Targeting of Enzymes with Quantum Dots for Light-Driven Renewable Biochemical Synthesis  JOHN BERTRAM (Presenter), PRASHANT NAGPAL, YUCHEN DING, University of Colorado, Boulder — Living cells do not interface naturally with nanoscale materials, although such artificial organisms can have unprecedented multifunctional properties, like wireless activation of enzyme function using electromagnetic stimuli. Realizing such interfacing in a nanobiohybrid organism (or nanorg) requires (1) chemical coupling via affinity binding and self-assembly, (2) the energetic coupling between optoelectronic states of artificial materials with the cellular process, and (3) the design of appropriate interfaces ensuring biocompatibility. We have shown that many different core–shell quantum dots (QDs) couple with targeted enzyme sites in bacteria. When illuminated by light, these QDs drive the renewable production of different biofuels and chemicals using carbon dioxide, water, and nitrogen (from air) as substrates. Together, these nanorgs catalyze light-induced air–water–CO2 reduction to synthesize biofuels like isopropanol, 2,3-butanediol, C11–C15 methyl ketone, hydrogen gas; and valued chemicals such as formic acid, ammonia, ethylene, and degradable bioplastics polyhydroxybutyrate. Therefore, these resting cells function as nano-microbial factories that synthesize valuable chemicals from abundant small molecules powered by the sun.

Ref: JACS, 2019, 141, 10272

4:54PM P21.00013: Building quantum dot-bacteria nano-biohybrids for light-driven renewable biochemical synthesis  YUCHEN DING (Presenter), JOHN BERTRAM, University of Colorado, Boulder — Live cells do not interface naturally with nanostructures, although such artificial organisms can have unprecedented multifunctional properties, like wireless activation of enzyme function using electromagnetic stimuli. Realizing such interfacing requires (1) chemical coupling via affinity binding and self-assembly, (2) energetic coupling between material optoelectronic states and the cellular process, and (3) design of appropriate interfaces ensuring biocompatibility. Here we show different core-shell quantum dots (QDs), with excitations ranging from UV to NIR, couple with targeted enzyme sites in bacteria. When illuminated by light, these QDs drive the renewable production of different biofuels and chemicals using CO2, water, and N2 as substrates. These QDs use their zinc-rich shell facets for affinity binding to the enzymes. Cysteine zwitterion ligands enable uptake through the cell, facilitating cell survival. Together, these nanorgs catalyze light-induced air-water-CO2 reduction with a high turnover number of \(~10^6\)-\(10^8\) (mols/mol of cells) to biofuels like C2H4, 2-propanol, 2,3-butanediol, methyl ketones, and H2; and chemicals such as formate, NH3, and bioplastics. Therefore, these resting cells function as nano-microbial factories powered by light. 
5:06PM P21.00014: Alcohol Synthesis on MoS$_2$-supported Gold Nanoparticle*  
TAO JIANG  
(Presenter), DUY LE, TALAT S. RAHMAN, Univ of Central Florida — Alcohol synthesis from syngas (CO, H$_2$) is an important part of an economy based on renewable fuels. Rational designing of efficient catalyst material for such synthesis is in great demand because of the limitation of the current state-of-the-art catalysts. We report our density functional theory based calculations of the hydrogenation of CO on 31-atom, bilayer Au cluster supported on single-layer MoS$_2$ (Au$_{31}$/MoS$_2$). In accordance with previous investigations [1], we found that the gold atoms at the edge were most affected by substrate interaction and had strong affinity for CO. Furthermore, molecular H$_2$ could only physisorb on Au$_{31}$/MoS$_2$ and the activation barrier of H$_2$ dissociation was 0.63 eV, lower than that on Au$_{13}$ [2]. We found that Au$_{31}$/MoS$_2$ offers excellent activity toward methanol synthesis, via two competitive reaction pathways: 1) CHO$^*$→CH$_2$O$^*$→CH$_3$O$^*$→CH$_3$OH$^*$; 2) CHO$^*$→CHOH$^*$→CH$_2$OH$^*$→CH$_3$OH$^*$, the former being kinetically more favorable. We compare our findings with that on Au$_{13}$ [2] to elucidate the influence of size and shape of nanoparticles on their catalytic performance.  
*This work is supported in part by DOE grant DE-FG02-07ER15842

5:18PM P21.00015: Analytical electron billiards model of geometric diodes  
JEREMY LOW  
(Presenter), JAMES P CUSTER JR., JAMES CAHOON, Univ of NC - Chapel Hill — Unlike traditional diodes that require a potential barrier to generate electrical asymmetry, geometric diodes operate simply by breaking the structural symmetry on a scale comparable to the mean-free-path length of charge carriers. This gives geometric diodes unique properties that allow them to function as long wavelength energy harvesters and ultra-high speed signal processors. These devices exhibit nonlinear charge transport that is largely dictated by geometric parameters and position-dependent mean-free-path. We aim to predict the device’s dependence on these parameters through analytically calculating the proportion of possible paths ballistic charge carriers can travel through the device. Trajectories of up to an arbitrary number of internal reflections are integrated over all space inside the device. To account for the effect of applied electric field on the electron momentum distribution, a spatial distribution weighted in one direction is used and the impact on diode asymmetry is evaluated. The model is able to simulate nonlinear charge transport in both 2D and 3D nanowire geometric diodes. The model has excellent agreement with experiment, matching trends of IV curve asymmetry versus geometric parameters in silicon nanowire geometric diodes.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P22 DBIO GSNP DCOMP: Inference, Information, and Learning in Biophysics: I  
303 - Pankaj Mehta, Boston University
2:30PM P22.00001: What can and can't Machine Learning do for Physics? [Invited] PANKAJ MEHTA (Presenter), Physics, Boston Univ — This speaker is on last year's program for invited talk but in fact that talk was given by someone else, due to a death in the family, making him eligible this year.

3:06PM P22.00002: Coarse scale representation of spiking neural networks: from dynamics to backpropagation through spikes ANGEL YANGUAS-GIL (Presenter), Argonne National Laboratory — Leaky integrate and fire neurons have long been used as a model system to understand the dynamics of spiking neural networks, recently becoming the underlying model of neuromorphic chips such as Intel's Loihi. One of the interesting features of this type of models is the presence of an absolute refractory period, which essentially limits the maximum spike rate that can be attained by the system. This is also the largest time interval that guarantees that at most a single spike is produced per neuron. In this work we have explored the development of coarse scale representations of leaky integrate and fire neurons that operate at this timescale. Our coarse scale approximation is obtained by approximating spike arrival times as being homogeneously distributed over our time interval, and results on a discrete representation that exhibits equivalent dynamics on randomly connected networks. Moreover, the coarse scale model allows us to implement stochastic gradient descent methods for spiking neurons that take advantage of backpropagation. This provides a useful baseline with which to compare more bio-inspired approaches based on local learning rules, as well as the impact of different codings on the network's ability to learn and generalize.

3:18PM P22.00003: Towards a grammar of probabilistic models for large biological networks PHILIPP FLEIG (Presenter), University of Pennsylvania, ILYA M NEMENMAN, Emory University — Biological interaction networks such as biological neural networks, amino acid sequences in proteins, etc. are critical to the functioning of any living system. The trend of modern experiments is to record data with a rapidly increasing number of simultaneously measured network variables. Inferring models for such complex data is becoming increasingly more difficult, since one is confronted with a combinatorial explosion in the number of possible interactions between variables. Here we present first steps of an approach to overcome this obstacle. We investigate the question whether a small set of carefully chosen statistical models suffices to describe rich phenomenology in data of biological networks. As candidate models for this grammar we consider low-rank approximation, clustering, sparsity, etc.. We discuss the distribution of eigenvalues and pairwise correlations characteristic for each model, working under the assumption that they serve as key indicators for the phenomenology described by a model. We provide examples of modelling data of Ising spin systems and outline a vision for how combinations of models in the grammar cover a large part of model space occupied by biological networks.

*This work was supported in part by NIH Grant R01-NS099375 and NSF Grant BCS-1822677.
3:30PM P22.00004: Different noise assumptions yield qualitatively different landscapes and transition paths in gene regulation models*  JOHN VASTOLA (Presenter), WILLIAM R. HOLMES, Vanderbilt Univ — Intrinsic gene expression noise is a major source of phenotypic variability in cancer biology, and noise-induced transitions are thought to contribute to everything from developmental error correction to drug resistance. It is increasingly common to incorporate noise into mathematical models of gene networks, but limited experimental knowledge forces noise to be modeled in a phenomenological/approximate way. Do the different ad-hoc ways noise is included in these models qualitatively affect their predictions? Building on earlier work that analyzed one and two gene toy models, we present results on how noise assumptions affect landscapes and transition paths in models of the epithelial-to-mesenchymal transition (EMT) and early T cell development. We focus on two aspects of modeling noise: its functional form (constant/additive, multiplicative/linearly dependent on concentration, or the ‘canonical’ Gillespie-like prescription) and its symmetry (whether different genes have the same amount of noise). We find that different assumptions about noise can dramatically impact (i) the relative occupancy of different states, (ii) the stability/existence of intermediate states, and (iii) transition rates and paths.

*This work was supported by NSF Grant # DMS 1562078.

3:42PM P22.00005: Stochastic Modelling of Dynein Motors on a One-Dimensional Lattice: Dynamics and Stationary State*  RIYA NANDI (Presenter), PRIYANKA ., Department of Physics & Center for Soft Matter and Biological Physics, Virginia Tech — The motion of molecular motors inside cells constitutes an exciting and biologically motivated non-equilibrium physics problem. Experimental studies in recent years have shown that dynein motors can move with variable step sizes along the microtubule, depending on the load and ATP concentration. Inspired by the dynamics of dyneins, we have developed a model of an exclusion process on a one-dimensional lattice, where the motors can move in the forward direction up to four steps depending on the load attached to it. We study the dynamics of the mean-square displacement, stationary state current, and gap distribution for both open and periodic boundary conditions. In the transient regime, the fluctuation grows as t.log(t) for the periodic boundary conditions and is ballistic for open boundary conditions. The gap distribution between the motors in the stationary state for periodic boundary conditions shows discrete peaks of exponentially decaying amplitude at multiples of four gap size. We have also verified these interesting results using a mean-field analysis.

*Research was sponsored by the U.S. Army Research Office and was accomplished under Grant Number W911NF1710156.
3:54PM P22.00006: Limits to biochemical signalling in a changing environment as an inference problem*  THIERRY MORA (Presenter), Ecole Normale Superieure, ILYA M NEMENMAN, Physics, Emory — Cells must sense concentrations of external ligands as well as internal signalling molecules in order to adapt to environment changes and execute developmental programs. Berg and Purcell calculated an upper bound to the accuracy of concentration sensing by physical objects, due to the particle nature of molecules and finite sensor size. However, that bound assumed that the concentration to be sensed was constant. In realistic situations, concentrations may vary quickly over orders of magnitude. Here, we calculate a new bound to concentration sensing of a changing concentration by mapping the problem onto a field theory through Bayesian inference, which we solve using a Gaussian approximation. We find that the inverse square root dependency of the error as a function of concentration, ligand diffusivity, sensor size and time in the classical Berg and Purcell bound is replaced by a quartic root. The solution to the inference problem provides dynamical inference equations which can be mimicked by simple biochemical downstream networks, providing a plausible biological implementation of optimal inference.

*Agence National pour la Recherche (ANR) grant No. ANR-17-ERC2-0025-01 “IRREVERSIBLE”. NSF Grants No. PHY-1410978 and IOS-1822677

4:06PM P22.00007: Human information processing in complex networks  CHRISTOPHER LYNN (Presenter), EVANGELIA PAPADOPOULOS, ARI KAHN, DANIELLE BASSETT, University of Pennsylvania — Humans communicate using systems of interconnected stimuli or concepts - from language and music to literature and science - yet it remains unclear if and how the structure of these networks supports the communication of information. Although information theory provides tools to quantify the information produced by a system, traditional metrics do not account for the inefficient and biased ways that humans process this information. Here we develop an analytical framework to study the information generated by a system as perceived by a human observer. We demonstrate experimentally that this perceived information depends critically on a system's network topology. Applying our framework to several real networks, we find that they communicate a large amount of information (having high entropy) and do so efficiently (maintaining low divergence from human expectations). Moreover, we show that such efficient communication arises in networks that are simultaneously heterogeneous, with high-degree hubs, and clustered, with tightly-connected modules - the two defining features of hierarchical organization. Together, these results suggest that many real networks are constrained by the pressures of information transmission, and that these pressures select for specific structural features.
4:18PM P22.00008: Information tradeoffs in sensing and sampling* CAROLINE HOLMES (Presenter), WILLIAM S BIALEK, Princeton University — Organisms sense the world through arrays of receptor cells. In some cases, such as the compound eyes of insects, these arrays are nearly crystalline. In other cases, including the human retina, sampling is much less regular. While ordered sampling typically gathers more information, this comes at the cost of specifying the positions of all the cells. We explore this tradeoff, asking about the maximum entropy of the sampling lattice that is consistent with gathering a certain amount of information from a Gaussian random signal; bits of sensory information are traded against bits of positional information. This problem maps to an equilibrium statistical mechanics problem for the positions of the receptor cells, with interactions that depend on the correlation structure of the input signal. In some limits we find that the information cost of disorder is surprisingly small. In other limits there are transitions where an ordered sampling lattice melts as we change the parameters of the sensory environment.

*This work was supported by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030) and the Graduate Research Fellowship Program.

4:30PM P22.00009: Optical reservoir computing with tumor spheroids* DAVIDE PIERANGELI, Univ of Rome La Sapienza, VALENTINA PALMIERI, University Cattolica, GIULIA MARCUCCI, Univ of Rome La Sapienza, CHIARA MORICONI, GIORDANO PERINI, MARCO DE SPIRITO, MASSIMILIANO PAPI, University Cattolica, CLAUDIO CONTI (Presenter), Univ of Rome La Sapienza — Photonics enables the implementation of many modern neural network architectures, like deep learning and random neural networks. When a multiple scattering medium is adopted for mixing optical signals and perform computations, one can realize optically different conventional applications of artificial intelligence, like image recognition or time-series prediction. Optical reservoir computing may have other applications beyond computing. We demonstrate a random optical network realized by tumor spheroids. The tumor spheroids are samples of human tumors, like glioblastoma. The characterization of tumor spheroids is commonly done by optical imaging, and it is time-consuming and resource-demanding. We experimentally realize a random optical network that uses a tumor spheroid as a computing reservoir. We train the device by data from conventional imaging to infer tumor metabolism and the growth rate. After the training, the network can predict the time-dynamics of the metabolism and also the effect of hyperthermia and chemotherapy.[1] Our bio-random optical network represents a new kind of smart device for cancer morphodynamics and biophysical applications.


*QuantERA QUOMPLEX (731473), PhoQus (820392).
4:42PM P22.00010: Stochastic Force Inference* PIERRE RONCERAY (Presenter), Princeton University, ANNA FRISHMAN, Technion — Brownian dynamics is ubiquitous in biophysics, from the motion of single molecules and cytoskeletal filaments to effective models for cell and small animal behavior. We propose a principled framework, Stochastic Force Inference, for the inverse problem of Brownian dynamics: reconstruct spatially dependent force and diffusion fields from individual trajectories. It consists in a linear regression of these fields with a basis of smooth functions. We show that it is data efficient and successfully addresses the many challenges associated to real biological data: localization error, high dimensionality of phase space, out-of-equilibrium currents, multiplicative noise, complex force fields.


*PR is supported by a Center for the Physics of Biological Function fellowship.

4:54PM P22.00011: Predicting the future from the past in visual object motion: optimal representations of mixed stochastic/deterministic trajectories* VEDANT SACHDEVA (Presenter), University of Chicago, ALEKSANDRA MARIA WALCZAK, THIERRY MORA, Ecole Normale Superieure, STEPHANIE PALMER, University of Chicago — Making predictions about the future state of the external world confers benefits to biological systems that can translate to increased fitness. This requires that sensory systems encode information about the stimulus in a manner suitable for prediction. However, physical constraints, such as finite metabolism and finite computing power, result in additional evolutionary pressures. These favor organisms that compress the representation of the input stimulus statistics along particular readout dimensions, creating an underlying tension between representing the statistics of a stimulus while preserving the information relevant to prediction. Here, we propose that the encoding scheme used by such biological systems can be predicted by the information bottleneck method. Using this technique, we can compute the optimal form of the encoding distribution for a variety of mixed stochastic and deterministic stimuli and demonstrate that these encoding distributions are optimized for prediction tasks at different timescales. We also consider the optimal encoding distribution when the underlying parameters of the stimulus evolve in time.

*VS, AW, TM, and SEP acknowledge FACCTS, CNRS, and NSF PHY-1734030 for support for this project. SEP also acknowledges NSF CAREER award 1652617.
5:06PM P22.00012: Quantifying success and failure in simple models of large neural populations  LEENOY MESHULAM (Presenter), Massachusetts Institute of Technology MIT, JEFFREY GAUTHIER, Swarthmore College, CARLOS BRODY, DAVID TANK, WILLIAM S BIALEK, Princeton University — In statistical physics we routinely study models for collective behaviors that are simpler than the underlying microscopic mechanisms. In biological systems, one systematic implementation of this idea is the maximum entropy method, where we match some features of the data but otherwise the model has as little structure as possible. To understand whether this approach “works”, it would be attractive to have a testing ground where we could see the same model succeed or fail to describe different but related systems. Recent experiments monitor the activity of 1000+ cells in the mouse hippocampus as the animal runs through a virtual environment. The scale of these data allows us to construct models for many different subsets of neurons drawn out of the whole population. We test many predictions of these models, and find that quantitative agreement with experiment is best when the group of cells is spatially contiguous; if we draw the same number of cells at random from large regions, the agreement gets systematically worse. Strikingly, the different predictions fail in an ordered way, so we can rank the different collective behaviors of the network activity by the degree of difficulty in getting them right. This serves to make precise what it means for these models to work.

5:18PM P22.00013: Quantifying temporal information accumulation for biochemical signaling dynamics  YING TANG (Presenter), ADEWUNMI ADELAJA, Institute for Quantitative and Computational Biosciences, University of California, Los Angeles, XIAOFENG YE, Department of Applied Mathematics & Statistics, Johns Hopkins University, ERIC DEEDS, ROY WOLLMAN, ALEXANDER HOFFMANN, Institute for Quantitative and Computational Biosciences, University of California, Los Angeles — The temporal patterns of intracellular signaling contains information for cell decision making. When signaling is initiated by a stimulus, circuits that decode the temporal patterns to control biological effectors must make decisions based on available information within the timecourse. Quantifying information flow through signaling networks thus requires a dynamical framework to estimate information transmission in a time-dependent manner. We find that a type of stochastic process can be used to represent the signaling activities that show a high degree of cell-to-cell variability. Based on the model, we extract the time-dependent channel capacity of signaling pathways. When the transcription factor NFκB is activated by diverse immune threats in macrophages (e.g. virus, gram negative or positive bacteria, or cytokine), the channel capacity reaches 1 bit of information around 1 hour and 2 bits of information within 10 hours. By knocking down the feedback regulation in the signaling pathway, the information accumulation was reduced, which uncovers that information transmission is enhanced by feedback control. The result demonstrates that the method allows quantification on the learning rate of decoding circuits for rapid cellular decision making.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P23 DBIO GSNP: Physics of the Brain: Structure and Dynamics
II 304 - Marek Cieplak, Institute of Physics, Polish Academy of Sciences - Tag(s): Focus
When we make reach-directed movements to an object, like a cup, there is an infinite number of possible trajectories that an arm could take to go from its initial position to the final target. These are not given by solving Newton’s equations but are controlled by the brain. Humans show highly stereotyped random trajectories with hand velocity profiles that appear smooth to the naked eye. However, by using high definition motion capture MEM sensors we have found that at finer millisecond time scales, away from naked eye detection, the kinematic variables have clear random peak fluctuations that were unknown previously. We have been able to directly connect, in an individualized way, these random fluctuations to the nature of the Neurodevelopmental Disorders (NDD) of children with autism or attention hyperactive disorders. These random peak fluctuations are very different, though, in healthy individuals. In this lecture I will describe the nature of experiments we carry out, the importance of fully filtering out the external electronic noise from neuronal noise. We measure angular velocity, linear acceleration, and the time derivative of the acceleration, known as jerk of importance in human kinematics. Based on the data measured over thousands of arm movement trials we developed a detailed statistical analysis that allowed us to uncover quantitative NDD biomarkers that a posteriori agreed with the clinical diagnoses for each individual studied. We further hypothesize that the brain tries to minimize the associated stochastic kinematic variable fluctuations describing the motions. The identified biomarkers quantitatively determine the illness severity, that could be used as a diagnostic tool by clinicians.


*National Science Foundation #79413515
Latent fields lead to emergence of scaling in simulated neurons

MIA MORRELL (Presenter), AUDREY SEDERBERG, ILYA M NEMENMAN, Emory University — Understanding activity of large populations of neurons is difficult due to the combinatorial complexity of possible cell-cell interactions. A remedy is to note that many systems may be macroscopically described with models simpler than the system's microscopic behavior. This has been probed via a coarse-graining procedure on experimental neural recordings, which shows over two decades of scaling in free energy, variance, eigenvalue spectra, and correlation time [1], hinting that a mouse hippocampus operates in a critical regime. We investigated whether this scaling behavior could be explained as a result of coupling the neural population to latent dynamic stimuli. We conducted simulations of conditionally independent binary neurons coupled to a small number of long-timescale stochastic fields with and without periodic spatial stimuli (depicting neural place cells) and replicated the coarse-graining shown in [1]. In a biologically relevant regime, we find that much of the observed scaling [1] may be recreated by this model. This suggests that aspects of the scaling may be explained by coupling to hidden dynamic processes, a ubiquitous trait of neural systems.


Architectural Principles and Predictive Modeling of the Mammalian Connectome

ZOLTAN TOROCZKAI (Presenter), FERENC MOLNAR, University of Notre Dame, ANA-RITA RIBEIRO GOMES, Neuroscience, l'Université Claude Bernard Lyon 1, MARIA ERCSEY-RAVASZ, Physics, Babes-Bolyai University, Cluj-Napoca, KENNETH KNOBLAUCH, HENRY KENNEDY, INSERM Stem Cell & Brain Research Institute U1208 — Although mammalian brains show a massive, 5 orders of magnitude variation in weight, they present common processing features, implying that cortical computing is built on a scalable architecture. We hypothesize the existence of network architectural organizational principles in the mammalian brain, critical for efficient and hierarchically modular information processing. Extending our empirical, consistent tract-tracing network databases, we confirm the validity of the Exponential Distance Rule (EDR) in the macaque cortex, showing that the EDR is an architectural network invariant. We have also developed and cross-validated novel, machine learning based imputation algorithms, suitable for dense interareal networks, exploiting the weighted, directed and the spatially embedded nature of these networks. As we show, these algorithms can efficiently be used to guide further tract-tracing experiments, for example by identifying potential injection targets that would generate the largest information gain, after every new injection.


NSF grant IIS-1724297 and ANR-17-FLAG-ERA-HBP-CORTICITY
3:30PM P23.00004: A 2D Stochastic Lattice Model Describing the Self-Assembly of Synaptic Membrane Protein Domains*  EVerest law (Presenter), Univ of Southern California — The regulation of neurotransmitter receptor domains on the postsynaptic membrane plays an important role in signal transduction across synapses. Inspired by the interactions between glycine receptors and gephyrin scaffolds, we present a stochastic lattice reaction-diffusion model explaining receptor domain formation. Using reaction and diffusion rates consistent with experimental observations, our model reproduces the receptor/scaffold copy numbers and domain areas observed in nanoscopy experiments. The Turing instability in our model intuitively explains the pattern formation observed, without assuming the existence of patterns a priori. The present work is an extension of previous work where the same model is only studied in 1D.

*This work was supported by National Science Foundation (NSF) award number DMR-1554716 and the USC Center for High-Performance Computing.

3:42PM P23.00005: Dynamics of the intrinsically disordered proteins and neurodegeneration* [Invited] Marek Cieplak (Presenter), Institute of Physics, Polish Academy of Sciences — The equilibrium dynamics of the intrinsically disordered proteins is thought to consist of transitions between many basins in the free energy landscape whereas structured proteins stay in the vicinity of one native basin. We demonstrate this picture explicitly by studying networks defined on the discretized plane: conformational end-to-end distances vs. radii of gyration. The bin sizes are defined by time scales that span orders of magnitude. The networks, derived from all-atom and coarse-grained molecular dynamics simulations, are nearly scale invariant. The bin representation also provides insights into the folding process of the structured proteins and identifies regions that hinder folding. Intrinsically disordered proteins often lead to neurodegenerative diseases through a variety of mechanisms. Here, we focus on one such mechanism: jamming of the proteasomal protein degradation by transient conformations that contain knots. We show that such conformations arise at least for sufficiently long polyglutamine tracts and α-synuclein. The polyglutamine tracts are fused within huntingtin protein that is associated with the Huntington neurodegenerative disease. We show that the presence of knots in the tracts obstructs translocation through a model proteasome, especially when the knots are deep. The knots in polyglutamine may form in tracts that exceed about 40 residues. This fact explains the existence of a similarly sized length threshold above which there is an experimentally observed toxicity at the monomeric level. We also discuss emergence of knots in α-synuclein – the protein associated with the Parkinson disease. We show that these knots are either shallow or deep and last for about 3 – 5 µs, as inferred from an all-atom explicit-solvent 20 and 30 µs trajectories. We argue that their presence enhances aggregation of α-synucleins. In collaboration with: M. Chwastyk, L. Mioduszewski, and B. de Aquino.

*National Science Centre, Poland, grant No. 2018/31/B/NZ1/00047
4:18PM P23.00006: Alpha rhythm shapes the correlation landscape of avalanche dynamics across resting wakefulness*  FABRIZIO LOMBARDI (Presenter), Institute of Science and Technology Austria, LUCILLA DE ARCANGELIS, University of Campania "L. Vanvitelli", HANS JURGEN HERRMANN, ESPCI Paris, OREN SHRIKI, Ben Gurion University — Brain rhythms and neuronal avalanches form a fascinating dichotomy in the universe of emergent brain dynamics. The former have characteristic times and amplitudes, whereas the latter are scale-free, i.e. they lack characteristic spatio-temporal scales. Yet, they coexist and can be independently measured across different physiologic states, such as sleep and resting wake. However, underlying dynamics and functional role of such emergent dichotomy, as well as the dynamic relationship between brain rhythms and avalanches, remain not understood. In this talk I will show that, while the scale-free properties are universal and preserved across sleep and wake, avalanche dynamics is intimately connected to the dominant brain rhythm characterizing each of those physiologic states, and shows unique features in the resting awake state. Our results indicate that the alpha rhythm induces a dynamic transition in the functional organization of neuronal avalanches, and crucially determines the relationship between consecutive avalanches to balance the spatio-temporal dynamics of spontaneous brain activity.

*FL acknowledge support from the Marie Sklodowska-Curie grant No. 754411

4:30PM P23.00007: Non-perturbative renormalization group analysis of strongly-coupled spiking networks  BRADEN BRINKMAN (Presenter), Neurobiology and Behavior, Stony Brook University — To fully explain how neural dynamics transmit information and perform computations, we need to understand the structure of the coordinated activity of neurons and their responses to external inputs. Given a model of neural dynamics and their synaptic connections, we would in principle achieve this goal by calculating the statistical and response functions of the network---a notoriously intractable task for all but the simplest models. While diagrammatic series have been successfully used to correct mean field predictions in weakly-coupled network models, they break down in networks with strong nonlinear behavior, demanding new approximation methods.

Here, we employ `non-perturbative renormalization group" methods to analyze strongly-coupled spiking networks. We show that the true mean firing rates of the network satisfy a nonlinear system of equations formally similar to the mean-field system but with a different effective nonlinearity. We explicitly derive a differential equation for this nonlinearity and solve it numerically. Our results predict the distribution of firing rates in simulated networks of neurons reasonably well, even in strong coupling regimes in which perturbative calculations begin to break down.
4:42PM P23.00008: Representation of nearby and infinitely far reference frames in the brain   SHONALI DHINGRA (Presenter), MINA SHAHI, MAYANK MEHTA, University of California, Los Angeles — While navigating the world, our brain needs to keep track of the space around us. A brain region called the Hippocampus plays a significant role in our perception of space. Our work shows that hippocampal cells recognize space as a vector! Hippocampal Place Cells have been shown to keep track of the subject's absolute position. Using GLM, we show that hippocampal cells also keep track of the direction of the rat's position with respect to various frames of reference. These frames include infinitely far frames, thus keeping track of the canonical Head Direction[1]. We also show that these cells utilize various frames of reference at finite distances from the rat's current position. We call the origin of these reference frames as Anchor Points. We see that these cells code for such anchor points in coherent and stable ways, and we call such tuning of these cells as Anchor Fields. We observe that visual cues are capable of affecting various properties of these anchor tunings, including position of Anchor Points, size of Anchor Fields, percentage of cells tuned, and the direction of tuning with respect to these anchor points. We posit that hippocampal cells utilize these tunings to create a vectorial map of space in our brains.


4:54PM P23.00009: How behavioral and evolutionary constraints sculpt early visual processing* [Invited] STEPHANIE PALMER (Presenter), University of Chicago — While efficient coding has been a successful organizational principle in visual neuroscience, to make a more general theory behavioral, mechanistic, and even evolutionary constraints need to be added to this framework. In our work, we use a mix of known computational goals and detailed behavioral measurements to add constraints to the notion of 'optimality' in vision. Accurate visual prediction is one such constraint. Prediction is essential for interacting fluidly and accurately with our environment because of the delays inherent to all brain circuits. In our work, we explore how our visual system makes these predictions, starting as early as the eye. We use techniques from statistical physics and information processing to assess how efficient, predictive vision emerges from these imperfect component parts. To test whether the visual system performs optimal predictive compression and computation, we compute the past and future stimulus information in populations of retinal ganglion cells, and in the vertical motion sensing system of the fly. In the fly, we anchor our calculations with published measurements of fast evasive flight maneuvers. This survival-critical behavior requires fast and accurate control of flight, which we show can be achieved by visual prediction via a specific wiring motif involving gap junction coupling. Developing a general theory of the evolution of computation is also a current research direction in our group. We use the repeated evolution of tetra-chromatic color vision in butterflies to test hypotheses about whether extant neural computations contain shadows of the evolutionary history of the organism.

*This work was supported by the National Science Foundation: CAREER award 1652617, and the Center for the Physics of Biological Function (PHY-1734030). This work was also supported by NIH grant R01EB026943.

Wednesday, March 4, 2020 2:30 PM - 5:18 PM
2:30PM P24.00001: Flow-Arrest Transition in Granular Materials* [Invited] ISHAN SRIVASTAVA (Presenter), GARY GREST, JEREMY LECHMAN, Sandia National Laboratories, LEO SILBERT, Central New Mexico Community College — Flowing granular materials can abruptly arrest if the applied stresses are smaller than a friction-dependent critical value. Such a phenomenon is commonly observed in geophysical scenarios and industrial practice, often with deleterious consequences. However, the statistical and rheological properties of this non-equilibrium transition are not well-understood. In this talk, I will describe our stress-controlled granular simulations that indicate a highly stochastic nature of this transition with long-tailed distributions of flowing times before arrest, which diverge as a power law at a critical stress ratio. We construct a flow-arrest state diagram that clearly distinguishes between shear flow and shear arrest in granular systems in terms of microstructural and rheological properties, with inter-particle friction being an important ingredient. Furthermore, granular flows in the vicinity of this transition exhibit rheological features that are not captured by the traditional \( \mu(I) \) model, such as the presence of normal stress differences. I will describe our recently developed 3D constitutive model that captures these features and is fully compatible with more complex flow scenarios beyond simple shear, such as extensional and so-called triaxial flows.

*Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE’s National Nuclear Security Administration under contract DE-NA-0003525.

3:06PM P24.00002: Shear thickening and jamming of dense suspensions: the importance of rolling friction ABHINENDRA SINGH (Presenter), University of Chicago, CHRISTOPHER NESS, University of Edinburgh, JUAN DE PABLO, HEINRICH M. JAEGGER, University of Chicago — The mechanism of shear thickening in dense suspensions has been linked to a stress-controlled transition from a lubricated ``frictionless'' to an unlubricated ``frictional'' rheology. Recent particle simulations that constrain the sliding motion between particles have been successful to reproduce both the discontinuous shear thickening (DST) and shear jamming (SJ) observed experimentally but cannot account for the surprisingly low SJ volume fraction (often below 50%) measured in real-life suspensions in which particles are rough. However, an additional way to build up and maintain stress-carrying paths across a suspension, particularly relevant to rough particles, is by constraining particle rolling. We show via simulations that using rolling friction together with sliding friction can significantly decrease the volume fraction required for the onset of DST and SJ leading to enhanced shear thickening. Moreover, rolling friction drastically affects the structure of the underlying network of frictional particle-particle contacts, while from a dynamical perspective it leads to an increase in the velocity correlation length, in part responsible for the increased dissipation.
Tuning Solvent Chemistry to Suppress Shear-Jamming in Dense Suspensions  
MICHAEL VAN DER NAALD (Presenter), LIANG ZHAO, GRAYSON JACKSON, HEINRICH M. JAEGER, University of Chicago — Mechanical stress can transform a free flowing suspension of solid particles in a Newtonian liquid into a shear jammed, solid-like state. While recent work highlighted how particle surface chemistry contributes to the shear jamming transition,[1] much less is known about the suspending liquid. We here report both steady state rheology and the transient impact response tracked by high-speed ultrasound imaging [2] for silica nanoparticles dispersed in polyethylene glycols (PEGs) of varied chain lengths. For suspensions with identical silica volume fractions and impact conditions, decreasing the solvent molecular weight (MW) suppresses shear jamming. We attribute these results to stronger solvation layers in low MW PEG which keep contacts between particles lubricated even under high stress.


Yielding and Rigidity of Sheared Columns of Hexapod Granules*  
YUCHEN ZHAO (Presenter), Department of Physics, Duke University, JONATHAN BARÉS, Laboratoire de Mécanique et Génie Civil, Université de Montpellier, JOSHUA SOCOLAR, Department of Physics, Duke University — Granular packings of non-convex or elongated particles can form free-standing structures like walls or arches. For some particle shapes, such as staples, the rigidity arises from interlocking of pairs of particles, but the origins of rigidity for non-interlocking particles remain unclear. We report on experiments and numerical simulations of sheared columns of “hexapods,” particles consisting of three mutually orthogonal rods whose centers coincide. We vary the length-to-diameter ratio, $\alpha$, of the rods and subject the packings to quasistatic direct shear. For small $\alpha$, we observe a finite yield stress. For large $\alpha$, however, column is rigid against shear, and stresses within it increase with increasing strain. Analysis of X-ray micro-computed tomography data collected during the shear, reveals that the stiffening is associated with a tilted, oblate cluster of hexapods near the nominal shear plane in which particle deformation and average contact number both increase. Simulation results show that geometric cohesion effects are negligible for small $\alpha$. For large $\alpha$ ($\alpha=10$), we directly observe that particles are collectively under tension even though they do not interlock pairwise. The tensile stress counteracts the tendency to dilate in direction normal to the shear plane.

*NSF-DMR1809762
Chaotic particle dynamics above and below yield in a 2D jammed material* LARRY GALLOWAY (Presenter), DOUG JEROLMACK, PAULO ARRATIA, University of Pennsylvania — Amorphous materials, often fail catastrophically, just beyond yield. This is a problem not just in design engineering (harnessing high strength glasses without the chance of ruinous breakdowns), but also in predicting the failure of non-constrained, natural systems (averting damage caused by mudslides). The yielding transition has previously been observed in both experiments and simulations to present via the emergence of specific particle trajectories, known as reversibly or irreversibly plastic. Here we present detailed quantification of Lagrangian properties (displacement lengths, arc-lengths, and enclosed area) of experimentally obtained particle trajectories for the purpose of illuminating where plasticity occurs in space and time both above and below yield. Our findings suggest plastic trajectories, both reversible and irreversible, predominantly occur in specific regions as a function of the strain amplitude, but not time. These findings imply that the yield transition is of the first order and that mean field and thermodynamic models are attainable. In this direction, we introduce a non-dimensional measure of plastic dissipation that applies both above and below yield and captures the rheological yield point.

*ARO: W911-NF-16-1-0290

NSF MRSEC: DMR17-20530

The precursors to stick-slip events in sheared granular systems* CHAO CHENG (Presenter), RITUPARNA BASAK, New Jersey Inst of Tech, MIROSLAV KRAMAR, Department of Mathematics, University of Oklahoma, LOU KONDIC, New Jersey Inst of Tech —

The stick-slip transition of granular systems is related to earthquakes and avalanches, and therefore understanding the conditions leading to slip events is of general importance. Although stick-slip behavior has been studied extensively, what triggers a slip event still remains unclear. The purpose of our study is to explore the existence of precursors to slip events. For this purpose, we study a sheared system in a stick-slip regime via two-dimensional discrete element simulations. Particular focus is on the evolution of force networks before and during slip events. We will show that some features of force network evolution could be used to gain insight into the occurrence of a slip event.

*Supported by ARO Grant No. W911NF1810184
4:06PM P24.00007: Jamming and tiling in fragmentation of rectangles  ELI BEN-NAIM (Presenter), Los Alamos Natl Lab, PAUL KRAPIVSKY, Boston University — We investigate a stochastic process where a rectangle breaks into smaller rectangles through a series of horizontal and vertical fragmentation events. We focus on the case where both the vertical size and the horizontal size of a rectangle are discrete variables. Because of this constraint, the system reaches a jammed state where all rectangles are sticks, that is, rectangles with minimal width. Sticks are frozen as they can not break any further. The average number of sticks in the jammed state, $S$, grows as $S \approx A/(2\pi \ln A)^{1/2}$ with rectangle area $A$ in the large-area limit, and remarkably, this behavior is independent of the aspect ratio. The distribution of stick length has a power-law tail, and further, its moments are characterized by a nonlinear spectrum of scaling exponents. We also study an asymmetric breakage process where vertical and horizontal fragmentation events are realized with different probabilities. In this case, there is a phase transition between a weakly asymmetric phase where the length distribution is independent of system size, and a strongly asymmetric phase where this distribution depends on system size.

4:18PM P24.00008: Contact breaking in packings of frictional disks  YAN CHEN (Presenter), PHILIP WANG, QIKAI WU, Yale University, MARK SHATTUCK, City College of New York, COREY SHANE O'HERN, Yale University — We employ discrete element modeling simulations of the geometrical asperity or "bumpy particle" model to study the nonlinear vibrational response of jammed packings of frictional disks. We first calculate the eigenmodes of the dynamical matrix for each bumpy-particle packing. We then perturb the packing by a given velocity along a single and multiple eigenmodes of the dynamical matrix, run the simulations at constant total energy, and measure the Fourier transform of the translational and rotational velocities of the particles. For small velocity perturbations, contacts do not break, and the peaks in the power spectrum occur at frequencies that match the eigenfrequencies of the dynamical matrix. We determine the characteristic temperature $T_c$ above which the interparticle contact network breaks, and compare the density of vibrational modes from dynamical matrix to the power spectrum for $T > T_c$. We show that perturbing along eigenmodes with primarily translational velocities gives rise to qualitatively different behavior of the vibrational response compared to that after perturbing along eigenmodes with primarily rotational content.
Modelling granular fragmentation in compacted systems

JOEL CLEMMER (Presenter), DAN STEFAN BOLINTINEANU, JEREMY LECHMAN, Sandia National Laboratories — The jamming of hard particles in the zero-pressure limit has been well studied, however many applications are far from this limit. As pressure increases, granular rearrangement is no longer the only mechanism for densification as grains deform and fracture. This breakdown of granular matter, or comminution, produces irregular shapes and sizes and changes macroscopic properties including rheology. We explore the compaction of brittle granular systems using large-scale discrete element simulations. Each grain is composed of many small, fundamental particles. These particles are interconnected by bonds which break under sufficient stress allowing grains to fragment into smaller grains. During loading, we monitor the evolution of stress, porosity, and distributions of grain size and shape. We characterize trends and explore the effect of strain rate and material properties. We also identify the pressure at which individual grains fracture and compare to theoretical models.

Electrostatic Attraction between Like-Charged Particles

BENJAMIN REGGIO (Presenter), SHUBHA TEWARI, Univ of Mass - Amherst — A point charge Coulomb force model provides an inadequate description of the interaction between finite-sized particles. Experiments find that dielectric particles of like charge can polarize one another, causing effective attractive forces between them that lead to clumping. To more accurately model the origin of these attractive forces, we study the effective interaction between two dielectric spherical shells with like charge as a function of their size and charge ratios, and the dielectric constant of each. We base our work on a model developed by Bichoutskaia et. al. [1] in which the authors map a phase diagram of attractive interactions between like-charged spheres at touching. We extend the phase diagram to finite separations between the particles, determining the boundary at which the force becomes repulsive. Though a closed form expression for the force between particles does not exist, we find an effective force in certain parameter regimes that can be used as an input in simulations of charged granular particles. The form of this force is found to vary depending on whether we are in the small size ratio or the small charge ratio regime.

4:54PM P24.00011: Unforgettable random walks: forces and displacements distributions in granular systems.*  
ANTON PESHKOV (Presenter), Department of Physics and Astronomy, University of Rochester, ZACKERY A BENSON, IREAP, University of Maryland, DEREK C RICHARDSON, Department of Astronomy, University of Maryland, WOLFGANG LOSERT, Affiliation: Departments of Physics, IPST and IREAP, University of Maryland — Granular systems are known to exhibit memory effects characterized by the remembrance of the past states and preparation history, which affect its future evolution. At the same time there exist a consensus that the force distributions of granular systems follow exponential and gamma distributions; a hallmark of the memory independent Brownian motion. Both of these assertions are mutually contradicting. We resolve this incongruity by experimentally and numerically verifying that the forces, as well as translational and rotational displacements of dense granular systems are governed by log-normal and power law distributions; consequence of a history dependent geometrical Brownian motion. We show the latter to be a natural product of contacts that reign between particles.

*This work was supported by National Science Foundation grant DMR5244620.

5:06PM P24.00012: Weakening, compaction and creep from vibration in sheared granular materials*  
STEPHANIE TAYLOR (Presenter), University of California, Santa Cruz, ABE CLARK, Naval Postgraduate School, EMILY BRODSKY, University of California, Santa Cruz — The strength and stability of granular materials like sands and powders corresponds to the strength and stability of soils, asphalt, building and industrial materials, gouge filled earthquake faults, hillslopes, and more. Passing vibrations and transient perturbations have been thought to play a role in determining dynamic friction during sliding in such systems as well as trigger failure in static grain packs. With laboratory experiments and discrete element method simulations, we show that low amplitude high frequency vibrations are capable of significantly reducing frictional resistance over a range of velocities in actively shearing systems. Near yield, coefficient of friction decreases with increasing acoustic energy raised to a power of -0.2. Susceptibility to creep, compaction and weakening depends on grain shape, vibration amplitude, frequency, system resonances and system pressure. Exposure to (and generation of) vibration during shear of granular materials is common in many industrial and transport processes, and granular materials’ susceptibility to vibrational weakening may play a pivotal role in these processes.

*Army Research Laboratory. Grant Number: W911NF 15 1 0012

Wednesday, March 4, 2020 2:30 PM - 5:06 PM

Session P25 GSNP DSOFT: Fabric, Knits and Knots II / Complex Networks 402 - Mark Shattuck, The City College of New York - Tag(s): Focus
2:30PM P25.00001: String Contraction via Twisting: Ideal and Nonideal Behavior  JESSE HANLAN (Presenter), University of Pennsylvania, GABRIELLE DAVIS, Department of Physics, University of Maryland, DOUGLAS DURIAN, University of Pennsylvania — Strings are an ancient and extremely common tool for force delivery. They may also be used to deliver torque via twisting, according to tension times the rate of length contraction versus twist angle $\Theta$, and this is important for twisted string actuators in robotics as well as for button-on-a-string toys and hand-powered centrifuges. Idealized behavior for length contraction is predicted to be $L^2 = L_0^2 - (r\Theta)^2$ where $L_0$ is the initial string length and $r$ is its radius. Here we compare this model with data for single, double and triple stranded strings of parachute cords, rattail cord, nylon, kevlar, monofilament fishing line, and metal wire. We also examine deviation from ideality at small and large twist angles in order to probe the internal structure of our strings. At small angles, we see a systematic decrease in the effective cord radius compared to expectation, as individual strands compress into each other, while at large twist angles we see less contraction than expectation due to the coiling of the strands. In all cases, nonideal effects may be quantified by an effective string radius indicative of internal geometry and string-string interaction, which could play a role in the mechanics of real knots and fabrics.

2:42PM P25.00002: Contact geometry of equidistant tubes  HARMEET SINGH (Presenter), PAUL GRANDGEORGE, TOMOHIKO SANO, PEDRO REIS, JOHN MADDOCKS, École polytechnique fédérale de Lausanne — We consider equilibrium configurations of two flexible tubes arranged in space such that their centrelines are separated by a constant distance. Depending on their configuration, the two centrelines may exhibit single or double contact. We will discuss the contact geometry of one such configuration that exhibits double contact, called the orthogonal clasp, where the two centrelines are assumed to lie in orthogonal planes. Based on this example, we will motivate a “capstan” like equation governing tension decay along the centreline of a flexible tube wrapped around a rigid hook with friction.

2:54PM P25.00003: Fibered by fibers: the geometry and elasticity of frustrated filaments*  DARIA ATKINSON (Presenter), Univ of Mass - Amherst, CHRISTIAN SANTANGELO, Syracuse University, GREGORY GRASON, Univ of Mass - Amherst — Filamentous and columnar assemblies are a ubiquitous motif in materials, from microscopic and biological materials, like discotic liquid crystals and biopolymer bundles, to familiar macroscopic materials like yarns, cables, and ropes. Ordered ground states in filament bundles, however, are highly geometrically constrained. We show that only two families of filament textures permit equidistance between the constituent filaments: the developable domains, which can bend, but not twist, and the helical domains, which can twist uniformly, but not bend. The elastic response of non-equidistant filament bundles is then frustrated, and cannot adequately be described by a linearized energy. To describe nonequidistant configurations, we derive a geometrically nonlinear, coordinate invariant, gauge-like theory for the elasticity of filamentous materials. Within this framework, we discuss the impact of filament texture on bundle elasticity, and calculate the stable states for non-equidistant bundles with small curvature.

*NSF DMR-1507377
NSF DMR-1608862
3:18PM P25.00005: Disease outbreak as stochastic resonance: interplay between host-seeking behavior and heterogeneous human/vector interactions results in system amplification*  
JOSHUA PARKER (Presenter), U.S. Army Engineer Research and Development Center, DAVE PECOR, Smithsonian Institution, NICOLE WAYANT, U.S. Army Engineer Research and Development Center — We perform phase space analysis on a mathematical model of mosquito-borne disease that incorporates the full mosquito life cycle. We also include the cessation of host-seeking after obtaining a blood meal, and heterogeneous interactions between the human and mosquito populations. We find that under these conditions, stochastic resonance results in the emergence of a dynamic phase of episodic outbreak, where the proportion of the human and mosquito populations susceptible to disease exposure varies wildly from year to year. The results of this work suggest that interventions to screen vector and human populations from disease leads to intermittent exposure to infection, which may lead to these populations becoming more sensitive to outbreaks.

*Funding for this project has been provided in part by funding from the Global Emergin Infection Surveillance program of Army Health Services Branch and the Engineer Research and Development Center, a division of US Army Corps of Engineers

3:30PM P25.00006: Impact of initial seeds in cooperative contagion processes  
BYUNGJOON MIN (Presenter), Department of Physics, Chungbuk National University — Many types of contagion phenomena are often strongly influenced by cooperative effects among multiple pathogens. When a node has been infected with one of the diseases, the probability of the second disease’s transmission grows, compared to single pathogen spreading. It remains unclear how to predict epidemic outbreaks from the location of the initial seeds. In this work, we modulate the probability of infection depending on the state of nodes taking into account the cooperativity between different pathogens. Defining the transmission probabilities of the first and of the second infecting disease, we derive message-passing equations for cooperative contagion processes. By using the message-passing equations, we assess the impact of seeds in cooperative coinfections and also provide explanation how cooperative epidemic occurs.
3:42PM P25.00007: Degree-preserving Network Growth* SHUBHA RAJ KHAREL (Presenter), University of Notre Dame, TAMÁS RÓBERT MEZEI, Alfréd Rényi Institute of Mathematics, SUKHWAN CHUNG, University of Notre Dame, DÁNIEL SOLTÉSZ, PETER ERDOS, Alfréd Rényi Institute of Mathematics, ZOLTAN TOROCZKAI, University of Notre Dame — Real-world networks evolve over time via the addition or removal of vertices and edges. In current network evolution models, vertex degree varies or can even grow arbitrarily, yet there are many networks in which it saturates (e.g., social networks) or is fixed (e.g., chemical complexes), thus requiring an entirely different description. We introduce a novel class of models that encapsulates degree preserving dynamics in the simplest form, resulting in structures significantly different from previous ones. We discuss their properties as function of the evolution of the network’s matching number and present several generative models based on this framework, from growing uniform degree distribution graphs to growing random regular graphs, which, to our best knowledge, is the first model of this kind. Within this approach, we also introduce configuration-like models that realize given degree sequences, with tunable degree-mixing properties. Moreover, this process can generate scale-free networks with arbitrary exponents, but without involving any degree-based preferential attachment.

*The project was supported in part by the NSF grant IIS-1724297 (ZT), Natl. Research, Development and Innovation Office-NKFIH grants K 116769, KH 126853 (ELP, TRM, DS) and by K 120706, KH 130371 (DS).

3:54PM P25.00008: Synchronization of Coupled Kuramoto Oscillators under Resource Constraints* KEITH WILEY (Presenter), University of Pennsylvania, PETER J MUCHA, University of North Carolina at Chapel Hill, DANIELLE BASSETT, University of Pennsylvania — A fundamental understanding of synchronized behavior in multi-agent systems can be acquired by studying analytically tractable Kuramoto models. Yet, such models typically diverge from many real systems whose dynamics evolve under marked resource constraints. Here we construct a system of coupled Kuramoto oscillators that consume or produce resources as a function of their oscillation frequency. At high coupling, we observe strongly synchronized dynamics, whereas at low coupling, we observe independent oscillator dynamics, as expected. For intermediate coupling which typically induces a partially synchronized state, we demonstrate that the system can exist in either an oscillatory synchronization state or a bistable synchronization state depending on whether the oscillators consume or produce resources, respectively. Relevant for systems as varied as coupled neurons and social groups, our study lays important groundwork for future efforts developing quantitative predictions of synchronized dynamics for systems embedded in environments marked by resource constraints.

*ARO MURI (Falk) W911NG-18-1-0244; Paul G. Allen Family Foundation.
Model reduction of large networked systems using the Manifold Boundary Approximation Method

BENJAMIN FRANCIS (Presenter), JACOB R NUTTALL, MARK TRANSTRUM, Brigham Young Univ - Provo, ANDRIJA SARIĆ, University of Novi Sad, ALEKSANDAR STANKOVIĆ, Tufts University — Complex systems are often described by a network. Models of these systems are often constructed from physical first principles by accounting for the interaction network among the components.

For large systems, model complexity grows faster than the richness of the available data, leading to many more tunable parameters than can be reliably estimated from measurements. The resulting models are often sloppy and amenable to effective descriptions in which mechanistic details are intentionally ignored in favor of the relevant collective degrees of freedom governing system behavior.

We consider the case of a small network model from electric power systems and show that sloppiness is manifest in both dynamic and network parameters.

Using techniques of information geometry, we derive reduced models of the network that act as effective theories in cases where only partial system measurements are available using the Manifold Boundary Approximation Method (MBAM).

Leveraging insights from this model, we apply a linearized version of MBAM to a much larger system.

We demonstrate that this method can identify the effective network of interactions, and discuss implications for modeling of other networked systems.

*This work was supported by the US National Science Foundation under Award EPCN-1710727.

Path-dependent Dynamics Induced by Rewiring Networks of Kuramoto Oscillators with Inertia

WILLIAM QIAN (Presenter), EVANGELIA PAPADOPOULOS, ZHIXIN LU, DANIELLE BASSETT, University of Pennsylvania — In networks of coupled oscillators, it is of wide interest to understand how interaction topology affects synchronization. Many studies have gained key insights into this question by studying the classic Kuramoto oscillator model on static networks. However, new questions arise when network structure is time-varying or when the oscillator system is multistable, which can occur by adding an inertial term to the Kuramoto model. While the consequences of evolving topology and multistability have been examined separately, real-world systems such as the brain may exhibit these properties simultaneously.

This motivates investigation into how rewiring of network connectivity affects synchronization in systems with multistability, where different paths of network evolution may differentially impact collective behavior. To this end, we study the effects of evolving network topology on coupled Kuramoto oscillators with inertia. We find that certain fixed-density rewiring schemes induce significant changes to the level of global synchrony, and that these changes are robust to a wide range of network perturbations. Our findings suggest that the specific progression of network topology can play a considerable role in modulating the collective behavior of systems evolving on complex networks.
4:30PM P25.00011: Distribution of the Sizes of the Blackouts in Power Grids, Synthetic Models, and the Motter and Lai Model under different Dynamical Rules and Criteria of Overload  GABRIEL CWILICH (Presenter), SERGEY BULDYREV, Physics, Yeshiva University, YOSEF KORNBLUTH, Mechanical Engineering, Massachusetts Institute of Technology — Studies of the sizes of the blackouts in real grids and computer simulation models of them using the direct current approximation suggest that the resulting blackout sizes are distributed as a power law when using the standard criterion of resilience, the so-called N-1 condition: The grid must safely operate in the event of a failure of any single line. At any stage of the cascade, one of the lines whose load exceeds the maximum values imposed by the N-1 condition fails and immediately all the currents in the grids are redistributed adjusting to the new topology. On the contrary, when the grid is modeled with a uniform tolerance proportional to its initial current for all the nodes and one removes all the overloaded lines simultaneously at each stage of the cascade, the distribution of the sizes of the blackouts is bimodal as in a first the order phase transition, resulting in either a very small blackout or a very large blackout. Here we reconcile both approaches by looking at how the blackout distribution changes with model parameters and different dynamic rules of failure of the overloaded lines. We also study the Motter and Lai model of betweenness overload and find similar results, suggesting that the physical laws of flow are not the determinant factor in the problem.

4:42PM P25.00012: Generating individual aging trajectories with a network model  SPENCER FARRELL (Presenter), ARNOLD MITNITSKI, KENNETH ROCKWOOD, ANDREW RUTENBERG, Dalhousie Univ — Aging is characterized by the stochastic accumulation of damage. We model this process with a set of health attributes as nodes that interact in a network leading to mortality. Health decline and mortality occur stochastically with a set of complex rates that are trained along with the interaction network using data from observational aging studies. Our model generates synthetic-individuals with health trajectories and lifespan resembling real individuals. The trajectories and lifespans generated with this method also let us model both health events and health interventions so as to better understand their effects on the future health and lifespan of individuals.
4:54PM P25.00013: Modeling the Dynamics of Belief in Climate Change with Statistical Physics

ERNEST AIGNER, Wirtschaftsuniversität Wien, JACKIE BROWN, York University, KYLE FURLONG, MITRE, DAVID GIER, University of California, Davis, LUDVIG HOLMÉR (Presenter), Stockholm School of Economics, RITWIKA VALLOMPARAMBATH PANIKKASSERYSU, Physics, University of California, Merced — We simulate the dynamics of belief in climate change using agents on a social network who update their beliefs according to a classical XY Model Hamiltonian. The initial conditions of the model are set by contemporary empirical insights in the social distribution of climate beliefs (Hornsey et al. 2016). The social network dynamics are inspired by dispersion rules proposed by Galesic and Stein (2019) but extend with additional social and environmental rules. Environmental effects include extreme weather events and disasters. The frequency, spatial-distribution, and intensity of extreme weather events are calibrated with real world data on climate impacts (Siscoe et al. 2017). The model enables us to analyse the interactions between social belief dynamics in networks and climate impacts and suggest when and if a consensus about climate change will form in the wake of extreme climate-related weather events.

*This research was supported in part by the Santa Fe Institute.

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Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P26 DBIO DCP: Immune Sensing and Response

2:30PM P26.00001: Universality of biochemical feedback and its application to immune cells* [Invited] AMIR EREZ (Presenter), Princeton University, TOMMY A. BYRD, Purdue University, ROBERT M VOGEL, IBM T. J. Watson Research Center, GREGOIRE ALTAN-BONNET, National Institutes of Health, ANDREW MUGLER, Purdue University — Positive feedback is ubiquitous in biochemical networks and can lead to a bifurcation from a monostable to a bistable cellular state. One such example is the immune self/foreign decision, which is manifested in a complex biochemical cascade. We consider a coarse-grained view of this cascade, its output and response to inhibition, and propose a theory which maps the stochastic dynamics to thermodynamic state variables. Our mapping allows experimental data analysis without curve fitting and highlights previously unknown features in the data. Beyond steady state, our theory reveals critical slowing down and a universal scaling of the response to changing stimulus. Finally, motivated by the immunological synapse, where a pair of cells communicate with each other through molecule exchange, we consider a pair of sensing/responding cells and how they might communicate effectively.

*This work was supported by Human Frontier Science Program Grant No. LT000123/2014 (A.E.), National Institutes of Health (NIH) Grant No. R01 GM082938 (A.E.), Simons Foundation Grant No. 376198 (T.A.B. and A.M.), and the Intramural Research Program of the NIH, Center for Cancer Research, National Cancer Institute.
3:06PM P26.00002: Optimal non-equilibrium decision making to store immune memory
OSKAR SCHNAACK (Presenter), Max Planck Institute for Dynamics and Self-Organization, ARMITA NOURMOHAMMAD, University of Washington — Our adaptive immune system consists of highly diverse immune receptors to mount specific responses against a multitude of pathogens. During an infection, a fraction of these receptors forms a memory for later encounters. Here, we address a key question: which of the immune receptors should be kept as memory so that they can mount a response against evolved forms of the original pathogen in future infections? To do so, we have developed a theoretical framework, where memory storage is a non-equilibrium decision-making process between an adaptive exploration to mount a specific response and exploitation of existing yet suboptimal memory that can be utilized immediately to suppress an infection. To achieve a long-term benefit for the host, we show that memory generation should involve feedback from receptors' affinity and should favor cross-reactive receptors with a moderate affinity over high-affinity receptors against the infecting pathogen. The recipe for memory generation should be tuned over the host's evolutionary timescale based on the pathogenic evolutionary rates. Our results are consistent with recent experiments that suggest cell fate decisions during memory generation are highly regulated to balance the affinity and cross-reactivity of immune receptors.

3:18PM P26.00003: Visualizing and controlling immune response to gut microbes*
BRANDON SCHLOMANN (Presenter), TRAVIS J WILES, ELENA S WALL, KAREN GUILLEMIN, RAGHUVEER PARTHASARATHY, Univ of Oregon — Trillions of bacteria reside in the intestine where they are largely kept away from epithelial surfaces. When this spatial confinement is broken, the resulting immune responses can be damaging and lead to disease. Understanding the processes that spatially restrict gut bacteria will open new avenues for microbiome-based therapies. I will present work that investigates interactions between immune cells and resident gut bacteria through live imaging of naturally transparent, larval zebrafish. We discovered that flagella-based swimming motility enables a native Vibrio species to govern its own spatial organization within the gut and stimulate a potent immune response. Mutants that cannot swim become aggregated and confined to the interior lumen of the gut. Loss of motility also leads to reduced expression of the proinflammatory cytokine TNFα in gut-associated macrophages and in the liver. Externally-inducible genetic switches enabled in situ manipulation of bacterial motility, and therefore external control of both bacterial spatial distribution and proinflammatory potential. Our findings reveal connections between the physical activity of bacteria, their spatial organization, and host inflammatory activity.

*This work was supported by the NIH, NSF, and Kavli Foundation.
Adoptive cell transfers have emerged as a disruptive approach to treat diseases in a manner that is more specific than using small molecule drugs. However, unlike traditional drugs, cells are living entities that can alter their function in response to subtle environmental cues. In this talk, I will present a class of particles, referred to as “backpacks”, that can regulate the phenotype of adoptively transferred macrophages in vivo. Backpacks are able to robustly adhere to macrophage surfaces and evade phagocytosis for several days. Once attached, backpacks can release encapsulated pro-inflammatory cytokines to potentiate antitumor (M1) phenotypes in macrophages, even in tumor-mimicking conditions. When injected intratumorally into mice bearing breast tumors, a potent immunosuppressive (M2) environment, backpacks allowed macrophages to maintain their M1 phenotypes. Conserved phenotypes led to significantly reduced metastatic burdens and slowed tumor growths compared to those of mice treated with an equal dose of free cytokine. Overall, controlled release of cytokines from backpacks may enable a new strategy to regulate phenotypes of adoptively transferred cells to aid in the treatment of a variety of inflammatory and autoimmune diseases.

Cells such as natural killer cells and macrophages can recognize and eliminate targets with aberrant surface ligand expression without antigen specificity. This innate mechanism of activation must be tightly regulated to prevent autoimmunity. We describe a quantitative model of the regulation of nonspecific activation that is grounded in Bayesian inference. Our model captures known behaviors of innate immune cells, including adaptation to changing environments and the development of hyposensitivity after prolonged exposure to activating signals. Our analysis reveals a tradeoff between precision and flexible adaptation to different environments. Maintaining the ability to adapt naturally leads to heterogeneous responses, even for hypothetical populations of immune cells and targets that have identical surface receptor and ligand expression. Collectively, our results describe an adaptive algorithm for self/nonself discrimination that functions even in the absence of antigen restriction and supports biological observations of single-cell heterogeneity in response to cell-cell interactions. The same model could also apply more broadly to the adaptive regulation of activation for other immune cell types.
A mathematical model of aging in the immune system

ERIC JONES (Presenter), University of California, Santa Barbara, JIMING SHENG, SHENSHEN WANG, University of California, Los Angeles, JEAN M CARLSON, University of California, Santa Barbara — The adaptive and innate branches of the vertebrate immune system work in close collaboration to protect organisms from harmful pathogens. As the organism ages the immune system undergoes immunosenescence, characterized by declined performance or malfunction in either branch, which can lead to various diseases and death. In this study we develop a mathematical model of the immune system that couples the innate and adaptive components of the immune system, allowing investigation of the mutual modulation of the innate and adaptive immune branches over time. Our results capture the clinically-observed chronic inflammatory response affiliated with aging (“inflamm-aging”), and find that the timing of this persistent inflammatory response is dependent on the history of pathogen encounters. By consolidating complex immune feedbacks into a mathematical model, our results inform the mechanisms responsible for immunosenescence and offer opportunities for their further exploration through quantitative modeling.

This work was supported by the David and Lucile Packard Foundation and the Institute for Collaborative Biotechnologies through contract no. W911NF-09-D-0001 from the U.S. Army Research Office.

B cells use mechanical energy to distinguish affinity and speed up adaptation

HONGDA JIANG (Presenter), SHENSHEN WANG, Department of Physics and Astronomy, University of California, Los Angeles — Generation of potent antibodies relies on positive selection of germinal center (GC) B cells expressing high affinity receptors. Effective selection during the rapid evolutionary process called affinity maturation requires efficient ranking of affinity. Yet, the mechanism by which affinity discrimination is achieved and how it affects B cell evolution remains unclear. Growing evidence shows that B cells use mechanical forces to actively extract antigens from the surface of antigen-presenting cells. Here we study the stochastic process of antigen extraction using theory and simulations. We find that application of mechanical force alters the energy landscape of molecular interactions and consequently extends the range of distinguishable affinities. Integrating this extraction model on the molecular scale with GC dynamics on the population level, we demonstrate that exertion of cytoskeletal forces for antigen extraction can accelerate the rate of affinity maturation.
Aging in the immune system is a loss of balance

Jiming Sheng (Presenter), Physics and Astronomy, University of California, Los Angeles; Eric Jones, Jean M Carlson, Physics, University of California, Santa Barbara; Shenshen Wang, Physics and Astronomy, University of California, Los Angeles — The innate and adaptive arms of the vertebrate immune system work in close collaboration to protect organisms from harmful pathogens. As an organism ages its immune system undergoes immunosenescence, characterized by degraded performance or malfunction, in either arm, that leads to diseases and even death. However, a system-level mechanism of immunosenescence is not understood.

In this talk, I introduce a mathematical model of immune response that integrates the innate and adaptive components, which enables studies of their mutual modulation over an individual's lifetime. Our results capture the clinically-observed chronic inflammation associated with aging, demonstrating that this “inflamm-aging” could be of protective origin by compensating for weakened adaptive immunity. We show that the timing of onset of persistent inflammatory response depends strongly on the temporal pattern of pathogen encounter and uncover potential determinants of the timing. Finally we examine the bipartite role of adaptive immunity in a balance between removing pathogens and mitigating inflammation. In all, our work suggests that aging in the immune system exemplifies a failure of coordination between adaptive and innate immunity and the timing of failure is strongly shaped by the infection history.

Influenza virus geometry shapes the immune response against it

Assaf Amitai (Presenter), Massachusetts Institute of Technology MIT; Maya Sangesland, Daniel Lingwood, The Ragon Institute of Massachusetts General Hospital, The Massachusetts Institute of Technology and Harvard University; Arup K Chakraborty, Massachusetts Institute of Technology MIT — Influenza surface glycoprotein – Hemagglutinin (HA) is the main target of the immune system following exposure to the virus. Most antibodies elicited following vaccination or infection are created against the head, which is highly mutable. A vaccination approach that would target immune response towards evolutionarily conserved residues on hemagglutinin stem can elicit broadly neutralizing antibodies capable of fighting many flu strains.

Using mice experiments, in-silico models of designed immunogens (nanoparticles) and of antibody development against flu, we study how a targeted response against conserved stem residues can be elicited. We find that because of the high density of HA molecules on the virus, infection by the virus drives the proliferation of B cells targeting mutable residues while suppressing those targeting conserved sites. Strong response against the conserved residue can be achieved by vaccinating with nanoparticles presenting the stem part of HA alone, of flu strain different from those to which the system was already exposed to.
4:42PM P26.00010: Spurious higher-order correlations from non-linearities in a receptor-ligand model  RICHARD ZHU (Presenter), ARVIND MURUGAN, University of Chicago — Multi-body correlations arise frequently in analyses of biological systems, such as antibiotic interactions in cell growth rate, mutational interactions on protein function and ligand interactions in the immune system. In particular, it is common practice to measure the 1st and 2nd-moments of quantities of interest, and fit a maximum-entropy model to the data. We demonstrate that pairwise and higher-order interactions emerge naturally from mismatches between the fitted model and the underlying physical system, as well as ignorance of unmeasured quantities. We study a simple receptor-ligand model and demonstrate that spurious higher-order interactions can arise from simpler interactions combined with non-linearities not accounted for. Our analysis shows how careful accounting for the underlying biology is needed to conclude the existence or absence of complex interactions within the system.

4:54PM P26.00011: To die or not to die: Cell decision-making in the face of viral threat*  [Invited]  JENNIFER OYLER-YANIV (Presenter), California State University, Los Angeles — Paradoxically, the pro-inflammatory cytokine Tumor Necrosis Factor α (TNFα) simultaneously activates opposing pro-apoptotic and pro-survival signaling. We show that the activation of antagonistic pathways changes the properties of cell fate decision transitioning cells from a “slow and accurate” to “fast and error-prone” decision mode. Mathematical modeling predicts, and experiments in vitro and in vivo validate, that the regulation of the decision mode of non-immune cells by innate immune cell production of TNFα is key to prevent viral spread. Overall our results demonstrate how a collective phenotype emerges from the regulation of fundamental tradeoffs within cellular cognitive processes.

*This work is supported by the National Eye Institute by the following two grants:
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2.) R01EY024960-06

Wednesday, March 4, 2020 2:30 PM - 5:18 PM

Session P27 FIAP DCMP: Synthesis and Characterization of Electronic Thin Films  404 - Amber Reed, Air Force Research Lab - WPAFB
2:30PM P27.00001: Effect of Scandium Nitride Film Orientation on Growth and Electrical Properties

AMBER REED (Presenter), Air Force Research Lab - WPAFB, DAVID LOOK, Semiconductor Research Center, Wright State University, HADLEY SMITH, ZACHARY BIEGLER, RACHEL ADAMS, MADELYN HILL, TYSON BACK, JOHN CETNAR, Air Force Research Lab - WPAFB — Scandium nitride (ScN) is a degenerate semiconductor with great potential as a complementary material to enhance GaN performance in high-power and high-speed electronic applications. Electron mobilities up to 130 cm$^2$/Vs have been reported for (100)-ScN on (100)-MgO substrates. The values reported for (111)-ScN, however, are significantly lower. In this work, we investigate the effect of ScN orientation on film growth, composition and electrical properties. A series of thin ScN films were deposited on (111)-, (110)- and (100)-MgO substrates using reactive magnetron sputtering. X-ray diffraction showed that ScN grew with the same orientation as the MgO and crystalline growth and quality was dependent on growth conditions. Secondary ion mass spectroscopy showed that while the variation in the oxygen concentration was negligible, the fluorine and hydrogen concentrations differed between ScN orientations. Hall-effect measurements showed that mobility, carrier concentration, and resistivity were dependent on orientation. In this presentation we will discuss the correlation between the measured electrical properties and the ScN crystallinity and composition.

*This research was supported by the Air Force Office of Scientific Research through project FA9550-RY17COR490.

2:42PM P27.00002: High-Mobility Two-Dimensional Electron Gases at Al$_x$Ga$_{1-x}$N/GaN Heterostructures Grown by Plasma-assisted Molecular Beam Epitaxy

YUXING REN (Presenter), YONGJIN CHO, AUSTIN HICKMAN, REET T CHAUDHURI, PHILLIP DANG, MENYOUNG LEE, WENWEN ZHAO, ZEXUAN ZHANG, HUILI GRACE XING, DEBDEEP JENA, Cornell University — Polarization-induced high-mobility two-dimensional electron gases (2DEGs) at AlGaN/GaN heterostructures have been studied and used for ultrafast transistors. They offer an interesting platform to study quantum transport in the high electron effective mass regime. At room temperature, the mobility is dominated by optical phonon scattering, but at low temperatures, the mobility is determined by defect and imperfection based scattering mechanisms, and weakly by acoustic phonons. In this talk, we will present how gate control of the 2DEG density helps us identify the impact of dislocations on the mobility. We have used a range of samples in which the dislocation densities vary over 4 orders of magnitude. With the help of high magnetic field oscillation studies at low temperatures we extract the effect of dislocations on the low temperature scattering processes.

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2:54PM P27.00003: Electrical Properties of Highly Functionalized Ultrathin, 2-Dimensional Hexagonal Boron Nitride* DANIEL CHOI (Presenter), National Research Council, STANISLAV TSOI, EVGENIYA LOCK, BORIS FEYLGELSON, United States Naval Research Laboratory — Hexagonal boron nitride (h-BN), an excellent dielectric material with a wide band gap value of ~6 eV, is widely used as insulating layer and gate dielectric in a wide variety of current electrical systems as well as emerging quantum based applications. Thus, much efforts have been invested in looking into modulating electrical properties of h-BN systems. However, much of the current state of the art h-BN studies have focused around larger flakes rather than thin films due to difficulty in uniform synthesis and surface chemistry, leading to low degree of functionalization. In this talk, we present electrical and tunneling properties of highly functionalized, ultrathin, 2D h-BN. Our h-BN are functionalized with TFPA-NH$_2$ and TFPA-SH molecules and electrical properties probed via conductive atomic force microscopy. Our approach reveals previously unachieved, high degree of functionalization, as well as electrical and tunneling properties of this novel system. Our results provide basis for understanding effects of high degree functionalization on h-BN thin films as well as additional incorporation method of h-BN into other 2D van der Waals heterostructure systems.

*This work was partially supported by the Office of Naval Research through Naval Research Laboratory Base Program.

3:06PM P27.00004: Mobility fluctuation Controlled Linear Positive Magnetoresistance in 2D Semiconductor Bi$_2$O$_2$Se nano-plates PENG LI (Presenter), University of Waterloo, CHENHUI ZHANG, King Abdullah University of Science and Technology, GUOXING MIAO, University of Waterloo, XIXIANG ZHANG, King Abdullah University of Science and Technology — Bi$_2$O$_2$Se is a promising 2D semiconductor with ultrahigh mobility and excellent stability in ambient conditions. We report the observation of positive and linear magnetoresistance in both Se-poor and Se-rich Bi$_2$O$_2$Se nano-plates grown by chemical vapor deposition. In Se poor Bi$_2$O$_2$Se nano-plates, the pronounced Shubnikov-de Hass oscillations lie in the linear magnetoresistance background. The Se-poor Bi$_2$O$_2$Se nano-plates show a typical 2D conduction feature with a small effective mass of 0.032m$_0$. The average transport Hall mobility, i.e. less than 5500 cm$^2$V$^{-1}$s$^{-1}$, is significantly reduced, compared to the ultrahigh quantum mobility that is as high as 16260 cm$^2$V$^{-1}$s$^{-1}$. The spatial mobility fluctuation leads to the linear magnetoresistance, which are strongly supported by inhomogeneity in the scanning near-field microscopy images and Shubnikov-de Hass oscillation analyses. On the contrary, Se-rich Bi$_2$O$_2$Se samples with the transport mobility less than 300 cm$^2$V$^{-1}$s$^{-1}$ show a smaller linear magnetoresistance ratio, which is controlled by the average mobility. Our finding expands the understanding of this 2D semiconductor and explores its potential magnetoresistive device application.
3:18PM P27.00005: First-principles study of adatom interactions on the $\beta$-Ga$_2$O$_3$(010) surface*  
MENGEN WANG (Presenter), SAI MU, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — Monoclinic $\beta$-Ga$_2$O$_3$ is a wide-gap (~4.8 eV)$^{1}$ semiconductor with a high breakdown field. This renders Ga$_2$O$_3$ a promising candidate for high-power electronics and deep ultraviolet detectors. However, the growth rate and crystal quality of Ga$_2$O$_3$ thin films are limited by etching of the Ga$_2$O$_3$ surface due to suboxide (Ga$_2$O) formation. It has been reported that the growth rate of Ga$_2$O$_3$ in molecular beam epitaxy can be enhanced by an additional indium supply.$^{2}$ However, the mechanism by which In impacts growth remains elusive. To address this puzzle, we use density functional theory to explore the adsorption and diffusion of Ga and O adatoms on the Ga$_2$O$_3$(010) surface. The low-energy adsorption structures are studied for various Ga coverages. We illustrate the effect of the co-adsorption of In and Ga on the adsorption energetics and the diffusion barriers of O atoms. Our study holds clues to understanding the growth and etching mechanism of the Ga$_2$O$_3$ surface.


*The work was supported by the GAME MURI of the Air Force Office of Scientific Research.

3:30PM P27.00006: Temperature coefficient of resistance (TCR) measurement on vanadium pentoxide (V$_2$O$_5$) nanoparticles*  
GANGA NEUPANE (Presenter), PARAMESWAR HARI, Univ of Tulsa — In this work, we varied molar concentrations (0.05M, 0.1M, 0.15M, and 0.2M) of vanadium pentoxide (V$_2$O$_5$) to synthesize nanoparticles by hydrothermal method. Structural properties were studied using X-ray diffraction spectroscopy (XRD) and Transmission electron microscopy (TEM). XRD and TEM confirmed the increase in particle size with increasing molar concentrations with no secondary phases. Optical properties were studied using Photoluminescence and absorption measurements. Bandgap energy of nanoparticles was found to decrease from 2.25 eV to 2.20 eV with increasing molar concentration. Elemental composition was analyzed by X-ray photoelectron spectroscopy (XPS). The electrical conductivity of nanoparticles was found to increases with increasing molar concentration and also with increasing annealing temperature. The resistivity of nanoparticles (0.05M, 0.1M, 0.15M, and 0.2M) with different temperatures from 293K to 393K was measured. The temperature coefficient of resistance (TCR) value of -2.39%/K and resistivity of 0.1 Ohm-cm for 0.2 M concentration of vanadium pentoxide nanoparticles were obtained. We will discuss the significance of TCR obtained in the microbolometer application.

*NASA EPSCoR  
The University of Tulsa
3:42PM P27.00007: Multiscale Modeling for MOCVD Synthesis and Characterization of Transition Metal Dichalcogenides*  NADIRE NAYIR (Presenter), YUANXI WANG, YUAN XUAN, Pennsylvania State University, KASRA MOMENI, Louisiana Tech University, MERT YIGIT SENGUL, YANZHOU JI, TANUSHREE HOLME CHOU DHURY, DANIELLE REIFSNYDER HICKEY, NASIM ALEM, JOAN M REDWING, VINCENT CRESPI, LONG Q. CHEN, ADRI C.T. VAN DUIN, Pennsylvania State University — MOCVD enables to synthesize high-quality TMD layers from vaporized precursors by providing flexibility in the selection of the precursors and their flow rate. Herein, we develop a multiscale approach as a combination of ReaxFF, continuum fluid dynamics, phase-field (PF) and machine learning (ML) to model the gas-phase kinetic of the MOCVD growth and to connect further the MOCVD control parameters to the morphology, size, and distribution of the synthesized TMD materials. The results of the model that we developed, first, for MOCVD gas-phase kinetic of 2D-WSe2 correlate well with the experimental thickness measurements of 2D-WSe2 and show that the model is capable of simulating the experimentally observed trend [1]. We further extend this model to the combination of ReaxFF, ML, and PF, in progress. A systematic representative data set is generated based on the ReaxFF potential to train an ML-model describing the edge energies and edge-growth rates of 2D-WSe2 flakes as a function of key parameters, then to incorporate them into the PF simulations. The target of this work is to bridge spatial scales that range from 10−9 to 10-3 m in space and explore the optimal growth conditions resulting in high-quality TMD materials.


*NSF DMR-1539916

3:54PM P27.00008: DISTORTED PHASE OF SINGLE LAYER JANUS MoSTe*  MEHMET YAGMURUKARDE S (Presenter), Department of Physics, University of Antwerp, CEM SEVIK, Anadolu University, FRANCOIS M PEETERS, Department of Physics, University of Antwerp — Recently synthesized monolayer of Janus MoSSe structure has attracted great attention on those out-of-plane anisotropic materials. Here, we investigate the electronic, vibrational, elastic, and piezoelectric properties of two dynamically stable crystal phases of monolayer Janus MoSTe, namely 1H-MoSTe and 1T'-MoSTe. The 1H-MoSTe phase is found to be an indirect band-gap semiconductor while 1T'-MoSTe is predicted as small-gap semiconductor. The calculated Raman spectrum of each structure shows unique character enabling us to clearly distinguish the stable crystal phases via Raman measurements. The systematic piezoelectric stress and strain coefficient analysis reveals that out-of-plane piezoelectricity appears in 1H-MoSTe and the noncentral symmetric 1T'-MoSTe has large piezoelectric coefficients. Static total-energy calculations show clearly that the formation of 1T'-MoSTe is feasible by using 1T'-MoTe2 as a basis monolayer. Therefore, we propose that the Janus MoSTe structure can be fabricated in two dynamically stable phases which possess unique electronic, dynamical, and piezoelectric properties.

*Flemish Science Foundation (FWO-VI)
4:06PM P27.00009: Synthesis and properties of hexagonal GaBN/BN heterostructure and quantum wells. 6.3.6* QINGWEN WANG (Presenter), JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech Univ — Hexagonal boron nitride \((h\text{-}BN)\) is the only layer-structured or quasi-2D material with bandgap \(>6.0\) eV among the members of the III-nitride semiconductor family. The unique features of \(h\text{-}BN\) make it highly attractive in novel device applications, which includes high optical emission efficiency, possibility of \(p\)-type conductivity control, promising host for single photon emitter, as well high detection efficiency for thermal neutrons. Like all other compound semiconductors, achieving the ability of bandgap tuning through alloying will further expand the applications of \(h\text{-}BN\). Here, we report the synthesis of \(h\text{-}GaBN\) alloys using metal organic vapor deposition (MOCVD) growth. By utilizing \(h\text{-}BN\) epilayers as templates, we have successfully achieved \(h\text{-}GaBN\) alloys and \(h\text{-}GaBN/BN\) quantum wells with Ga-content up to 7%. The effects of phase separation and critical thickness have been investigated in detail and will be reported. The present study provides insights into possible ways to synthesize layered GaBN and would open up many new applications.

*This work is supported by ARO (W911NF-16-1-0268) and monitored by Dr. Michael Gerhold. Jiang and Lin are grateful to the AT&T Foundation for the support of Ed Whitacre and Linda Whitacre endowed chairs.

4:18PM P27.00010: Temperature influence in the electrical conductivity of graphite oxide platelets* DIEGO SANCHEZ (Presenter), JOHN PRIAS, HERNANDO ARIZA, Optoelectronics, Universidad del Quindío — Graphite oxide platelets from bamboo pyrolygenous acid (GO-BPA) synthesized by using the double thermal decomposition (DTD) method at 973 K as carbonization temperature, exhibit temperature influence in the electrical conductivity like a semiconductor material. Samples were characterized by using Raman, FTIR, XRD, XPS, HR-TEM and I-V curves (two and four-points at temperatures of 20 to 300 K) techniques. Electrical measurements suggest that increased temperature increases electrical conductivity like a semiconductor material. Conduction mechanism was described mainly by 3D-variable range hopping.

*We would like to thank the Interdisciplinary Institute of Sciences, the Doctorate program in Physical Sciences at Universidad del Quindío for the financial support.
4:30PM P27.00011: Thermal Expansion and Residual Strain in AlN Thin Film Sensor Materials  
ROBERT LAD (Presenter), MORTON G GREENSLIT, DAVID T PLOUFF, MAURICIO PEREIRA DA CUNHA, Univ of Maine — Aluminum nitride films are attractive materials for high temperature sensor devices because of their stable piezoelectric and semiconducting properties up to 800°C in air, above which the films degrade by oxidation. In this work, epitaxial AlN (002) films were grown at 930°C on c-cut sapphire substrates by N₂-plasma-assisted Al evaporation and were characterized up to 1000°C in air using an X-ray diffraction (XRD) sample hot stage. The coefficient of thermal expansion (CTE) and homogeneous strain were determined from accurate measurements of the c-axis lattice parameter for AlN and sapphire vs. thermal processing up to 800°C, and film oxidation was evaluated above 800°C from the relative decrease in the AlN (002) XRD intensity and degradation of the (002) pole figure. AlN films grown to 200nm thickness have c-axis compressive strain, but this residual strain can be relieved by thermal cycling between 25-700°C. The CTE value of 2.5x10⁻⁶/°C for the as-deposited films decreased as the film strain was released and is below the value of 5.3x10⁻⁶/°C reported for bulk AlN. Understanding the level of residual film strain and thermal expansion matching across the relevant interfaces is key for preventing delamination, cracking, and failure of sensor packaging or sensor function itself.

4:42PM P27.00012: Effects of growth parameters on faceting and defects in confined epitaxial lateral overgrowth*  
ARANYA GOSWAMI (Presenter), SIMONE TOMMASO ŠURAN BRUNELLI, BRIAN MARKMAN, Electrical and Computer Engineering Department, University of California, Santa Barbara, DAN J PENNACHIO, Materials Department, University of California, Santa Barbara, HSINYING TSENG, SUKGEUN CHOI, Electrical and Computer Engineering Department, University of California, Santa Barbara, AIDAN TAYLOR, Materials Department, University of California, Santa Barbara, JONATHAN KLAMKIN, MARK RODWELL, CHRIS J PALMSTROM, Electrical and Computer Engineering Department, University of California, Santa Barbara — Laterally grown III-V epitaxial semiconductor layers offer multiple advantages over conventional vertically-grown layers for fabricating novel semiconductor devices and III-V on Si integration for photonics. In confined epitaxial lateral overgrowth (CELO), pre-fabricated dielectric templates are used to control the growth and its direction. Such grown nano-structures however, often suffer from high densities of stacking faults and rotational twins, which limit the performance of the devices made using these materials. Here, we use scanning electron microscopy (SEM), transmission electron microscopy (TEM) and electron channeling contrast imaging (ECCI) to characterize these nano-structures grown by metal organic chemical vapor deposition (MOCVD) on patterned InP substrates. Using a combination of plan-view and cross-sectional TEM on the same nano-structure, we explore the influence of growth conditions (growth temperature and V/III ratio), template direction and substrate orientations on the evolution of facets and the nature of defects. We further show growth and characteristics of heterostructures and superlattice structures grown using CELO, as well as electrical measurements of these nanostructures.

*This work was supported by NSF and SRC.
4:54PM P27.00013: Controlled Fractal Growth of Transition Metal Dichalcogenides* PEIJIAN WANG (Presenter), HAO ZENG, Physics, State Univ of NY - Buffalo, SHAOMING HUANG, School of Materials and Energy, Guangdong University of Technology — We report controlled fractal growth of atomically thin transition metal dichalcogenides (TMDCs) by chemical vapor deposition, with morphological evolution from dendritic to triangular. Based on experimental observations, we tuned several important growth parameters, including the relaxation rate, adhesion coefficient, diffusion anisotropy and growth time to fabricate TMDCs with controllable fractal dimensions. Furthermore, a model based on the steps of nucleation, diffusion limited aggregation, and relaxation, was proposed to explain the morphological evolution. The computational simulation based on this model yielded good agreements with the experiments results. Our study sheds light on the growth mechanism of TMDs, which is fundamental to improving controllability of growth.

*Nature Science Foundation of China (NSFC 51420105002, 51672193, 51902061 and 51920105004) and US National Science Foundation DMR-1104994 and CBET-1510121

5:06PM P27.00014: Properties of SPEED Grown FTO Thin Films Deposited at Various Solution Concentrations and Ageing time* GBADEBO TAOFEEK YUSUF (Presenter), Science Laboratory Technology, Osun State Polytechnic — There have been various reports on the scarcity of indium element which is one of the constituents of indium tin oxide (ITO). Alternative TCO material is therefore necessary before the supply eventually runs out. This research therefore focused on fluorine-doped tin oxide thin films (FTO) as a possible alternative to the ITO. FTO thin films were grown using the Streaming Process for Electrodeless Electrochemical Deposition (SPEED) technique. The structural and optical properties of the films were determined at various fluorine to tin (F: Sn) concentrations and aging time. The results, as revealed by SEM and XRD analysis show that the properties of FTO films improve as the solution concentration and aging time were jointly increased to 0.85 and 12 hours. All FTO thin films except those deposited at solution concentration (F: Sn) of 0.55 and 4 hours aging time show optical transmission above 80 % in the Visible-UV region. This study has shown that the SPEED technique is a promising technique for depositing high-quality FTO thin films for solar photovoltaic applications.

**Keywords:** Ageing time, FTO, Optical, concentration, SPEED

*Tertiary Education Trust Fund

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

**Session P28 FIAP: Fellows of FIAP** 405-407 - Michael Gordon, IBM Thomas J. Watson Research Center - Tag(s): Industry, Invited, Undergrad Friendly

2:30PM P28.00001: Semiconductor and Nanostructured Materials and Devices [Invited] NAZIR P KHERANI (Presenter), University of Toronto — TBD
3:06PM P28.00002: The Taming of the Superconducting Qubit: A Tale of Loss [Invited]  CONAL MURRAY (Presenter), IBM T.J. Watson Research Center — The potential of quantum computing to enable new ways of solving problems considered intractable on classical computing platforms relies on our understanding of how qubits operate. Qubit scaling follows different metrics than those associated with classical computing, driven by the requirement that the fragile states they possess can be retained for sufficiently long times. After a brief introduction into superconducting transmon qubits, I will discuss how dielectric loss impacts their relaxation times and how we can effectively model such behavior using analytical and computational approaches. The resulting analysis provides guidance into the design aspects associated with such qubits. A secondary issue that follows from manufacturing greater numbers of qubits involves unwanted communication among them. In particular, resonance modes generated in the substrate on which they reside can limit their operating frequencies. It is known that incorporating grounded, through-silicon vias can increase the corresponding cutoff frequency within the substrate. I will show how we can predict the resulting spectrum by considering the array of vias as an effective photonic crystal to arrive at a fundamental frequency dependent on the particulars of the via geometry.

3:42PM P28.00003: Addtive Manufacturing of Magnetic Materials for Clean Energy Applications* [Invited]  MARIAPPAN PARANTHAMAN (Presenter), Oak Ridge National Lab — The main goal of this research is to develop a process to print near-net shape NdFeB polymer bonded magnets and to minimize the cost associated with manufacturing. One of the ways in which we can achieve this goal is by using an additive manufacturing technique to create complex shapes and geometries of polymer bonded magnets from a computer aided design which requires no tooling but little post-field-annealing and reducing the amount of waste generated. We have successfully demonstrated the fabrication of near-net shape magnets with complex geometries and high energy product using over 70vol% of NdFeB in nylon polymer composite magnets. A higher energy product of over 18 MGOe have been achieved. We will discuss in detail about thow materials chemistry aspects are used to improve the mechanical, magnetic and thermal stability of printed magnets.

*This research was supported by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.

4:18PM P28.00004: Startups: The Place to Be [Invited]  MATT KIM (Presenter), QuantTera — TBD

4:54PM P28.00005: Application of Atomic Layer Deposited Films to Cultural Heritage Objects [Invited]  RAYMOND PHANEUF (Presenter), University of Maryland, College Park — TBD

Wednesday, March 4, 2020 2:30 PM - 5:06 PM

Session P29 DSOFT DBIO GSNP DPOLY: Active Matter and Liquid Crystals in Biological Systems I  501 - Zvonimir Dogic, University of California, Santa Barbara -

Tag(s): Focus
2:30PM P29.00001: Dipolar Extensile Dynamics in Microtubule-Based 2D Active Nematics
LINNEA LEMMA (Presenter), Physics Department, Brandeis University, ZVONIMIR DOGIC, Physics Department, University of California Santa Barbara — Theories describe 2D active nematics in terms of liquid crystals, hydrodynamics and chaotic fluids. However, the experimental system is inherently hierarchical and connecting the microscopic forces to the macroscopic flows remains an open challenge. Using an \textit{in vitro} 2D active nematic composed of microtubules and kinesin motors, we probe the microscopic dynamics under varying active stresses. We find that locally, flows are dipolar extensile whose strain rate can be tuned by ATP concentration. Additionally, we uncover a velocity distribution of microtubules along the director which indicates the importance of many body interactions in bridging the length scales of the system.

2:42PM P29.00002: Design of active nematic systems with controllable defect dynamics and flows [Invited] RUI ZHANG (Presenter), ALI MOZAFFARI, JUAN DE PABLO, University of Chicago — Active matter encompasses a wide spectrum of non-equilibrium condensed matter systems, the constituents of which convert energy into mechanical work. They exhibit intriguing collective behaviors, such as flocking and activity-induced phase transitions. In the particular case of anisotropic particles or molecules, these materials can enter an active nematic state, which displays intricate motions of topological defects, characteristic of nematic liquid crystals, accompanied by chaotic-like flows. Active nematics are encountered in numerous biological systems, ranging from cytoskeletal polymer extracts, to tissue cells and dense bacterial suspensions. The dynamics of active nematics are not fully understood, and efforts to control and manipulate the structure and flow of this class of materials have been limited. In this talk, I will summarize our recent progress in active nematics research, with an emphasis on the interplay between molecular interactions, elasticity, and hydrodynamic forces. In particular, I will discuss an experimentally realizable approach, which relies on spatiotemporal patterning of activity, to manipulate defects and flows in active nematics. I will show how simulations can be harnessed to guide design of well-controlled dynamics, paving the way towards engineering active matter for practical applications.
3:18PM P29.00003: Control of bacterial dynamics by splay and bend in nematic vortices*
RUNA KOIZUMI (Presenter), TARAS TURIV, Kent State Univ - Kent, MIKHAIL GENKIN, Cold Spring Harbor Laboratory, ROBERT LASTOWSKI, HAO YU, Kent State Univ - Kent, IRAKLI CHAGANAVA, Georgian State Teaching University of Physical Education and Sport, QIHUO WEI, Kent State Univ - Kent, IGOR ARONSON, Pennsylvania State University, OLEG D LAVRENTOVICH, Kent State Univ - Kent — Microswimmers exhibit collective behavior that can be controlled by an anisotropic environment such as a lyotropic chromonic liquid crystal. We explore the effect of splay and bend of the director field on the individual and collective behavior of motile *Bacilli subtilis*. The director field, imposed through photoalignment, is designed in the form of vortices of topological charge +1. Their geometry changes from pure radial to spiral and to the circular, representing thus deformations of a pure splay, splay-bend mix, and pure bend, respectively. In dilute dispersions, the bacteria follow the pre-imposed director field, but after their concentration reaches some threshold, they engage in a collective unipolar circulation. This collective behavior is controlled by the splay-to-bend ratio: vortices with dominating splay condense the bacterial swarms towards the center, while vortices with dominating bend push them away to the periphery. Vortices with splay-bend parity formed by 45-degree spiraling director produce the most stable swarming with a time-independent radius as long as the bacterial activity is constant. The change in swimming scenario as a function of splay-to-bend ratio is reminiscent of an unstable limit cycle.

*The work is supported by NSF DMS-1729509.

3:30PM P29.00004: Spatiotemporal Optimal Control of an Extensile Active Nematic Suspension*  
MICHAEL M NORTON (Presenter), Center for Neural Engineering, Pennsylvania State University, PIYUSH GROVER, Mechanical Engineering, University of Nebraska-Lincoln, APARNA BASKARAN, MICHAEL HAGAN, SETH FRADEN, Physics, Brandeis University — Active nematic suspensions are self-driven fluids that exhibit rich spatiotemporal dynamics characterized by director field buckling, defect nucleation/annihilation and chaotic trajectories of those defects. Towards developing experimental methods for controlling these dynamics, we consider an optimal control problem which seeks to find the spatiotemporal pattern of active stress strength required to drive the system towards a desired director field configuration. As an exemplar, we consider an extensile active nematic fluid confined to a disk. In the absence of control, the system produces two topological defects that perpetually circulate. Optimal control identifies a time-varying active stress field that drives the defects to orbit in the opposite direction.

*We acknowledge support from NSF MRSEC, Bioinspired Soft Materials, DMR-1420382
3:42PM P29.00005: Self propelling nematic microcapsules*  
CORINNA MAASS (Presenter), BABAK VAJDI HOKMABAD, Max Planck Institute for Dynamics and Self-Organization, KYLE A BALDWIN, SOFT Group, School of Science and Technology, Nottingham Trent University, CHRISTIAN BAHR, Max Planck Institute for Dynamics and Self-Organization — The ability to produce controllable, self propelling microcapsules is of great interest to synthetic biology and the design of smart microreactors. Inactive fluid shells are already widely used as artificial cell models, micro-reactors, and in food and drug applications. However, combining activity, stability, and control remains a significant challenge. Building on an established active emulsion platform, we have developed a new approach to the problem of encapsulation by using nematic active double emulsions, where a solubilization mechanism induces activity and the molecular nematicity provides stability. We show that using a nematic liquid crystal as the shell material with homeotropic anchoring at both interfaces will result in a nematoelastic force on a displaced core droplet and act as a topological barrier against the coalescence of the core droplet with the outer phase. We further present a peculiar self-propulsion mode where the interplay of spontaneous symmetry breaking and autochemotaxis results in a "shark-fin meandering" motion of the shell in a 2D-confined geometry and helical swimming in 3D. This behavior can be controlled or switched off by introducing chemical gradients, topographical guidance or by changing the shell topology.

*DFG SPP1726, Microswimmers

3:54PM P29.00006: The Dynamics of Active Nematic Defects on The Sphere Surface*  
YIHENG ZHANG (Presenter), Beijing Normal Univ, MARKUS DESERNO, Carnegie Mellon Univ, ZHANCHUN TU, Beijing Normal Univ — A nematic liquid crystal confined to the surface of a sphere exhibits topological defects of total charge +2 due to the topological constraint. In equilibrium, the nematic field forms four +1/2 defects, located at the corners of a tetrahedron inscribed within the sphere, since this minimizes the Frank elastic energy. Here we study the active counterpart of such a system, in which a self-driven directional motion of the individual nematogens creates a large-scale flow that drives the system out of equilibrium. In this new state, defects exhibit complex dynamics which, depending on the strength of the active forcing, can be simple and periodic (for weak forcing) or chaotic (for strong forcing). We show that Onsager's variational principle offers an exceptionally transparent way to derive the exact dynamical equations of the defects in such an active spherical nematic, and we explain its mobility at the hydrodynamics level.

*We thank for the financial support from the National Natural Science Foundation of China (Grant No. 11675017).
4:06PM P29.00007: Emergent dynamics of large scale collective rotations in 2D active nematic  DAVID QUINT (Presenter), Department of Physics, University of California, Merced, DALI E CHAPMAN, Department of Molecular and Cellular Physiology, Stanford University, STEVEN P. GROSS, Department of Developmental and Cell Biology, University of California, Irvine, DANIEL BELLER, AJAY GOPINATHAN, JING XU, Department of Physics, University of California, Merced — Motivated by recent work on active nematics we employ here a microtubule and kinesin motor gliding assay system to examine dynamic collective order in 2D. Without the need for a depletion agent, our system exhibits the classic nematic order transition that depends on microtubule and active motor density. However in the regime of very flexible microtubules nematic order is lost, suggesting that this ordering is a consequence of both microtubule stiffness and density. We demonstrate that the ordered state exhibits large scale coherent rotations and that the introduction of a time varying director is necessary for proper characterization of the active nematic system. We show that the rate of this collective rotation of the nematic order is strongly dependent on activity induced microtubule fluctuations.

4:18PM P29.00008: Defect dynamics of 3D active nematic turbulence  ZIGA KOS (Presenter), Faculty of Mathematics and Physics, University of Ljubljana, JACK BINYSH, University of Warwick, SIMON COPAR, JURE APLINC, SLOBODAN ZUMER, Faculty of Mathematics and Physics, University of Ljubljana, GARETH ALEXANDER, University of Warwick, MIHA RAVNIK, Faculty of Mathematics and Physics, University of Ljubljana — Three-dimensional active nematics are exciting new materials characterized by a network of continuously evolving defect lines and loops [1]. We report on detailed numerical investigation of confined 3D active nematics [2]. At sufficient activity, such system transitions into active turbulence with irregular dynamics of multiple defect loops with distinct topological events of loop crossover, annihilation, splitting and merging occurring in time. The dynamics of a single active defect loop depends on the local crosssection of the director profile that can span from +1/2 or -1/2 winding numbers to twist profiles. Depending on the loop orientational profile, we observe spontaneous shrinking, growing, and bending of a single zero-charge loop [3]. Our work aims to provide insight into 3D active turbulence from the perspective of the topology of the emergent 3D defects and their self-induced dynamics.

Topological Defects in Cell Monolayers Guided by Topography

Kirsten EndreSEN (Presenter), Minsu Kim, Francesca Serra, Johns Hopkins University — Many types of cells display long-range alignment like nematic liquid crystals (LCs), and have topological defects. These defects are characterized by their topological charge, the number of rotations of the alignment around the defect. In 2D cell culturing, only +/- 1/2 defects are typically observed, although other defects exist in living systems. Topological defects in cell layers have been associated with increase in cell apoptosis [1] and clustering [2]. We induce alignment of cells via contact guidance into formations that impose arbitrary topological charges. We survey multiple cell types (EpH-4 and 3T6) to characterize their alignment, density, and dynamics near defects of various topological charges, and define LC parameters such as defect core sizes and elastic constants. We observe a large change in density of fibroblasts (3T6) near the topological defects, where our tunable confinement allows us to identify the isotropic defect cores.


This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1746891.

Clustering, jamming, and topological defects in growing bacterial colonies at liquid interfaces

Blake Langeslay (Presenter), Gabriel Juarez, University of Illinois at Urbana-Champaign — Active nematic matter encompasses a broad variety of systems including confined vibrating rods, flocks of birds, and colonies of bacteria. Here, we present experimental results on growing colonies of rod-shaped bacteria confined in two dimensions by adsorption at an oil-water interface. Using microfluidics and time-lapse microscopy, we investigate the roles of motility and growth on cluster formation, topological defects, and jamming. As colonies grow on finite liquid interfaces, we observe cluster formation where regions of tightly packed bacteria that display notably low swimming velocities increase in number and size over time. As the surface coverage increases, a densely packed monolayer of bacteria with long-range orientation order is observed and topological defects are quantified. This setup functions as a useful model system for low-friction confinement of a growing active nematic comprised of discrete particles as well as carrying important implications for the study of biofilm formation at liquid interfaces.

Topological defects drive layer formation in bacteria colonies

Katherine Copenhagen (Presenter), Ricard Alert, Ned Wingreen, Joshua Shaevitz, Princeton University — The starvation-induced development of macroscopic fruiting bodies in Myxococcus xanthus begins with the formation of layered cell structures. Cells in these layers are densely packed, aligned via their rod shape, and retain their motility so that the population forms an active nematic liquid crystal. We investigate the origin of layering by looking at the formation of second layers and holes from cellular monolayers. These events occur at discontinuities in the cell direction field known as topological defects. Layers form at positive defects while holes open at negative defects. By measuring cell flows, we find an influx of cells towards positive defects and an outflux away from negative defects. We find that a model of monolayers as an active, dry extensible nematic with anisotropic friction can reproduce the measured flow fields and change in cell density at defects. Overall, we conclude that the conversion from a 2D cell layer to a 3D droplet is triggered by the formation of layers of cells at topological defects.
Pulsating air bubbles can swim in anisotropic fluids*  
SUNG-JO KIM (Presenter), EUJIN UM, JOONWOO JEONG, Ulsan National Institute of Science and Technology — Small-scale locomotion in fluids has been of great interest, from microorganisms to active matter and spermbots. Here we explore the swimming of a spherical bubble with a periodic change in its radius. Its spatial symmetry and the scallop theorem [1] tell us that the bubble with the reciprocal motion cannot achieve propulsion. In anisotropic fluids, however, the bubbles can swim. The spherical bubble dispersed in homogeneously aligned nematic liquid crystals (LCs) accompanies either a hyperbolic point defect or a disclination ring called a Saturn-ring. The pulsating bubble generates LC flow of which spatial and time-reversal symmetry are broken because of LC’s director configuration and viscoelastic response, respectively. The bubble with the point defect exhibits the net propulsion, while the swimming of the other one depends on the shape of the ring defect. We also introduce our theoretical understanding of this propulsion mechanism, with ideas to maximize swimming efficiency.


*This work is supported by IBS-R020-D1, NRF-2018R1C1B6002811, NRF-2018R1A6A3A01010921, and NRF-2017R1A6A3A04006179.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P30 DSOFT DPOLY: Soft Mechanics via Geometry III 502 - Michael Czajkowski, Georgia Inst of Tech
2:30PM P30.00001: Geometrically-frustrated wrinkle patterns 1: Defects and mesoscale structure*  
JOSEPH PAULSEN (Presenter), Physics, Syracuse University, OLEH TOVKACH, Physics,  
University of Massachusetts, Amherst, MONICA RIPP, Physics, Syracuse University, JUNBO CHEN, TENG  
ZHANG, Mechanical & Aerospace Engineering, Syracuse University, BENJAMIN DAVIDOVITCH, Physics,  
University of Massachusetts, Amherst — Thin films readily buckle to relax compression, creating  
wrinkle patterns that can have considerable morphological complexity. Some of this complexity  
stems from a basic geometric conflict, arising when wrinkles that would otherwise prefer a fixed  
wavelength are formed in geometries where the lines of tension are splayed, for example when  
wrinkles emanate radially from a point. We study such frustrated states within an annular region  
of an elastic sheet subjected to unequal tensions at its inner and outer boundaries. Using  
experiments and simulations, we demonstrate two distinct solutions: (i) states with  
approximately constant wavelength, enabled by “defects” in the wrinkle pattern where new  
wrinkles begin, and (ii) “defect-free” states consisting of a fixed number of wrinkles of non-  
constant wavelength. We show how these two morphological types reflect distinct minima of a  
suitable coarse-grained elastic energy. We further predict a mesoscopic lengthscale for patches  
of nearly-parallel wrinkles separated by defect-rich regions, in agreement with our observations.  
This work unravels an organizing principle with analogs in liquid crystalline and superconducting  
states of matter. (This is part 1 in a 3-talk series).

*Support from NSF-DMR and NSF-CMMI is gratefully acknowledged.

2:42PM P30.00002: Geometrically-frustrated wrinkle patterns 2: cascades versus defects*  
MENG XIN (Presenter), Univ of Mass - Amherst, DOIREANN O'KIELY, University of Oxford, BENJAMIN  
DAVIDOVITCH, Univ of Mass - Amherst, DOMINIC VELLA, University of Oxford — Cascades and  
localized defects are characteristic motifs of wrinkle patterns in  
elastic sheets, appearing when a array of uniformly-spaced wrinkled is incom-  
patible with a confining topography, boundary conditions, or gradients in the  
sheet's thickness or the stiffness of a supporting substrate. Inspired by a recent  
experimental study (J. Schleifer et al. Soft Matter 15 1405 (2019)), we employ  
numerical simulations to study the wrinkle patterns in a uniaxially-compressed  
sheet, floating on a liquid bath whose density in non-uniform, implying a gra-  
dient in the locally-favored value of the wrinkle wavelength in the direction  
orthogonal to the axis of compression. This simple model enables a systematic  
study of the basic mechanisms through which the wrinkle density and wave-  
length vary in space. Exploring the parameter regimes that correspond to weak  
and strong gradient of the liquid density, we show that the meso-scale features  
of the pattern may be determined by distinct physical mechanisms that involve  
cascade-like structures and localized defects

*NSF DMR 1822439
**2:54PM P30.00003: Geometrically-frustrated wrinkle patterns**

Experimental realisation of defect patterns

LUCIE DOMINO (Presenter), DOIREANN O'KIELY, DOMINIC VELLA, University of Oxford — In the previous talks, the role of geometry in forcing the creation of defects in wrinkle patterns has been discussed. Here, we present a series of experimental systems that exhibit different mechanisms for introducing new wrinkles, including smooth cascades and localised defects. We discuss the influence of the underlying preferred wrinkle pattern on which of these mechanisms is observed in reality. (This is part 3 in a 3-talk series).

*This research has received funding from the European Research Council under the European Union's Horizon2020 Programme

**3:06PM P30.00004: Curvature in Compressed Thin Cylindrical Shells Approaching the Isometric Limit**

NICOLE E VOCE (Presenter), CASSIDY ANDERSON, Physics and Astronomy, James Madison University, MARCELO DIAS, Engineering - Mechanical Metamaterials and Soft Matter, Aarhus University, KLEBERT FEITOSA, Physics and Astronomy, James Madison University — We study the buckling of a thin cylindrical shell constrained to slide onto an inner non-deformable pipe. Our goal is to characterize the relationship between the shell thickness and the localization of stresses by using curvature measurements. First, we induce surface buckling by immobilizing one end of the shell and applying force to the other end. Then, we obtain a virtual reconstruction of the surface from 3D optical scanning and compute the Gaussian curvature for every point on the mesh. We find that as the shell gets thinner, the distribution of Gaussian curvatures becomes broader. However, surprisingly, the mean of the Gaussian curvature distribution increases. Furthermore, measurements of areas enclosed by the parabolic lines around protruding vertices from the buckled surface show that the transitions between regions of positive and negative Gaussian curvature are more localized. Finally, the Gaussian curvature reveals the formation of substructures within the lobes around the vertices. These results demonstrate that the evolution of the cylindrical shell towards the isometric limit represented by the well-known Yoshimura pattern is non-trivial.

*This research was funded by 4-VA, a collaborative partnership for advancing the Commonwealth of Virginia.

**3:18PM P30.00005: Topological Floppy Modes in Epithelial Tissue Network**

HAROLD LIU (Presenter), Univ of Michigan - Ann Arbor, DI ZHOU, Georgia Inst of Tech, LEYOU ZHANG, DAVID LUBENSKY, XIAOMING MAO, Univ of Michigan - Ann Arbor — The ordering, structure formation, and mechanical response in epithelial cells are essential to the functioning of many tissues. In this talk, we explore topological mechanics in a simple epithelial cell sheet described by a vertex model. We find that floppy modes in this model can become polarized based on the geometry of the cells, and domain boundaries with localized floppy modes can be observed. This simple model indicates a possible role for epithelial cell structure in directing mechanical responses. This topological mechanical polarization may be related to the mechanism of formation of Planar Cell Polarization (PCP), an intriguing phenomenon often seen in animal development, which is a polarization of a field of cells within the plane of a cell sheet to obtain directional information that is essential for diverse cellular processes.
3:30PM P30.00006: Twisting, buckling, and tension in elastic helices with multiple perversions* ADAM FORTAIS (Presenter), KARI DALNOKI-VERESS, McMaster Univ — A telephone cord and the coils of cucumber tendrils; these are two examples of elastic beam-like systems that take on the shape of soft, helical springs. By unwinding such a spring and holding its ends fixed, an elastic instability forms, causing the spring to form both chiralities of the helix, meeting at defects called perversions. We investigate this phenomenon in an idealized experiment using highly uniform, microscopic, elastic fibers with cylindrical cross-sections. We measure the force of extension as a function of geometry, material properties, and twist. Previous work has shown that multiple perversions may form as a result of a spring's prismatic cross-section. Here we observe that, surprisingly, multiple perversions still form, despite the uniform cylindrical cross-section of our fibers.

*NSERC

3:42PM P30.00007: Simulations of buckling and crumpling in twisted ribbons* MADELYN LEEMBRUGGEN (Presenter), Physics, Harvard University, JOVANA ANDREJEVIC, School of Engineering and Applied Sciences, Harvard University, ARSHAD KUDROLLI, Physics, Clark University, CHRISTOPHER RYCROFT, School of Engineering and Applied Sciences, Harvard University — A twisted ribbon exhibits at least five deformation phases, with transitions facilitated by tuning the tension applied or twist angle. When driven from one of these self-avoiding phases into a disordered regime of self-contact, the ribbon develops ridges as it folds or crumples. Here, we develop a computational model of this complex, dynamic process, which reproduces the transitions seen in experimental tests. Our simulations illuminate the details of folding and crumpling transitions induced via twisting; allow careful analysis of the ribbon's topography and curvature; and potentially reveal a state variable by which the disordered system may be quantified.

*We acknowledge support from the National Science Foundation under Grant No. DMR-1420570.
3:54PM P30.00008: Statistical mechanics of 2D sheets under uniaxial tension*  MOHAMED EL HEDI BAHRI (Presenter), ANDREJ KOSMRLJ, Princeton University — Atomically thin sheets, such as graphene, are widely used in nanotechnology. Recently they have also been used in applications including kirigami and self-folding origami, where it becomes important to understand how they respond to external loads. Motivated by this, we investigate how isotropic sheets respond to uniaxial tension by employing the renormalization group. Previously, it was shown that for freely suspended sheets thermal fluctuations effectively renormalize elastic constants beyond a characteristic thermal length scale (a few nanometers for graphene at room temperature), beyond which the bending rigidity increases, while the in-plane elastic constants reduce with universal power law exponents. Under uniaxial tension, we find that the bending rigidity along the axis of tension diverges with a different power law exponent beyond a stress-dependent length scale whereas the Young's modulus in the orthogonal direction renormalizes to zero. As a consequence, for moderate tensions we find a universal nonlinear force-displacement relation and the universal Poisson's ratio. For large tensions, in-plane fluctuations longitudinal with the axis of tension are suppressed and classical mechanics along this axis is recovered.

* Work was supported by the NSF Career award DMR-1752100

4:06PM P30.00009: Isigami: sheet reconfiguration driven by cone interactions*  BENJAMIN KATZ (Presenter), VINCENT CRESPI, Pennsylvania State University — A novel class of surfaces holds the possibility of reversible reconfiguration into a large family of distinct, stable shapes. This property stems in part from their topological defects—they have equal numbers of cones and saddles. Exploring these surfaces with an example constructed out of a graphene monolayer with the defects arranged in a kagome-like superlattice, we model its mechanical response with semiclassical molecular dynamics. The cones possess a two-fold degree of freedom in their up/down orientation, yielding a reconfigurable surface with a large number of metastable shapes. Enumerating a complete 'zoo' of such shapes for a small patch of this material reveals that not only are the interactions between these degrees of mechanical freedom long-range enough to produce a gaussian-like 'density of states' for given cone orientations, but also that the surface possesses other hidden degrees of freedom in certain orientations—further increasing the number of stable shapes it can hold. These shapes cover a broad range of physical forms and a scale comparable to important biomolecules, raising the possibility of biological applications.

*Research performed under a training fellowship for CoMET, an NRT at Penn State funded by NSF.
4:18PM P30.00010: Indentation of ellipsoidal and cylindrical shells: new insights from shallow-shell theory  WENQIAN SUN (Presenter), JAYSON PAULOSE, Univ of Oregon — Pressurized elastic shells are ubiquitous in nature, from pollen grains to the outer walls of yeast and bacterial cells. Indentation measurements provide a means of simultaneously probing the internal pressure and elastic properties of thin shells, which in turn can be relevant to understanding cellular function. We study the effects of geometry and pressure-induced stress on the indentation stiffness of ellipsoidal and cylindrical elastic shells using shallow shell theory. The key advance in our work lies in reducing the linear indentation response to a single integral with two dimensionless parameters which encode the asphericity and internal pressure. This integral can be numerically evaluated in all regimes, and is used to generate analytical expressions in various limits. Our results provide theoretical support for previous scaling and numerical results on the stiffness of ellipsoids, and give new insights to the linear indentation response of pressurized cylinders.

4:30PM P30.00011: Statistical mechanics of dislocation pileups  GRACE ZHANG (Presenter), DAVID R. NELSON, Harvard University — Dislocations experiencing applied stress in two dimensions can order when trapped in a single glide plane with aligned Burgers vectors. These dislocation queues, called dislocation pileups, are critical in the initiation and propagation of deformations in materials. We study the static and dynamical properties of this class of defect ordering, where the dislocations themselves form inhomogeneous quasilattices in one dimension, with spatially varying lattice spacings whose spatial profile depends on the form of the applied stress. We study these dislocation pileup lattices using an intriguing connection with recent generalizations of random matrix ensembles, and examine the crystallization of these dislocations at low temperatures. We use random matrix theory to probe the equilibrium statistical mechanics, which allows us to extract the spatial correlation functions and structure factors of two distinct types of dislocation pileups, those in uniform stress fields and those in stress fields linear in space. Our formalism provides an analytical formulation for these correlations generalizable to other inhomogeneous crystals in one dimension. Finally, we analyze the low temperature excitation spectrum of these dislocation pileups and the spatial properties of their excitation modes.
4:42PM P30.00012: Statistical ensemble inequivalence for flexible polymers under confinement in various geometries* PANAYOTIS BENETATOS (Presenter), Department of Physics, Kyungpook National University, Rep. of Korea, SANDIPAN DUTTA, Center for Soft and Living Matter, Institute for Basic Science, Rep. of Korea — The problem of statistical ensemble inequivalence for single polymers has been the subject of intense research. In a recent publication, we show that even though the force-extension relation of a free Gaussian chain exhibits ensemble equivalence, confinement to half-space due to tethering to a planar substrate induces significant inequivalence [S. Dutta and P. Benetatos, Soft Matter, 2018, 14, 6857-6866]. In this talk, we extend that work to the conformational response to confining forces distributed over surfaces. We analyze in both the Helmholtz and the Gibbs ensemble the pressure-volume equation of state of a chain with free ends in rectangular, spherical, and cylindrical confinement. We especially consider the case of a directed polymer in a cylinder. We also analyze the case of a tethered chain in various geometries. In general, confinement causes significant ensemble inequivalence. Remarkably, we recover ensemble equivalence at the limit of squashing confinement. Our work may be useful to the interpretation of single molecule experiments and caging phenomena.

*P.B. acknowledges support by the National Research Foundation of Korea (NRF No-2019R1F1A1062360) funded by the Ministry of Science and ICT, Korea (MSIT).

4:54PM P30.00013: Soft actively contractile cylinders and spheres* MICHELE CURATOLO, PAOLA NARDINOCCHI, Structural Engineering and Geotechnics, Sapienza, University of Rome, Italy, LUCIANO TERESI (Presenter), Mathematics and Physics, University Roma Tre, Italy — In the last years, contractile gels have been the subject of intense research activity. Active gel microtubules have been produced to investigate how the dynamics of diffusion can be enhanced when gel activity is driven by molecular motors (Phil.Trans.R.Soc. A 372, 2014). Likewise, buckling shapes of thin sheets made of active polymers have been presented and discussed (Nature Communications 9, 2018). On a different side, microfluidic applications based on polymer microtubules have been investigated (Lab on a Chip 18, 2018).

In all those examples, active contraction of the gels as well as solvent release and flows contribute to the dynamics of the active gel structures and determine the smoothly or suddenly change of the original geometric shapes. Our mathematical model can describe some of the key features of these dynamics. We view active contraction as a change in the material metric of the structures, and describe it within a theory of stress-diffusion with remodeling of the polymeric network. The results of the model will be compared and contrasted with the observations of actual experiments on microtubules and microspheres.

*MIUR - Italian Ministry of University and Research, grant PRIN 2017
Non trivial deformation structures in confined elastic membrane under stretching

DEBANKUR DAS (Presenter), TIFR Centre for Interdisciplinary Sciences, JÜRGEN HORBACH, Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, SURAJIT SENGUPTA, TIFR Centre for Interdisciplinary Sciences, TANUSRI SAHA-DASGUPTA, S.N. Bose National Centre, Kolkata — Two dimensional elastic networks when stretched, deform plastically by producing pleats; system spanning linear structures with width comparable to lattice spacing, where the network overlaps on itself. When a similar elastic membrane is confined within rigid walls and allowed to have out of plane fluctuations, similar unconventional deformation modes appear upon stretching. Within these structures, which we call ripplocations, the height field becomes multivalued. These distinct structures are separated by large free energy barriers from a phase with only smooth ripples, that are always present at non-zero temperatures. To understand these structures and their interrelation, we introduce an external field that couples to local non-affine fluctuations measured from the flat reference. Using sequential umbrella sampling Monte Carlo involving sophisticated, non Boltzmann sampling, we obtain conditions under which ripplocations are formed. We obtain a finite temperature phase diagram in the strain-field plane. We also describe experimental signatures such as typical stress strain curves for membranes by which transitions from rippled to ripplocated membranes may be probed.

Mechanical response of wrinkled structures

SIJIE TONG (Presenter), ANDREJ KOSMRLJ, Princeton University — Wrinkling instability of compressed stiff thin films bound to soft substrates has been studied for many years and the formation and evolution of wrinkles is well understood. Recently, the wrinkling instability has been exploited to create structures with tunable drag, wetting and adhesion. While these studies successfully demonstrated the proofs of concepts, the quantitative understanding is still lacking, because we don't know how wrinkled surfaces deform in response to interactions with environment. To address this issue, we systematically study how wrinkled structures respond to infinitesimal surface forces both in the vertical and horizontal directions. We find that the linear response diverges near the onset of wrinkling instability and then decays away from this critical threshold. The mechanical response near the critical threshold is dominated by the characteristic mode of wrinkles. In analogy with the critical phenomena in ferromagnets, we can introduce the critical exponents for the response of the characteristic mode of wrinkles, which are consistent with the Landau theory. Our theory can be further used to study the response of wrinkled structures to more complicated distributions of external forces and can thus provide insights for the above-mentioned applications.
2:30PM P31.00001: Multi-scale relaxation dynamics of arrested patchy particle gels  JAKE SONG (Presenter), Massachusetts Institute of Technology MIT, MARC PIQUETTE, Tufts University, FELIPE DE QUESADA, Massachusetts Institute of Technology MIT, MEHEDI RIZVI, North Carolina State University, QINGTENG ZHANG, SURESH NARAYANAN, Argonne National Laboratory, JOSEPH TRACY, North Carolina State University, EMANUELA DEL GADO, Georgetown University, NIELS HOLTEN-ANDERSEN, GARETH H MCKINLEY, Massachusetts Institute of Technology MIT — Patchy particle interactions enable the design of so-called ‘equilibrium gels’, a system where arrest is achieved without an underlying phase separation, resulting in structurally equilibrated gels which do not undergo coarsening-induced aging. Here, we study the multi-scale relaxation dynamics of a model patchy particle gel consisting of nanoparticles linked with end-functionalized polymers by using stopped-flow spectro-photometry, x-ray photon correlation spectroscopy, and linear viscoelastic measurements. We show that, despite the fast dissociation dynamics of an individual polymer linker from the nanoparticle, the relaxation of the system becomes slow and arrested at larger length-scales due to multi-functional associations between the nanoparticles. We show that the nanoscale primary clusters undergo a combination of super-diffusive and diffusive relaxation modes, which is contrasted by the sub-diffusive and stretched-exponential relaxation of the network at the macroscale. We show that the super-diffusive dynamics of the primary clusters are highly intermittent, which supports the interpretation that avalanche dynamics is a general feature associated with the microscopic dynamics of arrested soft materials, irrespective of the material's route to arrest.

2:42PM P31.00002: Nanosheets and Metallo-Hydrogel Formed by 2-nm Metal-Organic Cages based on Electrostatic Interaction*  YUQING YANG (Presenter), HUI LI, TIANBO LIU, JIAHUI CHEN, TING-ZHENG XIE, YI FENG, XINYU SUN, polymer science, the university of akron — Macroionic solutions, including metal-organic cages, would form the single layered hollow sperical blackberry-type structure based on counterion-mediated attraction. Here, we observed a hydrogel formation process from 2-nm emissive, low molecular-weight metal-organic cages at low concentrations (>15 mg/mL) based on counterion-mediated attraction and π-π/hydrophobic interactions. With addition of small electrolytes, the cages in aqueous solution will follow the counterion-mediated attraction and self-assemble into 2D nanosheets, like normal macroionic solutions. However, the unique molecular structure and the charge distribution of the cages make the bending of nanosheets into spheres difficult, leading to stable, standing alone MOC nanosheets in solution and their very large excluded volumes lead to gelation at very low (~1.5 wt%) cage concentrations, with the helps from hydrophobic and partially π-π interactions similar to the gelation of graphene oxides.

*CHE1904397
2:54PM P31.00003: Emergence of Multiscale Dynamics in Colloidal Gels   JAE HYUNG CHO  
(Presenter), Massachusetts Institute of Technology MIT, ROBERTO CERBINO, University of Milan, IRMGARD BISCHOFBERGER, Massachusetts Institute of Technology MIT — To gain insight into the kinetics of colloidal gel evolution at low particle volume fractions $\phi$, we utilize differential dynamic microscopy to investigate particle aggregation, geometric percolation, and the subsequent transition to nonergodic dynamics. We report the emergence of unexpectedly rich multiscale dynamics upon the onset of nonergodicity, which separates the wave vectors $q$ into three different regimes. In the high-$q$ domain, the gel exhibits $\phi$-independent internal vibrations of fractal clusters. The intermediate-$q$ domain is dominated by density fluctuations at the length scale of the clusters, as evidenced by $q$-independence of the relaxation time $\tau$. In the low-$q$ domain, the scaling of $\tau$ as $q^{-3}$ suggests that the network appears homogeneous. The transitions between these three regimes introduce two dynamical characteristic length scales, distinct from the cluster size.

3:06PM P31.00004: Size-Dependent Tracer Diffusion in Colloidal Gels*   BRIAN KANG RYU  
(Presenter), ROSEANNA ZIA, Department of Chemical Engineering, Stanford University — Colloid diffusion in porous media is ubiquitous in industrial and biophysical systems, such as the extracellular matrix hydrogels of cell tissues and the nucleoid region inside prokaryotic cells, where specific pore morphologies enable selective filtering. Obtaining a relation between pore size and colloid diffusion in porous media will lead to the development of models that will elucidate how cells regulate biomolecule transport. In this study, we seek a fundamental understanding of how the diffusion of tracer colloids of various sizes are hindered by a porous medium. We present our results from simulations of tracer colloids undergoing Brownian diffusion in the voids of a colloidal gel. Detailed characterization of tracer diffusion reveals that all tracers experience sub-diffusive motion over short to intermediate length scales. Small tracers eventually recover the diffusive regime over longer length scales while large tracers remain in a local cavity. We additionally present algorithms to identify the characteristic length scale that marks the onset of the recovery to normal diffusion and the cutoff tracer size that determines whether a tracer is too large to break through the void network.

*This work was supported in part by a National Science Foundation DGE grant No. 1656518.
3:18PM P31.00005: Connecting the viscoelastic response of nanosheet gels to the elastic properties of the particles* SEBASTIAN BARWICH, MATTHIAS MOBIUS (Presenter), School of Physics, Trinity College Dublin — Micron-sized nanosheets such as graphene, graphene oxide or clay platelets can be used to make conducting inks or as fillers in composites to enhance their mechanical properties. At high concentrations beyond rigidity percolation, nanosheet suspensions become yield stress fluids with a finite storage modulus. In this regime the elastic response of nano-sheet suspensions appears to be universal. The storage modulus plateau of few-layer graphene in NMP solvent, aqueous graphene oxide gels and clays exhibit a power law exponent close to 3 as a function of relative volume fraction.

We present a new analytical model that explains this behaviour and connects the bulk response to the elastic properties of single nanosheets and their size. This allows is to infer the magnitude of the bending stiffness of single nano-sheets from our rheological data.

This model opens up the possibility to infer elastic properties of different nanosheets from rheological data of the suspension rather than performing AFM experiments on single nanosheets. Furthermore, this model may explain the mechanical enhancement of nanosheet composites where a similar exponent can be observed.

*The authors aknowledge funding from Science Foundation Ireland (SFI) under grant 17/CDA/4704

3:30PM P31.00006: Tunable viscoelasticity of double gel networks: colloidal gels embedded in a hydrogel matrix IPPOLYTI DELLATOLAS (Presenter), JAE HYUNG CHO, THIBAUT DIVOUX, IRMGARD BISCHOFBERGER, Massachusetts Institute of Technology MIT — We create double gel networks consisting of a colloidal gel embedded within a hydrogel matrix. Depending on the relative strength between the two networks, we can tune the rheology to be either dominated by the colloidal gel, the hydrogel, or to exhibit features characteristic of both systems. This allows us to adjust both the sample modulus and the yielding behavior. Looking beyond the macroscopic mechanical characteristics, we discuss the changes in the microscopic dynamics of the colloidal gel occurring as the hydrogel network forms around it. We use differential dynamic microscopy and confocal fluorescence microscopy to access the variations in the structure and network fluctuations of the colloidal gel.
Tuning vaporization threshold of perfluorocarbon by interfacial melting in endoskeletal droplets

GAZENDRA SHAKYA (Presenter), Department of Mechanical Engineering, University of Colorado, Boulder, SAMUEL HOFF, SHIYI WANG, HENDRIK HEINZ, Department of Chemical and Biological Engineering, University of Colorado, Boulder, XIAOYUN DING, MARK BORDEN, Department of Mechanical Engineering, University of Colorado, Boulder — Perfluorocarbon (FC) droplets have been extensively used as phase-change contrast agents for biomedical ultrasound imaging and therapy. Several studies have aimed at understanding the vapor embryo nucleation and vaporization behavior of these droplets. However, these studies have not looked at tuning the thermodynamic limit of stability (spinodal) by using multiphase mixtures. We investigated the vaporization behavior of endoskeletal perfluoropentane ($C_5F_{12}$) droplets by incorporating solid FC and solid hydrocarbon (HC) skeletons. Multiple geometries were generated, including endoskeletal (solid-in-liquid) as well as exoskeletal (liquid-in-solid) droplets. Vaporization of these droplets was measured over a range of temperatures both optically using a microscope and acoustically with clinical ultrasound scanner. We show that $C_5F_{12}$ stability can be tuned by controlling the intermolecular interactions, as captured quantitatively by the exchange parameter. Using a simple statistical thermodynamics lattice model, we demonstrate that the presence of the FC strengthens the intermolecular attraction and the presence of HC breaks the intermolecular attraction between the liquid molecules, making it possible to finely tune the spinodal and consequently the vaporization temperature.

Flow of Quasi-2D Emulsion Droplets Through Small Openings*

ANISA HOFERT (Presenter), YONGLUN JIANG, ERIC WEEKS, Emory University — We examine how various parameters affect the flow rate of quasi-2D soft particles moving through tight openings. To observe this, we create thin hopper-shaped chambers which have a small exit for the particles to flow through. We fill the chambers with monodisperse oil-in-water emulsions with a soap surfactant. We use microscopy to observe the droplets moving through the chamber. We find faster flow rates when there are more droplets in the chamber (providing a larger pressure head) and with larger exit sizes. We fit the flow rate to a modified Beverloo equation with an extra term for the height of the particles pushing the droplets through the opening.

*This work was supported by NSF CBET-1804186.
A granular material spreading as a liquid: growth dynamics of 3D aggregates of oil droplets

JEAN-CHRISTOPHE ONO-DIT-BIOT (Presenter), TANEL LORAND, KARI DALNOKI-VERESS, Physics and Astronomy, McMaster University — A continuous medium like a puddle has a characteristic critical height set by the capillary length, a balance between gravity and surface tension. In this study, monodisperse frictionless and lightly attractive oil droplets (radius approximately 10 microns) are produced one-by-one in an aqueous solution. Droplets are buoyant and accumulate underneath a glass slide which acts as the top of a liquid cell, forming 3D aggregates. The droplets initially accumulate vertically. As a critical height is reached, the aggregate collapses and spreads horizontally on the glass slide. Despite the aggregates being granular in nature, we find that the equilibrium shape of such aggregates follows the physics of continuous media. Indeed, the height of the aggregate reaches a critical value which is set by a balance between adhesion between the droplets and buoyancy. Both parameters can be tuned in the experiment to vary the geometry of the droplet aggregates. We developed a model that captures the shape of the aggregate with a simple parameter analogous to the capillary length.

Spreading of a 2D granular analogue of a liquid puddle: Predicting structure through a “granular capillary length”

JOHNATHAN HOGGARTH (Presenter), JEAN-CHRISTOPHE ONO-DIT-BIOT, KARI DALNOKI-VERESS, McMaster Univ — The structure of an accumulation of granular material, such as a pile of sand, is understood through the balance between gravity, which acts to limit the height, and inter-grain friction, which holds the particles together. In contrast, for the case of a continuous medium, the height of a puddle is dictated by the capillary length which balances gravity and surface tension. Here we develop an experimental model that allows us to probe the structure of a 2D pile of monodisperse microscopic oil droplets. The droplets are buoyant, adhesive, and friction is negligible. Oil droplets are deposited within a chamber and accumulate at a barrier. The droplets accumulate to a certain critical height at which point the pile collapses and spreads across the barrier. This process is reminiscent of the spreading of a liquid even though the pile is granular and 2D in nature. We define a parameter, analogous to the capillary length, which determines the height of the pile and is dictated by the balance between buoyant and adhesive forces. These parameters can be controlled experimentally in order to modify the height of the pile. We developed a simple model that can predict the shape of the pile based on the balance of adhesion and buoyancy.
4:30PM P31.00011: Characterizing the effects of Temperature and Ethanol Concentration on the louche of Absinthe. *  JESSICA BICKEL (Presenter), ANNA ELLIS, ANDREW H RESNICK, Cleveland State University — Oil flavored alcohols are traditionally served by mixing them with cold water to form a louche: a microemulsion that turns the drink opaque because of the interactions of the alcohol with water, which it dissolves, and the oil, which is disperses. When there is sufficient water the oil phase precipitates, forming the louche. Thus, characterization of the louche depends on the concentrations of water, alcohol and oil. Absinthe has not been as well characterized as other oil flavored alcohols such as Limoncello or Ouzo with no studies on either a ternary phase diagram or on the louche phase. This work examines the emergence of the louche phase in absinthe by measuring the optical transmittance of the solution as a function of both: (1) the concentration of ethanol and (2) the temperature, which can be separately varied. The laser transmission was measured through a temperature-controlled sample of absinthe. The change in transmission was recorded as water was added to the sample, revealing an inverse relationship between temperature and ethanol concentration at which louche forms. There are also two different steps in the louche suggesting two different micro-emulsions form depending on the concentrations.

*CSU Office of Research

4:42PM P31.00012: Surface active microgels: dual functioning soft stabilisers  DAVID CROSBY (Presenter), VINCENT MARTINEZ, TIFFANY WOOD, ALEX LIPS, WILSON POON, Univ of Edinburgh — Emulsions are stabilised by either surfactants or solid particles which sit at the interface between the phases. Particles irreversibly adsorb to an interface whereas surfactants detach under small perturbations. Due to their enhanced stability, particle-stabilised emulsions are used as a base for many products such as foods and pharmaceuticals. Furthermore, particles impart elasticity to interfaces, a quality which enhances the sensory performance of foods without the need for excessive amounts of fat [1]. Personal care products are another potential application as they require enhanced sensory properties and tuneable stability.

However, particle-stabilised interfaces can become unstable when dilated or compressed, processes which are common in processing. This instability, known as buckling, occurs when colloids jam together causing films to collapse.

We present work done on a commercial microgel system, composed of an amphiphilic polymer called Sepimax Zen (SZ). We show that SZ microgels stabilise an oil-water interface forming elastic films which are immune to buckling and can also be used to thicken suspensions.

4:54PM P31.00013: Clustering Colloids with Polymer Bridges  THEODORE HUECKEL (Presenter), New York Univ NYU, JOERI OPDAM, Eindhoven University of Technology, THOM SNOEREN, New York Univ NYU, REMCO TUINIER, Eindhoven University of Technology, STEFANO SACANNA, New York Univ NYU — Colloidal model systems are typically highly uniform, yet structurally simple. One design principle inspired from organic chemistry is to take rudimentary atomic building blocks and combine them into more complex and functional molecules. An analogous colloidal reaction is the heteroaggregation of core and shell particles into clusters that have new shapes, which can foster assembly in a directional fashion. Some colloidal pairings are naturally complementary, such as oppositely charged particles, but it is difficult to combine distinct like-charged suspensions in a similar manner. Highly tailored surface chemistry can bind particles together, however, severely impact throughput along the way. Here, a general approach to heteroaggregation is described where particles are speciated as either polymer-coated or bare and made to bind specifically to their counterpart through polymer bridging. Flexibly selecting from a variety of materials for the cores and shells creates a veritable zoo of different cluster products with large-scale production potential. Harnessing this colloidal bond has led to advancements in particle shape, surface pattern, and regioselective binding, which are all necessary control parameters for furthering our capabilities in synthetic self-assembling systems.

5:06PM P31.00014: Universal elasticity in nearly floppy soft matter  BRIAN TIGHE (Presenter), Delft University of Technology — In many soft matter systems, mechanics is governed by the balance between microscopic degrees of freedom and internal constraints on motion. Constraints on relative motion parallel to the bond between two particles, or between two nodes in a network, can be modeled with springs. However, other, non-central force constraints are often present as well — examples include constraints on sliding in frictional granular media and composites, constraints on bending in biopolymers and covalent glasses, and constraints on shape distortions in confluent tissues, foams, and emulsions. We consider the case where non-central force constraints are present, but carry a weaker energetic cost than their spring-like counterparts. We will show that the elasticity of these systems has universal features, independent of the origin of the non-central force constraint. These features can be explained in terms of the floppy modes that appear in the limit where non-central forces are "turned off." We derive scaling relations for the shear modulus and validate them numerically in three model systems — pre-tensioned spring networks, semi-flexible fibre networks, and composite packings of hard and soft particles.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P32 DPOLY DSOFT DCP DMP: Molecular and Polymer Glass Dynamics  504 - Mark Ediger, University of Wisconsin - Madison - Tag(s): Focus
Evidence for heterogeneous bulk melting dominating the transition of organic stable glasses

MARTA GONZALEZ-SILVEIRA (Presenter), ANA VILA-COSTA, MARTA RODRÍGUEZ-LOPEZ, AITOR F. LOPEANDÍA, JAVIER RODRIGUEZ-VIEJO, Physics Department, Autonomous University of Barcelona — For over a century, scientists have tried to understand the mechanisms behind the glass transition and the dynamics of glassy systems. Part of the difficulty arises from the time scales involved in these processes. The low stability of conventional glasses, obtained by cooling down a melted material, have determined for years how we study glass dynamics, focused basically on the aging regime, i.e., performing isothermal treatments below the limiting fictive temperature ($T_f$) of the glass, allowing the glass to evolve towards a more stable configuration. But the evolution of glasses above their $T_f$ in isothermal regime, what we could call softening of rejuvenation as the glass progressively loses stability, has been barely explored at temperatures not far above the conventional glass transition temperature of the material, $T_g$. The time scales in this case are extremely short for conventional glasses, and in order to study rejuvenation one would need either glasses of high stability (to increase the measuring time) or advanced instrumentation (able to work in very short times). This scenario has changed with the ability to prepare glasses of a wide range of stabilities by means of PVD and the development of fast scanning nanocalorimetry. By performing isothermal treatments at temperatures spanning more than 30 K above the conventional $T_g$ of the material we show that the rejuvenation process in stable glasses takes place via two different mechanisms: i) a homogeneous softening of the glass and ii) the formation of liquid patches in the bulk of the glass, which grow transforming the glass straight into the liquid, dominating the pace of the transformation and resembling the nucleation and growth process characteristic of the melting of crystals. Surprisingly, these two mechanisms are present even in glasses with stabilities close to those of the conventional glass, although clear differences can be found in the number of initial liquid patches and the transformation rate.

Solvent vapor annealing of stable glasses

SHIVAJEE GOVIND (Presenter), HAOQIANG ZHAO, PATRICK WALSH, ZAHRA FAKHRAAI, University of Pennsylvania — Stable glasses (SG) are highly dense, low energy glasses that are made by physical vapor deposition (PVD). Because of their desirable properties and wide range of applications, they are extensively studied glasses. However, measuring their dynamics can be difficult since they are produced directly into a SG state on a substrate during the process of PVD. We have introduced a novel and indirect method of measuring the dynamics of SG using solvent vapor annealing (SVA). Using this technique, together with in-situ ellipsometry, we have shown that even at low solvent vapor pressure, the surface of SG swells more quickly, in an analogous Fickian type diffusion, compared to that of the bulk. Above a certain threshold of vapor pressure, the bulk of the film swells linearly with time, which demonstrates a Case II type of diffusion. This shows the diffusion of the solvent molecule through the film is limited by the relaxation of the molecules such that the solvent uptake is governed by a two-layer model; one swollen with solvent and the other the dry medium. By monitoring the solvent front moving across the film, we compare the dynamics of the SG films of different stability produced at different deposition temperatures.

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NSF-MRSEC DMR-1720530
3:18PM P32.00003: Secondary Dynamics in Ultrastable Polystyrene Thin Films Studied by $\beta$-NMR

IAIN MCKENZIE, TRIUMF, DANAAN CORDONI-JORDAN, Chemistry, Simon Fraser University, DEREK FUJIMOTO (Presenter), Physics and Astronomy, University of British Columbia, VICTORIA KARNER, Chemistry, University of British Columbia, ROBERT F KIEFL, Physics and Astronomy, University of British Columbia, PHILIP C. P. LEVY, TRIUMF, W ANDREW MACFARLANE, RYAN M. L. MCFADDEN, Chemistry, University of British Columbia, GERALD MORRIS, MATT PEARSON, TRIUMF, ADAM RAEGEN, Physics and Astronomy, University of Waterloo, JOHN TICKNOR, Chemistry, University of British Columbia, JAMES A FORREST, Physics and Astronomy, University of Waterloo — Ultrastable, highly mono-disperse polystyrene (PS) thin films can be produced by physical vapor deposition. These films can exhibit properties similar to those of a normal glass that has been aged for thousands of years. $\beta$-detected nuclear magnetic resonance ($\beta$-NMR) of implanted $^8\text{Li}^+$ probes can be used to study dynamics in thin polymer films, which is not possible with conventional magnetic resonance techniques [I. McKenzie et al. Soft Matter 14, 7324 (2018)]. We have used $\beta$-NMR to study the temperature dependence of the secondary $\gamma$-relaxation process in an ultrastable PS film and a normal PS film that was produced by rejuvenating an ultrastable film by heating to $T_g + 25$ K for 2 minutes. The $\gamma$-relaxation is $\sim 38\%$ slower at 295 K, and the activation energy is $\sim 20\%$ larger in the ultrastable glass compared with the normal glass. Our interpretation of the results is that the denser packing in the ultrastable glass hinders motion of the phenyl rings.

*We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC).

3:30PM P32.00004: Uncovering $\beta$-relaxations in amorphous phase-change materials

SHUAI WEI (Presenter), RWTH Aachen University, SI-XU PENG, Huazhong University of Science and Technology, YUDONG CHENG, JULIAN PRIES, RWTH Aachen University, HAI-BIN YU, Huazhong University of Science and Technology, MATTHIAS WUTTIG, RWTH Aachen University — Relaxation processes are decisive for many relevant physical properties of amorphous materials. For amorphous phase-change materials (PCMs) employed in non-volatile memories, relaxation processes are, however, difficult to characterize due to the lack of bulk samples. Here, instead of bulk samples, we use powder mechanical spectroscopy for powder samples to detect the prominent excess wings – a characteristic feature of $\beta$-relaxations – in a series of amorphous PCMs at temperatures below the glass transition. By contrast, $\beta$-relaxations are vanishingly small in amorphous chalcogenides of similar composition, which lack the characteristic features of phase-change materials. This conclusion is corroborated upon crossing the border from PCMs to non-PCMs, where $\beta$-relaxations drop significantly. Such a distinction implies that amorphous PCMs belong to a special kind of covalent glasses whose locally fast atomic motions are preserved even below the glass transitions. These findings also suggest a correlation between $\beta$-relaxation and crystallization kinetics of PCMs, which may have technological implications for phase-change memory functionalities.
3:42PM P32.00005: A direct static scattering evidence on the dynamic nature of glass formation process in polystyrene*  HE CHENG (Presenter), GUIHENG JIAO, TAISEN ZUO, CHANGLI MA, ZEHUA HAN, JUNRONG ZHANG, Chinese Academy of Sciences, JUNPENG ZHAO, south china university of technology, CHARLES C HAN, Chinese Academy of Sciences — The combination of neutron total scattering, high concentration labelling and molecular dynamics (MD) simulation enable us to visualize the temperature dependence most-probable all-atom positions in atactic polystyrene (PS), and find out the dynamic nature of its glass forming. The scattering profiles from MD simulation are in agreement with all of the neutron scattering curves, as well as the X-ray scattering data in literatures at different temperatures. Two main scattering peaks at ~0.6 Å⁻¹ and 1.4 Å⁻¹ can thus be allocated. The peak at ~0.6 Å⁻¹ is from the segment-segment interaction, which is a combination of backbone-backbone and backbone-phenyl interactions. And the peak at 1.4 Å⁻¹ is mainly from phenyl-phenyl interaction. Below glass formation temperature, both peaks keep almost constant. Their heights jump during glass formation, revealing the melting of the configuration variation and development of dynamic heterogeneity.

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3:54PM P32.00006: Effects of aromatic side-group structure on thermal transitions of polyzwitterions* ANDREW CLARK (Presenter), YAJNASENI BISWAS, AYSE ASATEKIN, MORGAN E TAYLOR, MATTHEW J PANZER, Tufts Univ, CHRISTOPH SCHICK, Physics, University of Rostock, PEGGY CEBE, Tufts Univ — Aromatic structures can have a pronounced effect on the glass forming properties of ionic liquids and polymers. Polyzwitterions are polymers with side groups that contain a covalently linked anion and cation. Depending upon side chain structure, this can lead to high glass transition temperatures, occurring near the onset of degradation. In this study we are using fast scanning calorimetry to investigate how aromatic structures in the side-group alters the glass formation of polyzwitterions. Poly(sulfobetaine vinylimidazole) (PSBVI) and poly(sulfobetaine-4-vinylpyridine) (PSB4VP) were synthesized and cast into films. Both polymers contain identical sulfonate anions allowing for a good comparison of the effect of aromatic structure variations in the side-group. The glass transition could not be observed prior to degradation in either polymer using conventional slow scan DSC. Using fast scanning calorimetry, degradation was avoided by heating and cooling at 2000 K/s which allowed the first measurement of the glass transition process in these materials. We found that PSBVI has a T_g of 250 °C while PSB4VP has T_g at 215 °C. Analysis of the fragility reveals that PSBVI is a stronger glass former than PSB4VP.

*NSF DMR-1608125, DAAD, Tufts Collaborates Seed Grant, NSF CBET-1802729
Rigorous analysis of the linear viscoelastic behavior of thermo-rheologically complex amorphous materials

GRIGORI MEDVEDEV (Presenter), JAMES M CARUTHERS, Purdue Univ — It is well-known that linear viscoelastic response of amorphous materials, including both low molecular weight and polymeric, as probed in mechanical and dielectric relaxation experiments is thermo-rheologically complex. A common approach to analyzing viscoelastic data is to use a combination of phenomenological functions such as stretched exponential, Havriliak-Negami, etc. manifesting as distinct peaks in the relaxation spectrum. Unfortunately, not only the location on the time axis but also the shape and the spectral strength of these peaks is required to change with temperature rendering such representation merely a curve fit. A brute force Prony series expansion has also been tried, where the relaxation times are typically assumed to be evenly spaced on the logarithmic scale. The resulting set of Debye peaks of varying strength also lacks physical interpretation. We propose a different approach where all processes have the same strength, but the corresponding relaxation times are dictated by the data. When broad temperature interval comprising sub-Tg and above Tg regions is investigated a complete relaxation map emerges. Examples of the relaxation map will be shown for several materials, including epoxy systems of varying architecture.

Relaxation processes in polymer glasses: a hierarchical approach

PETER OLMSTED (Presenter), Department of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown University, DANIEL L BAKER, MATTHEW REYNOLDS, JOHAN MATTSSON, Department of Physics & Astronomy, University of Leeds, ROBIN MASUREL, Department of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown University — The glass transition temperature Tg in polymers increases with increasing molecular weight M, but the detailed Tg(M) dependence in polymers is not well understood. Here, we present experimental results of the M-dependence of both the structural (alpha) relaxation process, which controls the glass transition, and faster (beta and gamma) secondary relaxation processes for a range of polymers of varying chain flexibility. Based on our results, we propose a hierarchical relaxation scenario that links these relaxations and controls Tg in polymers, where the fundamental metric is linked to ‘local’ flexibility. We identify regimes in M where intra and inter-molecular relaxation dynamics play different roles in defining the dynamics (and thus Tg). We argue that dihedral barriers play a crucial role in controlling the dynamics, which gives rise to distinct differences in behaviour from what is observed in glass-formers with simpler ‘rigid’ structures, or in simplified bead-spring models of polymers.

*Funding from UK Engineering and Physical Sciences Research Council (EPSRC), Georgetown University (Ives Foundation)
4:30PM P32.00009: Unusual Viscoelasticity in Polyrotaxane Glasses  KARAN DIKSHIT (Presenter), CARSON J BRUNS, University of Colorado, Boulder — This work characterizes the viscoelastic properties of glasses made from polyrotaxanes, a class of mechanically interlocked polymers possessing a bead-on-a-string structure. The rheology of polyrotaxane-based glasses in the devitrified state reveals an absence of elastic plateau over a large range of frequencies. The motivation for this investigation stems from a need to understand the processability of polyrotaxanes. These “molecular necklaces”, without any modification, are crystalline due to the presence of strong hydrogen bonding between the cyclodextrin-based molecular beads. Similar to cellulose, which also exhibits strong hydrogen bonding, these materials do not flow when heated. Chemical modification of the cyclodextrins leads to the breakdown of hydrogen bonding which, in turn, reduces crystallinity and renders the polyrotaxanes amorphous and glassy. XRD and DSC data confirm the amorphous nature of these polymers and reveal their glass transition temperatures. Understanding the rheology of these polyrotaxane glasses will help characterize their mechanical behavior over different temperatures and time scales while identifying optimal processing conditions for applications in advanced materials.

4:42PM P32.00010: Volume recovery and physical aging of pressure-densified glasses  DANIEL FRAGIADAKIS (Presenter), ADAM HOLT, CHARLES M. ROLAND, United States Naval Research Laboratory — When a glass is formed by cooling under high pressure, the resulting pressure densified glass exhibits a higher density and different thermal and mechanical properties than the corresponding glass prepared by conventional cooling at low pressure. Understanding, manipulating, and exploiting the full potential of pressure densified glasses offers the possibility of better properties. The effects of pressure densification on 1,3,5-tri(1-naphthyl)benzene (TNB) are assessed from volumetric and calorimetric measurements. The pressure densified glass (PDG) exhibits anomalous physical aging. Rather than evolving monotonically towards the equilibrium density, there is an overshoot to a lower density state. Only when the density of the PDG becomes equivalent to the corresponding CG does the density begin a slow approach towards equilibrium. Using molecular dynamics simulations of a simplified model of TNB, we show that the effects of vitrification pressure and subsequent volume recovery and aging of the glass are comparable to experimental results for real TNB. A two-parameter description of the underlying non-equilibrium structure, entailing a fictive temperature and fictive pressure, appears adequate to interpret the “anomalous” aging behavior of pressure-densified TNB.
Understanding aging phenomena by the free-energy-landscape approach

TAKASHI ODAGAKI (Presenter), Research Institute for Science Education & Kyushu University — Aging phenomena have been observed in many non-equilibrium systems such as polymers and glasses, where physical properties depend on the waiting time before observation. It is not known what causes the aging, nor what information can be extracted from them. Exploiting the free-energy-landscape (FEL) theory[1], which explains dynamic and thermodynamic properties of non-equilibrium systems in a unified framework, I argue the physical origin of the aging phenomena for the first time. The FEL depends on temperature and, thus, will respond to a temperature modulation with delay. I consider physical quantities observed after a waiting time $t_w$ when the temperature is modulated at time $t = 0$ and show that the delayed response of the FEL manifests itself in an additional aging. As an example, I investigate aging phenomena of dielectric relaxation represented by a two-level model. I show that the relaxation function and the linear susceptibility show non-trivial dependence on $t_w$ from which one can deduce the relaxation time of the FEL.


This work was supported in part by the Grant-in-Aid for Scientific Research from MEXT.

Lifetime of Rate Domains: Comparison of Simulations and Single-Molecule Experiments in o-Terphenyl

HARVEEN KAUR, Chemistry and Biochemistry, Univ of South Carolina, KEEWOOK PAENG, LAURA KAUFMAN, Chemistry, Columbia University, MARK BERG (Presenter), Chemistry and Biochemistry, Univ of South Carolina — Supercooled liquids have domains with different relaxation rates. The lifetime of those domains is not well understood. The usefulness of single-molecule measurements has been limited by conventional, molecule-by-molecule analysis, which suffers from excessive noise. An alternative, ensemble-based analysis using multidimensional correlation functions is applied to single-molecule dichroism results in o-terphenyl near $T_g$ ($T_g$+4.5–1.5 K, $T_{rot}$ = 3–15 s). It yields a detailed rate-exchange correlation function, which is biphasic. The slow, main component is 22 times slower than the alpha-relaxation time, implying that single-particle relaxation does not fully equilibrate the liquid. A small, fast phase of rate exchange is attributed to molecules on the boundaries of rate domains. The same analysis was applied to a ms-long, all-atom simulation of o-terphenyl from the D. E. Shaw group [J. Phys. Chem. B 117, 12898 (2013)]. It is at a higher temperature (272.5 K, $T_{rot}$ = 16 μs), but it is still well below the mode-coupling temperature (290 K). There are clear differences from the results near $T_g$, suggesting that time–temperature superposition does not hold for rate exchange.

This material is based upon work supported by the National Science Foundation under CHE-1707813.
5:18PM P32.00013: Unified description of the Arrhenian and super-Arrhenian behavior of OTP by the excess internal energy model  JAMES M CARUTHERS (Presenter), JACK YUNGBLUTH, GRIGORI MEDVEDEV, BRET SAVOIE, Purdue Univ — As previously reported (Caruthers, Medvedev 2018), the excess internal energy model, $1/U_x$, unlike the excess entropy model of Adam and Gibbs, is able to describe the mobility of liquids in the super-cooled state as a function of temperature and pressure. The $1/U_x$ model prediction of the temperature effect on mobility was validated for 21 molecular glass formers and of the temperature and pressure – for ortho-terphenyl (OTP) – the only material for which there was sufficient data. In the current work MD simulations were performed on model OTP in the high temperature region that includes the onset of the super-Arrhenian behavior. The excess internal energy was obtained at pressures from 0.1 MPa to 5 GPa. The translational and rotation diffusivities were determined at these temperatures and pressures. The MD mobility data (including extremely long time 0.1 MPa simulations from Eastwood et al. 2013) were combined with experimental data, where it was shown that in both the high temperature Arrhenian region and the lower temperature super-Arrhenian region the mobility is a linear function of $1/U_x$, albeit with different proportionality constants; the transition between the Arrhenian and super-Arrhenian behaviors is relatively sharp at a critical internal energy $U_{x,α}$.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P33 DPOLY DSOFT: Hierarchical Structural Emergence in Elastomer Nanocomposites: Dispersion, Dynamics, Structure, Modeling, and Simulation II 505 - Greg Beaucage, Univ of Cincinnati - Tag(s): Focus

2:30PM P33.00001: WITHDRAWN ABSTRACT —
2:42PM P33.00002: Quantification of dispersion for weakly and strongly correlated fillers in polymer nanocomposites*  ALEX M MCGLASSON (Presenter), KABIR RISHI, GREG BEAUCAGE, MICHAEL CHAUBY, Univ of Cincinnati, VIKRAM KUPPA, University of Dayton — The dispersion of nanoparticles in viscous polymers is dictated by kinetics; interaction potentials between particles; and interfacial compatibility between the matrix and dispersed phases. An analogy has been made between thermally dispersed colloids and kinetically dispersed nanoparticles for cases where only weak interactions exist between particles allowing for a mean field description under the Ginzburg criterion such as for carbon black dispersed in polybutadiene. For these cases the pseudo- second virial coefficient can be used to quantify the quality of dispersion. However, this approach fails for nanoparticles with surface charges or other specific interactions that display strong correlations such as precipitated silica in styrene-butadiene rubber. Here, these strongly correlated systems are investigated in the context of the mean-field systems in order to gain a comparative description of dispersion using the network mesh size and a derived virial coefficient. In the proposed approach, the correlations in nanoaggregates are described by a combined semi-empirical function based on the Born-Green theory and a distribution function that accounts for the non-uniform accumulated strain in nanocomposites.

*NSF CMMI- 1635865, 1761420, 1636036; DOE APS (9ID-C) DE-AC02-06CH11357

2:54PM P33.00003: Recent Study of Small-Angle Neutron Scattering Spectrometer Suanni on Elastomer Nanocomposites* YUE SHUI, LIZHAO HUANG, TINGTING WANG, GUANGAI SUN, JIAN GONG, JIE CHEN, DONG LIU (Presenter), Key Laboratory of Neutron Physics and Institute of Nuclear Physics and Chemistry (INPC), China Academy of Engineering Physics (CAEP) — The small-angle neutron scattering (SANS) spectrometer Suanni at CMRR has been brought into operation since 2014 [1]. The SANS-Suanni can achieve a maximum-q up to 10.5 nm⁻¹. In this report, we will discuss some applications on the polymeric materials. By combining extensional rheological and in situ SANS techniques, the correlation between chain deformation and morphology of flow-induced crystallization has been studied [2]. The structure decomposition of silica-filled silicone rubber via the contrast variation SANS technique was presented. SANS results suggested unambiguously the existence of a bound rubber layer with thickness of ca. 8.5 nm [3]. Recently, the correlation between macroscopic mechanical properties and microscopic structures of an optimized silica fraction in silicone rubber was investigated. An optimum filler fraction ranges from 40~50 phr was found, in which the best performances of reinforcement and themorpholog were shown. [4].

Reference:

*National Key R&D Program of China (2018YFB0704200)

3:06PM P33.00004: WITHDRAWN ABSTRACT —
3:18PM P33.00005: Effect of Initial Dispersion State on the Structure and Property of Polymer Nanocomposites*  
GA YOUNG KIM (Presenter), SO YOUN Y KIM, Ulsan Natl Inst of Sci & Tech — In the colloids-polymer mixture system, the microstructure of particles and polymers are strongly dependent upon their interactions, which can vary systemically with the component concentrations. When the colloidal system is concentrated by solvent evaporation with drying, the continuous change of component concentrations also causes a continuous change in the interparticle interaction. Previous studies have been conducted to control the rate of evaporation or drying conditions of the system. In this study, we show how the initial dispersion of the colloidal system can influence the final structure and property of the polymer nanocomposites. To vary the initial dispersion state, we first set different initial dispersion concentrations to find the effect of polymer and particle volume fractions on the interaction. Second, we provide different equilibrium time for particles to be aggregated. Ensemble-averaged microstructures were analyzed by SAXS measurement and rheological properties were analyzed by rheometer.

*This work was supported by the National Research Foundation of Korea grant funded by Korea Government (NRF-2018R1A5A1024127)

3:30PM P33.00006: Thermodynamic model for dispersion in nanocomposites.*  
GREG BEAUCAGE (Presenter), KARSTEN VOGTT, KABIR RISHI, Univ of Cincinnati, HANQIU JIANG, The China Spallation Neutron Source (CSNS), Institute of High Energy Physics, ANDREW MULDERIG, Univ of Cincinnati — Dispersion of nanoparticles can involve thermally driven diffusion of particles or kinetically driven mixing. On the nano- to colloidal scale a virial expansion of osmotic pressure can be used to quantify dispersion. Scattering can be used to measure the osmotic compressibility associated with concentration fluctuations which are related to the second virial coefficient. These fluctuations might be created thermally or by kinetic mixing. For multi-hierarchical materials such as aggregates which cluster to form a macroscopic network, each level of structure contributes to the free energy. This can be quantified in terms of the total number of free particles contributed by each of the levels of structure. For different levels in a hierarchy the energy of aggregation can be associated with an aggregation equilibrium or an apparent equilibrium. The resulting number of particles can be related to the energy of aggregation. This approach is demonstrated for three systems, pigments dispersed with nonionic surfactants; worm-like micelles; and condensation polymerization.


*NSF CMMI-1635865; DOE APS (beamline 9ID-C) DE-AC02-06CH11357
3:42PM P33.00007: Scattering Studies on Hierarchically Self-Organized Filler Particles in Polymers [Invited] MIKIHITO TAKENAKA (Presenter), Kyoto Univ, SHOTARO NISHITSUJI, Yamagata University, TAKEJI HASHIMOTO, Kyoto Univ — In this study, we investigated the self-organization of nanoparticles dispersed in polymer melts under applied mechanical energy imposed to mixtures that are composed of a bulk of the particle powder and a bulk of the polymer melt. Using various scattering methods that enable the exploration of structures that exist over a length scale that spans from ~0.1 nm to ~20 mm, we elucidated that the self-organized particles had hierarchical structures with various hierarchical levels as follows: primary particles (PPs), aggregates of the PPs fused together, clusters of the aggregates, and partially interdigitating mass-fractal structures built up by the clusters.

4:18PM P33.00008: First principles Study of Interaction of Polymer Molecules with Flat Carbon Nanotubes GEETA SACHDEVA (Presenter), RAVINDRA PANDEY, Department of Physics, Michigan Technological Univ, GREGORY M. ODEGARD, Department of Mechanical Engineering and Engineering Mechanics, Michigan Technological Univ — Polymer composites possess an integrated combination of structures and properties associated with the host matrix and fiber material (e.g. carbon nanotubes), and thus holding the potential as high strength materials. In general, the load transfer from the matrix to the fiber depends upon the strength of bonding at the interface which characterizes the mechanical strength. In this talk, we present the results based on density functional theory for the composite consisted of epoxy/BMI resins and flat carbon nanotubes with an aim to provide atomistic description of the interface which determines the mechanical strength of the polymer composite.

4:30PM P33.00009: Multiscale Modeling of Fracture in Epoxy/CNT Nanocomposites HAYDEN HOLLENBECK (Presenter), CHENGYUAN WEN, RALPH ROMERO, TABASSUM AHMED, NESLIHAN GENCKAL, NISHANT SHIRODKAR, GARY SEIDEL, SHENGFENG CHENG, Virginia Tech — Modeling fracture in a polymer nanocomposite with molecular resolution is a big challenge. We have developed a multiscale modeling framework on the basis of coarse-grained molecular dynamics (CG-MD) simulations and peridynamics to study fracture initiation and propagation in epoxy/CNT nanocomposites. The CG model constructed via a hierarchical coarse-graining scheme enables us to model an epoxy network at micrometer scale and still capture its mechanical properties including various moduli. A jointed-tube model is developed for CNTs that overcomes the corrugation issue in traditional CG potentials between CNTs and polymers. Peridynamics simulations of CG CNT bundles dispersed in CG epoxy are used at the microscale to generate statistical distributions of moduli and fracture properties to be used in macroscale peridynamics simulations of fracture toughness tests. The calculations are validated against physical experiments at a given macroscale volume fraction. Successful validation of our hybrid hierarchical-concurrent modeling framework integrating CG-MD and peridynamics models paves the way to designing epoxy/CNT nanocomposites with desired fracture properties via tuning CNT loading and dispersion state.

4:42PM P33.00010: Molecular Dynamics Investigation of the Structural and Mechanical Properties of Off-Stoichiometric Epoxy Resins  CHANG WOON JANG (Presenter), JOHN LAWSON, NASA Ames Research Center — We carried out molecular dynamics (MD) simulations to measure the mechanical properties of various off-stoichiometric polymers regarding amine to epoxy ratios (r) and to understand the stiffness of the polymers in terms of their structures. The aerospace-grade API-60 epoxy resin is used as an adhesive bond for assembling large-scale composite structures via the co-curing-ply bonding method. This method will produce a reliable and certifiable composite joint without additional fasteners. Calculated Young's modulus was measured from the uniaxial tension simulation with several high strain rates, and the experimental modulus was estimated by extrapolating the simulation results. We found that the stiffness was associated with molecular packing caused by chemical cross-linking. We also found that the number of network clusters gradually decreased as the ratio approached r = 1.0, which made the tighter cluster and the system much stiffer with an increase in the molecular weight and the degree of cross-linking. Structural properties such as Rg, MSD were measured to figure out the degree of stiffness with respect to the r.

4:54PM P33.00011: Deformation of Epoxy Nano-Composites  SURESH AHUJA (Presenter), materials, xerox corporation — Polymeric materials show properties which come from the interplay of phenomena at various length and time scales. The presence of layered silicates in polymers (PNC) changes the viscoelastic behavior of the unfilled matrix from liquid-like to solid-like because of the formation of a three-dimensional percolating network of exfoliated or intercalated stacks. This gel-like behavior is a direct consequence of the highly anisotropic nature of the nano-clays which prevents their free rotation and the dissipation of stress. Particle to particle interactions is the dominant mechanism in fumed silica nanocomposites whereas particle to polymer interaction is the dominant one in colloidal silica nanocomposites at identical filler concentrations.

Nano clays organically treated were mixed with Epoxy in a high shear mixer. Viscosity, normal stresses and dynamic viscoelastic measurements at various temperatures were determined. Relaxation modulus as function of time at different temperatures was used to get power law fits. Relaxation modulus at different crosslinking level in the nanocomposite shows large difference from nanocomposite with un-crosslinked epoxy. These structures by X-ray diffraction and TEM showed significant exfoliation.
Effect of interface modifiers on the cure, mechanical and viscoelastic properties of hierarchical carbon nanotube composites.  AJAY KRISHNAMURTHY (Presenter), RAN TAO, QI AN, AARON M FORSTER, National Institute of Standards and Technology — Addition of carbon nanotubes (CNTs) to traditional fiber-reinforced polymer composites (FRPs) has led to significant improvements in multifunctional capabilities of these materials. However, achieving these superior properties require incorporating relatively large CNT mass fractions (greater than 1%) where methods of dispersing CNTs in polymer matrix fail. Directly grafting CNTs onto fiber surfaces prior to resin infusion is a viable alternative and here this is achieved by using an electrophoretic deposition (EPD) process. To deposit the CNTs on fiber surfaces, they are first oxidized and mixed with a polyelectrolyte (such as polyethyleneimine (PEI)) which upon protonation is used to drive the CNTs onto fiber surfaces. In our previous study, we observed that the presence of small percentages of PEI affects the viscoelastic properties and the hydrogen dynamics of the composite. Here we aim to isolate the effect of PEI in the absence of CNTs and glass fibers and study its effect on the cure kinetics, mechanical properties and viscoelastic characteristics of the resin system. The cure process is understood using differential scanning calorimetry, the viscoelastic characteristics using dynamic mechanical thermal analysis and the mechanical properties using tensile testing.

Adhesion Strength of Block Copolymer Modified Epoxy Adhesives

VINCENT PANG (Presenter), University of Minnesota, ZACHARY JOHN THOMPSON, GUY D. JOLY, 3M Company, FRANK S BATES, LORRAINE F. FRANCIS, University of Minnesota — Epoxies are widely used as coatings and structural adhesives in the aerospace, automotive, and consumer goods industries. Prior studies have shown that the addition of block copolymers (BCPs) to epoxy resins can increase bulk fracture toughness, but little work has been done to understand the adhesive properties of these modified epoxy systems. In this work, the influence of self-assembled BCP nanostructures on the adhesion strength of epoxy thermosets was evaluated. Poly(ethylene-alt-propylene)-b-poly(ethylene oxide) BCP modifiers of various molecular weights and weight fractions were mixed into an epoxy resin, forming well dispersed nanoscale structures. Two self-assembled morphologies were studied: spherical micelles and bilayer vesicles. For both nanostructure morphologies, the modified epoxies exhibited significant improvements in bulk fracture toughness, with no reduction in elastic modulus. Single-lap-joint shear tests showed a significant (~50%) increase in the adhesion strength when spherical micelle modified epoxies were used on surface roughened aluminum. In contrast, vesicle-forming modifiers were detrimental, with a 36% reduction in adhesion strength. Possible mechanisms for the adhesion strength results will be discussed.

*This work was funded by the 3M Company.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P34 DPOLY DSOFT: Characterization of Non-Equilibrium or Exotic Structures of Polymers 506 - Douglas Tree, Brigham Young Univ - Provo - Tag(s): Focus
2:30PM P34.00001: Non-equilibrium laser annealing derived mesostructured silicon templated in mesoporous thin film network structures from block copolymer self-assembly

FEI YU (Presenter), QI ZHANG, ULRICH WIESNER, Cornell University — Block copolymer self-assembly derived network structures are combined with non-equilibrium transient laser heating to serve as nanotemplates for directing structures of inorganic materials, which otherwise are difficult to achieve mesoscale order. Amphiphilic block copolymers swelled by carbon precursors self-assemble into equilibrium bicontinuous gyroidal phases via solvent vapor annealing. After pyrolysis in nitrogen, the resulting mesoporous gyroidal carbon thin films are backfilled with amorphous Si (a-Si). The poor tolerance of carbon toward high temperature in air and the high melting points of inorganic materials present an enormous challenge in preparing crystalline mesostructured Si in the carbon templates. The carbon templates' stability is significantly enhanced, however, using nanosecond laser heating. Melting and recrystallization of Si (a-Si melts at \( \sim 1250 \) °C) during this ultrafast, highly non-equilibrium process allow conformal template backfilling so that crystallized Si inherits the templates' mesostructural order. Such non-equilibrium nanostructure formation approaches in conjunction with equilibrium self-assembly process open up opportunities for novel materials in catalysis and photonics.

*Funding from the National Science Foundation (DMR-1707836) is appreciated.

2:42PM P34.00002: Probing Block-Copolymer Self-Assembly Kinetics with In-Situ Spectroscopic Ellipsometry*

CONNOR BILCHAK (Presenter), GUILLERMO CONTREAS, SHIVAJEE GOVIND, Department of Chemistry, University of Pennsylvania, SHAWN MAGUIRE, RUSSELL COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania, ZAHRA FAKHRAAI, Department of Chemistry, University of Pennsylvania — Understanding the assembly of block copolymers during various processing procedures is critical for the development of functional materials, as well as providing information on the underlying polymer physics. However, direct observation of the assembly process in-situ is exceedingly challenging and time-consuming. In this work, we develop and implement a novel characterization method to monitor the assembly of cylinder- and lamellar- forming block copolymers using spectroscopic ellipsometry, which tracks the optical anisotropy that results from microphase separation of the assembled domains. Measurements of the birefringence are well-correlated with surface AFM images and are in good agreement with the birefringence expected from simple geometric arguments. Furthermore, the fast sampling rate (1 sec) permits in-situ measurements of the polymer self-assembly during both thermal and solvent vapor annealing in a single, rapid measurement, and correlate with the . Ellipsometry thus presents a means to not only obtain information to inform future experimental parameters for obtaining ordered phases, but also may be utilized as a novel technique to study the assembly kinetics of soft materials.

*NSF PIRE #1545884
2:54PM P34.00003: A fluorescence-based method for determining order-disorder transition temperatures in block copolymers  MUZHOU WANG (Presenter), ZHE QIANG, LINGQIAO LI, JOHN TORKELSON, Northwestern University — We present a technique for observing the order-disorder transition (ODT) in block copolymers through changes in the temperature-dependent behavior of an optically fluorescent probe. This technique provides potential advantages over existing strategies such as scattering and rheology, as it is non-invasive and can be directly applied to thin films. Pyrene molecules were covalently attached to the styrene block of a PS-b-PMMA copolymer through addition of trace levels of functionalized monomer during synthesis by controlled radical polymerization. We observed a discontinuous change in the intensity ratio of the pyrene vibronic emission bands as the polymer was heated through its ODT. As this intensity ratio is sensitive to the chemical environment surrounding these molecules, we hypothesized that this change occurs as the pyrenes are in contact with only PS when the polymer is ordered, but experiences an averaged effect of both PS and PMMA in the disordered state. We then applied this ODT measurement technique to thin films, where an increase in $T_{ODT}$ is observed when the substrate preferentially interacts with the PMMA and the film thickness is sufficiently small. Further experiments tuned this effect by modulating the surface energy of the substrate.

3:06PM P34.00004: Evolution of disordered hyperuniformity in block copolymers thin films by homopolymer dilution  URI GABINET (Presenter), CHANGYEON LEE, CHINEDUM OSUJI, University of Pennsylvania — Disordered hyperuniform materials display long range order despite their seemingly random structure – long range density fluctuations are suppressed as reflected in a vanishing structure factor at zero wavevector. Close-packed micelles of block copolymers (BCPs) display such behavior. Here, we explore the degree of structural order in BCP thin films and manipulation of such order, through the lens of disordered hyperuniformity. We explore the effect of gradually increasing disorder by increasing the nearest-neighbor distance between micelles by homopolymer addition. The hyperuniformity of the system is evaluated as a function of BCP concentration via numerical image analysis of AFM or SEM images of the BCP films. We observe a continuous transition from a DH state to randomly disordered, as characterized by the change in scaling of particle number density with increasing BCP dilution. These results offer a new perspective on structural order in BCP thin films and add to the understanding of the evolution and emergence of hyperuniform states in disordered materials. The findings are also relevant for improved engineering of nanoscale arrays based on BCP templates towards ‘designer made’ DH materials.
3:18PM P34.00005: Fluctuation/Correlation Effects in Symmetric Diblock Copolymers: On the Disordered Phase  YAN WANG (Presenter), Chemical and Biological Engineering, Colorado State University, JING ZONG, Chemical Engineering, Mississippi State University, DELIAN YANG, Synopsys, QIANG WANG, Chemical and Biological Engineering, Colorado State University — While the polymer self-consistent field theory has gained great success in describing various inhomogeneous polymeric systems, particularly the self-assembled morphologies of block copolymers, for spatially homogeneous systems it reduces to the Flory-Huggins theory and gives the simplest, yet often qualitatively incorrect, predictions. We compare, without any parameter-fitting, the thermodynamic and structural properties of the disordered phase of symmetric diblock copolymers obtained from fast off lattice Monte Carlo (FOMC) simulations [Q.Wang and Y.Yin, J.Chem.Phys.130,104903(2009)], reference interaction site model (RISM) and polymer reference interaction site model (PRISM) theories, and Gaussian-fluctuation theory for the same model system of discrete Gaussian chains interacting with soft, finite-range repulsion used in the dissipative particle dynamic simulations. We compared the internal energy, entropy, Helmholtz free energy, pressure, constant-volume heat capacity, chain/block dimensions, and various structure factors in the systems, which unambiguously and quantitatively reveal the consequences of various theoretical approximations and validity of these theories in describing the fluctuations/correlations in disordered diblock copolymers.

3:30PM P34.00006: Multiscale Modeling of Multicompartment Micelle Consisting of Block Copolymers*  MACKENZIE MALLARD, SEUNG MIN LEE, SEUNG SOON JANG (Presenter), Georgia Inst of Tech — In this work, we present a procedure for estimating the Flory-Huggins χ-parameter for use in atomistic and mesoscale molecular simulations for multicompartment micelle consisting of multiblock copolymers. In particular, we propose improvements upon traditional Flory-Huggins theory by considering coordination number correction, dielectric screening, and molecular volume normalization. We apply this technique to several test systems. Our results demonstrate that the newly developed procedure offers high precision and consistency in predicting the Flory-Huggins χ-parameter for miscibility analysis. In addition, we discuss the application of multicompartment micelle for nano-reactor. For this, 1) we characterize the transport of small molecules through the multicompartment micelle; 2) we introduce photo-responsive chemical structure to transform the structure of micelle. From this study, we conclude that a set of well-determined χ-parameters enables the molecular design of multiblock copolymer for variety of applications utilizing molecular self-assembly.

*We thank the U.S. Department of Energy, Office of Basic Energy Sciences, for funding this work through Catalysis Contract DE-FG02-03ER15459.
**3:42PM P34.00007: Direct Observation of Block Copolymer Micelle Fragmentation in Ionic Liquids**  
JULIA T EARLY (Presenter), University of Minnesota, KEVIN YAGER, Brookhaven National Laboratory, TIMOTHY LODGE, University of Minnesota — Recently, attention has been directed to quantifying the relaxation kinetics of block copolymer micelles, such as micelle fragmentation and fusion. Studies on block copolymer micelle fragmentation typically involve indirect techniques such as small angle scattering and *ex-situ* transmission electron microscopy. In this work, the direct observation of fragmentation in 1,2-polybutadiene-*block*-poly(ethylene oxide) (PB-PEO) micelles in the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide was achieved using high-temperature liquid-phase transmission electron microscopy. The kinetics of PB-PEO fragmentation were also studied for various molecular weights in one ionic liquid using time-resolved small-angle X-ray scattering and dynamic light scattering. By combining these experimental techniques, a detailed analysis of the effect of molecular weight on micelle fragmentation kinetics, along with the observation of intermediate structures during fragmentation events, was conducted. These experiments provide further insights into the equilibration kinetics of block copolymer micelles via fragmentation and the mechanism of fragmentation itself.

**3:54PM P34.00008: The Effects of the Size of Crystal Domains to the Polymorphism of Close-Packed Micelles**  
SANGWOO LEE (Presenter), LIWEN CHEN, Chemical and Biological Engineering, Rensselaer Polytechnic Institute, HAN SEUNG LEE, Characterization Facility, University of Minnesota, MIKHAIL ZHERNENKOV, National Synchrotron Light Source-II, Brookhaven National Laboratory — Polymorphism is technologically important, but its mechanistic origin is not well understood. We recently investigated the transitional structures of strongly-segregated block copolymer micelles in water in the liquid-to-solid and solid-to-solid transitions. In both transition processes, we found that the polytypes of close-packed block copolymer micelles are regulated by the size of crystal domains. In the liquid-to-solid phase transition, the crystallization of micelles proceeds by forming metastable hexagonal close-packed (HCP) structures that transform into stable face-centered cubic (FCC) structures via intermediate randomly stacked two-dimensional hexagonal close-packed (RHCP) structures. In the solid-to-solid transformation, the martensitic shear transformation of metastable FCC structures could be initiated by heating that reduces the size of metastable FCC crystal domains. These observations suggest that the polymorphism of crystalline solids is likely regulated by the size of crystal domains.
4:06PM P34.00009: Quasiperiodic Ordering of Minimally Hydrated Ionic Surfactant Micelles*  
ASHISH JAYARAMAN (Presenter), CARLOS BAEZ-COTTO, TYLER J MANN, MAHESH MAHANTHAPPA, University of Minnesota — Minimally hydrated surfactant micelles, by analogy to hard spheres, pack into high-symmetry body-centered cubic, face-centered cubic and hexagonally closest-packed structures. Recently, hydrated dianionic surfactant micelles were shown to self-assemble into low-symmetry Frank-Kasper (FK) σ and A15 morphologies. These FK phases are well-known periodic approximants of dodecagonal quasicrystals (DDQC), which possess 12-fold rotational symmetry yet lack translational symmetry. We report the formation of a well-ordered DDQC formed by oil-swollen aqueous dispersions of alkylphosphonate surfactants. Our studies show that the DDQC formation is strongly path dependent, and that different processing approaches to the same final composition instead yield periodic σ and A15 approximants. These findings coupled with the observations of irreversible thermal transformation of the DDQC into a σ phase suggest the metastability of these soft quasicrystals. This discovery illustrates avenues to tune the subtle free-energy balance prevalent among complex micellar phases and exemplifies the universality of quasiperiodic order in soft matter self-assembly.

*NSF CHE 1608115, CHE 1807330

4:18PM P34.00010: Processing Path-Dependent Complex Micelle Packings of Hydrated Diblock Polymer Amphiphiles [Invited] MAHESH MAHANTHAPPA (Presenter), University of Minnesota — Water drives the self-assembly of short diblock polymer amphiphiles into spatially periodic lyotropic liquid crystalline (LLC) mesophases, including lamellae, polycontinuous networks, hexagonally-packed cylinders (HEX), and 3D sphere packings. Beyond high symmetry body-centered cubic (BCC) and cubic close-packed micellar phases, diblock oligomers also form tetrahedrally closest-packed Frank-Kasper (FK) A15 phases. In spite of the low molecular weight of the constituent amphiphile, we recently demonstrated that judicious thermal processing of an A15 LLC enables formation of a surprisingly long-lived, non-equilibrium state. Specifically, heating an A15 phase drives transitions to BCC and HEX phases at elevated temperatures. Quenching these LLCs unexpectedly drives formation of a remarkably well-ordered, tetragonal FK sigma phase comprising 30 quasispherical micelles per unit cell as a metastable state, which takes ~150 days at 22 °C to revert to the original A15 structure. The formation and metastability of the sigma phase is contingent on sample quench rate, quench depth, and annealing temperature. These slow order-order phase transformation kinetics stem from a complex interplay of temperature-dependent phase nucleation and growth rates, which are coupled to the molecular-level rate of particle size reconfiguration and mesoscale rate of spatial rearrangement of the micelles. These findings highlight the importance of processing path-dependence on the observed mesophases of self-assembled soft materials.
Expanding spherical regions of block copolymers via designed chain architectures* YICHENG QIANG, WEI-HUA LI (Presenter), Macromolecular Science, Fudan Univ — Recently, the self-assembly of block copolymers into spherical phases has attracted renewed interest due to the discovery of Frank-Kasper spherical phases. Experiment and theory unravel that the formation of Frank-Kasper phases mainly results from the expansion of spherical region. However, it is generally believed that the spherical domains self-assembled from AB-type block copolymers are composed of the minority blocks. Breaking this generic rule so that the spherical domains are formed by the majority blocks requires new mechanisms to drastically expand the stable region of spherical packing phases. Herein, we propose a useful mechanism, and thus we design a series of dendron-like AB-type block copolymers. Our self-consistent field theory calculations predict that all these dendron-like copolymers exhibit a spherical region extending to $f > 0.5$. In particular, the maximal spherical region even approaches $f \sim 0.7$. Interestingly, such a phase diagram exhibits multiple reentrant transitions of Frank-Kasper phases.

*This work was supported by the National Natural Science Foundation of China (NSFC) (Grants No. 21774025)

Exotic Phase Behaviors of Purposely Designed Dendron-Like Block Copolymers* YICHENG QIANG (Presenter), WEI-HUA LI, Department of Macromolecular Science, State Key Laboratory of Molecular Engineering of Polymers, Fudan University — Within a series of purposely designed dendron-like AB-type block copolymers, self-consistent field theory (SCFT) calculations reveal that the regions of spherical phases can be extended to a volume fraction over 0.5, along with the vanishing of most traditional phases and the emergence of bicontinuous P phase as well as some exotic cylindrical phases. By changing the control parameter $\tau$ from 0 to $\infty$, these dendron-like copolymers can be reduced to dendritic block copolymers or miktoarm $AB_n$ block copolymers, respectively, which both exhibit similar phase behaviors to that of the simplest AB diblock copolymer. To demonstrate how spherical regions change non-monotonically as $\tau$, we construct a large set of phase diagrams for different $\tau$ values. We observe many exotic phase behaviors in these phase diagrams, especially about the change of the stability regions of different spherical phases including the classical BCC phase and complex Frank-Kasper phases.

*This work was supported by the National Natural Science Foundation of China (NSFC) (Grants No. 21774025)

Abstract Withdrawn

*This work was supported by the National Natural Science Foundation of China (NSFC) (Grants No. 21774026) and Ministry of Science and Technology of the People's Republic of China (No.2016YFA0203301)
2:30PM P35.00001: Modeling of complexation of oppositely charged polyelectrolytes in aqueous solutions*    MOHSEN GHASEMI (Presenter), Univ of Michigan - Ann Arbor, SEAN FRIEDOWITZ, JIAN QIN, Stanford University, RONALD LARSON, Univ of Michigan - Ann Arbor — The association of oppositely charged polyelectrolytes in aqueous solutions can lead to formation of polyelectrolyte complexes (PECs) whose properties are governed by many physiochemical parameters. PECs can be divided into overcharged complexes, where one type of polyelectrolyte charge is present in excess, and neutral ones, which contain equimolar ratios of polyanion and polycation. Using a theory, which captures the effects of chain connectivity and ion-specificity of charged species, here we rationalize why in non-stoichiometric mixtures, excess polyelectrolyte appears in the PEC and we pinpoint theoretical underpinnings of the overcharging phenomenon. Further, using the same theory, we investigate “doping” of stoichiometric PECs, in which salt concentration is increased, leading to the breaking of ion-pairs between oppositely charged groups of polyelectrolytes and their replacement with counterions. We find that the predictions of the level of counterion replacement during doping follow a similar trend to data from doping experiments. The development of such theories to could lead to methods of rational design of practical applications of PECs.

*We acknowledge the financial support from the National Science Foundation.

2:42PM P35.00002: ``Looping-back'' complexation in stoichiometrically asymmetric polyelectrolyte solutions    SEAN FRIEDOWITZ (Presenter), JUNZHE LOU, YAN XIA, JIAN QIN, Stanford Univ — The complexation of ionic polymers is typically studied in model systems lacking compositional heterogeneity that is often unavoidable in realistic systems. We address this by examining the coacervation behavior of synthetic, homologous polyions over a range of stoichiometric asymmetry between polyanions and polycations. An unexpected, narrow ``looping-back'' coexistence window is observed at low salt concentrations, and is captured by a theoretical model incorporating reversible ion-binding and chain connectivity, revealing the importance of the competition between charge neutrality and mixing entropy. Partitioning of both small ions and polyions between the supernatant and coacervate phases is measured, and theoretically analyzed.
The first report on a synthetic polyelectrolyte, polyacrylic acid, was published by W. Kern (1939). Ten years later, Fuoss and Sadek reported the first complex between two synthetic, oppositely-charged polyelectrolytes. At the time, it seemed evident that “strong electrostatic interactions would lead to mutual precipitation.” However, Michaels could not measure an enthalpy of complexation and concluded it was driven by entropy or the “escaping tendency of microions.” With more sensitive calorimetric measurements, complexation enthalpies were again ascribed to the coulombic forces assembling the component polyelectrolytes. In this talk I will show how polyelectrolyte coacervates, complexes and multilayers rely on the loss of counterions, an entropic driving force, to assemble. This overall driving force is moderated by an enthalpic contribution attributed to changes in the structure of water around counterion-compensated polyelectrolyte repeat units. The experimentally-determined relative ion concentrations within and external to a PEC are predicted by the Donnan equilibrium.

*This work was supported by the National Science Foundation, Division of Materials Research

Polyelectrolyte complexation opens new territory for polymer self-assembly. Micelles with complex cores are formed from neutral-charged block copolymers complexing with oppositely charged homopolymers and copolymers. The resulting objects bear a physical resemblance to micelles formed from solvophobic self-assembly of block copolymers. However, the details of formation, exchange, dissociation and scaling laws are all different. These characteristics will be discussed. The cores of these micelles can be used as depots and delivery vehicles for oppositely charged macromolecules. When these macromolecules are biologically active, such as proteins and nucleic acids, polyelectrolyte complex micelles can be used as therapeutic delivery vehicles. We have studied such micelles with nucleic acid-containing cores in detail with some unexpected results. At high concentrations of these micelles, when they begin to impinge on one another, they form as series of ordered phases with varying structures from bcc to hexagonal to lamellar. This set of structures and their associated properties will be discussed at length.

*The work has been supported by the Center for Hierarchical Materials Design funded by the National Institute of Standards and Technology of the US Department of Commerce.

Measurements on a common linear oppositely-charged polyelectrolyte complex, potassium-poly(styrene sulfonate) and poly(diallyl dimethyl ammonium bromide), shows liquid-liquid phase separation upon heating, or lower critical solution temperature behavior. The experimental accessibility of the binodal temperature occurs for a narrow range of monovalent salt concentration. We will report new results on the kinetics of phase separation studied by scattering techniques as a function of quench depth from the binodal. The growth rate of concentration fluctuations will be discussed and compared to available theories.
3:54PM P35.00006: Quantification of the lower critical solution temperature phase diagram of polyelectrolyte complex coacervates  YUANCHI MA (Presenter), SAMIM ALI, YIMIN MAO, DEBRA AUDUS, VIVEK PRABHU, National Institute of Standards and Technology, Gaithersburg, MD — Measurements on a common aqueous oppositely-charged polyelectrolyte complex, potassium-poly(styrene sulfonate) and poly(diallyl dimethyl ammonium bromide), shows liquid-liquid phase separation upon heating, or lower critical solution temperature behavior. The experimental accessibility of the apparent critical temperatures occurs for a narrow range of monovalent KBr salt concentration. We will show new static and dynamic light scattering and small-angle neutron scattering results and discuss how the correlation length, osmotic compressibility, and relaxation times change as the coexistence curve is approached by increasing temperature. The measurements of the binodal and spinodal curves from these associating polyelectrolyte solutions are compared to available mean field models.

4:06PM P35.00007: An Anomalous Small Angle X-ray Scattering Study of Counterion Distribution around Macroion*  JIAHUI CHEN (Presenter), Univ of Akron, MRINAL BERA, NSF’s ChemMatCARS Sector 15, The University of Chicago, TIANBO LIU, Univ of Akron — Counterion condensed around marcoion is important for solution behavior. While other techniques can hardly achieve, anomalous small angle X-ray scattering (ASAXS) can provide numbers and spatial distribution of counterions around macroion. (Mo_{132}), a negatevely charged sphere of ~3 nm diameter, was used as model of macroions to investigated by ASAXS. The result shows: 1. Extra Rb^{+} can neutralize most of negative charges and induce coagulation. 2. Extra Sr^{2+} can effectively screen the electrostatic interaction between macroions, while contrary to DLVO or Debye-Huckel theory, it only loosely associate with macroion and cannot induce coagulation. While the Coulomb force dominate the interactions between macroions and counterions in most cases, the energy penalty of break the hydration shell of divalent cation upon counterion-macroion association is important.

*The ASAXS were conducted at NSF’s ChemMatCARS, which is supported by the Divisions of Chemistry and Materials Research, National Science Foundation, under grant number NSF/CHE 1834750. Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.
The Complexation of oppositely charged polyelectrolytes through electrostatic interaction is ubiquitous in both natural and synthetic systems. One of the microscopic properties of interest in polyelectrolyte complexes (PEC) is the polymer chain conformation of a labeled chain. Recent literature studies on polycation/polyanion chain conformation in PECs using small-angle neutron scattering reported Gaussian chain statistics. Such scaling behavior is unlike polymer chains dissolved in good solvents, which show Gaussian statistics only at very high polymer concentrations (semidilute state). This behavior appears to be independent of chain length, salt concentration, and polymer concentration. We performed coarse-grained Langevin dynamics simulations of symmetric and flexible PECs and counterions, with and without salt added. As we gradually increase polymer concentration, the polymer chains transition from a globule-like state and level off to a Gaussian chain conformation. Qualitatively, similar behavior was also observed in the presence of salt. The polycations and polyanions have been observed to be highly overlapped in both cases. Such a qualitative agreement with experiments is observed because of the strong electrostatic driving force for complexation.

Constraint Release in Entangled Liquid Coacervates Made from Oppositely Charged Polyelectrolytes

Mixtures of oppositely charged polyelectrolytes can phase separate to form a polymer rich coacervate phase, important in many technological applications and biological systems. Many studies focus on formation of the coacervate, but less work has focused on predicting their dynamics. We developed a scaling theory predicting the dynamics of unentangled and entangled liquid coacervates, finding that the structure of asymmetric coacervates results in a dynamic coupling between the high and low charge density polymers. The high charge density polymer can either reptate along the tube formed by other high charge density chains or along the tube formed by low charge density chains. In the latter, topological constraints imposed by the low charge density chains onto the high charge density chains vary with time by reptation of low charge density chains through the process called constraint release. In this work, we develop a scaling model to predict the effects of constraint release on entangled asymmetric coacervates, finding that the dynamic coupling broadens regimes dominated by tube rearrangement as compared to symmetric coacervates. Furthermore, constraint release weakens the concentration dependence of viscosity in regimes dominated by reptation of the high charge density chains.
Solid-to-Liquid Phase Transition in Polyelectrolyte Complexes: Structural Evolution, Dynamics, and Phase Behavior

SIQI MENG (Presenter), JEFFREY M TING, HAO WU, MATTHEW TIRRELL, Pritzker School of Molecular Engineering, University of Chicago — The physical states of polyelectrolyte complexes (PECs), formed by mixing together solutions of oppositely charged polyelectrolytes, can span from glassy solids to low viscosity liquids. Transformation between these two states can be readily achieved by altering salt concentration and temperature, but our understanding towards this process is still incomplete. To fill this gap, we here study a model PEC system comprising two controllably synthesized styrenic polyelectrolytes. We first employed rheology to determine phase and evaluate mechanical properties of this PEC under different conditions. Surprisingly, we detected a counterintuitive trend that in the solid regime, these complexes became stiffer as temperature and salt concentration increased. Above certain threshold, viscoelastic liquid responses appeared. Next, we used small-angle X-ray scattering and cryogenic electron microscopy to unveil the structural evolution of this PEC. Additionally, thermogravimetric analysis was adopted to quantitatively probe water composition and phase behavior. Together, structures, dynamics and phase behavior demonstrated excellent agreement and dictated an integrated mechanism for the physical responses of this PEC system during solid-to-liquid phase transition.

Free Energy Profile of Complexation of two oppositely charged Polyelectrolytes

SOUMIK MITRA (Presenter), ARINDAM KUNDAGRAMI, IISER Kolkata — We report a study of the complexation process of two oppositely charged polyelectrolyte (PE) chains in dilute solution interacting through screened Coulomb potential within the DLVO framework. The two PE chains, as well as the neutral complex, are considered to be hypothetical spheres whose radii quantitatively denote the sizes of the respective chains, and the system is characterized by its free energy, calculated within the uniform spherical expansion approximation. Detailed comparative study of the effect of entropy gain of free counterions due to complexation and enthalpy change due to the reorganization of ion-pairs into two types—both of the monomer-counterion type and oppositely charged monomer-monomer type—is shown. We have looked into both salt-free and salty conditions and how it affects the complex formation process. Several factors drive the mutual adsorption of the two PEs to form a neutral coacervate. The full free energy profile of complexation, including the intermediate stages, is found to be monotonic at all conditions. A free energy landscape for the pathway of the complexation process may also be employed in studying the quantitative time scales in the kinetics of complex coacervation of two PEs.

*Ministry of Human Resource Development (Govt. of India)
5:06PM P35.00012: Scaling relation of Complex Coacervate Core Micelles  
TAEYOUNG HEO  
(Presenter), Hongik University, DEBRA AUDUS, National Institute of Standards and Technology,  
SOOHYUNG CHOI, Hongik University — Complex coacervation is a liquid-liquid phase separation  
when two oppositely charged polyelectrolytes are mixed in an aqueous solution. Because of the  
nature of electrostatic interaction, the coacervates are highly responsive to solution condition  
such as ionic strength. In this study, complex coacervate core micelles (C3Ms) are prepared by  
simple mixing of AB and A'B diblock copolyelectrolyte solutions in an aqueous solution where A  
and A' are oppositely charged blocks, and B is PEO block. Owing to the coacervate cores, C3Ms  
have been used for stimuli-responsive vehicles in the field of food, cosmetics and biomedical  
industry. For wider utilization of C3Ms, understanding the scaling relation is significant. We have  
developed the scaling relation for C3Ms such as core dimension as a function of charged block  
length and ionic strength, and compared to experimental data obtained by light, x-ray, and  
neutron scattering measurements. These results are discussed in terms of current understanding  
of complex coacervates including free energy and interfacial tension.

5:18PM P35.00013: Ionic-group-dependent phase behavior of polyelectrolyte coacervates  
SOJEONG KIM  
(Presenter), MINHWAN LEE, WON BO LEE, Seoul Natl Univ, SOOHYUNG CHOI, Hongik  
University — Complex coacervates are polymer-rich phases generated by liquid-liquid phase  
separation when oppositely charged polyelectrolytes are mixed in aqueous solutions. Since the  
previous Voorn-Overbeek model does not account for the chain connectivity and chemistry-  
specific details, advanced models have been suggested up to now. However, experimental data  
of well-defined model system is rare to compare with the theoretical description. In this study, 4  
polyelectrolytes are prepared (e.g., strong/weak and polyanion/polycation) from identical parent  
polymer using anionic polymerization, and thus 4 pairs of polyelectrolyte complex coacervates  
are investigated to map out the phase diagrams as a function of the pair of ionic group. It is  
found that the phase diagram shows distinctive features including salt resistance, the area of a  
two-phase region and the shape of binodal curves depending on the pairs of polyelectrolytes. In  
addition, atomistic MD simulations give molecular-level insight into the interaction of two  
charged moieties and especially show a clear difference in the ability to form hydrogen bonds.  
We believe chemistry specific parameters play an important role in control phase behavior and  
these findings shed new light on the biologically important topic of complex coacervation.

Wednesday, March 4, 2020 2:30 PM - 5:06 PM

Session P39 DCOMP DMP DCP: First-Principles Modeling of Excited-  
State Phenomena in Materials VIII: TDDFT and Nonadiabatic  
Dynamics  
703 - David Strubbe, University of California, Merced - Tag(s): Focus
2:30PM P39.00001: Heterogeneous proton-coupled electron transfer at nanoparticle and electrode interfaces [Invited] SHARON HAMMES-SCHIFFER (Presenter), Yale University — Interfacial proton-coupled electron transfer (PCET) reactions play a vital role in a wide range of energy conversion processes. A general theory of PCET that includes the quantum mechanical effects of the active electrons and transferring protons, as well as the motions of the proton donor-acceptor mode and solvent environment, has been developed. This formulation enables the calculation of rate constants and kinetic isotope effects for homogeneous as well as heterogeneous processes at nanoparticles and electrode surfaces. This theory has been applied to experimentally studied photoreduced ZnO nanocrystals reacting by PCET with the nitroxyl radical TEMPO. The calculations indicate that the electron transfers from the conduction band of the ZnO nanocrystal to TEMPO concertedly with proton transfer from a surface oxygen of the ZnO nanocrystal to the oxygen of TEMPO. Proton diffusion from inside the nanocrystal to reactive sites on the surface was found to explain the experimentally observed nonexponential kinetics. This PCET theory has also been applied to experimentally studied proton discharge from triethylammonium to a gold electrode in acetonitrile. These experiments demonstrated an isotope-dependent Tafel slope or, equivalently, a potential-dependent kinetic isotope effect. The calculations explain the potential-dependent kinetic isotope effect in terms of contributions from excited electron-proton vibronic states that depend on both isotope and applied potential. Proton discharge to a gold electrode in acidic and alkaline aqueous solution has also been studied. These applications highlight the importance of using a vibronically nonadiabatic theory that quantizes the transferring proton and includes the effects of hydrogen tunneling and excited electron-proton vibronic states. These studies are also assisting in the interpretation of experimental data and the design of more effective catalysts for energy conversion processes.

3:06PM P39.00002: Excitation Dynamics in Water under Proton Irradiation: Time-dependent Maximally-Localized Wannier Function Approach* CHRIS SHEPARD (Presenter), DILLON C YOST, YI YAO, YOSUKE KANAI, Univ of NC - Chapel Hill — Proton irradiation of liquid water has many important medical applications, including proton beam therapy. However, understanding the quantum dynamical details of the electronic excitations of water induced by the energetic protons has long been intangible. Using the approach of propagating maximally localized Wannier functions (MLWFs) in real-time TDDFT, we study the molecular-level dynamics of the electronic excitations\(^1\). These time-dependent MLWFs (TD-MLWFs) are localized in space, offering a convenient ‘chemical moiety’ picture of liquid water and allow for understanding of the electron dynamics in terms of bond centered and lone pair electrons of water molecules. The spatially-localized nature of the TD-MLWFs allows us to study the secondary electronic excitations from the electrons initially excited by the proton. The MLWF gauge also enables usage of the length-gauge to describe the homogeneous electric field to model photo-excitation, and analyze proton and photo- irradiation on equal footing.

\(^{1}\)J. Chem. Phys. 150, 194113 (2019)

*Work financially supported by NSF under Award No. CHE-1565714/OAC-1740204. Computer time provided by the INCITE program. This research used resources of the ALCF, a DOE Office of Science User Facility supported under Contract No. DE-AC02-06CH11357.
3:18PM P39.00003: Time-dependent exciton wave functions from TDDFT*  JARED R. WILLIAMS (Presenter), CARSTEN A. ULLRICH, Physics and Astronomy, Univ of Missouri - Columbia — Time-dependent density-functional theory (TDDFT) is a computationally efficient alternative to the Bethe-Salpeter equation for calculating optical spectra in insulators and semiconductors, including excitonic effects. We show how time-dependent exciton wave functions can be obtained from TDDFT via the time-dependent Kohn-Sham transition density matrix. The method is illustrated using one-dimensional model solids.

*This work was supported by NSF Grant No. DMR-1810922.

3:30PM P39.00004: Transient X-ray absorption spectra in solids from generalized Kohn-Sham real-time TDDFT.*  SRI CHAITANYA DAS PEMMARAJU (Presenter), SLAC - Natl Accelerator Lab — Simulating transient X-ray absorption spectra in solids with TDDFT requires at a minimum, a balanced treatment of both localized core and possibly delocalized valence excitations. To this end range-separated hybrid exchange-correlation functionals offer improved accuracy by mitigating self-interaction errors across multiple length-scales [1,2]. In this work the velocity-gauge formulation of real-time TDDFT is combined with multiply-range-separated hybrid functionals to simulate transient soft X-ray near-edge absorption spectra in solids where excitonic effects are important. Immediately following laser excitation by few femtosecond pump pulses, soft X-ray probe spectra are shown to exhibit characteristic features of population induced bleaching and transient energy shifts of exciton peaks. Simulation results are assessed for accuracy by comparison with experimental data on prototypical solid state systems.


*This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515.

3:42PM P39.00005: TD-DFT without wavefunctions  KAILI JIANG (Presenter), XUECHENG SHAO, MICHELE PAVANELLO, Rutgers University, Newark — We present an extension of Orbital-Free Density Functional Theory (OFDFT) to the time domain (TD-OFDFT). The method hinges upon approximating the wavefunction of the system by a single effective orbital augmented by a position-dependent phase factor. We find that such a simplified picture still delivers good optical spectra and response properties for metal clusters, surfaces and bulk systems. Specifically, we show that the method delivers plasmonic collective electronic excitations of metal clusters in reasonable agreement with Kohn-Sham TD-DFT. Because of the simplicity of the model, and the efficient codebase [1], the simulations are extremely computationally efficient delivering converged results in wall-times two or more orders of magnitude smaller than conventional Kohn-Sham TD-DFT.

3:54PM P39.00006: Pre-equilibrium stopping power mechanisms in proton-irradiated aluminum sheets* ALINA KONONOV (Presenter), ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Although ion-irradiation is a standard tool for imaging and altering materials' surfaces, most existing knowledge concerning an energetic ion's interaction with solids is limited to bulk materials. As an ion approaches and traverses a surface, it is expected to exchange charge with the material and transition into bulk conditions resembling a steady-state. To gain insight into this so-called pre-equilibrium behavior, we use real-time time-dependent density functional theory to simulate protons with 6 - 60 keV of kinetic energy impacting few-layer aluminum sheets. We find up to 25% stopping power enhancement in aluminum sheets compared to bulk, particularly near the entrance surface, and we examine several possible explanations for this behavior including pre-equilibrium projectile charge dynamics, polarization induced in the sheet during the proton's approach, and surface plasmon excitations. Our analysis suggests that surface plasmons are a plausible source of stopping power enhancement, while the contribution of the other potential mechanisms is either small or inconclusive. Such pre-equilibrium behavior has particularly important implications for optimizing focused ion beam techniques for 2D materials.

*NSF OAC 17-40219

4:06PM P39.00007: Quantitative electronic stopping power from localized basis set* IVAN MALIYOV (Presenter), XIXI QI, JEAN-PAUL CROCOMBETTE, FABIEN BRUNEVAL, Service de Recherches de Métallurgie Physique, CEA-Saclay — In charged particle irradiation, the electronic excitations are the prevailing phenomenon. The energy transfer from the projectile to the electrons of the target material is measured by the so-called electronic stopping power. Today, it can be obtained from time-dependent density functional theory [1]. Most implementations rely on a plane-wave approach, however, at the expense of very cumbersome calculations.

In this work, we show that localized orbitals, especially Gaussian-type orbitals, can be an practical alternative [2]. They can yield electronic stopping powers in quantitative agreement with the plane-wave results, while retaining the computational burden relatively low. These positive results are only possible with the use of Gaussian basis sets specially designed for the stopping power evaluation. With this tool, we investigate the discrepancy between TDDFT calculations and experiment at large velocity, the role of core excitations in the total stopping power. We rule out the wide-spread centroid path approximation as soon as some core excitations are involved.


*HPC resources from GENCI-TGCC and GENCI-CINES (project gen6018) are acknowledged.
4:18PM P39.00008: New Simulation Method for Temperature Dependent Magnetic Circular Dichroism with Non-Perturbative Treatment of Magnetic Field*  SHICHAO SUN (Presenter), XIAOSONG LI, University of Washington — Magnetic circular dichroism (MCD) is an important experimental tool for probing open shell molecules, but the simulation is challenging. First, simulating MCD involves multiple perturbations, such as magnetic field, spin-orbit coupling and circularly polarized light. Second, the ground state Zeeman splitting comparable with kT makes MCD temperature dependent. Scientists used to parameterize temperature dependence, and evaluate the perturbation by sum over states or excited state gradient method. However, such perturbations increase the computational cost and fail in strong magnetic field. We developed a non-perturbative treatment of magnetic fields and spin-orbit coupling in linear response non-collinear TDDFT formalism, which simplifies the perturbation. It is especially advantageous for strong magnetic field. In order to resolve the temperature dependence of MCD, excitations are weighted by temperature dependent occupation number. This method is applied in Mo(CN)$_8^{3-}$ and gives correct MCD-temperature dependence.

*The development of two-component electronic structure method is funded by the US Department of Energy (DE-SC0006863). The development of non-perturbative spectroscopic methods is supported by the National Science Foundation (CHE-1856210).

4:30PM P39.00009: Polarization dependence of optical excitations in anisotropic metal/insulator heterostructures*  MARKUS ERNST GRUNER, ROSSITZA PENTCHEVA (Presenter), Department of Physics, University of Duisburg-Essen — In the framework of real-time time-dependent density functional theory (RT-TDDFT) we unravel the layer-resolved dynamics of a Fe$_1$/(MgO)$_3$(001) multilayer after optical excitations. Short optical pulses with two polarization directions of light and a frequency smaller than the band gap of bulk MgO induce strong anisotropic dynamic response: Substantial transient changes to the electronic structure, which persist after the duration of the pulse, are only observed for in-plane polarized electric fields. We find the largest effect in the Fe-layer, but time-dependent changes in the occupation numbers are visible in all layers, promoted by the presence of interface states. The time evolution of the layer-resolved occupation numbers indicates transfer from in-plane to out-of-plane orbitals that support the propagation of optically induced excitations into the interface region. We also see a small net charge transfer away from oxygen towards the Mg sites even for MgO layers, which are not directly in contact with the metallic Fe.


*German Science Foundation, CRC1242, project C02.
4:42PM P39.00010: Dissociation Path Competition of Radiolysis-Ionization induced Molecule Damage under Electron Beam Illumination  ZENGHUA CAI, SHIYOU CHEN (Presenter), East China Normal University, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The radiolysis ionization under electron beam illumination induces dissociation and damage of organic and biological molecules, which causes the inability of transmission electron microscopy (TEM) in imaging the related materials. We developed a procedure based on the real-time time-dependent density functional theory (rt-TDDFT) for simulating the radiolysis damage processes of molecules, which can describe the ionization cross sections of electronic states and the fast dissociation processes caused by the hot carrier cooling and the Auger decay on deep levels. For the radiolysis damage of C$_2$H$_6$O$_2$, our simulation showed unexpectedly that there is strong competition among three different dissociation paths, including the fast dissociation caused by the hot carrier nonadiabatic cooling; the fast dissociation caused by Auger decay induced double ionization and Coulomb explosion; the slow dissociation caused by the increased kinetic energy. As the energy of incident electron beam changes, the time scales of these dissociation paths and their prudency in causing the molecule damage change significantly. These results explained the measured mass spectra of the C$_2$H$_6$O$_2$ dissociation fragments, and revealed the dissociation paths in the TEM imaging of organic and biological materials.

4:54PM P39.00011: Generalized nanoquanta exchange-correlation kernel and nonhydrogenic Rydberg series of excitonic binding energies in monolayer WS$_2$  VOLODYMYR TURKOWSKI (Presenter), JOSE MARIO GALICIA-HERNANDEZ, Department of Physics, University of Central Florida, Orlando, FL 32816, GREGORIO HERNANDEZ-COCOLETZI, Instituto de Fisica Ing. Luis Rivera Terrazas, Benemerita Universidad Autonoma de Puebla, Puebla 72550, Mexico, TALAT S. RAHMAN, Department of Physics, University of Central Florida, Orlando, FL 32816 — We have formulated a methodology to derive a generalized nanoquanta (nanoquanta+) TDDFT exchange-correlation (XC) kernel that is capable of describing excitonic properties of extended systems. Compared to the standard nanoquanta XC kernel, the generalized one takes into account screening effects more accurately through the usage of exact (beyond one-loop) electron susceptibility in the formalism. As we demonstrate for the example of monolayer WS$_2$, such an improved XC kernel allows one to reproduce accurately the experimentally-observed nonhydrogenic Rydberg series in the excitonic spectrum, [1] which has so far not been possible with other familiar kernels. We also calculate the effective electron-hole potential that enters the TDDFT eigen-energy equation of excitons, and demonstrate that the reason for the nonhydrogen Rydberg energy series is a non-Coulomb structure of the potential. We discuss the general properties of the nanoquanta+ kernel and compare them to that of other XC kernels employed for extracting properties of excitons.


*Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354

Wednesday, March 4, 2020 2:30 PM - 5:18 PM
2:30PM P40.00001: Matter in Extreme Environments: Novel Chemistry under Pressure

MAOSHENG MIAO (Presenter), Chemistry and Biochemistry, California State University, Northridge — Thanks to the developments of high-pressure techniques and quantum mechanics based crystal structure prediction methods, numerous novel compounds with atypical compositions have been obtained or predicted in the past decade. Differing from conventional solid materials, many of these new compounds consist of various homonuclear chemical species such as dimers, trimers, pentagonal and heptagonal rings, polymer chains, atomic layers, and three-dimensional networks, unexpectedly telling a story of rich chemistry under pressure. More strikingly, pressure can alter the chemical characteristics of elements by activating the core electrons, the unoccupied orbitals and the quantum orbitals at the interstitial sites, leading to many new surprising phenomena. In this talk, I will outline the novel compounds and the new chemical phenomena within one conceptual framework based on the change of quantum states of electrons under high pressure. In contrast to the conventional view and chemical intuition, the quantum mechanics features of electrons such as directional bonds, inhomogeneous distribution, lower symmetry etc. are actually magnified by the increasing pressure, giving rise to rich moieties and variations in novel inorganic compounds. One striking example is that the core electrons can be activated to form bonds, violating a primary principle of chemistry. Other examples include electrons detaching from all atoms to play the role of anions at the interstitial sites (electrides), noble gases behaving as anions because their outer-shell $d$ orbitals gain electrons, and noble gases reacting with ionic compounds without forming any chemical bonds. The influence of this new picture on future studies that is destined to higher pressures, more complex compositions and applicable materials is discussed.

*We acknowledge the support of NSF CAREER award 1848141 and ACF PRF 50249-UN16. Calculations were performed on XSEDE resources (TG-DMR130005) especially on the clusters run by TACC.
Theoretical phase diagram of boron carbide $B_xC$ from ambient to high pressure ($P$) and high temperature ($T$): the “single phase” regime in the light of the density functional theory (DFT) results*

antoine jay, Laboratoire d'analyse et d'architecture des systèmes, CNRS, Toulouse, olivier hardouin duparc, jeleña sjakste, cnrs, laboratoire des solides irradiés, nathalie vast (Presenter), cea-saclay, laboratoire des solides irradiés — the phase diagram of boron carbide is calculated within the DFT as a function of $T$ and $P$ up to 80 GPa, accounting for icosahedral, graphite- and diamond-like atomic structures [1]. Only some icosahedral phases turn out to be thermodynamically stable with atomic carbon concentrations ($c$) of resp. 8.7% ($B_{10.5}C$), 13.0% ($B_{6.7}C$), 20% ($B_{4}C$) and 28.6% ($B_{2.5}C$). Their respective ranges of stability under pressure and temperature are calculated, and the theoretical $T$-$P$-$c$ phase diagram boundaries are discussed. At ambient conditions, the introduction in the phase diagram of the new phase $B_{10.5}C$, with an ordered crystalline motif of 414 atoms, is shown to bring the theoretical solubility range of carbon in boron close to the experimental one. The introduction of configurational entropy heavily changes the convex hull at finite temperature. We discuss the occurrence of the “single phase regime” in the light of these new results.

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Novel tunable band gap BC8/ST12 Si$_x$Ge$_{x-1}$ alloys: insights from first-principles calculations*

johnes wagner (Presenter), helmholtz-centre potsdam (gfz), maribel nunez valdez, goethe university frankfurt am main & helmholtz-centre potsdam (gfz) — the cubic $Ia\-3$ (BC8) and tetragonal $P4_{3}2_{1}2$ (ST12) modifications of Si and Ge are promising candidates for applications in optoelectronic, thermoelectric or plasmonic devices. However the indirect and narrow band gaps are a limiting factor of the pure phases. Si-Ge alloys in these modifications could overcome this drawback and enable tailoring for specific use-cases. To that end, high pressure BC/ST12 Si$_x$Ge$_{x-1}$ solid solutions for $0 \leq x \leq 1$ have been synthesized and reported to be stable at ambient conditions[1]. Here we employ ab initio calculations to further investigate the electronic properties of these alloys as a function of $x$. We show how atomic site occupancy affects the band gap and which atomic arrangements stabilize intermediate compositions. We find that the ST12 phase is energetically favorable up to $x$=0.75 and that the indirect band gap of the ST12 Ge end-member can be tuned to become direct for $0.05 \leq x \leq 0.2$. Furthermore, we obtain the effective band structure of intermediate random alloys by calculating special quasi random structures (SQS) for selected compositions.


*Funded by the Helmholtz Association and the John von Neumann Institute for Computing (NIC), Project ID AblInitioModMatsGeo
3:30PM P40.00004: First-Principles Simulation of Strain Effects on Lanthanum Monopnictides
CHIA-MIN LIN (Presenter), WEI-CHIH CHEN, CHENG-CHIEN CHEN, Department of Physics, Univ of Alabama - Birmingham — Rare-earth monopnictides have attracted significant attention due to their exotic electronic and topological properties with potential thermoelectric and spintronic applications. Here, we theoretically investigate strain effects on lanthanum monopnictides LaX (X = N, P, As, Sb, and Bi) by first-principles simulations using hybrid density functionals with spin-orbit coupling. In particular, the phonon properties, electronic bandstructures, and topological natures of these materials under compressive and tensile strains are computed. It is shown that strain engineering is an effective approach to manipulating the properties of LaX for improved performance and device applications.

3:42PM P40.00005: A First-Principles Exploration of Na$_x$S$_y$ Binary Phases at 1 atm and Under Pressure
NISHA GENG (Presenter), TIANGE BI, NILOOFAR ZARIFI, Chemistry, University at Buffalo, YAN YAN, School of Science, Changchun University, EVA ZUREK, Chemistry, University at Buffalo — Interest in Na-S compounds stems from their use in battery materials at 1 atm, as well as the potential for superconductivity under pressure. Evolutionary structure searches coupled with Density Functional Theory calculations were employed to predict stable and low-lying metastable phases of sodium poor and sodium rich sulfides at 1 atm and within 100–200 GPa. At ambient pressures, four new stable or metastable phases with unbranched sulfur motifs were predicted: Na$_2$S$_3$ with C2/c and Imm2 symmetry, C2 -Na$_2$S$_5$ and C2 -Na$_2$S$_8$. Van der Waals interactions were shown to affect the energy ordering of various polymorphs. At high pressure, several novel phases that contained a wide variety of zero-, one-, and two-dimensional sulfur motifs were predicted, and their electronic structures and bonding were analyzed. At 200 GPa, P4/mmm -Na$_2$S$_8$ was predicted to become superconducting below 15.5 K, which is close to results previously obtained for the β-Po phase of elemental sulfur. The structures of the most stable M$_3$S and M$_4$S, M = Na, phases differed from those previously reported for compounds with M = H, Li, K.
Tuning Magnetic and Electronic Properties in Exotic Silver(II) Fluorides Using Pressure

WOJCIECH GROCHALA (Presenter), ADAM GRZELAK, JAKUB GAWRACZYNSKI, Center of New Technologies, University of Warsaw, DOMINIK KURZYDLOWSKI, Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszynski Univ., ZORAN MAZEJ, Dept. of Inorg. Chem. and Techn., Jozef Stefan Institute, VITALI PRAKAPENKA, Center for Advanced Radiation Sources, University of Chicago, MARIANA DERZSI, Center of New Technologies, University of Warsaw, VIKTOR STRUZHUKIN, Geophysical Laboratory, Carnegie Institution for Science, PAOLO BARONE, SPIN, CNR, JOSE LORENZANA, Dept. of Physics, ISC-CNR and Univ. of Rome — Silver(II) fluorides exhibit unique structural, electronic and magnetic features which render them similar to parent compounds of high-TC oxocuprate superconductors. These encompass the reduced structural and magnetic dimensionality, the persistence of the Jahn-Teller effect, substantial covalence of chemical bonding between metal and nonmetal (d-p hybridization), potent magnetic superexchange via nonmetal atom, insulating charge-transfer character within the Zaanen-Sawatzky-Allen classification, small energy band gap at the Fermi level, comparable Debye frequencies, etc. Here I will discuss the behaviour of some of these materials (including doped systems) at elevated pressure conditions as obtained from combined experimental and theoretical studies. Influence of high pressure on bonding, as well as electronic and magnetic properties, will be discussed. Possibility to achieve metallization and superconductivity will also be addressed.

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Slovenian Research Agency (ARRS) (P1-0045 Inorganic Chemistry and Technology)
ICM UW supercomputers (ADVANCE++, GA76-19)
GeoSoilEnviroCARS (The University of Chicago, Sector 13) is supported by the National Science Foundation - Earth Sciences (EAR-1128799) and the Department of Energy - GeoSciences (DE-FG02-94ER14466). This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Portions of this work were performed at the HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory. HPCAT operation is supported by the DOE-NNSA under Award No. DE-NA0001974, with partial instrumentation funding by the NSF.
Italian MAECI under collaborative Projects SUPERTOP-
**4:30PM P40.00007: The change of basic chemical behavior of elements under high pressure**

*YUANHUI SUN (Presenter), MAOSHENG MIAO, California State University, Northridge —

The chemistry at ambient condition has implicit boundaries rooted in the atomic shell structure: The inner-shell electrons and the unoccupied outer-shell orbitals do not involve as major component in chemical reactions and in chemical bonds. The chemical properties of atoms are determined by the electrons in the outermost shell; hence, these electrons are called valence electrons. These general rules govern our understanding of chemical structures and reactions. Using first principles calculations, we demonstrate that under high pressure, the above doctrines can be broken. Our previous studies showed that both the inner shell electrons and the outer shell empty orbitals of Cs and other elements can involve in chemical reactions. The formation of CsF\(_n\) (\(n > 1\)) compounds demonstrates that Cs atom can behave like a \(p\)-block element under high pressure.[1] Besides, we found that Hg in Hg-F compounds transfers charge from the \(d\) orbitals to F atoms, thus behaving as a transition metal.[2] We have extended the above study and found that the involvement of core electrons in forming chemical bonds is a common phenomena while the external pressure is high enough.


*NSF CAREER award 1848141 and ACF PRF 50249-UN16.

**4:42PM P40.00008: Ultrahigh-pressure induced decomposition of silicon disulfide into high coordination number silicon-sulfur compounds**

*YUANZHENG CHEN (Presenter), School of Physical Science and Technology, Southwest Jiaotong University, Chengdu 610031, China., XIAOLEI FENG, SIMON A. T. REDERN, Department of Earth Sciences, University of Cambridge, Cambridge, CB2 3EQ, UK, HANYU LIU, College of Physics, Jilin University, Changchun 130012, China — SiS\(_2\) is thought to occur in inter-stellar dust and is of interest more generally among the silicon chalcogenides as a comparator to SiO\(_2\), an important component of terrestrial planets. However, the high-pressure behaviors of silicon sulfides are unclear. Here, using an efficient structure search method, we systematic explore the structural evolution of different Si-S stoichiometries up to 250 GPa. We find that SiS\(_2\) is only stable below 155 GPa, which then decomposes into two previously-unreported compounds, SiS and SiS\(_3\), at higher pressures. SiS adopts a high symmetry \(Pm\)-3\(m\) structure consisting of 8-fold coordinated silicon in face-sharing SiS\(_8\) polyhedra, while SiS\(_3\) crystallizes in \(R3m\) structure containing 9-fold coordinated SiS\(_9\) polyhedra. Analysis suggests the new Si 8-fold coordination environment could be a common feature for group IV-VI compounds under high pressure. Our findings provide key insights on the nature of the Si-S compounds under ultrahigh pressure.

*We acknowledge funding from the National Natural Science Foundation of China (No. 11604270, 11704050), and the Fundamental Research Funds for the Central Universities (2682017CX052; 2018GF08).
4:54PM P40.00009: A novel all-nitrogen molecular crystal as promising high-energy density material LEI ZHAO (Presenter), California State University, Northridge, SHIJIE LIU, School of Physics and Engineering, Henan University of Science and Technology, YUANZHENG CHEN, School of Physical Science and Technology, Southwest Jiaotong University, WENCAI YI, Department of Physics, Qufu Normal University, FENGLONG GU, School of Chemistry and Environment, South China Normal University, YONGHAO ZHENG, School of Optoelectronic Science and Engineering, University of Electronic Science and Technology of China, BINGBING LIU, State Key Laboratory of Superhard Materials, Jilin University, MAOSHENG MIAO, California State University, Northridge — In the decades-long search for energy-dense materials capable of greater energy output, many studies have focused on nitrogen rich compounds, which have the advantages of relative stability at ambient conditions, high-energy output when broken down, and a clean gas product (N₂) that is inert, non-toxic, and a non-contributor to the greenhouse effect. The most stable form of nitrogen under ambient condition is N₂ molecular crystal, because of its exceedingly stable triple bond in nature. Besides N₂, there is not any report of other all nitrogen molecular crystals either at ambient condition or under high pressure, except a recently reported N₈ crystal. Here, using ab initio calculations combined with an intelligence structure-searching, we report the discovery of a thermodynamically stable nitrogen molecular crystal, which has perfect packing and more energetic stability at lower pressure range, compared with the N₈ crystal. While decompose at ambient pressure, this all nitrogen molecular crystal can release great amount of energy (~2.90 kJ/g).

5:06PM P40.00010: Structure and Stability of Oxyfluorides and Oxychlorides and Their Relations to Catalytic Activities in Oil Refining Reactions DALAR KHODAGHOLIAN (Presenter), California State University, Northridge — Metal oxides have long been used as catalysts or supporters of catalysts in petroleum refining processes. Mixing anions such as fluorine into the structures of these compounds can greatly enhance their structural stability. Therefore, metal oxyfluorides are potential candidates for such catalysts due to their stability, atomic and electronic properties. The stability of several compositions of these compounds has been investigated, combining different anions or replacing them partially or fully. Since synthesizing mixed anion compounds is challenging, automatic crystal structure search together with density functional theory, particle swarm optimization algorithm and geometry relaxation calculations have been performed to obtain information regarding the stability and properties of these compounds. Plotting convex hull has revealed that FeOF, Fe₂OF₄, and AlOF have low formation energies, therefore can be used in synthesizing the catalyst materials. Based on structures obtained, electronic properties of these structures have been studied. Also, the effects of pressure on these compounds have been explored. Under pressures such as 10 GPa, fluorine rich compound Fe₂OF₄ and AlOF become highly destabilized, leaving FeOF more likely to be a candidate compound under higher pressures.
P40.00011: Physical property modulation in 2D TMDs homo- and hetero-structures via pressure engineering  

JUAN XIA (Presenter), University of Electronic Science and Technology of China — 2D TMDs and their van der Waals heterostructures (vdWs HSs), exhibit attractive optical and optoelectronic properties thanks to the different band alignments and interlayer interactions. Their sensitivity to interlayer distance allows effective tuning of material properties through external modulation of lattice parameters. Therefore, it is of both fundamental and practical importance to explore interlayer excitons in vdWs HSs, especially their dynamic response and underlying mechanisms to different tuning techniques. So far, only limited changes in lattice parameters have been achieved, hampering effective tuning of physical properties in vdWs HSs. In this talk, we demonstrate effective tuning of the excitonic states by controlling the interlayer distance in TMDs vdWs HSs, and further tune the interlayer spacing and thus the band structure using hydrostatic pressure. In addition, we perform DFT calculations and achieve good agreement with the experimental observations, revealing a pressured-induced changeover in the band structure of the HSs. This may offer new insights into the strong interlayer interaction and electron-phonon coupling in TMDs via pressure engineering, which can be exploited for designing new excitonic devices based on 2D vdWs HSs.

Wednesday, March 4, 2020 2:30 PM - 5:18 PM

Session P41 GMAG DMP FIAP DCOMP: Spins in Non-magnetic Semiconductors 707 - Raphael Daveau, Cornell University

2:30PM P41.00001: Band structure probe of near Surface InAs Quantum Wells*  

BRENDEN A MAGILL (Presenter), GITI KHODAPARAST, Virginia Tech, SUNIL K THAPA, CHRISTOPHER J STANTON, Univ. of Florida, JOSEPH YUAN, MEHDI HATEFIPOUR, WILLIAM MAYER, MATTHIEU DARTIALH, KASRA SARDASHTI, KAUSHINI S WICKRAMASINGHE, JAVAD SHABANI, New York University, Y. H. MATSUDA, ZHUO YANG, YOSHIMITSU KOHAMA, Univ. of Tokyo — Near surface InAs quantum wells (QW) have recently attracted a great deal of interest as tools to explore mesoscopic and topological superconductivity. These shallow QWs can interact strongly with superconducting layers which can be epitaxially grown on their surfaces. In this talk, we present a combined experimental and theoretical approach to study the band structure of these QWs. The effective mass and g-factors in these QWs were determined using high field cyclotron resonance (CR). Unlike GaAs, narrow gap systems like InAs have large nonparabolicity in their band structures. The band parameters extracted from our CR experiments are consistent with those obtained from Shubnikov de Hass measurements and agree remarkably well with the theoretical calculations. Our band structure models include strong mixing of the conduction and valence bands which leads to a large non-parabolicity. The calculations accurately describe the experimental observations and allowing us to accurately map the effective mass and g-factor as a function of magnetic field, Landau level index, and the well width for different near surface InAs QWs.

*Supported by the AFOSR FA9550-17-1-0341 and partially by NSF EAGER DMR-1836687 and the NSF- MRSEC DMR-1420073.
2:42PM P41.00002: Weak-antilocalization Induced by Spin-orbit Interaction in Two-dimensional Tellurium* CHANG NIU, ZHUOCHENG ZHANG (Presenter), GANG QIU, YIXIU WANG, WENZHUO WU, PEIDE (PETER) YE, Purdue Univ — Tellurium (Te) is an intrinsic p-type semiconductor with a narrow bandgap of 0.35eV, whose hexagonal crystal structure is formed by van der Waals interaction between each helical atom chains. Through controllable atomic layer deposition (ALD) grow dielectric doping, we can access transport properties of Te conduction band. Here we report experimental results regarding weak-antilocalization (WAL) effect in n-type two-dimensional (2D) Te films at cryogenic temperatures. The gate and temperature dependence on WAL shows D'yakonov-Perel (DP) mechanism plays the main role in spin relaxation and electron-electron (e-e) interaction is dominant for phase relaxation, which matches well with Iordanskii, Lyanda-Geller, and Pikus (ILP) theory. Also, phase coherence length of Te extracted from WAL feature reaches 573nm at T=1K and transition from weak-localization (WL) to weak-antiocalization (WAL) is observed by tuning the gate bias, indicating its potential for future tunable spintronic applications.

*This work was supported by NSF/AFOSR 2DARE Program, ARO, and SRC.
The synthesis of 2D Te materials is supported by the National Science Foundation under Grant CMMI-1762698.

2:54PM P41.00003: Magneto-optical properties of n-type InAsP films in ultrahigh magnetic fields* SUNIL K THAPA (Presenter), CHRISTOPHER J STANTON, University of Florida, BRENDEN A MAGILL, RATHSARA R HERATH MUDIYANSELAGE, GITI KHODAPARAST, Virginia Tech, Y. H. MATSUDA, ZHUO YANG, YOSHIMITSU KOHAMA, University of Tokyo, SUKGEUN CHOI, CHRIS J PALMSTROM, Univ. of California, Santa Barbara — InAsP ternary alloys have immense prospect for optoelectronic and quantum communication devices due to their variable band gap of 0.35-1.35 eV and tunability in the g-factors. We present a theoretical/experimental study of the magneto-optical properties of n-type InAs\(_x\)P\(_{1-x}\) films (x=0.07,0.34) in ultrahigh magnetic fields in the Faraday's geometry at T=300 K using k.p method with modified 8-band Pidgeon-Brown model. The calculated Landau-level Fan diagram for x=0.34 suggests a near-zero g-factor. Moreover, the Field-dependent Fermi levels and the absorption coefficients show a very strong corroboration with the Cyclotron Resonance (CR) measurements, both in position and the strength. In this study, we also employed ultrafast Time Resolved Differential Reflectivity (TRDR) and ultrafast time resolved Magneto-optic Kerr Effect (MOKE) to provide information on the carrier and spin relaxation dynamics.

*This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0341, and DURIP funding (FA9550-16-1-0358).
3:06PM P41.00004: Ultralong spin coherence in MAPbI$_3$ single crystals revealed by ultrafast optics  
YUE YAO (Presenter), MATTHEW SHEFFIELD, HESHAN HEWA WALPITAGE, ISAAC P BROWN HEFT, University of Utah, YE LIU, ZHENYI NI, JINSONG HUANG, University of North Carolina at Chapel Hill, YAN LI, University of Utah — Hybrid organic-inorganic perovskites (HOIPs) have demonstrated remarkable optoelectronic properties with their unprecedented rate of increase in solar cell efficiency, and their applications have been quickly extended to many areas, including light emitting diodes, lasing, and photo detection. Recent studies have also revealed their great potential in spintronics because of spin-dependent optical transitions, long spin lifetimes, and predicted large spin-orbit coupling effects for potential spin manipulation. Our previous study revealed long spin lifetimes ($T_{2^*}$) exceeding 1 ns at 4 K on MAPbI$_3$ polycrystalline films despite the presence of large spin-orbit coupling. Here, in order to exclude the influence of the polycrystalline structure and obtain intrinsic spin dynamics, we investigate spin dynamics on high quality MAPbI$_3$ single crystals by time-resolved Faraday rotation (TRFR). The spin lifetime improved by an order of magnitude when compared to polycrystalline films, which suggests the long spin lifetime is an intrinsic property of MAPbI$_3$. Combining the TRFR measurements with circularly-polarized photoluminescence, we analyze the interplay between carrier dynamics and spin dynamics upon optical excitation of spin-polarized carriers in this HOIP.

3:18PM P41.00005: Probing the cubic crystal anisotropy and spin-orbit interaction in GaAs heterostructures using hole quantum point contacts  
KARINA HUDSON (Presenter), ASHWIN SRINIVASAN, Univ of New South Wales, DMITRY MISEREV, Department of Physics, University of Basel, QINGWEN WANG, OLEH KLOCHAN, Univ of New South Wales, IAN FARRER, Department of Electronic and Electrical Engineering, University of Sheffield, DAVID A RITCHIE, Cavendish Laboratory, University of Cambridge, ALEX HAMILTON, Univ of New South Wales — Understanding the form of the spin-orbit interaction (SOI) in semiconductors such as GaAs is a prerequisite for engineering of topological superconducting and insulating states in these materials. Zeeman spin-splitting transport measurements in p-type 1D quantum point contacts (QPCs) are an effective probe of the SOI. Previous measurements have shown that there is a strong anisotropy in the in-plane g-factors in hole QPCs due to SOI ($g_{||} > g_{\perp}$), which can be explained as arising from a second $k^2B$ Zeeman term in addition to the established $k^4B$ Zeeman term$^1$. Here we present the first study of the effect of cubic crystal anistropies on the anisotropy of the g-factor. By rotating the QPC with respect to the crystal axes, we change the effect of the cubic crystal terms. We find the anisotropy of the g-factor is strongly dependent on QPC orientation, and present a theoretical framework describing the SOI terms arising from cubic crystal anisotropy. We identify four additional Zeeman terms that describe the dependence of the anisotropy of the in-plane g-factors with respect to QPC orientation. Our model shows that SOI is highly dependent on crystal asymmetries with implications for topological systems such as artificial graphene.

3:30PM P41.00006: Origin of Rashba-Dresselhaus effect in a Pb-free ferroelectric nitride perovskite. SUBHADEEP BANDYOPADHYAY (Presenter), INDRA DASGUPTA, School of Physical Science, Indian Association for the Cultivation of Science — First principles electronic structure calculations have been employed to investigate the Rashba-Dresselhaus spin splitting of the bands in a Pb-free non-toxic ferroelectric nitride perovskite. Our first principles results are supplemented with effective k.p model analysis. A systematic study of orthorhombic and rhombohedral phases of this system reveal the importance of symmetry in realizing the nature of the splitting of bands around the time reversal invariant k-points. In the orthorhombic structure it shows linear Rashba-Dresselhaus splitting where nonsymmorphic symmetries play an important role in enhancing the band splitting in the \( k_z = \pi/c \) plane. While the rhombohedral phase shows existence of unique higher order Rashba-Dresselhaus term which mixes with the linear Rashba-Dresselhaus term to produce unusual pattern of out-of-plane spin component in the spin texture that may find application in spintronics.

3:42PM P41.00007: Efficient spin to charge conversion at strained amorphous-Si thin film interfaces RAVINDRA G BHARDWAJ, ANAND KATAIHA, PAUL C LOU, SANDEEP KUMAR (Presenter), University of California, Riverside — Interfacial asymmetry in conjunction with strain engineering can provide an alternate pathway to achieve efficient and controllable spin to charge conversion. This hypothesis is experimentally verified using spin-Seebeck effect measurement in case of B-doped amorphous-Si thin film interface. The spin-Seebeck voltage and spin-Hall angle in amorphous-Si is found to be an order of magnitude larger than the corresponding value for Pt thin film spin detector. Further, the spin-Seebeck effect is greatly enhanced in the multilayer heterostructures and it diminishes when the strain effects in the sample are reduced. The inhomogeneous strain induces strong interfacial Rashba-Dresselhaus spin-orbit coupling in the two-dimensional electron gas at the metal-Si interface. The resulting intrinsic inverse spin-Hall effect is the underlying cause of efficient spin to charge conversion, which is of the same order as the topological surface states. This study gives a new direction of research for spin-caloritronics applications using strain engineering and amorphous materials.
3:54PM P41.00008: Dephasing in quasi-1D wires: Non-Markovian noise and correlations due to itinerant spin interactions*

MATTHEW FOSTER (Presenter), SETH M DAVIS, Rice Univ —

Motivated by the interest in many-body localization, we revisit the problem of dephasing due to electron-electron scattering in quasi-1D (many channel) wires. The effectively Markovian bath due to Coulomb interactions dephases at any nonzero temperature [1]. The effect of short-ranged (e.g. spin exchange) electron-electron scattering is more subtle. The latter induces a non-Markovian, diffusive noise kernel. Formally the field theory describing the dephasing in the presence of a purely diffusive bath has an upper critical spatial dimension of \( d = 4 \), and is strongly coupled in \( d = 1 \) [2]. We show that a perturbative expansion in the diffusive noise kernel is well-defined but unphysical at long times. We also consider the case of both Coulomb and spin-exchange scattering, using the former to physically regularize the latter. In this case we find "rephasing" contributions at second order that are in contrast to the Markovian limit [3]. We discuss possible experimental signatures.


*NSF CAREER Grant No. DMR-1552327
Welch Foundation, Grant No. C-1809

4:06PM P41.00009: Radial spin texture in elemental tellurium with chiral crystal structure*

MASATO SAKANO, Univ of Tokyo, MOTOAKI HIRAYAMA, RIKEN, TAKANARI TAKAHASHI, Tokyo Institute of Technology, SHUNTARO AKEBI, MITSUHIRO NAKAYAMA, KENTA KURODA, Univ of Tokyo, KAZUAKI TAGUCHI, TOMOKI YOSHIKAWA, KOJI MIYAMOTO, TAICHI OKUDA, Hiroshima University, KANTA ONO, High Energy Accelerator Research Organization, HIROSHI KUMIGASHIRA, Tohoku University, TOSHIYA IDEUE, YOSHIHIRO IWASA, MITSUISHI NATSUKE (Presenter), KYOKO ISHIZAKA, SHIK SHIN, Univ of Tokyo, TAKASHI MIYAKE, AIST, SHUICHI MURAKAMI, TAKAO SASAGAWA, Tokyo Institute of Technology, TAKASHI KONDÔ, Univ of Tokyo — Trigonal tellurium has a chiral crystal structure which is characterized by a lack of mirror symmetry and an inversion center, resulting in the inequivalent right- and left-handed structures. To reveal the spin textures of chiral crystals, here we investigate the spin and electronic structure in \( p \)-type semiconductor elemental tellurium by using spin- and angle-resolved photoemission spectroscopy. Our data demonstrate that the highest valence band crossing the Fermi level has a spin component parallel to the momentum of electron around the Brillouin zone corners. Significantly, we have also confirmed that the spin polarization is reversed in the crystal with the opposite chirality. The results indicate that the spin textures of the right- and left-handed chiral crystals are hedgehog-like, leading to unconventional magnetoelectric effects and nonreciprocal phenomena.

*This research was partly supported by CREST projects (Grant No. JPMJCR16F2, No. JP-MJCR14F1) from Japan Science and Technology Agency (JST) and JSPS KAKENHI (Grants-in-Aid for Scientific Research) (Grant No. JP18H03678, JP19H00651).
4:18PM P41.00010: Prediction of momentum dependent spin splitting in antiferromagnetic compounds without spin-orbit coupling*  LINDING YUAN (Presenter), ZHI WANG, University of Colorado, Boulder, JUN-WEI LUO, Chinese Academic of Science, ALEX ZUNGER, University of Colorado, Boulder — The Conventional way of creating spin splitting entails the involvement of spin orbit coupling (SOC). The latter entails heavy elements that lead to weak bonds and undesirable defects. Can one generate spin splitting without relying on SOC? We identify the magnetic symmetry conditions that produce AFM prototypes having spin splitting even at TRIM points without external magnetic field and even when SOC is set to zero. The resulting spin splitting in AFM arises from the coupling between electron spin and the position coordinates which is k dependent and of the same order as the Thomas term. Band structures of specific compounds are worked out within DFT showing the effects.

*Funded by DOE-BES- MSE to CU Boulder

4:30PM P41.00011: Response of Bloch Electrons to Electric Fields  WILLIAM KERR (Presenter), Wake Forest Univ — We consider the response of spinful Bloch electrons to external electric fields; the electrons’ unperturbed Hamiltonian is the one given by Dresselhaus [1], including the spin-orbit interaction. We write matrices for the system observables with respect to the Bloch basis states of the unperturbed Hamiltonian, truncate them to two bands, and use them to obtain their Heisenberg equations of motion. The equation for the velocity contains not only the anomalous velocity term obtained by Karplus and Luttinger [2] [expressed in terms of the now-familiar (position operator) Berry connection [3]], but also additional terms involving “quasi-connections” from the momentum and spin operators. We apply the equations of motion resulting from this procedure to a two-dimensional model of a ferromagnet with the Dresselhaus linear-in-wavevector spin-orbit interaction and an exchange field term. We find for this model that the anomalous velocity is dominated by the term coming from the spin operator rather than the position operator.

Introducing spin-polarized carriers in semiconductor lasers reveals an alternative path to realize room-temperature spintronic applications, beyond the usual magnetoresistive effects[1]. Through carrier recombination, the angular momentum of the spin-polarized carriers is transferred to photons, thus leading to the circularly polarized emitted light. Surprisingly, a large birefringence[2], considered detrimental in both conventional and spin-lasers, has been demonstrated to lead to ultrafast operation with an order of magnitude faster modulation frequency [3] than in the best commercial lasers. By using transparent rate equations we explain how the birefringence can provide key differences in the modulation frequency of the intensity and polarization of light emitted from a laser. We reveal that for such ultrafast operation it is important to have a short spin relaxation time in the active region of the semiconductor lasers, typically made of quantum wells.


*NSF ECCS-1810266, US ONR 000141712793.
Colloidal Nanoplatelet is a two-dimensional semiconductor nanocrystal heterostructure that allows for wavefunction engineering by controlling their composition and or thickness. With the inclusion of a shell doped with magnetic ions around a non-magnetic core, there exists a carrier mediated exchange interaction between the excitonic spin density and the Mn spins. Through the exchange interaction, magnetic effects such as Zeeman splitting and the excitonic photoluminescence circular polarization can be controlled by varying the shell thickness and or Mn content [1,2]. The previous works did not take into account on how the exitonic wavefunction is affected by the addition of the magnetically doped shell. Here, we present a model that includes the carrier mediated exchange interaction and study its effect on the excitonic wavefunction. [1] S. Delikanl et al., ACS. Nano 2015 9, 12, 12473-12479 [2] F. Muckel et al., Nano Lett. 2018, 18, 2047–2053.
Correlated States and Frustration in Magnetic Quantum Dots with Multiple Occupancy*  

TIAGO CAMPOS (Presenter), State Univ of NY - Buffalo, JAMES PIENTKA, St Bonaventure Univ, ALEX MATOS ABIAGUE, Wayne State Univ, JONG E HAN, IGOR ZUTIC, State Univ of NY - Buffalo — Magnetically doped semiconductor quantum dots (QDs) provide an enhanced control of magnetic ordering as compared to their bulk-like counterparts [1]. Unlike in the bulk structures, adding a single carrier in a magnetic QD can have important ramifications. An extra carrier can both strongly change the total carrier spin and the temperature of the onset of magnetization. Recent experiments reveal how multiple carrier occupancy is optically controlled in Mn-doped II-VI QDs [2] and motivate studies of strongly-correlated states in these systems. While Wigner molecules, as the nanoscale manifestation of correlation effects in Wigner crystals, have been extensively studied in nonmagnetic QDs, their generalizations in magnetic QDs are largely unexplored [3]. Using exact diagonalization and conditional probability density we reveal peculiar manifestations of strongly-correlated states in Mn-doped QDs. The spatial control of Mn-dopants provides a platform to examine the role of magnetic frustration and the shell-structure formation with the change in the strength of Coulomb interaction.


*US DOE, BES DE-SC0004890.

Theory of Excitonic Phases in an Electron-Hole Double-Layer System with Relativistic Spin-Orbit Interaction  

YEYANG ZHANG (Presenter), KE CHEN, RYUICHI SHINDOU, Peking Univ — We propose helicoidal and helical excitonic insulator phases in a Coulomb-coupled two-dimensional electron-hole double layer (EHDL) system with relativistic spin-orbit interaction. Previously, it was proposed that layered InAs/AlSb/GaInSb heterostructure is an ideal experimental platform for searching excitonic dense phases, while its electron layer has non-negligible Rashba interaction. We clarify that due to the Rashba term, the spin-triplet (spin-1) and spin-singlet (spin-0) excitonic fields in the EHDL system forms either helicoidal or helical structure, depending on its coupling with an in-plane Zeeman field. We provide a comprehensive understanding of electric and magnetic properties of these condensed phases as well as their low-energy collective modes.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P42 GMAG DMP: Complex Oxide Interfaces & Heterostructures - Skyrmions and Novel Magnetism  

709/711 - Sanghoon Kim
2:30PM P42.00001: Topological Hall Effect in SrTiO$_3$/SrIrO$_3$/SrRuO$_3$ Superlattices*  JOSE FLORES (Presenter), ADAM S AHMED, BINBIN WANG, NURIA BAGUES SALGUERO, DAVID W. MCCOMB, FENGYUAN YANG, Ohio State Univ - Columbus — Ferromagnet(FM)/heavy-metal(HM) bilayers films have been found to able to host topological magnetic structures like skyrmions stabilized by exchange and interfacial Dzyaloshinskii-Moriya interactions. Electrical measurement by the topological Hall effect (THE) has been a primary method of detection of these features. Perovskites multilayers are an excellent platform for investigating these systems due to the wide range of electrical and magnetic properties and very low lattice mismatch allowing for the growth of high-quality films. Here we investigated the topological hall effect in STO(001)/SrRuO$_3$/SrIrO$_3$/SrTiO$_3$ superlattices where SrTiO$_3$ acts as a spacer layer that seperates the FM/HM layers SrRuO$_3$/SrIrO$_3$. As the spacer thickness was increased, the magnitude of the topological Hall resistivity decreased suggesting interlayer coupling. Superlattices with thinner spacer layers show a transition between two topological hall peaks corresponding to before and after the magnetization has switched and an intermediate temperature where both signal are observed. This behavior appears to be unique to the superlattices and is not seen in bilayer structures.

*Funding for this research was provided by the Center for Emergent Materials: an NSF MRSEC under award number DMR-1420451

2:42PM P42.00002: Tunable real- and momentum-space topological properties in SrRuO$_3$ ultrathin films  LINGFEI WANG (Presenter), TAE WON NOH, Department of physics and astronomy, Seoul National University — In perovskite-structured SrRuO$_3$ (SRO), a fine balance between the electron-electron correlation and spin-orbit coupling gives rise to a variety of exotic topological properties. Here, we will show our recent results about tunable real-and momentum-space topological properties in SRO ultrathin films. First, we report the discovery of ferroelectrically tunable skyrmions in ultrathin BaTiO$_3$/SRO bilayer heterostructures. The ferroelectric proximity effect at the BaTiO$_3$/SRO heterointerface can trigger a sizable Dzyaloshinskii-Moriya interaction, thus stabilizing a real-space topological spin texture: magnetic skyrmion. By locally manipulating the ferroelectric polarization, we can achieve local, switchable, and nonvolatile control of both skyrmion density and thermodynamic stability. Second, we will focus on the highly tunable anomalous Hall effect (AHE) in SRO single layers. We found the AHE exhibit a clear sign reversal as the SRO film thickness decreases to 4 unit-cells due to the changes in momentum-space Berry curvatures. By harnessing the step-flow growth, we can induce an artificial thickness inhomogeneity and a two-channel AHE in SRO films. We developed several experimental methods for distinguishing the skyrmion-induced topological Hall effect from the two-channel AHE.
2:54PM P42.00003: Investigating the Skyrmion Phase Diagram in Polycrystalline Chemically Substituted Cu\(_2\)OSeO\(_3\) with Small Angle Neutron Scattering*  PAUL NEVES (Presenter), Department of Physics, University of Maryland, College Park, DUSTIN GILBERT, National Institute of Standards and Technology Center for Neutron Research, SHENG RAN, I-LIN LIU, SHANTA SAHA, JOHN COLLINI, Department of Physics, University of Maryland, College Park, MARKUS BLEUEL, National Institute of Standards and Technology Center for Neutron Research, JOHNPIERRE PAGLIONE, Department of Physics, University of Maryland, College Park, JULIE ANN BORCHERS, NICHOLAS BUTCH, National Institute of Standards and Technology Center for Neutron Research — The chiral helimagnet Cu\(_2\)OSeO\(_3\) is now understood to host a variety of interesting magnetic phases. The stability of these phases is sensitive to many parameters, including magnetic field and temperature history, magnetic field direction, and chemical tuning. Here, we discuss results studying the magnetic phase diagram of chemically substituted polycrystalline (Cu\(_{1-x}\)M\(_x\))\(_2\)OSeO\(_3\), M = (Ag, Zn), and Cu\(_2\)(O\(_{1-x}\)S\(_x\))\(_2\)SeO\(_2\) with bulk magnetization and small angle neutron scattering (SANS). Notably, we perform SANS measurements after rotation of our powdered samples in a magnetic-field to resolve 6-fold symmetric skyrmion lattice diffraction patterns. This allows us to gleam information about the skyrmion lattice order and magnetocrystalline anisotropy. Bulk magnetization suggests an enhancement of skyrmion temperature stability in the Ag and S substituted samples, while SANS suggests a generic decrease in the ability of field rotation to align skyrmion lattices in chemically disordered systems. Additionally, we are unable to confirm the presence of a second skyrmion phase in Zn substituted samples.

*DMR-1508249

3:06PM P42.00004: Theoretical investigations of Topological Hall Effect at Manganite/Iridate Oxide Interfaces*  NARAYAN MOHANTA (Presenter), Oak Ridge National Lab, ELBIO DAGOTTO, Department of Physics and Astronomy, University of Tennessee at Knoxville, SATOSHI OKAMOTO, Oak Ridge National Lab — We study topological Hall effect at the interface between La\(_{1-x}\)Sr\(_x\)MnO\(_3\) and SrIrO\(_3\). We show that the ferromagnetism at the manganite layer, in conjunction with the Dzyaloshinskii-Moriya (DM) interaction which arises at the interface due to broken inversion symmetry and strong spin-orbit coupling from the iridate layer produces a skyrmion crystal (SkX) phase in the presence of an external magnetic field. Using the Monte Carlo technique and a two-orbital spin-fermion model for manganites, we obtain phase diagrams which reveal, at low temperatures, a clear SkX phase and also a low-field spin-spiral phase. Increasing temperature, a skyrmion-gas phase, precursor of the SkX phase upon cooling, was identified. The topological Hall effect primarily appears in the SkX phase. We also show that a planar topological Hall effect can robustly appear at oxide interfaces from conical spin spirals at oxide interfaces, without skyrmions, when the magnetic field is applied parallel to the interface plane.


*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division.
3:18PM P42.00005: Investigation of Domain Walls in Single Crystal Cr$_2$O$_3$ Using Nitrogen Vacancy Scanning Magnetometry  NATASCHA HEDRICH (Presenter), KAI WAGNER, BRENDA SHIELDS, Department of Physics, University of Basel, Klingelbergstrasse 82, Basel 2056, Switzerland, TOBIAS KOSUB, DENYS MAKAROV, Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328, Dresden, Germany, PATRICK MALETINSKY, Department of Physics, University of Basel, Klingelbergstrasse 82, Basel 2056, Switzerland — Magnetolectric antiferromagnets are promising candidates for spintronic devices that have been used to demonstrate electrical reading and writing [1]. Chromia, in particular, has drawn attention due to its room temperature ordering. While domain structures in thin-film Cr$_2$O$_3$ have been studied in detail [2], domains in single crystals prove more elusive and less well understood. Second harmonic generation and magnetic force microscopy have been used to study these structures, but these techniques have provided primarily qualitative images [3,4]. Here, we present a quantitative study of domain walls in single crystal chromia using nitrogen vacancy (NV) magnetometry, performed with all-diamond scanning probes, where we make use of the sub 1 uT/$\sqrt{\text{Hz}}$ sensitivity and sub 50 nm spatial resolution of these structures to investigate the domain wall properties at the nanoscale. Our measurements demonstrate the unique possibility offered by NV magnetometry to study single crystalline antiferromagnetic systems and reveal fundamental properties of the crystal and its spin textures.

References

3:30PM P42.00006: Spin Dynamics in the Antiferromagnetic Oxy- and Fluoro- Pnictides: LaMnAsO, LaMnSbO, and BaMnAsF*  FARHAN ISLAM (Presenter), PINAKI DAS, YONG LIU, ELIJAH GORDON, LIQIN KE, Ames Laboratory, Iowa State University, DOUGLAS L ABERNATHY, Oak Ridge National Laboratory, ROBERT MCQUEENEY, DAVID VAKNIN, Ames Laboratory, Iowa State University — Inelastic neutron scattering (INS) from polycrystalline LaMnAsO, LaMnSbO, and BaMnAsF are analyzed using $J_1$-$J_2$-$J_c$ Heisenberg model in the framework of the linear spin-wave theory. All three systems show clear evidence that $J_1$ and $J_2$ are both antiferromagnetic (AFM) with a ratio of $2J_2/J_1 < 1$. Thus, the competing interactions do not lead to the stripe structure, preserving the square lattice checkerboard AFM structure. The inter-plane coupling $J_c$ in all three systems is on the order of $\approx 3\times10^{-4}J_1$, rendering the magnetic properties of these systems quasi-two-dimensional. The substitution of Sb for As significantly lowers the in-plane exchange coupling, which is also reflected in the Néel temperature $T_N$. Although BaMnAsF shares similar MnAs sheets as LaMnAsO, their $J_1$-$J_2$ values are substantially different. Using density functional theory, we calculate exchange parameters $J_{ij}$ to rationalize the differences between these systems.

*This work is supported by U.S. Department of Energy, Office of Basic Energy Sciences, Contract No.~DE-AC02-07CH11358
3:42PM P42.00007: Magnetic structure and spin dynamics of a buckled-honeycomb antiferromagnet Co4Ta2O9

SUNGYUN CHOI (Presenter), VALERY KIRYUKHIN, Department of Physics and Astronomy, Rutgers University, New Brunswick, MATTHIAS J GUTMANN, DAVID J VONESHEN, ISIS Neutron and Muon Source, SHANGKE PAN, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University, New Brunswick — Controlling magnetism by the electric field is one of the most important topics in correlated materials, which could be realized via magnetoelectric (ME) coupling. The discovery of ME in Cr2O3 [1] initiates intense research on related ME materials for practical applications. However, there are not many real materials that show strong ME coupling due to rather strict symmetrical conditions: the absence of the inversion and time-reversal symmetry.

The interest was renewed when the Co4Nb2O9 study found a large ME coupling with an antiferromagnetic ordering [2]. Keeping this interest, we present a combined measurement of magnetic susceptibility, neutron diffraction and inelastic neutron scattering on Co4Ta2O9 [3]. We determined a magnetic order by single-crystal neutron diffraction and also performed inelastic neutron scattering to prove spin dynamics. We will discuss the implication of our results on the magnetic structure and spin excitations in the context of the magnetoelectricity of this material.


3:54PM P42.00008: Direct visualization of domain dynamics in Ni$_2$MnTeO$_6$ antiferromagnet using X-ray Bragg diffraction Phase contrast Imaging.*

MIN GYU KIM (Presenter), SUNGYUN CHOI, Rutgers University, Piscataway, HU MIAO, Brookhaven National Lab., CHOONGJAE WON, Pohang University of Science and Technology, JUNJIE YANG, New Jersey Institute of Technology, WEN HU, CLAUDIO MAZZOLI, Brookhaven National Lab., SANG-WOOK CHEONG, Rutgers University, Piscataway, ANDI BARBOUR, STUART B WILKINS, IAN KEITH ROBINSON, MARK DEAN, Brookhaven National Lab., VALERY KIRYUKHIN, Rutgers University, Piscataway — Magnetic phase transitions provide one of the important testbeds in condensed matter physics. Development of the magnetic domains lies at the heart of any such transitions. Generally, antiferromagnetic (AFM) domains can evolve with temperature, through the phase transition from the paramagnetic phase to the ordered state, or between states with different AFM orders. However, the study of such dynamics of AFM domain was impossible due to the lack of temporal resolution in the existing techniques. Using recently developed X-ray Bragg diffraction Phase contrast Imaging (XBPI) technique that can visualize AFM domains and domain walls in real-time and real-space, we present the growth and merging of the AFM domains in real-time as a function of temperature in Ni$_2$MnTeO$_6$ where two AFM states with different Q vectors exist.

*Work at the Rutgers University was supported by the U.S. Department of Energy (DOE) under Grant No. DOE: DEFG02-07ER46382.
4:06PM P42.00009: Random Telegraph Noise in Ferromagnetic Garnets∗ ROBERT SPONSEL (Presenter), E. DAN DAHLBERG, University of Minnesota — Magnetic noise in ten garnet samples is reported. The magnetic noise, fluctuations in the transmitted light intensity using the Faraday effect to observe the magnetization, was measured when the samples were driven by an applied AC magnetic field. The data were taken as a function of the area sampled, the magnitude of the AC magnetic field, and the AC frequency (40-250 Hz). In zero applied magnetic field, the magnetization of the samples consisted of either stripe or serpentine domains. The measured noise is white at fields somewhat below and somewhat above the coercive field for all length scales. Intermediate fields, close to the coercive field of a sample, exhibit a Lorentzian power spectral density (PSD) as would be expected for random telegraph noise (RTN). This PSD was seen at all length scales. Surprisingly, the Lorentzian noise exhibits the same characteristic frequency at all positions measured in a given sample. With increasing area the magnitude of the Lorentzian noise decreases following a 1/area relation consistent with the Lorentzian noise arising from many uncorrelated RTN oscillators. The results will be discussed in terms of random pinning of domains to create complex domain structures.

∗This work was supported by NSF grant DMR 1609782.

4:18PM P42.00010: Magnetic structure and electronic properties in Layered BaMn$_2$Sb$_2$ and Ba$_2$Mn$_3$Sb$_2$O$_2$∗ QIANG ZHANG (Presenter), Louisiana State University, Baton Rouge, LA 70803 USA and Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*, ZHENYU DIAO, Louisiana State University, Baton Rouge, LA 70803 USA, HUIBO CAO, Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, AHMAD IKHWAN US SALEHEEN, RAMAKANTA CHAPAI, DONGLIANG GONG, SHANE STADLER, RONGYING JIN, Louisiana State University, Baton Rouge, LA 70803 USA — We present the structural, electronic, and magnetic properties of BaMn$_2$Sb$_2$ and Ba$_2$Mn$_3$Sb$_2$O$_2$ single crystals, both with the layered structure analogous to high-temperature Fe- and/or Cu-based superconductors. While the Mn moment in the MnSb$_4$ tetrahedral environment forms a long-range G-type antiferromagnetic (AFM) ordering in both BaMn$_2$Sb$_2$ ($T_{N1}$ ≈443 K) and Ba$_2$Mn$_3$Sb$_2$O$_2$ ($T_{N1}$ ≈314 K), a short-range AFM order is found in the intercalated MnO$_2$ layer at a much lower temperature ($T_{N2}$ ≈60 K) coexisting with long-range G-type order in MnSb$_4$ layer in Ba$_2$Mn$_3$Sb$_2$O$_2$. The directions of the ordered moments in these two magnetic sub-lattices of Ba$_2$Mn$_3$Sb$_2$O$_2$ are perpendicular to each other. The G-type AFM order in MnSb$_4$ layers in both compounds is distinct from the stripe-like order in Fe-based superconductors, but the in-plane magnetic structure in MnO$_2$ layers of Ba$_2$Mn$_3$Sb$_2$O$_2$ is found to be similar to that in the Cuprates. Our study reveals the significant and distinct roles of the CuO$_2$- and FeAs$_4$-type transition metal layers in the structure, novel magnetic and electronic properties.

∗This work was primarily supported by the U.S. Department of Energy under EPSCoR Grant No. DE-SC0012432. A portion of this research used resources at the High Flux Isotope Reactor, a DOE Office of Science User Facility.
**4:30PM P42.00011: Calculated magnetic exchange interactions in the Dirac magnon material Cu3TeO6**  
DI WANG (Presenter), XIANGYAN BO, FENG TANG, XIANGANG WAN, Nanjing Univ — Recently, topological aspects of magnon band structure have attracted much interest, and especially, the Dirac magnons in Cu3TeO6 have been observed experimentally. In this work, we calculate the magnetic exchange interactions J's using the first-principles linear-response approach and find that these J's are short range and negligible for the Cu-Cu atomic pair longer than 7 Å. Moreover, there are only five sizable magnetic exchange interactions, and according to their signs and strengths, modest magnetic frustration is expected. Based on the obtained magnetic exchange couplings, we successfully reproduce the experimental spin-wave dispersions. The calculated neutron scattering cross section also agrees very well with the experiments. We also calculate Dzyaloshinskii-Moriya interactions (DMIs) and estimate the canting angle of the magnetic noncollinearity based on the competition between DMIs and J’s, which is consistent with the experiment. The small canting angle agrees with that current experiments cannot distinguish the DMI-induced nodal line from a Dirac point in the spin-wave spectrum. Finally, we analytically prove that the “sum rule” conjectured in W. Yao et al. [Nat. Phys. 14, 1011 (2018)] holds but only up to the 11th-nearest neighbor.

**4:42PM P42.00012: Elucidation of spin reorientation and short-range ferromagnetic correlations in double perovskite Ho2FeCoO6**  
THOMAS HEITMANN (Presenter), MU Research Reactor, Univ of Missouri - Columbia, MO 65211 USA, HARIPRIYA G R, K. SETHUPATHI, V. SANKARANARAYANAN, Low Temperature Physics Laboratory, Department of Physics, Indian Institute of Technology, Madras, Chennai-600036, India, R. PRADHEESH, the Racah Institute of Physics, the Hebrew University of Jerusalem, Jerusalem, 91904 Israel, HARIKRISHNAN S NAIR, Department of Physics, University of Texas at El Paso, El Paso, TX 79968 USA — We report on energy resolved neutron diffraction and inelastic neutron scattering studies of double perovskite Ho2FeCoO6. The B-site moments have been shown previously to order antiferromagnetically near 250 K with a spin reorientation transition at 45 K. We use energy resolved neutron diffraction of a Ho2FeCoO6 powder to establish the order parameter of these two phases and to characterize a diffuse scattering signal observed surrounding q ≈ 1.3 Å⁻¹. The diffuse part is determined to result from short-range ferromagnetic correlations of the Ho-moments. The development of Ho correlations coincides in temperature with the spin reorientation transition so it is likely that exchange between sublattices is becoming important in this temperature range. We have also explored this system via inelastic scattering and report on a crystalline electric field that is detected at E = 9.8 meV. Both the diffuse and inelastic signals were found to be absent in non-A-site magnetic La2FeCoO6 confirming the origin of these effects as the Ho sublattice.
4:54PM P42.00013: Precursor effects to the Verwey transition of Fe₃O₄: a MaxEnt-μSR study.* CARLOS MORANTE (Presenter), CAROLUS BOEKEMA, San Jose State University — The magnetic fields of Fe₃O₄ have been previously studied using muon-spin rotation (μSR). [1,2] The Verwey transition at Tᵥ (~123 K) and a transition at T₃ (~247 K) are observed. Using Maximum Entropy (MaxEnt, ME) the single-crystal Fe₃O₄ μSR data are analyzed with improved precision. [3] Extra signals are found, indicating 2 signals at room temperature (RT) and 2 at 205 K. [4] These frequencies are found at B_{ext} // <110> and B_{ext} smaller than the demagnetization B. At RT, the upper signal follows the trend seen in the Tᵥ-T₃ region. At 205 K, the lower signal follows the extension above T₃. Short-range ordering could be interpreted as precursor effects to the Tᵥ transition. [1,2] This short-range ordering relates to the “extra” 3d-electron (3d*) behavior. We re-examine the T dependence of fields with B (720 Oe) // <110>. Our Fe₃O₄ MEμSR study of the 3d* spin-phonon interaction could lead to a better understanding of the magnetism of this Mott-Wigner glass. [1] C Boekema et al, Hpf Interactions 31 (1986) 487; 17-19 (1984) 305. [2] C. Boekema et al, Phys Rev B33 (1986) 2102; Phys Rev B31 (1985) 1233. [3] C Boekema and MC Browne, MaxEnt 2008, AIP Conf Proc #1073 (2008) 260. [4] C Morante and C Boekema, MMM19 Las Vegas (2019) submitted.

*Research supported by DOE-LANL, AFC & SJSU.

5:06PM P42.00014: Spin waves above and below the Verwey transition in TbBaFe₂O₅*

DANIEL PAJEROWSKI (Presenter), Oak Ridge National Lab, DANIEL K. PRATT, National Institute of Standards and Technology, STEVEN E HAHN, WEI TIAN, GARRETT E GRANROTH, ALEXANDER KOLESNIKOV, Oak Ridge National Lab, ALEXEY A TASKIN, YOICHI ANDO, Osaka University, ROBERT MCQUEENEY, Iowa State University — TbBaFe₂O₅+δ (TBFO) is a mixed valence compound with antiferromagnetic order (T_N = 450 K) that changes along with the crystal structure and conductivity upon cooling below a Verwey-like transition (Tᵥ = 280 K). This type of double-cell-layered-perovskite is useful to study putative charge ordering in fractional valence systems because the crystal structure develops unique sites for the different valence states. While the static magnetic structure of TBFO is known, in this study we investigate the magnetic interactions. Single crystal inelastic neutron scattering experiments at T = 4 K < Tᵥ and T = 320 K > Tᵥ show spin-waves that are modeled with linear spin wave theory to extract magnetic anisotropy and superexchange parameters. Below Tᵥ there is a sizable magnon gap due to an easy-axis magnetic anisotropy that closes above Tᵥ resulting from the evolution to easy-plane anisotropy. The magnetic interactions are found to be highly three-dimensional and change across Tᵥ. Above Tᵥ, where the conductivity is greater, a damping term is required to model the spin waves.

*Research conducted at ORNL’s Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U. S. Department of Energy.
Localized electron spins can couple magnetically via the Ruderman-Kittel-Kasuya-Yosida interaction even if their wave functions lack direct overlap. Theory predicts that spin-orbit scattering leads to a Dzyaloshinskii-Moriya type enhancement of this indirect exchange interaction, giving rise to chiral exchange terms. Here we present a spin-polarized scanning tunneling microscopy study of transition metal oxide chains on the (001) surfaces of Ir and Pt. Our STM results confirm that deposition of Co, Fe, Mn, and Cr on the (2×1) oxygen-reconstructed Ir(001) surface leads to the formation of quasi-one-dimensional chains with a (3×1) unit cell. In contrast, preparation on Pt(001) required deposition onto the cold substrate with subsequent annealing in an oxygen atmosphere. In particular, for MnO$_2$ chains we found highly complex spin structures. Whereas we find an almost antiferromagnetic Mn–Mn coupling along the chains, the inter-chain coupling across the non-magnetic substrates turns out to be chiral. We will show that some of the magnetic structures observed for MnO$_2$ can be viewed as highly anisotropic Skyrmions.
2:30PM P43.00001: Inverse Design of Soft Materials: Crystals, Quasi Crystals, Liquid Crystals*  [Invited] MARJOLEIN DIJKSTRA (Presenter), Debye Institute for Nanomaterials Science, Utrecht University — In 1960, Feynman challenged us to think “from the bottom up” and to create new functional materials by directing and manipulating the arrangements of individual atoms ourselves. With recent advances in the synthesis of colloidal nanoparticles and the bottom-up fabrication of nanostructured materials using colloidal self-assembly, we are tantalizingly close to realizing this dream. In this talk, I will show using theory and simulations how one can structure matter over multiple length scales using hierarchical self-assembly. The prediction and design of these structures remains an important challenge for nanomaterials science. I will present a method to predict which structures are stable assuming the shape and interactions between the constituent particles are known, and I will show that particle shape alone can already give rise to a wide variety of structures such as (plastic) crystals [1,2], quasi crystals [3], and liquid crystals [4,5], which can be classified using machine learning techniques. Subsequently, I will show how one can reverse-engineer the particle shape to stabilize highly exotic liquid crystal phases.


*NWO Netherlands Organisation for Scientific Research

3:06PM P43.00002: Hard Particle Colloidal Clathrates with Rotating Guest  SANGMIN LEE (Presenter), SHARON C GLOTZER, Chemical Engineering, University of Michigan — Clathrate crystal consisting of polyhedral cages is usually found in gas hydrate or intermetallic systems where the size of particles forming the structures is mostly atomic or molecular length scale. In this work, we report a design strategy of hard colloidal particles that self-assemble into various colloidal clathrate crystals with single or multiple rotating guests. Monte Carlo simulations show that a single component system of hard truncated triangular bipyramids (TBPs) self-assembles into five different clathrates with rotating guests depending on the truncation of the TBP. Truncation of the TBP creates a cavity at the center of the clathrate cage-like motifs, and the cavity is occupied by guest particles when the size of the cavity reaches a comparable size of the guest. Thermodynamic stability of the clathrates is confirmed by Frenkel-Ladd free energy calculations. The dynamics of the guests can be categorized as free rotation, rotation around a fixed axis, or quantized rotation and rattling, with the mode determined by guest/cavity size ratio, prolateness of the cavity and shape of the guest. In addition, when the TBPs are mixed with other hard shapes, clathrates encapsulate these different guest particles.
3:18PM P43.00003: Symmetry-based discovery of multicomponent, two-dimensional colloidal crystals  NATHAN MAHYNSKI (Presenter), National Institute of Standards and Technology, EVAN PRETTI, Lehigh University, VINCENT SHEN, National Institute of Standards and Technology, JEETAIN MITTAL, Lehigh University — We present a systematic method for computing the ground state phase behavior of multicomponent colloidal materials. In two-dimensions there are exactly 17 “wallpaper groups” which represent distinct combinations of isometries of the Euclidean plane. Using properties of these groups, we develop an algorithm to cover the plane with a fixed number of arbitrary components in all ways that satisfy a desired stoichiometric ratio. These combined symmetry-stoichiometry rules dramatically reduce the number of possible configurations, which generally suffer from a so-called “combinatorial explosion” otherwise making extensive, random structure searching computationally infeasible. With subsequent continuum relaxation, this enumeration approach can predict crystal structures in silico for multicomponent colloidal mixtures. We use this approach to investigate the ground state phase behavior of multicomponent systems inspired by DNA-coated colloidal mixtures, with a focus on stable, low-density “open” crystals. We demonstrate the approach for binary and ternary mixtures at zero ambient pressure to explore how complexity can be achieved through the combination of several components with simple interactions rather than a single component with a more complicated interaction potential.

3:30PM P43.00004: Why integer valence point-charge model works so well  RUOSHI JIANG (Presenter), Tsung-Dao Lee Institute, XIANG LI, Shanghai Jiao Tong University, XINYAO ZHANG, Tsung-Dao Lee Institute — Integer valence counting works extremely well in determining stability of chemical compounds. It comes as a surprise that the same integer valence counting also works very well in comparing energies of different lattice structures of the same composition, even though an incomplete (non-integer) charge transfer is expected in realistic systems. Then, why is the point charge model reasonably accurate (even more than employment of real partial charge)? Here, by partitioning the charge density via atom-centered Wannier functions, we justify the integer valence counting approach through a systemic analysis of multi-pole expansion of the Coulomb energy. Our results demonstrate the dominance of the point charge contribution over the finite moment ones, and reveal the important role of local point group symmetry in suppressing first few low-order moments. While the inaccuracy grows expectedly as the system’s covalency increases from LiF, ZnO, GaAs to Si, surprisingly a reasonable accuracy is still achieved by an effective ionic assignment even for Si (as Si$^{4+}$Si$^{4-}$). Our formulation also illuminates the removal of the infamous self-interaction in such a simple approach, further explaining its unexpected success in numerous applications.
3:42PM P43.00005: Integrated Particle and Field-Theoretic Simulations: A Multiscale Approach to Complex Soft Matter Formulations*  NICK SHERCK (Presenter), KRIS T DELANEY, SCOTT SHELL, GLENN H FREDRICKSON, University of California, Santa Barbara — Our work investigates the phase-behavior of complex polymeric solutions leveraging the strengths of both particle and polymer field-theoretic simulations. Mesostructured polymeric solutions are difficult to simulate using traditional particle-explicit approaches due to the disparate time and length scales, while the predictive capability of field-theoretic simulations is hampered by the need to specify emergent parameters (e.g., chi parameters) with nonobvious connections to molecular architecture. To overcome the weaknesses of both, we discuss an original way to use small-scale, atomistic simulations to parameterize statistical field theory models. Subsequently, field-theoretic simulations can probe behavior at larger length scales in polymeric solutions efficiently while maintaining a connection to the underlying polymer chemistry. This synergistic approach to polymer simulations opens the door to explore–de-novo–a wide variety of polymeric solution phase behavior. We demonstrate the predictive capability of this approach by reproducing the high-temperature, aqueous, PEO phase diagram, without any experimental data.

*Funded by BASF California Research Alliance

3:54PM P43.00006: First principles investigations of orthorhombic-cubic phase transition and its effect on thermoelectric properties in cobalt-based ternary alloys.  HEM KANDPAL (Presenter), Chemistry, Indian Institute of Technology Roorkee — We screened six cobalt-based 18-VEC systems CoVSi, CoNbSi, CoTaSi (Si-group) and CoVGe, CoNbGe, CoTaGe (Ge-group) by the first-principles approach, with the motivation of stabilizing these orthorhombic phases into the cubic symmetry -- favorable for thermoelectrics. We account the cubic ground state of the Si-group to the interplay of internal pressure and covalent interactions. The principle of reducing covalent interactions will provide insight and could be vital in speeding the search of missing cubic half-Heusler alloys. Meanwhile, the calculated transport properties of all the systems on p-type doping, except CoVSi, are more promising than the well-known CoTiSb. We also provide conservative estimates of the figure of merit, exceeding the CoTiSb. Based on our findings, we suggest possible new phases of ternary compounds for thermoelectric applications.
4:06PM P43.00007: Unexpected Photonic Band Gaps in 3D Crystal Structures*  ROSE CERSONSKY (Presenter), Macromolecular Science and Engineering Program, University of Michigan, JAMES A. ANTONAGLIA, BRADLEY DICE, Department of Physics, University of Michigan, SHARON C GLOTZER, Department of Chemical Engineering, University of Michigan — Photonic crystals are materials composed of mixed dielectric media that result in the reflection of all electromagnetic waves within a range of wavelengths commensurate with the length scale of the crystal. Such complete photonic band gaps allow for light to be controlled through materials design. Since first theorized in 1987, much effort has been made to define and synthesize photonic crystal structures. In the decades since, many photonic structures have been discovered, often by using naturally occurring crystal structures as templates for design. However, these studies have yet to answer the question: what features of a 3D structure will produce a complete photonic band gap? Here, we present data on over 150,000 potential photonic crystals, and show that complete photonic band gaps are possible for many unexpected structures that have yet to be explored. Our simulations suggest that when designing novel photonic materials, the toolbox of structural templates may be larger and richer than previously thought, widening the field of target crystal structures.

*Center for Bio-Inspired Energy Science, # DE-SC0000989206
Dept. of the Navy, ONR #N00014-18-1-2497
UM Rackham Predoctoral Fellowship Program
NSF Grad. Research Fellowship, # DGE2131256260
Adv. Research Computing at UM

4:18PM P43.00008: A mesoscale lattice model and atomistic simulations of controlled drug release*  KULVEER SINGH, RATNA SANDEEP KATIYAR, SOUMITRA SATAPATHI, PRATEEK JHA (Presenter), Indian Institute of Technology Roorkee — Excipients such as polymers are used for the delivery of poorly soluble drugs to enhance drug bioavailability by limiting drug aggregation/crystallization. I will discuss two distinct approaches, which target different time and length scales of the excipient design problem. First, a two-dimensional lattice model is developed of “ants” (drug) performing a random walk in a lattice containing “walls” (excipient). Ants can be “blind” or “friendly”, corresponding to hydrophilic or hydrophobic drug molecules, respectively. Second, atomistic molecular dynamics simulations are performed on an example system containing acrylic acid oligomers as excipient and doxorubicin as the drug. We mimic drug release by matrix swelling in atomistic simulations using a sequential water removal approach that is a crude but simpler alternative of grand canonical ensemble simulations. Drug release by polymer erosion and drug release in a non-swellable, non-eroding matrix is mimicked in our simulations by variations in polymer/drug concentrations. Together, these two simulation approaches provides design rules for choosing polymer-drug combinations for controlled release.

*PKJ thanks DST-INSPIRE grant IFA14-ENG72 of Department of Science and Technology, India.
**4:30PM P43.00009: Van der Waals Metamaterials**

SYEDA MINHAL GARDEZI (Presenter), HARRIS PIRIE, WILLIAM DORRELL, NATHAN C DRUCKER, FAN DU, JENNIFER E. HOFFMAN, Harvard University — Van der Waals (vdW) heterostructures are a fertile frontier for discovering emergent condensed matter phenomena. They are constructed by stacking elements of a large library of two-dimensional materials, which couple together through vdW interactions. However, fully exploring the vast number of possible combinations within this library is a daunting task. Here we introduce vdW metamaterials to rapidly prototype and screen their quantum counterparts. These layered metamaterials reshape the flow of ultrasound to mimic electron motion. We first present a method to recreate the vdW interaction between layered phononic metamaterials using interlayer coupling membranes, which we can tune to create acoustic analogs of well-known vdW heterostructures, including all configurations of bilayer and trilayer graphene. We then twist coupled metamaterial layers to induce interesting phononic behavior mimicking twisted bilayer graphene. We anticipate vdW metamaterials will inform future electronic devices. Equally, they allow the transfer of useful electronic behavior to acoustic systems, such as flat bands in magic-angle twisted bilayer graphene, which may advance super-resolution ultrasound imaging.

*This work was supported by NSF DMR-1231319 and the Gordon and Betty Moore Foundation grant 4536.*

**4:42PM P43.00010: Development of an implicit solvent model for the interfacial configuration of colloidal nanoparticles and application to the interfacial self-assembly of truncated cubes**

UNMUKT GUPTA (Presenter), FERNANDO A ESCOBEDO, Cornell University — This study outlines the development of an implicit solvent model that reproduces the behavior of colloidal nanoparticles at a fluid-fluid interface. The center-point of this formulation is the generalized Quaternion-based Orientational Constraint (QOCO) method. The model captures 3 major energetic characteristics that define the nanoparticle configuration – position (orthogonal to the interfacial plane), orientation, and inter-nanoparticle interaction. The framework encodes physically relevant parameters that provide an intuitive means to simulate a broad spectrum of interfacial conditions. For a wide range of shapes, we are able to replicate the behavior of an isolated nanoparticle at an explicit fluid-fluid interface, both qualitatively and quantitatively. Using the family of truncated cubes as test-bed, we analyze the effect of change in the degree of truncation on the potential landscape. Furthermore, we model the self-assembly of an array of cuboctahedra to provide corroboration to the experimentally observed honeycomb and square lattices. Finally, by exploring a broader range of interfacial conditions, we identify and suggest the assembly mechanism for a set of novel superlattice configurations.

*NSF Grant CBET 1803878*
First-principles study on the stable hydrogen configuration in SrVO$_2$H

MASAYUKI OCHI (Presenter), KAZUHIKO KUROKI, Department of Physics, Osaka University — Mixed-anion compounds, which contain multiple anionic species in a single phase, such as oxyfluorides and oxyhydrides, have been gathering growing attention as a new platform of materials science [1]. While it is an attracting idea to employ the anionic degrees of freedom for tuning the cation environment, much less is known about mixed-anion compounds than oxides. In particular, understanding and controlling the stable configuration of multiple anions in crystal is one of the most challenging issues. For example, hydrogen atoms are aligned along one direction in some oxyhydrides such as SrVO$_2$H [2-3], but are randomly distributed in some oxyhydrides such as SrCrO$_2$H [4]. In this study, we investigate the stable hydrogen configuration in SrVO$_2$H by performing first-principles calculation of the total energy for several hundreds of possible crystal structures with different hydrogen configurations. In this talk, we will discuss what determines the stability of the hydrogen configuration in this material. References: [1] H. Kageyama et al., Nat. Commun. 9, 772 (2018). [2] F. D. Romero et al., Angew. Chem. Int. Ed. 53, 7556 (2014). [3] J. Bang et al., JACS 136, 7221 (2014). [4] C. Tassel et al., Angew. Chem. Int. Ed. 53, 10377 (2014).

Understanding Li-ion Diffusion Through Artificial SEI Coating Layers

ANGELA HARPER (Presenter), Univ of Cambridge, STEFFEN EMGE, Chemistry, University of Cambridge, ANDREW J MORRIS, Metallurgy and Materials, University of Birmingham — Li-ion batteries show promise for storing large amounts of energy, yet, they are limited by the capacity of the graphite anode. High capacity alternatives, such as Li or Si, pose additional issues due to volume expansion and dendrite growth. In both Si and Li, Al$_2$O$_3$ coatings can be used as a protective layer on the anode [1,2]. We apply a combined theoretical and experimental study to both predict and confirm the structure of this interface, a combination which has been applied numerous times in this field [3]. Using Al K-edge X-Ray absorption spectroscopy calculated with DFT, we have shown how individual layers of Al$_2$O$_3$ grow via atomic layer deposition, and how the structure of the layers is dependent on the number of layers. This result was confirmed experimentally, and suggests that the performance of this coating layer is dependent on the number of layers grown. Finally, we calculate the Li$^+$ diffusivity across the interface, and show how the interface changes during ion diffusion. These results provide both a computational and experimental explanation for the enhanced performance of Al$_2$O$_3$ coated high-capacity anodes.

Fingerprints based biasing for finding complex reaction pathways. *

DEB DE (Presenter), MARCO KRUMMENACHER, BASTIAN SCHAEFER, STEFAN A C GOEDECKER, University of Basel — Determining the pathway of a reaction/transformation is of great importance in chemistry, physics and materials sciences. However, due to the indistinguishability of atoms, finding complex reaction and transformation pathways, containing a large number of intermediate states, is difficult within the existing methods at the density functional theory level. We have resolved this issue by introducing a bias that is invariant under atomic index permutations and that can target a single well defined configuration as the final configuration of a chemical reaction or physical transformation. In this way we can overcome the index mapping problem. The forces arising from the bias, by construction, do not depend on the indexing of the atoms. We have thus reduced the combinatorial atomic indexing problem, that has an exponential scaling, to a global minimization problem on a biased PES involving an indexing invariant penalty function. The later problem can be solved easily in practice. The penalty function we propose is universal and can be applied to any reaction or transformation. We expect that this method will give atomistic insight into complex reaction pathways i.e. in catalysis as well as complex phase and shape transformations.

*This work was done within the NCCR MARVEL.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P44 DCOMP DMP: Electrons, Phonons, Electron Phonon Scattering, and Phononics III - 704 - Olivier Delaire, Duke University - Tag(s): Focus
2:30PM P44.00001: Theoretical Spectroscopy of 2D Materials: Exciton-phonon coupling in resonant Raman and luminescence spectroscopy* [Invited] LUDGER WIRTZ (Presenter), FULVIO PALEARI, Department of Physics and Materials Science, University of Luxembourg, ALEJANDRO MOLINA-SANchez, QuantaLab, International Iberian Nanotechnology Laboratory, PIER LUIGI CUDAZZO, Department of Physics and Materials Science, University of Luxembourg, SVEN REICHARDT, Department of Materials, University of Oxford — 2D materials are known to exhibit very pronounced excitonic effects due to the confinement of electrons and holes in a layer and due to the weak dielectric screening of the electron-hole interaction. In spectroscopy involving vibrational degrees of freedom, the exciton-phonon coupling must therefore be included in order to obtain a qualitative understanding of the spectra and in order to obtain quantitative results. We present our methods for the calculation of exciton-phonon coupling via a finite displacement [1] and via a diagrammatic approach [2,3], both using many-body perturbation theory.

We present results for the phonon-assisted luminescence spectrum of bulk hexagonal boron nitride (hBN), where the combination of indirect band gap and strong excitonic effects leads to a complex peak structure due to coupling of excitons with various phonon branches [1]. Furthermore, we present calculations of resonant Raman intensities with the combined inclusion of both excitonic and non-adiabatic effects. In bulk hBN, which has high phonon-frequencies due to the light atoms, we demonstrate the emergence of strong quantum interference between different excitonic resonances due to non-adiabatic effects. In MoS\textsubscript{2} and MoTe\textsubscript{2}, our calculations explain the observed different intensity dependences of the A\textsubscript{1}' and E' modes on the energy of the exciting laser [3].


*We acknowledge support from the National Research Fund, Luxembourg through project INTER/ANR/13/20/NANOTMD

3:06PM P44.00002: Strong phonon-assisted Auger recombination in PbSe* XIE ZHANG (Presenter), JIMMY SHEN, CHRIS VAN DE WALLE, University of California, Santa Barbara — It is commonly believed that direct Auger recombination dominates in narrow-gap semiconductors. With the example of the prototypical narrow-gap semiconductor PbSe, we demonstrate that this is not necessarily the case. By explicitly calculating both the direct and phonon-assisted indirect Auger recombination coefficients of PbSe from first principles, we show that a number of puzzling anomalies in the Auger recombination in PbSe can be well understood. These insights shed new light on the impact of electron-phonon coupling on Auger recombination in IV-VI semiconductors, which is critical for improved device design.

*This work was supported by DOE.
3:18PM P44.00003: Fully Anharmonic, Non-Perturbative First-Principles Theory of Electronic-Vibrational Coupling in Solids

MARIOS ZACHARIAS, MATTHIAS SCHEFFLER, CHRISTIAN CARBOGNO (Presenter), Fritz Haber Institute of the Max Planck Society, Berlin — The coupling between nuclear vibrations and the electronic structure plays a pivotal role for many material properties, including optical absorption and electronic transport. In this regard, however, today’s state-of-the-art methodologies rely on two approximations [1]: the harmonic (phonon) approximation for the nuclear motion and the linear response description of the electronic structure with respect to harmonic displacements. In this work, we overcome both these approximations by performing fully anharmonic ab initio molecular dynamics (aiMD) calculations and by accounting for the non-perturbative, self-consistent response of the wavefunctions along the aiMD trajectory. By this means, we obtain fully anharmonic, vibronically renormalized spectral functions, from which macroscopic material properties like temperature-dependent band gaps and electronic transport coefficients are obtained. We validate our approach using silicon as an example, for which the traditional electron-phonon coupling formalism is recovered. Using cubic SrTiO$_3$ as example, we further demonstrate that anharmonic electronic-vibrational coupling effects not captured in traditional formalisms play a decisive role in complex materials like perovskites.


3:30PM P44.00004: Phonon-mediated Optical and Electronic Transport Properties of BAs*

KYLE BUSHICK (Presenter), KELSEY MENGLE, SIEUN CHAE, ZIHAO DENG, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — While boron arsenide (BAs) has attracted attention for its ultrahigh thermal conductivity, open questions remain about its use in semiconducting devices. To address this problem, we apply density functional and many body perturbation theory to understand its electronic and optical properties and guide device applications. Since BAs has an indirect band gap of approximately 2 eV and a direct gap of 4.1 eV, absorption of visible light is exclusively mediated by phonons. We therefore calculate the indirect and direct optical absorption spectra to assess its potential in photovoltaics and examine how excitonic effects alter the absorption. Our results are in excellent agreement with experimental data. We also calculate the effect of strain on the band alignment and the electron and hole mobilities, and show that bi-axial tensile strain increases the mobilities of both carriers by over 50%. Finally, we determine the band offsets of BAs heterostructures with nearly lattice-matched ZnSnN$_2$ and InGaN to guide heterostructure design. Our work elucidated the functional properties of BAs for technologically relevant device applications.

*This work was supported by NSF DMREF program (1534221) and DOE grant DE-SC0020347. Computational resources provided by DOE NERSC (DE-AC02-05CH11231).
3:42PM P44.00005: Electron and Phonon Hydrodynamics in Antimony  ALEXANDRE JAOUI (Presenter), BENOIT FAUQUE, KAMRAN BEHNIA, ESPCI Paris — We present a study of the electrical and thermal resistivities in millimetric samples of the semimetal Sb down to sub-Kelvin temperatures. By applying a large magnetic field, we can clearly separate the electronic and phononic thermal resistivities. The Wiedemann-Franz (WF) law is recovered at low temperature ($T \approx 4K$) in all samples. Yet, a size-dependent departure from the WF law is observed at higher temperatures. We show that this deviation is due to a mismatch between the prefactors of the thermal and electrical $T^2$-resistivities. By analogy with the case of normal-state liquid $^3$He, where fermion-fermion collisions generate a thermal conductivity inversely proportional to temperature [1], we can associate the larger $T^2$-thermal resistivity to the momentum-conserving electronic collisions [2]. In this scenario, the size-dependence of the ratio of the thermal to the electrical $T^2$-prefactors in Sb points to a hydrodynamic flow of electrons [3]. Furthermore, in the 1K-7K range, we also report on a large increase of the thermal diffusivity of phonons, in the same samples, i.e. a signature that the flow of phonons is partially hydrodynamic.


3:54PM P44.00006: Unraveling a New Heat Transport Regime at The Nanoscale.* GIUSEPPE BARBALINARDO (Presenter), ZEKUN CHEN, SHUNDA CHEN, DAVIDE DONADIO, University of California, Davis — The understanding of heat transport in nanoscale semiconductors is of fundamental importance because of its huge technological impact in electronics and renewable energy harvesting and conversion. A particularly interesting question is related to the understanding of how thermal properties of dielectrics, like silicon, change when their size of the order of a few hundred nanometers, which is the characteristic size of state of the art electronic circuits. In this size range heat transport is in a regime in between ballistic and diffusive, which is inaccurately described by either approximation.

In this work, we analyze the current state of the art of heat transport in semiconductor nanostructures. We identify substantial gaps in the theoretical treatment of the quasi-ballistic transport regime, and we propose a new atomistic model to compute the thermal conductivity of nanoscale systems, including both quantum and finite boundaries effects. Our novel approach is implemented in a computational environment, which gives to the powerful framework of anharmonic lattice dynamics, the ability to perform high accuracy predictions for finite size systems, and provide a rigorous alternative to non-equilibrium molecular dynamics.

*The Molecular Sciences Software Institute (MolSSI)
4:06PM P44.00007: Electron wind force in an atomistic non-equilibrium molecular dynamics simulation*  DAVIDE MANDELLI, Istituto Italiano di Tecnologia, FRANCO PELLEGRINI (Presenter), Ecole Normale Superieure Paris, GIUSEPPE E. SANTORO, ERIO TOSATTI, International School for Advanced Studies — We demonstrate electronic friction on metals by addressing the reverse process – the force imparted on the atoms by the flow of an electronic current in the metal. By well established Ehrenfest dynamics we implement a quantum-classical simulation of the motion of a chain of classical atoms forming a contactless monatomic ring, where electrons flow by nearest neighbor hopping between atomic-like orbitals in an electric field generated by a linearly growing external magnetic field threading the ring. In the real time dynamics, electron-phonon scattering events take the form of Landau-Zener processes, each of them imparting momentum to the classical atoms, that can vibrate and also dissipate to a bath. The realistic features of electron conduction and resistivity are recovered in this model, plus a microscopic description of the current-induced momentum transfer to the atoms which vibrate and to the whole chain which drifts. When one additional adatom is added to the chain, the quantum mechanics of the wind force and the resulting electromigration drift are controlled by the weak hybridization of the adatom orbital to the chain atomic orbitals where the current flows, suggestive of a rather general mechanism.

*Supported by ERC Advanced Grants 320796 MODPHYSFRICT and 824402 ULTRADISS

4:18PM P44.00008: Thickness-dependent electron-phonon coupling and transport in metals from first principles  SUSHANT KUMAR (Presenter), RAVISHANKAR SUNDARARAMAN, Rensselaer Polytechnic Institute — Recent strides in thin-film deposition technology have made the next generation of ultrathin plasmonic devices and ultrascaled metallic interconnects plausible. It has led to a renewed interest in the study of properties of metals and semiconductors in the low dimensional limit. Here, starting with a single layer, we systematically investigate the effect of thickness on the electronic properties and electron-phonon (e-ph) coupling of ultrathin metallic films. Such ab initio studies have typically been challenging because of the inability of the state-of-the-art DFT codes to correctly predict the phonon dispersion curves of finite thickness materials, especially in the $q \to 0$ limit. We propose a new computationally-inexpensive correction scheme for the phonon force matrix based on rotational invariance of the elasticity tensor. This scheme facilitates accurate computation of phonon bandstructures and e-ph coupling for arbitrary film geometries. Using this capability, we determine the variation of electronic transport properties as a function of layer number, fully accounting for effects such as phonon confinement. These ab initio calculations give us an insight into the effect of surface and interfacial strain on the e-ph scattering in thin metallic films.
**4:30PM P44.00009: Phonon interactions in rock salt and fluorite structures**  
LYUWEN FU (Presenter), MARK ALAN MATHIS, ENDA XIAO, CHRIS MARIANETTI, Columbia Univ — Space group irreducible derivatives of the Born Oppenheimer potential are computed from density functional theory for materials with the rock salt and fluorite structures, including PbTe and ThO2. We utilize our recently developed group theoretical approach which allows the extraction of the irreducible derivatives from finite displacement calculations on the smallest possible supercells using the smallest possible number of calculations. Quadratic (i.e. phonons), cubic, and quartic irreducible derivatives have been computed. The fidelity of the irreducible derivatives is tested via comparison to strain derivatives of the phonons. Both dynamics and thermodynamics are evaluated using our irreducible Taylor series, yielding observables such as phonon linewidths, thermal conductivity, thermal expansion, mean square displacements, etc. Results on PbTe and ThO2 are compared to experiment.

**4:42PM P44.00010: Predictive calculations of electron and heat transport in ultra-wide-band-gap semiconductors**  
EMMANOUIL KIOUPAKIS (Presenter), KELSEY MENGLE, Univ of Michigan - Ann Arbor — Ultrawide-band-gap semiconductors are used for energy-efficient power electronics, but there is a pressing need to improve on current materials. Beta gallium oxide (β-Ga2O3) outperforms materials such as Si, SiC, and GaN due to its wide band gap and corresponding large breakdown field. However, three drawbacks of β-Ga2O3 are its lack of p-type doping, its low thermal conductivity, and its inferior electron mobility. Using first-principles calculations we calculate the electron-phonon coupling of β-Ga2O3 to understand the origin of the limits to the electron mobility and thermal conductivity. We also explore rutile germanium dioxide (r-GeO2) as a semiconductor for power-electronic applications. The calculated band gap and optical absorption spectrum is in good agreement with optical measurements. We also determine the phonon-limited carrier mobilities and lattice thermal conductivity as a function of temperature and crystal orientation. We find that the electronic and thermal transport properties of r-GeO2 outperform current materials, while it can also be ambipolarly doped. Our results highlight the potential of r-GeO2 for power electronics.

*This work was supported by NSF DMR-1534221 DGE-1256260. Computational resources provided by the DOE NERSC facility.*
Optical absorption in gallium oxide

HARTWIN PEELAERS (Presenter),
Department of Physics and Astronomy, University of Kansas, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — Transparent conducting oxides (TCOs) are a technologically important class of materials used in optoelectronic devices, as TCOs balance two conflicting properties: transparency and conductivity. The requirement of transparency is typically tied to the band gap of the material being sufficiently large to prevent absorption of visible photons. This is a necessary but not sufficient condition: indeed, the high concentration of free carriers, required for conductivity, can also lead to optical absorption. This absorption can occur through direct absorption to higher-lying conduction band states, or by an indirect process, for example mediated by phonons or charged impurities.

We performed a detailed first-principles study of these absorption processes in Ga$_2$O$_3$ [1,2], a material with promising applications in high-power devices and UV photodetectors. Our results elucidate the fundamental limitations of optical absorption in Ga$_2$O$_3$ and shed light on experimental observations.


*Work supported by DOE and AFOSR.

Low and high field transport in 2-dimensional electron gas in β-(Al$_x$Ga$_{1-x}$)$_2$O$_3$/Ga$_2$O$_3$ heterostructures

AVINASH KUMAR (Presenter), UTTAM SINGISETTI, State Univ of NY - Buffalo — β-Ga$_2$O$_3$ is an emerging wide-bandgap semiconductor for potential application in power and RF electronics. The 2-dimensional electron gas (2-DEG) in β-(Al$_x$Ga$_{1-x}$)$_2$O$_3$/Ga$_2$O$_3$ heterostructures show the promise for high speed transistors. We will present both the low- and high- field 2-DEG transport properties in the AlGa$_2$O$_3$/Ga$_2$O$_3$ heterostructure. A self-consistent Poisson-Schrodinger simulation of heterostructure is used to obtain the subband energies and wavefunctions. Intra-subband, inter-subband, 2D-3D, 3D-2D and 3D-3D scattering rates are calculated for all the different scattering mechanisms. The electronic structure, assuming confinement in a particular direction, and the phonon dispersion is calculated based on first principle methods under DFT and DFPT framework. Phonon confinement is not considered for the sake of simplicity. The different scattering mechanisms that are included in the calculation are phonon (polar and non-polar), remote impurity, alloy and interface-roughness. We include the full dynamic screening in polar optical phonon scattering. We will use Full Band Monte Carlo to calculate the velocity-field profile in different crystal directions. We will also report the low field mobility by solving the Boltzmann transport equation using Rode's iterative method.
Phonon RIXS calculations using Green's function Momentum Average technique

KRZYSZTOF BIENIASZ (Presenter), MONA BERCIU, Stewart Blusson Quantum Matter Institute, University of British Columbia, STEVEN JOHNSTON, University of Tennessee in Knoxville —

Spectroscopic experiments are the most extensively used probes for characterizing the physical properties of condensed matter. However, their understanding often requires a theoretical calculation of the spectra in question, usually starting from some simplified model of the underlying system. One of the problems that are key to the understanding of many properties of materials is the physics of phonons and their interaction with the conduction electrons. These are the issues lying at the base of conventional superconductivity and it is hoped that their better understanding in high temperature superconductors might help elucidate some of the mysteries still surrounding those materials. The RIXS spectroscopy is a novel, emerging technique, that only recently started to approach the resolving power necessary to observe the phononic features. Thus, theoretical predictions concerning phonon RIXS are now becoming timely in this rapidly progressing field of research. Our aim is to use the Momentum Average Green's function technique and apply it to the problem of phonon RIXS calculations, thus going beyond the current dichotomy of exact diagonalization vs. perturbative expansion methods that are the two dominating methodologies in RIXS theory.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P45 DCOMP GDS DSOFT DPOLY: Emerging Trends in Molecular Dynamics Simulations and Machine Learning IV 706 - Maria Chan, Argonne Natl Lab -

Tag(s): Focus
KURT KREMER (Presenter), Max Planck Institute for Polymer Research — Most biological systems and a huge class of everyday products ranging from simple plastics to complex functional systems and to most foods are made of soft matter. Its generic properties are mostly governed by the statistical mechanics of strongly fluctuating huge molecules, such as polymers. For this the plain fact that polymer chains cannot cross through each other introduces significant constraints and is of central importance, e.g. for polymer rheology where entanglements dominate the dynamics or for chromosome territories in the cell nucleus in biophysics, where “topological repulsion” plays a role. Such constraints can be permanent, as for gels and networks or ring polymers or temporary but long lived as in polymer melts or for chromosome organization in the cell nucleus. By manipulating entanglements new non-equilibrium materials can be made. Based on computer simulations new morphologies are predicted, and are tested experimentally. Currently there is no comprehensive analytic theory, which links topological constraints to material properties. The talk will give an overview of recent developments and point to some challenging opportunities based on advances in computational physics of soft matter and experiment.

The author acknowledges a very fruitful collaboration with H.P. Hsu and M.K. Singh

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Transfer learning is a subfield of machine learning that leverages proficiency in one or more prediction tasks to improve proficiency in a related task. For chemical applications, transfer learning models represent a promising approach for addressing intrinsic data scarcity by utilizing potentially abundant data across adjacent domains. For chemical applications, it is still largely unknown how correlation between the prediction tasks affects performance, the limitations on the number of tasks that can be simultaneously trained in these models before incurring performance degradation, and if transfer learning positively or negatively affects ancillary model properties. In this talk we investigate these questions using an autoencoder latent space as a latent variable for transfer learning models trained on the QM9 dataset that have been supplemented with quantum chemistry calculations. We explore how property prediction can be improved by utilizing a simpler linear predictor model, forces the latent space to reorganize linearly with respect to each property. The linear organization of the latent space has further applications to novel structure generation by increasing the quality of generated species and facilitating targeted structure searching.

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3:18PM P45.00003: Neural Network Based Molecular Dynamics to Study Polymers
CHRISTOPHER KUENNETH (Presenter), RAMAMURTHY RAMPRASAD, School of Materials Science and Engineering, Georgia Institute of Technology — Polymers are an important class of materials that display morphological complexity and diverse inter-atomic interactions. These two factors have defied large-scale and long-time quantum-accurate atomic-level simulations of polymer dynamics. Traditional simulation methods utilize parameterized classical potentials or force fields which often lack accuracy, transferability, and versatility. Moreover, although these methods are known to fail in notable circumstances, it is not clear how the traditional methods can be systematically improved using the known failures. Neural network based models for molecular dynamics, the subject of this study, are capable of learning from reference quantum mechanical data. Once learned, these models can emulate the parent quantum calculations in accuracy, but be about a billion orders of magnitude faster. Neural network based molecular dynamics simulations can thus reach length-scales and time-scales previously inaccessible using quantum mechanical methods. In this work, we develop a new class of first-ever neural network models for the prototypical case of hydrocarbons and provide several meticulous and diverse validation tests. Challenges that remain are discussed and pathways to overcome such challenges are presented.

3:30PM P45.00004: Applications of Automatic Differentiation to Materials Design* ELLA KING (Presenter), CARL GOODRICH, Harvard University, SAM SCHOENHOLZ, EKIN DOGUS CUBUK, Google, MICHAEL PHILLIP BRENNER, Harvard University — Developments in automatic differentiation (AD) have opened the door to an array of new possibilities throughout the physical sciences. However, AD in materials design has largely been out of reach. Simulations of novel materials were far too computationally intensive for a tool that requires running hundreds of thousands of simulations. Recent work has begun to integrate molecular dynamics simulations with AD, bringing the developments in AD to a new and exciting domain. We demonstrate the power of AD in materials design by building on a seminal paper by Torquato. The prior work begins with a specific model pair potential, and varies four parameters to achieve a honeycomb lattice. Through AD, we are able to start from an entirely arbitrary pair potential, optimize that potential, and ultimately reach a honeycomb lattice with fewer defects.

*Harvard Materials Research Science and Engineering Center Grant DMR-1420570 and ONR Grant N00014-17-1-3029

3:42PM P45.00005: Trainable Molecular Dynamics Models CARL GOODRICH (Presenter), ELLA KING, Harvard University, SAMUEL SCHOENHOLZ, EKIN DOGUS CUBUK, Google, MICHAEL PHILLIP BRENNER, Harvard University — The development of automatic differentiation is motivated by the desire to train computational models with non-trivial architectures that more accurately reflect the underlying structure of the data. This is especially desirable when studying complex physical phenomena, which are governed by fundamental principles (e.g. conservation of energy) that are well understood. By applying automatic differentiation to well-established physics simulations, one can in principle obtain machine trainable models with the physics built in. We will discuss the first steps towards Trainable Molecular Dynamics Models (TMDMs): how they work, their significant potential for scientific and technological discovery, and initial discoveries of non-trivial self-assembly pathways.
3:54PM P45.00006: Hydrogen-Oxygen Combustion: Data-Driven Generation of Quantum-Accurate Interatomic Potentials*  
ALLAN AVILA (Presenter), University of California, Santa Barbara, 
LUKE BERTELS, University of California, Berkeley, IGOR MEZIC, University of California, Santa Barbara, 
MARTIN P HEAD-GORDON, University of California, Berkeley — Although quantum scale simulations of hydrogen-oxygen combustion offer an accurate description of the process, a multi-atom quantum simulation of combustion is unfeasible as it would not terminate in a scientist's lifetime. Multi-atom simulations of combustion are feasible at the molecular scale, however, the potential bond energies are inaccurate and results often fail to match quantum data. We demonstrate how the programmable potentials methodology can be utilized to develop quantum accurate molecular level potentials for several intermediate reactions involved in hydrogen-oxygen combustion. Sparse Electronic Structure Theory (EST) simulation data is utilized to train our programmable potentials. The developed potentials are then inputted into the molecular dynamics simulation package LAMMPS for verification. Our results demonstrate that the developed programmable potentials generalize beyond the sparse EST training dataset. Most importantly, the developed potentials lead to feasible and quantum-accurate molecular dynamics simulations of hydrogen-oxygen combustion.

*Army Research Office

4:06PM P45.00007: Toward optimal descriptors for accurate machine learning of flexible molecules  
VALENTIN VASSILEV GALINDO (Presenter), IGOR POLTAVSKYI, ALEXANDRE TKATCHENKO, University of Luxembourg Limpertsberg — Robust machine learning (ML) models should be able to reliably predict global molecular potential-energy surfaces (PES) including equilibrium and “far-from-equilibrium” geometries. However, existing molecular ML models are substantially biased towards “close-to-equilibrium” geometries. Indeed, the difficulty of the learning task increases with increasing flexibility of a molecule, due to a vast manifold of configurations with a complex interplay of covalent and non-covalent interactions to be learned.

Our objective is to test how the ability to accurately reproduce PES depends upon the choice of a molecular descriptor. We use azobenzene, aspirin and salicylic acid molecules as our test systems, and the sGDML code¹ for building ML force-fields. We found that the descriptors which demonstrate excellent performance for “close-to-equilibrium” parts of PES are inefficient for building global PES models. To resolve this challenge, we propose new descriptors that allow building accurate and data-efficient ML models for flexible molecules.

4:18PM P45.00008: Towards transferable parametrization of Density-Functional Tight-Binding with machine learning  LEONARDO MEDRANO SANDONAS (Presenter), MARTIN STOEHR, ALEXANDRE TKATCHENKO, Physics and Materials Science Reasearch Unit, University of Luxembourg — Machine learning (ML) has been proven to be an extremely valuable tool for simulations with ab initio accuracy at the computational cost between classical interatomic potentials and density-functional approximations. Similar efficiency can only be achieved by semi-empirical methods, such as density-functional tight-binding (DFTB). One of the limiting factors in terms of the accuracy and transferability of DFTB parametrizations is the so-called repulsive potential, which plays a considerable role for the prediction of energetic, structural, and dynamical properties. Few attempts of using ML-techniques to address this issue have been proposed recently but, up to now, evidence of transferability and scalability is still scarce. Using the QM7-X database of small organic molecules, we demonstrate that the DFTB repulsive energy can be effectively learned by means of ML-approaches including neural networks and kernel ridge regression. We further show how the resulting DFTB+ML model can also be used for more complex systems like molecular dimers and crystals, and modeling techniques like (global) structure search or vibrational analysis. DFTB+ML thus opens a route to the simultaneous access to reliable electronic and structural/dynamical properties of diverse molecular systems.

4:30PM P45.00009: Active learning of fast Bayesian force fields with mapped gaussian processes - application to stability of stanene  YU XIE (Presenter), JONATHAN VANDERMAUSE, LIXIN SUN, ANDREA CEPELLOTTI, BORIS KOZINSKY, Harvard University — Machine learning force-fields can reach accuracy comparable to ab-initio molecular dynamics and simulate much larger systems. Gaussian process (GP) regression has remarkable advantage due to its built-in uncertainty quantification based on Bayesian posterior inference, which can be used to monitor the quality of predictions. A limitation is that the prediction cost grows linearly with the training set size, making accurate GP predictions slow. To solve this, we exploit the special structure of an n-body kernel function to construct interpolation functions based on the trained GP, mapping both forces and uncertainties. To demonstrate the capability of this mapped GP Bayesian force field (BFF) method, we perform active learning and large-scale simulation of stanene. We reveal the decomposition mechanism of stanene and identify the range the phase transition temperature. The application shows that we can reach classical potential prediction speed while keeping quantum accuracy, at the same time incorporating uncertainty quantification. We present progress in implementing automated active learning workflows for training BFFs, aimed at large-scale simulations of rare event dynamics in complex materials.
4:42PM P45.00010: Nuclear quantum delocalization enhances non-covalent intramolecular interactions: A machine learning and path integral molecular dynamics study  
HUZIEL SAUCEDA (Presenter), Tech Univ Berlin, VALENTIN VASSILEV GALINDO, Physics and Materials Science Research Unit, University of Luxembourg, STEFAN CHMIELA, KLAUS-ROBERT MÜLLER, Tech Univ Berlin, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, University of Luxembourg — It is of common knowledge that nuclear quantum effects generates delocalized molecular dynamics. In this study, we present evidence that nuclear delocalization can enhance electronic and electrostatic interactions that promote localized dynamics. These results were obtained from the reconstructed potential-energy surfaces using the symmetrized gradient-domain machine learning (sGDML) framework[1] trained on coupled cluster with single, double, and perturbative triple excitations (CCSD(T)) data combined with path integral molecular dynamics simulations. The physical process responsible for this phenomenon is the effective reduction of the interatomic distances between non-covalently bonded atoms or functional groups. This potentiates intramolecular interactions such as the \( n\to\pi^* \) and electrostatic interactions[2]. These results diverge from the general assumption that nuclear quantum effects just tend to lower energetic barriers or to smoother the energy landscape, opening new avenues into possible explanations of complex processes in chemistry and biology.


4:54PM P45.00011: Active learning identifies optimal \( \pi \)-conjugated peptide chemistries for optoelectronics*  
KIRILL SHMILOVICH (Presenter), ANDREW L FERGUSON, University of Chicago — In this work we perform active learning discovery within an embedded chemical space of \( \pi \)-conjugated peptides using coarse-grained molecular dynamics simulation to discover molecules with emergent optoelectronic behavior. Molecules with oligopeptide wings flanking a \( \pi \)-conjugated core have surfaced as an extensible building block for self-assembling electronic devices due to overlaps between \( \pi \)-orbitals in supramolecular assemblies leading to optical and electronic properties with the potential to operate in bio-compatible frameworks. However, a combinatorial explosion in the molecular design space of possible peptide sequences render brute force trial-and-error discovery impossible through either experiment or simulation. By deploying an activate learning procedure over a variational autoencoder learned space of \( \pi \)-conjugated peptides molecules are iteratively selected for computational screening by balancing exploration of undersampled regions and exploitation in high confidence regions of chemical space. This protocol efficiently navigates this large chemical space to ultimately identify promising \( \pi \)-conjugated peptide chemistries with optimal optoelectronic behavior for further computational testing and experimental synthesis.

*DMR-184180  
DGE-1746045  
DMR-1828629
5:06PM P45.00012: A Self-consistent Artificial Neural Network Inter-atomic Potential for Li/C Systems  
YUSUF SHAIDU (Presenter), RUGGERO LOT, International School for Advanced Studies, FRANCO PELLEGRINI, Laboratoire de Physique Statistique, École Normale Supérieure, Université PSL, EMINE KUCUKBENLI, Harvard University, STEFANO DE GIRONCOLI, International School for Advanced Studies — Graphene-based structures, due to their large surface area, have been suggested as suitable anode materials for Li-ion batteries. In a previous study[1] we examined Li adsorption on graphene at finite temperature with a site-based potential and identified the temperature and Li coverage at which a transition can be expected from disperse Li ion to clustered Li atoms configuration on graphene surface. To extend this study to a wide range of Li coverage on realistic anode materials, a more flexible and accurate Li-C potential is needed. In this talk we first present a self-consistent approach to construct a neural network potential for Carbon using the PANNA code[2]. Our potential performs excellently in ranking the energies of distinct sp3 networks and reproduces the equation of state of graphite, diamond and graphene, as well as elastic and vibrational properties of these phases. We then extend our potential to Li/C systems incorporating long range electrostatics and test its performance on a wide range of Li adsorbed carbon allotropes.


5:18PM P45.00013: Active Learning Driven Machine Learning Inter-Atomic Potentials Generation: A Case Study for Hafnium dioxide*  
GANESH SIVARAMAN (Presenter), Argonne Leadership Computing Facility, Argonne National Laboratory, ANAND NARAYANAN KRISHNAMOORTHY, MATTHIAS BAUR, CHRISTIAN L. HOLM, Institute for Computational Physics, University of Stuttgart, MARIUS STAN, Applied Materials Division, Argonne National Laboratory, GÁBOR CSÁNYI, Department of Engineering, University of Cambridge, CHRIS BENMORE, X-ray Science Division, Argonne National Laboratory, ALVARO VAZQUEZ-MAYAGOITIA, Computational Science Division, Argonne National Laboratory — We propose a novel active learning scheme to automate the configuration selection to fit the Gaussian Approximation Potential (GAP). The proposed scheme consists of an unsupervised active sampler coupled to a Bayesian optimization to evaluate the GAP model. We apply this scheme to \textit{ab initio} molecule dynamics trajectories of Hafnium dioxide. We will show that this scheme leads to a much lower number of training configuration that arrives at near \textit{ab initio} energy fit accuracy as evaluated by an error metric. With the active learned GAP model, we performed molecule dynamics (MD) simulation. We show that the MD simulation calculated x-ray structural factors are in the good agreement with experiments.

*Argonne National Laboratory's work was supported by the U.S. Department of Energy, Office of Science, under contract DE-AC02-06CH11357.

Wednesday, March 4, 2020 2:30 PM - 5:18 PM

Session P46 GMAG DMP DCOMP: Unconventional Order and Phase Behaviors in Complex Oxides 708 - Arun Paramekanti, Univ of Toronto - Tag(s): Focus
2:30PM P46.00001: Collective Spin and Charge Behavior in Ni\textsuperscript{1+}-Rich Layered Nickelates\*  
[Invited] JOHN MITCHELL (Presenter), Argonne Natl Lab — For more than 30 years nickel oxides have been explored in vain as potential cuprate-like superconductors. The recent report of superconductivity in a nickelate film by Hwang et al (Nature 572, 624 (2019)) brings new urgency to this quest. Unlike that of their cuprate analogs, the electronic phase diagram of layered nickelates, R\textsubscript{2-x}Sr\textsubscript{x}NiO\textsubscript{4} (R=rare earth) is populated not by metals and superconductors, but rather with insulating charge- and spin-stripe phases. The absence of superconductivity can be rationalized by factors such as d-p mixing, lack or planar orbital polarization, among others. Each of these traces ultimately to the markedly different electronic configuration of d\textsuperscript{8} Ni\textsuperscript{2+} in octahedral coordination vis-à-vis d\textsuperscript{9} Cu\textsuperscript{2+} in an essentially square planar environment. Ni\textsuperscript{1+}-containing solids are rare and difficult to synthesize. However, a family of such materials with square planar Ni does exist, with formula R\textsubscript{n+1}Ni\textsubscript{n}O\textsubscript{2n+2}, where the Ni\textsuperscript{1+} fraction is given by (n-1)/n. Indeed, the reported nickelate superconductor thin film derives from the Sr-doped ‘infinite layer’ endmember of this series, Nd\textsubscript{0.8}Sr\textsubscript{0.2}NiO\textsubscript{2}. Here we discuss the phase behavior of the n=3 member of this series, R\textsubscript{4}Ni\textsubscript{3}O\textsubscript{8}(R=La,Pr) made possible by advances in high pressure crystal growth. Specifically, we show the emergence in this system of several characteristics of cuprates that have been missing in nickelates, including strong in-plane x\textsuperscript{2}-y\textsuperscript{2} orbital polarization, significant 3d-2p mixing at E\textsubscript{F}, and competition between metallic and antiferromagnetic insulating stripe phases. We present an expanded phase diagram of the reduced, layered nickelates and suggest ways in which these materials might be made into superconductors.

\*This work was supported by the U.S. DOE Office of Science, Basic Energy Sciences, Division of Materials Science and Engineering.

3:06PM P46.00002: An \textit{ab initio} study of electron-hole pairs in the insulating single layer cuprates and nickelates\*  
CHRISTOPHER LANE (Presenter), JIAN-XIN ZHU, Los Alamos National Laboratory — Advanced density functionals have proven to be an indispensable tool in studying correlated materials exhibiting the delicate interplay between complex charge and non-collinear magnetic order. We perform a comparison study of the electronic and magnetic structure of a prototypical high-temperature superconductor La\textsubscript{2}CuO\textsubscript{4} with the isostructural single-layer nickelate La\textsubscript{2}NiO\textsubscript{4}. We find key differences in the low-energy electronic structure, where in particular, La\textsubscript{2}NiO\textsubscript{4} exhibits an enhanced Hund’s coupling. Additionally, utilizing our accurate \textit{ab initio} ground state, we obtain the excitonic dispersion for each material. Excitons in La\textsubscript{2}CuO\textsubscript{4} are delocalized and can freely move in the CuO\textsubscript{2} plane without disturbing the antiferromagnetic order. In contrast, in La\textsubscript{2}NiO\textsubscript{4} we find the low-lying excitonic states to be extremely localized, producing a nearly flat dispersion. Our results are in excellent agreement with RIXS observations, and give insights into the excited state dynamics of the cuprates and nickelates. Finally, we will briefly connect our results to the newly discovered superconducting infinite-layer nickelates.

\*This work was supported by the U.S. DOE NNSA under Contract No. 89233218CNA000001 and by the Center for Integrated Nanotechnologies, a DOE BES user facility.
3:18PM P46.00003: Low Temperature Specific Heat of Doped SrTiO$_3$: Doping Dependence of the Effective Mass and Kadowaki-Woods Scaling Violation*  ERIC MCCALLA, McGill University, MARIA NAVARRO GASTIASORO, GUY CASSUTO, RAFAEL FERNANDES, CHRIS LEIGHTON (Presenter), University of Minnesota — We discuss wide-doping-range (8 x 10$^{17}$ to 4 x 10$^{20}$ cm$^{-3}$ Hall electron density) low temperature specific heat measurements on single crystal SrTiO$_3$:Nb, correlated with electronic transport data and tight-binding modeling [1]. Lattice dynamic contributions to specific heat are shown to be well understood, albeit with unusual sensitivity to doping, likely related to soft modes. Electronic contributions to specific heat provide effective masses that increase substantially, from 1.8 to 4.8$m_e$, across the two SrTiO$_3$ Lifshitz transitions. It is shown that this behavior can be quantitatively reconciled with quantum oscillation data and calculated band structure, establishing a doping-independent mass enhancement factor of 2.0. With the doping-dependent $\tau^2$ resistivity prefactor and Sommerfeld coefficient known, Kadowaki-Woods scaling has been tested over the entire doping range. Despite Fermi liquid behavior in electronic specific heat, standard Kadowaki-Woods scaling is dramatically violated, highlighting the need for new theoretical descriptions of $\tau^2$ resistivity in SrTiO$_3$.


*Work supported by DOE through the UMN Center for Quantum Materials. E.M. thanks Fonds de Recherche du Québec and NSERC for fellowship support.

3:30PM P46.00004: Influence of structural distortions on the magnetic order of rare-earth titanates*  ANA NAJEV (Presenter), Faculty of Science, Department of Physics, University of Zagreb, DAMJAN PELC, SAJNA HAMEED, JOSEPH JOE, MARTIN GREVEN, School of Physics and Astronomy, University of Minnesota, MIROSLAV POZEK, Faculty of Science, Department of Physics, University of Zagreb — Perovskite oxides feature fundamentally and technologically alluring properties such as magnetism, superconductivity and colossal magnetoresistance. How structural distortions and disorder influence the electron system in these materials is an important open question. Rare-earth titanates show promise in shedding new light on this problem through the study of their magnetic ground states, which are controlled by distortions induced by different-sized rare-earth ions. The compounds exhibit an interplay among charge, orbital, spin and lattice degrees of freedom, which produces a complex phase diagram that includes ferromagnetic and antiferromagnetic phases (e.g., in $Y_{1-x}La_xTiO_3$) and metal-insulator transitions (e.g., $Y_{1-x}Ca_xTiO_3$, $La_{1-x}Sr_xTiO_3$). We have conducted NMR measurements on select rare-earth titanates. Our results point to unusual local behavior well above magnetic ordering temperatures, which is not seen by macroscopic probes. Additionally, we have modified the structural distortions by uniaxial pressure and investigated their effect via magnetic susceptibility measurements.

*This work was funded by the Croatian Science Foundation (Project IP-01-2018-2970) and by the US Department of Energy through the University of Minnesota Center for Quantum Materials under DE-SC-0016371.
3:42PM P46.00005: Multipolar orders in Kondo materials [invited] Sungbin Lee, Korea Adv Inst of Sci & Tech, Arun Paramekanti (Presenter), Univ of Toronto — Recent experiments on a series of Pr-based heavy fermion cage compounds have found evidence of complex quadrupolar and octupolar orders emerging from interactions between localized non-Kramers doublets. This talk will discuss our recent work, employing Landau theory and Monte Carlo simulations, showing that incorporating multispin interactions is important to understanding such ordered states. We argue that such interactions might become increasingly important near the small-to-large Fermi surface transition.

4:18PM P46.00006: Changes in phonon dispersion across metal-insulator transition in a Pr-containing cobaltite* Daniel Phelan (Presenter), Matthew Krogstad, Materials Science Division, Argonne National Laboratory, Nathaniel Schreiber, Department of Materials Science and Engineering, Cornell University, Raymond Osborn, Materials Science Division, Argonne National Laboratory, Ayman Said, Advanced Photon Source, Argonne National Laboratory, Hong Zheng, Stephan Rosenkrantz, Materials Science Division, Argonne National Laboratory — A group of praseodymium-containing cobaltites are known to undergo 1st order metal-insulator transitions that are correlated to valence shifts that involve both Pr and Co cations. We have measured the dispersion of acoustic phonons in a single crystal of (Pr$_{0.85}$Y$_{0.15}$)$_{0.7}$Ca$_{0.3}$CoO$_{3-\delta}$ in both the metallic and insulating states and have observed differences which arise at the phase transition temperature. We interpret changes in the mode energies in terms of changes in the elastic constants. Anomalous damping of the phonons is observed near the phase transition. Elastic diffuse scattering, symptomatic of precursory behavior in the metallic phase is observed.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Science, Materials Science and Engineering Division. This research used resources of the Advanced Photon Source, a US Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.
4:30PM P46.00007: Phonon density of states of the infinite layer nickelate Nd$_{0.8}$Sr$_{0.2}$NiO$_2$*

STEPHAN ROSENKRANZ (Presenter), DANIEL PHELAN, BIXIA WANG, HONG ZHENG, Materials Science Division, Argonne National Laboratory, DOUGLAS L ABERNATHY, Neutron Scattering Division, Oak Ridge National Laboratory, JOHN MITCHELL, RAYMOND OSBORN, Materials Science Division, Argonne National Laboratory — One of the main mysteries of high-temperature superconductivity in oxides is why this has so far only been observed for cuprates, but not for other oxides with transition metals exhibiting similar electronic properties. The recent report of superconductivity up to 15K in a thin film nickelate with similar crystal and electronic structures to that of the cuprates, suggests that these infinite-layer nickelates could harbor superconductivity with the same underlying pairing mechanism as the cuprates. Here we report inelastic neutron scattering measurements performed on a bulk sample of Nd$_{0.8}$Sr$_{0.2}$NiO$_2$, the same nominal composition for which superconductivity was observed in thin film form grown on a SrTiO$_3$ substrate. We will discuss the implications of our results, in particular the measured phonon density of states, on possible superconducting mechanisms in this compound.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. Work at ORNL’s Spallation Neutron Source was sponsored by the U.S. DOE, Office of Basic Energy Sciences, Scientific User Facilities Division.

4:42PM P46.00008: Study of competing order parameters and relaxation dynamics in La$_{1/3}$Sr$_{2/3}$FeO$_3$ using first-principles  
NAM NGUYEN (Presenter), VIJAY SINGH, HYOWON PARK, Univ of Illinois - Chicago — La$_{1/3}$Sr$_{2/3}$FeO$_3$ is a strongly correlated material exhibiting the strong interplay between spin, charge, and lattice degrees of freedom. It is an antiferromagnetic Mott insulator at low temperature below 200K accompanying a charge ordering with the Fe-O bond disproportionation. The charge ordering driven by magnetism shows the Fe$^{3+}$/Fe$^{5+}$/Fe$^{3+}$/Fe$^{3+}$/Fe$^{5+}$/Fe$^{3+}$ structure along the [111] direction, and it disappears above 200K as the magnetic order is suppressed. Using first-principles calculations, we identify two charge ordering structures can occur in this material. With close energetics near the ground state and study electronic and structural orders along the energy path obtained using method of climbing image nudged elastic band. We then solve the time-dependent Landau equation along the Free energy path and study the non-equilibrium dynamics of those competing order parameters. Our results can provide an insightful explanation to the slow dynamics of this material observed in the recent ultra-fast experimental measurement.
4:54PM P46.00009: Synthesis and characterization of bulk polycrystalline Nd\textsubscript{1-x}Sr\textsubscript{x}NiO\textsubscript{3} and 
Nd\textsubscript{1-x}Sr\textsubscript{x}NiO\textsubscript{2}\textsuperscript{*}  

BIXIA WANG (Presenter), HONG ZHENG, STEPHAN ROSENKRANZ, DANIEL PHELAN, 
JOHN MITCHELL, Argonne Natl Lab — Recently, superconductivity has been reported for Sr-doped nickelate NdNiO\textsubscript{2} thin films [1]. This intriguing result represents a realization of the long-sought superconductivity in oxides that possess low-valence nickel cations in square planar coordination. In this work, we have synthesized bulk polycrystalline Nd\textsubscript{1-x}Sr\textsubscript{x}NiO\textsubscript{3} and Nd\textsubscript{1-x}Sr\textsubscript{x}NiO\textsubscript{2} compounds. The electrical, magnetic and structural properties of these compounds are discussed.


*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Science, Materials Science and Engineering Division.

5:06PM P46.00010: Quantum Materials for Energy Efficient Neuromorphic Computing: 
Defective La\textsubscript{1-x}Sr\textsubscript{x}CoO\textsubscript{3-d}\textsuperscript{*}  

SHENLI ZHANG (Presenter), GIULIA GALLI, University of Chicago — We present a first principle study of La\textsubscript{1-x}Sr\textsubscript{x}CoO\textsubscript{3-d}, a promising candidate material to build devices for neuromorphic computers. In particular we investigate how the generation of oxygen vacancies can drive a metal-to-insulator transition in the system, with focus on the interplay between structural, electronic and magnetic properties.

Using DFT+U and the Quantum Espresso package (https://github.com/QEF/q-e/releases/tag/qe-6.1.0), we found that increasing the oxygen vacancy concentration from 0 % to ~11 % leads to a change of the cobalt’s oxidation state and of the magnetic state of the system, accompanied by a variation of the octahedral tilt angle and lattice parameters. Altogether these changes determine the opening of the fundamental gap. For x = 0 (no Sr doping) and d varying from 0 to 0.5, we observe a structural transformation from a perovskite phase (semiconductor) to a brownmillerite phase (insulator), consistent with experiments.

*This work was supported as part of the Quantum-Materials for Energy Efficient Neuromorphic-Computing (Q-MEEN-C), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award # DE-SC0019273.
P46.00011: Protonation-induced magnetic phase transition in SrRuO$_3$* WEIDONG LUO (Presenter), ZIJUN TIAN, School of Physics and Astronomy, Shanghai Jiao Tong University, ZHUOLU LI, SHENGCHUN SHEN, PU YU, Department of Physics, Tsinghua University — In transition metal oxides, the subtle modulation of charge carrier triggers the emergence of exotic electronic and magnetic properties. In the ferromagnetic metal SrRuO$_3$, experiment has shown a systematic and reversible control of both carrier density and crystalline symmetry through the ionic liquid gating induced protonation. The insertion of protons dopes the SrRuO$_3$, leading to a ferromagnetic to paramagnetic phase transition. In order to understand the protonation induced structural and magnetic phase transformations in SrRuO$_3$, we performed first-principles calculations. The proton intercalation leads to a significant splitting of the degenerated Ru t$_{2g}$ bands, resulting in dramatically modified density of states. The lattice also shows a significant expansion with the intercalation of proton, consistent with the XRD results. The observed ferromagnetic to paramagnetic transition in SrRuO$_3$ can be understood within the Stoner model.

*This work is supported by the National Natural Science Foundation of China (Grant Nos. U1632272, 11521404, and 51788104).

Wednesday, March 4, 2020 2:30 PM - 5:06 PM

Session P47 GMAG: Magnetism of 2D Semiconductors, Dichalcogenides and Graphene 710/712 - Scott Crooker, Los Alamos Natl Lab

2:30PM P47.00001: Magnetic interactions in the 2D layered van der Waals semiconductor CrPS$_4$ STUART CALDER (Presenter), Oak Ridge National Lab, AMANDA HAGLUND, University of Tennessee, YAOHUA LIU, DANIEL PAJEROWSKI, HUIBO CAO, TRAVIS WILLIAMS, VASILE O GARLEA, Oak Ridge National Lab, DAVID MANDRUS, University of Tennessee — Compounds with two-dimensional layers weakly connected by van der Waals bonding offer routes to enhanced quantum behavior in the bulk as well as in reduced layer materials achieved through exfoliation analogous to graphene. The presence of magnetic ions in the layers can provide new fundamental insights and possible functionality. Consequently the search and investigation of such "beyond graphene" materials has proved a recent focus for research efforts. CrPS$_4$ is such a semiconducting magnetic van der Waals material, however has undergone only limited experimental investigations to date. Here we present a series of neutron scattering measurements that allow the magnetic structure to be determined and exchange interactions extracted. The results reveal the subtle role of competing interactions, which manifest in a non-trivial magnetic transition and a tunable magnetic structure with small applied fields. Our results in the bulk compound provide intriguing insights that can be applied to an understanding of the behavior of reduced layer CrPS$_4$. 
2:42PM P47.00002: High Curie temperature and strain-induced spin reorientation transition in two dimensional CrPbTe3* IMRAN KHAN, JISANG HONG (Presenter), Pukyong National Univ — We investigated the strain-induced magnetic properties of two-dimensional CrPbTe3 (CPT) monolayer belonged to the members of Cr based two-dimensional family. We explored the possibility of fabrication of 2D layer through the mechanical stability, dynamical stability, formation energy, cohesive energy, and thermal stability calculations. We found ferromagnetic ground state and the pristine CrPbTe3 monolayer had an indirect band gap of 0.25 eV with an in-plane magnetic anisotropy of -1.37 meV/cell. The Curie temperature was 110 K and this is much larger than that of CrI3, CrSiTe3, and CrGeTe3. Under the 4 % tensile strain, the band gap was increased to 0.45 eV and also the Curie temperature was enhanced to 150 K. We found strain-induced semiconductor-metal transition under the compressive strain and also the spin reorientation transition from in-plane to perpendicular magnetic anisotropy at 4 % compressive strain and the perpendicular magnetic anisotropy energy was almost three times larger than that of the CrGeTe3 layer. Our finding may suggest that the CrPbTe3 system can be utilized for spintronics and straintronic applications.

*This research was supported by the National Research Foundation of Korea (NRF) (2019RA21B5B01069807).

2:54PM P47.00003: Magnetic Properties of Proton Irradiated van der Waals Magnets* SRINIVASA RAO SINGAMANENI (Presenter), LUIS M MARTINEZ, HECTOR ITURRIAGA, OLMOS RUBYANN, University of Texas, El Paso, QIANG WANG, West Virginia University, SHAO LIN, Texas A&M, YU LIU, CEDOMIR PETROVIC, Brookhaven National Laboratory — The advent of two-dimensional (2D) van der Waals (vdWs) magnetic crystals such as ABTe3 (A = Fe, Cr, Mn; and B = Si, Ge) creates new possibilities in exploring their magnetic properties as they are easily exfoliable. They retain their magnetic nature, chemical stability and structural integrity down to monolayers and, are readily tuned by various kinds of external stimuli, and opened enormous opportunities in controlling their magnetic states through coupling with external perturbations. Irradiation with protons has been shown to be an effective versatile method in inducing and manipulating the magnetic and electronic properties. In this work, we present and discuss the magnetic properties of proton irradiated vdWs magnets such MnSiTe3 and CrSiTe3 as a function of proton fluence (10^15 to 10^18/cm^2). Our findings show that it is possible to tune the saturation magnetization by about 53% in both these crystals. As evidenced from complementary measurements, spin-lattice coupling is strongly modified upon proton irradiation and that could cause the observed changes in the magnetic properties.

*Nuclear Regulatory Commission, 31310018M0019.
3:06PM P47.00004: Optical Characterizations of Magnetic Phases in Two-Dimensional Ferromagnetic Semiconductor CrSBr  KIHONG LEE (Presenter), AVALON DISMUKES, EVAN TELFORD, CORY DEAN, XIAOYANG ZHU, XAVIER ROY, Columbia University —
The advent of two-dimensional (2D) magnetic materials has not only altered our understanding of magnetism in low-dimensional systems, but invites numerous applications in nanoscale transport, optoelectronics, and quantum devices. However, the library of materials has been limited to metals and insulators with strong air-sensitivity, limiting the potential scope of utilization. Here, we present 2D ferromagnetic semiconductor CrSBr, which possesses in-plane magnetic anisotropy and interlayer antiferromagnetic coupling. Magnetic phase transitions in CrSBr are probed with second- and third-harmonic generations in various thicknesses to the monolayer limit. With decreasing number of layers, CrSBr displays unconventional increase in magnetic transition temperature. Linear spectroscopy and transport measurements demonstrate the semiconducting nature of the material. Lastly, Raman spectroscopy reveals complex magnetic phases in bulk CrSBr, some of which are suppressed at the atomically thin limit.

3:18PM P47.00005: Magnetic anisotropy of two-dimensional ferromagnetic insulator MnBi$_2$Te$_4$*  YANG LI (Presenter), WENHUI DUAN, Department of physics, Tsinghua university —
MnBi$_2$Te$_4$ has attracted great interest recently due to its magnetic and topological properties. Based on the density functional theory calculation, we systematically study the magnetic anisotropy of the monolayer MnBi$_2$Te$_4$, which is vital for establishing the long-range magnetic order in two-dimensional system. We find the exchange interaction in monolayer MnBi$_2$Te$_4$ almost has no contribution to the magnetic anisotropy, as a result of the weak p-d hybridization between Mn and Te. The magnetic anisotropy originates from the single-ion anisotropy, leading to a ferromagnetic Curie temperature of about 20 K. Interestingly, the emergence of the single-ion anisotropy cannot be induced solely by the spin-orbit coupling of Mn atoms, but also involves the spin-orbit coupling of ligand Te. This behavior is very different from that in monolayer CrI$_3$ and CrGeTe$_3$. Our findings may provide a comprehensive understanding of the magnetic behavior in monolayer MnBi$_2$Te$_4$ and motivate further research on its potential applications.

*This work was supported by the Ministry of Science and Technology of China (Grant No. 2016YFA0301001), the National Natural Science Foundation of China (Grant Nos. 11674188 and 51788104), and the Beijing Advanced Innovation Center for Future Chip (ICFC).
Ferrimagnetic excitations in the layered hexagonal compound $\text{Mn}_3\text{Si}_2\text{Te}_6^*$

MATTHEW STONE (Presenter), GABRIELE SALA, JIAO LIN, ANDREW MAY, Oak Ridge National Laboratory — The layered ferrimagnet $\text{Mn}_3\text{Si}_2\text{Te}_6$ orders below $T_c=78$ K. The $S=5/2$ Mn sites are arranged in alternating honeycomb and triangular lattice layers. Each honeycomb layer is ferromagnetically ordered with the moments pointing in a singular direction in the ab-plane. The triangular lattice layer has the moments also pointing in the ab-plane but in the opposite direction. A net moment is generated due to an imbalance in the Mn content within the different layer types. We examine single crystal inelastic neutron scattering measurements of the excitations in $\text{Mn}_3\text{Si}_2\text{Te}_6$ below $T_c$. We use super-resolution image correlation techniques to refine the resolution convolved spin-wave spectrum in order to determine the exchange interactions in this system. We find significant exchange interactions orthogonal to the ab-plane, produce a network of geometrically frustrated interactions. The potential for Dirac nodes in the dispersion of the coupled ferromagnetic hexagonal layers will also be considered.

*This research was supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. A portion of this research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

Large scale synthesis of monolayer ferromagnetic $\text{Fe}_3\text{GeTe}_2^*$

RYAN ROEMER (Presenter), CHONG LIU, KE ZOU, University of British Columbia — Until now, the two-dimensional ferromagnets remain limited to exfoliated micron-sized samples. Large-scale thin films are desirable for the fabrication of integrated devices for spintronic and memory storage applications. We show, by molecular beam epitaxy, the synthesis of high-quality $\text{Fe}_3\text{GeTe}_2$ (FGT) films, a promising candidate that carries ferromagnetic states at room temperature upon ionic liquid gating. The FGT unit cell consists of two weakly coupled quintuple layer substructures with hexagonal symmetry, confirmed by surface x-ray diffraction.

*Quantum Electronic Science & Technology (QuEST) scholarship
Magnetism tunability in wafer-scale few-layered van der Waals ferromagnetic Fe₃GeTe₂ films

SHANSAN LIU (Presenter), KE YANG, ZIHAN LI, Department of Physics, Fudan Univ, WENQING LIU, Department of Electronic Engineering, Royal Holloway University of London, ENZE ZHANG, HUA WU, FAXIAN XIU, Department of Physics, Fudan Univ — Two-dimensional (2D) ferromagnetic materials have been discovered with tunable magnetism and nodal-line properties. 2D magnetism modulation in exfoliated nanoflakes via electrostatic gating introduces the boosted Tₘ. One of the most intriguing challenges, however, is still the realization of high Tₘ materials that are tunable, robust. Here, we report the effective manipulation of magnetic properties of wafer-scale 2D ferromagnetic Fe₃GeTe₂ films by changing the sample composition and utilizing the proximity effect in ferromagnetic/antiferromagnetic heterostructures. With the film thickness decreasing, Tₘ drops continuously from 220 K (bulk-like) down to 130 K (few-layer). By varying the sample compositions, Tₘ will monotonously increase as the ratio changing. Tₘ behaves a rising trend as the ferromagnetic/antiferromagnetic heterostructure period increases. Our experiments have confirmed the room-temperature Tₘ and the phase transition, which are consistent with the DFT calculations. The large-scale high-Tₘ film growth and controllable ferromagnetism of Fe₃GeTe₂ promise the practical spintronic applications. It also opens unprecedented opportunities to explore rich physics in heterostructures of van der Waals ferromagnets with 2D superconductors and topological materials.

Magnetic interactions in two-dimensional single-layer transition-metal dichalcogenides*

TATSUYA SHISHIDOU (Presenter), MICHAEL WEINERT, University of Wisconsin - Milwaukee — The transition-metal dichalcogenides (TMD), a class of two-dimensional layered van der Waals materials, have attracted extensive interest because of the wide variety of physical properties that they exhibit. An important recent addition is the intrinsic ferromagnetic order found in atomic single layers of VSe₂ [1] and MnSe₂ [2] that persists above room temperature. This discovery opens up exciting opportunities [3] to study strong spin fluctuations in reduced dimensionality, as well as to engineer novel spintronic devices. In this talk, using a density-functional spin-spiral approach [4], we address the magnetic interactions in two-dimensional TMD films in the ultrathin limit.


*This work is supported by the U.S. National Science Foundation, EFMA-1741673.
4:18PM P47.00010: High Curie temperature in magnetically doped tungsten diselenide
SABYASACHI TIWARI (Presenter), MAARTEN L VAN DE PUT, Department of Materials Science and Engineering, The University of Texas at Dallas, BART SOREE, imec, WILLIAM G VANDENBERGHE, Department of Materials Science and Engineering, The University of Texas at Dallas — Two-dimensional (2D) magnets have attracted immense attention recently because of their possible use in future energy-efficient spintronic devices. A class of 2D magnetic materials are transition-metal dichalcogenides (TMDs) that are substitutionally doped with magnetic transition metals like Cr, Fe, and Mn. Especially, TMDs based on heavy elements like tungsten (W) and selenium (Se). In this work, we investigate magnetism in magnetically doped WSe$_2$ monolayers using Density Functional Theory (DFT). In particular, we simulate the magnetic phase transition using Monte-Carlo simulations of a classical Heisenberg Hamiltonian, built for randomly doped samples of WSe$_2$. Specifically, we investigate the effect of dopant-atom clustering on the magnetic properties of doped monolayer WSe$_2$. To take into account the effect of the clustering of the dopant atoms, we introduce a functional form for the exchange interaction and obtain the parameters of our classical Heisenberg Hamiltonian from total energy DFT calculations. From the Monte-Carlo calculations, we extract the doping-density-dependent Curie temperature for each dopant atom. Finally, we show a high Curie temperature of about 300 K in Fe/Mn-doped WSe$_2$ at a doping concentration of 7-8%.

4:30PM P47.00011: Magnetic Response of Graphene Flakes*
SEAN DEYO (Presenter), SELMAN P HERSHFIELD, Physics, University of Florida — The orbital diamagnetism and spin paramagnetism of graphene flakes is computed as a function of size, shape, boundary type, and temperature, using a nearest-neighbor tight binding Hamiltonian. In general the orbital magnetization per atom grows as the size of the flake increases, but not necessarily monotonically. Flakes with "open" boundaries, where open means there are atoms on the edges of the flake with only one nearest neighbor, exhibit a smaller magnetization than flakes with "closed" boundaries, where closed means every atom has at least two nearest neighbors. The orbital susceptibility increases with temperature for open flakes, whereas the closed flakes show little change at low temperatures.

The paramagnetic spin response also depends on the boundaries. In particular, for certain types of edge defects states near zero energy are created. The wave functions of these states are not localized to the boundary. They produce a paramagnetic response that looks like an isolated spin so that the net magnetization of the flake is paramagnetic at low fields and diamagnetic at higher fields. Such magnetization vs. B plots have been observed.

*We thank the University of Florida's University Scholars Program for funding this research.
4:42PM P47.00012: Computational challenges in the characterization of magnetism for atomically precise nanographenes on noble metal substrates.*  
CARLO ANTONIO PIGNEDOLI (Presenter), KRISTJAN EIMRE, SHANTANU MISHRA, Empa, Swiss Federal Laboratories for Materials Science and Technology, DOREEN BEYER, Faculty of Chemistry and Food Chemistry & Center for Advancing Electronics Dresden, Technical University of Dresden, Dresden, Germany, OLIVER GRÖNING, PASCAL RUFFIEUX, ROMAN FASEL, Empa, Swiss Federal Laboratories for Materials Science and Technology — On-surface synthesis techniques have demonstrated high flexibility and atomic precision in the fabrication of carbon-based nanomaterials, with recent examples ranging from graphene nanoribbons hosting topological quantum phases\(^1\) to specifically shaped nanographenes (NGs).\(^2\)-\(^5\) NGs may exhibit a magnetic, open-shell structure as a result of their peculiar topology, which makes them highly attractive for applications in molecular electronics. Furthermore, unpaired spins in open-shell NGs may be used to perform spin logic operations. I will discuss present challenges for ab-initio simulations in understanding recent experiments reporting evidence of magnetism for specific nanographenes supported on gold substrates. I will present both, cases of non-Kekulé NGs where sublattice imbalance is responsible for magnetism, and of NGs where - despite absence of sublattice imbalance - topological frustration in the underlying π-electron network generates uncompensated radicals.


*This work was supported by the Swiss National Science Foundation, NCCR MARVEL*
Increased Curie temperature and enhanced perpendicular magneto anisotropy of Cr$_2$Ge$_2$Te$_6$/NiO heterostructure*  

ANDRES LLACSAHUANGA ALLCCA (Presenter), Physics and Astronomy, Purdue University, HIROSHI IDZUCHI, XING-CHENG PAN, KATSUMI TANIGAKI, Advanced Institute for Material Research, Tohoku University, YONG CHEN, Physics and Astronomy, Purdue University — Van der Waals (vdW) materials with ferromagnetic properties down to few layers such as CrI$_3$ and Cr$_2$Ge$_2$Te$_6$ have recently attracted a lot of attention due to their potential in spintronic applications. However, the Curie temperature (T$_C$) of these vdW has remained relatively low. Here, we report increased T$_C$ and enhanced perpendicular magnetic anisotropy in Cr$_2$Ge$_2$Te$_6$ (CGT) flakes interfaced with antiferromagnetic insulator NiO for a wide range of CGT thicknesses (5-200 nm).

Measurements of the same flake by polar magneto optic Kerr effect (MOKE) microscopy before and after coating NiO reveal a hysteresis loop with a square shape and larger coercive field for the CGT/NiO heterostructure. Furthermore, the maximum T$_C$ observed for CGT/NiO reached ~120K, almost double the T$_C$ of CGT alone (~60K). These observations suggest that interfacing van der Waals ferromagnets with other materials could provide a venue to engineer their magnetic properties. [1]


*We acknowledge partial support of the work by NSF, Sumimoto Foundation, WPI-AIMR, and JSPS.
**P47.00014: 2D Layered Ferromagnet: the Emergence of Skyrmions in Transition Metal Dichalcogenides**

*YUNBO OU (Presenter), Francis Bitter Magnet Laboratory, Plasma Science and Fusion Center, Massachusetts Institute of Technology, NORBERT MARCEL NEMES, Unidad Asociada ICMM-CSIC "Laboratorio de Heteroestructuras con Aplicación en Espintronica", Complutense University of Madrid, JOSE LUIZ MARTINEZ, Instituto de Ciencia de Materiales de Madrid ICMM-CSIC, MIRKO ROCCI, HANG CHI, Francis Bitter Magnet Laboratory, Plasma Science and Fusion Center, Massachusetts Institute of Technology, DANIEL LARSON, Department of Physics, Harvard University, AUSTIN AKEY, Center for Nanoscale Systems, Harvard University, WENBO GE, Department of Physics and Astronomy, Rutgers University, DHAVALA SURI, Francis Bitter Magnet Laboratory, Plasma Science and Fusion Center, Massachusetts Institute of Technology, DAVID CHARLES BELL, School of Engineering and Applied Sciences, Harvard University, WEIDA WU, Department of Physics and Astronomy, Rutgers University, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University, JAGADEESH MOODERA, Department of Physics, Massachusetts Institute of Technology — Recently there is great attraction drawn towards Van der Waals (vdW) ferromagnet since the discovery of ferromagnetism in monolayer CrI$_3$. Due to the extraordinary topology driven properties, magnetic transition metal dichalcogenides (TMDCs) appear to behave more exotically. In this work, utilizing molecular beam epitaxy, a stable CrTe$_2$, one of TMDCs, films are fabricated down to monolayer (ML) level. Ferromagnetism is exhibited even down to the 2D insulating limit - 1 ML film. Surprisingly, the topological Hall effect (THE), which manifests the real space topology of magnetic structure in TMDCs, is observed in thicker films (> 6 ML) up to 130 K, a first such observation. Electric transport data and magnetometry data indicate a high possibility of presence of magnetic Skyrmions, real space nanometer-sized quasi-particles with topological spin textures. Although they are found in many systems even at room temperature, but not in TMDCs, until now. The discovery of magnetism in monolayer CrTe$_2$ and topological magnetic structure in thicker CrTe$_2$ not only enriches the 2D magnet family and the capability of TMDCs, but also pave a way for all vdW materials based spintronic devices.

*Supported by NSF (NSF-DMR 1700137), ONR (N00014-16-1-2657), CIQM (DMR-1231319) and ARO (ARO W911NF1920041).

**Wednesday, March 4, 2020 2:30 PM - 5:06 PM**

**Session P48 DCMP: Superconductivity: Transport Properties II** Mile High

Ballroom 1A - Jose Vicent, Univ Complutense
2:30PM P48.00001: Study on the pressure-induced superconducting phases of antimony*
ZHENG WU (Presenter), LIANGZI DENG, MELISSA GOOCH, SHUYUAN HUYAN, PAUL C. W. CHU, Texas Center for Superconductivity and Department of Physics, University of Houston — Pressure-induced superconductivity in antimony was investigated electrically using a diamond anvil cell up to 61 GPa. A semimetal to metal transition was observed in the pressure range of 22 to 28 GPa at room temperature, which coincides with the transition from an incommensurate tetragonal host-guest structure to a body-centered cubic (bcc) structure. The high pressure metal phase was found to be superconducting and the transition temperature ($T_c$) was non-monotonous with regard to the applied pressure while in the bcc structure. The empirical rule, lighter elements having higher $T_c$s in a homologous series in non-transition elements in the periodic table, was found not to hold for bcc Sb when compared with Bi. A controlled pressure quench of the superconducting phase in the incommensurate composite phases at temperatures up to 77 K was also performed and the zero resistance was retained in the quenched phase with the midpoint of the superconducting transition above 3.4 K and a transition width of 0.2 K.

*The work performed at Houston is supported by USAFOSR Grant FA9550-15-1-0236, TLL Temple Foundation, JJ&R Moores Endowment, and State of Texas through TCSUH.

2:42PM P48.00002: Andreev quantum dot chain in an InSb nanowire  HAO WU (Presenter), PO ZHANG, JUN CHEN, University of Pittsburgh, SASA GAZIBEGOVIC, ROY OP HET VELD, GHADA BADAWY, ERIK BAKKERS, Eindhoven University of Technology, SERGEY M FROLOV, University of Pittsburgh — We built a chain of quantum dots in a semiconductor nanowire to study the Kitaev model of a one dimensional topological superconductor. Three quantum dots are electrostatically confined in an InSb nanowire. Each dot is strongly coupled to a superconducting NbTiN electrode. We observe Andreev bound states in each of these quantum dots and study their magnetic field dependence with fields parallel to the nanowire axis. Having two normal contacts at the wire ends and three superconducting leads, we are able to perform non-local measurements. We study spatial separation of Andreev bound states in this three dots chain with various inter-dot coupling strengths. Our experiments may provide insights on non-locality of zero modes in Majorana wires.
2:54PM P48.00003: Quantum Hall Effect in an Epitaxial Nitride Semiconductor/Superconductor Heterostructure*  PHILLIP DANG (Presenter), GURU BAHADUR KHALSA, Cornell University, D. SCOTT KATZER, NEERAJ NEPAL, BRIAN DOWNEY, VIRGINIA D. WHEELER, U.S. Naval Research Laboratory, ALEXEY SUSLOV, National High Magnetic Field Laboratory, ANDY XIE, EDWARD BEAM, YU CAO, CATHY LEE, Qorvo, HUILI XING, Cornell University, DAVID MEYER, U.S. Naval Research Laboratory, DEBDEEP JENA, Cornell University — The quantum Hall effect (QHE) is a paragon of topological protection in electronic states, exhibiting exceptional precision in resistance, while superconductivity allows exceptional precision in voltage due to flux quantization. To create seamless heterostructures of these two electronic phases is highly desirable for the discovery of new physics and use in quantum information science. To this end, we design an all-epitaxial superconductor/semiconductor nitride heterostructure, based on GaN two-dimensional electron gases (2DEGs) and superconducting NbN, using an industrial device process that is compatible with silicon and nitride semiconductor technology. The heterostructure is demonstrated to simultaneously exhibit the integer QHE in the GaN 2DEG and superconductivity in the NbN. Such a demonstration in an all-epitaxial nitride heterostructure is the first of its kind and paves the way for new quantum technologies.

*This work was supported by ONR Grant No. N00014-17-1-2414 monitored by Dr. Paul Maki and by NSF Grant Nos. E2CDA 1740286 and NewLAW EFRI 1741694. P.D.’s support by NSF GRFP Grant No. DGE-1650441 is acknowledged. The National High Magnetic Field Laboratory is supported by the NSF Cooperative Agreement No. DMR-1644779 and the State of Florida.

3:06PM P48.00004: Transport properties of double quantum dots coupled to a superconductor  PO ZHANG (Presenter), HAO WU, University of Pittsburgh, SABBIR AHMED KHAN, PETER KROGSTRUP, University of Copenhagen, DAVID PEKKER, SERGEY M FROLOV, University of Pittsburgh — Superconductor/semiconductor hybrid systems have drawn a lot of attention due to their rich physics and the potential to demonstrate topologically protected qubits. We experimentally investigate transport properties of a double dot electrostatically defined in an InAs nanowire by metallic gates under the wire. Superconductivity is provided by epitaxial Al shell grown in-situ after nanowire growth. The shell induces a hard gap and sharp spectral features of Andreev bound states in the nanowire. The source of the double dot is a normal metal while the drain is a superconductor. We study the spectra of the resulting normal-Andreev double dot and search for the recently proposed Andreev blockade upon which current is blocked in the triplet (1,1) configuration which is unable to form a Cooper pair and enter the drain superconductor.
Angular dependence of the magnetoresistance in HgBa$_2$CuO$_{4+\delta}$.*

KATHERINE SCHREIBER (Presenter), ERIC BAUER, NEIL HARRISON, MUN KEAT CHAN, Los Alamos Natl Lab — The Fermi surface in the cuprates is known to undergo significant changes with temperature and doping, from Fermi arcs to small pockets reconstructed by charge density wave order. In general the shape of the Fermi surface for a particular phase reveals information about its place in the phase diagram; for example, the symmetries broken by the charge density wave. Such information is valuable to understanding the relationship of these phases to high temperature superconductivity. The pseudogap phase is of particular interest because superconductivity and the charge density wave emerge from this phase as temperature is lowered.

Here we present measurements of the angular dependence of the c-axis magnetoresistance in the pseudogap regime of underdoped single layer cuprate HgBa$_2$CuO$_{4+\delta}$. We have performed transport measurements up to 65 T at many angles of the c-axis with respect to the applied field. From this data we are able to extract details about the structure of the Fermi surface in the pseudogap regime and discuss its morphology.

*NHMFL is supported by the National Science Foundation through NSF/DMR-1644779, the state of Florida and the U.S. Department of Energy. This work is also funded by the DOE BES “Science of 100 Tesla” grant.

Hall effect measurements under high pressure for Pr$_2$Ba$_4$Cu$_7$O$_{15-\delta}$

FUMIHIRO ISHIKAWA (Presenter), Faculty of Science, Niigata University, MASAYA SAWADA, Graduate School of Science and Technology, Niigata University, AYAKO OHMURA, Faculty of Science, Niigata University, TAKASHI NAKA, National Institute for Materials Science, ANTHEUNIS DE VISser, Univ. of Amsterdam — It is well known that the Pr-substitution for Y-site in YBa$_2$Cu$_3$O$_{7-\delta}$ and YBa$_2$Cu$_4$O$_8$ dramatically suppresses the superconducting transition temperature $T_c$ and superconductivity in CuO$_2$ planes disappears. However, Pr$_2$Ba$_4$Cu$_7$O$_{15-\delta}$ (Pr247) oxide shows superconductivity with $T_c = 15$ K after reduction treatment [1]. Pr247 has the same crystal structure as Y$_2$Ba$_4$Cu$_7$O$_{15-\delta}$ with an alternative repetition of the single and double chains along the c-axis. As-sintered sample of Pr247 shows metallic conductivity at low temperatures owing to the conduction in the CuO double chains. Reduction treatment on Pr247 caused the electron carrier density change by controlling the amount of oxygen deficiency. Applying high pressure on superconductive Pr247 suppresses the superconductivity. This is well explained by the one-dimensional conduction mechanism based on Tomonaga-Luttinger liquid theory [2]. High pressure study on Hall effect reveals the effect of pressure on electron carrier concentration for Pr247.


*This work is supported by the JSPS (Japan Society for the Promotion of Science) Program for Fostering Globally Talented Researchers, Grant No. JPMXS05R2900003.
Influence of plastic deformation on the transport and magnetic properties of strontium titanate

SAJNA HAMEED (Presenter), DAMJAN PELC, ZACHARY ANDERSON, School of Physics and Astronomy, University of Minnesota Twin Cities, CHRIS LEIGHTON, Chemical Engineering and Materials Science, University of Minnesota, MARTIN GREVEN, School of Physics and Astronomy, University of Minnesota Twin Cities — Strontium titanate (SrTiO$_3$, STO) is one of the most important transition metal oxides: it is a model perovskite with a structural phase transition, and also one of the most commonly used single crystal substrates for epitaxial growth of oxide thin films. Superconductivity in STO occurs at unusually low carrier densities at temperatures well below 1 K and is not understood, even five decades after its discovery.

Building on our recent work on oxide superconductors [1], we explore another interesting property of STO: its high ductility at room temperature, which allows us to plastically deform single crystals using uniaxial pressure. We report on the influence of this compressive plastic deformation on the transport and magnetic properties of STO, with particular emphasis on the superconducting state.


Work supported by the Department of Energy through the University of Minnesota Center for Quantum Materials under DE-SC0016371.

Anomalous transverse magnetoresistance in superconductor/ferromagnet multilayers

XAVIER PALERMO, SALVATORE MESORACA, NICOLAS REYREN, ANKE SANDER, SOPHIE COLLIN, FLORIAN GODEL, KARIM BOUZEHOUANE, Unité Mixte de Physique CNRS/Thales, Palaiseau, France, JACOBO SANTAMARIA, GFMC, Universidad Complutense de Madrid, Spain, VINCENT CROS, Unité Mixte de Physique CNRS/Thales, Palaiseau, France, ALEXANDRE BUZDIN, LOMA, Université de Bordeaux, France, JAVIER VILLEGAS (Presenter), Unité Mixte de Physique CNRS/Thales, Palaiseau, France — We have studied the magnetoresistance of metallic multilayers composed of a low-$T_c$ superconductor (MoSi) and different ferromagnets (from single Co layers to combinations of these with heavy-elements) which present variable magnetic anisotropy and domain structure. In some cases, the longitudinal magnetoresistance shows a strong magnetic hysteresis that results from the interaction of flux quanta in the superconductor and the stray field from the ferromagnet's domains. Interestingly, that behavior is accompanied by an anomalous transverse magnetoresistance whose parity depends on the direction of the magnetic field relative to the ferromagnet's easy axis. We will discuss the different scenarios allowing for an understanding of these effects.

Work supported by ERC grant 647100 “SUSPINTRONICS” and French ANR grant ANR-15-CE24-0008-01 “SUPERTRONICS"
4:06PM P48.00009: Higgs mode and tr-ARPES in Non-equilibrium Superconductors with a Moving Condensate*  ANKIT KUMAR (Presenter), ALEXANDER F KEMPER, North Carolina State University — When a superconducting state is perturbed, one of the resulting excitations gives rise to the amplitude oscillation mode known as the Higgs mode. The existence of the Higgs mode in a perturbed broken-symmetry state is one of the fundamental phenomena in condensed matter systems. However, the Higgs mode is hard to measure experimentally due to the spin-less and charge-less nature of the condensate. Recently, it was proposed that the Higgs mode in superconductors can be coupled to light in the linear regime if there is a non-zero supercurrent present in the system. Motivated by that, we study the dynamics of the Higgs mode in the presence of supercurrent. We find that the supercurrent creates an asymmetry of the electron distribution in the momentum space which leads to a momentum-dependent superconducting spectral gap. When we pump the system with an ultra-fast light pulse, the frequency of the Higgs mode gains momentum dependence. We analyze the dynamics of the Higgs mode through the electron spectral function which can be measured using angle-resolved photoemission spectroscopy (ARPES), and propose that the presence of supercurrent may help in the observation of the Higgs mode through time-resolved ARPES.

*This work was supported by NSF DMR-1752713.

4:18PM P48.00010: Magnetoconductance of planar cuprate superconductor/graphene junctions*  KEVIN SEURRE (Presenter), VINCENT HUMBERT, Unité mixte de physique CNRS-Thales, Palaiseau, France, DAVID PERCONTE, Cold temperature laboratory, Universidad autonoma de Madrid, Madrid, Spain, CHRISTIAN ULYSSE, C2N-CNRS, Palaiseau, France, ANKE SANDER, JUAN TRASTOY QUINTELA, BRUNO DLUBAK, PIERRE SENEOR, JAVIER VILLEGAS, Unité mixte de physique CNRS-Thales, Palaiseau, France — Graphene/superconductor junctions have been extensively studied using low-Tc superconductors, but studies involving high-Tc temperature cuprates are scarce despite their interest for instance the rich physics expected from the d-wave order parameter. Here we study planar high-Tc superconductor/graphene junctions fabricated by transferring CVD graphene onto optimally doped c-axis PDL grown YBaCuO_{7-x} films, which are patterned using electron lithography and ion irradiation. Transport measurements at low temperature revealed an interesting, anomalous behavior of the magnetoconductance, which first increases at low magnetic fields before remaining constant or decreasing depending on the samples. This effect highly depends on temperature and voltage bias applied to the junction. We will discuss the different scenarios allowing for an understanding of this behavior.

*Work supported by the ERC grant n° 647100 “SUSPINTRONICS”
4:30PM P48.00011: Non-Majorana quantized zero-bias conductance peaks in semiconductor nanowire devices
MAKSIM GOMANKO (Presenter), PENG YU, Univ of Pittsburgh, GHADA BADAWY, SASA GAZIBEGOVIC, ROY OP HET VELD, ERIK BAKKERS, Eindhoven University of Technology, JUN CHEN, SERGEY M FROLOV, Univ of Pittsburgh — Quantized zero bias conductance peaks are predicted and reported in InSb nanowire devices coupled to NbTiN superconductors under certain conditions that are compatible with Majorana zero modes. These conditions include induced superconductivity, spin-orbital coupling, and an external magnetic field. We observed quantized zero bias conductance peaks at one end of similar nanowire devices, without observing matching zero bias peak of any height on the other side. These results imply either a topological segment shorter than the superconducting segment which is 400 nm, or a non-Majorana origin of the observed quantized zero-bias peaks.

4:42PM P48.00012: Versatile and selective platform for high-quality hybrid semiconductor-superconductor nanowire devices.*
NICK LOO (Presenter), GREG P. MAZUR, Delft University of Technology, SEBASTIAN HEEDT, MARINA QUINTERO PEREZ, Microsoft station Q Delft, FRANCESCO BORSOI, Delft University of Technology, ALEXANDRA FURSINA, Microsoft station Q Delft, MAY AN VAN DE POLL, Delft University of Technology, KEVIN VAN HOOGDALEM, Microsoft station Q Delft, GHADA BADAWY, SASA GAZIBEGOVIC, ERIK BAKKERS, Department of Applied Physics, Eindhoven University of Technology, LEO P. KOUWENHOVEN, Microsoft station Q Delft — Majorana bound states and topological superconductivity are highly anticipated candidates for decoherence-free quantum computation. To achieve this goal, high-quality semiconductor-superconductor hybrid systems are the most promising platform. Here, we combine high-mobility semiconductor nanowires with selective deposition of a superconducting material, resulting in state-of-the-art hybrid devices. We benchmark our devices by investigating InSb/Al Josephson junctions. In voltage-bias spectroscopy, we observe multiple Andreev reflections indicating a highly-transparent interface. Furthermore, in current-bias spectroscopy we observe remarkably high critical currents. Finally, we emphasize that we have developed a versatile platform which can easily be used to investigate different material combinations. In addition, it can be used to create sophisticated quantum circuits for the purpose of demonstrating the proof of principle of a topological qubit.

*European Research Council, Dutch Organization for Scientific Research, and Microsoft Corp. Station Q.
4:54PM P48.00013: Design and discovery of CaKRu$_4$P$_4$: a new member of the generalized 1144 structure.* MINGYU XU (Presenter), Iowa State University, PALASYUK ANDRIY, Ames Lab, SERGEY L. BUD’KO, BOQUIN SONG, KAI-MING HO, PAUL C CANFIELD, Iowa State University — AeAFe$_4$As$_4$ (Ae=Ca, Sr; A=K, Rb, Cs) compounds were discovered as a new structural type [1] which has alternate stacking of the Ae and A layers. The AeAFe$_4$As$_4$ structure is stabilized by the combination of large $\Delta c = (c^{A122} - c^{Ae122})$ and small $\Delta a = (a^{A122} - a^{Ae122})$, where a and c are lattice parameters of the AFe$_2$As$_2$ and AeFe$_2$As$_2$ parent structures. In this presentation we extent this idea to similar, phosphorus-based 122 compounds with large $\Delta c$ and small $\Delta a$ values, identifying CaKRu$_4$P$_4$ as a promising candidate. The stability of a CaK1144 type ruthenium phosphide was also recently predicted by combining first principle calculations [2]. We synthesize polycrystalline CaKRu$_4$P$_4$ by solid state reaction of CaRu$_2$P$_2$ and KRu$_2$P$_2$. The crystallographic structure and physical properties of CaKRu$_4$P$_4$ will be presented.

[2], Song Boqun, et al., APS March Meeting (2019)

*This work is supported by the US DOE, Basic Energy Sciences, Materials Science and Engineering Division under contract No.DE-AC02-07CH11358.

Wednesday, March 4, 2020 2:30 PM - 5:06 PM

Session P49 DCMP DMP: Metals: Actinide, Nuclear Related and Rare Earth Physics Mile High Ballroom 1B - Krzysztof Gofryk, Idaho National Laboratory

2:30PM P49.00001: Plutonium in high magnetic fields. MARK WARTENBE (Presenter), PAUL H TOBASH, NEIL HARRISON, JOHN SINGLETON, LAUREL E WINTER, Los Alamos National Laboratory — High magnetic field studies of plutonium have been limited up until now. The complex behavior of plutonium’s 5f electrons are thought to be responsible for the elements unusual behavior, making it possibly the strangest element in the periodic table. Here we review data from a new set of various experiments involving high magnetic field and extremes of temperature. High magnetic fields are especially effective in probing electronic states and is the highlighted method of this study. We present the data in the context of gaining in site into the 5f electrons physics of the material and its ephemeral magnetic moment.
2:42PM P49.00002: Ab initio study of the properties of liquid uranium for temperatures up to 2050 K* LUIS GONZALEZ (Presenter), BEATRIZ GONZALEZ DEL RIO, DAVID GONZALEZ, Univ de Valladolid — Uranium compounds are used as fissile materials in nuclear reactors. Nowadays the most used nuclear fuel is UO$_2$, but in generation-IV reactors other compounds are being considered, such as UC and UN [1].

Upon possible loss of coolant accidents, the core of the reactor would get heated up to very high temperatures, and it is essential to understand the behaviour of the nuclear fuel in such conditions for proper risk assessment. UO$_2$ and UC would eventually melt, but UN would not reach a melting process since at high temperatures it is thermochemically unstable, and decomposes into gaseous N$_2$ and liquid U.

The experimental study of liquid U is difficult and scarce. For instance, there is no experimental information about its static structure factor. In this contribution we analyze the properties of liquid U, studied through ab initio methods, for three temperatures in the temperature range between its melting point (1405 K) and 2050 K. We show results for the static structure and also for several dynamic properties, including atomic diffusion and viscosity.

**References:**

*Funding provided by spanish Ministry of Economy and Competitiveness and EU FEDER funds (PGC2018-093745-B-I00) and by Junta de Castilla y Leon (VA124G18).

2:54PM P49.00003: Theoretical investigations of the tritium diffusion pathways in γ-LiAlO$_2$ pellets HARI P PAUDEL, TING JIA, YUHUA DUAN (Presenter), Natl Energy Technology Lab — In tritium-producing burnable absorber rods (TPBAR), γ-LiAlO$_2$ is used in the form of an annular ceramic pellet enriched with $^6$Li isotope and is located between the zircaloy-4 liner and nickel-plated zircaloy-4 tritium getter with a gas gap in between. When irradiated in a pressurized water reactor (PWR), the $^6$Li pellets absorb neutrons and produce tritium ($^3$H) through $^6$Li + n → $^3$H + α. However, accurate analysis of the $^3$H transport through the ceramic pellets and the barrier/cladding system is hampered by the lack of fundamental data about the hydrogen isotope solubility and diffusivity. For TPBARs to enable effective tritium production in PWRs and to improve the performances of these components, we are investigating the $^3$H solubility and diffusion pathways in the bulk and surface of γ-LiAlO$_2$ with different concentrations of lithium defects. The calculated results for bulk and low-index surfaces properties, thermal conductivity, $^3$H activation energy barriers, and the diffusion coefficients in γ-LiAlO$_2$ are in good agreement with the available experimental values. With a better knowledge of $^3$H transport properties within γ-LiAlO$_2$ pellets through our modeling, its performances and higher $^3$H production rate can be further evaluated experimentally with a higher confidence.
3:06PM P49.00004: Complex Phase Behavior of U$_3$O$_8$  ANDREW MISKOWIEC (Presenter), JENNIFER NIEDZIELA, TYLER SPANO, Oak Ridge National Lab, SARAH FINKELDEI, University of California - Irvine, RODNEY HUNT, MICHAEL AMBROGIO, Oak Ridge National Lab — Oxidation of UO$_2$ produces U$_3$O$_8$. During oxidation, the unit cell undergoes a significant expansion (approx. 17%). This reaction must be considered in technological applications of UO$_2$ (such as nuclear fuel). U$_3$O$_8$ itself has multiple crystal phases, including an orthorhombic Amm2 phase that occurs below 300 °C, and a hexagonal P-62m phase above 300 °C. Although these phases are nearly isomorphic, one fact is that the Amm2 phase has two crystallographic uranium sites, and the oxidation configuration is 2U(V) + U(VI). But, the P-62m phase has only one crystallographic site, and so each of the three uranium atoms must carry 16/3 charge. We present preliminary investigations into possible resolutions of this observation, including temperature dependent Raman and x-ray diffraction measurements. Coupled with density functional theory calculations, we show an intimate relationship between phonon softening and local U-O structural re-arrangements. In particular, softening of one strong Raman-active mode near 420 cm$^{-1}$ appears to be the driving effect in the orthorhombic-to-hexagonal phase transition. We also explore the possibility of coupling between this phonon and the electronic structure and whether this phonon facilitates an electron-hopping mechanism.

3:18PM P49.00005: Crystal-field states of UO$_2$ probed by directional dependence of nonresonant inelastic x-ray scattering*  MARTIN SUNDERMANN (Presenter), Institute of Physics II, University of Cologne, GERRIT VAN DER LAAN, Magnetic Spectroscopy Group, Diamond Light Source, ANDREA SEVERING, Institute of Physics II, University of Cologne, LAURA SIMONELLI, ALBA Synchrotron Light Source, GERARD H LANDER, European Commission, Joint Research Centre (JRC), MAURITS HAVERKORT, Institute for Theoretical Physics, Heidelberg University, ROBERTO CACIUFFO, European Commission, Joint Research Centre (JRC) — Core-level nonresonant inelastic x-ray scattering (NIXS) [1-3], also called x-ray Raman scattering, has been performed on single crystals of UO$_2$ to study the directional dependence of higher-order multipole scattering from the uranium O$_{4,5}$ edges (90-110 eV). By comparing the experimental results with theoretical calculations the symmetry of the ground state is confirmed directly as the crystal-field Γ$_5$ triplet state within the $J = 4$ manifold [4] as had been suggested by inelastic neutron scattering [5]. The results demonstrate that the directional dichroism of the NIXS spectra is sensitive to the CF strength and establish NIXS as a tool for probing crystal-field interactions quantitatively.


*NIXS data were taken at the beamline ID20 at the ESRF in Grenoble under proposal HC-743. M.S. and A.S. benefited from the financial support of the Deutsche Forschungsgemeinschaft (DFG) under grant SE-1441-5-1.
Excess Electrons on Reduced AnO$_2$ (111) Surfaces (An = Th, U, Pu) and Their Impacts on Catalytic Water Splitting

GAOXUE WANG (Presenter), ENRIQUE BATISTA, PING YANG, Los Alamos National Laboratory — Excess electrons from intrinsic oxygen vacancies play a key role in the surface chemistry and catalytic properties of metal oxides. This effect is particularly critical in actinide dioxides (AnO$_2$), the most common nuclear fuels, where radiation can induce the formation of vacancies. However, the behavior of excess electrons on AnO$_2$ surfaces has not been fully explored. In this talk, I will discuss our first-principle study of the electronic structure of excess electrons from oxygen vacancies on AnO$_2$ (111) surfaces. The low-energy electronic structure is searched via U-ramping and occupation matrix control. The excess electrons are found to localize at the vacancy site on ThO$_2$, move to the metal 5f orbitals on PuO$_2$ surface, with UO$_2$ as an intermediate case. In the presence of water, the excess electrons lead to the exothermic splitting of H$_2$O and formation of H$_2$ on ThO$_2$ and UO$_2$ surfaces, while on PuO$_2$ surface the formation of H$_2$ is thermodynamically unfavorable. This work has important implications in the surface chemistry and corrosion of AnO$_2$, and hence the handling and long-term storage of spent nuclear fuels.

LANL LDRD and Director's Postdoc Fellow

First Principles Investigation of the electronic and magnetic structure of Pu$_6$Fe

SARAH HERNANDEZ (Presenter), JOHN M WILLS, Los Alamos National Laboratory — Chemical impurities within δ-plutonium (Pu) arises due to the casting and processing of the material. One impurity, iron (Fe), is believed to segregate to the grain boundaries and forms an intermetallic compound ζ-Pu$_6$Fe. This compound was determined by X-ray diffraction (XRD) to be body-centered tetragonal with a space group of I4/mcm and to date, very little is known about its physical properties, other than it has a low melting temperature at 410°C. Using density functional theory, we can predict equilibrium properties and begin to understand the fundamental electronic and magnetic structure of Pu$_6$Fe. This work will present density functional theory calculations using the all-electron full-potential linearized augmented-plane-wave plus local orbital basis method as implemented in the WIEN2k code. Calculations included a non-magnetic, ferromagnetic, and anti-ferromagnetic arrangement at the respective optimized structures with no-spin-orbit-coupling, spin-orbit-coupling, and spin-orbit-coupling with orbital polarization to gauge the different level of theories.

This work is funded by LDRD.
3:54PM P49.00008: Magnetic torque of USb single crystals  XIAXIN DING (Presenter), KESHAV SHRESTHA, Idaho National Laboratory, INGRID ZIMMERMANN, ROSS MCDONALD, FRANZISKA WEICKERT, NEIL HARRISON, MARCELO JAIME, MYRON B SALAMON, Los Alamos National Laboratory, J-C. GRIVEAU, DG Joint Research Centre, Germany, JAMES L SMITH, Los Alamos National Laboratory, KRZYSZTOF GOFRYK, Idaho National Laboratory — Over 40 years, uranium monoantimonide (USb) has been investigated by a variety of experimental and theoretical methods. This compound crystallizes in the cubic NaCl-type of crystal structure and is known to order antiferromagnetically with a non-collinear triple-k magnetic structure below $T_N \sim 214$ K. This high-symmetry complex magnetic structure consists of three equivalent $<0 0 1>$-type of wave vectors, with spins that point along $<1 1 1>$ direction. During the talk we will present results of our recent magnetic torque measurements performed on high-quality single crystals of USb at temperatures below and above $T_N$. The measurements have been carried out in both DC and pulsed magnetic fields up to 60 T. The results obtained are crucial in understanding of magnetic interactions, anisotropy, and their coupling to the lattice in this material. We will discuss implications of these results.

4:06PM P49.00009: 5f-electron localization in metallic PuPdSn*  KRZYSZTOF GOFRYK (Presenter), Idaho National Laboratory, J-C. GRIVEAU, ERIC COLINEAU, ROBERTO CACIUFFO, DG Joint Research Centre, Directorate G-Nuclear Safety and Security, Karlsruhe, Germany, JAMES L SMITH, Los Alamos National Laboratory — While the effect of electronic correlations is relatively well studied in Ce, Yb and U based materials, there is still lack of knowledge on how these collective phenomena impact magnetic, transport, and thermodynamic properties in transuranium intermetallics. Depending upon the strength of the interactions, many unusual properties such as complex magnetism, Kondo effect, heavy fermion ground state, valence fluctuations, and/or unconventional superconductivity have been observed in these materials. Here we present our detailed studies on the structural, magnetic, thermal, and transport properties of PuPdSn. This compound crystalizes in the hexagonal ZrNiAl-type of structure [space group P62m]. It orders antiferromagnetically at $T_N = 21$ K that is followed by another AF-like transition at 9.6 K. The low-temperature linear specific heat coefficient is small, $\gamma \sim 8$ mJ/mol K$^2$. All the results obtained strongly suggest the presence of well localized 5f-states in this material, which is rare among U and Pu intermetallics.

*We are grateful to R. Jardin and J. Rebizant for sample preparation and characterization. This work is supported by DOE's Early Career Research Program.
Equiatomic GdNi and HoNi are ferromagnetic materials with a Curie temperature $T_c = 69$ K and $T_c = 36$ K, respectively. These compounds exhibit a large magnetocaloric effect and are suitable for low temperature magnetic refrigerator applications. We investigate the electronic structure of GdNi and HoNi using Hard X-ray photoemission spectroscopy (HAXPES). HAXPES of the Gd and Ho 3d, 4d, 4s and 5p core level spectra confirm the atomic multiplets of Gd$^{3+}$ and Ho$^{3+}$.

Valence band HAXPES of GdNi and HoNi shows Ni 3d features at the Fermi level, confirming a partially filled 3d band, while the Gd 4f/ Ho 4f states occur at high binding energies away from the Fermi level. For GdNi, we have also carried out XAS and XMCD studies in the ferromagnetic phase at $T = 25$ K. We analyze the Gd $M_{4,5}$-edge and Ni $L_{2,3}$-edge spectra using atomic multiplet and cluster model calculations, respectively. The Gd $M_{4,5}$-edge XMCD spectrum is consistent with a ground state configuration of $S = 7/2$ and $L=0$. The Ni $L_{2,3}$-edge XMCD results indicate that the antiferromagnetically aligned Ni moments exhibit a small but finite magnetic moment ($m_{\text{tot}} \sim 0.19 \mu_B$). The results indicate that the Ni 3d band is not fully occupied and invalidates the charge-transfer model for GdNi and HoNi.
Magnetic frustration and magnetic correlations in YbMn$_2$Sb$_2$ single crystals

RAQUEL RIBEIRO (Presenter), JULIAN MUNEVAR, FABIANA R ARANTES, LETICIE MENDONÇA-FERREIRA, MARCOS A AVILA, Univ Federal do ABC, ELVEZIO MORENZONI, Paul Scherrer Institut — The crystal growth and the structural, transport and magnetic characterization of the magnetically frustrated YbMn$_2$Sb$_2$ single crystals are reported. The crystals show a trigonal symmetry, where corrugated honeycomb layers of MnSb are separated by Yb atoms. No structural transition was observed down to 22 K. The resistivity measurements show a predominantly insulating behavior. The combined resistivity, dc and ac susceptibility, and heat capacity measurements confirm successive transitions at 230 K, 116 K and 40 K, being the transition at $T_N = 116$ K due to the Mn$^{2+}$ lattice antiferromagnetic ordering. Muon spin rotation experiments ($\mu$SR) reveal a more complicated scenario, with a complex temperature dependence of the magnetic volume fraction and a several order of magnitude variation of the relaxation rate, with its maximum at approximately 40 K.

This work was supported by European Community's Seventh Framework Programme (FP7/2007-2013) under Grant 290605 (PSI-FELLOW/COFUND) and from the Brazilian funding agencies CNPq, FAPESP (Grants No. 2011/19924-2 and 2014/20365-6) and CAPES. RAR was supported by the Gordon and Betty Moore Foundation.

Study of the Band Structure and the Origin of the XMR Effect in La$_{1-x}$Ce$_x$Bi

YUJIE HAO (Presenter), XIAO-MING MA, BIN LI, YANPING GUO, FENG YUE, RUI'E LU, CHANG LIU, Southern University of Science and Technology — Extremely high magnetoresistance (XMR) [1] in the rare earth monopnictides LnX (Ln = La, Ce, X = Sb, Bi) has recently received considerable interest [2-3]. These compounds with simple rock salt structure and electronic band structure are ideal model systems to search for the origin of the XMR effect. In this work, La$_{1-x}$Ce$_x$Bi single crystals with $x$ ranging from 0 to 0.2 is studied. By combining transport, magnetic and angle-resolved photoemission measurements, we performed a systematic investigation on the magnetotransport property and electronic structure of La$_{1-x}$Ce$_x$Bi. We clearly observe that the XMR effect in LaBi is gradually suppressed with increasing Ce doping level. The field-induced resistivity upturn and plateau disappear before the XMR effect is completely suppressed. On the other hand, the band structures near the Fermi surface barely changed with increasing Ce doping level. According to our results, whether the XMR effect originates from particular bands near the Fermi surface still needs further investigation.

Reference

*National Natural Science Foundation of China (NSFC) (Nos. 11504159 and 11874195).
P49.00014: The interplay of electronic, magnetic and structural properties of GdB₆ from first principles*  
SHAOWEN XU (Presenter), Physics Department, International Centre of Quantum and Molecular Structures, Shanghai University, Shanghai, 200444 China — Gadolinium hexaboride (GdB₆) is a well-known field emitter material that has been investigated for more than three decades. We perform a systematical density-functional theory (DFT) study of GdB₆ by using the generalized-gradient approximation and considering the electron interaction parameter U. The basic structural and electronic properties are carefully revised, as well as a strong U-value dependence in determining the antiferromagnetic (AFM) magnetic structures of Gd 4f electronic states. We found a small U (0~3eV) showing the most consistent experimental ground-state properties, which gives rise to a magnetic structure with a ground state of C-AFM and a second stable E-AFM. Moreover, we find the distortion modes of boron octahedron play an important role in the interaction between spin and lattice structures in this system. These results will deepen our understanding of the boron-based correlated rare earth compounds.

*the National Natural Science Foundation of China (Grants No. 51672171, No.51861145315, and No. 51911530124), the National Key Basic Research Program of China (Grant No. 2015CB921600), Work at the University of Missouri was supported by the U.S. Department of Energy, Award No. DE-SC0019114.

Wednesday, March 4, 2020 2:30 PM - 5:18 PM

Session P50 DCMP: Floquet and Nonequilibrium Models Mile High Ballroom 1C - 
Maxim Dzero, Kent State Univ - Kent

2:30PM P50.00001: Floquet control of indirect exchange interaction in periodically-driven magnetic lateral heterostructures*  
MAHMOUD M. ASMAR (Presenter), WANG KONG TSE, Physics and Astronomy, University of Alabama — Controlling the indirect exchange interaction between ferromagnetic impurities is pivotal for spintronic information transfer and storage. We present a theory for the RKKY interaction in a monochromatically irradiated magnetic lateral heterostructure (MLH). The MLH is composed of a left-side ferromagnet, a two-dimensional electron gas, and a right-side ferromagnet. Using the Keldysh-Floquet formalism, we calculate the time-averaged spin susceptibility and RKKY interaction mediated by the irradiated MLHs. Our results show that the emergence of non-equilibrium Floquet states under periodic driving leads to two qualitatively different RKKY regimes: 1) when the n ≤ 0 Floquet bands intersect the Fermi level, the sign and period of oscillation of the RKKY interaction are controllable by the frequency and amplitude of the laser; 2) when the n ≤ -1 Floquet bands intersect the Fermi level, the RKKY coupling does not display oscillations and remains ferromagnetic, resembling the exchange interaction mediated by insulating spacers. Our work demonstrates the feasibility of optically controlling the indirect exchange interaction with coherent laser fields.

*This work was supported by the US Department of Energy, Office of Science, Basic Energy Sciences under Early Career Award No. DE-SC0019326.
Nonequilibrium susceptibility in photoinduced Floquet states

ATSUSHI ONO (Presenter), SUMIO ISHIHARA, Department of Physics, Tohoku University — We investigate the nonequilibrium spin susceptibility in an electron system subject to a time-periodic electric field [1]. The spin susceptibility is formulated on the basis of the Floquet Green’s function method, and is calculated numerically in a wide range of amplitude and frequency of light. When the frequency is larger than the bandwidth, the susceptibility is enhanced by the dynamical localization effect, and their peak positions in the momentum space are shifted due to the Fermi surface deformation. In the case of the small frequency and amplitude, a multiple-peak structure emerges in the susceptibility, originating from the electron-hole excitation in and between the Floquet sidebands. To confirm those numerical results and provide the interpretation, a perturbative expression of the susceptibility is derived for small electric-field amplitude.


*This work was supported by JSPS KAKENHI Grant Numbers JP15H02100, JP17H02916, JP18H05208, and JP18J10246.

Promoting spontaneous symmetry breaking through Floquet band engineering

ILIYA ESIN (Presenter), GAURAV KUMAR GUPTA, Technion - Israel Institute of Technology, EREZ BERG, Weizmann Institute of Science, MARK RUDNER, Niels Bohr Institute, University of Copenhagen, NETANEL LINDNER, Technion - Israel Institute of Technology — In itinerant electronic systems, spontaneous symmetry breaking results from an interplay between interactions and density of states: a large density of states allows electrons to form long-range correlations by reducing the associated kinetic energy cost. The prospect of realizing new correlated states of electrons motivates us to seek methods for engineering band structures exhibiting large densities of states. We show that "Floquet engineering" via application of strong electromagnetic fields provides means for obtaining the necessary density of states to realize a novel nonequilibrium spontaneous symmetry breaking transition. We show that the transition occurs in the steady-state of the system achieved due to interplay between the coherent external drive, electron-electron interactions, and dissipative processes due to coupling to phonons and the electromagnetic environment. We obtain the phase diagram of the system using numerical calculations that match predictions obtained from a phenomenological treatment and discuss the conditions on the system and the external drive under which spontaneous symmetry breaking occurs. Our results imply that Floquet engineering of the density of states provides a new route for obtaining correlated states of electrons "on-demand".
Observation of Floquet prethermalization in dipolar spin chains

PAI PENG (Presenter), CHAO YIN, XIAOYANG HUANG, Massachusetts Institute of Technology MIT, CHANDRASEKHAR RAMANATHAN, Dartmouth College, PAOLA CAPPELLARO, Massachusetts Institute of Technology MIT — Periodically driven (Floquet) quantum systems provide a promising platform to study physics out of equilibrium, such as time crystalline phase and Floquet topological structure. However, the drive generically heats up the system to infinite temperature. Still, it was shown theoretically that the heating rate is exponentially small in the driving frequency, giving rise to a long-lived prethermal stage that exhibits all the intriguing properties of Floquet systems.

Here we present nuclear magnetic resonance observation of Floquet prethermalization in dipolar spin chains. We first show that the system quickly converges to a prethermal state that agrees with the equilibrium statistics of a time-independent “prethermal” Hamiltonian (PTH). We then observe the exponentially slow heating of quasi-conserved quantities, by measuring the time-autocorrelation of the PTH itself. Intriguingly, we find that at timescale when the PTH is no longer conserved, the system may still possess other symmetries.

The results improve our understanding of thermalization in driven quantum systems and demonstrate the possibility to realize novel Floquet phases of matter and robust Floquet engineering in the prethermal regime.

*We are supported by the National Science Foundation PHY1734011 and PHY1915218.

Approaching a Floquet Time Crystal phase in the periodically driven O(N) model

MUATH NATSHEH (Presenter), New York Univ NYU, ANDREA GAMBASSI, SISSA, Italy, ADITI MITRA, New York Univ NYU — Results are presented for the dynamics of the periodically driven O(N) model starting from a prescribed initial state. This model is known to host ferromagnetic phases that, depending on microscopic parameters, are period doubled or period synchronized, the former being an example of a Floquet Time Crystal. Employing numerical simulations, and analytic calculations within a large-N approach, we study how an initial paramagnetic phase evolves into the Floquet time crystal phase following a quench. We identify regimes where the transient dynamics is characterized by an effective mass that approaches steady state as a universal power-law. Results for the one-loop corrections to correlations functions in this transient regime are presented. Analogies to transient dynamics at the critical point of the static O(N) model are highlighted. The possibility of universality in the transition from the paramagnetic and Floquet time crystal phase is discussed.

*This work was supported by the US National Science Foundation Grant NSF-DMR 1607059 and partially by the MRSEC Program of the National Science Foundation under Award Number DMR-1420073.
3:30PM P50.00006: Quantum butterfly effect in polarized Floquet systems with conservation laws*  
XIAO CHEN (Presenter), RAHUL M NANDKISHORE, ANDREW LUCAS, University of Colorado, Boulder — We explore quantum dynamics in Floquet many-body systems with local conservation laws in one spatial dimension, focusing on sectors of the Hilbert space which are highly polarized. We numerically compare the predicted charge diffusion constants and quantum butterfly velocity of operator growth between models of chaotic Floquet dynamics (with discrete time translation invariance) and random unitary circuits which vary both in space and time. We find that for any non-zero polarization per length (in the thermodynamic limit), the random unitary circuit correctly predicts the butterfly velocity but incorrectly predicts the diffusion constant. We argue that this is a consequence of quantum coherence on short time scales. Our work clarifies the settings in which random unitary circuits provide correct physical predictions, and the origin of the slow down of the butterfly effect in highly polarized systems.

*XC acknowledges support from DARPA DRINQS program. RMN is supported by the Air Force Office of Scientific Research under grant number FA9550-17-1-0183 and by the Alfred P. Sloan Foundation through a Sloan Research Fellowship.

3:42PM P50.00007: Floquet Conformal Field Theory*  
RUIHUA FAN (Presenter), YINGFEI GU, ASHVIN VISHWANATH, Harvard University, XUEDA WEN, Massachusetts Institute of Technology — Conformal field theory provides an ideal platform to discuss examples of Floquet dynamics in an analytic and exact way. Earlier work solved for the Floquet dynamics using a particular driving Hamiltonian (the sl(2,R) generators) and restricted initial state (eigenstates). In this talk, we will generalize the original set-up to go beyond the sl(2,R) algebra and also discuss driving a thermal state. We will discuss the entanglement pattern and energy profile in these generalized set-ups and also describe some non-universal features of the Floquet dynamics.

*Y.G. is supported by the Gordon and Betty Moore Foundation EPIQS Initiative through Grant (GBMF-4306) and DOE grant, de-sc0019030. X.W. is supported by the Gordon and Betty Moore Foundations EPIQS initiative through Grant (GBMF-4303) at MIT. AV and RF are supported by the DARPA DRINQS program (award D18AC00033) and by a Simons Investigator Award.
3:54PM P50.00008: Positivity of the Spectral Densities of Retarded Floquet Green Functions*  JAMES FREERICKS (Presenter), Physics, Georgetown University, MONA KALTHOFF, Physics, University of Hamburg, GOETZ S UHRIG, Physics, University of Dortmund — Periodically driven nonequilibrium many-body systems are interesting because they have quasi-energy spectra, which can be tailored by controlling the external driving fields. We derive the general spectral representation of retarded Green functions in the Floquet regime, thereby generalizing the well-known Lehmann representation from equilibrium many-body physics. The derived spectral Floquet representation allows us to prove the non-negativity of spectral densities and to determine exact spectral sum rules, which can be employed to benchmark the accuracy of approximations to the exact Floquet many-body Green functions.

This work appears in Phys. Rev. Lett. 122, 130604 (2019).

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4:06PM P50.00009: Floquet dynamics under spatially inhomogeneous drive*  ZHOUSHEN HUANG (Presenter), AASHISH CLERK, IVAR MARTIN, Argonne Natl Lab — Floquet engineering has been shown to be a promising mechanism in realizing quantum information manipulations. While spatially homogeneous drives allow for block diagonalization in momentum, and have thus often been invoked in theoretical studies, in realistic systems, translation symmetry is typically broken. In this work, we discuss features of Floquet systems under inhomogeneous spatial drives, in the context of band theory, such as nondispersing traveling wave packets, simplification of dynamical Hilbert space, and a machine learning scheme which can predict time dynamics of arbitrary temporal driving profiles.

*Argonne LDRD
4:18PM P50.00010: Long-lived interacting phases of matter protected by multiple time-translation symmetries in quasiperiodically-driven systems  DOMINIC ELSE (Presenter), Department of Physics, Massachusetts Institute of Technology MIT, WEN WEI HO, Department of Physics, Harvard University, PHILIPP DUMITRESCU, Center for Computational Quantum Physics, Flatiron Institute — We show how a large family of interacting nonequilibrium phases of matter can arise from the presence of multiple time-translation symmetries, which occur by quasiperiodically driving an isolated quantum many-body system with two or more incommensurate frequencies. These phases are fundamentally different from those realizable in time-independent or periodically-driven (Floquet) settings. Focusing on high-frequency drives with smooth time-dependence, we rigorously establish general conditions for which these phases are stable in a parametrically long-lived `preheating' regime. We develop a formalism to analyze the effect of the multiple time-translation symmetries on the dynamics of the system, which we use to classify and construct explicit examples of the emergent phases. In particular, we discuss time quasi-crystals which spontaneously break the time-translation symmetries, as well as time-translation symmetry protected topological phases.

4:30PM P50.00011: Non-equilibrium steady state solutions of time-periodic driven Luttinger liquids* SERENA FAZZINI (Presenter), University of Kaiserslautern, Germany, PIOTR CHUDZINSKI, School of Mathematics and Physics, Queens Univ. Belfast, CHRISTOPH DAUER, IMKE SCHNEIDER, SEBASTIAN EGGERT, University of Kaiserslautern, Germany — The recent development of Floquet engineering has made periodic driving a versatile tool for achieving new phases not accessible in static equilibrium systems. We now study the exact Floquet steady states of the periodically driven Tomonaga-Luttinger liquid without resorting to any high frequency approximations. We show that the time-dependent Schrödinger equation can be solved analytically for a large class of driven interacting 1D systems, which give the resulting non-equilibrium steady states. Remarkably, we observe regions of instabilities as a function of total momentum where the solution is not of Floquet form, which implies a loss of time translational invariance and therefore heating of excitations. For small driving amplitudes the instabilities are close to the naively expected resonance condition $nu=2vq$, but for stronger driving the heating regions separate a rich structure of bands of steady state solutions. Physical consequences are discussed.

*Supported by the Deutsche Forschungsgemeinschaft (DFG) via SFB/TR185 "OSCAR"
4:42PM P50.00012: Spontaneously broken discrete time translation symmetry in driven quantum Brownian motion*  JYONG-HAO CHEN (Presenter), Physics, University of California, Berkeley, MASAKI OSHIKAWA, ISSP, University of Tokyo — Spontaneously broken discrete time translation symmetry (DTTS) in Floquet systems, often be dubbed as discrete time crystal or Floquet time crystal, draws a lot of attention in recent years. While most experimental realizations and theoretical studies of the DTTS breaking involve many-body localization to avoid heating, the effect of dissipation is an obvious alternative to prevent heating. In this work, we consider the quintessential model of quantum dissipation — the Caldeira-Leggett model and take into account the presence of a periodically driven external potential. Employ a perturbative approach within the framework of Feynman-Vernon influence functional enables us to demonstrate analytically that DTTS breaking would occur in such a simple model. The interplay between the driving frequency, the strength of dissipation, and the temperature are studied in detail. A crossover between the quantum and classical limit is examined as well. Owing to the ubiquitousness of the ordinary Caldeira-Leggett model, our findings pave a new avenue toward exploring the novel phenomena of DTTS breaking in broad systems.

*Japan Society for the Promotion of Science and Swiss National Science Foundation.

4:54PM P50.00013: Dynamic Control of Metal-Insulator Transitions Out of Equilibrium*  JOSEPH KLEINHENZ (Presenter), IGOR KRIVENKO, Physics, University of Michigan, GUY COHEN, Chemistry, Tel Aviv University, EMANUEL GULL, Physics, University of Michigan — Dynamic switching between different phases of quantum matter offers many exciting theoretical and practical possibilities. We present recent results from our studies of switching across the Mott metal-insulator transition in the Hubbard model within the framework of non-equilibrium DMFT. We find that the metal to insulator transition is relatively easy to drive but for many quenches the insulator to metal transition occurs over a very long timescale. We present quench protocols that are able to overcome this difficulty and demonstrate controllable switching across the phase boundary in both directions.

*DOE ER 46932

5:06PM P50.00014: Photo-induced superconductivity in the Kondo lattice  TOMONORI SHIRAKAWA (Presenter), SHOHEI MIYAKOSHI, SEIJI YUNOKI, RIKEN — The non-equilibrium dynamics can induce many interesting phenomena in strongly correlated quantum systems. For example, recent experiments have observed the photoinduced superconducting-like behavior in some of the high-$T_c$ cuprates and the alkali-doped fullerenes even above $T_c$. In this context, we have previously studied theoretically the photo-excited states from the Mott insulating state in the Hubbard model and found that the pulse irradiation can induce the enhancement of superconducting correlations, which is attributed to eta-pairing formation [1]. Here, we show that the same mechanism can be applied to the Kondo lattice model, an effective model for heavy fermion systems, by demonstrating that the photo-irradiation indeed enhances the eta-pairing correlations. As in the Hubbard model, the non-linear optical process is essential to increase the number of photo-induced eta-pairs and thus enhance the superconducting correlations.

2:30PM P51.00001: Fully tunable Magic Angle Twisted Bilayer Graphene Josephson Junction

DANIEL RODAN-LEGRAIN (Presenter), YUAN CAO, JEONG MIN PARK, Massachusetts Institute of Technology MIT, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology MIT — Superconductivity and correlated insulating states have recently been observed in ‘magic-angle’ twisted bilayer graphene (MATBG) heterostructures at twist angles close to 1.1 degrees, featuring nearly-flat bands owing to strong interlayer coupling. MATBG offers a new playground to study superconductivity and strongly correlated physics with an unprecedented degree of tunability. One of the elemental superconducting devices are Josephson Junctions, where two superconductors are coupled by a non-superconducting weak link. In this work, we exploit such tunability to create a fully tunable 2D Josephson Junction allowing to independently control the electronic state of the weak link and the rest of the junction via multiple electrostatic gates. The MATBG electrodes can thus be brought into a superconducting state, either in the hole regime or the electron regime, while the narrow junction at the center of the device can be tuned into any possible state of the phase diagram of MATBG (from metal, band insulator, charge neutrality, correlated insulator, superconductor). Such devices may pave the way towards new geometries in the study of strongly correlated systems, tunable superconducting qubits, and fully-integrated 2-dimensional electronics for the future nanodevice technology.

2:42PM P51.00002: Chiral twist on the high-T\textsubscript{c} phase diagram in moiré heterostructures\textsuperscript{*}

YU-PING LIN (Presenter), RAHUL NANDKISHORE, Department of Physics, University of Colorado, Boulder —

We show that the large orbital degeneracy inherent in moiré heterostructures naturally gives rise to a ‘high-\text{\textsubscript{T_c}}’ like phase diagram with a chiral twist - wherein an exotic quantum anomalous Hall insulator is flanked by chiral $d+id$ superconducting domes. Specifically, we analyze repulsively interacting fermions on hexagonal lattices near Van Hove filling, with an SU(4) flavor degeneracy. At this point, a nested Fermi surface and divergent density of states give rise to strong $\ln^2$ instabilities to correlated phases, the competition between which can be controllably addressed through a combination of weak coupling parquet renormalization group and Landau-Ginzburg analysis. We uncover an unambiguous and rich behavior, wherein at weak coupling the leading instability is to a Chern insulator, characterized by a spontaneous breaking of time reversal symmetry and a quantized Hall response. Upon doping this phase gives way to a chiral $d+id$ superconductor. We further consider deforming this minimal model by an orbital splitting, and discuss the resulting RG flow and phase diagram. Our analysis thus bridges the minimal model and the practical moiré bands, thereby elucidates transparently how the correlated phases arise.

\textsuperscript{*}Supported by the Army Research Office under Grant No. W911NF-17-1-0482.
We present a systematic classification and analysis of possible pairing instabilities in graphene-based moiré superlattices. Motivated by recent experiments on twisted double-bilayer graphene showing signs of triplet superconductivity, we analyze both singlet and triplet pairing separately, and describe how these two channels behave close to the limit where the system is invariant under separate spin rotations in the two valleys, realizing an SU(2)$_+$ $\times$ SU(2)$_-$ symmetry. Further, we discuss the conditions under which singlet and triplet can mix via two nearly degenerate transitions, and how the different pairing states behave when an external magnetic field is applied. We find that an approximate SU(2)$_+$ $\times$ SU(2)$_-$ symmetry can generically account for the linear increase of the critical temperature with small magnetic fields, and we map out the possible forms of the phase diagram as a function of temperature and magnetic field. Finally, we also detail the differences in the classification when the additional microscopic or emergent symmetries relevant for twisted bilayer graphene and ABC trilayer graphene on hexagonal boron nitride are taken into account.

*This research was funded by the NSF (Grant DMR-1664842) and the German National Academy of Sciences Leopoldina (Grant LPDS 2016-12).

We use scanning tunneling microscopy to explore several non-encapsulated twisted bilayer graphene devices with different nominal twist angles. In this talk, I present quantitative results of the homogeneity on different length scales.

*This work was supported by the Netherlands Organisation for Scientific Research (NWO/OCW), as part of the Frontiers of Nanoscience program.
3:18PM P51.00005: Tunable electron interactions in moiré graphene: extinction of Mott order in the presence of screening  ALI FAHIMNIYA (Presenter), MIT, DMITRI EFETOV, PETR STEPANOV, ICFO Barcelona, LEONID LEVITOV, MIT — Magic-angle twisted bilayer graphene (TBG) is a strongly-correlated system that hosts different ordered states, notably Mott-insulating and superconducting, stabilized by the electron-electron (e-e) and electron-phonon (el-ph) interactions. Understanding the individual roles of these interactions, as well as their interplay, is a central question of the moiré graphene physics. To that end, we explore the robustness of the Mott order in the presence of a screened e-e interaction, as is the case in currently studied heterostructures comprised of TBG, hexagonal boron nitride (hBN), and graphite layers. Screening of electron charges in TBG by image charges in graphite weakens e-e interactions as the hBN spacer width decreases. The suppression of the Mott order due to enhanced screening sets in at the hBN widths on the order of the Wannier orbital radius (~10nm) and is followed by complete extinction of the Mott order. At the same time, el-ph coupling strength remains unchanged. The experiments, too, show a drastic change of the Mott insulator phase upon varying hBN width but find that the superconducting phase survives in the absence of long-range e-e interactions. Comparison of theory and experiment sheds new light on the origin of Mott order and superconductivity in the TBG system.

3:30PM P51.00006: Tunable bandwidths and gaps in twisted double bilayer graphene system on the verge of correlations*  PRATAP ADAK (Presenter), SUBHAJIT SINHA, UNMESH GHORAI, L. D. VARMA SANGANI, Tata Institute of Fundamental Research (TIFR), KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Tsukuba, RAJDEEP SENSARMA, MANDAR M DESHMUKH, Tata Institute of Fundamental Research (TIFR) — Recently, superlattices in graphene have gained much interest due to its ability to tune its band structure. In particular, it has been demonstrated that when two copies of monolayer graphene are stacked with a ‘magic’ angle twist between them, flat bands appear. Flat bands give birth to a plethora of electronic interaction governed phenomena like superconductivity, ferromagnetism, etc.

When two copies of bilayer graphene are put on top of each other with a relative twist, it allows electrical control over the flatness of the bands and the gaps between them. Even before studying interaction driven physics, it is useful to study the tunability of bands in such a system. We perform transport measurements on dual gated twisted double bilayer graphene device (TDBG) and use simple model calculations to understand important experimentally observed features. Specifically, we will discuss how the bandwidth of the bands can be tuned electrically and how an electron-hole asymmetric model can explain some observations. A discussion on some observations which may be precursors to correlation will conclude the presentation.

*We acknowledge funding from Department of Atomic Energy, India and Department of Science and Technology, India.
Observation of charging peaks near the flat band in magic-angle twisted bilayer Graphene

NIKHIL TILAK (Presenter), XINYUAN LAI, Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, Piscataway, NJ 08855 USA, YUHANG JIANG, JINHAI MAO, Department of Physics and Astronomy, University of Chinese Academy of Sciences, CMSJ+7X, Huabeiizhen, Huairou, Beijing, China, MINGYU XU, RAQUEL DE ALMEIDA RIBEIRO, PAUL C CANFIELD, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011, USA, EVA ANDREI, Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, Piscataway, NJ 08855 USA — Magic-angle twisted bilayer Graphene (MA-tBLG) has emerged as a highly tunable platform to study correlation physics. Numerous transport experiments have shown the existence of correlated insulating states, unconventional superconductivity and emergent ferromagnetism as the filling of the flat moire bands in MA-tBLG is tuned. More recently, several Scanning Tunneling Microscopy/Spectroscopy (STM/STS) experiments have also observed correlated-insulator like behavior, charge order and broken C3 symmetry in this system. Here, using Low temperature STM/STS measurements, we report the observation of sharp charging peaks which appear in the LDOS as the Fermi level is tuned close to the edges of the flat band. We perform a systematic study of these states to see their evolution in space using STS mapping. The observation of these states hints at the formation of local compressible regions surrounded by a gapped incompressible region because of tip induced band bending.

Work supported by DOE-FG02-99ER45742, NSF DMR 1708158

Experimental Observation of Tunable Chern insulator and Ferromagnetism in ABC-Trilayer Graphene on hBN Moiré Superlattice

GUORUI CHEN (Presenter), University of California, Berkeley, AARON SHARPE, ELI J FOX, Stanford, YAHUI ZHANG, MIT, SHAOXIN WANG, LILI JIANG, University of California, Berkeley, BOSAI LV, Shanghai JiaoTong University, HONGYUAN LI, University of California, Berkeley, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, ZHIWEN SHI, Shanghai jiaoTong University, SENTHIL TODADRI, MIT, DAVID GOLDHABER-GORDON, Stanford, YUANBO ZHANG, Fudan University, FENG WANG, University of California, Berkeley — Haldane theorized that Chern insulators with integer QH effects could appear in lattice models with complex hopping parameters even at zero magnetic field. The ABC-trilayer graphene/hexagonal boron nitride (TLG/hBN) moiré superlattice provides an attractive platform to explore Chern insulators because it features nearly flat moiré minibands with a valley-dependent electrically tunable Chern number. Here we report the experimental observation of a correlated Chern insulator in a TLG/hBN moiré superlattice. We show that reversing the direction of the applied vertical electric field switches TLG/hBN’s moiré minibands between zero and finite Chern numbers, as revealed by dramatic changes in magneto-transport behavior. The Hall resistance is well quantized at h/2e2, i.e. C = 2, for B > 0.4 T. The correlated Chern insulator is ferromagnetic, exhibiting significant magnetic hysteresis and a large anomalous Hall signal at zero magnetic field. Our discovery of a C = 2 Chern insulator at zero magnetic field should open up exciting opportunities for discovering novel correlated topological states, possibly with novel topological excitations, in nearly flat and topologically nontrivial moiré minibands.
Spin-triplet superconductivity and ferromagnetism in moire systems: A case study for twisted double bilayer graphene

YI-TING HSU (Presenter), FENGCHENG WU, University of Maryland, College Park — Recent experiments have observed possible ferromagnetism and spin-triplet superconductivity in twisted double bilayer graphene that comprises a pair of AB-stacked bilayer graphene under a displacement field. We show that ferromagnetism and spin-triplet pairing can naturally be the dominant instabilities in such systems as a general consequence of the valley-dependent van Hove physics when the nesting is weak. Specifically, by performing a renormalization group analysis for all possible pairing, magnetic, and charge instabilities, we find ferromagnetism or spin-triplet pairing to be dominant throughout a broad parameter space of interactions and low-energy band structure properties we consider. Finally, we discuss the possibility of topological superconductivity and relevance to the experimental findings.

Ferromagnetism in twisted bilayer graphene

AARON SHARPE (Presenter), ELI J FOX, ARTHUR W BARNARD, JOE FINNEY, Stanford Univ, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, MARC KASTNER, DAVID GOLDHABER-GORDON, Stanford Univ — When two sheets of graphene are stacked at a small twist angle, the resulting flat superlattice minibands are expected to strongly enhance electron-electron interactions. These enhanced interactions have led to the observation of interesting correlated electronic states, such as superconductivity, where metallic behavior would otherwise be expected. Here we present evidence that near three-quarters (3/4) filling of the conduction miniband these enhanced interactions drive the twisted bilayer graphene into a ferromagnetic state. We suggest that the system is a Chern insulator. We further present magneto transport measurements in tilted field that may hold clues to the nature of the magnetism.

*This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.

Ferromagnetism in narrow bands of moiré superlattices

CECILE REPELLIN, DONG ZHIHUAN (Presenter), Department of Physics, Massachusetts Institute of Technology, YAHUI ZHANG, Department of Physics, Harvard University, SENTHIL TODADRI, Department of Physics, Massachusetts Institute of Technology — Many graphene moiré superlattices host narrow bands with non-zero valley Chern numbers. We provide analytical and numerical evidence for a robust spin and/or valley polarized insulator at total integer band filling in nearly flat bands of several different moiré materials. In the limit of a perfectly flat band, we present analytical arguments in favor of the ferromagnetic state substantiated by numerical calculations. Further, we numerically evaluate its stability for a finite bandwidth. We provide exact diagonalization results for models appropriate for ABC trilayer graphene aligned with hBN, twisted double bilayer graphene, and twisted bilayer graphene aligned with hBN. We also provide DMRG results for a honeycomb lattice with a quasi-flat band and non-zero Chern number, which extend our results to larger system sizes. We find a maximally spin and valley polarized insulator at all integer fillings, which can be destabilized by interaction-induced effective dispersive terms. These results still hold in the case of zero valley Chern number. We give an intuitive picture based on extended Wannier orbitals, and emphasize the role of the quantum geometry of the band, whose microscopic details may enhance or weaken ferromagnetism in moiré materials.
Transport experiments in twisted (double) bilayer graphene

PETER RICKHAUS, FOLKERT DE VRIES (Presenter), ELIAS MARIN PORTOLES, GIULIA ZHENG, Physics, ETH Zurich, MING-HAO LIU, National Cheng Kung University, Taiwan, JOSE LADO, Aalto University Helsinki, JOHN WALLBANK, Centre for Ecology and Hydrology, Oxfordshire, SERGEY SLIZOVSKIY, The University of Manchester, MARCIN KURPAS, University of Silesia in Katowice, RICCARDO PISONI, HISKE OVERWEG, YONGJIN LEE, ANNIKA KURZMANN, MARIUS EICH, CHUYAO TONG, REBEKKA GARREIS, CAROLIN GOLD, MICHELE MASSERONI, Physics, ETH Zurich, KLAUS RICHTER, University of Regensburg, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, Japan, THOMAS IHN, KLAUS ENSSLIN, Physics, ETH Zurich — We study signatures in electronic transport in twisted (double) bilayer graphene. Specifically, we are interested in the coupling and decoupling between single- and bilayer graphene layers as a function of twist angle. For large twist angles, the wavefunction of the layers are decoupled. Using twisted double bilayer graphene, we determine the intrinsic energy difference between inner and outer layers of the stack. Such a crystal field opens a gap in the groundstate [1]. Since the two layers are strongly capacitively coupled but their wavefunctions can be independently tuned, the geometric capacitance between the layers is heavily affected by the finite thickness of graphene, which we determine [2]. We also show transport data at small angles, where the layers are strongly coupled. At tiny twists, we detect a topological network [3] in twisted bilayer graphene and correlated states in twisted double bilayer graphene. Finally, we study the crossover between the coupled and decoupled regime, where the wavefunctions start to spread over all layers.


*European Graphene Flagship
NCCR QSIT
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4:54PM P51.00013: Colossal mid-infrared photoresponse in small-twist-angle bilayer graphene* BINGCHEN DENG (Presenter), CHAO MA, Yale University, QIYUE WANG, University of Texas at Dallas, SHAOFAN YUAN, Yale University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, FAN ZHANG, University of Texas at Dallas, FENGNIAN XIA, Yale University — Small-twist-angle bilayer graphene has drawn much attention recently due to its exotic transport properties such as superconductivity and correlated insulating phase. The Brillouin zone folding and the formation of flat moiré bands significantly modify the density of states (DOS). Here we demonstrate the colossal and gate-tunable mid-infrared (5 ~ 12 μm) photoresponse leveraging the enhanced DOS and the emergence of superlattice-induced bandgaps. At liquid nitrogen temperature, we achieve a maximum extrinsic responsivity of 26 mA W⁻¹ at 12 μm in a 1.81° twist angle bilayer graphene, when the Fermi level is tuned to the middle of the superlattice gap in the electron branch. Together with transport study, we reveal the bolometric origin of the photoresponse. Moreover, the colossal photoresponse critically relies on the formation of superlattice gaps as it is vanishingly small in ultrasmall twist angle (< 0.5°) device, where the gaps are absent in our measurement range. Our results show the desirable properties and promising applications of twisted bilayer graphene for mid-infrared optoelectronics.

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Office of Naval Research
Army Research Office (W911NF-18-1-0416)
Natural Science Foundation (DMR-1921581) through the DMREF program

5:06PM P51.00014: Nano-photocurrent mapping of twisted bilayer graphene SAI SUNKU (Presenter), ALEXANDER MCLEOD, Columbia Univ, TOBIAS STAUBER, ICMM-CSIC, HYOBIN YOO, Harvard Univ, DORRI HALBERTAL, GUANGXIN NI, AARON STERNBACH, Columbia Univ, BOR-YUAN JIANG, UC San Diego, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, PHILIP KIM, Harvard Univ, MICHAEL M FOGLER, UC San Diego, DMITRI BASOV, Columbia Univ — We report a combined nano-photocurrent and infrared nanoscopy study of twisted bilayer graphene. We show that the photocurrent as a function of carrier density changes sign at twist-induced insulating states. We use this property to identify domains of varying local twist angle in our sample. Consistent with the photocurrent study, infrared nano-imaging experiments reveal optical conductivity features dominated by twist-angle dependent interband transitions. Nano-photocurrent imaging can be broadly applied to moiré superlattices occurring in various other van der Waals heterostructures.
**5:18PM P51.00015: Nano-optical study of Moire superlattice domains in twisted graphene heterostructures**

DORRI HALBERTAL (Presenter), NATHAN FINNEY, SAI SUNKU, SHAOWEN CHEN, CHARLES ZHANG, NICOLA CURRELI, MATTHEW A YANKOWITZ, ALEXANDER MCLEOD, GUANGXIN NI, ALEXANDER KERELSKY, CARMEN RUBIO VERDU, LEO MCGILLY, ABHAY NARAYAN, CORY DEAN, JAMES C HONE, DMITRI BASOV, Physics, Columbia University — Twisted graphene heterostructure have attracted a considerable amount of attention, realizing a plethora of physical phenomena including strongly interacting correlated states, superconductivity, magnetism and more. In this work we used several nano-optical techniques to study the formation and reconstruction of domain walls in several twisted graphene heterostructures. The techniques are uniquely suited to provide a nanometric spatial map of the domains, over an entire flake scale, which allowed us to study domain formation and internal structure on all relevant scales, and to gain insight into the reconstruction problem in several system of interest, including the twisted bilayer graphene and the twisted double bilayer graphene.

*Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences (BES), under award DE-SC0019443n

**Wednesday, March 4, 2020 2:30 PM - 5:18 PM**

**Session P52 DMP: Focus Topic: Surface, Interface, and Thin Film Science of Organic Molecular Solids II** Mile High Ballroom 1E - Jeffrey Guest, Argonne Natl Lab - Tag(s): Focus

**2:30PM P52.00001: Detecting Stable Surface Adsorbates with Bayesian Optimization**

JARI JÄRVI (Presenter), MILICA TODOROVIC, PATRICK RINKE, Department of Applied Physics, Aalto University — Determining stable structures of organic molecules at inorganic surfaces requires both quantum mechanics and thorough exploration of the potential energy surface (PES). This is prohibitively expensive with density-functional theory (DFT). We combine DFT with artificial intelligence (AI) for global atomistic structure search of stable adsorbates. Bayesian Optimization Structure Search (BOSS) [1] is a new AI tool, which accelerates the structure search via a strategic sampling of the PES. BOSS minimizes the number of expensive DFT simulations to compute the complete PES. This allows a clear identification of the most stable minimum energy structures and the barriers between them.

We apply BOSS to study the adsorption of a camphor molecule on the Cu(111) surface as a function of molecular orientation and translations. We identify the optimal structure and 8 unique types of stable adsorbates, in which camphor chemisorbs via oxygen (global minimum) or physisorbs via hydrocarbons to the Cu(111) surface. This study demonstrates that the new cross-disciplinary tools, like BOSS, allow us to identify complex interface structures and properties, and tune the functionality of advanced materials.

2:42PM P52.00002: Unusual self-assembly of chloroaluminium phthalocyanine on graphite
HAIYANG MA (Presenter), JINFENG JIA, Shanghai Jiao Tong Univ, RUIQIN ZHANG, Physics, City University of Hong Kong — We report an unusual self-assembled layer structure of chloroaluminium phthalocyanine (ClAlPc) molecules on highly ordered pyrolytic graphite (HOPG), in which a close-packed well-ordered monolayer is separated from the substrate by a relatively disordered buffer layer, as revealed using scanning tunneling microscopy (STM). Our close-packed monolayer has a nearly rectangular lattice, instead of the distinctly different square lattice for the more commonly observed well-ordered bilayer structure. This may be due to the dominance of intermolecular interactions within the monolayer when the influence from the substrate is shielded by the buffer layer. Density Functional Theory (DFT) calculations and Reduced Density Gradient (RDG) analysis indicate that the dominant intermolecular interaction within the unusual layer is likely the London dispersion force.

2:54PM P52.00003: Coherent X-ray measurement of local step-flow propagation during growth on polycrystalline organic semiconductor thin film surfaces*  RANDALL HEADRICK (Presenter), JEFFREY G ULBRANDT, Department of Physics and Materials Science Program, University of Vermont, PECO MYINT, Division of Materials Science and Engineering, Boston University, JING WAN, Boston University, YANG LI, Department of Physics and Materials Science Program, University of Vermont, ANDREI FLUERASU, YUGANG ZHANG, LUTZ WIEGART, National Synchrotron Light Source II, Brookhaven National Laboratory, KARL F LUDWIG, Division of Materials Science and Engineering and Department of Physics, Boston University — Vapor deposition of C\textsubscript{60} on a graphene coated surface is investigated in real-time by utilizing coherent hard X-rays. X-ray Photon Correlation Spectroscopy is performed in grazing incidence to achieve surface-sensitivity. Local step-flow is monitored through the observation of oscillatory correlations in the later stages of growth after crystalline mounds have formed. Coherent X-rays do not average over complex structures, and this allows us to monitor growth on polycrystalline surfaces without loss of information. The results show that the step-flow velocity is nonuniform, and we model the velocity of each step-edge as being a simple function of the lengths of the terraces above and below it. Sensitivity to local step-flow is enhanced by coherent mixing of X-rays scattered from the average mound structure with those scattered from the step array. This effect is a version of heterodyne scattering, where the scattering from the average step array can be considered to be a quasi-static reference signal. This work shows that the use of coherent X-ray scattering provides an approach to better understand surface dynamics and fluctuations during crystal growth.

*This material is based upon work supported by the U.S. Department of Energy Office of Science under Grant No. DE-SC0017802.
3:06PM P52.00004: Realizing nearly-free-electron like conduction band in a molecular film through mediating intermolecular van der Waals interactions* [Invited] MIN FENG (Presenter), School of Physics and Technology and Key Laboratory of Artificial Micro- and Nano-Structures of Ministry of Education, Wuhan University — The degree of electron delocalization in organic semiconductors is critical for their adoption in electronic and optoelectronic applications. Electron delocalization, however, is usually facile through chemical bonds in conjugated organic materials, but is rarely optimal when the noncovalent intermolecular vdW forces define the self-assembly and the intermolecular electronic coupling. As a typical vdW material, C_{60} molecules form solids through the attractive vdW force, thus are characterized with flat electronic bands with inconsequential dispersions and hopping transport, which is unfavourable for their practical applications.

To enhance intermolecular electronic hybridization, we introduce a method to mediate the vdW interactions between C_{60} molecules through a substrate control of intermolecular interactions. We show by STM and theory that the black phosphorus (BP) substrate organizes C_{60} molecules into a compressed monolayer that optimizes the intermolecular π-π couplings, resulting in a nearly-free-electron (NFE) like LUMO band in C_{60} monolayers, acquiring an effective mass of 0.53-0.70 and has carrier mobility of ~200 to 440 cm^2V^{-1}s^{-1}. The fact that the π-π vdW interactions does trigger the NFE like electronic band formation implies that templating of intermolecular interactions by vdW forces on otherwise weakly interacting substrates provides a promising strategy for tailoring remarkable electronic properties in organic materials for electronics and optoelectronics.

Reference:

*This work is supported National Key R&D Program of China (2017YFA0303500, 2017YFA0303504); the Strategic Priority Research Program of Chinese Academy of Science (XDB30000000); the NSFC 11574364, 11622437 and 61674171.
3:42PM P52.00005: Predicting $\chi$ of polymer blends using atomistic "morphing" simulations

SHREYA SHETTY (Presenter), ENRIQUE D GOMEZ, SCOTT MILNER, Pennsylvania State University — The Flory Huggins interaction parameter $\chi$ governs phase behavior in polymer blends and block copolymers. We have previously used molecular dynamic (MD) simulations and thermodynamic integration during the morphing of one species to another, to compute the excess free energy of mixing in coarse-grained, bead-spring model of polymer blends. Using this method, we have studied the effect on $\chi$ of factors like stiffness mismatch, chain architecture and Lennard Jones interactions. In this work, we use united-atom MD simulations and the morphing method to calculate $\chi$ for real polymer blends: (1) poly(ethylene) - poly(ethylene oxide), (2) poly(styrene) - poly(2-vinyl pyridine), (3) poly(isoprene) - saturated (polyisoprene) and (4) poly(styrene) - poly(α-methyl styrene). These examples require different kinds of morphing- LJ interactions and partial charges of atoms (cases 1 and 2), transform double bond to single bond (case 3) and disappearance of atoms (case 4). All simulations used force field parameters adopted from TRAPPE. Our $\chi$ values from simulations are in reasonable agreement with experiment, but are sensitive to force field parameters used in the simulation.

*Financial support from the National Science Foundation under Award DMREF-1629006 is acknowledged.

3:54PM P52.00006: Visualizing Molecular Orientational Ordering and Electronic Structure in Cs$_n$C$_{60}$ thin films

SHA HAN (Presenter), Physics, Tsinghua University, MENGXUE GUAN, Chinese Academy of Sciences, CANLI SONG, Physics, Tsinghua University, YILIN WANG, Shandong University, MINGQIANG REN, Physics, Tsinghua University, SHENG MENG, Chinese Academy of Sciences, XUCUN MA, QIKUN XUE, Physics, Tsinghua University — Alkali-doped fullerides exhibit a wealth of unusual phases that remain controversial by nature. Here a cryogenic scanning tunneling microscopy and first-principles calculation are combined to investigate the sub-molecular structural and electronic properties of expanded fullerene C$_{60}^{n^-}$ films on inert graphene with various cesium (Cs) doping. By varying the discrete charge states and film thicknesses, we reveal a large tunability of orientational ordering of C$_{60}^{n^-}$ anions, yet the tunneling conductance spectra are robustly characteristic of energy gaps, hallmarks of the Jahn-Teller distortions and electron correlations. The Fermi level lies halfway within the insulating gap for stoichiometric Cs doping level of $n = 1, 2, 3$ and $4$, apart from which it moves toward the band edges with concomitant electronic states in the gap. Our findings establish the universality of Jahn-Teller instability, and clarify the relationship among the doping, structural and electronic structures in Cs$_n$C$_{60}$ fullerides.

*Ministry of Science and Technology of China (Grants No. 2017YFA0304600, No. 2016YFA0301004, No. 2015CB921001)
National Natural Science Foundation of China (Grants No. 11774192, No. 11427903, No. 11634007)
Beijing Innovation Center for Future Chips, Tsinghua University
Facet Specific Adsorption as a Route to Remediation of Chlorinated Organic Contaminants

HAO GUO (Presenter), Univ of Akron, EMILY GERSTEIN, University of Wisconsin-Milwaukee, KSHITIJ C JHA, MESFIN TSIGE, Univ of Akron — The deployment of Palladium (Pd) based technologies in contaminant removal would require multiples of improvement in reactivity specific to a given feed. Control in Pd nanostructure has shown as an approach that would allow scalable realization of gains in it. We report the behavior of two common chlorinated organic contaminants, trichloroethylene (TCE) and 1,3,5-trichlorobenzene (TCB), on three facets of Pd in terms of their adsorption, structural organization. We separate the adsorption organic molecules to atop, bridge and hollow types. Effects of temperature are additionally provided to correlate to adsorption isotherms. The Pd {110} surface templates an interlocked structure for both TCE and TCB, while having the least favorable adsorption energies. The Pd {111} surface provides stability to TCB. All the energy calculation has been done for each adsorption type and is consistent with the result of Potential of Mean Force (PMF).

This work was supported by NSF CHE-1665284.

Evidence for an accumulation layer at the donor-acceptor interface in organic solar cells

XINRUI ZHU (Presenter), CHRISTINA MCGAHAN, ALEXI C. ARANGO, KATHERINE AIDALA, Physics, Mount Holyoke College — Expected band bending at typical donor-acceptor interfaces in solar cells suggests an accumulation layer could develop for sufficiently high bias, though this is rarely discussed in the photovoltaic literature. There is evidence from bilayer organic field effect transistors as well as organic light emitting transistors that high mobility interfacial accumulation layers exist [1], as well as a report on unexpectedly long diffusion lengths in a solar cell [2]. Our model of dark current in solar cells, which carefully considers multiple physical contributions to the total current, suggests the role of an accumulation layer in supporting observed high current densities. Here we present bulk electrical measurements on bilayer transistors, along with scanning Kelvin probe force microscopy capable of measuring band bending and density of states. Materials studied include CuPC/NTCDA bilayer transistors.


*DMR-1708970
DMR-1231319
Controlling energy level alignment at a chromophore/TiO$_2$ interface using a co-adsorbed helical peptide*  

JONATHAN VIERECK (Presenter), Physics and Astronomy, Rutgers University, YUAN CHEN, RYAN HARMER, ELENA GALOPPINI, Chemistry, Rutgers University - Newark, SYLVIE RANGAN, ROBERT ALLEN BARTYNISKI, Physics and Astronomy, Rutgers University — The sensitization of wide band gap transition metal oxide semiconductors by chromophores has become ubiquitous in the field of photovoltaic devices. Since performance hinges on the charge transfer across the interface, which in turn depends upon the alignment of the chromophore frontier orbitals with respect to the substrate band edges, it is crucial to find ways of controlling this energy alignment.

Here, we present a novel and versatile approach of controlling this energy alignment via a “mixed-layer” solution sensitization process, where a monolayer of a dipole containing helical peptide is prepared on a single crystal TiO$_2$(110) surface and successively exposed to a solution of a Zinc Tetrphenylporphyrin (ZnTPP) derivative. Using UV and X-ray photoemission spectroscopies, we find that (1) repeated exposure to the ZnTPP derivative progressively displaces the peptides on the surface, and (2) the highest occupied molecular orbital and N 1s core level of the ZnTPP derivative within the mixed layer are located 300 meV lower in energy than their respective counterparts on a pure ZnTPP-derivative monolayer. These results are consistent with a simple parallel plate capacitor model of the intermixed peptide dipole layer.

*The authors acknowledge funding from DOE-FG02-01ER15256.

Investigating the monolayer structure of caffeine molecules on Au(111)*

MALTE SCHULTE (Presenter), Experimental Physics 1, TU Dortmund University, ANDREAS JEINDL, Institute for Solid State Physics, TU Graz, ISMAIL BALTACI, MARIE SCHMITZ, Experimental Physics 1, TU Dortmund University, PETER ROESE, ULF BERGES, DELTA, TU Dortmund University, OLIVER T. HOFMANN, Institute for Solid State Physics, TU Graz, CARSTEN WESTPHAL, Experimental Physics 1, TU Dortmund University — Polymorphism is an important property of pharmaceutical ingredients in terms of their bioavailability. As a bottom-up approach we investigated the formation of monolayers of caffeine molecules on a Au(111) surface to understand caffeine's polymorph behavior.

In this work we analyzed the structure formation of caffeine molecules on Au(111) by scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), x-ray photoelectron spectroscopy (XPS), and density functional theory (DFT) calculations. All investigations were conducted at monolayer coverage at room temperature.

By combining these powerful surface science techniques, we demonstrate successful formation of caffeine monolayers including molecular alignment in two mirrored directions of the Au(111) surface. We propose a structure model for the two found surface domains in a three-molecular unit cell. This contributes to an understanding of the driving forces for surface structure formation which is essential for potential applications.

*The authors are grateful for financial support by the Land Nordrhein-Westfalen and by the Austrian Science Fund (FWF): P28631-N36 and Y1157.
4:54PM P52.00011: Spiropyran/Merocyanine adsorption on a Gold Surface  ANDREAS RIEemann (Presenter), LUCAS BROWNING, HUNTER GOFF, NELSON TATE, Western Washington Univ — Spiropyran is a photochromic, three-dimensional molecular switch which can be converted to Merocyanine, a planar isomer of Spiropyran where the central C-O bond has been broken. The adsorption behavior of a specific molecule, namely naphtho-merocyanine on an Au(111) substrate has been investigated using Scanning Tunneling Microscopy (STM) and computational chemistry methods. The experiments show a strong preference of dimer formation of the merocyanine molecule. Topographical and spectroscopic measurements are used to identify two distinguished configurations, an elongated dimer and a compact dimer. With the help of DFT and Molecular Mechanics calculations these two configurations as well as the specific merocyanine isomer can be identified and energy calculations including adsorption geometries could be performed. This is a first step in investigating possible pathways toward the switching behavior of merocyanine and spiropyran on this substrate.

5:06PM P52.00012: Investigating Electronic structure at Nano-Bio Interface to optimize Excitonic Solar cell architecture  SUBHABRATA DAS (Presenter), Langmuir Center of Colloids and Interfaces, Columbia Univ, XIAOJiANG YU, Synchrotron Light Source, National University of Singapore, LIANG CAO, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, ABHIRUP PATRA, Chemistry, University of Pennsylvania, XINGyu GAO, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, MARK BREESE, Synchrotron Light Source, National University of Singapore, PONISSERIL SOMASUNDARAN, Langmuir Center of Colloids and Interfaces, Columbia Univ, ZHAONING SONG, Physics and Astronomy, University of Toledo, BERNARDO BARBIELLINI, Physics, LUT University of Technology, VENKATESAN RENUGOPALAKRISHNAN, Chemical Biology, Northeastern University — A study of the Bacteriorhodopsin/TiO₂ and Bacteriorhodopsin/Perovskite interfaces associated with the photoactive chromophore in bacteriorhodopsin (bR) and its various mutant (D96N, triple glutamic mutations E9Q/E194Q/E204Q) forms allowed the explanation of the effective coupling existing between the π electrons of the chromophore and the local environment of the Schiff base when adsorbed to a substrate (Das et al., ACS applied materials & interfaces 11.34 (2019)). X-ray Photoemission Spectroscopy (XPS) and X-ray Absorption Spectroscopy (XAS) experiments have been used to explain some of the optical properties for various substrates such as Mesoporous TiO₂ and Perovskite. Density functional calculations (DFT) for both the ground state and the excited state has been carried in parallel with the experimental measurements. We discussed how to compensate the charge offset, to restore the Valence Band and XPS of C1s while mapping the occupied and unoccupied states around both sides of the Fermi level. In specific, we calculated the electronic band structure of the bR Chromophore using DFT+U methodology. The goal of this investigation is to optimize future Solar cell architecture (Das et al., The Journal of Physical Chemistry C (2019)).
P52.00013: Light-induced molecular dipole reordering in halide perovskites* YA-PING CHIU (Presenter), HUNG-CHANG HSU, National Taiwan University, BO-CHAO HUANG, Academia Sinica, SHU-CHENG CHIN, National Taiwan University, CHENG-RONG HSING, DUC-LONG NGUYEN, Academia Sinica, MICHAEL SCHNEDLER, Forschungszentrum Jülich, RAMAN SANKAR, Academia Sinica, RAFAL E. DUNIN-BORKOWSKI, Forschungszentrum Jülich, CHING-MING WEI, Academia Sinica, CHUN-WEI CHEN, National Taiwan University, PHILIPP EBERT, Forschungszentrum Jülich — Light-induced molecular dipole's orientation has been suggested to be a critical degree of freedom to affect the performance of hybrid perovskite-based optoelectronic devices. In this work, we utilized light-illuminated cross-sectional scanning tunneling spectroscopy to map simultaneously the organic cation's dipole orientation and the corresponding electrostatic potential with atomic resolution. Our discovery provides real space experimental evidence of the dipole reordering under illumination to create a deep one-dimensional potential energy well. The result may be directly responsible for the efficient carrier transport and suppressed carrier recombination of hybrid perovskite as an excellent photovoltaic and optoelectronic material.

*This work was financially supported by the Ministry of Science and Technology of Taiwan (Contract No. MOST 106-2628-M-002 -011 -MY3), National Taiwan University (Contract No. NTU-107L7848), and the Center of Atomic Initiative for New Materials from the Featured Areas Research Center Program within the framework of the Higher Education Sprout Project by the Ministry of Education (MOE) in Taiwan. Bo-Chao Huang acknowledges financial support from Academia Sinica through the investigator award (AS-IA-107-M03) given to Prof. Yuh-Lin Wang.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P53 DCMP: Physical properties of carbon nanotubes, 1D structures derived from 2D materials, and nanowires Mile High Ballroom 1F - Masa Ishigami, Univ of Central Florida
2:30PM P53.00001: Band-Gap-Dependent Electronic Compressibility of Carbon Nanotubes in the Wigner Crystal Regime  
NEDA LOTFIZADEH (Presenter), University of Utah, DANIEL R. MCCULLEY, MITCHELL SENGER, Oregon State University, HAN FU, University of Chicago, ETHAN D. MINOT, Oregon State University, BRIAN SKINNER, Ohio State University, VIKRAM V DESHPANDE, University of Utah — Electronic compressibility, the second derivative of ground-state energy with respect to total electron number, is a measurable quantity that reveals the interaction strength of a system and can be used to characterize the orderly crystalline lattice of electrons known as the Wigner crystal. Here, we measure the electronic compressibility of individual suspended ultraclean carbon nanotubes in the low-density, Wigner crystal regime. Using low-temperature quantum transport measurements, we determine the compressibility as a function of carrier number in nanotubes with varying band gaps. We observe two qualitatively different trends in compressibility versus carrier number, both of which can be explained using a theoretical model of a Wigner crystal that accounts for both the band gap and the confining potential experienced by charge carriers. We extract the interaction strength as a function of carrier number for individual nanotubes and show that the compressibility can be used to distinguish between strongly- and weakly- interacting regimes.

2:42PM P53.00002: Beating the Detailed Balance Limit in Ideal Carbon Nanotube pn diodes*
PRATHAMESH DHAKRAS (Presenter), College of Nanoscale Science and Engineering, SUNY Polytechnic Institute, EVERETT COMFORT, Intel, JI UNG LEE, College of Nanoscale Science and Engineering, SUNY Polytechnic Institute — The detailed balance (DB) limit developed by Shockley-Queisser has been the guiding principle for the design of modern solar cells. According to the DB limit, a single junction pn diode exhibits the maximum open-circuit voltage (\(V_{OC}\)) when it operates in the ideal diode limit. An ideal pn diode is characterized by an ideality factor \(n=1\) which correlates to a specific generation and recombination (GR) process in a diode. Though \(V_{OC}\) is directly proportional to \(n\), typically a higher \(n\) does not correspond to a larger \(V_{OC}\). This is due to higher GR process for diodes with \(n\) that directly correspond to an increased diode leakage current, which reduces the diode's open-circuit voltage. Here, we exploit a previously overlooked parameter, the diode ideality factor \(n\), to increase the \(V_{OC}\) above the ideal diode limit. We use dynamic gate modulation in a single-walled carbon nanotube diode to engineer a digitally tunable effective ideality factor that is decoupled from the diode leakage current. We show that the open-circuit voltage can be tuned in direct proportion to \(n\) and achieve a \(V_{OC}\) that is 3 times higher than that given by the DB limit of an ideal pn diode.

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DTRA/NRL Grant No. N00173-14-1-G017
2:54PM P53.00003: Electrical Transport of One-Dimensional Atomic Tellurium Nanowires Scaling Down to Two Nanometer Limit  PAI-YING LIAO (Presenter), JINGKAI QIN, GANG QIU, MENGWEI SI, Purdue Univ, SIQI ZHANG, YOKE KHIN YAP, Department of Physics, Michigan Technological University, PEIDE (PETER) YE, Purdue Univ — Due to the capability of forming air-stable thin films with high carrier mobility up to 800 cm$^2$ V$^{-1}$ s$^{-1}$ at room temperature, tellurium (Te) as a chalcogen has shown its excellent potential in the field of semiconductor devices. As a narrow-bandgap p-type semiconductor, bulk Te has a direct bandgap of $\sim$0.35 eV. Besides, Te has a unique crystal structure composed by helical chains. Each Te atom is covalently bonded with the other two adjacent Te atoms to form a spiral chain, and bulk crystal is consist of numerous chains stacked by van der Waals interaction. Here, we systematically studied the electronic transport properties of 1D Te devices scaling down to 2 nm limit in diameter. Since the native oxidation and degradation of 1D Te nanowires (NWs), the limit of bare Te NWs to exhibit stable electronic signal is around 6-7 nm. In order to further explore the performance of thinner Te NWs, we grew Te atomic chains into boron nitride nanotubes (BNNTs) and realized its field effect successfully down to 2 nm limit. Due to the encapsulation of BNNTs, the on-state current can even be dramatically increased. Moreover, the phonon responses of 1D Te NWs have also been investigated from bulk form down to a single atomic chain limit by encapsulation of carbon nanotubes (CNTs).

3:06PM P53.00004: Fabrication and characterization of ultrathin Ta$_2$(Pd or Pt)$_3$Se$_8$ nanowires*  ABIN JOSHY (Presenter), YUN LING, Tulane Univ, XUE LIU, Physics and Applied Physics, Nanyang Technological University, ANDREW STEELY, GAVIN R BLAIR, Tulane Univ, LIUBOV YU ANTIPINA, PAVEL B. SOROKIN, Technological Institute for Superhard and Novel Carbon Materials, ANA M. SANCHEZ, University of Warwick, ZHIQIANG MAO, Pennsylvania State University, JIANG WEI, Tulane Univ — Miniaturization of semiconductor devices has been a prime focus of the electronics industry to address the requirements of next-generation electronic devices. One possible solution to tackle this problem is semiconducting one-dimensional (1D) van der Waals(vdW) wires. Here we present quasi 1D semiconducting Ta$_2$(Pd or Pt)$_3$Se$_8$(TPS) crystals, composed of weakly bound molecular ribbons. Inter-ribbon bonding energy(0.34eV/atom) of TPS bulk is 17 times weaker than the intra ribbon bonding energy(5.7eV/atom). In this work, we used cost-effective and easily processable liquid phase exfoliation technique to achieve molecularly thin wires. The thinnest nanowire we have readily achieved is around 1 nm, corresponding to a bundle of one or two molecular ribbons. Optimum solvent for the dispersion is investigated and found Di-acetone alcohol gives strong dispersion. High-resolution TEM, SEM and AFM studies were done to investigate the morphology and crystallinity of the ultrathin wires obtained. Our electrical transport measurements have shown that these thin wires are gatable and preserve the intrinsic bulk characteristics. The fabricated 1D transistors exhibit high switching performance and excellent ambient environment stability.

*This work is supported by NSF grant #1752997
3:18PM P53.00005: Carbon nanotube photocurrent quantum yield greater than 100%*
MITCHELL SENG (Presenter), DANIEL R. MCCULLEY, Physics, Oregon State University, ANDREA
BERTONI, Istituto Nanoscienze, Consiglio Nazionale delle Ricerche, VASILI PEREBEINOS, Electrical
Engineering, University at Buffalo, ETHAN D. MINOT, Physics, Oregon State University — Carbon
nanotubes (CNTs) have been identified as a candidate material to surpass the Shockley-Queisser
limit, however, early measurements of photocurrent quantum yield (PCQY) in CNT photodiodes
found PCQY < 100%. We studied CNT photodiodes made from individual suspended CNTs with
the goal of elucidating the role of nanotube diameter, dielectric environment, axial electric field,
and the optical excitation energy. When photons of energy approximately twice the band gap are
absorbed in the intrinsic region of a CNT photodiode, it is possible to extract a photocurrent that
 corresponds to more than one electron-hole pair per absorbed photon. We observed this high-
quantum-yield process by increasing CNT diameter to > 2.6 nm and increasing the axial electric
field to > 10 V/µm (a previously unstudied regime). Higher energy optical excitation gives even
higher PCQY. The observed dependence on diameter and dielectric environment is consistent
with theoretical models for exciton binding energy and exciton dissociation rates. Our work
suggests there are conditions for which efficient exciton dissociation co-exists with efficient
impact ionization.

*This material is based upon work supported by the National Science Foundation under Grant
No. 1709800.

3:30PM P53.00006: Temperature-Dependent Thermoelectric Transport in Polymer-Sorted
Semiconducting Carbon Nanotube Networks with Different Diameter Distributions*
MARTIN STATZ (Presenter), Univ of Cambridge, SEVERIN SCHNEIDER, FELIX BERGER, University of
Heidelberg, LIANGLUN LAI, WILLIAM ADAM WOOD, Univ of Cambridge, JANA ZAUMSEIL, University of
Heidelberg, HENNING SIRRINGHAUS, Univ of Cambridge — We report carrier density and
temperature dependent field-effect mobility and on-chip Seebeck coeff. measurements of small
diameter (6,5) (0.76 nm), ttmgb treated (6,5) and large diameter plasma torch (RN, 1.17-1.55 nm)
SWCNT networks with different network densities to provide insights into their charge transport
mechanisms and potential for thermoelectric applications. The Seebeck coeff. offers insights into
transport energetics, potential contributions from electron-electron and electron-phonon
interactions and the relative contributions of inter- versus intra-CNT transport.¹ A pure
percolation theory and VRH description cannot explain both transport coefficients and instead
intra-CNT transport depending on chirality needs to be considered as well. In the high network
density regime, the density influences neither electric nor thermoelectric transport strongly,
indicating both are dominated by tubes rather than tube-tube junctions. Despite generally lower
mobilities, (6,5) SWCNTs show comparable power factors to RN networks. These findings provide
design guidelines towards narrow DoS distr., large diameter SWCNT networks for both electronic
and thermoelectric applications.²


*ERC SC2 (610115)
**3:42PM P53.00007: Applying Machine Learning to Thermal Conductance**

ALEXANDER KERR (Presenter), KIERAN MULLEN, Homer L Dodge Department of Physics and Astronomy, Univ of Oklahoma, DANIEL T GLATZHOFER, Department of Chemistry and Biochemistry, Univ of Oklahoma, LIANGLIANG HUANG, School of Chemical, Biological and Materials Engineering, Univ of Oklahoma — Machine learning provides a new approach in materials design. Recent years have seen the use of generative models to algorithmically produce candidate molecules for a variety of tasks. One such model is the variational autoencoder (VAE), which can map discrete information to a continuous, low-dimensional space. We study the ability of these methods to design nanostructures for thermal conductivity: from idealistic harmonic chains to functionalized carbon nanotubes (CNTs). Designing the latter’s side-chains is of particular interest for overcoming the severe Kapitza resistance of CNTs and accessing their promising thermal properties. We also highlight the ability of a genetic algorithm (GA) enhanced with a discriminating neural network to optimize molecules for their thermal conductance. Because discriminating GAs are forced to consider a diverse field of molecules, they are an effective way to generate a varied dataset for analysis. It can be shown that molecules sampled in this manner are clustered based on their thermal properties in the latent space learned by the VAE. In addition, studying the GA trajectory may reveal design rules that can narrow the search for good conductors.

*This work was supported by NSF grant DMR-1310407.

**3:54PM P53.00008: Carbon Nanotube Alignment Dynamics under Electric Fields in Different Solutions**

ATIQUR RAHMAN, AHMED ZUBAIR (Presenter), Electrical and Electronic Engineering, Bangladesh University of Engineering and Technology — Controlled macroscopic assembly of carbon nanotubes (CNTs) while preserving their excellent optoelectronic properties still remain a key challenge. Here, we investigated the molecular dynamics of single-wall carbon nanotube (SWCNT) alignment inside various viscous media under electric fields. An analytical model based on dielectrophoresis induced torque considering the viscosity and conductivity of the medium was used to obtain molecular dynamics of the SWCNTs. An alternating current (AC) electric field was applied to SWCNT containing liquid solutions of several solvents/surfactants such as DIW, DMF, DPSF, SDS, and DOC. Time required for the SWCNTs to get aligned to the applied AC electric field were calculated for different initial conditions for all the solutions. The effects of CNT length, CNT diameter, and frequency of the electric field on the SWCNT network formation were theoretically studied. Longer and thinner SWCNTs prompted to faster alignment in SWCNT network. Furthermore, the effect of concentration of surfactant on arrangement time was examined. Slower SWCNT alignment was observed in medium with higher viscosity. The findings of this report will be helpful for establishing an effective technique of producing large-scale aligned CNT films for diverse applications.
4:06PM P53.00009: Achieving Global Alignment of Single-Wall Carbon Nanotube Films through Electrostatic Control*  JOSHUA S. WALKER (Presenter), Physics, University of Wyoming, JEFFREY A. FAGAN, ADAM BIACCHI, National Institute of Standards and Technology, VALERIE KUEHL, Chemistry, University of Wyoming, THOMAS A SEARLES, Howard University, ANGELA HIGHT WALKER, National Institute of Standards and Technology, WILLIAM D. RICE, Physics, University of Wyoming — Single-wall carbon nanotubes (SWCNTs), known for their exceptional mechanical, thermal, electrical, and optical properties, present a platform for next generation opto- and thermo-electronics. The difficulty, however, lies in the ability to reproducibly form aligned SWCNT films from aqueous nanotube solutions, which continues to be a significant scientific and technological challenge. Although multiple research groups have achieved high nematic ordering from SWCNT solutions, the mechanism driving this alignment, as well as optimization of it, remains elusive. Here, we use an automated filtration platform and superhydrophobic glass to create globally aligned films from solution-based SWCNTs. We show how SWCNT alignment is impacted by the filtration flow rate and SWCNT electrostatic environment. Additionally, we find that the SWCNT nematicity can be enhanced via buffing of the polymeric membrane coating and hindered by reducing the Debye interaction length of the SWCNTs, both of which show the importance of electrostatics in the alignment mechanism. These results have direct implications for achieving and optimizing the alignment of single- and few- chirality SWCNT films.

*JSW and WDR acknowledge support from the UW School of Energy Resources and Academic Affairs.

4:18PM P53.00010: Electron-phonon and phonon-phonon interaction in low-dimensional carbon materials  IOANNIS CHATZAKIS (Presenter), Physics and Astronomy, Texas Tech University — Low-dimensional (e.g. atomically thin) materials continue to gain prominence in applications ranging from electronics to photonics and alternative energy generation systems. Critical to efficiently developing these systems is the understanding of the fundamental processes related to the dynamics of charge carriers, phonons, and other excitations (i.e. excitons, polaritons). In this talk, I will focus on electron-phonon interactions in low dimensional carbon materials. Through these interactions the electrons lose all their excess energy above the band edge and become thermally equilibrated with the most strongly coupled optical phonon modes. Subsequently the optical phonons modes through unharmonic phonon-phonon scattering processes decay to lower-energy phonon modes.
4:30PM P53.00011: A Raman study of G-bands in isolated and bundled triple-walled carbon nanotubes  JIA WERN HUE (Presenter), Department of Physics & Astronomy, The University of Alabama, THOMAS CH HIRSCHEMANN, Attocube Systems AG, YOONG AHM KIM, School of Polymer Science and Engineering, Chonnam National University, NEWTON M BARBOSA NETO, Instituto de Ciências Exatas e Naturais – Programa de Pós-graduação em Física, Universidade Federal do Pará, PAULO T ARAUJO, Department of Physics & Astronomy, The University of Alabama — The G-band is a Raman-active phonon mode, caused by tangential and longitudinal stretching of the two dissimilar carbon atoms in the unit cell. This mode is well studied in other forms of carbon, e.g. graphite, graphene, single-walled and double-walled carbon nanotubes. Building on that knowledge, a study on bundled and isolated triple-walled carbon nanotubes (TWNT) is presented. Of particular interest is how many G-band peaks are present, their lineshapes, and how the G-band frequencies of the constituent tubes are affected from being in a TWNT system compared to if they were just SWNTs.

4:42PM P53.00012: High pressure Raman spectroscopy of Linear carbon chain encapsulated in isolated multiwall carbon nanotube*  KESHAV SHARMA (Presenter), Univ of Alabama - Tuscaloosa, NATHALIA L.M. COSTA, ALEXANDRE ROCHA PASCHOAL, Departamento de Física, Universidade Federal do Ceará, Fortaleza, PAULO T ARAUJO, Univ of Alabama - Tuscaloosa — Elusive measurements of the Longitudinal optical (LO) phonon mode frequency of isolated Cn@MWCNT systems (linear carbon chains encapsulated by multi-wall carbon nanotubes) were studied under extreme high pressure via Resonance Raman spectroscopy. The pressure-dependent frequency softening with increasing pressure is discussed in terms of a simple force constant model in which the spring constants present a dependence with pressure. The model allowed us to easily obtain both the Young's modulus and the Gruneisen parameter associated to such LO mode. In particular, the Gruneisen parameter was found to be much higher than that of Graphene and CNTs. Additionally, the LO phonon lifetime was found to be decrease with increasing stress.

*The authors want to acknowledge The Sociedade Brasileira de Física (SBF) and the American Physical Society (APS) for the Brazil-U.S. Physics Ph.D. Student and Postdoc Visitation Program award.
4:54PM P53.00013: Raman Spectra of Vertical Graphene Nanosheets*  CHUNYU LU  (Presenter), ABDULRAHMAN AL-HAGRI, NITUL RAJPUT, MATTEO CHIESA, Khalifa University — Raman spectroscopy studies have been demonstrated their importance in providing a quantitative measure on different carbon-based samples, such as graphene, carbon nanotube, and sp3 amorphous carbon. Recently, plasma-enhanced chemical vapor deposition grown vertical graphene nanosheets (VGNs) have attracted much attention owing to their abundant edges, surface, and enhanced electrochemical activity, which are potentially applicable to a wide of fields. However, due to its complexity of the vertical structures, the knowledge gained in previous carbon-based materials has not fully been extended to VGNs. In this work, we review the recent advance of Raman characterization results on PECVD-grown VGNs. With the insights from interference in graphene nanosheets and their electrical field distribution, we are able to extend the knowledge from the Raman spectroscopy of conventionally flat graphene layer to vertical graphene nanosheets. A feasible way to distinguish and evaluate the quality and structures of the VGNs from Raman spectra is presented in combination with the transmission electron microscopy characterization.

*the Cooperative Agreement between the Khalifa University, UAE and the Massachusetts Institute of Technology, MA, USA, Reference Number FR2017-000001.

5:06PM P53.00014: Manipulating high-harmonic generation in single walled carbon nanotubes*  KAZUHIRO YANAGI (Presenter), HIROYUKI NISHIDOME, Tokyo Metropolitan Univ, KOHEI NAGAI, KENTO UCHIDA, YOTA ICHINOSE, YOHEI YOMOGIDA, KOICHIRO TANAKA, Physics, Kyoto university — High-harmonic generation (HHG), which is the generation of multiple optical harmonic light, is an unconventional nonlinear optical phenomenon beyond the perturbation regime. The HHG in solid state materials is strongly influenced by the presence of nonlinearity in transport and optical transitions, but how to engineer these parameters has not yet been elucidated. Here, we demonstrate manipulation of HHG by tuning the electronic structure and carrier densities using single-wall carbon nanotubes with tuned electronic structures and Fermi levels. We reveal systematic changes in the HH spectra of carbon nanotubes with a series of electronic structures from a zero band-gap metal to a semiconductor. We demonstrate enhancement or reduction of harmonic generation by more than one order of magnitude by tuning electron and hole injection into the semiconductor carbon nanotubes through static electric field application.

*K.Y. acknowledges support by JSPS KAKENHI through Grant Numbers JP17H06124, JP17H01069, and JP18H01816 and JST CREST through Grant Number JPMJCR17I5, Japan.
5:18PM P53.00015: Polymer Host for Optical and Terahertz Spectroscopy of Low-Aggregation Nanoparticle Films*  HENRY WLADKOWSKI (Presenter), JULIAN A. DUARTE, Univ of Wyoming, JEFFREY A. FAGAN, National Institute of Standards and Technology, JEFFREY L BLACKBURN, National Renewable Energy Laboratory, SHASHANK RAM NANDYALA, JON M PIKAL, WILLIAM D. RICE, Univ of Wyoming — Preparation techniques for producing films of individualized nanoparticle for low-temperature optical spectroscopy are often challenging to execute and specific for a particular nanoparticle system. Here, we present a rapid, facile, and low-cost technique for producing 100 μm-thick nanoparticle-polymer films that exhibit high uniformity, low aggregation, excellent optical transparency, and low terahertz absorption. These films are both robust at cryogenic temperatures and exhibit a high laser damage threshold of 0.3 TW/cm², which make them ideal for pulsed laser measurements. Additionally, we show that free-standing flexible films can be made from 0D quantum dots and 1D single-wall carbon nanotubes (SWCNTs). Using absorption, Raman scattering, and photoluminescence excitation spectroscopy we show that SWCNT individualization is maintained from solution to film. Finally, we perform optical pump, terahertz probe measurements on SWCNT films to demonstrate pulsed spectroscopic investigation across a broad electromagnetic regime. This polymer host presents spectroscopists with a straightforward method for producing free-standing and flexible nanoparticle films with low aggregation.

*HVW and WDR acknowledge support from the Ivers Fellowship and the UW School of Energy Resources.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P54 DCMP: Geometric and Fluid Properties of Quantum Hall States  Mile High Ballroom 2A

2:30PM P54.00001: Free surface boundary dynamics of compressible and dissipationless fluids with Hall viscosity  SRIRAM GANESHAN (Presenter), Simons Center for Geometry and Physics, GUSTAVO MONTEIRO, The City College of New York, ALEXANDER ABANOV, Simons Center for Geometry and Physics, TANKUT CAN, Initiative for the Theoretical Sciences, The Graduate Center, CUNY — In this talk, we consider non-dissipative and compressible two-dimensional broken parity fluids with odd viscosity and magnetic field with a free surface boundary condition. We solve the linearized hydrodynamic equations for the deepwater case and derive the dispersion of chiral surface waves. We show that in the long-wavelength limit the flow profile exhibits an oscillating vortical boundary layer near the free surface. The thickness of the layer is controlled by the length scale given by the ratio of odd viscosity to the sound velocity. In the incompressible limit, the vortical boundary layer becomes singular with the vorticity within the layer diverging as the velocity of sound. The boundary layer is formed by odd viscosity coupling the divergence of velocity to vorticity. It results in non-trivial chiral free surface dynamics even in the absence of external forces. The structure of the odd viscosity induced boundary layer is very different from the conventional free surface boundary layer associated with dissipative shear viscosity.
2:42PM P54.00002: Variational principle for free surface boundary dynamics of dissipationless fluids with Hall viscosity  GUSTAVO MONTEIRO (Presenter), SRIRAM GANESHAN, The City College of New York, ALEXANDER ABANOV, Simons Center for Geometry and Physics, TANKUT CAN, Initiative for the Theoretical Sciences, The Graduate Center, CUNY — In this talk, we present the variational principle for non-dissipative and compressible two-dimensional broken parity fluids with odd viscosity with a free surface boundary condition. In the absence of shear viscosity, the boundary layer is formed by odd viscosity coupling the divergence of velocity to vorticity. The dissipationless nature of the boundary layer allows us to construct an effective action that gives both bulk hydrodynamic equations and free surface boundary conditions. The free surface boundary conditions require an additional boundary term in the action which resembles a 1+1D chiral boson field coupled to the background geometry. We discuss generalizations of this action to quantum Hall fluids and nearly incompressible fluids.

2:54PM P54.00003: Hall viscosity in systems with discrete symmetry: point group and lattice anisotropy*  PRANAV RAO (Presenter), BARRY BRADLYN, University of Illinois at Urbana-Champaign — Inspired by recent experiments on graphene, we examine the non-dissipative viscoelastic response of anisotropic two-dimensional quantum systems. We pay particular attention to electron fluids with point group symmetries, and those with discrete translational symmetry. We extend the Kubo formalism for viscosity to systems with internal degrees of freedom and discrete translational symmetry, highlighting the importance of properly considering the role of internal angular momentum. We analyze the Hall components of the viscoelastic response tensor in systems with discrete point group symmetry, focusing on the hydrodynamic implications of the resulting forces. We show that though there are generally six Hall viscosities, there are only three independent contributions to the viscous force density. To compute these coefficients, we develop a framework to consistently write down the long-wavelength stress tensor and viscosity for multi-component systems, and apply our formalism to a few examples.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE 1746047
3:06PM P54.00004: Geometric response of fractional quantum Hall states to anisotropy*  
AKSHAY KRISHNA (Presenter), Princeton University, MATTEO IPPOLITI, Stanford University, FAN CHEN,  
RAVINDRA NAUTAM BHATT, Princeton University — Fractional quantum Hall states possess a  
geometric degree of freedom that is usually hidden in the case of rotationally symmetric  
Hamiltonians. When this symmetry is broken, for example by means of an anisotropic electron  
band mass or electron-electron interaction, the many-body wavefunction optimizes over this  
degree of freedom to obtain the lowest energy. This is manifested as a partial transference of the  
anisotropy of Hamiltonian to observable properties of the ground state. In some cases, the  
fractional quantum Hall phase is unstable to the application of anisotropy and there is a  
transition to a broken symmetry phase. We use a combination of exact diagonalization and the  
infinite density matrix renormalization group (iDMRG) algorithm to quantify the extent of the  
anisotropic response and find a remarkable dependence on filling fraction, Landau level index,  
interaction type and particle statistics [1].  
*This work was supported by DOE BES Grant DE-SC0002140.

3:18PM P54.00005: Non-trivial edge profile of the Laughlin wave function*  
GABRIEL JOSE GOULART CARDOSO (Presenter), ALEXANDRE ABANOV, Department of Physics and Astronomy, Stony  
Brook University, JEAN-MARIE STÉPHAN, CNRS, University of Lyon 1 — The wave function proposed by  
Laughlin in 1983 led to a great advance in understanding the many-body quantum physics of the  
Fractional Quantum Hall Effect (FQHE). Laughlin's plasma analogy maps the distribution of  
electron densities in the FQHE state to the one of the classical 2-dimensional One-Component  
Plasma (2DOCP), with the temperature of the 2DOCP corresponding to the filling fraction of the  
FQHE state. We explore this connection further to investigate the non-trivial behavior of the  
electron density close to the edge of a FQHE droplet. Using a mix of recent Monte Carlo results  
and analytical methods we show that the observed profile of overshoot plus damped oscillations  
of the density near the edge can be explained in terms of the partial crystallization of the  
corresponding 2DOCP close to a boundary. We analyze the dependence of this effect on the  
proximity to the boundary and on the FQHE filling fraction.  
*NSF DMR-1606591
3:30PM P54.00006: Contactless pulsed tunneling spectroscopy of exciton superfluid phase in a quantum Hall bilayer*  HEUN MO YOO (Presenter), Massachusetts Institute of Technology MIT, K. W. BALDWIN, KENNETH WEST, LOREN PFEIFFER, Princeton University, RAYMOND ASHOORI, Massachusetts Institute of Technology MIT — A quantum Hall (QH) bilayer with sufficiently small interlayer separation $d$ is predicted to host an exciton superfluid phase. Here, we use a contactless pulsed tunneling technique to search for novel superfluid properties of the QH bilayer. As our method does not require ohmic contacts to the layers, it permits access the entire range of density imbalances ($\Delta \nu$) at a total filling factor $\nu_T = 1$. At a small magnetic field ($d/l_B = 1.49$), zero-bias interlayer tunneling is maximized at $\Delta \nu = 0$ and is consistent with prior DC tunneling measurements. On the other hand, at a larger magnetic field ($d/l_B = 1.82$), we observe the maximum of zero-bias tunneling near a full density imbalance $\Delta \nu = 1$. The observed behavior near $\Delta \nu = 1$ contradicts the simple theoretical expectation, based on the pseudospin stiffness going to zero, that the system would evolve into a trivial $\nu = 1$ QH-state in one layer. In addition to the full density imbalance dependence, future pulse tunneling measurements can reveal high-frequency dynamical response of the exciton superfluid phase.

*This work is supported by the Basic Energy Sciences Program of the Office of Science of the U.S. Department of Energy through contract no. FG02-08ER46514 and by the Gordon and Betty Moore Foundation through grant GBMF2931.

3:42PM P54.00007: Observation of a new reentrant integer quantum Hall state in the N=0 Landau level*  GABOR CSATHY (Presenter), VIDHI SHINGLA, Purdue Univ, KENNETH WEST, LOREN PFEIFFER, Princeton Univ — We report the observation of a reentrant integer quantum Hall state in the $N = 0$ Landau level near the Landau level filling factor $\nu = 2 - 1/5$. Unlike similar reentrant states in high $N \geq 2$ Landau levels, the reentrant state reported here is interpreted as a Wigner solid that is the particle-hole conjugate of the reentrant Wigner solid forming at $1/5 < \nu < 2/9$. Our results indicate that Wigner solids in the GaAs/AlGaAs system commonly straddle the partial filling factor $1/5$ and paint a complex picture of the competition of the Wigner solid with fractional quantum Hall states.

*Measurements at Purdue University were supported by NSF grants DMR 1505866 and 1904497. Sample growth efforts at Princeton University were supported by Gordon and Betty Moore Foundation Grant No. GBMF 4420, and the National Science Foundation MRSEC Grant No. DMR-1420541.
3:54 PM P54.00008: Collective excitations of quantum Hall states under tilted magnetic field

KANG YANG (Presenter), Department of Physics, Stockholm University, MARK OLIVER GOERBIG, Laboratoire de Physique des Solide, Paris-Sud University, BENOÎT DOUÇOT, Sorbonne University — We study the neutral excitations of quantum Hall systems under external anisotropy introduced by tilting the magnetic field. In the isotropic case, the neutral collective excitation can be worked out through the conserving method of composite fermions satisfying integer quantum Hall effects in the Hamiltonian theory. We show how such a computation can be carried out perturbatively for an anisotropic interaction. We find that unlike the charge gap, the neutral collective gap is much more easily destroyed by the parallel component of the magnetic field. We also address the issue about the convergence of the collective spectrum to the activation gap.

4:06 PM P54.00009: Hall viscosity in abelian gauge theories*

UMANG MEHTA (Presenter), DAM THANH SON, University of Chicago — We investigate the Hall viscosity of U(1) gauge theories. Starting with the Maxwell-Chern-Simons theory, by explicitly constructing the ground state wave functional, we show that the Hall viscosity is zero. We also add Lorentz-breaking parity-odd terms to the Lagrangian and observe that the Hall viscosity remains zero. We argue that the result is general and discuss the implications for the Hall viscosity of the composite fermions in the fractional quantum Hall effect.

*This work is supported by the Simons Foundation through a Simons Investigator grant and the Simons Collaborations on Ultra-Quantum Matter, US Department of Energy grant No. DE-FG02-13ER41958 and a Big Ideas Generator (BIG) grant from the University of Chicago.

4:18 PM P54.00010: Pseudopin transition of two-dimensional hole systems in hydraulic pressure*

YANG LIU (Presenter), KE HUANG, Peking Univ, LOREN PFEIFFER, KENNETH WEST, K. W. BALDWIN, Electrical engineering, Princeton university, XI LIN, Peking Univ — We preform transport measurement of high quality two-dimensional hole systems in a pressure cell at low temperatures. We find that the hydraulic pressure can induce phase transition to fractional quantum Hall effect near $\nu = 3/2$. The discovered phenomenon is consistent with spin polarization transitions when the energy separation between the lowest two Landau levels is quenched by the large hydraulic pressure. Our finding reveal subtle dependence of spin degree of freedom on hydraulic pressure in hole systems.

*We acknowledge support from the National Key Research and Development Program of China (No. 2017YFA0303301), the National Natural Science Foundation of China (Grant No. 11674009 and No. 11921005), the National Basic Research Program of China (Grants No. 2015CB921101), the Beijing Natural Science Foundation (JQ18002), and the Key Research Program of the Strategic Priority Research Program of Chinese Academy of Sciences (Grant No. XDB28000000) for measurements, the NSF (Grants No.DMR-1305691 , and No. MRSEC DMR-1420541), the Gordon and Betty Moore Foundation (Grant No. GBMF4420), and the Keck Foundation for the material growth and characterization.
4:30PM P54.00011: Anomalous nematic states in half-filled Landau levels in tilted magnetic fields

MICHAEL ZUDOV (Presenter), XIAOJUN FU, QIANHUI SHI, University of Minnesota, GEOFF C GARDNER, JOHN WATSON, MICHAEL MANFRA, Purdue University, K. W. BALDWIN, LOREN PFEIFFER, KENNETH WEST, Princeton University — In this talk we examine the effect of in-plane magnetic fields on anomalous nematic phases in half-field high Landau levels which are characterized by unexpected minima (maxima) in \( R_{xx} \) \( (R_{yy}) \) and plateau-like features in \( R_H \) emerging at low temperatures. In particular, we have found that these features quickly disappear upon application of in-plane magnetic field, regardless of its orientation with respect to the native anisotropy axis, and that conventional quantum Hall stripe phase is restored.

*The work at Minnesota (Purdue) was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award \# ER 46640-SC0002567 (DE-SC0020138). L.N.P. and K.W.W. of Princeton University acknowledge the Gordon and Betty Moore Foundation Grant No. GBMF 4420, and the National Science Foundation MRSEC Grant No. DMR-1420541. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement Nos. DMR-1157490, DMR-1644779 and the State of Florida.

4:42PM P54.00012: Interlayer exciton condensates in high Landau levels in bilayer WSe2

QIANHUI SHI (Presenter), EN-MIN SHIH, DANIEL A RHODES, BUMHO KIM, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ZLATKO PAPIC, University of Leeds, JAMES C HONE, CORY DEAN, Columbia University — Exciton condensates (EC) have been realized in the quantum hall regime in GaAs double quantum wells and graphene double layers separated BN, appearing in the lowest Landau level (LL) with index \( N = 0 \). In these systems, the barrier thickness has to be carefully chosen in order to preserve strong interlayer Coulomb interaction but suppress tunneling at the same time. In bilayer WSe2, the spin-valley locking together with the valley misalignment in natural AB stacking, results in suppressed interlayer tunneling and allows independent control of the layer population. We observe signatures consistent with interlayer EC when the two layers have matched LL orbital wavefunctions. Unlike previous systems with intentional tunnel barrier, the natural bilayer has the interlayer spacing \( d \) as small as the lattice constant and the strong interlayer Coulomb interaction allows EC to be realized in \( N > 0 \) LLs. Compared to EC in the lowest LL, EC in high LLs turn out to be more robust in the low \( d/l_B \) limit (\( l_B \) is the magnetic length), and the charge gap demonstrates an opposite dependence against interlayer density imbalance.

*Supported by US Department of Energy (DE-SC0016703).
4:54PM P54.00013: Properties of Reentrant Integer Quantum Hall States in High Landau Levels*  
DOHYUNG RO (Presenter), NIANPEI DENG, MICHAEL MANFRA, Purdue Univ, LOREN PFEIFFER, KENNETH WEST, Princeton University, GABOR CSATHY, Purdue Univ — Reentrant integer quantum Hall states in two-dimensional electron gases are commonly associated with electronic bubble phases, novel electronic solids predicted by Hartree-Fock theories. Various measurements were all consistent with the Hartree-Fock theory, with the exception of predictions of proliferation of such ground states in high Landau levels. This has recently changed with observations of double reentrance in the N=3 Landau level. We will discuss the filling factor and the temperature dependence of magnetotransport of the reentrant integer quantum Hall states in the N=3 Landau level. Our findings significantly strengthen the bubble interpretation of the reentrant integer quantum Hall states and provide insight into details of the competition of electron-electron interaction and disorder effects in the formation of the electronic bubbles.

*Our work was supported by the NSF grant DMR 1904497. Sample growth work of M.J.M. was supported by the DOE contract no. DE-SC0006671, while that of K.W.W. and L.N.P. by the National Science Foundation MRSEC Grant DMR-1420541 and the Gordon and Betty Moore Foundation Grant GBMF 4420.

5:06PM P54.00014: From Casimir Effect to Quantum Atmosphere*  
QINGDONG JIANG (Presenter), Stockholm Univ, FRANK WILCZEK, MIT — By altering the propagation of virtual photons, materials can influence the behavior of objects in their vicinity. They can cause forces on macroscopic bodies (Casimir effect), or perturb the spectra of nearby molecular complexes. I'll briefly show how to make repulsive Casimir force by using chiral materials, but mainly discuss how symmetry breaking states of matter can transmit symmetry breaking effects to spectra. I'll discuss a few such effects, which involve the “axion electrodynamics” relevant to topological insulators, quantitatively. Then I'll describe an operator framework whereby effects of this kind can be analyzed systematically, qualitatively, and discuss possible experimental implications.

*This work was supported by the Swedish Research Council under Contract No. 335-2014-7424. Frank Wilczek’s work is supported by the U.S. Department of Energy under grant Contract No. DE-SC0012567 and by the European Research Council under grant 742104.

5:18PM P54.00015: Spinning Radiation from Topological Insulator*  
EMROZ KHAN (Presenter), EVGENII NARIMANOV, Purdue Univ — Axion coupling in topological insulator (TI) gives rise to unusual electromagnetic phenomena such as induction of image magnetic monopole, Faraday rotation etc. Here we show this coupling also leads to emergence of spin angular momentum (SAM) in the thermal radiation from TI (Phys. Rev. B 100, 081408(R)). A slab of TI with a thin magnetic coating would radiate light with the same degree of circular polarization in all directions, in contrast to conventional thermal emitters with structured interface. Through the control of emission of SAM, TIs may, therefore, find potential applications in generation of structured light from thermal sources.

*The authors acknowledge support for this work from the National Science Foundation under Grant No. DMREF- 1629276 and the Gordon and Betty Moore Foundation.
2:30PM P55.00001: THz Emission Spectroscopy of Surface Photogalvanic Effects in a Chiral Weyl Semimetal  
DARIUS TORCHINSKY (Presenter), BAOZHU LU, Temple Univ, DYLAN REES, University of California, Berkeley, KAUSTUV MANNA, HORST BORRMANN, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, JOSEPH ORENSTEIN, University of California, Berkeley — Topological materials, and Weyl semimetals in particular, exhibit diverse optical effects. If inversion symmetry is broken, second order responses are allowed, expanding the number of methods that can be used to probe the optical properties of a material. These second order effects are also allowed at material interfaces, providing a unique tool to study their topologically important surface states. Here, we present photogalvanic effect data collected via terahertz emission spectroscopy on a chiral Weyl semimetal as a function of polarization and incident wavelength and discuss how our data reveal signatures of the topologically relevant surface states.

2:42PM P55.00002: Non-linear Optical Response of an Exactly Soluble Model of Topological Insulators*  
PETER RISEBOROUGH (Presenter), Temple Univ — We examine an exactly soluble model of time-reversal and inversion symmetric Topological Insulators and calculate the linear optical conductivity. For frequencies smaller than the bulk gap, the response is quantized and yields information on the surface Weyl cones and their energies. The inclusion of many-body interactions changes the result and may cause an instability due to the spontaneous emission of spin-one k=0 excitations, if the Fermi-energy is in close proximity to the vertex of the Weyl cone. For topological insulators, the low-frequency conductivity is caused by metallic states and the conductivity is highly non-local. The non-linear response functions are shown to diverge at low-frequencies, due to the 1/√ω coupling that lead to the well-known infra-red divergences found in Brehmstrahlung. We show that the infra-red divergences in the response functions due to the interaction with the surface states at both surfaces of the slab, cancel analogously to Furry's Theorem. Cancellation of the divergences seems to requires that the non-local Maxwell's equations are solved and the systematic inclusion many-body interactions.

*This work was funded by the US Department of Energy, Office of Basic Energy Sciences, Materials Science, through award DE-FG02-01ER45827
2:54PM P55.00003: Circular photogalvanic effect in interacting Weyl semimetals
ALEKSANDR AVDOSHKIN (Presenter), VLADYSLAV KOZII, JOEL MOORE, University of California, Berkeley — The circular photogalvanic effect (CPGE) is a photocurrent that depends on the sense of circular polarization. In a disorder-free, non-interacting chiral Weyl semimetal, the magnitude of the effect is approximately quantized with a material-independent quantum e^3/h^2 for reasons of band topology. We study the first-order corrections due to the Coulomb and Hubbard interactions in a continuum model of the Weyl points. We find that the inclusion of interactions generically breaks the quantization yet the corrections are non-divergent. The corrections are similar in spirit to the case of interaction corrections to the (non-topological) linear conductivity of graphene. Thus, we conclude that, unlike the quantum Hall effect or the chiral anomaly in field theories, the quantization of the CPGE is not protected but has perturbative corrections in interaction strength.

3:06PM P55.00004: Electronic band structure and free carrier properties of strained tin-germanium alloys on InSb from FTIR ellipsometry*
RIGO CARRASCO (Presenter), STEFAN ZOLLNER, New Mexico State Univ, ARNOLD KIEFER, BRUCE CLAFLIN, Wright-Patterson Air Force Base, STEPHANIE CHASTANG, JINSONG DUAN, GORDON GRZYBOWSKI, KBR Wyle — From Fourier-transform infrared ellipsometry, we provide spectroscopic evidence about the valence band structure of α-tin. The mid-infrared dielectric function of α-tin grown pseudomorphically by molecular beam epitaxy shows a strong peak near 0.41 eV. The peak can be attributed to the allowed intra-valence band transitions from the Γ(7) (electron-like) to the Γ(8) +υ heavy hole valence band and/or interband transitions from the Γ(7) band to the Γ(8) +c light “hole” conduction band. Possible sources for the strength of the peak and its temperature dependence will be discussed. Our results are significant, because intra-valence band transitions have not previously been reported as a peak in ellipsometry spectra. This peak cannot be described as a van Hove singularity with a critical point lineshape. It should be universal, i.e., common to all zero-gap semiconductors. We will also show the dependence of this peak on composition and strain in Ge_{1-x}Sn_{x} alloys with up to 6% Ge. At photon energies below 0.4 eV, FTIR ellipsometry spectra are dominated by the Drude response of free carriers and a discussion on the species of the carriers will be provided.

*Supported by NSF (DMR-1505172, HRD-1305011), AFOSR (FA9550-16RYCOR296), and AFOSR Summer Faculty Fellowship Program 2018.
3:18PM P55.00005: SHG spectroscopy of the surface states of a chiral Weyl semimetal

DYLAN REES (Presenter), University of California, Berkeley, BAOZHU LU, Department of Physics, Temple University, KAUSTUV MANNA, CLAUDIA FELSER, Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Straße-40, 01187 Dresden, Germany, JOSEPH ORENSTEIN, University of California, Berkeley, DARIUS TORCHINSKY, Department of Physics, Temple University — Second harmonic generation (SHG) is an optical effect that has recently been extensively used to study the electronic band structure as well as lattice and electronic symmetry of various inversion-symmetry breaking solid state materials, including topological systems. Since the surface of any material is a locus of inversion symmetry breaking, SHG spectroscopy has traditionally been used to selectively probe the surface electronic properties of materials. We present an SHG study of a chiral Weyl semimetal as a function of incident photon energy to study SHG response deriving solely from the surface and discuss what our analysis of the nonlinear tensor elements reveals on the topological nature of the material.

*Gordon and Betty Moore Foundation's EPIQs Initiative, Grant No. GBMF4537.
Quantum Materials program supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
ERC Advanced 20 Grant No. 742068 “TOPMAT”

3:30PM P55.00006: Kerr and Faraday rotations in a Weyl semimetal in a strong magnetic field

JEAN-MICHEL PARENT (Presenter), RENE COTE, ION GARATE, Universite de Sherbrooke — One striking property of the Landau level spectrum of a Weyl semimetal (WSM) is the existence of a chiral Landau level (CLL) in which the electrons propagate unidirectional along the magnetic field. This linearly dispersive level influences the optical properties of WSMs. For example, it was shown that a complete optical valley polarization is achievable in a time-reversal symmetric WSM placed in a strong magnetic field [1]. This effect originates from interband transitions involving the CLL and requires a tilt of the Weyl cones in the Hamiltonian. In this talk, we show how the presence of the CLL changes the behavior of the Kerr and Faraday rotations of an electromagnetic wave incident on a WSM in a strong magnetic field with respect to a non-topological metal. To calculate the optical conductivity tensor \( \sigma_{\alpha\beta}(\omega) \), we use the minimal model of a WSM developed in Ref. [1] with four tilted Weyl nodes related by mirror and time-reversal symmetry. We present the dependency of the Kerr and Faraday angles on the tilt angle of the cones, the position of the Fermi level, the thickness of the WSM and the magnetic field intensity in both the resonant and non-resonant frequency regimes.

Connecting second-order optical response with the band structure geometry of Weyl semimetals*

TOBIAS HOLDER (Presenter), DANIEL KAPLAN, BINGHAI YAN, Weizmann Institute of Science — Nonlinear optical response is well studied in the context of semiconductors and has gained a renaissance in studies of topological materials in the recent decade. In non-magnetic materials the response is believed to root in the Berry curvature of the material band structure. Here, we revisit the general formalism for the second-order optical response with finite lifetimes, focusing on the consequences of the time-reversal-symmetry breaking. We identify three physical mechanisms to generate a dc photocurrent, i.e. the Berry curvature, the quantum metric and the diabatic motion. All three effects are non-zero when time-reversal symmetry is broken. They can be understood intuitively from the anomalous acceleration; the first two terms are respectively the antisymmetric and symmetric parts of the quantum geometric tensor. The last term is due to the dynamical antilocalization that refers to the phase accumulation between time-reversed fermion loops.

*This research was supported by the Willner Family Leadership Institute for the Weizmann Institute of Science, the Benoziyo Endowment Fund for the Advancement of Science, Ruth and Herman Albert Scholars Program for New Scientists, and the European Research Council (Grant No. 815869).

Probing quantum criticality using nonlinear Hall effect in a metallic Dirac system*

VLADIMIR JURICIC (Presenter), HABIB ROSTAMI, NORDITA — Interaction driven symmetry breaking in a metallic (doped) Dirac system can manifest in the spontaneous gap generation at the nodal point buried below the Fermi level. Across this transition linear conductivity remains finite making its direct observation difficult in linear transport. In this talk, we will show how the nonlinear Hall effect can be used as a direct probe of this transition when inversion symmetry is broken [1]. Specifically, for a two-dimensional Dirac material with a tilted low-energy dispersion, we first predict a transformation of the characteristic inter-band resonance peak into a non-Lorentzian form in the collisionless regime. Furthermore, we find that inversion-symmetry breaking quantum phase transition is controlled by an exotic tilt-dependent line of critical points. As this line is approached from the ordered side, the nonlinear Hall conductivity is suppressed owing to the scattering between the strongly coupled incoherent fermionic and bosonic excitations. Our results should motivate further studies of nonlinear responses in strongly interacting Dirac materials.


*H.R. acknowledges the support from the Swedish Research Council (VR 2018-04252).
Observation of bulk-to-surface optical transition in topological insulator Bi$_2$Se$_3$

JIWON JEON, KWANGNAM YU, JIHO KIM, Univ of Seoul, JISOO MOON, SEONGSHIK OH, Department of Physics and Astronomy, Rutgers, the state university of New Jersey, EUNJIP CHOI (Presenter), Univ of Seoul — We performed broadband optical transmission measurements of Bi$_2$Se$_3$ and In-doped (Bi$_{1-x}$In$_x$)$_2$Se$_3$ thin films, where in the latter the spin-orbit coupling (SOC) strength can be tuned by introducing In. An optical absorption peak located at E=1eV in Bi$_2$Se$_3$ becomes completely suppressed at the critical x=0.06 in correlation with the topological surface state (SS) quenched at the same x due to TI-NTI transition. When Bi$_2$Se$_3$ is electrically gated, the 1eV-peak becomes stronger(weaker) when electron is depleted from (accumulated into) the SS. These observations combined together demonstrate that under the 1eV photo illumination, electron is excited from a bulk band into the SS of Bi$_2$Se$_3$. The bulk-to-surface optical transition or equivalently the optical population of the SS, is the first kind of such phenomena observed in TI's, is not only of fundamental significance but also offers an opportunity for optoelectronic application.

Chiral Magnetic Photocurrent in Dirac and Weyl Materials

SAHAL KAUSHIK (Presenter), DAMITRI E KARZEEV, EVAN PHILIP, State Univ of NY - Stony Brook — Circularly polarized light (CPL) can induce an asymmetry between the number of left- and right-handed chiral quasiparticles in Dirac and Weyl semimetals. We show that if the photoresponse of the material is dominated by chiral quasiparticles, the total chiral charge induced in the material by CPL can be evaluated in a model-independent way through the chiral anomaly. In the presence of an external magnetic field perpendicular to the incident CPL, this allows to predict the linear density of the induced photocurrent resulting from the chiral magnetic effect. The predicted effect should exist in any kind of Dirac or Weyl materials, with both symmetric and asymmetric band structure. An estimate of the resulting chiral magnetic photocurrent in a typical Dirac semimetal irradiated by an infrared laser of intensity $\sim 5 \times 10^6$ W/m$^2$ and a wavelength of $\lambda \sim 10 \mu$m in an external magnetic field $B \sim 2$T yields a current $J \sim 50$ nA in the laser spot of size $\sim 50 \mu$m. This current scales linearly with the magnetic field and wavelength, opening up possibilities for applications in photonics, optoelectronics, and THz sensing.

*This work was supported in part by the U.S. Department of Energy under Awards DE-SC-0017662, DE-FG-88ER40388, and DEAC02-98CH10886.
4:30PM P55.00011: The Low Energy Second Harmonic Generation Spectrum of the Chiral Multifold Fermion System RhSi  
BAOZHU LU (Presenter), Temple Univ, DYLAN REES, University of California, Berkeley, KAUSTUV MANNA, HORST BORRMANN, Max Planck Institute for Chemical Physics of Solids, ADOLFO G GRUSHIN, Neel Institute (CNRS), CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, JOSEPH ORENSTEIN, University of California, Berkeley, DARIUS TORCHINSKY, Temple Univ — Lacking any mirror symmetries, the Weyl nodes of the multifold fermion system RhSi are offset in energy, permitting a spectroscopic study of the optical properties of a single node. The lack of any mirror symmetry also implies that RhSi lacks an inversion center and thus can support second order nonlinear optical processes in its bulk. Here, we present a spectroscopic study of one of these processes, the bulk second harmonic generation response as a function of incidence photon energy and measure the single SHG susceptibility tensor element $\chi_{xyz}$ over the 275 - 900 meV range. We describe how our results directly probe the nonlinear optical response of the isolated Weyl at the $\Gamma$ point in the Brillouin zone and discuss our findings in the context of the linear optical response of the material.

4:42PM P55.00012: Nonlinear optical response of graphene family materials near topological phase transitions*  
RAJESH MALLA (Presenter), Center for Nonlinear Studies and Theoretical Division, Los Alamos National Laboratory, WILTON J DE MELO KORT-KAMP, Theoretical Division, Los Alamos National Laboratory —  
The graphene family materials behave as topological insulators due to non-negligible spin-orbit coupling. The gaps at each Dirac cone can be tailored when static electric fields and/or non-resonant circularly polarized lasers are applied to the system. Various electronic phases, characterized by Chern numbers, have been explored by changing the external fields. In this work we study the interaction of graphene family materials with ultrashort (~10's of femtosecond) linearly polarized optical pulses both in time and frequency domain. In order to observe the nonlinear response of these materials, we develop a non-perturbative approach to solve the massive Dirac equation for each valley and spin. Then we compute the longitudinal and transverse currents to investigate signatures of the ultrafast dynamics of the material. We demonstrate that the asymmetry of different Dirac cones plays a crucial role in the nonlinear response of the graphene family materials near topological phase transition boundaries.

*The authors acknowledge financial support from LANL LDRD program and the Center for Nonlinear Studies.
4:54PM P55.00013: Femtosecond to Nanosecond Lifetimes in Optically-Excited Nodal-Line Semimetals

ROBERT KIRBY (Presenter), GREG SCHOLES, LESLIE SCHOOP, Princeton University — Topological semimetals, such as the Dirac semimetal Cd$_3$As$_2$, have been proposed as superior materials for the next generation of highspeed optoelectronic devices due to their previously-observed ultrafast response times and high carrier concentrations [1]. Nodal-line semimetals, such as ZrSiX, should be even better suited to these applications because they have a much higher carrier concentration in Dirac bands, since those bands extend over lines or loops in k-space instead of just around a single point. In this talk, we will discuss our ultrafast optical measurements of the response of ZrSiX ($X = S, Se, Te$) to narrowband near-infrared pulses. Unlike other studies into this class of materials, multiple time scales are observed in the response, from the femtosecond- to nanosecond-scale. The spectral and kinetic features are connected to the structure and bandstructure of the materials, particularly surrounding the nodal-line straddling the Fermi level.


5:06PM P55.00014: Colliding Electrons and Holes in Semiconductors to Reconstruct Berry Curvature

* JOSEPH COSTELLO (Presenter), SEAMUS O’HARA, DARREN VALOVCIN, Physics, University of California, Santa Barbara, QILE WU, MACKILLO KIRA, Electrical Engineering and Computer Science, University of Michigan, LOREN PFEIFFER, Electrical Engineering, Princeton University, MARK STEPHEN SHERWIN, Physics, University of California, Santa Barbara — Electron-hole recollisions occur when a probe laser beam excites electron-hole pairs in a semiconductor that is driven by sufficiently strong THz-frequency electric fields [1]. The THz accelerates the electron-hole pairs and causes recollision, leading to the release of photons at higher energy than the probe in a process called high order sideband generation (HSG).

The intensity and polarization of each sideband depends on the relative polarizations of the probe and THz [2]. One cause of this dynamical birefringence is quantum interference between electron-hole recollision pathways under non-Abelian Berry curvature from the coupling between valence bands. In this talk I will present HSG experiments done in GaAs and demonstrate how to extract parameters relating to hole dynamics. This procedure opens the door to measurements of the complete electronic structure of semiconductors, including Berry curvature, Bloch wavefunctions, and effective Hamiltonian parameters.

References:
Banks, H., et al., PRX, 7, 0401042 (2017)

*Supported by NSF DMR 1710639

Wednesday, March 4, 2020 2:30 PM - 5:30 PM
Session P56 DCMP: Uranium-Based Superconductors, Hidden Order, and Related Phases  Mile High Ballroom 2C - Firoza Kabir, Univ of Central Florida

2:30PM P56.00001: Polar Kerr effect measurements of UTe₂ using Sagnac interferometry.*
DI WEI (Presenter), Stanford University, JIAN ZHANG, Fudan University, SHENG RAN, JOHNPIERRE PAGLIONE, NICHOLAS BUTCH, University of Maryland, College Park & NIST, AHARON KAPITULNIK, Stanford University — The heavy fermion compound UTe₂ was recently found to superconduct with Tᵋ = 1.6K, showing paramagnetic behavior and closely resembling the family of uranium based ferromagnetic superconductors [Ran et al., Science, 2019]. This initial study presented strong evidence of spin-triplet superconductivity, likely mediated by ferromagnetic fluctuations, which have been shown to occur below Tᵋ in μSR experiments [Sundar et al., arXiv, 2019]. Additionally, a recent scanning tunneling microscopy experiment claims signatures of chiral modes inside of the superconducting gap, raising the possibility of topological superconductivity [Jiao et al., arXiv, 2019]. A direct measurement of possible time-reversal symmetry (TRS) breaking effects in this system can provide insight on the exact order parameter of UTe₂, as well as evidence for the possible topological nature of the system. We present measurements of the polar Kerr effect using Sagnac interferometry in search for a possible TRS breaking state, and to examine ferromagnetic fluctuations in the Meissner and vortex states of this material.

*Work at Stanford University was supported by the Department of Energy, Office of Basic Energy Sciences, under contract no. DE-AC02-76SF00515.

2:42PM P56.00002: Electrodynamic response of the unconventional superconductor UTe₂*
SIRAK MEKONEN, DAVID BARBALAS, DIPANJAN CHAUDHURI, Johns Hopkins University, SHENG RAN, WESLEY T FUHRMAN, University of Maryland, College Park, NICHOLAS BUTCH, NIST Center for Neutron Research, National Institute of Standards and Technology,, PETER ARMITAGE (Presenter), Johns Hopkins University — Evidence was recently reported that UTe₂ is a nonunitary spin-triplet superconductivity, which features a high (for this material family) transition temperature of 1.6 K and a remarkably large and anisotropic upper critical field exceeding 40 T. Here we report results of measurements on the electrodynamic response of this compound down to low frequencies and temperatures. We investigate the finite frequency response of this system and search for evidence for the ferromagnetic fluctuations that have been seen in the optical response of other exotic superconductors close to ferromagnetism.

*Work at Johns Hopkins was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331. Crystal growth work at UMD was supported by NIST. Wesley T. Fuhrman is grateful for the support of the Schmidt Science Fellows program, in partnership with the Rhodes Trust.
Electronic structure of ferromagnetic superconductor UGe$_2$ in comparison to UTe$_2$

JONATHAN DENLINGER (Presenter), Lawrence Berkeley National Laboratory, JAMES W ALLEN, U. of Michigan, A. D. HUXLEY, JACQUES FLOUQUET, CEA-Grenoble — The newly discovered spin-triplet superconductor UTe$_2$ [1] has a strong suggestive relationship to the family of ferromagnetic superconductors UGe$_2$, URhGe and UCoGe. Here we update studies [2] of the electronic bandstructure of UGe$_2$, experimentally measured by angle-resolved photoemission (ARPES) near the U 5$d$-5$f$ resonance, with comparisons to DFT calculations of ThGe$_2$ decomposed into subunit building block structures. A signature imprint of a 2D diagonal square-net plane of Ge atoms on the formation of large diamond-shaped Fermi surface contours is shown to agree well with ARPES and with dHvA orbit sizes. Similar theoretical decomposition of the UTe$_2$ structure into zig-zag U-Te chains and a plane of Te linear chains with strong $p$-orbital bonding-antibonding splitting identifies the origins of the underlying orthogonal quasi-1D band structures near the Fermi level, in agreement with recent ARPES measurements [3].


Systematics of uranium-based superconducting materials.

ETERI SVANIDZE (Presenter), Max Planck Inst — A large number of uranium-based materials are exotic – they show complex magnetic orders, coexistence of superconductivity with magnetism, enhanced effective electron masses, quantum critical behavior, and topological states. All of these peculiar phenomena are thought to arise from electrons’ dual nature, which is also believed to lie at the origin of high-temperature superconductivity. Among unconventional uranium-based systems, the most intriguing are in fact superconductors – UBe$_{13}$, URu$_2$Si$_2$, and UPt$_3$ [1-3]. In this talk, I will provide a brief historic overview of superconductivity in uranium-based compounds, and address several pertinent questions [4]: Is superconductivity in uranium-based materials always unconventional? Why are superconducting temperatures in uranium-based compounds so low, compared to other compounds, based on actinide or lanthanide elements? Is there a way to pinpoint crystallographic motifs, which are favorable for the emergence of superconducting state?

3:18PM P56.00005: Revealing the intrinsic properties of the heavy-fermion superconductor UBe\textsubscript{13} PRIMOZ KOZELJ (Presenter), ULRIKE STOCKERT, MARKUS KOENIG, ANDREAS LEITHE-JASPER, YURI GRIN, ELENA HASSINGER, ETERI SVANIDZE, Max Planck Institute for Chemical Physics of Solids — Even though UBe\textsubscript{13} was one of the first reported heavy-fermion superconductors, it continues to receive a considerable amount of attention due to its unconventional ground state [1 - 3]. While single crystals of UBe\textsubscript{13}, grown out of Al flux, have been available early on [1], it was recently shown that their physical properties are highly affected by the Al incorporation into the lattice [4]. Even though the amount of Al atoms in the UBe\textsubscript{13} structure is rather small (< 1 - 2 at. %), it leads to dramatic changes in the physical properties. Our work provides a novel way in which polycrystalline samples of UBe\textsubscript{13} can be studied. These samples, which are inherently free of Al inclusions, provide a comprehensive examination of the inherent crystallographic defects both at the atomic- and the micro-scale. We show that these defects have a rather strong influence on the critical temperature $T_c$, the Sommerfeld coefficient $\gamma$, and the size of the specific heat anomaly.


3:30PM P56.00006: Aluminium impurities in single crystals of the heavy-fermion superconductor UBe\textsubscript{13} ANDREAS LEITHE-JASPER (Presenter), ALFRED AMON, ETERI SVANIDZE, PAUL SIMON, MATEJ BOBNAR, IRYNA ZELENINA, MARCEL NAUMANN, PRIMOZ KOZELJ, ELENA HASSINGER, YURI GRIN, Max Planck Institute for Chemical Physics of Solids, MPG — We studied the influence of Al incorporation on the heavy fermion superconductor UBe\textsubscript{13} to explain the sample dependence of physical properties. Al which substitutes Be in the crystal structure of flux-grown UBe\textsubscript{13} single crystals can be detected by combining X-ray diffraction, nuclear magnetic resonance and X-ray spectroscopy. The minute amounts of Al (1-2 at. %) in the structure are located by atomic resolution transmission electron microscopy. Specific heat measurements complement this study and reveal strong influence of the incorporated Al on the physical properties of UBe\textsubscript{13}. 

3:42PM P56.00007: Generalized Spin Fluctuation Feedback in Heavy Fermion Superconductors* ADIL AMIN (Presenter), DANIEL AGTERBERG, University of Wisconsin - Milwaukee — Experiments reveal that the superconductors UPt$_3$, PrOs$_4$Sb$_{12}$ and U$_{1-x}$Th$_x$Be$_{13}$ undergo two superconducting transitions in the absence of an applied magnetic field. The prevalence of these multiple transitions suggests a common underlying mechanism. A natural candidate theory which accounts for these two transitions is the existence of a small symmetry breaking field, however such a field has not been observed in PrOs$_4$Sb$_{12}$ or U$_{1-x}$Th$_x$Be$_{13}$ and has been called into question for UPt$_3$. Motivated by arguments originally developed for superfluid $^3$He we propose that a generalized spin fluctuation feedback effect is responsible for these two transitions. In this talk, we show that a phenomenological theory which couples spin fluctuations to superfluidity correctly predicts that a high temperature broken time-reversal superfluid $^3$He phase can emerge as a consequence. This phenomenological approach is then applied to these three superconductors revealing that this naturally leads to a high-temperature time-reversal invariant nematic superconducting phase, which can be followed by a second transition into a broken time-reversal symmetry phase, as observed.

*Adil Amin and D.F.A acknowledge financial support through the UWM research growth initiative.

3:54PM P56.00008: Magnetic Field Dependent Low-Temperature Specific Heat in UCo$_{1-x}$Fe$_x$Ge* SANGYUN LEE (Presenter), ERIC BAUER, FILIP RONNING, ROMAN MOVSHOVICH, Los Alamos National Laboratory — We have investigated low-temperature specific heat of UCo$_{1-x}$Fe$_x$Ge with $x$ spanning a narrow region around the concentration $x=0.23$ of the purported Ferromagnetic Quantum Critical point (FM QCP), at temperatures from 60 mK to 2 K and in magnetic field up to 9 T. All investigated samples show a rise in specific heat at low temperature when external field is applied, interpreted as being due to the Co nuclear Schottky anomaly, as the magnitude of the low temperature anomaly scales with the Co content. The Schottky anomaly is absent when the external field is zero, and $x$ is close to 0.23, indicating paramagnetic ground state in these samples. The shallow rise of the Sommerfeld coefficient $\gamma = C/T$ with decreasing temperature for $x=0.22$ and $x=0.23$ samples is consistent with previously reported higher temperature specific heat data, which were interpreted as an evidence of an FM QCP. In this talk, we discuss about quantum criticality of UCo$_{1-x}$Fe$_x$Ge system.

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4:06PM P56.00009: Quantum phase transition and superconductivity in ferromagnetic heavy-fermion systems*  
HAOYU HU (Presenter), ANG CAI, QIMIAO SI, Rice University —  
Ferromagnetic Kondo lattice systems have been shown to display the phenomenon of Kondo destruction [1], raising the prospect of quantum criticality in ferromagnetic heavy fermion systems in parallel with their antiferromagnetic counterparts [2]. The issue becomes particularly pressing given the recent developments on UTe2. This system shows strong evidence for spin-triplet superconducting pairing and indications of quantum criticality in the normal state [3,4]. In this work, we study a periodic Anderson model with ferromagnetic RKKY interactions. We treat the model within the extended dynamical mean-field theory [5] and solve the self-consistency equations with the continuous-time quantum Monte Carlo method [6]. We present the results on the underlying quantum phase transition and the superconducting pairing correlations, showing that the system has a strong tendency to triplet pairing.


*Supported by NSF grant DMR-1920740 and Welch Foundation grant C-1411.

4:18PM P56.00010: Angle Dependence of the Field-Induced Phases in UPt$_2$Si$_2$*  
GRETA CHAPPELL (Presenter), DAVID E GRAF, KAYA WEI, YOU LAI, WILLIAM NELSON, BENNY SCHUNDELMIER, CHRIS MANN, RYAN BAUMBACH, Florida State Univ —  
The low temperature antiferromagnet ($T_N = 32$ K) UPt$_2$Si$_2$ exhibits complex magnetic field-induced phases. Previous studies have established magnetic phase diagrams for applied fields along the $a$- and $c$-axes and suggest that the metamagnetic phase transitions (PT) may be associated with an evolution of the Fermi surface [1,2]. Here, we examine the PT angle dependence with RF skin depth and torque magnetometry experiments at temperatures $T < 1$ K and in fields $H < 45$ T. We find that AFMI $\rightarrow$ III evolves with nearly $1/\cos\theta$ dependence, III $\rightarrow$ V is hysteretic and nearly angle independent, and an additional PT in region V that also follows a $1/\cos\theta$ dependence. We shall discuss these results and the implications for the metamagnetism in UPt$_2$Si$_2$ and similar uranium-based materials.


*Work performed at NHMFL is supported by the National Science Foundation through DMR-1644779 and the State of FL. A portion of work is supported by the Center for Actinide Science and Technology, an EFRC funded by the US DOE under DE-SC0016568.
**4:30PM P56.00011: Field induced phases in UCr$_2$Si$_2$**

YOU LAI (Presenter), Los Alamos National Laboratory, JONAS DIAZ, GRETA CHAPPELL, National High Magnetic Field Laboratory, PHILIP MOLL, Institute of Materials (IMX), EPFL, RYAN BAUMBACH, National High Magnetic Field Laboratory, ROSS MCDONALD, Los Alamos National Laboratory — In the broader family of (Ln-An)Cr$_2$Si$_2$ (Ln = lanthanide and An = actinide), UCr$_2$Si$_2$ is unique, where the system undergoes a structural (tetragonal to monoclinic) and antiferromagnetic phase transitions at $T_S = 210$ K and $T_N = 27$ K, respectively, and the U ions carry a magnetic moment. Here, we present an extensive study of the behavior in high magnetic fields. We have performed pulsed field torque magnetometry and resistivity measurements on single crystalline samples UCr$_2$Si$_2$ grown first time by molten flux method. Along the crystallographic c axis, at low temperatures, we find a metamagnetic-like transition in fields of the order 10 T, possibly indicating a first-order transition, the field induced phase transition moves to higher field and reaches maximum while the field is along the $<101>$ diagonal of the tetragonal lattice. From our analysis of the data we can distinguish new high-field phases above the AFM ground state, which indicate the UCr$_2$Si$_2$ is possibly similar to what is seen for URu$_2$Si$_2$ and UPt$_2$Si$_2$, where the emergence of these new phase is due to the Fermi surface effects.
Spectroscopic investigation of UFe$_2$Si$_2$, URu$_2$Si$_2$, UNi$_2$Si$_2$, and UPd$_2$Si$_2$: from Pauli paramagnetism to antiferromagnetism via the hidden order state.* ANDREA SEVERING (Presenter), Institute of Physics II, University of Cologne, ANDREA AMORESE, Max-Planck Institute for Chemical Physics of Solids Dresden, MARTIN SUNDERMANN, Institute of Physics II, University of Cologne, MAURITS HAVERKORT, Institute of Theoretical Physics, University of Heidelberg, YINGKAI HUANG, van der Waals Zeeman Institute, Amsterdam University, MARIA SZLAWSKA, DARIUSZ KACZOROWSKI, Polish Acadademy of Science, RAN SHENG, M BRIAN MAPLE, Department of Physics, University fo California, San Diego, ERIC BAUER, Los Alamos National Laboratory, ANDREAS LEITHE-JASPER, LIU TJENG, Max-Planck Institute for Chemical Physics of Solids Dresden — We have carried out hard x-ray photoelectron spectroscopy (HAXPES) measurements at the U 4$f$ core level and non-resonant inelastic x-ray scattering (NIXS) at the U O$_{4.5}$ edge of UT$_2$Si$_2$ compounds that all form in the tetragonal ThCr$_2$Si$_2$ structure but exhibit different ground state properties: UFe$_2$Si$_2$ is a Pauli paramagnet; URu$_2$Si$_2$ is the famous hidden order compound of which the order parameter is still fiercely debated despite 30 years of intense experimental and theoretical studies [1]; UPd$_2$Si$_2$ and UNi$_2$Si$_2$ are antiferromagnets with T$_N$ well above 100 K and sizeable ordered magnetic moments [2].

We have determined the degree of the 5$f$-electron localization (HAXPES [3]) as well as the symmetry of the 5$f$ ground state wave function (NIXS [4]) across these very different compounds. This enabled us to identify their systematics and to place them in an effective Doniach phase diagram.

[1] see e.g. references in J.A. Mydosh and P.M. Oppeneer in Rev. Mod. Phys. 83, 1301{1322 (2011) and in Phil. Magazine 94, 3642 (2014).
[2] see e.g. references in T. Endstra et al, PRB 48, 9595 (1993)

*Financial support of the DFG under grant SE-1441/5-1 is gratefully acknowledged.
**4:54PM P56.00013: Origin of the gap-like behavior in pure and doped URu$_2$Si$_2$: A combined study via quasiparticle scattering spectroscopy and resistivity measurements**

SHENZHI ZHANG (Presenter), GRETA CHAPPELL, RYAN BAUMBACH, National High Magnetic Field Lab, Florida State University, NAVEEN POUSE, M BRIAN MAPLE, physics, University of California, San Diego, LAURA GREENE, WAN KIYU PARK, National High Magnetic Field Lab, Florida State University — Using Quasiparticle scattering spectroscopy (QPS), we track the temperature dependence of the hybridization gap in URu$_{2-x}$Fe$_x$Si$_2$ and URu$_2$Si$_2$P$_x$ (URSP) [1,2,3] in all substitutions, whether the hidden order (HO) appears or not. This poses a challenge to the Fermi surface gapping scenario, due to the absence of drastic changes in the conductance spectra across the HO transition. As an alternative way to explain the gap-like behavior, we adopt a model based on gapped bosonic excitations in the ordered state [4]. With an unusual temperature dependence of their stiffness, the temperature-dependent resistivity can be reproduced well including the jump at the HO transition. The extracted gap increases with increasing Fe-content, which agrees with the behavior of the $E_1$ gap in inelastic neutron scattering under pressure. This implies that the $E_1$ gap might originate from the same gapped bosonic excitations.


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**5:06PM P56.00014: Structural studies of Fe-doped URu$_2$Si$_2$ near the hidden order transition using X-ray crystallography**

XIAOLAN SUN (Presenter), University of Illinois at Urbana-Champaign, JOHN A MYDOSH, Leiden University, NAVEEN POUSE, M BRIAN MAPLE, University of California, San Diego, SANGJUN LEE, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — The origin of hidden order (HO) in URu$_2$Si$_2$ has been debated for the past thirty years. An interesting observation in recent years is the phase transition into a large moment antiferromagnetic (LMAF) state under either high pressure or Fe substitution for Ru. We used low-temperature x-ray crystallography to study the structure of URu$_2$Si$_2$, both with and without Fe doping. We observed changes in the intensities of the Bragg peaks suggesting the HO transition is associated with a breaking of spacegroup symmetry not accompanied by a change in lattice parameters. The pattern of atomic displacements changes markedly when crossing into the LMAF phase via Fe doping. No structural superlattice reflections were observed, consistent with past studies. We will discuss how our results constrain the subgroups and physical origin of the HO and LMAF phases.

*This work was supported by DOE Office of Basic Energy Sciences grant no. DE-FG02-06ER46285.
Magnetostriction of URu$_{2-x}$Fe$_x$Si$_2$ in High Magnetic Fields

Alexander Breindel (Presenter), University of California, San Diego, Sheng Ran, University of Maryland, Naveen Pouse, Inho Jeon, University of California, San Diego, Marcelo Jaime, Los Alamos National Laboratory, M Brian Maple, University of California, San Diego — URu$_2$Si$_2$ is a compound of great interest due to its hidden order (HO) phase whose order parameter has remained a mystery for more than three decades. It has been discovered that the substitution of Fe for Ru produces a transition from the HO to an antiferromagnetic (AFM), similar to what occurs under the application of pressure. This provides an opportunity to study URu$_2$Si$_2$ in both the HO and AFM phases at atmospheric pressure using experimental techniques that cannot readily be performed under pressure. In that vein, we conducted high field magnetostriction measurements on URu$_{2-x}$Fe$_x$Si$_2$. Our results support the findings of other high field measurements on URu$_{2-x}$Fe$_x$Si$_2$. However, we do not see a signature of the HO transition in our data, suggesting that our probe is not sensitive to the HO transition.

*The National High Magnetic Field Laboratory is supported by the NSF through NSF/DMR-1157490/1644779 and the State of Florida. Research at UCSD was supported by the US DOE BES under Grant No. DE-FG02-04-ER46105 (materials synthesis and characterization) and the US NSF under Grant No. DMR-1206553 (low temperature measurements) This research is also funded by a QuantEmX grant from ICAM and the Gordon and Betty Moore Foundation through Grant GBMF5305 to Alexander Breindel

Wednesday, March 4, 2020 2:30 PM - 5:18 PM

Session P57 DMP: Electronic and Optical Properties of 2D Materials III
Mile High Ballroom 3A - Wencan Jin, Auburn University - Tag(s): Focus

2:30PM P57.00001: Valleytronics and excitonics in 2D materials. [Invited] Tony Heinzel (Presenter), Applied Physics and Photon Science, Stanford University — Selected by Focus Topic Organizer (Liuyan Zhao, Robert Hovden)
3:06PM P57.00002: High-temperature exciton condensation in two-dimensional atomic double layers [Invited]  
ZEFANG WANG (Presenter), Cornell University, DANIEL A RHODES, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Tsukuba, Japan, JAMES C HONE, Columbia University, JIE SHAN, KIN FAI MAK, Cornell University — Bose-Einstein condensate is the ground state of matter of a dilute gas of bosons, such as atoms cooled to temperatures close to absolute zero. With a much smaller mass than atoms, excitons have been predicted to condense at significantly higher temperatures. The small exciton binding energy in conventional semiconductors has so far limited the condensation temperature to below 1 K. In the past several years, a new class of two-dimensional (2D) semiconductors with much larger exciton binding energy has emerged. In this talk, I will discuss the development of transition metal dichalcogenide double layer structures and electrical injection of interlayer excitons up to $10^{12} \text{ cm}^{-2}$ in the system. We study the electron-hole double layers through the interlayer tunneling and electroluminescence (EL). We observe a threshold dependence of the EL intensity on exciton density, accompanied by a super-Poissonian photon statistics near the threshold, and a large EL enhancement peaked narrowly at equal electron-hole densities. These results provide compelling evidence for interlayer exciton condensation in atomic double layers.

3:42PM P57.00003: Comparative KPFM measurements on doped monolayer MoS$_2$*  
CHRISTINA MCGAHAN (Presenter), Mount Holyoke College, PIN-CHUN SHEN, YUXUAN LIN, Massachusetts Institute of Technology, ASHLEY CAVANAGH, Mount Holyoke College, TOMAS PALACIOS, JING KONG, Massachusetts Institute of Technology, KATHERINE AIDALA, Mount Holyoke College — Tuning the electrical properties of monolayer MoS$_2$ through doping allows better control and flexibility over future device design. Here we present electrical measurements on sulfur-rich and oxygen-rich MoS$_2$ flakes using kelvin probe force microscopy (KPFM) and a field effect transistor sample geometry, allowing us to resolve spatial variations. Preliminary KPFM measurements show that oxygen-rich MoS$_2$ has a larger work function than sulfur-rich MoS$_2$ and that the work function of monolayer MoS$_2$ differs from that of multilayer MoS$_2$. The trend in work functions between differently doped MoS$_2$ flakes observed via KPFM is consistent with the trend in threshold voltages extracted from bulk current-voltage measurements on the flakes as well as the trend in work functions calculated via density functional theory. The sensitivity of the shift in work function of the MoS$_2$ flakes from an applied gate voltage suggests that local density of states measurements can be extracted with KPFM to experimentally examine the energy levels of the differently doped monolayer MoS$_2$ flakes.

*NSF-DMR 1231319, NSF-1541959, NSF-DMR 1708970, NSF 0939514
3:54PM P57.00004: Tomonaga-Luttinger Liquid in MoSe₂ Twin Domain Boundaries*  YIPU XIAXUNQIU ZHANG, Physics Department, The University of Hong Kong, YUANJUN JIN, Physics Department, Southern University of Science and Technology, WINGKIN HO, Physics Department, The University of Hong Kong, HU XU, Physics Department, Southern University of Science and Technology, MAOHAIXIE (Presenter), Physics Department, The University of Hong Kong — In epitaxial MoSe₂ monolayer grown by molecular-beam epitaxy, dense networks of twin domain boundaries (DBs) have been observed [1]. They behave as metals. Being sandwiched between semiconducting pristine MoSe₂ domains, they represent an ideal one-dimensional (1D) system for studying the physics of 1D metals, such as the Peierls type instability and collective excitations of Tomonaga-Luttinger liquid (TLL). Indeed, there have already been reports of charge density waves (CDW) [2] and the TLL [3] in such systems. In this work, we report a low-temperature scanning tunneling spectroscopy study revealing the quantum confinement effect and signatures of the TLL in the 4|4P-type DB defects in MoSe₂. Notably, CDW is not observed at temperatures down to ~ 5 K. This finding is consistent with a recent study of another type (4|4E) 1D defect in MoS₂ [4].


*The work is supported by a Collaborative Research Grant (No. C7036-17W) from the Research Grant Council of Hong Kong Special Administrative Region, China.

4:06PM P57.00005: Probing Excitonic Resonances of Metal Films on Suspended 2D Membranes Using Electron Energy Loss Spectroscopy*  TODD BRINTLINGER (Presenter), JOSE FONSECA, JAMES CLIFFORD CULBERTSON, MAXIM ZALALUTDINOV, RHONDA MICHELE STROUD, JEREMY ROBINSON, United States Naval Research Laboratory — We characterize Oriented Porous mEtallic Networks (OPEN) with aberration-corrected scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS). These OPEN films are synthesized by annealing metal films on 2D layers, which causes lattice registry between the metal layer and the 2D materials. We are studying the morphological influence that MoS₂ monolayers have on relatively thick (13-25nm) gold thin films during annealing. Ex-situ annealing experiments of MoS₂/Au on SiO₂ substrates shows that the Au films can become textured (oriented), as revealed through electron beam scattering diffraction, and that the Au film can locally dewet beneath the MoS₂ layer to form a porous metal layer with suspended MoS₂ membranes. Further, 60 kV STEM imaging and EELS show that the metal and 2D lattices are aligned, with several EELS resonances in the low loss range. One resonance at ~ 2 eV is associated with the so-called A and B excitons. We will discuss the origin of these resonances, and how both the metal overlayer and disordered carbon contamination affect them.

*The authors acknowledge funding from the Office of Naval Research (Naval Research Laboratory Basic Research Program).
4:18PM P57.00006: Out-of-plane charge transport anomalies in polytypes of NbS$_2$*  
KONSTANTIN SEMENIUK (Presenter), EDOARDO MARTINO, CARSTEN PUTZKE, Ecole Polytechnique Federale de Lausanne, DAVID LEOBEUF, Laboratoire National des Champs Magnétiques Intenses, HELMUTH BERGER, PHILIP MOLL, LASZLO FORRO, Ecole Polytechnique Federale de Lausanne — Tuning interlayer coupling in quasi-two-dimensional materials is a powerful tool for realising novel electronic states for potential applications in electronic and optical devices. Crucial information regarding the underlying interactions can be obtained by probing the c-axis resistivity$^1$. We present the case of the 2H and 3R polytypes of NbS$_2$, which have the same in-plane structure but different stacking of the layers and as a result exhibit very contrasting charge transport properties. By utilising focused-ion-beam-assisted sample preparation we were able to unambiguously probe the in-plane and out-of-plane resistivities of the compounds. The corresponding anisotropies are substantially lower than has been thought before. Furthermore, we show a number of previously unobserved features, including non-monotonic temperature dependence of resistivity and negative longitudinal magnetoresistance. We suggest that the stacking faults, occurring naturally in the studied compounds$^2$, are the primary cause of the aforementioned behaviours.


*The work was supported by the Swiss National Foundation for Scientific Research

4:30PM P57.00007: Identification of select populations of single photon emitters in hexagonal boron nitride based on their zero phonon line and linewidth broadening footprint  
HAMIDREZA AKBARI (Presenter), WEI-HSIANG LIN, BENJAMIN VEST, HARRY ATWATER, Applied Physics, Caltech — Single photon emitters (SPE) in hexagonal boron nitride (hBN) have shown promising electrical and optical properties for utilization in quantum light source applications. The unpredictability of defect properties in hBN remains a significant challenge in order to reproducibly and more deterministically identify bright and robust emitters. In this presentation, we first investigate the characteristics of zero phonon line spectra (ZPLs) from defects found in hBN samples fabricated by chemical vapor deposition techniques. Depending on the growth conditions, the ZPL distribution of defects from the same sample can be significantly reduced. This suggests that defects exhibiting similar properties might be identified. Based on these observations, we carry out an in-depth study of the spectral properties and emission line broadening mechanisms for different sets of defects showing similar spectral features. In particular, we perform both low temperature spectroscopy of photoluminescence down to 4K and luminescence decay lifetime measurements. Mechanisms of line broadening for the different populations of defects will be discussed. These elements build a better understanding of the zoology of defects in hBN and of their potential and limitations for quantum light applications.
4:42PM P57.00008: Unraveling the Mystery of the 1.5 layer Raman Response in Exfoliated MoS2. ANDREY KRAYEV (Presenter), HORIBA Scientific, MATĚJ VELICKÝ, Chemistry and Chemical Biology, Cornell University — Recently a new method of exfoliation of large area monolayers of transition metal dichalcogenides (TMDC) was proposed. Confocal Raman characterization of exfoliated monolayers of MoS2 showed A' peak splitting, the components of this split peak corresponding to a standard A' peak of the monolayer and A1g peak of the bi-layer correspondingly. We further performed tip enhanced Raman Scattering (TERS) imaging of these exfoliated crystals. Thanks to greatly improved spatial resolution of TERS imaging, we discovered that some areas of what seemed to be a uniform monolayer, actually contained a network of tiny islands (few tens of nm across) having spectral signature closely matching TERS response of the bilayer while TERS spectra of areas in between these islands closely resembled standard Raman spectrum of the monolayer. Thanks to these observations we came to the conclusion that the gold-assisted exfoliation of MoS2 may result in inhomogeneous crystals featuring a network of tiny bilayer islands, and consequently, greatly increased crystal edge length per unit of area, a feature that may be useful for (photo)catalytic applications of TMDCs.

References
Velický, M.; et.al. ACS Nano 2018, 12, 10463-10472.

4:54PM P57.00009: Correlating 3D atomic defects and electronic properties of 2D transition metal dichalcogenides with picometer precision* XUEZENG TIAN (Presenter), DENNIS S KIM, University of California, Los Angeles, SHIZE YANG, Oak Ridge National Laboratory, CHRISTOPHER CICCARINO, Harvard University, YONGJI GONG, Rice University, YONGSOO YANG, YAO YANG, University of California, Los Angeles, BLAKE DUSCHATKO, Harvard University, YAKUN YUAN, University of California, Los Angeles, PULICHEL M AJAYAN, Rice University, JUAN-CARLOS IDROBO, Oak Ridge National Laboratory, PRINEHA NARANG, Harvard University, JIANWEI MIAO, University of California, Los Angeles — The field of research in two-dimensional (2D) transition metal dichalcogenides (TMD), has experienced extraordinary growth. To understand the structure-property relationship of these materials at the fundamental level, we must know their 3D atomic structure with high precision.

Here, we developed scanning atomic electron tomography (sAET) to localize the 3D atomic coordinates in 2D materials and heterostructures with picometer precision. Using a Re-doped MoS2 monolayer sample, we demonstrated a general sAET method to overcome several limitations and determined the 3D coordinates of individual atoms with precision down to 4 pm. We identified 3D crystal defects such as dopants, vacancies and atomic-scale ripples and measured the 3D atomic displacement and the full strain tensor of the Re-doped MoS2. Furthermore, the experimental 3D atomic coordinates were used as direct input to DFT to correlate crystal defects with the electronic band structure at the single-atom level. sAET is generally applicable to the determination of the 3D atomic coordinates of various 2D materials, heterostructures and thin films.

*DOE: DE-SC0010378; STROBE: DMR-1548924; NSF: DMR-1437263; MURI:18057522
5:06PM P57.00010: Transport Studies of Nanofabricated Tellurium Devices*  XINXIN CAI
(Presenter), CHENYU YU, School of Physics and Astronomy, University of Minnesota, PRAFFUL GOLANI,
Department of Electrical and Computer Engineering, University of Minnesota, YAN WANG, XINGLONG
REN, Department of Chemical Engineering and Materials Science, University of Minnesota, STEVEN J.
KOESTER, Department of Electrical and Computer Engineering, University of Minnesota, C. DANIEL
FRISBIE, Department of Chemical Engineering and Materials Science, University of Minnesota, VLAD S.
PRIBIAG, School of Physics and Astronomy, University of Minnesota — Tellurium is a narrow bandgap
semiconductor with high hole mobility of several hundred cm²(Vs)⁻¹. It has attracted great
interest due to its unique crystal structure, consisting of 1D helical chains interconnected by van
der Waals type bonds. A recent development is the successful synthesis of two-dimensional
tellurium, or tellurene, using a solution-based process. Various interesting transport phenomena
have been experimentally demonstrated since then, such as anisotropic magnetoresistance,
quantum Hall effect and gate-tuned insulator-metal transition, revealing its potential for
fundamental studies and future applications of nanoscale devices. We discuss the fabrication and
electrical measurements of few-layer and bulk tellurium flakes grown by the solution method. We
study anisotropic and nanoscale transport of the material.

*This work is supported by the Office of Naval Research.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P58 DCP: Journal of Chemical Physics Editor's Choice Awards
Mile High Ballroom 3B - Tag(s): Invited, Undergrad Friendly

2:30PM P58.00001: Electron transfer in confined electromagnetic fields* [Invited]  ALEXANDER
SEMENOV (Presenter), ABRAHAM NITZAN, University of Pennsylvania — The interaction between
molecular (atomic) electron(s) and the vacuum field of an optical cavity has drawn significant
attention thanks to the rapid developments in nano-optics. Such interaction which is a subject of
cavity quantum electrodynamic can substantially affect transport properties of molecular
systems. In this work we consider non-adiabatic electron transfer process in the presence of a
cavity mode. We present a generalized framework for the interaction between a charged
molecular system and a quantized electromagnetic field of a cavity and apply it to the problem of
electron transfer between a donor and an acceptor placed in a confined vacuum electromagnetic
field. The effective system Hamiltonian corresponds to a unified Rabi and spin-boson model
which includes a self-dipole energy term. Two limiting cases are considered: one where the
electron is assumed to be much faster than the cavity mode and another in which the electron
tunneling time is significantly larger than the mode period. In both cases a significant rate
enhancement can be produced by coupling to the cavity mode in the Marcus inverted region. The
results of this work offer new possibilities for controlling electron transfer processes using visible
and infrared plasmonics

*U.S. National Science Foundation (Grant No. CHE1665291 to A.N.), the Israel-U.S. Binational
Science Foundation (Grant No. 2014113).
3:06PM P58.00002: Laser-based imaging of gas phase molecules [Invited] ARNAUD ROUZÉE (Presenter), Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy — Watching a molecule at work, the so-called making a molecular movie, is a long standing goal in the physical chemistry community. With the recent advent of X-ray free electron lasers and relativistic electron guns, femtosecond diffractive imaging studies with intense short-wavelength pulses and with ultrafast electron bunchs became possible. In this talk, I will discuss alternative routes based on strong field ionization by intense femtosecond laser pulses to image molecular structures and dynamics. Two techniques, namely laser-induced Coulomb explosion imaging and laser-induced electron diffraction, will be presented and recent applications of these techniques to the retrieval of molecular structure and ultrafast molecular dynamics will be provided.

3:42PM P58.00003: Diffusion, plasticity, and excess entropy in complex colloidal fluids* [Invited] XIAOGUANG MA (Presenter), University of Pennsylvania — Excess entropy is the difference between the “true” system entropy and that of an equivalent ideal gas. Rosenfeld first observed that the diffusivity and viscosity of simple liquids scale exponentially with excess entropy. This intriguing discovery had motivated numerous studies of excess entropy scaling in a wide variety of materials spanning different particle type, size, density, interaction, temperature, and even shear rate, most of which are computer simulation work. In this talk, I will discuss our recent experiments utilizing excess entropy concept to understand the dynamics of complex fluids. In the first experiment, we investigate the structure and dynamics in dense colloidal fluids with tunable short-range attractions. From particle trajectory data we measure the two-body excess entropy and the long-time diffusion coefficients from samples with different packing fractions and attraction strengths. These results are found to follow Rosenfeld's excess entropy scaling that is independent of sample packing fraction and attraction strength. In the second experiment, we study plastically deformed colloidal solids. We directly imaged the dynamics and micro-structure induced by plastic shear flow in a series of amorphous solids under oscillatory shear. Data reveal novel scaling relationships between plastic flow, viscous response, and excess entropy. These findings extend the application of excess entropy concept from equilibrium to nonequilibrium systems.

*We gratefully acknowledge supports from the National Science Foundation through PENN MRSEC DMR1720530, NSF DMR1607378, and NASA 80NSSC19K0348.
Markov state models have become popular in the computational biophysics community as a technique for identifying stationary and kinetic information of protein dynamics from molecular dynamics (MD) simulation data. We extended the applicability of automated Markov state modeling to simulation data of molecular self-assembly by constructing collective coordinates from molecular descriptors that are invariant to permutations of molecular indexing. Understanding molecular self-assembly is of critical importance if we want to deepen our understanding of neurodegenerative diseases where the aggregation of disordered peptides or misfolded proteins is thought to be the main culprit. I will present the Markov state models that we obtained for the self-assembly of different peptides and demonstrate that the Markov state models clearly map out the different aggregation pathways, something which has not been possible with standard MD analysis tools.

Spin waves in the antiferromagnetic topological insulator MnBi$_2$Te$_4^*$

BING LI (Presenter), Ames Laboratory, Ames, IA 50011, USA; Iowa State University, Ames IA 50011, USA, SIMON RIBEROLLES, LIQIN KE, ELIJAH GORDON, Ames Laboratory, Ames, IA 50011, USA, DANIEL PAJEROWSKI, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, ANDREAS KREYSSIG, Ames Laboratory, Ames, IA 50011, USA; Iowa State University, Ames IA 50011, USA, BENJAMIN UELAND, Ames Laboratory, Ames, IA 50011, USA, JIAQIANG YAN, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, ROBERT MCQUEENEY, Ames Laboratory, Ames, IA 50011, USA; Iowa State University, Ames IA 50011, USA — MnBi$_2$Te$_4$ is proposed to be the first antiferromagnetic (AF) topological insulator (TI). The natural intergrowth of magnetic and TI layers, and the ground state tunability via a magnetic field provide a unique platform for studying the interplay between magnetism and topological electronic states, which give rise to the quantum anomalous Hall effect and axion electrodynamics. Here we present results from our inelastic neutron scattering (INS) study on MnBi$_2$Te$_4$ single crystals, where we determined the strength of the magnetic interactions and anisotropy in the AF state ($T_N = 24$ K). By comparing our INS data to the dynamic spin susceptibility calculated using a linear-response density functional theory, we find that magnetic interactions extending further than the Mn nearest-neighbor distance are necessary to understand the observed spin wave dispersion.

*This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.
Electronic states and magnetic response of MnBi$_2$Te$_4$ surface by scanning tunneling microscopy and spectroscopy

YONGHAO YUAN (Presenter), XINTONG WANG, Department of Physics, Tsinghua University, HAO LI, School of Materials Science and Engineering, Tsinghua University, JIAHENG LI, YU JI, ZHENQI HAO, Department of Physics, Tsinghua University, YANG WU, Department of Mechanical Engineering, Tsinghua University, KE HE, YAYU WANG, YONG XU, DUAN WENHUI, WEI LI, QIKUN XUE, Department of Physics, Tsinghua University — The newly discovered intrinsic magnetic topological insulator, MnBi$_2$Te$_4$, has demonstrated novel quantum phenomena. Quantized Hall conductance and topological axion state have been realized in its thin flakes. However, the measured band structures show deviations from calculation results and the reason is still in debate. In our studies, low-temperature scanning tunneling microscopy experiment is carried out to investigate its surface states and magnetic response. Unexpected electronic structures are obtained from quasiparticle interference patterns on the topmost layer, which show deviations from the prediction of out-of-plane A-type antiferromagnetic structure. Such differences presumably originate from the re-orientation of magnetic moments near the surface. Moreover, 5% of Mn substitutions at Bi sites are observed. They not only give rise to fluctuating electronic structures, but also affect the magnetism of the material. Our findings shed new lights on the magnetic property of MnBi$_2$Te$_4$ and the design of magnetic topological insulators.
2:54PM P59.00003: Gapless surface Dirac cone and its possible origin in antiferromagnetic topological insulator MnBi$_2$Te$_4$*  YU-JIE HAO, PENGFEI LIU, YUE FENG, XIAO-MING MA, Physics, Southern University of Science and Technology, EIKE F. SCHWIER, MASASHI ARITA, SHIV KUMAR, Hiroshima Synchrotron Radiation Center, Hiroshima University, CHAOWEI HU, Physics and Astronomy, University of California, Los Angeles, RUI'E LU, MENG ZENG, YUAN WANG, ZHANYANG HAO, HONG-YI SUN, Physics, Southern University of Science and Technology, KE ZHANG, Hiroshima Synchrotron Radiation Center, Hiroshima University, JIAWEI MEI, Physics, Southern University of Science and Technology, NI NI, Physics and Astronomy, University of California, Los Angeles, LIUSUO WU, Physics, Southern University of Science and Technology, KENYA SHIMADA, Hiroshima Synchrotron Radiation Center, Hiroshima University, CHAOYU CHEN, QIHANG LIU, CHANG LIU (Presenter), Physics, Southern University of Science and Technology — The recent discovered antiferromagnetic topological insulators in the Mn-Bi-Te family have rapidly drawn broad interest since its cleaved surface state is believed to be gapped, hosting the unprecedented axion states. However, we show by ARPES that a gapless Dirac cone at the (0001) surface of MnBi$_2$Te$_4$ exists inside the bulk band gap. Such unexpected surface state remains unchanged across the bulk Néel temperature, and is robust against severe surface degradation, indicating additional topological protection. Through symmetry analysis and \textit{ab initio} calculations we consider different types of surface magnetic reconstruction as possible origins giving rise to such linear dispersion. Our results reveal that the intrinsic magnetic topological insulator hosts a rich platform to realize various topological phases, and thus pushed forward the comprehensive understanding of magnetic topological materials.

*Work at SUSTech was supported by the National Natural Science Foundation of China (NSFC) (Nos. 11504159 and 11874195), the Guangdong Innovative and Entrepreneurial Research Team Program (Nos. 2016ZT06D348 and 2017ZT07C062), etc. Work at UCLA was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0011978.
Intrinsic magnetic topological insulators are stoichiometric materials with both magnetic ordering and topological electronic states. Due to its inherent magnetism, this class of materials processes rich topological quantum phases that induced by symmetry breaking, while maintaining good crystallinity and high purity of the material. We report the MBE synthesis and characterization of an intrinsic magnetic topological insulator MnBi$_2$Se$_4$. The MnBi$_2$Se$_4$ thin films are deposited with alternating layer growth of Bi$_2$Se$_3$ and a-MnSe(111). The high quality of the material is shown with cross-sectional TEM. Dirac surface state is demonstrated with angle-resolved photoemission spectroscopy above its magnetic ordering temperature. SQUID magnetometry measurement on films with different thicknesses shows layered-antiferromagnetic ordering in this material. Low-field SQUID measurement also shows a hysteresis loop, with magnetic moments preferred to stay within the lattice plane. The ferromagnetic signal is attributed to uncompensated magnetic moments at the surface. Its magnetic characterization is also confirmed with XMCD measurement. Furthermore, magnetometry measurement also shows that the magnetic ordering in MnBi$_2$Se$_4$ persists down to the monolayer limit.
3:18PM P59.00005: Scanning tunneling microscopy and spectroscopy investigation of the antiferromagnetic topological insulator MnBi$_2$Te$_4^*$  HONG LI (Presenter), HE ZHAO, Boston College, CHAOWEI HU, SCOTT MACKEY, Physics and Astronomy, UCLA, ZIQIANG WANG, Boston College, NI NI, Physics and Astronomy, UCLA, ILIJA ZELJKOVIC, Boston College — The interplay of topology and magnetism within the same material can give rise to exotic electronic phases, such as the quantum anomalous Hall state and the axion insulator state. Recently discovered MnBi$_2$Te$_4$ is believed to be the first intrinsic antiferromagnetic topological insulator. Using low temperature scanning tunneling microscopy and spectroscopy, we study the surface of high-quality single crystals of MnBi$_2$Te$_4$. From STM topographs, we visualize the spatial distribution of accidental Mn substitutions in the topmost Te layer. Moreover, by imaging the scattering of electrons on the surface, we track the evolution of the electronic band structure and compare it with angle-resolved photoemission spectroscopy experiments. Our measurements provide a nanoscale insight into the chemical inhomogeneity and the electronic structure of this novel system.

*Army Research Office Grant No. W911NF-17-1-0399.

3:30PM P59.00006: Strongly Gapped Topological Surface States in MnBi$_2$Te$_4$(Bi$_2$Te$_3$)$_n$ Family*  KYLE GORDON (Presenter), University of Colorado, Boulder, CHAOWEI HU, Physics, University of California, Los Angeles, PENGFEI LIU, Physics, Shenzhen Institute for Quantum Science and Technology, BARUN GHOSH, Physics, Indian Institute of Technology-Kanpur, ANDREW LINN, HAOXUANG LI, DUSHYANT NARAYAN, University of Colorado, Boulder, JINYU LIU, Physics, University of California, Los Angeles, HONGYI SUN, Physics, Shenzhen Institute for Quantum Science and Technology, BAHADUR SINGH, Physics, Northeastern University, AMIT AGARWAL, Physics, Indian Institute of Technology-Kanpur, SUYANG XU, Physics, Massachusetts Institute of Technology, HSIN LIN, Physics, Academia Sinica, TAY-RONG CHANG, Physics, National Cheng Kung University, QIHANG LIU, Physics, Shenzhen Institute for Quantum Science and Technology, NI NI, Physics, University of California, Los Angeles, DANIEL DESSAU, University of Colorado, Boulder — The MnBi$_2$Te$_4$(Bi$_2$Te$_3$)$_n$ family of materials are potential candidates for magnetic topological insulators (MTIs) that may show the Quantum Anomalous Hall Effect (QAHE). This class of materials are heterostructures of MnBi$_2$Te$_4$ and Bi$_2$Te$_3$ layers that are stacked together via van der Waals forces, with n number of Bi$_2$Te$_3$ layers interstitially placed between MnBi$_2$Te$_4$ layers. In this talk, we present Angular Resolved Photoemission Spectroscopy (ARPES) experiments on MnBi$_4$Te$_7$, MnBi$_6$Te$_{10}$, and MnBi$_8$Te$_{13}$, demonstrating the topological nature of each material. Furthermore, we deconvolve the surface spectra due to each possible surface termination for each stacking arrangement, demonstrating a rich transition from the gapless MnBi$_2$Te$_4$ surface, through a gapped Bi$_2$Te$_3$-like surface, and ending with an approximate pure Bi$_2$Te$_3$ surface.

*Work at CU Boulder was supported by NSF-DMR 1534734, work at UCLA was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0011978. Work at SUSTech was supported by the NSFC under Grant No. 11874195. This work was supported partially by the MOST, Taiwan, Grant MOST107-2627-E-006-001.
Competing Interactions in the Antiferromagnetic State of the Axion Insulator Candidate MnBi₂Te₄

VINCENT MORANO (Presenter), VERONICA STEWART, Johns Hopkins University, YIMING QIU, CRAIG BROWN, National Institute of Standards and Technology, TYREL MCQUEEN, COLLIN LESLIE BROHOLM, Johns Hopkins University — A new class of materials, antiferromagnetic topological insulators, has been predicted to realize the bulk axion insulator with a large and in some cases quantized magneto-electric coefficient. Hexagonal MnBi₂Te₄ is a candidate material and here we report neutron scattering experiments conducted at the NIST Center for Neutron Research to understand its magnetism. We confirm A-type antiferromagnetic order (alternating FM basal planes with spins along the hexagonal axis) with T_N=24 K. Inelastic scattering reveals an excitation spectrum with a bandwidth of 4.5 meV and gap \( \Delta <0.6 \) meV. Modelling these data using spin-wave theory, we obtain an effective spin Hamiltonian for MnBi₂Te₄ that features competing ferro- and antiferromagnetic interactions within the basal plane.

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331.

Investigation on the topological surface states of a superlattice-like magnetic topological insulator MnBi₄Te₇

XUEFENG WU (Presenter), YU ZHANG, XIAO-MING MA, CHUNSHENG ZHOU, KEDONG WANG, QIHANG LIU, CHANG LIU, YUE ZHAO, physics, Southern University of Science and Technology — The recently verified intrinsic magnetic topological insulator MnBi₂Te₄ has attracted tremendous research interest, as it is considered to be a promising platform for emergent quantum phenomena such as the quantum anomalous Hall effect, and the axion insulator state, etc. In a superlattice-like bulk of alternating MnBi₂Te₄ and Bi₂Te₃ layers, the antiferromagnetic exchanged coupling can be effectively weakened. Here, we investigate the surface states of MnBi₄Te₇ crystal via angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) techniques. Two different band structures are observed, both showing the Dirac point located at \(-280\) mV below the Fermi level and gapless feature at Dirac point. The two different band structures can be associated with the MnBi₂Te₄-terminated and Bi₂Te₃-terminated surfaces by STM study. We further analyze the quasi-particle interference scattering at various energies, which exhibit distinct \( \Gamma\)-\( M \) features corresponding to the scattering of topological surface states, showing good correspondence to ARPES data. Our results can help to understand the electronic structure and related phenomena in the emerging intrinsic magnetic topological insulators.
Dynamic magnetic properties of a magnetic topological insulator material MnBi₄Te₇

KAVITA MEHLAWAT (Presenter), ALEXEY ALFONSOV, ANNA ISAEVA, BERND BUECHNER, VLADISLAV KATAEV, Leibniz IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — A van der Waals compound MnBi₄Te₇ belongs to the family of (Bi₂Te₃)ₙ(MnBi₂Te₄), (n = 0, 1, 2) heterostructures and is a candidate magnetic topological insulator [1]. It is the first magnetic material that features both, the intrinsic net magnetization and a band inversion. Static magnetic susceptibility (χ) and magnetization (M) measurements as a function of the applied field (H) on MnBi₄Te₇ single-crystals show an antiferromagnetic state at Tₑ = 13 K and a ferromagnetic-like hysteresis occurring upon cooling below 5 K [1]. We performed electron spin resonance (ESR) spectroscopy measurements in wide frequency and temperature ranges to explore the dynamic magnetic properties of MnBi₄Te₇. From high-frequency ESR measurements, we obtain evidence that MnBi₄Te₇ is an easy-axis type ferromagnet and ferromagnetic spin correlations persist up to T = 30 K on the time scale of an ESR experiment (10⁻¹⁰ - 10⁻¹¹ s).


*K. Mehlawat acknowledges the Hallwachs Röntgen Postdoc Program of Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter ct.qmat EXC 2147

Topological Electronic Structure and Its Temperature Evolution in Antiferromagnetic Topological Insulators

LEXIAN YANG (Presenter), Tsinghua University, ZHONGKAI LIU, ShanghaiTech University, YONG XU, Tsinghua University, YULIN CHEN, Oxford University — Magnetic topological insulators represent a novel state of topological quantum materials with unique blends of non-trivial band topology and magnetism. Recently, Intrinsic magnetic topological insulator MnBi₂Te₄ is shown to exhibit rich topological effects such as quantum anomalous Hall effect and axion electrodynamics, which attracts tremendous research interests. Here, we carried out comprehensive and high-resolution angle-resolved photoemission spectroscopy studies on MnBi₂Te₄, and identified its topological electronic structure. In contrast to theoretical predictions and previous studies, we observe topological surface states with a diminished gap forming a characteristic Dirac cone. In addition, the temperature evolution of the energy bands reveals their interplay with the magnetic phase transition by showing interesting differences between the bulk and surface states, respectively. Our results provide important insights into not only the exotic properties of MnBi₂Te₄, but also the generic understanding of the interplay between magnetism and topological electronic structure in magnetic TQMs.

*Supported by the National Natural Science Foundation of China (Grant No. 11774190 and No. 11674229).
Characterization of the Layered Antiferromagnetic Topological Insulator MnBi2Se4 Using Scanning Tunneling Microscopy

ROBERT WALKO (Presenter), Ohio State Univ - Columbus, TIANCONG ZHU, University of California, Berkeley, ALEXANDER BISHOP, ROLAND KAWAKAMI, JAY A GUPTA, Ohio State Univ - Columbus — Recently, topological insulators have been an area of interest due to the existence of symmetry protected states. Those with broken time reversal symmetry are particularly interesting because they have been predicted to host several intriguing phenomena such as the quantum anomalous hall effect, magneto-electric effects, and topologically protected surface and edge states. MnBi2Se4 (MBS) is a predicted topological insulator formed of van der Waals separated septuple layers (SL) with a layered anti-ferromagnetic structure, which breaks time-reversal symmetry and could therefore potentially realize some of those phenomena. For this study, a Se capped 20SL MBS film was grown on a sapphire substrate using molecular beam epitaxy. After other measurements were taken ex-situ the sample was then de-capped and transferred via vacuum suitcase to a low-temperature (5K) scanning tunneling microscope (STM). In our STM images, we observed a triangular lattice with an average lattice constant of 3.85Å. Additionally, we see a semiconducting nature in scanning tunneling spectroscopy with a band gap of approximately 700meV.

Engineering MnBi2Te4 thin films by chemical dopants and tailoring structure

LIGUO ZHANG (Presenter), HAICHENG LIN, FENGREN FAN, YAN SUN, CLAUDIA FELSER, Max-Planck Institute for Chemical Physics of Solids — As the first realized intrinsic magnetic topological insulators, MnBi2Te4 (MBT) has been extensively studied and shows rich novel transport properties and magnetic properties. As MBT is layered material with antiferromagnetic coupling between adjacent layers, it is a challenge to realize the quantum anomalous Hall effect in MBT. With molecular beam epitaxy technique, we prepared MBT thin films and tried to modify the magnetic coupling by constructing multilayer structures and co-doping method. In this work we systematically studied the magneto-electrical transport properties with the bottom gate tuning method. In the multilayer films stacked with other magnetically doped topological insulators, we observed a diversity behaviors of magnetoresistance and Hall effect in different samples, which are likely due to the variable magnetic orders. Besides, we also discovered an evident evolution in Sb-doped MBT films with varying the ratio of Bi/Sb. Our study indicates that the magnetic order can be tuned in MBT based films and it paves a promising way to control different exotic topological states.
**Surface magnetism of antiferromagnetic topological insulator**

*MnBi$_2$Te$_4$*  WEIDA WU (Presenter), PAUL SASS, Physics and Astronomy, Rutgers University, New Brunswick, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Lab — MnBi$_2$Te$_4$ is a promising candidate of antiferromagnetic (AFM) topological insulator which might host fascinating quantized anomalous Hall effect or axion insulator state in few molecular layers$^{1,2}$. These quantum phenomena are induced by the mass gap on Dirac surface states opened by the A-type AFM order (alternating ferromagnetic layers)$^3$ with uniaxial anisotropy in MnBi$_2$Te$_4$. However, recent high resolution angle resolved photoemission spectroscopy studies reveal gapless surface states, indicating paramagnetic or non-uniaxial A-type AFM orders$^{4-7}$. Yet there is no direct evidence of such surface magnetism. Recently we demonstrated magnetic imaging of AFM domain walls in MnBi2Te4 family using our homemade cryogenic magnetic force microscope (MFM)$^8$. In this talk, we will present MFM studies of MnBi2Te4 single crystals to address the nature of surface magnetism.

**References**


*This work is supported by DOE BES under award DE-SC0018153.*
5:06PM P59.00014: Quantum transport in a dual-gated antiferromagnetic topological insulator* KENJI YASUDA (Presenter), ERIC SORIANO, XIRUI WANG, Massachusetts Institute of Technology MIT, JIAQIANG YAN, Oak Ridge National Laboratory, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology MIT — Magnetic topological insulator provides an exciting arena to investigate the interplay between magnetism and spin-momentum-locked Dirac surface state [1]. The recent discovery of the intrinsic antiferromagnetic topological insulators, MnBi2Te4, MnBi4Te7, and MnBi6Te10 has enabled us to study the quantum anomalous Hall effect and axion insulator in exfoliated crystals [2,3]. Especially interesting is the electric-field effect on the crystals due to the expected finite topological magnetoelectric effect. We here report the quantum transport properties of dual-gated antiferromagnetic topological insulator devices, which allow the independent control of the carrier density and the electric field.


*This work was partially supported as part of the Center for the Advancement of Topological Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

5:18PM P59.00015: Realizing intrinsic magnetic topological insulators with gapped topological surface states in MnBi2-xSb_xTe4* WONHEE KO (Presenter), MAREK KOLMER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, ANH PHAM, MINGMING FU, FELIX LUEPKE, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, SATOSHI OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory, PANCHAPAKESAN GANESH, ZHENG GAI, ANPING LI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — The interplay between magnetism and topology of materials could create a variety of exotic topological quantum states, including the quantum anomalous Hall (QAH) effect showing dissipationless chiral edge states, the topological axion states displaying quantized magnetoelectric effects, and Majorana fermions, obeying non-Abelian statistics. All of these quantum states are hopefully realizable in MnBi2Te4. However, the Fermi level is usually in the bulk conduction band of the materials, which is not ideal for revealing these topological properties in transport. Here we show that by doping MnBi2Te4 with Sb, the Fermi level can be shifted while the non-trivial topology is maintained. Scanning tunneling microscopy (STM) is utilized to observe electronic band structure by quasi-particle interference, which reveals surface states in the bulk band gap and a surface band gap at the Dirac point. The transport from multiprobe-STM further displays a surface dominant transport. Our results show that the MnBi2-xSb_xTe4 is an intrinsic magnetic topological insulator that would offer an ideal platform to observe various exotic topological phenomena.

*This research was performed at the Center for Nanophase Materials Sciences which is a DOE Office of Science User Facility.
2:30PM P60.00001: Recent progress of Majorana zero mode in iron-based superconductors

[Invited] HONG DING (Presenter), Chinese Academy of Sciences — In this talk I will report our recent progress of Majorana zero mode in iron-based superconductors. Following our original findings of superconducting topological surface state [1] and Majorana zero mode (MZM) [2] of Fe(Te, Se), we have recently observed a half-integer level shift of vortex bound states [3] and quantized Majorana conductance [4] in this material, which are hallmarks of MZMs. In addition, we have also found that most of iron-based superconductors [5], including monolayer Fe(Te, Se)/STO [6], have similar topological electronic structures. One of them, CaKFe$_4$As$_4$, an Fe-As bilayer superconductor (Tc ~ 35K), is found to possess MZM and other bound states that can be well reproduced by a simple theoretical model [7]. Our observations offer a new, robust platform for realizing and manipulating MZMs, which may be used for quantum computing at a relatively high temperature.

References
3:06PM P60.00002: Superconducting and topological properties of CoX (X = As, Sb and Bi)*
JIAQING GAO, SHUNHONG ZHANG, WENJUN DING (Presenter), PING CUI, ZHENYU ZHANG, ICQD, University of Science and Technology of China — Recent studies have revealed high transition temperature ($T_c$) topological superconductivity in FeSe-based superconductors in either monolayer or bulk form. Here we use first-principles approaches to demonstrate that the systems of CoX (X = As, Sb, and Bi) are not only isovalent to FeSe, but also adopt the same layered structure, thereby may serve as new promising platforms to realize high-$T_c$ superconductivity. Our detailed band structure analyses further show that these systems are topologically nontrivial, and can be exploited for materialization of topological superconductivity. Moreover, all these layered CoX structures can be stabilized on SrTiO$_3$(001), which not only could enhance $T_c$, but also preserve the topological nature. These findings characterize CoX as appealing new systems to achieve high-$T_c$ superconductivity and topological properties.

*Supported by NNSF of China and MOST.

3:18PM P60.00003: Effect of Zeeman coupling on the Majorana vortex modes in iron-based topological superconductors
POUYAN GHAEMI (Presenter), The City College of New York, AREG GHAZARYAN, Physics, Institute of Science and Technology Austria, PEDRO LOPES, Physics, University of British Columbia, PAVAN HOSUR, Physics, University of Houston, MATTHEW GILBERT, Electrical and Computer Engineering, University of Illinois at Urbana-Champaign — In the superconducting regime of FeTe(1−$x$)Sex, two types of vortices which are distinct by the presence or absence of zero energy states in their core are observed. To understand their origin, we examine the interplay of Zeeman coupling and superconducting pairings in three-dimensional metals with band inversion. Zeeman fields are found to suppress the intra-orbital spin-singlet pairing, known to localize the states at the ends of the vortices on the surface. On the other hand, an orbital-triplet pairing is shown to be stable against Zeeman interactions, leads to delocalized zero-energy Majorana modes. In contrast, the finite-energy vortex modes remain localized at the vortex ends for both types of pairings. Phenomenologically, this manifests as an observed disappearance of zero-bias peaks within the cores of topological vortices upon increase of the applied magnetic field. The presence of magnetic impurities in FeTe(1−$x$)Sex, which are attracted to the vortices, would lead to such Zeeman-induced delocalization of Majorana modes in a fraction of vortices that capture a large enough number of magnetic impurities. Our results provide an explanation to the dichotomy between topological and non-topological vortices recently observed in FeTe(1−$x$)Sex.
**3:30PM P60.00004: Exploring Higher-Order Topological Physics in FeTe\textsubscript{0.55}Se\textsubscript{0.45}**

MASON GRAY (Presenter), MEAGHAN DOYLE, JAZZMIN R VICTORIN, NARENDRA KUMAR, Boston College, RUIDAN ZHONG, Brookhaven National Laboratory, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, University of Tsukuba, GENDA GU, Brookhaven National Laboratory, KENNETH BURCH, Boston College — Higher order topological superconductors (HOTSC) are a new class of topological materials in which the “bulk-boundary correspondence” is generalized to higher dimensions. FeTe\textsubscript{0.55}Se\textsubscript{0.45} is an ideal candidate to search for and manipulate such higher-order topological modes due to its intrinsic non-trivial topology and anisotropic superconductivity. In this work, we expand upon recent experimental studies which provide evidence for higher-order modes in FeTe\textsubscript{0.55}Se\textsubscript{0.45}. Furthermore, we explore predictions for HOTSC in this recently emerging platform by studying the response of FeTe\textsubscript{0.55}Se\textsubscript{0.45} to various angles of applied magnetic field.

*National Science Foundation Award No. DMR-1709987

**3:42PM P60.00005: Topological Crystalline Superconductivity in Dirac Semimetal Phase of Iron-based Superconductors**

TAKUTO KAWAKAMI (Presenter), Osaka Univ, MASATOSHI SATO, Kyoto Univ — Recently, topological states of iron-based superconductors have attracted much attention. In Fe(Se, Te) and LiFeAs, triple band inversions occur between a $p_z$ orbital and three $d$ orbitals [1,2]. ARPES experiments showed that one of the inversions near the Fermi level forms topological insulating gap [1]. Furthermore, another inversion at higher energy causes a band touch with linear dispersion [2]. Therefore, these systems with carrier doping can be Dirac semimetal.

Motivated by these experiments, we theoretically investigated unconventional superconductivity of this Dirac semimetal in iron-based superconductors [3]. We found that the Cooper pair between the electrons with d- and p-orbitals in this system yields odd-parity superconductivity. In the presentation we will discuss its topological property and typical surface states, such as Majorana flat band, Majorana quartet, and Möbius twisted surface states.


*Supported by JSPS KAKENHI Grants Nos. JP15H05855, JP16K17755, JP17H02922, and JP17J08855; the JSPS Core-to-Core program; JSPS and ISF under the Japan-Israel Research Cooperative Program, and CREST, JST (Grant No. JPMJCR18T4).
Observation of conductance plateau of Majorana zero modes in Fe(Te,Se)

LINGYUAN KONG (Presenter), SHIYU ZHU, LU CAO, HUI CHEN, Institute of Physics, Chinese Academy of Sciences, MICHAL PAPAJ, Massachusetts Institute of Technology, SHIXUAN DU, YUQING XING, WENYAO LIU, DONGFEI WANG, CHENGMIN SHEN, FAZHI YANG, Institute of Physics, Chinese Academy of Sciences, JOHN SCHNEELOCH, RUIDAN ZHONG, GENDA GU, Brookhaven National Laboratory, LIANG FU, Massachusetts Institute of Technology, YUYANG ZHANG, HONG DING, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences —

Recently, iron-based superconductor turns to be a promising platform for studying Majorana quasiparticles. The sharp and isolated zero-bias conductance peaks (ZBCPs) were observed clearly by high-resolution scanning tunneling microscopy. The wavefunction behavior of the ZBCPs and the global behavior of vortex bound states series were well studied. It implies that the observed ZBCPs are most probably Majorana zero modes (MZMs), and its topological nature renders the global $\pi$-phase shift of vortex bounds states.

There is another long-sought-after fingerprint for MZMs, i.e. $2e^2/h$-quantized Majorana conductance induced by resonant Andreev reflection. That resonance nature is ensured by the particle-hole equivalence of MZMs and introduces a plateau feature of zero-bias conductance at zero temperature. Due to the large energy level spacing in the vortex core, the iron-based superconductor turns to be a good platform to check that expectation. Here, I will report our recent tunnel-couple tunable STM measurement on a topological vortex of Fe(Te,Se). We find that the conductance of ZBCP has plateau behavior with its value close to or even reach $2e^2/h$, while other finite energy vortex bound states do not have such exotic behavior.


FeTe$_{1-x}$Se$_x$: Magnetism, electronic coherence, superconductivity, and surface state

YANGMU LI (Presenter), NADER ZAKI, Brookhaven National Laboratory, DAVID MICHAEL FOBES, Los Alamos National Laboratory, ZHIJUN XU, National Institute of Standards and Technology, GENDA GU, RONGWEI HU, CEDOMIR PETROVIC, Brookhaven National Laboratory, ANDREI T SAVICI, VASILE O GARLEA, Oak Ridge National Laboratory, PETER JOHNSON, JOHN TRANQUADA, IGOR ZALIZNYAK, Brookhaven National Laboratory — Local inhomogeneity has a great impact on the electronic band structure and magnetic properties of correlated quantum materials. We apply neutron spectroscopy, together with spatially-resolved chemical and electrical analysis, to a topological superconductor candidate, FeTe$_{1-x}$Se$_x$. Combining with photoemission spectroscopy, we obtain detailed physical and chemical information, which points to an underlying connection among magnetism, electronic coherence, superconductivity, and the topological surface state.

*Work at Brookhaven is supported by the Office of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy (DOE) under Contract No. DE-SC0012704.
4:18PM P60.00008: High-T\textsubscript{c} Superconductor Fe(Se,Te) Monolayer: an Intrinsic, Scalable and Electrically-tunable Majorana Platform*  
XIANXIN WU (Presenter), Physics department, Pennsylvania State University, XIN LIU, Physics department, Huazhong University of Science and Technology, RONNY THOMALE, Physics department, University of Wuerzburg, CHAOXING LIU, Physics department, Pennsylvania State University — A monolayer of the high-T\textsubscript{c} superconductor FeTe\textsubscript{1-x}Se\textsubscript{x} has been predicted to realize a topologically non-trivial state with helical edge modes at its boundary, providing a novel intrinsic system to search for topological superconductivity and Majorana zero modes. Evidence in favor of a topological phase transition and helical edge modes has been given in recent experiments. We propose to create Majorana zero modes by applying an in-plane magnetic field to the FeTe\textsubscript{1-x}Se\textsubscript{x} monolayer and by tuning the local chemical potential via electric gating. We demonstrate that, for appropriate parameter regimes, Majorana zero modes can exist at several different locations, including the corner between two perpendicular edges, the domain wall of chemical potentials at one edge, and certain type of tri-junction in the 2D bulk. The scalability and electrical tunability of our proposal render FeTe\textsubscript{1-x}Se\textsubscript{x} monolayer a promising Majorana platform which is in reach of contemporary experimental capability.

*The Office of Naval Research (Grant No. N00014-18-1-2793), DOE grant (DE-SC0019064) and Kaufman New Initiative research grant of the Pittsburgh Foundation. The work in Wuerzburg is supported DFG-SFB 1170 and by the Wuerzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter.

4:30PM P60.00009: Zero-Energy Modes on Superconducting Bismuth Islands Deposited on Fe(Te,Se)*  
HAI-HU WEN (Presenter), Physics Department, Nanjing University — Topological superconductivity is one of the frontier research directions in condensed matter physics. One of the unique elementary excitations in topological superconducting state is the Majorana fermion (mode) which is its own antiparticle and obeys the non-Abelian statistics, and thus useful for constructing the fault-tolerant quantum computation. The evidence for Majorana fermions (mode) in condensed matter state is now quickly accumulated. Here we report the easily achievable zero-energy mode on the tunneling spectra on Bi islands deposited on the Fe(Te,Se) superconducting single crystals. We interpret this result as the consequence of proximity effect induced topological superconductivity on the Bi islands with strong spin-orbit coupling effect. The zero-energy mode is argued to be the signature of the Majorana modes in this size confined system.

*This work was supported by National Key R&D Program of China, Natural Science Foundation of China.
Yu-Shiba-Russinov states around an excess iron in FeSe$_{0.4}$Te$_{0.6}$

TADASHI MACHIDA (Presenter), RIKEN, YUE SUN, Department of Physics and Mathematics, Aoyama Gakuin University, SUNSENG PYON, Department of Applied Physics, The University of Tokyo, SHUN TAKEDA, Laboratory for Materials and Structures, Tokyo Institute of Technology, YUHKO KOHSAKA, TETSUO HANAGURI, RIKEN, TAKAO SASAGAWA, Laboratory for Materials and Structures, Tokyo Institute of Technology, TSUYOSHI TAMEGAI, Department of Applied Physics, The University of Tokyo — Zero-energy bound states have been detected at interstitial excess irons in the iron-based superconductor Fe(Se,Te) by using a scanning tunneling microscope (STM) [1], and its relationship to the Majorana quasiparticles (QP) has been discussed [2]. However, higher energy resolution of the order of ~10 μeV is necessary to make clear the origin of the bound states at the excess irons. Here, we performed high-energy resolution (~20 μeV) tunneling spectroscopy around excess irons, using a dilution-refrigerator STM [3]. We found that most of the excess irons indicate only finite energy peaks. We also found excess irons with the zero energy peak, but it splits into a pair of finite energy peaks with increasing the distance from the excess irons and with changing the set-point conductance. These findings suggest that the bound states at the excess irons are not Majorana QP in origin but associated with the conventional Yu-Shiba-Russinov state.


Field-free platform for Majorana modes in superconductors

SONGTIAN SONIA ZHANG (Presenter), JIAJIN YIN, Princeton University, GUANGYANG DAI, Chinese Academy of Sciences, KUN JIANG, Boston College, TAY-RONG CHANG, National Cheng Kung University, LINGXIAO ZHAO, Chinese Academy of Sciences, HSIN LIN, Academia Sinica, GUOQING CHANG, Princeton University, GENFU CHEN, Chinese Academy of Sciences, RAMAN SANKAR, National Taiwan University, CHANGQING JIN, Chinese Academy of Sciences, ZIQIANG WANG, Boston College, ZAHID HASAN, Princeton University — Superconducting materials exhibiting topological properties are emerging as an exciting platform to realize fundamentally new excitations from topological quantum states of matter. Finding a systematic and controllable path to generate nonabelian Majorana zero energy excitations has been the central task in this research direction. Here, we explore the possibility of a field-free platform by depositing magnetic impurities on the surface of candidate topological superconductors. We use scanning tunnelling microscopy to probe localised states induced at the Fe atoms on the atomic scale at sub Kelvin temperatures and find that each Fe adatom generates a striking zero-energy bound state inside the superconducting gap. Our findings point to magnetic adatoms evaporated on bulk superconductors with topological surface states as a new platform for exploring Majorana zero modes under field-free conditions.

*Work at Princeton was supported by the US DOE under Basic Energy Sciences programme (grant number DOE/BES DE-FG-02-05ER46200) and the Gordon and Betty Moore Foundation (GBMF4547/ Hasan).
**P60.00012: Topological superconducting and Majorana zero mode in a new Fe-As bilayer superconductor**  WENYAO LIU (Presenter), Chinese Academy of Sciences — By combining the topological band structure and superconductivity, Fe-based superconductor Fe(Te,Se) is found to host a Majorana Zero Mode (MZM) inside its vortex core. However, the strong intrinsic inhomogeneity induced by the difference between Te and Se atom constraints further researching and practical application of MZM in this material. Recently, we found a Fe-As bilayer superconductor (Tc~35 K), CaKFe$_4$As$_4$, which could host the topological nontrivial surface state and homogeneous bulk meanwhile. Here I will introduce our observation in CaKFe$_4$As$_4$. Our ARPES and STM results mention that MZM and other bound states are derived from the topological surface state, which can be well reproduced by a simple theoretical model for topological superconducting, thus CaKFe$_4$As$_4$ is promising to be a new and more practical Majorana platform.

**Wednesday, March 4, 2020 2:30 PM - 5:30 PM**

**Session P61 DMP DCMP: Spin-orbit coupled systems** Mile High Ballroom 4B -
Matthias Vojta - Tag(s): Focus

**2:30PM P61.00001: Valence bond glass state in the 4d$^1$ Mo$^{5+}$ fcc antiferromagnet Ba$_2$LuMoO$_6$**  OTTO MUSTONEN (Presenter), HEATHER MUTCHE, Materials Science and Engineering, University of Sheffield, PETER BAKER, HELEN WALKER, ISIS Pulsed Neutron and Muon Source, CHARLOTTE PUBH, Materials Science and Engineering, University of Sheffield, FIONA COOMER, Johnson Matthey Battery Materials, CHENG LIU, SIAN E DUTTON, Cavendish Laboratory, University of Cambridge, EDMUND J CUSSEN, Materials Science and Engineering, University of Sheffield — Ba$_2$LuMoO$_6$ is a 4d$^1$ Mo$^{5+}$ fcc antiferromagnet in the double perovskite structure. Here we show that it is a valence bond glass; similar to the well known isostructural Ba$_2$YMoO$_6$ compound. Muon spin rotation and relaxation measurements on Ba$_2$LuMoO$_6$ revealed the lack of magnetic order or spin freezing down to 60 mK, in contrast to Ba$_2$YMoO$_6$ where spin freezing occurs at 1 K. Inelastic neutron scattering measurements revealed a singlet-triplet gap of 28 meV similar to Ba$_2$YMoO$_6$. These results are interpreted as the formation of a valence bond glass, where spin singlets form in a disorganized manner. Some orphan spin do not form singlets and remain paramagnetic even at 60 mK.


*This work is supported by the Leverhulme Trust Research Project Grant RPG-2017-109.*
**2:42PM P61.00002: Tuning electron correlation strength by charge doping of 5d\(^1\) double perovskites**

ERICK GARCIA (Presenter), Brown University, PAOLA CATERINA FORINO, University of Bologna, RONG CONG, CHARLES SNIDER, Brown University, PHUONG TRAN, PATRICK WOODWARD, The Ohio State University, VESNA F MITROVIC, Brown University, SAMUELE SANNA, University of Bologna — Competing interactions between spin-orbit coupling (SOC) and strong electron correlations have recently led to widespread studies of various emergent novel quantum phases. Double perovskites, particularly those containing 5d transition metal ions, present a useful opportunity to study such interactions since they display comparable magnitudes of electron correlations, crystal field, and SOC. Here, we present a systematic study of the electron doped powder Mott insulator Ba\(_2\)Na\(_{1-x}\)Ca\(_x\)OsO\(_6\) through the Na/Ca partial substitution using \(^{23}\)Na nuclear magnetic resonance at various doping concentrations. These results complement our previous muon spin relaxation (μSR) and superconducting quantum interference device (SQUID) measurements. Ba\(_2\)Na\(_{1-x}\)Ca\(_x\)OsO\(_6\) displays a crossover from an exotic canted ferromagnetic state driven by multipolar ordering at \(x = 0\) to an antiferromagnetic state at \(x = 1\). Moreover, the magnetic transition increases monotonically from 5 K to 40 K with increasing Ca concentration. The experimental results will be compared to theoretical work and their implications will be discussed.

*This work was supported by NSF grant DMR-1608760 and DMR-1905532.

**2:54PM P61.00003: NMR study on single crystal Ba\(_2\)LiOsO\(_6\)**

CHARLES SNIDER (Presenter), RONG CONG, ERICK GARCIA, Brown University, SAMUELE SANNA, University of Bologna, SANATH RAMAKRISHNA, Florida State University, ARNEIL P REYES, National High Magnetic Field Laboratory, JIAQIANG YAN, Oak Ridge National Lab, VESNA F MITROVIC, Brown University — Nuclear magnetic resonance (NMR) measurements on single crystals of Ba\(_2\)LiOsO\(_6\) were carried out to test the universality of theoretical models based on anisotropic exchange interactions \[^1\]. The results are compared with NMR findings on its isostructural and isovalent compound Ba\(_2\)NaOsO\(_6\). Ba\(_2\)LiOsO\(_6\) displays significant line broadening at low temperature, but no well-defined line splitting like its Na counterpart \[^2\]. In addition, the spin-lattice relaxation and linewidth of its spectrum undergoes an abrupt change at 6 T. The implications of these findings will be discussed.


*We acknowledge funding from NSF grant DMR-1608760 and DMR-1905532.
On the charge transfer energy in iridates: a hard x-ray photoelectron spectroscopy study

DAISUKE TAKEGAMI (Presenter), DEEPA KASINATHAN, KLAUS WOLFF, SIMONE G ALTENDORF, CHUN-FU CHANG, KATHARINA HOFER, ANNA MELÉNDEZ-SANS, YUKI UTSUMI, Max Planck Institute for Chemical Physics of Solids, FEDERICO MENEGHIN, Politecnico di Milano, THAI DUY HA, Department of Electrophysics, National Chiao Tung University, CHIEN-HAN YEN, Department of Physics, National Tsing Hua University, KAI CHEN, Institute of Physics II, University of Cologne, CHANG-YANG KUO, Y. F. LIAO, KU-DING TSUEI, National Synchrotron Radiation Research Center, RYAN MORROW, SABINE WURMEHL, Leibniz Institute for Solid State and Materials Research IFW Dresden, B.E. PRASAD, Max Planck Institute for Chemical Physics of Solids, MARTIN JANSEN, Max Planck Institute for Solid State Research, ALEXANDER KOMAREK, PHILIPP HANSMANN, LIU HAO TJENG, Max Planck Institute for Chemical Physics of Solids — We have investigated the electronic structure of iridates in the double perovskite crystal structure containing either Ir$^{4+}$ or Ir$^{5+}$ using hard x-ray photoelectron spectroscopy (HAXPES). The experimental valence band spectra can be well reproduced using tight binding calculations including only the Ir 5$d$, O 2$p$ and O 2$s$ orbitals with parameters based on the down-folding of the density-functional band structure results. We found that regardless the A and B cations, the A$_2$BIrO$_6$ iridates have essentially zero O 2$p$ to Ir 5$d$ charge transfer energies. They are extremely covalent systems with the consequence is that the magnetic exchange interactions become very long-ranged, thereby hampering the materialization of the Kitaev model. Nevertheless, it still would be possible to realize a spin-liquid system using the iridates with a proper tuning of the various competing exchange interactions.

We acknowledge supported by the Deutsche Forschungsgemeinschaft through SFB 1143 (project-id 247310070) and Grant No. 320571839.

Monte Carlo simulation of a strong SOC model for d$^1$ double perovskite

RONG CONG (Presenter), JOHN BRADLEY MARSTON, VESNA F MITROVIC, Brown University — Recent NMR experiments have revealed exotic quantum phases in the magnetic Mott insulator with strong spin orbit coupling (SOC) Ba$_2$NaOsO$_6$[1]. To investigate the possible spin and orbital order patterns consistent with the NMR observations, we performed Monte Carlo simulations of a microscopic model for d$^1$ double perovskites magnetic Mott insulators with multipolar spin interactions[2] . We obtained the low temperature phase diagram involving both spin and orbital degrees of freedom by magnetic annealing. We found that the zero temperature phase diagram consists of a fluctuating xyAFM, a canted FM[100] and a magnetic quadrupolar state each with distinct corresponding orbital ordering pattern. Furthermore, the xyAFM and the quadrupolar state are also found at intermediate temperatures as a result of enhanced thermal fluctuations. We demonstrate that the ground state evolves from the canted FM[100] state to the quadrupolar state as electric quadrupole-quadrupole interaction increases.


We acknowledge funding from NSF grant DMR-1608760, DMR-1905532 and NSF grant No. ACI-1548562.
3:30PM P61.00006: Ground state in the novel dimer iridate $\text{Ba}_{13}\text{Ir}_6\text{O}_{30}$ with Ir$^{6+}(5d^3)$ Ions*

HENGDI ZHAO (Presenter), University of Colorado, Boulder, FENG YE, Neutron Scattering Division, Oak Ridge National Laboratory, HAO ZHENG, BING HU, YIFEI NI, YU ZHANG, ITAMAR KIMCHI, GANG CAO, University of Colorado, Boulder — We have synthesized and studied a new iridate, $\text{Ba}_{13}\text{Ir}_6\text{O}_{30}$, with unusual Ir oxidation states: 2/3 Ir$^{6+}(5d^3)$ ions and 1/3 Ir$^{5+}(5d^4)$ ions. Its crystal structure features dimers of face-sharing IrO$_6$ octahedra, and IrO$_5$ monomers, that are linked via long, zigzag Ir-O-Ba-O-Ir pathways. Nevertheless, $\text{Ba}_{13}\text{Ir}_6\text{O}_{30}$ exhibits two transitions at $T_{N1} = 4.7$ K and $T_{N2} = 1.6$ K. This magnetic order is accompanied by a huge Sommerfeld coefficient 200 mJ/mole K below $T_{N2}$, signaling a coexisting frustrated/disordered state persisting down to at least 0.05 K. This iridate hosts unusually large $J_{\text{eff}}=3/2$ degrees of freedom, which is enabled by strong spin-orbit interactions (SOI) in the monomers with Ir$^{6+}$ ions and a joint effect of molecular orbitals and SOI in the dimers occupied by Ir$^{5+}$ and Ir$^{6+}$ ions. Features displayed by the magnetization and heat capacity suggest that the combination of covalency, SOI and large effective spins leads to highly frustrated ferrimagnetic ordering, a novelty of this new high-spin iridate.

*This work was supported by the National Science Foundation via grant DMR-1712101 and No. DMR-1903888.
3:42PM P61.00007: Spin-orbital-entangled quantum magnet on a honeycomb lattice [Invited]
TOMOHIRO TAKAYAMA (Presenter), Max Planck Inst — In heavy transition-metal compounds containing 4d or 5d elements, strong spin-orbit coupling often yields spin-orbital-entangled $J_{\text{eff}}$-states for $d$-electrons. The magnetic interactions between such states may give rise to an exotic ground state due to their bond-sensitive character. In particular, quantum liquid state of spin-orbital-entangled objects have been expected to emerge in a simple honeycomb lattice.

Honeycomb-based iridates with $J_{\text{eff}} = 1/2$ pseudospins have been intensively investigated as a potential realization of Kitaev spin liquid. Although the honeycomb iridates such as Na$_2$IrO$_3$ and α-Li$_2$IrO$_3$ are shown to undergo magnetic ordering likely due to the additional magnetic interactions other than Kitaev-type exchange, a quantum liquid state has been identified in the hydrogen-exchanged material H$_3$LiIr$_2$O$_6$. No magnetic order or spin-glass freezing is not seen in H$_3$LiIr$_2$O$_6$ down to 50 mK. However, clear evidence for Kitaev-type spin liquid is lacking so far, and the prime driving force for the liquid state remains elusive. In order to investigate the critical role of hydrogen, we synthesized an isotopic material D$_3$LiIr$_2$O$_6$. D$_3$LiIr$_2$O$_6$ displays a large isotope effect in structural and magnetic properties; the antiferromagnetic Weiss temperature increases from 100 K for H$_3$LiIr$_2$O$_6$ to 170 K for D$_3$LiIr$_2$O$_6$. Nevertheless, the quantum liquid state was found to be robust. We argue that the disordered OH/OD bonds likely play a role to stabilize the quantum liquid state.

Another exotic honeycomb magnet is expected for systems with $d^4$ configuration. In the case, the spin-orbit coupling produces nonmagnetic $J_{\text{eff}} = 0$ singlet ground state. However, the $d^4$ ions magnetically interact with each other via the excited $J_{\text{eff}} = 1$ levels, and such magnetic interactions are also shown to inherit bond-dependent character. We argue that a honeycomb ruthenate Ag$_3$LiRu$_2$O$_6$ has the spin-orbit induced singlet ground state and discuss the possible pressure-induced electronic phase transitions.

4:18PM P61.00008: Jahn-Teller effect and spin-orbit coupling in $t_{2g}$ systems* SERGEY STRELTSOV (Presenter), Institute of Metal Physics, DANIEL KHOMSKII, Univeristy of Cologne — In this talk we will discuss a very general problem of interplay between the Jahn-Teller (JT) effect and the spin-orbit coupling (SOC). It will be shown that the result of competition strongly depends on the specific situation: for some cases, such as $d^4$ and $d^5$, but also $d^2$ configurations, strong SOC may sometimes reverse, but finally completely suppresses JT distortion, whereas in other cases, notably $d^3$, SOC generates JT effect in the configuration which is usually considered as “orbitally dead”.

*We thank Russian Foundation for Basic Researchers (projects 20-32-70019 and 20-52-S52003).
**4:30PM P61.00009: Thermodynamics of Spin-Orbital Coupled Magnets: The Case of Dimers and Timers**  STEPHEN WINTER (Presenter), YING LI, ROSER VALENTI, Institute for Theoretical Physics, Goethe University Frankfurt — Recently, there has been great interest in 4d and 5d magnetic insulators with strong spin-orbit coupling (SOC) - which have shown the potential to realise low-energy spin Hamiltonians featuring a variety of complex anisotropic couplings of fundamental interest. In this contribution, we focus on the theoretical description of recently reported spin-liquid candidate materials based on mixed valence $M_2O_9$ dimers [1] and $M_3O_{12}$ trimers [2,3]. The challenge of modelling these materials lies in their complex local electronic structures, which should manifest in e.g. complex spin-orbital ground states, instabilities towards charge order, and strong structural sensitivity of the magnetic response. We focus, in particular, on experimental signatures and consequences of various possible ground states as a function of SOC strength and electronic filling. Of particular experimental importance is the inapplicability of Curie-Weiss analysis due to the non-commutability of SOC with magnetic fields.


**4:42PM P61.00010: Effect of disorder in Kitaev materials** [Invited]  NATALIA PERKINS (Presenter), University of Minnesota, JOHANNES KNOLLE, Physics, Technical University of Munich, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, WEN-HAN KAO, University of Minnesota — Recent years have seen remarkable progress in identifying candidate materials that can realize Kitaev quantum spin liquid [1]. In particular, a significant experimental and theoretical effort has been devoted to the study of magnetic properties of 4d and 5d systems, such as iridates and ruthenates, in which the interplay of strong spin-orbit coupling and electronic correlations gives rise to highly anisotropic and spatially dependent Ising-like interactions between effective moments $J=1/2$. Many of these materials show the presence of various forms of disorder, such as site disorder (magnetic or non-magnetic impurities), bond disorder and layer stacking faults. This is why these systems offer a remarkable playground for new phenomena that can be realized as a cooperative manifestation of disordered topological condensed matter systems. Recently we argued [2] that a minimal model of a bond disordered Kitaev quantum spin liquid can account for most of the salient experimental findings in $H_3LiIr_2O_6$ [3]. However, other implications of disorder might be crucial to account for all observations in this material. Here we discuss how include vacancies in this consideration and consider combined effect of bond disorder and vacances at finite temperature properties of the Kitaev quantum spin liquid.


*We acknowledge the US Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0018056.*
Resonant elastic x-ray scattering on the molecular orbital in Li$_2$RuO$_3$

SEOKHWAN YUN (Presenter), Department of Physics and Astronomy, Seoul National University, BEOM HYUN KIM, Korea Institute for Advanced Study, KI HOON LEE, Department of Physics and Astronomy, Seoul National University, DAN G. PORTER, Diamond Light Source, Harwell Science and Innovation Campus, SERGIO DI MATTEO, Universite de Rennes, SOONMIN KANG, JAEHONG JEONG, Department of Physics and Astronomy, Seoul National University, ALESSANDRO BOMBARDI, Diamond Light Source, Harwell Science and Innovation Campus, JE-GUEN PARK, Department of Physics and Astronomy, Seoul National University — In solid, the $d$-orbital electrons of transition metal (TM) elements are generally described in the atomic orbital limit because an overlap between adjacent orbitals is much smaller than other perturbations like $d$-$p$ hybridization or Coulomb $U$. However, when ionic radii increase with the rise of periodicity or adjacent ions are getting closer like ones in edge-sharing or face-sharing octahedra, the enhanced overlap of orbitals can lead the molecular behavior of orbital clusters.

Li$_2$RuO$_3$ has a layered honeycomb structure composed of edge-sharing RuO$_6$ with strong dimerization. It enhances the orbital overlap so induces the spin-singlet, molecular orbital state. We measured the Bragg-forbidden (010) reflection in Li$_2$RuO$_3$ single crystal using resonant elastic x-ray scattering to identify the spatial distribution of the molecular orbitals. The peak was measured at the $\sigma$-$\pi$ polarization change, but it is not a magnetic reflection as Li$_2$RuO$_3$ has no long-range magnetic order. We observed a distinct phase difference in the polarization dependence between Ru 2$p$-4$d$ ($t_{2g}$) and 2$p$-4$d$ ($e_{g}$) process. It also shows a fine structure from the crystal-field effect only at Ru $L_3$ edge but not at $L_2$ edge. This result elucidates the local shape of the molecular orbital of the Ru dimer.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P62 DMP: Electron-Phonon Coupling and Transport in Nanostructures

Mile High Ballroom 4C - Shixiong Zhang, Indiana Univ - Bloomington - Tag(s): Focus
It has been known for some time that a perfect (delta-function) energy filter allows, in principle, thermal-to-electric energy conversion near ideal (Carnot) efficiency. [1,2] I will introduce this concept and report on a recent experiment where we realized a near-ideal quantum-dot heat engine in devices based on single nanowires, realizing power production at maximum power with Curzon-Ahlborn efficiency, and reaching more than 70% of Carnot efficiency at maximum efficiency settings [3]. This proof-of-performance of efficient energy harvesting from electrons is directly relevant to the concept of hot-carrier or thermophotovoltaics, where the aim is to boost energy conversion efficiency by harvesting heat from non-equilibrium electrons [4]. I will present our progress towards implementing this principle in heterostructure nanowires. [4]

References

*Funded by the Knut and Alice Wallenberg Foundation, the Swedish Research Council, the European Commission, and NanoLund.
3:06PM P62.00002: Cooling and self-oscillation in a nanotube electromechanical resonator
CARLOS URGELL (Presenter), WEI YANG, SERGIO DE BONIS, CHANDAN SAMANTA, ICFO-The Institute of Photonic Sciences, MARIA JOSÉ ESPLANDIU, Catalan Institute of Nanoscience and Nanotechnology, QUAN DONG, YONG JIN, Centre de Nanosciences et de Nanotechnologies, ADRIAN BACHTOLD, ICFO-The Institute of Photonic Sciences — Nanomechanical resonators are used with great success to couple mechanical motion to other degrees of freedom, such as photons, spins and electrons [1,2]. The motion of a mechanical eigenmode can be efficiently cooled into the quantum regime using photons [2,3,4], but not other degrees of freedom. Here, we demonstrate a simple yet powerful method for cooling, amplification and self-oscillation using electrons. This is achieved by applying a constant (d.c.) current of electrons through a suspended nanotube in a dilution refrigerator. We demonstrate cooling to 4.6±2 quanta of vibrations. We also observe self-oscillation, which can lead to prominent instabilities in the electron transport through the nanotube. We attribute the origin of the observed cooling and self-oscillation to an electrothermal effect. This work shows that electrons may become a useful resource for cooling the mechanical vibrations of nanoscale systems into the quantum regime.


3:18PM P62.00003: Theory of hot-carrier generation and relaxation in plasmonic nanoparticles
YU ZHANG (Presenter), Theoretical Division, Los Alamos National Laboratory — Hot-carrier generation from surface plasmon decay has attracted much recent attention due to its promising applications in physical, chemical, materials and energy science. However, the detailed mechanisms of plasmonic hot-carrier generation and relaxation are less studied or treated by the semiclassical model. In this work, we develop and apply a quantum-mechanical model and coupled master equation method to study the generation, relaxation, and extraction of hot-carriers. And the connection with the semiclassical model is discussed. The initial distribution of hot-carriers and lifetimes of hot-carriers induced by different excitation are investigated. The relaxation due to electron-electron and electron-phonon scatterings are treated on the equal footing. Heat generation from hot-carriers decay is also described. We also generalize the model to study the extraction of hot-carriers to attached molecules or semiconductors. The quantum yield of extracting hot-carriers from the plasmonic nanoparticles is found to be size-dependent.

*The work at Los Alamos National Laboratory (LANL) was supported by the LANL Directed Research and Development Funds (LDRD). LANL is operated by Triad National Security, LLC, for the NNSA of the U.S. DOE (Contract No. 89233218NCA000001).
3:30PM P62.00004: Nanoimaging of surface waves in 2D materials  DMITRI VORONINE (Presenter), Univ of South Florida — Propagating surface waves such as surface-plasmon polaritons and exciton-polaritons have recently been of interest in a variety of optical, electronic and quantum communication applications. Nano-optical imaging of surface waves in two-dimensional (2D) transition-metal dichalcogenide (TMD) materials has been realized in several cavity-coupled systems. In this work, new nanoimaging schemes based on tip-enhanced photoluminescence (TEPL) and Kelvin-probe force microscopy (KPFM) are presented, revealing the optical and electric components of surface waves in 2D TMD heterostructures, respectively. These results could be used in novel nanophotonic coupling schemes for quantum emitters in 2D materials.

3:42PM P62.00005: Coupled electron-phonon thermal transport across metal-nonmetal interfaces and superlattices  CHENG SHAO (Presenter), JUNICHIRO SHIOMI, Univ of Tokyo — Understanding the thermal transport across metal/nonmetal interface is of great importance for applications like electronic and thermoelectric devices. In nonmetal phonons are the dominant heat carriers; while in metal both electrons and phonons conduct heat. The nonequilibrium carrier populations and the complicated coupling channels at the interfaces make our current understanding yet to be completed. In this work, we utilize the fully coupled Monte Carlo simulations to study thermal transport across the metal-nonmetal interfaces and superlattice. The mode-wise electron and phonon relaxation times and their coupling strengths are obtained from first-principles calculations, while the phonon transmissions at interfaces are obtained from the Green's function methods. The simulation results show that the thermal transport at metal/nonmetal interface can be enhanced by inserting an intermediate metal layer with high electron-phonon coupling strength. For metal-nonmetal superlattice structure, thin metal layers with weak electron-phonon coupling can largely impede the thermal transport. The simulation results reveal the importance of mode-wise scattering channel and the nonequilibrium between electron, acoustic phonon, and optical phonon at the interface to thermal transport.
Modification of Electron-Phonon Coupling by Micromachining and Suspension*  
OLLI SAIRA (Presenter), Brookhaven National Laboratory, MATTHEW MATHENY, California Institute of Technology, LIBIN WANG, JUKKA P PEKOLA, Aalto University, MICHAEL ROUKES, California Institute of Technology — Weak electron-phonon interaction in metals at low temperatures forms the basis of operation for cryogenic hot-electron detectors. Standard power laws, describing the heat flow in the majority of experiments, have been identified and derived theoretically. However, a full picture encompassing experimentally relevant effects such as reduced dimensionality, material interfaces, and disorder is in its infancy, and has not been tested extensively.

Here [1], we study the electron-phonon heat flow in a thin gold film on a suspended SiO$_2$ platform at temperatures below 100 mK using supercurrent thermometry. We observe a half-integer power law that has been recently predicted by theory [2], defying conventional results for bulk (semi-infinite) systems. The novel thermometry method we employ addresses some of the shortcomings of conventional nanoscale thermal measurement schemes. Similar behavior has been reported in earlier work [3].


*We acknowledge support from the U.S. Army Research Laboratory and the U.S. Army Research Office (contracts W911NF-13-1-0390 and W911NF-18-1-0028) and Academy of Finland (contract 312057).
4:06PM P62.00007: Influence of Highly Non-Equilibrium Electron-Phonon Transport on Heat Conduction across Metal-Insulator Superlattice  Kyoungjung Kim (Presenter), Mechanical Engineering, Univ of Tokyo, Yosuke Kurosaki, Naoto Fukatani, Shin Yabuuchi, Research & Development Group, Hitachi Ltd., Yosuke Ira, Cheng Shao, Mechanical Engineering, Univ of Tokyo, Jun Hayakawa, Research & Development Group, Hitachi Ltd., Junichiro Shiomi, Mechanical Engineering, Univ of Tokyo — Nanostructuring is often utilized to improve figure-of-merit of thermoelectric materials by reducing thermal conductivity (TC). There, thermal boundary conductance at nanostructure interfaces is important, and population of heat carriers can be highly non-equilibrium. One strategy to further reduce TC is to utilize metal–semiconductor interfaces, such as in metal-semiconductor superlattice with the electron-phonon scattering mean free path being comparable or longer than the nanostructure length-scale. There, the nonequilibrium interfacial regions are expected to make phonons the dominant heat carrier even in the metal part, which should contribute to the reduction of TC. In this study, we take metal-insulator(MgO) superlattice as a model case and measure the TC by the time-domain thermoreflectance method. We prepare two kinds of samples with different metal layers (AuSi or Ta) with relative difference in the electron-phonon coupling strength. As a result, for both kinds of samples, TC of superlattice was reduced as the unit-layer of the superlattice was made thinner. While the reduction of TC is expected due to the increase in the number of interfaces, the different trends of reduction between AuSi and Ta samples suggest roles of non-equilibrium phonon-electron transport.

4:18PM P62.00008: Ultrafast investigation of electronic and vibrational dynamics of via pump-degenerate four-wave mixing  Joseph Avenoso (Presenter), Univ of Delaware, Daniela Zahn, Ralph Ernstorfer, Fritz Haber Institute, Lars Gundlach, Univ of Delaware — Phonon dynamics and their coupling to electronic excitations in bulk tungsten disulfide is investigated. Pump-degenerate four-wave mixing is used to measure the femtosecond dynamics of the phonons, which when combined with transient absorption spectroscopy, provides an energy-resolved picture of phonon dynamics and their lifetimes. Measurements suggest the LA(M) phonon mitigates electron scattering from the K point to the Σ valley in under 100 fs. Pump-degenerate four-wave mixing is hereby shown to be an effective tool to compliment momentum-resolved methods for studying coupling in tungsten disulfide and other transition metal dichalcogenides.
4:30PM P62.00009: Acoustoelectric charge transport at the LaAlO$_3$/SrTiO$_3$ interface by surface acoustic waves*  YIGITCAN UZUN (Presenter), SANDER SMINK, M. P. DE JONG, HANS HILGENKAMP, WILFRED G. VAN DER WIEL, Univ of Twente — Surface acoustic waves (SAWs) are capable of transporting free charge carriers along their propagation path, resulting in an acoustoelectric current or voltage. This has been explored intensively in AlGaAs/GaAs heterostructures. Here, we integrate SAWs with the LaAlO$_3$/SrTiO$_3$ 2-dimensional electron system, which is known to exhibit high mobility at low temperature, magnetism and superconductivity under the appropriate conditions. Despite the non-piezoelectric nature of SrTiO$_3$ (and LAO) we can make use electrostriction for SAW generation. We measure the acoustoelectric effect both at room temperature and at 150 K, and observe a considerable enhancement at lower temperatures. Our results suggest robust coupling between the SAWs and the interfacial free electrons, which opens the way for applying the same approach in other non-piezoelectric (complex-oxide) systems.

*This project was financially supported by the European Union’s Horizon 2020 research and innovation programme under the Marie-Curie grant agreement No. 642688 (SAWtrain). The authors also acknowledge financial support of the Netherlands Organisation for Scientific Research (NWO) through a Vrij Programma grant (QUAKE, 680.92.18.04/7566) and the DESCO programme.

4:42PM P62.00010: Hot-carrier induced above-threshold light emission in plasmonic tunnel junctions*  LONGJI CUI, YUNXUAN ZHU (Presenter), MAHDIYEH ABBASI, ARASH AHMADIVAND, BURAK GERISLIOGLU, PETER JAN ARNE NORDLANDER, DOUGLAS NATELSON, Rice Univ — Light emission from electrically driven tunnel junctions, mediated by localized surface plasmons, have attracted much recent interests, showing that the emitted photon energies are limited by the applied voltage bias. Recent works have reported the above-threshold light emission in which the emitted photons have energies significantly above the applied voltage. However, the physical mechanism underlying this phenomenon, is elusive. Here we report systematic measurements of light emission from tunneling junctions made of different plasmonic materials and proposed a hot-carrier induced light emission mechanism. The characteristics and dynamics of the hot carriers is found to be set by the non-radiative plasmonic process. The reported light emission and electrically driven hot carrier generation opens new possibility in plasmonic chemistry and optoelectronic energy conversion applications.

*Robert A. Welch Foundation Grant No. C-1636; J Evans Atwell Welch Postdoctoral Fellowship
4:54PM P62.00011: Ultrafast hot carrier injection in Au/GaN: the role of band bending and the interface band structure* FAN ZHENG (Presenter), LIN-WANG WANG, Lawrence Berkeley National Laboratory — Plasmon photochemistry can potentially play a significant role in photocatalysis. To realize this potential, it is critical to enhance the plasmon excited hot carrier transfer and collection. However, the lack of atomistic understanding of the carrier transfer across the interface, makes it challenging to design more efficient system. In this work, we apply the non-adiabatic molecular dynamics simulation to study hot carrier dynamics in the system of Au nanocluster on top of GaN surface. By setting up the initial excited hole in Au, the carrier transfer from Au to GaN is found to be on a sub-pico second time scale. After the hole has cooled down to the band edge of GaN, we find some of the charges can return back to Au. By applying different external potentials to mimic the Schottky-barrier band bending, the returning charge can be reduced effectively. Finally, with the understanding of the carrier transfer's pathway, we suggest that a ZnO layer between GaN and Au can effectively block the "cold" carrier from returning back to Au but still allow the hot carrier to transfer.

*This work is funded by the Joint Center for Artificial Photosynthesis, supported through DOE under Award number DE-SC0004993. NERSC and Oak Ridge Leadership Computing Facility provide computational support.

5:06PM P62.00012: Tunable plasmonic hot carrier dynamics in noble metal alloys ADELA HABIB (Presenter), RAVISHANKAR SUNDARARAMAN, Rensselaer Polytechnic Institute — Noble metal alloys exhibit promise as a tunable plasmonic material with an 'on-demand optical response' [1]. However, the performance of these metal alloys for plasmonic hot carrier harvesting remains unknown. In particular, disorder in the alloys is expected to lead to increased scattering and inhibit transport of low energy carriers in metal alloys, but the corresponding situation for hot carriers is not yet known. Moreover, hot carrier generation and injection across a metal-semiconductor interface depend sensitively on the band structure [2], and alloys may provide an opportunity to tune the band structure for increasing injection. This talk will present first-principles predictions of hot carrier generation and transport properties of ordered and random structures of gold-silver alloys. The density of states and phase space for both optical excitation and hot carrier scattering depend critically on composition and disorder, providing an additional knob for generating and harvesting hot carriers with desired energy distributions.

Recent developments in nanotechnology enable us to control and observe electron transfer with high accuracy fulfilling needs for quantum metrology. One of its important instances is an electron pump driven by a time periodic bias voltage between source and drain electrodes attached to a microscopic system such as a quantum dot (J. P. Pekola et al., Rev. Mod. Phys. 85, 1421 (2013)). In conventional studies, the electron pump has been mostly formulated in an adiabatic regime, where the time-dependent bias is described by an infinitely slow modulation of electrochemical potentials of electrodes (T. Yuge et al., Phys. Rev. B 86, 235308 (2012)). This formalism is, however, practically useless because the pumped current generated by the infinitely slow modulation is zero in a strict sense. The purpose of the present study is to provide a more realistic formalism describing the pumping under a finite speed continuous modulation of the bias voltage. To this end, we propose an extended formalism of the pumping based on the full counting statistics with quantum master equation taking into account a temporal shift of single-particle energy of electrons in source and drain induced by the voltage modulation.

*This study is supported by KAKENHI No. 19K14611.

Wednesday, March 4, 2020 2:30 PM - 5:18 PM

Session P63 DMP DCOMP FIAP: Defects: Structure and Strain 1 Mile High Ballroom 4D - Kunal Mukherjee, University of California, Santa Barbara - Tag(s): Focus

2:30PM P63.00001: Defects in Chalcogenide Compound Semiconductors for Photovoltaics [Invited] ANGUS ROCKETT (Presenter), Colorado Sch of Mines — This talk briefly reviews recent progress in solar cell energy generation to set the stage. The most promising include the thin film chalcogenide compound based devices. The talk then reviews the characterization and understanding of defects in the two primary materials classes used in solar cells (photovoltaics), CdTe and CuInSe$_2$ and related compounds. The characterization methods discussed include scanning tunneling microscopy, nuclear magnetic resonance, and capacitance methods including scanning microwave impedance microscopy. The implications of the results for device performance are described.
Does lattice expansion really occur in defected low-temperature GaAs?

MARY CLARE ESCANO (Presenter), Research Center for Development of Far-Infrared Region, University of Fukui, Japan, TIEN QUANG NGUYEN, Institute of NanoScience Design, Osaka University, Japan, HIDEAKI KASAI, National Institute of Technology, Akashi College, Japan, MASAHIKO TANI, Research Center for Development of Far-Infrared Region, University of Fukui, Japan — A prominent example of lattice expansion caused by point defects is that of GaAs grown at low temperature (LT-GaAs). A linear correlation between the lattice expansion and concentration of As-antisite ($\text{As}_{\text{Ga}}$) point defect is obtained experimentally by XRD. However, using full first-principles method (DFT-LDA) on a large 512-atom supercell of GaAs bulk, we found that, in the limit of small concentrations of $\text{As}_{\text{Ga}}$ (less than 1%), the lattice does not expand but the As-As bond length near the defect increased. DFT-LDA method is tested vis-a-vis the more sophisticated DFT-hybrid functionals and the former yields the same lattice changes as the latter. We propose that the observed expansion maybe due to the increased bonds near the defect. We also found that $\text{As}_{\text{Ga}}$ point defects do not prefer isolated structure even at low concentration. Using molecular dynamics simulation, we confirm that the above results hold true even at room temperature. Study of electronic properties reveals that, in this low concentration regime, abrupt changes in density of states near the fermi level occur. These findings pose impact in the use of LT-GaAs for optoelectronic/terahertz devices, where fundamental understanding of defect concentration's relation with material structure/functionality is vital.

Off-centered Pb Interstitials in PbTe*

SUNGJIN PARK (Presenter), BYUNGKI RYU, Korea Electrotech Res Inst — The nature of off-stoichiometry of PbTe has not been fully understood yet though many studies existed by investigating its intrinsic defects. We reinvestigated the formation of intrinsic defects of PbTe by DFT study. From this, Te vacancy ($V_{\text{Te}}$) was the major defect under Pb-rich condition. Due to experiments that reported the increase of the lattice parameter as the Pb excess content grew up, a controversy between the DFT and the experimental results existed since the existence of $V_{\text{Te}}$ could not explain the volume increase. So we assumed Pb interstitial ($\text{Pb}_{\text{Int}}$) as the major defect in PbTe instead $V_{\text{Te}}$ because it not only exhibited the second-lowest formation energy, but also could be responsible for the lattice parameter increase. From this, all possible $\text{Pb}_{\text{Int}}$ positions in PbTe were first investigated to understand its off-stoichiometry. As a result, we found new stable positions of $\text{Pb}_{\text{Int}}$ other than the conventional one at the subcubic center. Moreover, among the various locations, $\text{Pb}_{\text{Int}}$ toward the nearest Te and Pb dimer with $\text{Pb}_{\text{Int}}$ were the ground and a metastable state. Finally, we believed that the many local minima of $\text{Pb}_{\text{Int}}$ might be responsible for the off-stoichiometry of PbTe during the sintering of thermoelectric PbTe.

*KERI (19-12-N0101-22), KETEP and MOTIE (20188550000290).
3:30PM P63.00004: Quantifying Cation Disorder in ZnGeP$_2$ Thin Films Using Resonant Energy X-ray Diffraction  
REKHA SCHNEPF (Presenter), Colorado School of Mines, BEN LEVY-WENDT, Stanford University, BROOKS TELLEKAMP, National Renewable Energy Lab, BRENDEN ORTIZ, CELESTE MELAMED, Colorado School of Mines, LAURA SCHELHAS, KEVIN STONE, MICHAEL TONEY, SLAC National Accelerator Laboratory, ERIC TOBERER, Colorado School of Mines, ADELE TAMBOLI, National Renewable Energy Lab — II-IV-V$_2$ materials, ternary analogs to III-V’s, are emerging for their potential applications in devices such as LEDs and solar cells. Controlling cation ordering in II-IV-V$_2$'s offers the potential to tune properties at nearly fixed compositions and lattice parameters. Cation disorder is prevalent in many II-IV-V$_2$'s and has a profound effect on properties – however, quantification of disorder remains difficult. In this work, we investigate two different methods to quantify cation ordering in ZnGeP$_2$ thin films: a stretching parameter calculated from lattice constants ($c/a$), and an order parameter determined from the cation site occupancies ($S$). We use high resolution X-ray diffraction (HRXRD) to determine $c/a$ and resonant energy X-ray diffraction (REXD) to extract $S$. REXD is critical to distinguish elements with similar Z-number (e.g. Zn and Ge) through X-ray diffraction. We found that samples with a $c/a$ corresponding to the ordered chalcopyrite structure had only partially ordered $S$ values. The optical absorption onset for these films occurred at lower energy than expected for fully ordered ZnGeP$_2$, indicating that $S$ better captures disorder in these samples. This work highlights the importance of nuanced techniques (e.g. $S$) when analyzing more complex ternary systems.

3:42PM P63.00005: Phonon Dispersion in Anisotropic Dilute Alloys by Weighted Dynamical-Matrix Approach  
MINA AZIZIHA (Presenter), SAEED AKBARSHAHI, Physics and Astronomy, West Virginia University, SAYANDEEP GHOSH, PRATIVA PRAMANIK, Physics, Indian Institute of Technology, JAMES PATRICK LEWIS, ALDO H ROMERO, Physics and Astronomy, West Virginia University, SURESH PITTALA, Physics, Indian Institute of Science, SUBHASH THOTA, Physics, Indian Institute of Technology, MOHINDAR S SEEHRA, MATTHEW BRUCE JOHNSON, Physics and Astronomy, West Virginia University — The calculation of phonon frequencies in dilute anisotropic alloys is not a simple undertaking and the successful methodologies are not well developed. We propose weighted dynamical-matrix (WDM) approach for calculating optical phonon spectra that is applicable to such complex alloys for a large range of alloying elements. Our WDM approach forms the dynamical-matrix for random alloys using the weighted average of parent structures mass and calculated force constants that allows us to calculate the phonon spectra. This WDM approach is computationally efficient and easily implemented. We demonstrate its use for the effect of Fe-doping on the phonon modes in dilute alloy of CuAl$_{1-x}$Fe$_x$O$_2$ delafossite powders whose structural and magnetic properties have been reported previously$^{1,2}$ and the phonon frequencies are measured using Raman and FTIR spectroscopies. The observed phonon modes are in good agreement with our WDM approach calculations. These results are consistent with the lattice expansion accompanying the Fe-doping, weakening the bonds. Also, Fe-doping effect on optical properties of these alloys is explored and explained by the first-principle calculated band structures.

Simulations of Nitrogen Incorporation into GaAsN Alloys: The Role of Lattice Relaxation*

EMILY OLIPHANT (Presenter), Physics, University of Michigan and Idaho State University, RACHEL GOLDMAN, Physics and Materials Science and Engineering, University of Michigan, LIANG QI, TIMOTHY JEN, ALBERT TSUI, Materials Science and Engineering, University of Michigan, DRIMIK CHOWDHURY, Mathematics, University of Michigan, YONGQIANG WANG, Materials Science and Technology Division, Los Alamos National Laboratory — Due to the significant band gap narrowing induced by dilute fractions of N in III-V semiconductors, dilute nitride semiconductor alloys are of significant interest for long-wavelength optoelectronics. However, rapid thermal annealing (RTA) is often needed to achieve suitable transport properties and emission efficiencies. Therefore, identification of the local N environments and the influence of RTA on those environments is needed. For GaAsN, it has been suggested that N shares an As site with either As or N, with N-As and N-N pairs (split interstitials) aligned along [010] and [111] directions, respectively. However, the effect of lattice relaxation in the vicinity of incorporated N has not been considered. Here, we utilize density functional theory to compute minimum energy positions of NAs and surrounding neighbors. To identify N incorporation sites, we compare nuclear reaction analysis (NRA) spectra with Monte Carlo-Molecular Dynamics simulations along the [100], [110], and [111] directions. The measured NRA spectra exhibit the highest (lowest) yields in the [111](100) directions. Similar trends are observed for simulations of (N-As)As, confirming the presence of interstitial complexes, predominantly (N-As)As, in GaAsN.

*NSF-DMR#1810280

Diffusion of Acceptor Dopants in Atomically Precise Devices*

JEFFREY IVIE (Presenter), EVAN ANDERSON, SCOTT W SCHMUCKER, LISA A TRACY, DEANNA CAMPBELL, DAVID SCRYMGEOUR, AARON KATZENMEYER, JUAN P MENDEZ, PING LU, XUJIAO GAO, DAN R. WARD, EZRA BUSSMANN, TZU-MING LU, SHASHANK MISRA, Sandia National Laboratories — Atomically precise (AP) electrical devices, fabricated using hydrogen depassivation lithography in a scanning tunneling microscope, offer a potential pathway to ultra-efficient transistors. Almost all previous work regarding AP devices has been focused on understanding the properties of phosphorus-based donor devices integrated into intrinsic or donor-implanted substrates. Equivalent knowledge for integration on to substrates having acceptor dopants is critically lacking. Here, we present our work in understanding the diffusion processes of acceptor dopants during CMOS compatible AP processing, which demonstrates highly counterintuitive behavior compared to donor dopants. We speculate on the origin of this diffusion mechanism, which is neither thermally-driven nor concentration gradient-driven.

*This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.
**4:18PM P63.00008: p-Type Doping of Pyrite FeS$_2$**  
BRYAN VOIGT (Presenter), WILLIAM MOORE, Chemical Engineering & Materials Science, University of Minnesota, DEBMALYA RAY, Chemistry, University of Minnesota, MICHAEL MANNO, Chemical Engineering & Materials Science, University of Minnesota, JEFF D JEREMIASON, Chemistry, Gustavus Adolphus College, LAURA GAGLIARDI, Chemistry, University of Minnesota, ERAY AYDIL, CHRIS LEIGHTON, Chemical Engineering & Materials Science, University of Minnesota — Pyrite FeS$_2$ is a potentially ideal absorber for thin film solar cells as it is composed of earth-abundant, inexpensive elements, has a suitable band gap (0.95 eV), and is strongly absorptive. Lack of doping control, however, has precluded $p$-$n$ homojunctions. Heterojunction solar cells have disappointing efficiencies (≤3 %), likely limited by a leaky surface inversion layer. The ability to controllably $n$- and $p$-dope FeS$_2$ would make possible a homojunction solar cell that could, uniquely, avoid this surface inversion entirely. Recently, we established S vacancies as $n$-dopants in FeS$_2$ and achieved transport control in bulk crystals. Here, we demonstrate $p$-doping by introducing phosphorus (P) during growth. Increasing P concentrations above ~40 ppm triggers a majority carrier inversion from $n$- to $p$-type. Thermal activation energy, room temperature hole density, and mobility in $p$-type crystals are ~170 meV, $\sim 10^{18}$ cm$^{-3}$, and 1 cm$^2$V$^{-1}$s$^{-1}$, respectively. Density functional theory confirms that P substitution for S creates an acceptor level 100’s of meV from the valence band, in agreement with experiment. With $p$-type control thus achieved, $p$-$n$ FeS$_2$ homojunctions now become possible.

*This work was supported by the customers of Xcel Energy through a grant from the Renewables Development Fund.

**4:30PM P63.00009: Insulator-Metal Transition in Co-Doped Pyrite FeS$_2$ Single Crystals**  
BHASKAR DAS (Presenter), BRYAN VOIGT, MOUMITA MAITI, WILLIAM MOORE, MICHAEL MANNO, University of Minnesota, ERAY AYDIL, New York University, CHRIS LEIGHTON, University of Minnesota — Iron pyrite (FeS$_2$) is a low-cost, earth-abundant, non-toxic semiconductor with attractive electronic and optical properties, both for fundamentals, and applications (e.g. photovoltaics). Sulfur vacancies ($V_S$)[1] and Co[2] are the only well-established $n$-dopants in FeS$_2$. $V_S$ are deep donors, however, preventing facile study of phenomena such as the insulator-metal transition (IMT), while surface conduction complicates transport at low Co doping. In this work the problem of surface conduction is circumvented via a contacting scheme that provides access to the bulk, enabling wide-$T$-range transport studies of Co-doped FeS$_2$ single crystals. An IMT is found at ~4X$10^{17}$cm$^{-3}$ Hall density, with Efros-Shklovskii variable-range hopping and/or activated transport below this, and electron-electron interaction-corrected metallic conductivity above it. A number of unexpected features also occur, however, including non-monotonic $T$ dependence of the Hall coefficient, resistivity anomalies at intermediate $T$, and non-saturating non-parabolic positive magnetoresistance. These will be discussed in detail.


*Work supported by the customers of Xcel Energy through grant from the Renewables Development Fund.
Toward Deterministic Doping of Silicon via Dopant Containing Homopolymer

MICHELE PEREGO (Presenter), GABRIELE SEGUINI, ELISA ARDUCA, ANDREA NOMELLINI, FRANCESCO CARUSO, IMM-CNR, KATIA SPARNACCI, DIEGO ANTONIOLI, VALENTINA GIANOTTI, RICCARDO CHIARCOS, MICHELE LAUS, Università del Piemonte Orientale — Manipulation of isolated impurity atoms in semiconductors fostered a vision of novel classical and quantum single atom devices. The main roadblock toward their exploitation is the lack of strategies to control the positioning of dopant impurities within the semiconductor lattice by a methodology compatible with current semiconductor technology. Recently, we developed a doping strategy using self-assembled monolayers of polymers terminated with P-containing moieties, used as dopant-carrying molecules.(1,2) Their self-limiting “grafting-to” reaction from melt determine the areal density of the grafted molecules and consequently the number of P atoms in the dopant source. Subsequent injection and activation of P atoms into the Si substrate is achieved by high temperature annealing.(1) Control of the lateral distribution of P atoms over the substrate could be achieved by integrating these materials with suitable lithographic techniques. In this talk, we will review our results on this topic providing preliminary data on the development of a deterministic doping strategy based on self-assembly materials.

References

2) R. Chiarcos et al., ACS Appl. Electron. Mater. 2019, 1, 1807-1816

Epitaxial growth, structure, and properties of MgZrN$_2$, an emerging nitride semiconductor

SAGE BAUERS (Presenter), National Renewable Energy Laboratory, JOHN S MANGUM, Metallurgical and Materials Engineering, Colorado School of Mines, JOHN PERKINS, STEPHAN LANY, ANDRIY ZAKUTAYEV, National Renewable Energy Laboratory — Inorganic nitrides are important technological materials, many of which belong to one of two families: hexagonal main-group metal nitride semiconductors and cubic transition-metal nitride superconductors. We break this dichotomy with our discovery of several new semiconducting Mg-TM-N (TM=Ti, Zr, Hf, Nb, Ta) nitrides which adopt rocksalt crystal structures. Ab-initio calculations on this family of mid-gap semiconductors reveal extremely large dielectric constants (up to 80 $\varepsilon_0$), and a striking tolerance to structural defects relative to other ternary nitrides. This talk will focus on Mg$_x$Zr$_{2-x}$N$_2$. We find that this material forms over a broad metal composition range. At stoichiometric MgZrN$_2$ compositions, this material behaves as a heavily-doped n-type semiconductor exhibiting a negative temperature coefficient of resistivity and thermally-activated carriers. The transport properties can be radically tuned with Mg:Zr ratio from metallic (Zr-rich) to non-degenerately-doped (Mg-rich). X-ray diffraction and electron microscopy reveal that MgZrN$_2$ can be epitaxially grown on both GaN and MgO substrates. The combination of elemental abundance, compelling properties, and structural compatibility highlights the potential of these materials for integration with known nitrides.
5:06PM P63.00012: Proton radiation-induced enhancement of conductivity of composite amorphous/nanocrystalline silicon thin films* ZVIE RAZIELI, NATHAN BOSCH, School of Physics and Astronomy, University of Minnesota, LAGY T BABY, Department of Physics, Florida State University, LIS STOLIK VALOR (Presenter), School of Physics and Astronomy, University of Minnesota, RACHEL YOHAY, Department of Physics, Florida State University, ROGER W RUSACK, JAMES KAKALIOS, School of Physics and Astronomy, University of Minnesota — While most semiconductor devices are susceptible to radiation damage, we report here observations of an enhancement of the conductivity of undoped composite hydrogenated amorphous silicon thin films containing silicon nanocrystalline inclusions (a/nc-Si:H) following irradiation with high-energy protons. A series of films with varying nc content, synthesized in a unique dual-chamber co-deposition system, were irradiated with 16 MeV protons from a superconducting linear accelerator for fluences ranging from $2 \times 10^{13}$ cm$^{-2}$ to $10^{15}$ cm$^{-2}$. For the highest irradiation doses, the dark conductivity is enhanced by over an order of magnitude. Unlike the persistent photoconductivity effect observed in amorphous semiconductors, the radiation-induced enhancement is permanent and is not removed by annealing, remaining unchanged at least eight months after irradiation. Various mechanisms are tested to explain the irradiation-induced conductivity enhancement, but none are found to be able to fully account for our observations.

*This work was partially supported by NSF grants PHYS-1344251 and DMR-1608937, the NINN Characterization Facility, the Minnesota Nano Center and, the University of Minnesota.

P63.00013: Impurity diffusion induced dynamic electron donors in semiconductors* WEN-HAO LIU, JUN-WEI LUO (Presenter), SHU-SHEN LI, State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, LIN-WANG WANG, Materials Science Division, Lawrence Berkeley National Laboratory — Low-energy impurity diffusion in a host material is often regarded as an adiabatic process. Here, we present that the diffusion process in semiconductors can involve nonadiabatic electron excitations, rendering it to be a more complicated process. Impurity diffusion in a device at working temperature can pump one electron up from localized impurity state into the host conduction band and causes the impurity to be a dynamic donor since it temporarily loses its electron to the host. This nonadiabatic process, against a common belief, fundamentally change the diffusion behavior, including its barrier height and diffusion path. Although we mainly demonstrate this process with Au metal impurity in bulk Si through time-dependent density functional theory simulations, we believe this could be a rather common phenomenon as it is shown that the similar phenomena also exist in Zn, Cd impurities diffusion in bulk Si, and Ti diffusion in TiO2. We believe this study can open up a new direction of inquiry for such diffusion behavior in semiconductor.

*L.W.W. was supported by the Director SC-BES-MSED-DOE under Contract No. DE-AC02-05CH11231 through the Materials Theory program (KC2301). The work in China was supported by NSFC under Grant No. 61888102.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM
GUOXIANG HU, Center for Nanophase Materials and Sciences, Oak Ridge National Laboratory, CHANDLER BENNETT, QIYANG LU, Materials Science and Technology Division, Oak Ridge National Laboratory, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory, PAUL KENT, Center for Nanophase Materials and Sciences, Oak Ridge National Laboratory, HO NYUNG LEE, JARON KROGEL, Materials Science and Technology Division, Oak Ridge National Laboratory, PANÇHAPAKEŞAN GANESH (Presenter), Center for Nanophase Materials and Sciences, Oak Ridge National Laboratory — A subclass of ABO$_x$ perovskites undergoes metal-to-insulator transitions (MITs) when n-doped either via oxygen vacancies concomitant with ordering, chemical substitution or strain. For example, the oxygen-rich perovskite SrCoO$_3$ is a ferromagnetic metal, while the oxygen-deficient brownmillerite SrCoO$_{2.5}$ is an anti-ferromagnetic insulator. The precise mechanism driving the MIT, and its relation to the electronic-structure of the metallic phase, remains unknown. Here we hypothesize that metallic ABO$_3$ that are more susceptible to a MIT via n-doping are self-hole doped negative charge transfer metals; n-doping fills these pre-existing holes and gives rise to an insulating state. Magnetism is a secondary effect that may or may not assist in the gap opening. Moreover, this tendency to remain self-hole doped determines a universal electronic response to modulations in stoichiometry/composition/pressure. In this work, we use *ab-initio* density functional theory (DFT), DFT+U, DFT+hybrid as well as many-body quantum Monte Carlo (QMC) calculations to shed light on the hypothesis, with comparison to experiments where possible.

*This work was supported by the Center for Predictive Simulation of Functional Materials, a DOE-BES center.*
Pressure-induced metal-insulator transition in degenerately doped ferroelectrics*  CHENGLIANG XIA (Presenter), YUE CHEN, The University of Hong Kong, HANGHUI CHEN, NYU-ECNU Institute of Physics, New York University Shanghai — We perform first-principles calculations to study oxygen vacancies in two important types of ferroelectric oxides (LiNbO₃ as the prototype of R3c-type ferroelectrics and BaTiO₃ as the prototype of perovskite-type ferroelectrics). Under ambient conditions, with a low concentration of oxygen vacancies, both LiNbO₃₋δ and BaTiO₃₋δ become metallic; the polar distortions are reduced in both compounds but do not disappear. However, under pressures, the polar distortions in BaTiO₃₋δ are completely suppressed and the system remains metallic with itinerant electron uniformly distributed on Ti atoms. By contrast, the polar distortions in LiNbO₃₋δ increase under pressures and above a critical pressure, the system turns into an insulating state. The increased polar displacements in LiNbO₃₋δ reduce the band width even though the overall volume decreases under pressures, which localizes the itinerant electrons onto a defect state and eventually leads to a metal-insulator transition.

*H.C. acknowledges the funding of National Natural Science Foundation of China (Grant No. 11774236) and NYU University Research Challenge Fund.

Can free charge carriers enhance polarization?*  SHUTONG LI (Presenter), TURAN BIROL, University of Minnesota — Ferroelectricity and metallicity has long been thought to be mutually exclusive because of the screening of the long range coulomb force. After the observation of ferroelectric-like transitions in metals recently, there has been a surge of interest in the study of `ferroelectric metals‘ and the stabilizing forces of structural polarization therein. Nevertheless, addition of carriers to semiconducting or insulating ferroelectrics is still usually thought to be detrimental to ferroelectricity. In this talk we show, by using first principles calculations, that ferroelectric polarization can actually be strengthened by introduction of free carriers in a series of oxide ferroelectrics. We consider introduction of carriers through electrostatic gating, which can alter the carrier concentration without changing the level of disorder.

*This work was supported by the National Science Foundation through the UMN MRSEC under DMR-1420013.
3:06PM P64.00004: Dielectric Conduction in the Post-breakdown Region Predicted Using a Charge Transport Model  YUEMING XU (Presenter), JOEL L PLAWSKY, TOH-MING LU, Rensselaer Polytechnic Institute — A Charge Transport Model was developed originally in our group to predict time-dependent dielectric breakdown (TDBB) in the back end of line (BEOL) interconnects. Both ramped voltage stress tests (RVS) and constant bias stress tests (CVS) data could be simulated with a same set of fitting parameters by the model.

To investigate what happens post-breakdown, we removed the industrially defined breakdown condition that was used to stop the simulation and with adjustments to the voltage response of both the Schottky barrier height and of the electron at the metal/dielectric interface, the model has now been extended into the post-breakdown region. The revised model can now predict the entire current vs. time history from the breakdown to ohmic behavior post-breakdown.

The linear I-V behavior agrees with the experimental observations of the current behavior of various resistive random-access memories (ReRAM) at low resistive state (LRS) after the generally required ‘Forming’, which is essentially a dielectric breakdown process. The extended charge transport model, therefore, provides a possible explanation for the ReRAM conduction mechanism at LRS by treating it as an incompressible electronic flow system.

3:18PM P64.00005: A high-throughput search of antiferroelectric perovskites.*  HUGO ARAMBERRI (Presenter), Luxembourg Inst of Science and Technology, JORGE INIGUEZ, Luxembourg Inst of Science and Technology; University of Luxembourg — Despite the perovskite family of compounds showing a plethora of polymorphs with rich ferroic behaviors, the quest for an antiferroelectric perovskite oxide with a simple displacive behavior remains fruitless (but for maybe PbZrO3). By means of first principles calculations, we carry out a high-throughput study of non-magnetic perovskites (ABO3), comparing their leading instabilities in their vibrational spectra and their known experimental polymorphs. Most remarkably, this search has allowed us to identify a family of perovskite-derivative compounds that display a rich variety of polar and non-polar polymorphs and seem promising candidates for antiferroelectric behavior.

*We acknowledge financial support from the Luxembourg National Research Fund through grant No. INTER/ANR/16/11562984/EXPAND/Kreisel.
3:30PM P64.00006: Frustrated Dipole Order Induces Noncollinear Proper Ferrielectricity in Two Dimensions*  LING-FANG LIN (Presenter), YANG ZHANG, ADRIANA MOREO, ELBIO DAGOTTO, University of Tennessee, SHUAI DONG, Southeast University — Achieving novel physical properties in two-dimensional (2D) materials should enable numerous functionalities in nanoscale devices. In recent years, interest in high-performance 2D ferroelectric materials has also grown rapidly across multiple scientific and engineering disciplines. Here, dioxydihalides MO\textsubscript{2}X\textsubscript{2} materials (where M= Mo and W; X= Cl and Br) are studied based on density functional theory calculations. For dioxydihalides MO\textsubscript{2}X\textsubscript{2} monolayers, we predict that they should display noncollinear ferrielectricity, induced by competing ferroelectric and antiferroelectric soft modes [1]. More importantly, this intrinsic noncollinearity of dipoles generates unique physical properties, such as Z\textsubscript{2}xZ\textsubscript{2} topological domains, atomic-scale dipole vortices/anti-vortices, and negative piezoelectricity. Our investigations should open the door to a new branch of 2D materials in the pursuit of intrinsically strong noncollinear ferrielectricity.


*Supported by the National Natural Science Foundation of China (Grants No. 11834002 and No. 11674055) and the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Science and Engineering Division.

3:42PM P64.00007: A room-temperature ferroelectric semimetal  PANKAJ SHARMA (Presenter), University of New South Wales; ARC Centre of Excellence in Future Low-Energy Electronics Technologies, UNSW, Sydney, NSW, Australia — Ferroelectricity has often been associated with and observed in materials that are insulating or semiconducting rather than metallic because conduction electrons in metals screen out the static internal fields arising from a long-range dipolar order. In the 1960s, Anderson and Blount proposed materials with these seemingly incompatible characteristics, i.e., metals with a polar axis termed ferroelectric metals. Since then, ferroelectric metals were merely a theoretical construct until recent experimental observations suggesting otherwise. Despite the progress, electrically switchable intrinsic electric polarization, together with the direct observation of ferroelectric domains, has not yet been realized in a bulk crystalline metal, although incomplete screening by mobile conduction charges should, in principle, be possible.

Here, we provide evidence that native metallicity and ferroelectricity coexist in bulk crystalline van der Waals WTe\textsubscript{2}. We show that, despite being a Weyl semimetal, WTe\textsubscript{2} has switchable spontaneous polarization and a natural ferroelectric domain structure at room temperature. This new class of materials has tantalizing potential for functional nanoelectronics applications.
3:54PM P64.00008: The Role of Oxide Surface Structure and Polarity in Flexoelectricity*
CHRISTOPHER MIZZI (Presenter), LAURENCE D. MARKS, Northwestern University — Interest in flexoelectricity has grown significantly over the past decade owing to its universality and importance at the nanoscale. Unlike many other oxide properties, a material's macroscopic flexoelectric response is predicted to be highly surface sensitive. This surface sensitivity has been demonstrated with first principles calculations on (100) SrTiO$_3$ bulk terminations [PRB 90, 201112(R) (2014)]. However, experimentally observed oxide surfaces often possess structural and chemical differences from the corresponding bulk material, the effects of which remain unclear in the context of flexoelectricity. Using density functional calculations, we compare the flexoelectric response of a number of low-energy (100) SrTiO$_3$ reconstructions to assess the impact of surface stoichiometry and periodicity on flexoelectricity. Additionally, we address the role of polar surfaces with calculations on (100) and (111) MgO surfaces. Our calculations on experimentally observed oxide surface structures corroborate previous work highlighting the importance of surfaces in flexoelectricity and have important implications for flexoelectric measurements and thin film growth.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, award no. DE- FG02-01ER45945.

4:06PM P64.00009: Uniqueness of the Polarization in Crystals and Nanostructures*
SHOHAM SEN (Presenter), YANG WANG, Carnegie Mellon Univ, PRADEEP SHARMA, Mechanical Engineering, University of Houston, KAUSHIK DAYAL, Carnegie Mellon Univ — Ionic crystals such as solid electrolytes and complex oxides are central to modern technologies for energy storage, sensing, actuation, and other functional applications. An important fundamental issue in the atomic and quantum scale modeling of these materials is the question of defining the macroscopic polarization. In a periodic crystal, the usual definition of the polarization as the first moment of the charge density in a unit cell is found to depend qualitatively and quantitatively on the choice of the unit cell.

We examine this issue using a rigorous approach based on the framework of two-scale convergence. By examining the continuum limit of when the lattice spacing is much smaller than the characteristic dimensions of the body, we prove that accounting for the boundaries consistently provides a route to uniquely compute electric fields and potentials despite the non-uniqueness of the polarization. Specifically, different choices of the unit cell in the interior of the body leads to correspondingly different partial unit cells at the boundary; while the interior unit cells satisfy charge neutrality, the partial cells on the boundary need not; the net effect is that these changes compensate each other.

*We thank the DOD MURI program for financial support.
4:18PM P64.00010: Multiferroic Quantum Criticality [Invited] AWADHESH NARAYAN (Presenter), Indian Institute of Science — Phase transitions are ubiquitous in nature -- water turning to steam is an everyday example. A special kind of phase transition can occur at zero temperature by changing a non-thermal control parameter. Such a quantum phase transition is the driver for exotic quantum critical physics that extends to elevated temperatures [1]. In this talk, I will begin by introducing quantum phase transitions in magnets, which have been widely explored [2]. I will next discuss, the very recently established, ferroelectric quantum critical behavior [3]. Finally, I will present the concept of multiferroic quantum criticality -- in which both magnetic and ferroelectric quantum criticality occur in the same system -- that we have recently proposed [4]. I will describe the associated experimental signatures and material systems to realize it, and highlight possible future directions.


4:54PM P64.00011: Dynamical hybrid improper ferroelectricity in incipient ferroelectric SrTiO\textsubscript{3} * MINGQIANG GU (Presenter), JAMES RONDINELLI, Northwestern University — SrTiO\textsubscript{3} (STO) has been intensively studied, in part, because of its ‘incipient’ ferroelectricity. A small perturbation, such as strain, stress, chemical variation, or surface truncation, can induce a paraelectric to ferroelectric phase transition. Recent optical pump-probe experiments found that even THz light excitations can trigger the transition in STO. The underlying mechanism for the light-mediated ferroelectricity remains controversial; explaining it is crucial for both ultrafast manipulation and control. Here, we explain this process as a form of dynamical hybrid improper ferroelectricity. The inversion symmetry is lifted by the trilinear coupling between a polar mode, a zone-center antiferrodistortive mode, and a zone-boundary in-phase rotation mode activated under THz pumping. With density functional theory calculations, we compute the free energy profiles of the coupled modes. With the fitted coupling coefficients, we estimate the time evolution of the inversion symmetry lifting and compare our model with the experimental results. Our understanding extends the scope of improper ferroelectricity, and may open a new route to manipulate inversion symmetry of other materials in the time domain.

*Supported by the U.S. DOE under Grant numbers DE-AC02-06CH11357 and DE-SC0012375.
Multiferroic Switching Dynamics in BiFeO$_3$  

ERIC PARSONNET (Presenter), YEN-LIN HUANG, University of California, Berkeley, CHIA-CHING LIN, TANAY GOSAVI, Intel Corporation, ALEXANDER QUALLS, University of California, Berkeley, IAN YOUNG, Intel Corporation, LANE WYATT MARTIN, JEFFREY BOKOR, RAMAMOORTHY RAMESH, University of California, Berkeley — With room temperature coupling between magnetic and electric degrees of freedom, BiFeO$_3$ (BFO) has attracted much attention as a leading candidate for magnetoelectric applications. There has been extensive work studying quasi-static magnetoelectric coupling in BFO, but the magnetoelectric coupling dynamics, their fundamental speed limits and intrinsic mechanisms of switching have yet to be explored. We are studying time-domain switching dynamics of the ferroelectric state as the first step in understanding magnetoelectric dynamics. Such studies are challenging, often limited by the platform on which the experiment is performed. Using short electrical pulses with rise time $\sim$100ps and pulse widths of the order of 10ns, we are able to probe the switching of the ferroelectric state on timescales much shorter than previous studies. The data reveal low-nanosecond switching, faster than any formerly reported switching times in (La)BFO. We probe the effects of chemical composition on magnetoelectric switching by studying two model systems, namely BFO and La-doped BFO. We study to what extent multiferroic switching conforms to existing models for classical ferroelectric switching and analyze deviations in the context of magnetoelectric coupling.

Multiferroic LuFeO$_3$ on GaN, Studies of Band Offsets and a Polar-Polar Interface  

JOSEPH CASAMENTO (Presenter), DARRELL SCHLOM, HUILI GRACE XING, DEBDEEP JENA, Cornell University — The ability to integrate epitaxial ferroelectrics on GaN, an established wide bandgap semiconductor platform, has been recently demonstrated [Li et al, Advanced Materials Interfaces 5, 1700921 (2018)] by pulsed laser deposition (PLD) of Pb$_x$Zr$_{1-x}$TiO$_3$. LuFeO$_3$, a room temperature ferroelectric and low temperature (~147K) multiferroic material, has been integrated with LuFe$_2$O$_4$ layers in a superlattice that demonstrated near room temperature (~281K) magnetoelectric multiferroic behavior [Mundy et al, Nature 537, 7621 (2016)]. Its hexagonal crystal symmetry makes it promising for epitaxial integration with III-nitrides. Here, we report the molecular beam epitaxy (MBE) growth, ferroelectricity, and band offsets of hexagonal LuFeO$_3$ on GaN. Piezoresponse force microscopy (PFM) results of LuFeO$_3$-n type GaN interface indicate ferroelectric switching behavior. X-ray photoelectron spectroscopy (XPS) of core levels of LuFeO$_3$-GaN interfaces was utilized to determine the valence band offset. Preliminary results indicate a valence band offset of $\sim$1.3 eV. Assuming a bandgap of $\sim$ 1 eV for LuFeO$_3$, this gives a conduction band offset of $\sim$ 1 eV. These studies highlight a potential avenue of epitaxial LuFeO$_3$-GaN based multiferroic-semiconductor heterojunctions for memory and logic applications.

Wednesday, March 4, 2020 2:30 PM - 5:06 PM

Session P65 DCMP: 2D Materials: Twisted Bilayers

Mile High Ballroom 4F - Peter Jacobse, University of California, Berkeley
Tunable correlated insulator behavior in twisted double bilayer graphene

Sergio de la Barerra (Presenter), Samuel Aronson, Yuan Cao, Daniel Rodan-Legrain, Oriol Rubies-Bigorda, Pablo Jarillo-Herrero, Raymond Ashoori, Massachusetts Institute of Technology MIT — Recent evidence for correlated physics in moire superlattice systems has motivated numerous theoretical studies and predictions relating flat bands, interactions, topology, and the underlying dependence on twist angle. In particular, twisted structures of two Bernal-stacked graphene bilayers display transport signatures of correlated insulating states at quarter- and half-filling of the superlattice bands that appear at finite displacement fields. Here, we explore the detailed evolution of these features in the electronic structure via sensitive measurements of the electronic compressibility. By varying carrier density and displacement field in a dual-gate capacitor geometry, we tune the bands into the various incompressible regimes to shed light on the possible correlations. By applying in- and out-of-plane magnetic fields, we probe the spin character and Landau level spectrum of the moire bands and comment on the correspondence to existing theoretical predictions.

This work was supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319.

Ferromagnetism and its stability from the one-magnon spectrum in twisted bilayer graphene

Yahya Alavirad (Presenter), Jay Sau, University of Maryland, College Park — We study ferromagnetism and its stability in twisted bilayer graphene. We show that in the perfectly flat band limit and at filling fractions $\pm 3/4$, the saturated ferromagnetic (spin and valley polarized) states are ideal ground state candidates in the large band-gap limit. By assuming a large enough substrate (hBN) induced sub-lattice potential, the same argument can be applied to filling fractions $\pm 1/4$. We estimate the regime of stability of the ferromagnetic phase around the chiral limit by studying the spectrum of one-magnon excitations. The instability of the ferromagnetic state is signaled by a negative magnon excitation energy. This approach allows us to deform the results of the idealized chiral model towards more realistic systems. Furthermore, we use the low energy part of the exact one-magnon spectrum to calculate the spin-stiffness of the Goldstone modes throughout the ferromagnetic phase. The value of spin-stiffness can determine the energy of charged skyrmions. We further calculate the spectrum of the gapped single valley-flip excitations. The valley-mode gap can be used to estimate the transition temperature of quantum anomalous Hall state.

This work was supported by the NSF-DMR1555135 (CAREER), JQI-NSF-PFC (PHY1430094) and the Sloan research fellowship.
2:54PM P65.00003: Recovery of massless Dirac fermions at charge neutrality in strongly interacting twisted bilayer graphene with disorder*  
ALEX THOMSON (Presenter), JASON F. ALICEA, Caltech — Stacking two graphene layers twisted by the `magic angle' generates flat energy bands, which in turn catalyzes various strongly correlated phenomena. At charge neutrality, transport measurements reveal superficially mundane semimetallicity in some samples yet robust insulation in others. We propose that the interplay between interactions and disorder admits either behavior, even when the system is strongly correlated and locally gapped. We argue that strong interactions supplemented by weak, smooth disorder stabilize a network of gapped quantum valley Hall domains with spatially varying Chern numbers determined by the disorder landscape --- even when an entirely different order is favored in the clean limit. Sufficiently small samples that realize a single domain are insulating. Conversely, multi-domain samples exhibit re-emergent massless Dirac fermions formed by gapless domain-wall modes, yielding semimetallic behavior. Our results highlight the crucial role that randomness can play in ground-state selection. We discuss experimental tests of our proposal.

*ARO, W911NF-17-1-0323; NSF, DMR-1723367; Caltech IQIM, an NSF Physics Frontiers Center w support of Moore Foundation, GBMF1250; Walter Burke Institute for Theoretical Physics; Moore Foundation's EPIQS Initiative, GBMF8682 to JA

3:06PM P65.00004: Evolution of charge modulation in twisted bilayer graphene near the magic angle*  
XINYUAN LAI (Presenter), NIKHIL TILAK, Rutgers University, New Brunswick, YUHANG JIANG, JINHAI MAO, University of Chinese Academy of Sciences, MINGYU XU, RAQUEL DE ALMEIDA RIBEIRO, PAUL C CANFIELD, Iowa State University, EVA ANDREI, Rutgers University, New Brunswick — Twisting and stacking two layers of graphene with a twist-angle near "magic angle" flattens the energy band and significantly slows down the movement of charge carriers. The resulting strong electron-electron interactions favors the emergence of novel correlated phases, including a charge ordered stripe phase\[1\]. Using STM on magic-angle twisted bilayer graphene with a gate tunable doping dependence, we study the evolution of the band structure with doping and its effect on the charge ordered state. When the flat band is empty or full it produces a pronounced STS spectroscopy peak which corresponds to a peak in the density of states. Bringing the Fermi level within the flat band we observe a correlation induced pseudogap at the Fermi energy accompanied by a spatial variation of the charge distribution that breaks the C3 symmetry. We will report on the evolution of the charge ordered phase with temperature, magnetic field and on its relation to the pseudogap.


*Work supported by DOE-FG02-99ER45742, NSF DMR 1708158
Emergent quantum phases driven by electronic interactions can manifest in materials with narrowly dispersing, i.e. “flat”, energy bands. Recently, flat bands have been realized in a variety of graphene-based heterostructures using the tuning parameters of twist angle, layer stacking and pressure, and resulting in correlated insulator and superconducting states. Here we report the experimental observation of similar correlated phenomena in twisted bilayer tungsten diselenide (tWSe$_2$), a semiconducting transition metal dichalcogenide (TMD). Unlike twisted bilayer graphene where the flat band appears only within a narrow range around a “magic angle”, we observe correlated states over a continuum of angles, spanning 4° to 5.1°. Hall measurements supported by ab initio calculations suggest that the strength of the insulator is driven by the density of states at half filling, consistent with a 2D Hubbard model in a regime of moderate interactions. At 5.1° twist, we observe evidence of superconductivity upon doping away from half filling, reaching zero resistivity around 3 K. Our results establish twisted bilayer TMDs as a model system to study interaction-driven phenomena in flat bands with dynamically tunable interactions.

Emergent quantum phases driven by electronic interactions can manifest in materials with narrowly dispersing, i.e. “flat”, energy bands. Recently, flat bands have been realized in a variety of graphene-based heterostructures using the tuning parameters of twist angle, layer stacking and pressure, and resulting in correlated insulator and superconducting states. Here we report the experimental observation of similar correlated phenomena in twisted bilayer tungsten diselenide (tWSe2), a semiconducting transition metal dichalcogenide (TMD). We observed that a Mott-like insulator appears at half band filling that can be sensitively tuned with displacement field over a continuum of angles, spanning 4° to 5.1°. We further study the system under high magnetic field. The interleaved Landau fans coming from band edge and full-filling of Moiré cell show the first observed Hofstadter butterfly pattern in TMD. The strength of correlated insulating state is modulated by magnetic field in an unusual way and the extra Landau fan coming from half-filling shows complex patterns. These exotic features allow us to study the interplay between topology, electronic correlations and magnetism in the flat band platform.
3:42PM P65.00007: Magic continuum in twisted bilayer WSe$_2$: critical phenomena and phase transitions  AUGUSTO GHIOTTO (Presenter), LEI WANG, EN-MIN SHIH, Columbia Univ, LEDE XIAN, Max Planck Institute for the Structure and Dynamics of Matter, DANIEL A RHODES, CHENG TAN, Columbia Univ, MARTIN CLAASSEN, Simons Foundation, DANTE M. KENNES, Max Planck Institute for the Structure and Dynamics of Matter, BUMHO KIM, YUSONG BAI, Columbia Univ, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, XIAOYANG ZHU, JAMES C HONE, Columbia Univ, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter, CORY DEAN, ABHAY PASUPATHY, Columbia Univ — Emergent quantum phases driven by electronic interactions can manifest in materials with narrowly dispersing, i.e. “flat”, energy bands. Recently, flat bands have been realized in a variety of graphene-based heterostructures using the tuning parameters of twist angle, layer stacking and pressure, and resulting in correlated insulator and superconducting states. Here we report the experimental observation of similar correlated phenomena in twisted bilayer tungsten diselenide (tWSe$_2$), a semiconducting transition metal dichalcogenide (TMD). Unlike twisted bilayer graphene where the flat band appears only within a narrow range around a “magic angle”, we observe correlated states over a continuum of angles, spanning 4° to 5.1°. Hall measurements supported by ab initio calculations suggest that the strength of the insulator is driven by the density of states at half filling, consistent with a 2D Hubbard model in a regime of moderate interactions. At 5.1° twist, we observe evidence of superconductivity upon doping away from half filling, reaching zero resistivity around 3 K. This talk will focus on the critical phenomena and phase transitions in this system in an attempt to convey the uniqueness of its quantum phases.

Reference: arXiV: 1910.12147

3:54PM P65.00008: Designing quantum geometry and nonlinear responses in van der Waals homostackings  HUITAO SHEN (Presenter), YANG ZHANG, SUYANG XU, LIANG FU, Massachusetts Institute of Technology — The recent discovery of magic-angle twisted bilayer graphene has attracted tremendous interest. Despite the excitement, an important open question is that whether layer stacking can enable other new dimensionalities that can be utilized to discover fundamentally new physics and functionalities. In this talk, I will show that van der Waals (vdW) homostackings can be used to very effectively design the quantum geometry and nonlinear or nonreciprocal responses of many vdW materials. Specifically, carefully designed homostackings can generate strong Berry curvature in the electronic structures of 2D materials. As a result, exotic nonlinear responses such as nonlinear Hall and circular photogalvanic effects are enabled in materials. Moreover, homostackings can turn many vdW materials, even graphene and transition metal dichalcogenides, into being ferroelectric, paving the way for realizing nonvolatile memory devices. The results are applicable to a wide range of vdW materials and therefore provide a new means to discover, control and harness emergent quantum phenomena in 2D devices.
In twisted bilayer systems, the breaking of the mono-layer Bravais lattice translation symmetry induces off-diagonal couplings between monolayer Bloch States. In an effort to model the coarse-grained couplings we establish new integral results for the two dimensional Fourier Transforms of generalized Slater-Koster hopping amplitudes, for various radial scaling functions, in the form of a series which rapidly converges over the entire parameter space.

Applied with a first-order gradient expansion of the strain fields, we evaluate this continuum model approach in relation to commensurate band structure calculations for a variety of appropriate Van-der Waals bilayer structures.

*Office of Naval Research

4:18PM P65.00010: Phonons in Twisted Transition Metal Dichalcogenide Bilayers ("Twistnonics"): Ultra-soft Phasons, and a transition from Superlubric to Pinned Phase

INDRAJIT MAITY (Presenter), MIT H. NAIK, PRABAL K MAITI, SRIRAM RAMASWAMY, HULIKAL KRISHNAMURTHY, MANISH JAIN, Indian Institute of Science - Dept of Physics — The tunability of the interlayer coupling by twisting one layer with respect to another layer of two-dimensional materials provide a unique way to manipulate phonons and related properties. We refer to this engineering of phononic properties as "Twistnonics". We study the effects of twisting on low-frequency shear (SM) and layer breathing (LBM) modes in transition metal dichalcogenide (TMD) bilayer using atomistic classical simulations. We show that these low-frequency modes are extremely sensitive to twist and can be used to infer the twist angle. We find unique “ultra-soft” phason modes (frequency ≤ 1 cm⁻¹) for any non-zero twist, corresponding to an effective translation of the moiré lattice by relative displacement of the constituent layers in a non-trivial way. Unlike the acoustic modes, the velocity of the phason modes is quite sensitive to twist angle. As twist angle decreases, (θ ≤ 3°, & ≥ 57°) the ultra-soft modes represent the acoustic modes of the “emergent” soft moiré scale lattice. Also, new high-frequency SMs appear, identical to those in stable bilayer TMD (θ = 0°/60°). Our study reveals the possibility of an intriguing θ dependent superlubric to pinning behavior and of the existence of ultra-soft modes in all two-dimensional materials.
4:30PM P65.00011: Particle-Hole Duality, Emergent Fermi Liquids and Fractional Chern Insulators in Moiré Flatbands

AHMED ABOUELKOMSAN (Presenter), Department of Physics, Stockholm University, ZHAO LIU, Zhejiang Institute of Modern Physics, Zhejiang University, EMIL BERGHOLTZ, Department of Physics, Stockholm University — We consider the core problem of Coulomb interactions within fractionally filled Moiré flat bands and demonstrate that the dual description in terms of holes, which acquire a non-trivial hole-dispersion, provides key physical intuition and enables the use of standard perturbative techniques for this strongly correlated problem. We find that the single-hole dispersion has a profound impact on the phase diagram: in experimentally relevant examples such as ABC stacked trilayer and twisted bilayer graphene aligned with boron nitride, it leads to emergent Fermi liquid states at band filling fractions down to $1/3$ and $2/3$ respectively. At even lower filling fractions, the electron density still faithfully tracks the single-hole dispersion while exhibiting distinct non-Fermi liquid behaviour. We also show that fractional Chern insulators can form in twisted bilayer graphene aligned with boron nitride at band filling $1/3$.

*This work was supported by the Swedish Research Council (VR) and the Wallenberg Academy Fellows program of the Knut and Alice Wallenberg Foundation.

4:42PM P65.00012: Valley Jahn-Teller effect in Twisted Bilayer Graphene

MATTIA ANGELI (Presenter), ERIO TOSATTI, MICHELE FABRIZIO, SISSA — The surprising insulating and superconducting states of narrow-band graphene twisted bilayers have been mostly discussed so far in terms of strong electron correlation, with little or no attention to phonons and electron-phonon effects. We found that, among the 33492 phonons of a fully relaxed $\theta=1.08^\circ$ twisted bilayer, there are few special, hard, and nearly dispersionless modes that resemble global vibrations of the moiré supercell (‘moiré phonons’). One of them, doubly degenerate at $\Gamma$, couples very strongly with the valley degrees of freedom, also doubly degenerate, realizing a so-called Exe Jahn-Teller (JT) coupling. The JT coupling lifts very efficiently all degeneracies which arise from the valley symmetry, and may lead, for an average atomic displacement as small as 0.5 mÅ, to an insulating state at charge neutrality. In addition, freezing the same phonon at a zone boundary point brings about insulating states at most integer occupancies of the four ultraflat electronic bands.

Ref:


*This research is partially funded by the European Research Council (ERC) under H2020 Advanced Grant No. 692670 “FIRSTORM”.
Electron pairing instability in magic angle twisted bilayer graphene*
MING XIE (Presenter), ALLAN MACDONALD, University of Texas at Austin — Superconductivity is one of the most intriguing properties observed recently in magic angle twisted bilayer graphene. Its origin is evidently closely tied to the nearly flat low energy bands at magic angle, which possess both spin/valley flavor symmetries and unique topological properties. The precise mechanism of pairing remains unclear however. Here we make an unbiased assessment of different pairing models, taking both Coulomb interactions and effective interactions induced by electron-phonon coupling into account. We find that it is essential to account for the screening of Coulomb interactions by remote metallic gates which increase the momentum dependence of Coulomb interactions and open the door to unconventional pairing channels. I will also comment on orbital suppression of superconductivity by an in-plane magnetic field, and on the possibility of using the magnetic-field dependence of superconductivity to identify the pairing mechanism.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award# DE-SC0019481.

Wednesday, March 4, 2020 2:30 PM - 5:30 PM

Session P70 DCMP DMP: Metals: Magnetism, Semi-metals and Topology 208 - Hans Hallen, North Carolina State University

Computing Transport Coefficients of Many-Body Hamiltonians by Equilibrium Averages*
ASSA AUERBACH (Presenter), Physics, Technion - Israel Institute of Technology, ILIA KHAIT, Physics, University of Toronto, NOGA BASHAN, Physics, Technion - Israel Institute of Technology — DC transport coefficients of most strongly interacting Hamiltonians demand insurmountable computational challenges, e.g. large system sizes, long real-time evolution, and poorly controlled analytic continuation of quantum Monte Carlo data. In contrast, continued fractions expansions and the use of our new formulas for Hall-type resistivities, require only computations of equilibrium averages. These are amenable to well controlled methods, e.g. imaginary-time quantum Monte Carlo, high temperature series, and variational wavefunctions. We review continued fractions dynamical conductivity and Hall and Thermal Hall coefficients calculations for the Bose and Fermi Hubbard models, and the disordered Heisenberg chain.

*US-Israel Binational Science Foundation grant 2016168 and the Israel Science Foundation grant 2021367.
Investigation of the universal scattering rate in PdCrO$_2$ by high energy electron irradiation*  
**ELINA ZHAKINA** (Presenter), PHILIPPA MCGUINNESS, VERONIKA SUNKO, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, MARCUS KONCZYKOWSKI, Ecole Polytechnique, Palaiseau, France, SEUNGHYUN KHIM, MARKUS KOENIG, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — PdCrO$_2$ is an extremely pure magnetic delafossite metal. It combines both possibilities for the motion of electrons in a solid: a nearly free electron metal and a Mott insulating state. The resistivity of PdCrO$_2$ exhibits a $T$-linear dependence between 150 K and 300 K. In the region of the $T$-linear resistivity, the scattering rate per kelvin is well approximated by the ratio $k_B/h$. A number of other materials reveal similar results, in spite of large differences in the microscopic origins of the scattering [1].

To investigate the universal behaviour of the scattering rate, we conducted a study of the influence of point defects on the resistivity of PdCrO$_2$, the results of which we report here. We introduced point defects to FIB microstructures of PdCrO$_2$ by irradiating them with high-energy electrons. Comparing the results with those on PdCoO$_2$, we confirm that the increase in the resistivity is dominated by defects in Pd layers. Matthiessen's rule is obeyed in the $T$-linear region, indicating that the inelastic scattering events could be considered independent from the elastic ones.


*Max Planck society. PM and VS thank EPSRC for PhD studentship funding through grant number EP/L015110/1. The irradiation was supported by EMIR network.

Quantum Paracrystalline Shear Resonances in Metals  
**JUN YONG KHOO** (Presenter), Max Planck Institute for the Physics of Complex Systems, PO-YAO CHANG, National Tsing Hua University Taiwan, FALKO PIENTKA, INTI SODEMANN, Max Planck Institute for the Physics of Complex Systems — Unlike classical fluids, a quantum fermi liquid can support a long-lived and propagating shear sound wave, reminiscent of the transverse sound in crystals, despite lacking any form of long-range crystalline order. This mode is expected to be present in moderately interacting metals where the quasiparticle mass is renormalised to be more than twice the bare mass, but, it is hard to excite and detect because it does not involve charge density fluctuations, in contrast to the conventional plasma mode. We propose two strategies to excite and probe this unconventional mode. One is the appearance of sharp dips in the AC conductance of narrow channels when the frequency matches the energy dispersion of the shear sound. Another is the coupling of the mode to charge fluctuations under weak magnetic fields, that could allow to excite it using near field techniques such as those employed to excite plasma modes in two-dimensional metals.
3:06PM P70.00004: Polarizability and magnetoplasmons for the $\alpha$-T$_3$ model* GODFREY GUMBS (Presenter), DIPENDRA DAHAL, Physics and Astronomy, Hunter college, ANTONIOS BALASSIS, Fordham University, ANDRII IUROV, Medgar Evers college, DANHONG HUANG, Kirtland Air Force Research Lab — Godfrey Gumbs, Dipendra Dahal, Antonios Balassis, Andrii Iurov, and Danhong Huang

*The dynamical polarizability is calculated at zero temperature and then employed in the dielectric function to determine the dispersion relation for magnetoplasmons for the $\alpha$-T$_3$ model. In the absence of magnetic field, the low-energy spectrum consists of a pair of a pair of Dirac cones and a dispersionless (flat) band in the K and K' valleys, i.e., two inequivalent Dirac points in the first Brillouin zone. However, the corresponding wave functions are valley-dependent. The Dirac-Weyl Hamiltonian for this structure with pseudospin S=1 is characterized by a parameter alpha which is a measure of the coupling strength between an additional atom at the center of the honeycomb lattice for the A and B atoms on the rim. We present results for a doped layer in the integer quantum-Hall regime for fixed alpha and various magnetic fields, and chosen magnetic field and different alpha in the random-phase approximation.

3:18PM P70.00005: The origin of sub-room temperature ferromagnetism in VSe$_2$ monolayer: reduced dimension and electron correlation* TAEKJUNG KIM (Presenter), SIHEON RYEE, Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), SANGKOOK CHOI, Condensed Matter Physics and Materials Science Department, Brookhaven National Laborator, MYUNG JOON HAN, Department of Physics, Korea Advanced Institute of Science and Technology (KAIST) — Recently 1T-VSe$_2$ has been reported as one of the first room-temperature two-dimensional ferromagnets. However, this conclusion remains elusive both theoretically and experimentally. In this presentation we apply LDA+DMFT (local density approximation plus dynamical mean-field theory) approach to study the magnetic properties of bulk and monolayer VSe$_2$. Our results indicate that bulk 1T-VSe$_2$ is a paramagnetic material as well-known but the monolayer is ferromagnetically ordered. The calculated Curie temperature is ~250K. From the detailed analysis on the electronic structure and the local spin susceptibility, we attribute the formation of local moment and the monolayer ferromagnetism to the concerted effect of quasiparticle pre-localization caused by reduced dimensionality and the electronic correlation. Further analysis shows that this ferromagnetism is vulnerable to the formation of interlayer interaction or extra charge doping, which provides the useful insight to understand the controversial experiments.

*BK21plus program, Basic Science Research Program (2018R1A2B2005204), Creative Materials Discovery Program through NRF (2018M3D1A1058754) and the U.S Department of Energy, Office of Science, Basic Energy Sciences as a part of the Computational MaterialsScience Program.
3:30PM P70.00006: Modulation of magnetism across the van der Waals interfaces

HIDEKI MATSUOKA, MOHAMMAD SAEED BAHRAMY, YUE WANG, SATOSHI YOSHIDA, KYOKO ISHIZAKA, YOSHIHIRO IWASA, MASAKI NAKANO (Presenter), Univ of Tokyo — A van der Waals (vdW) heterostructure provides an indispensable material platform in modern condensed-matter researches. There, weak interlayer bonding nature ensures formation of an atomically-abrupt heterointerface beyond fundamental constraint imposed by lattice matching condition, while strong electronic coupling enables creation of an emergent electronic ground state that is missing in individual materials. Here we fabricated vdW heterostructures by molecular-beam epitaxy, where a new type of 2D magnet, vanadium selenide epitaxial thin film\(^1\), was incorporated. In the presentation, we will show transport properties of those magnetic heterostructures, and discuss the interface proximity effect on 2D magnetism. [1] M. Nakano et al, Intrinsic 2D ferromagnetism in V\(_5\)Se\(_8\) epitaxial thin films. arXiv:1910.01959.

*This work was supported by Grants-in-Aid for Scientific Research (Grant Nos. 19H05602, 19H02593, and 19H00653) and A3 Foresight Program from the Japan Society for the Promotion of Science.

3:42PM P70.00007: High-Temperature Ferromagnetic Resonance in FePt Thin Films

CHUANPU LIU (Presenter), Colorado State University, KUMAR SRINIVASAN, ANTONY AJAN, Western Digital Corporation, ETHAN MCCOLLUM, MINGZHONG WU, Colorado State University — Understanding of damping processes in ferromagnetic thin films at temperatures (T) near the Curie temperature (T\(_c\)) has significant implications for heat-assisted magnetic recording and magnetic sensors operating at elevated temperatures. Recent ferromagnetic resonance (FMR) studies [PR Applied 10, 054046 (2018)] using out-of-plane fields showed that there are two major relaxation processes in granular L1\(_0\)-odered FePt thin films at 10-45 K below T\(_c\); two-magnon scattering and spin-flip magnon-electron scattering; with a decrease in T, the FMR linewidth increases due to the enhancement of the two-magnon scattering. This presentation reports high-T FMR studies on continuous FePt thin films with cubic structures, rather than L1\(_0\) structures. The films are 6-nm thick and have T\(_c\)≈680 K; the FMR measurements were performed over 300-620 K in out-of-plane fields. As opposed to the L1\(_0\) FePt films, the cubic FePt films show an FMR linewidth that decreases with a decrease in T. This T dependence suggests that the spin-flip magnon-electron scattering is dominant over the two-magnon scattering; the two-magnon scattering is weak because it is expected to be absent in continuous films under out-of-plane fields.
3:54PM P70.00008: Structure and Magnetism of New Metastable Fe₈Co₈N₂ Compound*

BALAMURUGAN BALASUBRAMANIAN, RABINDRA PAHARI, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, SHAH VALLOPPILLY, XINGZHONG LI, Nebraska Center for Materials and Nanoscience, University of Nebraska, RALPH SKOMSKI, XIAOSHAN XU, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, DAVID SELLMYER (Presenter), Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska — Recently, the discovery of new magnetic materials with high magnetocrystalline anisotropy $K_1$, large saturation magnetic polarization $J_s$, and high Curie Temperature $T_c$ has been accelerated by efficient computational and non-equilibrium fabrication methods [1-4]. Guided by theoretical predictions [4], we have produced a new Fe₈Co₈N₂ compound in the form of nanoparticles using a cluster-deposition method and characterized it by XRD, XPS, STEM, EDS and magnetometry measurements. The nanoparticles have a stoichiometry of about Fe₈Co₈N₂ and exhibit a uniform elemental distribution of Fe, Co and N. A Rietveld refinement of XRD data shows that the new compound crystallizes in a tetragonal structure [space group I4/m (87), $a = 6.188$ Å and $c = 5.669$ Å]. Fe₈Co₈N₂ exhibits appreciable magnetic properties, $K_1 = 16$ Mergs/cm³, $J_s = 17.6$ kG, and $T_c = 650$ K, which are promising for a wide range of applications including information and energy processing.

References

*This research is supported by the NSF-DMREF: SusChEM (1729288), NSF-NNCI (1542182), and NCMN-NRI
4:06PM P70.00009: Topology on a new facet of bismuth*  HSIN LIN (Presenter), Academia Sinica, CHUANG-HAN HSU, National University of Singapore, XIAOTING ZHOU, TAY-RONG CHANG, National Cheng Kung University, QIONG MA, NUH GEDIK, Massachusetts Institute of Technology, ARUN BANSIL, Northeastern University, SUYANG XU, LIANG FU, Massachusetts Institute of Technology — Bismuth-based materials have been instrumental in the development of topological physics, even though bulk bismuth itself has been long thought to be topologically trivial. A recent study has, however, shown that bismuth is in fact a higher-order topological insulator featuring one-dimensional (1D) topological hinge states protected by three-fold rotational and inversion symmetries. In this talk, we uncover another hidden facet of the band topology of bismuth by showing that bismuth is also a first-order topological crystalline insulator protected by a two-fold rotational symmetry. As a result, its (1\(\bar{1}0\)) surface exhibits a pair of gapless Dirac surface states. Remarkably, these surface Dirac cones are unpinned in the sense that they are not restricted to locate at specific \(k\) points in the (1\(\bar{1}0\)) surface Brillouin zone. These unpinned 2D Dirac surface states could be probed directly via various spectroscopic techniques. Our analysis also reveals the presence of a distinct, previously uncharacterized set of 1D topological hinge states protected by the two-fold rotational symmetry. Our study thus provides a comprehensive understanding of the topological band structure of bismuth.

*Support by Academia Sinica and MOST in Taiwan and USDOE and NSF is acknowledged.

4:18PM P70.00010: The relation between ferromagnetism and structure in half-metallic transition metal oxides*  MOHAMMAD SAGHAYEZHIAN (Presenter), ZHEN WANG, HANGWEN GUO, RONGYING JIN, Louisiana State University, Baton Rouge, YIMEI ZHU, Brookhaven National Lab, JIANDI ZHANG, E WARD PLUMMER, Louisiana State University, Baton Rouge — Interface-driven magnetic properties such as exchange bias and inverted hysteresis are highly sought after in modern functional materials, where at least two magnetically active layers are required. Ability to achieve these functionalities in a single layer thin film (monolithic) reduces the dimensionality while enriching the magnetism. Here we uncover a previously unseen part of the phase diagram of a monolithic epitaxial thin film of \(\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3\) on \(\text{SrTiO}_3\) which exhibits inverted hysteresis, spontaneous magnetic reversal and exchange bias due to a structural gradient in oxygen octahedral network. We have mapped the phase diagram of this material and discovered that at a specific oxygen pressure and above a critical thickness, a complex magnetic behavior appears. Atomic-scale characterization shows that this peculiar magnetism is closely linked to continuous structural gradient that creates three distinct regions within the film, each with a different magnetism onset. Extracting oxygen octahedral geometry by electron microscopy, we found that the Curie temperature is directly correlated with the bond angle. This study illustrates the importance of octahedral geometry in the magnetic properties of the materials.

*US Department of Energy (DOE) under Grant No. DOE DE-SC0002136
**4:30PM P70.00011: Anomalous suppression of higher-order nonlinearities in 3D Dirac semimetals**  
JEREMY LIM (Presenter), YEE SIN ANG, LAY KEE ANG, Science and Math cluster, Singapore University of Technology and Design, LIANG JIE WONG, School of Electrical and Electronic Engineering, Nanyang Technological University — Three dimensional Dirac semimetals are often thought to share the same essential physics as 2D Dirac materials. Here, we present a counter-intuitive feature of 3D Dirac semimetals that sets them apart from their 2D counterparts: the absence of field-induced intraband nonlinearities beyond the third order at zero temperature at or near a critical field strength. Our closed-form intraband current expressions show that this effect is robust against changes in incident field polarization and phase, and remains significant at finite temperatures. Our theory is in excellent agreement with nonperturbative numerical simulations of the field-induced electron dynamics. Additionally, we identify regimes where 3D Dirac semimetals effectively function as bulk versions of 2D Dirac semimetals with the potential for superior performance in terms of high-harmonic generation. Our work fills a vital gap in understanding the nonlinear response of bulk Dirac electrons, and paves the way for the development of chip-integrable, nanophotonic devices and optoelectronics based on Dirac materials.

**4:42PM P70.00012: Topological Semimetal in a Chiral Crystal with Large Chern Numbers, Multifold Band Crossings, and Long Fermi-arcs**  
MAIA G VERGNIORY (Presenter), Donostia International Physics Center — Topological semimetals (TSs) in structurally chiral crystals (which possess a handedness due to a lack of mirror and inversion symmetries) are expected to display numerous exotic physical phenomena, such as new fermionic excitations with large topological charge, long Fermi-arc surface states, unusual magnetotransport and lattice dynamics, as well as a quantized response to circularly polarized light. Despite multiple recent photoemission studies of predicted material candidates, this maximal Chern number, measured by counting the number of Fermi-arcs, has not yet been observed experimentally. Using angle-resolved photoelectron spectroscopy and ab-initio calculations, here we show that the chiral topological semimetal candidate PdGa displays the required multifold nodes, which are connected by long surface Fermi-arcs. Due to large spin-orbit coupling and the high crystallinity of our sample surfaces, we are for the first time able to resolve 4 independent Fermi-arcs, proving experimentally that the observed multifold nodes – which are a generic feature of many chiral metals – display the maximal Chern number magnitude of 4.

****See continuation in Special Instructions.........
4:54PM P70.00013: Polar and Phase Domain Walls in Weyl Semimetallic MoTe$_2$: New Paradigm for Topological Interfacial States* FEI-TING HUANG, SEONG JOON LIM, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, SOBHIT SINGH, JINWOONG KIM, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, LUNYONG ZHANG, Laboratory for Pohang Emergent Materials and Max Plank POSTECH Center for Complex Phase Materials, Pohang University of Science and Technology, Pohang 37673, Republic of Korea, JAEOOK KIM, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, M.-W CHU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 106, Taiwan, China, KARIN M RABE, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, SANG-WOOK CHEONG (Presenter), Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — Much of the dramatic growth in research on topological materials has focused on topologically protected surface states. While the domain walls of topological materials such as Weyl semimetals with broken inversion or time-reversal symmetry can provide a new paradigm for exploring topological interfacial states, such investigations have received little attention to date. Utilizing in-situ cryogenic transmission electron microscopy combined with first-principles calculations, we discover intriguing domain-wall structures in MoTe$_2$, both between polar variants of the low-temperature(T) Weyl phase, and between this and the high-T higher-order topological phase. We demonstrate how polar domain walls can be manipulated with electron beams, and show that phase domain walls tend to form superlattice-like structures along the c axis. Scanning tunneling microscopy indicates a possible signature of a conducting hinge state at phase domain walls. Our results open new avenues for investigating topological interfacial states and unveiling multifunctional aspects of domain walls in topological materials.

*The work at Rutgers University was supported by the NSF under Grant No. DMR-1629059.

5:06PM P70.00014: Giant extrinsic anomalous Hall effect in the Kagome, Dirac Antimonide KV$_3$Sb$_5$ YAOJIA WANG (Presenter), Max planck institute of Microstructure physics — The electronic anomalous Hall effect (AHE), where charge carriers acquire a velocity component orthogonal to an applied electric field, is one of the most fundamental and widely studied phenomena in physics. There are several different AHE mechanisms known falling into intrinsic and extrinsic regimes. The skew scattering mechanism (extrinsic) applies to high conductivity materials and has traditionally focused on ferromagnetic metals. Here we report the observation of a giant extrinsic AHE in KV$_3$Sb$_5$, an exfoliable Dirac semimetal with a spin 1/2 Kagome layer of Vanadium atoms. Our exfoliated flake devices reach low resistivity $\sim$1.6 $\mu\Omega$ cm at low temperature and even though KV$_3$Sb$_5$ shows no magnetic ordering down to 0.25 K, the anomalous Hall conductivity (AHC) reaches $\sim$10000 $\Omega^{-1}$cm$^{-1}$ with a skew constant of 0.013, nearly an order of magnitude larger than Fe. Surprisingly, the AHE scales with the square of the longitudinal conductivity, defying expectations from skew scattering theory. This observation invites a wider variety of materials to be investigated for giant anomalous AHE including metallic magnetically frustrated materials and cluster magnets as well as posing new fundamental questions about high conductivity AHE mechanisms.
Quantum squeezing and coherence of magnons detected by spin transport

WOLFGANG BELZIG (Presenter), Univ Konstanz, AKASHDEEP KAMRA, Department of Physics, NTNU, QuSpin — We predict the emergence of novel magnetic quasiparticles, mediated by magnetic dipolar interactions, even for a uniform ground states. These quasiparticles exhibit a spin ranging from zero to above 1 [1]. Of particular interest is our finding that the eigenmodes in an easy-axis antiferromagnet are spin-zero quasiparticles instead of the widely believed spin-1 magnons [2]. These unusual properties originate from a competition between quantum mechanical squeezing (increasing the spin) and hybridization (decreasing the spin). We show that spin-current noise measurement can reveal this fundamental quantum phenomenon [1] in full analogy to the effective charge known from shot noise measurements. Antiferromagnetic magnons are shown to exhibit giant antanglement, which might be used as quantum battery [3]. Finally, we show that by adding two normal metal spin current detectors, the magnon coherence can be tested by measuring the cross correlations [4] in analogy to the well-known second-order coherence.


Wednesday, March 4, 2020 4:00 PM - 5:00 PM

Session Q01 APS: LGBTQ+ Roundtable  Hyatt Centennial B - Tag(s): Diversity, Undergrad Friendly

4:00PM Q01.00001: LGBTQ+ Roundtable — The LGBT+Physicists group welcomes all interested attendees to participate in a roundtable discussion on improving the professional and educational climate within physics with particular attention to those who identify as gender and sexual minorities (LGBTQQIAAP +).

Wednesday, March 4, 2020 5:00 PM - 6:00 PM

Session Q02 APS: NSBP Meetup  Hyatt Mineral D - Tag(s): Diversity, Undergrad Friendly

5:00PM Q02.00001: NSBP Meetup — The National Society of Black Physicists (NSBP) meetup will provide opportunities for NSBP members and those interested in the work of the societies to gather, network, and learn about NSBP initiatives. All are welcome. Students and postdoctoral researchers are especially encouraged to attend.

Wednesday, March 4, 2020 5:30 PM - 6:30 PM
Session Q28 FIAP: FIAP Business Meeting (5:30pm-6:30pm) 405-407 - Tag(s): Industry

5:30PM Q28.00001: FIAP Business Meeting (5:30pm-6:30pm) —

Wednesday, March 4, 2020 5:45 PM - 6:45 PM

Session Q03 APS: GSCCM Business Meeting (5:45pm - 6:45pm) 107

5:45PM Q03.00001: GSCCM Business Meeting (5:45pm-6:45pm) —

Wednesday, March 4, 2020 5:45 PM - 6:45 PM

Session Q10 GIMS: GIMS Business Meeting (5:45pm-6:45pm) 108

5:45PM Q10.00001: GIMS Business Meeting (5:45pm-6:45pm) —

Wednesday, March 4, 2020 5:45 PM - 6:30 PM

Session Q11 APS: March Meeting Task Force Town Hall 104

5:45PM Q11.00001: March Meeting Task Force Town Hall —

Wednesday, March 4, 2020 5:45 PM - 7:15 PM

Session Q12 APS: Scholarly Metrics in Research Assessment 201

5:45PM Q12.00001: Scholarly Metrics in Research Assessment — Scholarly metrics play a significant role in the way scientists and their research are assessed for funding, hiring, and promotion. The APS editors will host a special session in which three panelists with experience in university administration, bibliometrics research, computational social science, and science policy will present their perspectives on scholarly metrics and research assessment.

Wednesday, March 4, 2020 5:45 PM - 6:45 PM

Session Q15 GDS: GDS Business Meeting (5:45pm - 6:45) 706

5:45PM Q15.00001: GDS Business Meeting (5:45pm - 6:45pm) —

Wednesday, March 4, 2020 5:45 PM - 6:45 PM
Session Q31 DSOFT: DSOFT Business Meeting (5:45pm-6:45pm) 503

5:45PM Q31.00001: DSOFT Business Meeting (5:45pm-6:45pm) —

Wednesday, March 4, 2020 6:00 PM - 7:00 PM

Session Q32 APS: NSHP Meetup Hyatt Mineral E - Tag(s): Diversity, Undergrad Friendly

6:00PM Q32.00001: NSHP Meetup — The National Society of Hispanic Physicists (NSHP) meetup will provide opportunities for NSHP members and those interested in the work of the societies to gather, network, and learn about NSHP initiatives. All are welcome. Students and postdoctoral researchers are especially encouraged to attend.

Wednesday, March 4, 2020 6:30 PM - 8:00 PM

Session Q37 APS: 50 Years of Physical Review A-D: Enduring Discoveries. Tomorrow's Advances. 405/407 - Sarma Kancharla, American Physical Society - Tag(s): Undergrad Friendly

6:30PM Q37.00001: 50 Years of Physical Review A-D: Enduring Discoveries. Tomorrow's Advances. — In a special session celebrating 50 years of Physical Review A, B, C, and D, hear these widely cited and read Physical Review authors speak about both their personal experiences with PRA and PRB, and an overview of the scientific fields they have been working in.

Speakers: Sankar Das Sarma, University of Maryland; Immanuel Bloch, Max-Planck, Garching and LMU, Munich; Giulia Galli, University of Chicago

Wednesday, March 4, 2020 7:00 PM - 8:30 PM

Session Q33 APS: Diversity Reception (7:00pm - 8:30pm) Hyatt Centennial C - Tag(s): Diversity, Undergrad Friendly

7:00PM Q33.00001: Diversity Reception (7:00pm - 8:30pm) — Join us for an opportunity to learn about current diversity efforts spearheaded by the APS, the Committee on Minorities (COM), the Committee on the Status of Women in Physics (CSWP), and the LGBT+ physicists group. Students are also encouraged to attend to meet with representatives from Google about career opportunities at their company. Light refreshments will be served.

Co-sponsored by Google and the APS Forum on Education (FEd)

Wednesday, March 4, 2020 7:30 PM - 8:30 PM
Session Q34 APS: Thing Explain your Research Friendly

7:30PM Q34.00001: Thing Explain your Research

Wednesday, March 4, 2020 8:00 PM - 9:30 PM

Session Q35 APS: Staged Reading of the Play: Einstein's Wife Hyatt Centennial
FG - Tag(s): Outreach, Undergrad Friendly

8:00PM Q35.00001: Staged Reading of the Play: Einstein's Wife [Invited] — Sponsored by the Forum on the History of Physics
This new play Einstein’s Wife by the playwright scientist-historian David C. Cassidy is based on the true story of the courtship, marriage, and ultimately separation of Albert Einstein and his first wife Mileva Maric. Mileva confronts the challenges of disability and discrimination, love, fate, and marriage to Albert Einstein.
In the late 1800s, Mileva Maric, a young Serbian woman facing the exclusion of women from higher education in much of Europe, travels to Zurich, Switzerland where she meets another first-year physics student, Albert Einstein. Mileva and Albert soon fall in love and eventually marry, a romance and marriage spanning Albert’s ascent to the top of his profession by the eve of World War I. But fate is unkind to Mileva, challenging her love and career and bringing upon the lovers both triumph and tragedy. Based on actual events, letters, and poems. The play Einstein’s Wife was written and developed by David C. Cassidy in collaboration with Break A Leg Productions, NY and its artistic director, Teri Black. The play director is Susan Lyles, Artistic Director and Founder of the And Toto too Theatre Company. Some of the play’s actors as well the playwright will be available for a talkback discussion after the play reading.
Produced by Brian Schwartz, CUNY and Smitha Vishveshwara, University of Illinois, Urbana-Champaign. Co-Sponsored by: the Forum on Outreach and Engaging the Public, the Forum on Physics and Society, the Forum on Education, the Topical Group on Physics Education Research, the Committee on the Status of Women in Physics, the Division of Materials Physics, and the Division of Condensed Matter Physics.

Wednesday, March 4, 2020 8:00 PM - 9:00 PM

Session Q38 APS: Mental Health Roundtable
202 - Tag(s): Diversity, Undergrad Friendly

8:00PM Q38.00001: Mental Health Roundtable — This event is for those who identify as neurodivergent, having a mental illness, or dealing with mental health issues to meet others and to discuss challenges they face, resources they use, and ways to improve the community.

Wednesday, March 4, 2020 9:15 PM - 10:45 PM
Session Q36 APS: Rock-n-Roll Sing-a-long/Listen-a-long  Four Seasons 4 - Tag(s): Outreach, Undergrad Friendly

9:15PM Q36.00001: Rock-n-Roll Sing-a-long/Listen-a-long  —

Thursday, March 5, 2020 8:00 AM - 10:36 AM

Session R01 DAMOP DCMP: Topological States in AMO Systems II  103 -
Tag(s): Focus

8:00AM R01.00001: Non-Hermitian topological photonics and light steering* [Invited] LIANG FENG (Presenter), HAN ZHAO, XINGDU QIAO, TIANWEI WU, BIKASHKALI MIDYA, University of Pennsylvania, STEFANO LONGHI, Physics, Politecnico di Milano — Photonic topological insulators provide a route for disorder-immune light transport, which holds promise for practical applications. Flexible reconfiguration of topological light pathways can enable high-density photonics routing, thus sustaining the growing demand for data capacity. By strategically interfacing non-Hermitian and topological physics, we demonstrate arbitrary, robust light steering in reconfigurable non-Hermitian junctions, in which chiral topological states can propagate at an interface of the gain and loss domains. Our non-Hermitian–controlled topological state can enable the dynamic control of robust transmission links of light inside the bulk, fully using the entire footprint of a photonic topological insulator.

*ARO and NSF

8:36AM R01.00002: Floquet engineering with resonant drive and Application to symmetry-protected topological phases  KAORU MIZUTA (Presenter), Kyoto University, KAZUAKI TAKASAN, University of California, Berkeley, NORIO KAWAKAMI, Kyoto University — Recently periodically driven (Floquet) systems have attracted much interested, and Floquet engineering, control of phases by a periodic drive, is one of the most vigorous fields in Floquet systems. However, in conventional Floquet engineering, only high-frequency drives (=drives whose energy scale is much smaller than the frequency) are mainly utilized since it is based on high-frequency expansion theory, only applicable to Floquet systems under high-frequency drives. Therefore, we extend the conventional high-frequency expansion theory to the cases in the presence of resonant drives (= drives whose local energy scale is comparable to the frequency) and propose a new scheme of Floquet engineering done by high-frequency and resonant drives [1]. We clarify that the effective Hamiltonian describing long-time dynamics acquires an emergent $Z_N$ symmetry, and hence our scheme enables us to simultaneously control phases and add a symmetry to the system. With our Floquet engineering, we also propose a way to realize/control topological phases protected by a $Z_2 \times Z_2$ symmetry only in the presence of a $Z_2$ symmetry [2].

[References]
In my talk I will present a definition of topological invariants for driven dissipative lattices that relies on the singular value decomposition of non-Hermitian coupling matrices, $H$, or, equivalently, on the eigenstates of an effective Hamiltonian, $H_{\text{eff}} = \sigma^+ H + H^\dagger \sigma^-$. I will show that topological non-trivial phases of $H_{\text{eff}}$ correspond to steady-states in which the driven dissipative lattice behaves as a directional amplifier. Thus, our work leads to a connection between topological band theory and amplification in photonic lattices, which also leads to a physically motivated classification of topological phases non-Hermitian lattices. I will briefly sketch an implementation of our ideas with periodically driven superconducting circuits.


*I acknowledge support from Spanish project PGC2018-094792-B-100 (MCIU/AEI/FEDER, EU)
Quantum quench is nonequilibrium dynamics and its interplay with band topology gives rise to intriguing dynamical topological phenomena. We introduce the concept of loop unitary

\[ U_l \]

and its homotopy invariant

\[ W_3 \]

to fully characterize the quench dynamics of arbitrary two-band insulators in two dimensions, going beyond existing scheme based on Hopf invariant which is only valid for trivial initial states. The theory traces the origin of nontrivial dynamical topology to the emergence of

\[ \pi \]

-defects in the phase band of

\[ U_l \]

, and establishes that

\[ W_3 = C_f - C_i \]

, i.e. the Chern number change across the quench. We further show that the dynamical singularity is also encoded in the winding of the eigenvectors of

\[ U_l \]

along a lower dimensional curve where dynamical quantum phase transition occurs, if the pre- or post-quench Hamiltonian is trivial. The winding along this curve is related to the Hopf link, and shown to give rise to torus links and knots for quench to Hamiltonians with Dirac points. Our framework which can be generalized to multiband systems and other dimensions paves the way to study quench dynamics and its associated topology.

*This work is supported by AFOSR Grant No. FA9550-16-1-0006 and NSF Grant No. PHY-1707484.
9:12AM R01.00005: Quantum many-body scars from virtual entangled pairs*  SAMBUDDHA CHATTOPADHYAY (Presenter), Harvard University, HANNES PICHLER, California Institute of Technology, MIKHAIL LUKIN, WEN WEI HO, Harvard University — We study weak ergodicity breaking in a one-dimensional, non-integrable spin-1 XY model. We construct for it an exact highly excited eigenstate, which despite having a non-zero energy density, can be represented analytically by a finite bond-dimension matrix product state (MPS) with area-law entanglement. Upon a quench to a finite Zeeman field, the state undergoes periodic dynamics with perfect many-body revivals, in stark contrast to other generic initial states which instead rapidly thermalize. Remarkably, we find that the dynamics can be completely understood in terms of the evolution of entangled virtual spin-1/2 degrees of freedom, which in turn underpin the presence of an O(L) tower of strong-eigenstate thermalization hypothesis (ETH)-violating many-body eigenstates: quantum many-body scars. The scars we find are therefore of novel origin, and we provide insight into their nature and entanglement structure.

*Supported by the National Science Foundation (NSF), the Center for Ultracold Atoms, DOE., Office of Naval Research and the Vannevar Bush Fellowship, Herschel Smith Fellowship, Jacob Wendell Prize, the NSF through a grant for ITAMP and by the Gordon and Betty Moore Foundation’s EPiQS Initiative’s Grants GBMF8682 and GBMF4306 and NUS Development Grant AY2019/2020.

9:24AM R01.00006: Haldane Phase in Spin-1 Bose-Hubbard Model with Flat Band*  HONG YANG (Presenter), HAYATE NAKANO, HOSHO KATSURA, Univ of Tokyo — The Haldane phase has been widely discussed in spin chains. A famous rigorous example is the AKLT model. However, in itinerant spin systems which have both unfrozen spin and charge degrees of freedom, the Haldane phase has been rarely investigated, to say nothing of any rigorous results. Here we study the spin-1 Bose-Hubbard model on a sawtooth lattice with flat band. At half-unit filling with fine-tuned interaction strength, we prove that the ground state can be exactly written down in the form of a matrix product state (MPS) similar to that of the AKLT model. The ground state correlation lengths, edge states, string order parameters, etc. are analytically given for both spin and charge degrees of freedom. The entanglement spectrum also analytically shows perfect two-fold degeneracy. Moreover, with general interaction strength, when a parameter (related to hopping and on-site potential of the lattice) is sufficiently large, perturbation theory yields the spin-1 bilinear-biquadratic model as the effective spin model, which can be either symmetry-protected-topological (Haldane) or trivial, depending on the interaction strength.

*JSPS Grant-in-Aid for Scientific Research on Innovative Areas: No. JP18H04478 and JSPS KAKENHI Grant No. JP18K03445 (H.K.)
Detecting fractional Chern insulators in optical lattices through quantized displacement

ILYOUN NA (Presenter), Physics, University of California, Berkeley, JOHANNES MOTRUK, Lawrence Berkeley National Laboratory — The realization of interacting topological states of matter such as fractional Chern insulators (FCIs) in optical lattices with synthetic gauge fields has recently come within experimental reach. However, detecting their occurrence might prove difficult since transport measurements akin to those in solid state systems are challenging to perform in cold atom setups and alternatives have to be found. We consider a $\nu = 1/2$ FCI state realized in the lowest band of a Harper-Hofstadter model of hardcore bosons in a harmonic trapping potential. We demonstrate the stability of the topological state for a wide range of confining strengths by density matrix renormalization group simulations. Using matrix-product state algorithms, we study the time evolution when applying an effective electric field for the particles on top of the harmonic confinement. The movement of the particle cloud allows an accurate determination of the fractionally quantized Hall conductivity which provides an experimentally measurable signal to detect the topological nature of the state. Below a critical field strength, the particle displacement shows oscillations around the quantized value which abate as the field strength decreases.

Robustness of quantum scarred states to the presence of disorder and external drives

IAN MONDRAGON-SHEM (Presenter), Argonne National Laboratory, MAXIM G VAVILOV, Department of Physics, University of Wisconsin - Madison, IVAR MARTIN, Argonne National Laboratory — Recent experiments in Rydberg atom quantum simulators have found unexpected coherent and persistent oscillations in an ergodic system at infinite temperature. The origin of such oscillations has been explained in terms of quantum scarred states that are embedded in an ergodic spectrum. We examine the robustness of such quantum scarred states to the presence of inhomogeneous potentials as well as the action of external drives. We focus on models that exhibit approximate SU(2) symmetries, such as the PXP model, and explore conditions under which the dynamics of the system remains non-ergodic. To do this, we evaluate diagnostic quantities such as the revival probability, the spatial entanglement, and the average spin dynamics. Finally, we discuss similarities with the disordered Heisenberg spin chain in a regime in which anomalous non-ergodic dynamics can also be obtained.
10:00AM R01.00009: Topological effects in interacting Su-Schrieffer-Heeger chains  HELENA DRUEEKE (Presenter), DIETER BAUER, University of Rostock, Germany — The Su-Schrieffer-Heeger (SSH) model [1] describes a linear chain with two distinct topological phases. We investigate the behavior of two interacting particles in this one-dimensional system by simulating the equivalent system of a single particle in a two-dimensional system. Even though the two particles repel each other, doublon states, where both particles are on the same lattice site, are possible. By performing time-dependent simulations, we investigate transitions between the two topological phases of the two-dimensional SSH-like system. We focus on the doublon and surface states and the relation between them.

Optical waveguides are a possible experimental realization of such two-dimensional systems [2]. Realizing energetically separated surface and doublon states would allow the routing of light along specific paths within a bundle of waveguides. This could lead to increased bandwidth for fiber-optic communications.


10:12AM R01.00010: Topological photonic resonator for chiral quantum optics*  SABYASACHI BARIK (Presenter), AZIZ KARASAHIN, SUNIL MITTAL, EDO WAKS, MOHAMMAD HAFEZI, University of Maryland, College Park — Topological photonics has enabled unprecedented applications in the field of optics. The resulting topological structures exhibit chiral edge states that are robust to disorder and sharp bends. By coupling these photonic states to quantum emitters, one can generate directional light emission. Even though the previous works have investigated directional light emission in one-dimensional edge states, the extension of this concept to resonator structures has remained elusive. Here we demonstrate chiral light-matter interactions in a topological resonator. We use valley-Hall topological edge states to realize a helical resonator. Such a helical resonator is created at the interface of two distinct topological regions that supports two counter-propagating light modes with opposite polarizations. We show the chiral coupling of the resonator to a quantum emitter. Moreover, we achieve an intensity enhancement of 3.4 due to resonant coupling. Such robust resonators could provide a platform for studying novel many-body dynamics and designing complex nano-photonic circuits.

*This work is supported by NSF 1820938, 1430094 Physics Frontier Center at the Joint Quantum Institute and the Air Force Office of Scientific Research–Multidisciplinary University Research Initiative FA9550-16-1-0323).
R01.00011: Effective field theories at the edges of topological insulators  MANUEL VALIENTE (Presenter), XIN CHEN, Tsinghua University — We consider interacting two-dimensional time reversal invariant topological insulators with time reversal preserving (non-magnetic) disorder near their edges. These systems are known to fail to exhibit quantized spin currents even when the fermion-fermion interactions are weak, as was recently shown within Hartree-Fock theory (Novelli et al., Phys. Rev. Lett. 122, 016601). Here, we investigate the microscopic origin of the lack of quantization by considering the most relevant few-body processes at the edges of the system, and find that fermion-impurity resonances are responsible for backscattering. We build two different effective field theories for the interacting edge modes in the system near the Fermi energy that eliminate the bulk in two different ways: 1) by keeping the inhomogeneity explicitly and 2) by accounting for the width of the resonance in the dispersion relations.

10:24AM R01.00012: Dynamical Quantum Phase Transitions in U(1) Quantum Link Models in (1+1)d and (2+1)d*  YI-PING HUANG (Presenter), DEBASISH BANERJEE, MARKUS HEYL, the Max Planck Institute for the Physics of Complex Systems — Quantum link models (QLMs) are extensions of Wilson-type lattice gauge theories which realize exact gauge invariance with finite-dimensional Hilbert spaces. QLMs not only reproduce standard features of Wilson lattice gauge theories in equilibrium, but can also host new phenomena such as crystalline confined phases. The local constraints due to gauge invariance also provide kinetic restrictions that can influence substantially the real-time dynamics in these systems. We aim to characterize the nonequilibrium evolution in lattice gauge theories through the lens of dynamical quantum phase transitions, which provide general principles for real-time dynamics in quantum many-body systems. Specifically, we study quantum quenches for two representative cases, U(1) QLMs in (1+1)D and (2+1)D, for initial conditions exhibiting long-range order. Finally, we discuss the connection to the high-energy perspective and the experimental feasibility to observe the discussed phenomena in recent quantum simulator settings such as trapped ions, ultracold atoms, and Rydberg atoms.

* M. H. acknowledges support by the Deutsche Forschungsgemeinschaft via the Gottfried Wilhelm Leibniz Prize program.
**8:00AM R02.00001: Experimental and numerical studies on phase change under dynamic loadings: application to Tin.** [Invited] CAMILLE CHAUVIN (Presenter), Commissariat à l'énergie atomique et aux énergies alternatives — Polymorphic (structural) phase transformations of metals under dynamic high pressures is an area of fundamental scientific research at CEA which are studied through both experimental and theoretical/computational means. Experiments have long suggested that non-equilibrium behavior (kinetics) is an important part of the dynamic compression response of materials undergoing phase transformations. Both this deeper understanding, and quantitative data on specific metals, are needed to improve material models used in state-of-the-art hydrocodes. Only in recent years have experimental capabilities advanced sufficiently enough, in terms of diagnostics as well as drivers, that kinetics effects in dynamic phase transformations can begin to be quantified in a more rigorous manner. Empirical kinetic models can in a lot of cases reproduce the experimental velocity profiles but without clearly identifying the nature of the transition.

At CEA, we have developed preheating devices for gas gun and for HPP driver a promising testing on x-ray diffraction under shock. We propose to present our preliminary results to explore the phase diagram of Tin and how these experimental data help to understand kinetic models and EOS.

**8:36AM R02.00002: Unusual strength in tin under dynamic compression**

CAMELIA STAN (Presenter), ALEX ZYLSTRA, Lawrence Livermore Natl Lab, MATTHEW P HILL, Atomic Weapons Establishment, TOM LOCKARD, HYE-SOOK PARK, PHILIP POWELL, DAMIAN C SWIFT, JAMES M MCNANEY, Lawrence Livermore Natl Lab — Tin is a soft metal that undergoes several phase transitions at high pressure and temperature (1). These structural changes should lead to significant changes in both material microstructure and physical properties upon compression. Here, we use the Rayleigh-Taylor instability to measure its strength within the high-pressure BCC phase. A pre-machined rippled pattern seeds the instability, wherein a low density fluid pushing against a high density fluid causes growth of surface perturbations. We use a CH layer as the low density material, and the “push” is provided by the Omega EP laser facility, University of Rochester, which generates a ramped compression drive of ~1.5 Mbar in the sample. Ripple growth is measured using face-on radiography, and strength is interpreted based on the rate of growth relative to the undriven portion of the sample. We find that the growth rate is much less than that predicted in hydrodynamic simulations using a Steinberg-Guinan model. This suggests that BCC tin has unusually high strength, interpreted here as a resistance to plastic deformation. Lazicki, A et al. Phys. Rev. Lett. 115, (2015).

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.*
8:48AM R02.00003: Coupled Experiment and Theory to Explore the Limits of Material Strength at High Strain Rates  MITCHELL WOOD (Presenter), JAMES STEWART, JOSEPH D OLLES, Sandia National Laboratories — Experiments to study materials at high pressure are challenging and time consumptive, therefore we turn to modeling tools to refine and predict outcomes beforehand. Efficient models balance absolute physical accuracy against approximate but computationally lightweight constitutive inputs. By using a relatively small number of high fidelity simulations we have be able to broaden the predictive power of the shock response in metals and polymers. Analysis of these simulations has produced parameterizations of material strength, which can be used as constitutive inputs for continuum hydrodynamics codes. For shocked Cu, MD simulations show a yield strength from Richmyer-Meshkov Instability(RMI) jet growth of approximately 450MPa that depends on the details of the free surface geometry. This value is close to the yield strength of 500MPa parameterized from experiments at the Dynamic Compression Sector at Argonne National Lab. The same analysis applied to MD simulations of PMMA jetting resulted in no clear determination of yield strength, implying a more complex RMI process in polymeric materials. Simulations of both materials demonstrate the need for explicit strain rate dependence for future improvements in strength models used in continuum codes.

9:00AM R02.00004: Dynamic Strength in Polymers  JENNIFER JORDAN (Presenter), RACHEL HUBER, DANA DATTELBAUM, Los Alamos National Laboratory, DANIEL T. CASEM, CCDC Army Research Laboratory — Dynamic strength in polymers has been related to the underlying polymer structure in studies by Bourne, Millett, and co-workers. However, the majority of this work focused on changing the polymer chemistry. In this study, the effect of polymer structure, e.g. crystallinity, on dynamic polymer strength is investigated. The current understanding of polymer strength will be reviewed and recent results will be presented.

9:12AM R02.00005: Rayleigh-Taylor strength experiments in the high pressure and high strain rate regime on NIF*  HYE-SOOK PARK (Presenter), NATHAN R BARTON, ANDREW KRYGIER, BRUCE ALLEN REMINGTON, ROBERT E RUDD, PHILIP POWELL, SHON T. PRISBREY, DAMIAN C SWIFT, CHRISTOPHER WEHRENBERG, ALEX ZYLSTRA, JAMES M MCNANEY, Lawrence Livermore Natl Lab, MATTHEW P HILL, AWE — A solid material can be placed in the high energy density regime by compressing it to pressures >1 Mbar using a laser driven plasma piston drive. We create a ramped laser drive that keeps the material in the solid state during compression without shock melting. Understanding plastic deformation dynamics of materials under these extreme conditions is of high interest to a number of fields, including meteor impact dynamics and advanced inertial confinement fusion. We infer the strength of Ta, Pb [1,2] and Fe at high pressures (upto 8 Mbar), high strain rates (~10⁷ s⁻¹) and high strains (> 30%) by measuring the growth of Rayleigh-Taylor instabilities (RTI) under ramped compression. We find that the RTI growth for materials in the solid state, compressed under high pressure and high strain rates, is reduced compared to the no-strength case. We will describe the experimental results from NIF and compare them to various strength models.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
9:24AM R02.00006: Experimental studies of material strength in the high energy density regime*  PHILIP POWELL (Presenter), ANDREW KRYGIER, HYE-SOOK PARK, NATHAN R BARTON, CHANNING M HUNTINGTON, BRUCE ALLEN REMINGTON, ROBERT RUDD, SHON T. PRISBREY, DAMIAN SWIFT, CHRISTOPHER WEHRENBERG, ALEX ZYLSTRA, JAMES M MCNANEY, Lawrence Livermore Natl Lab — A solid material can be placed in the high energy density regime by compressing it to pressures > 1 Mbar using a laser driven plasma piston drive. We create a ramped laser drive that avoids shock melting, maintaining the material in the solid state during the full compression. Understanding plastic deformation dynamics of materials under these extreme conditions is of great interest in a number of fields, including meteor impact dynamics and advanced inertial confinement fusion. We infer the strength of Ta, Pb [1,2] and Fe at high pressures (up to 8 Mbar), high strain rates (~10^7 s^{-1}) and high strains (> 30%) by measuring the growth of Rayleigh-Taylor instabilities (RTI) under ramped compression. We find that the RTI growth for materials in the solid state, compressed under high pressure and high strain rates, is reduced compared to the no-strength case. We describe recent experimental results from NIF and compare them to various strength models. [1] H. -S. Park et al., Phys. Rev. Lett. 114, 065502 (2015). [2] A. Krygier et al., Phys. Rev. Lett., accepted (2019).

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

9:36AM R02.00007: Influence of Defects on the Shock Hugoniot of Tantalum*  SARYU FENSIN (Presenter), Los Alamos Natl Lab, ERIC N HAHN, University of California, San Diego — Using molecular dynamics simulations, we investigate the effect of vacancies and dislocations on the dynamic response of single crystal tantalum to shock loading. A Hugoniostat technique is employed, for which a series of states along the Hugoniot are sampled by many individual simulations. We show that defects have a limited effect on the shock/particle velocity relationship and that the shock pressure/volume relationship can be well predicted by taking into account the changes in the initial density and sound speeds of the samples. The principal effect of initial defects is the activation of heterogeneous dislocation nucleation and expedited dislocation multiplication during shock. The heat generated by plastic work, caused by defects moving through the lattice, is substantial. The result is significantly divergent final shock temperatures for different initial defect concentrations and pronounced changes in the resultant shock melting temperatures. The motion of dislocations also leaves behind a inconsequential concentration of vacancies that is quantified.

* Molecular dynamics simulations utilized resources were provided by the LANL Institutional Computing Program and funding was provided by Science Campaign 1.
9:48AM R02.00008: Experiments studying the flow strength of tantalum up to 30 GPa
FRANK CHERNE (Presenter), MATTHEW HUDSPETH, MICHAEL PRIME, BRIAN JENSEN, Los Alamos National Laboratory — In the recent years, there has been a number of experiments performed looking at different platforms or techniques to probe the strength of tantalum. The focus of this research has been to apply a shock/double shock drive conditions to determine the flow strength in tantalum up to about 30 GPa. The elastic/plastic response of tantalum and its interaction with typical lower impedance window materials complicates the design of these experiments. In this work, we present the results where we applied the shock/reloading technique to determine the flow strength of tantalum at initial loading stress states up to 30 GPa. Simulations with and without a PTW strength model are also compared to the experimental data.

10:00AM R02.00009: Simulating Tantalum Strength Measurements on the National Ignition Facility, Z-Machine, and Gas Gun Platforms* CORBETT BATTAILE (Presenter), Sandia National Laboratories, NATHAN R BARTON, Lawrence Livermore National Laboratory, JUSTIN BROWN, MATTHEW D LANE, HOJUN LIM, Sandia National Laboratories, PHILIP POWELL, Lawrence Livermore National Laboratory, MICHAEL PRIME, Los Alamos National Laboratory — The yield strengths of body-centered-cubic refractory metals (e.g. molybdenum, niobium, tantalum, and tungsten) can depend strongly on temperature, pressure, and strain rate. A variety of constitutive models have been proposed to describe these effects, but most are calibrated and/or validated in specific regimes of interest. In this work we used three recently-developed strength models, namely the Livermore Multiscale Model, the Preston-Tonks-Wallace model, and the Kink Pair model, to describe the response of tantalum subjected to elevated temperatures, pressures, and strain rates. We applied these models to predict strength measurements from Lawrence Livermore's National Ignition Facility, Los Alamos' gas gun facilities, and Sandia's Z-Machine, in order to explore a wide range of loading regimes. In this presentation we will outline each approach, and discuss validation results for the models' predictions of the strength of tantalum across a wide range of temperatures, pressures, and strain rates on these high-energy-density platforms.

*Sandia is managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a subsidiary of Honeywell International, for the US DOE's NNSA under contract DE-NA-0003525.
10:12AM R02.00010: Nonisentropic Release of a Shocked Solid  PATRICK HEIGHWAY (Presenter), MARCIN SLIWA, DAVID R MCGONEGLE, University of Oxford, CHRISTOPHER WEHRENBERG, Lawrence Livermore National Laboratory, CYNTHIA BOLME, Los Alamos National Laboratory, JON HENRY EGGERT, Lawrence Livermore National Laboratory, ANDREW HIGGINBOTHAM, York Plasma Institute, AMY E LAZICKI, Lawrence Livermore National Laboratory, HAEJA LEE, BOB NAGLER, SLAC National Accelerator Laboratory, HYE-SOOK PARK, ROBERT RUDD, RAYMOND SMITH, Lawrence Livermore National Laboratory, MATTHEW SUGGIT, University of Oxford, DAMIAN SWIFT, Lawrence Livermore National Laboratory, FRANZ TAVELLA, SLAC National Accelerator Laboratory, BRUCE ALLEN REMINGTON, Lawrence Livermore National Laboratory, JUSTIN STEPHEN WARK, University of Oxford — Shock release is the fundamental process that takes place when a material at high pressure undergoes rapid decompression. It is commonly accepted that rarefaction of this sort takes place isentropically, and is thus attended by substantial cooling due to the thermoelastic effect. However, this treatment fails to account for the fact that rapidly releasing material within the first few microns of the free surface typically exhibits material strength of order gigapascals, and therefore suffers copious plastic-work heating. Moreover, an isentropic treatment of release neglects the energy that can be recovered via the annihilation of crystal defects that ensues during rarefaction. Here, we present molecular dynamics simulations of shock and release in micron-scale tantalum crystals that exhibit release temperatures far exceeding those expected under the standard assumption of isentropic release. We show via an energy-budget analysis that this is due primarily to heating from material strength that largely counters thermoelastic cooling. The simulations are corroborated by experiments where the release temperatures of laser-shocked tantalum foils are deduced from their thermal strains via femtosecond x-ray diffraction, and are found to be close to those behind the shock itself.

10:24AM R02.00011: A model for twinning and plasticity in tantalum under shock conditions  NICOLAS BRUZY (Presenter), AURÉLIEN VATTRÉ, CHRISTOPHE DENOUAL, CEA de Bruyeres-le-Chatel — During deformation of tantalum at high strain rates, a competition takes place between plastic slip and twinning. The higher the strain rate, the harder it is to activate slip systems and twinning becomes predominant. In view of investigating this transition, a phase field model for phase changes including crystal plasticity, written in the finite strain format, is derived. It relies on the Reaction Pathway formalism, which is tailored for dynamic loadings since elastic and inelastic effects are properly split. First, all accessible variants are identified using point group symmetries of the parent phase. In the case of tantalum, two levels of transformation are considered (with 1+36 accessible variants in total), which makes it possible to reproduce secondary twinning. Then, the variants are taken as local minima of an energy landscape from which transformational energy and kinetic relations are obtained. A crystal plasticity model is further embedded at each variant to run polyphase plastic computations. Shock simulations on tantalum bars are performed using a 3D total Lagrangian code with an element-free Galerkin least-squares formulation. Results in terms of both variants repartition and plastic activity are consistent with past experimental works.
10:36AM R02.00012: Study of Hugoniot Elastic Limit in Tantalum single crystal using elastic precursor decay at normal and elevated temperature: Molecular Dynamics study
ANURADHA SINGLA (Presenter), ADITI RAY, Bhabha Atomic Res Ctr — Crystalline solids subjected to extremely high strain rates, as happens in shock wave propagation, is an important branch of material science. Knowledge of HEL is of fundamental importance in shock wave studies. Among BCC metals, Ta has several technological advantages due to its excellent mechanical property and thermodynamic phase stability at extreme conditions. This makes it useful in designing high impedance flyers for equation of state studies.

MD simulation of Ta has been performed in an effort to study formation of two-wave structure and its attenuation over distance. This leads to determination of HEL as a function of peak stress and sample thickness in two principle orientations. The work is mainly focused on studying decay of elastic precursor with advancement of shock along sample at normal and elevated temperature. The precursor decay for sub-micron sized sample has been modeled with empirical fitting relation. The fit predicts experimental result and other MD results for above-micron sized sample. This indicates that computationally intensive simulation for longer lengths can be avoided. Also, strong crystal anisotropy effect has been observed in onset of elastic-plastic wave.


R02.00013: Anisotropic shock response of single-crystalline β-phase tin* ROBERT SCHARFF (Presenter), NMO, Nevada National Security Site — Mesoscale simulations of the dynamic response of polycrystalline metals to shockwave compression can provide unique insight into the nature of the various physical mechanisms responsible for material failure. This approach requires a constitutive description for individual grains and boundaries, including defects such as dislocations, within an explicit representation of the microstructure geometry and evolving deformation fields. Computational models of the single-crystal constituents cannot be unambiguously constrained by traditional measurements of the shock or stress-strain response of polycrystalline metals. Instead, these models require comprehensive measurements of the anisotropic shock response of single crystals for their calibration and validation. We present a coordinated experimental and simulation campaign on the shock response of single-crystalline β-phase tin demonstrating a remarkable anisotropic elastic-plastic response of the metal.

*This work was done by Mission Support and Test Services LLC, under Contract No. DE-NA0003624 with the U.S. Department of Energy, and supported by the Site-Directed Research and Development Program. DOE/NV/03624—0391.
8:00AM R07.00001: Optimal approximate quantum error correction for quantum metrology*  SISI ZHOU (Presenter), Physics, Yale University, LIANG JIANG, Pritzker school of molecular engineering, University of Chicago — For a generic set of Markovian noise models, the estimation precision of a parameter associated with the Hamiltonian is limited by the $1/\sqrt{t}$ scaling where $t$ is the total probing time, in which case the maximal possible quantum improvement in the asymptotic limit of large $t$ is restricted to a constant factor. However, situations arise where the constant factor improvement could be significant, yet no effective quantum strategies are known. Here we propose an optimal approximate quantum error correction (AQEC) strategy asymptotically saturating the precision lower bound in the most general adaptive parameter estimation scheme where arbitrary and frequent quantum controls are allowed. We also provide an efficient numerical algorithm finding the optimal code. Finally, we consider highly-biased noise and show that using the optimal AQEC strategy, strong noises are fully corrected, while the estimation precision depends only on the strength of weak noises in the limiting case.

*We acknowledge support from the ARL-CDQI (W911NF15-2-0067, W911NF-18-2-0237), ARO (W911NF-18-1-0020, W911NF-18-1-0212), ARO MURI (W911NF-16-1-0349), AFOSR MURI (FA9550-151-0015), DOE (DE-SC0019406), NSF (EFMA-1640959), and the Packard Foundation (2013-39273).

8:12AM R07.00002: Multi-parameter metrology with the Holevo Cramer Rao bound; an explicit 2-qubit 3-parameter bound*  JAMIE FRIEL (Presenter), FRANCESCO ALBARELLI, ANIMESH DATTA, Univ of Warwick — Quantum metrology is essential for the rigorous analysis and optimisation of all quantum-limited experiments. Since no experiment is ever truly a single parameter one what is required is multi-parameter quantum metrology. It invokes the central axiom of quantum mechanics, that of incompatible observables. Hitherto, SLD quantum Fisher information matrix (QFIM) has largely been the Cramer-Rao bound of choice for examining multi-parameter metrology. In this work we show that the QFIM is an inadequate metric for multi-parameter problems. Further, we show that the Holevo Cramer-Rao (HCRB) bound is not only easier to calculate both numerically and analytically than previous thought but it is also essential for multi-parameter problems.

We point out new insights obtained from evaluating the HCRB for much larger Hilbert spaces than before, enabled by the convexity of the problem. We also show that previously known techniques allow us to calculate an explicit bound for 3D-magnetometry with 2 qubits, which again leads to new insight and further emphasises the pitfalls of the QFIM.

*Centre for Doctoral Training in Diamond Science and Technology, EP/L015315/1
8:24AM R07.00003: Parametrically-enhanced quantum sensing with effective non-Hermitian lattice dynamics  ALEXANDER MCDONALD (Presenter), AASHISH CLERK, University of Chicago — Systems whose dynamics are described by a non-Hermitian effective Hamiltonian have been suggested as platforms for improved sensing. Several experiments have already demonstrated the utility of exceptional points, a uniquely non-Hermitian feature, in setups consisting of a few resonant modes [1-3]. The phenomena exhibited by coupled multi-mode non-Hermitian systems, such as the non-Hermitian skin effect [4] and the existence of abnormally large susceptibilities, are also promising sensing resources. Here, we show how to harness the unusual lattice physics to build quantum sensing platforms with remarkable properties. In particular, the quantum Fisher information of our measurement scheme grows exponentially with system size, even when bounding the number of photons used for the measurement. This is achieved without coupling to dissipative baths or postselection. Our setup is realizable in a number of experimental platforms, including superconducting quantum circuits and quantum optical setups.


8:36AM R07.00004: Metrology near exceptional points from superconducting circuits with loss*  PATRICK HARRINGTON (Presenter), MARYAM ABBASI, Washington University, St. Louis, YOGESH JOGLEKAR, Indiana University - Purdue University Indianapolis, KATER MURCH, Washington University, St. Louis — The underlying mechanism of sensors, amplifiers, and metrological devices is a strong response to small perturbations. Such strong responses are expected for classical systems governed by non-Hermitian Hamiltonians. We use post-selection to create an effective non-Hermitian Hamiltonian for a superconducting quantum circuit and measure the sensitivity of the circuit to a coherent drive for different system parameters. We find that the quantum Fisher information about the drive amplitude diverges at the exceptional point, indicating enhanced sensitivity. However, enhanced sensitivity is achieved at the cost of additional experimental data due to post-selection statistics. With this experiment, we highlight the interplay of dissipation, dephasing, and loss near exceptional points of non-Hermitian open quantum systems and, we observe the role of quantum measurement backaction for quantum sensing.

*NSF Grant PHY-1607156, and NSF Grant PHY-1752844
8:48AM R07.00005: Macroscopic Quantum Tunneling Devices for Nanoscale Attonewton Force Sensing  
BENJAMIN SAFVATI (Presenter), YI-TING CHEN, MORGAN BRUBAKER, HARI C. MANOHARAN, Stanford Univ — The precision enabled by ultra-high vacuum, low temperature scanning tunneling microscopy for atomic manipulation has allowed the design of nanostructures that exhibit quantifiable quantum dynamics. This work presents a novel nanoscale probe of atomic-scale forces and enables new detection methods of the energy landscape in a Fermi gas. In a two-dimensional electron gas, the geometry of the boundaries on the surface will produce uniquely non-local alterations in the electronic wave function. By creating a device in which a single atom or molecule can macroscopically tunnel between degenerate states in a double potential well, we are able to detect quantum forces that break the degeneracy by measuring an asymmetry in the tunneling rates between each side. Our new method of two-dimensional nanoscale force measurement is able to detect forces with attonewton sensitivity, and the device's design permits the probing of quantum forces due to proximal nanostructures with atomic resolution. Designer boundary conditions can amplify the measured forces and further illustrate the non-local nature of quantum force fields. We will discuss ways to extend device sensitivity even further, below the attonewton level.

9:00AM R07.00006: Dissipation-based quantum sensing of magnons*  
SAMUEL WOLSKI (Presenter), DANY LACHANCE-QUIRION, YUTAKA TABUCHI, Research Center for Advanced Science and Technology, The University of Tokyo, SHINGO KONO, Center for Emergent Matter Science, RIKEN, KOJI USAMI, YASUNOBU NAKAMURA, Research Center for Advanced Science and Technology, The University of Tokyo — Magnons are the quanta of collective spin excitations. We introduce a novel technique for quantum sensing of magnons by leveraging the quantum coherence of a superconducting qubit which interacts with a magnetostatic mode. This is enabled by the realization of a strong dispersive coupling between the uniformly precessing magnetostatic mode in a ferromagnetic sphere and a superconducting qubit in a hybrid system [1,2]. A finite magnon population induces additional dephasing in the qubit, and can thus be inferred by probing the qubit coherence via Ramsey interferometry. A magnon detection sensitivity of around $10^{-3}$ magnons/√Hz is demonstrated, in good agreement with numerical simulations. The dissipation-based nature of our quantum sensor is confirmed by the dependence of the sensitivity on the detuning used in the Ramsey interferometry. The use of quantum sensing techniques in magnonics could find applications in fields such as magnon spintronics and magnetic field sensing.  

*This work is partly supported by JSPS KAKENHI (26220601, 18F18015), JST ERATO (JPMJER1601), JSPS and FRQNT Postdoctoral Fellowships, and the MEXT Monbukagakusho Scholarship.
9:12AM R07.00007: Quantum sensing with superconducting microwave circuits*  
MATTI PARTANEN (Presenter), KIRILL FEDOROV, STEFAN POGORZALEK, MICHAEL RENGER, QI-MING CHEN, ACHIM MARX, FRANK DEPPE, RUDOLF O GROSS, Walther-Meissner-Institut, Munich, Germany — Quantum mechanics offers intriguing opportunities for sensing applications with accuracies beyond the classically obtainable limits. An especially interesting approach is based on using entangled microwave photons for radar applications [Las Heras et al., Sci. Rep., 7, 9333 (2017)]. Here, we discuss a novel frequency-degenerate scheme for quantum sensing with superconducting microwave circuits. Our method is based on continuous variables that provide a convenient platform for quantum communication [Pogorzalek et al., Nat. Commun., 10, 2604 (2019)]. The same microwave regime is utilized in conventional radars owing to the transparency window of the atmosphere. Hence, our scheme suffers no conversion losses and, therefore, is promising for future real-world applications.

*We acknowledge the support by the Germany's Excellence Strategy EXC-2111-390814868, Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No. 820505).

9:24AM R07.00008: Quantum-Enhanced Noise Radar  
NIZAR MESSAoudi (Presenter), CHUNG WAI SANDBO Chang, A.M. Vadiraj, Insitute of Quantum Computingan Electrical and Computer Engineering, University of Waterloo, JEROME BOURASSA, Istitut Quantique, Universite de Sherbrooke, BHASYAM BALAJI, Radar Sensing and Exploitation Section, Defence R&D Canada, C.M. WILSON, Insitute of Quantum Computingan Electrical and Computer Engineering, University of Waterloo — Quantum Illumination (QI) promises improvement in the sensitivity of target detection technologies. The approach takes advantage of strong correlations that can be created in electromagnetic beams using quantum processes, through a form of entanglement. Notably, QI has proven to be very robust to the presence of noise and loss, suggesting that it may have practical applications. We have made a proof-of-principle demonstration of a novel QI protocol: quantum-enhanced noise radar (QENR). In QENR, we use a parametric amplifier to produce a two-mode squeezed (TMS) state, which exhibits continuous-variable entanglement between signal and idler beams. This state is the input to the radar system. Compared to existing proposals for QI, our protocol does not require joint measurement of the signal and idler. This greatly enhances the practicality of the system by eliminating the need for a quantum memory to store the idler. We compare the performance of a TMS source to an ideal classical source that saturates the classical bound for correlation, finding a quantum enhancement approaching a factor of 10. One of the main challenges to making QENR practical is bringing the quantum microwaves out of the cryostat. We will discuss progress towards overcoming this challenge.
Parametric quantum amplifiers are of paramount importance for quantum information processing with superconducting circuits. A promising route to design quantum amplifiers is based on parametric modulation of coupled modes, where the required mode-mixing processes are realized by utilizing Josephson junction-based tunable couplers. All designs face the challenge of higher-order nonlinearities, resulting in a limitation of the dynamical range of the amplifier. However, even without any higher-order nonlinearities, the amplification process is itself nonlinear, e.g., it involves the mixing of three waves: the pump, the idler and the signal. Only for weak enough signal intensity the pump can be considered stiff and the amplification process becomes linear. Once the signal strength grows this approximation does not hold true anymore. The nonlinear nature of the mixing process leads to back-action, limiting the dynamical range of the amplifier.

Here we present possible ways to face these challenges, and how to avoid unwanted back-action effects in engineered quantum systems. Furthermore, we discuss routes for optimizing the design of quantum-limited parametric amplifiers that one can avoid pump-depletion effects completely.
Near quantum limited Josephson traveling wave amplifiers I, Fabrication and characterization

LUCA PLANAT (Presenter), ARPIT RANADIVE, RÉMY DASSONNEVILLE, JAVIER PUERTAS, SEBASTIEN LEGER, CÉCILE NAUD, OLIVIER BUISSON, WIEBKE GUICHARD, Institut Neel, DENIS M BASKO, Laboratoire de Physique et Modélisation des Millieux Condensés, NICOLAS ROCH, Institut Neel — Efficient low noise amplification is a crucial component for any system dealing with low amplitude signals. Currently, Josephson parametric amplifiers (JPAs) can attain quantum limited amplification for microwave signals. However, JPAs based on resonant structures are limited to low bandwidth and saturation power. These limitations can be overcome using Josephson meta-materials forming traveling wave parametric amplifiers (TWPAs).

In part I, we will present in detail, our simplified aluminum-based two-step fabrication technique for TWPAs with low footprint[1], and discuss their linear characterization[2]. This technique paves the way for on-chip integration of broadband amplifiers with quantum devices.

In part II, we will present the performance of these amplifiers, exhibiting a large and near quantum limited gain over bandwidth larger than 2GHz; and conclude with a discussion on techniques for mitigating some of the limitations.


*This work was supported by the ANR CLOUD project No. ANR-16-CE24-0005 and EU Horizon 2020 program(grant no. MSC-754303 and EMP-824109). R.D. and S.L. ack support from the CFM foundation and the 'Investissements d'avenir' (ANR-15-IDEX-02) programs of the French ANR.
Performance and further development*  ARPIT RANADIVE (Presenter), LUCA PLANAT, REMY DASSONNENVILLE, JAVIER PUERTAS, SEBASTIEN LEGER, CÉCILE NAUD, OLIVIER BUISSON, WIEBKE HASCH-GUICHARD, Institut Neel, DENIS M BASKO, Laboratoire de Physique et Modélisation des Milieux Condensés, NICOLAS ROCH, Institut Neel — Efficient low noise amplification is a crucial component for any system dealing with low amplitude signals. Currently, Josephson parametric amplifiers (JPAs) can attain quantum limited amplification for microwave signals. However, JPAs based on resonant structures are limited to low bandwidth and saturation power. These limitations can be overcome using Josephson meta-materials forming traveling wave parametric amplifiers (TWPAs).

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Heisenberg-limited single-mode quantum metrology in a superconducting circuit  WEITING WANG (Presenter), YUKAI WU, YUWEI MA, WEIZHOU CAI, LING HU, XIANGHAO MU, YUAN XU, Tsinghua University, ZIJIE CHEN, University of Science and Technology of China, HAIYAN WANG, YIPU SONG, Tsinghua University, HAIDONG YUAN, Chinese University of Hong Kong, CHANGLING ZOU, University of Science and Technology of China, LUMING DUAN, LUYAN SUN, Tsinghua University — Quantum metrology is one of the most promising near-term applications of quantum technology. Reaching a quantum advantage in metrology usually requires hard-to-prepare two-mode entangled states such as NOON states. Instead of exploring quantum entanglement in the two-mode interferometers, a single bosonic mode also promises a measurement precision beyond the shot-noise limit (SNL) by taking advantage of the infinite-dimensional Hilbert space of Fock states. In this talk, we demonstrate such a single-mode phase estimation that approaches the Heisenberg limit (HL) unconditionally in a superconducting circuit by preparing the superpositions of Fock states (|0> + |N>) up to N=12. We realize a 9.1 dB improvement over the SNL at N=12, which is only 1.7 dB away from the HL. Our experimental architecture can be combined with quantum error correction techniques to fight against decoherence, and thus promises quantum-enhanced sensing in practical applications.
RAFAL DEMKOWICZ-DOBRZANSKI (Presenter), Faculty of Physics, University of Warsaw — A comprehensive overview of the most recent advances in theoretical methods of quantum metrology will be presented, that in particular benefit from the quantum information related concepts such as quantum error-correction or matrix product states formalism. The theory developed allows to determine whether the Heisenberg scaling of precision is possible for a quantum sensor subject to a general Markovian noise. The theory takes into account all the possible quantum strategies, including entangling the sensor with ancillary systems, adaptive strategies such as e.g. quantum error correction protocols. Moreover, effective algorithms, based on the matrix product states/matrix product operator formalism, are developed that allow to identify the optimal metrological protocols in presence of noise (also correlated noise) in the limit of large number of probes, inaccessible by the state-of-the-art methods. These results are highly relevant for modern developments of quantum enhanced sensing protocols, including NV-center magnetometry, squeezed states enhanced optical and atomic interferometry or stabilization protocols for atomic clocks.

References:

*Polish Ministry of Science and Higher Education Iuventus Plus program for years 2015-2017 No. 0088/IP3/2015/73
National Science Center (Poland) grant No. 2016/22/E/ST2/00559,
Simultaneous Measurement of 53 Superconducting Transmons on the Sycamore Processor

ZIJUN CHEN (Presenter), OFER NAAMAN, DANIEL T SANK, PAUL KLIMOV, CHRIS QUINTANA, JULIAN KELLY, ANTHONY E MEGRANT, Google Inc - Santa Barbara, HARTMUT NEVEN, Google Inc, JOHN M MARTINIS, Google Inc - Santa Barbara —

Progress in low-noise amplifiers, device design, and device calibration has enabled high fidelity readout in transmon qubits. However, challenges arise when scaling up to large numbers of qubits, where deleterious effects such as crosstalk and unwanted interactions can degrade readout fidelity. In this talk, I will discuss how we overcame some of these challenges to achieve simultaneous readout of 53 qubits on Google's Sycamore processor, enabling the demonstration of quantum supremacy. [1].


Single-shot readout and state preparation of a fluxonium qubit without the use of a parametric amplifier

DARIA GUSENKOVA (Presenter), MARTIN SPIECKER, RICHARD GEBAUER, LUKAS GRUENHAUPT, PATRICK WINKEL, FRANCESCO VALENTI, IVAN TAKMAKOV, DENNIS RIEGER, ALEXEY V. USTINOV, WOLFGANG WERNSDORFER, OLIVER SANDER, IOAN-MIHAI POP, Karlsruhe Institute of Technology —

High-fidelity qubit readout is an essential requirement for the implementation of quantum algorithms. A commonly used readout technique involves the dispersive interaction between a qubit and a resonator, which encodes the qubit state into the phase and amplitude of the microwave readout tone. In theory, the state discrimination can be substantially improved if the resonator is populated with high photon numbers [1]. In practice however, the optimal photon number, at which the best readout fidelity is obtained, is usually in the range of a few photons [2, 3], and parametric amplifiers with near quantum-limited noise are needed to overcome the noise of even the best commercial high electron mobility transistor amplifiers.

Using a fluxonium qubit with a granular aluminum superinductance [4], we demonstrate single shot qubit measurements without a parametric amplifier, at a readout power corresponding to hundreds of circulating photons. The dispersive shift decreases with photon number, and the qubit decay rate increases, resulting in a tradeoff between applied power and readout fidelity.

Measurement of quantum jumps of a fluxonium qubit using a Dimer Josephson Junction Array Amplifier operated at high power  

IVAN TAKMAKOV (Presenter), PATRICK WINKEL, Karlsruhe Institute of Technology, FARSHAD FOROUGHI, NEEL, MARTIN SPIECKER, LUKAS GRUENHAUPT, DARIA GUSENKOVA, Karlsruhe Institute of Technology, LUCA PLANAT, NEEL, DENNIS RIEGER, ALEXEY V. USTINOV, WOLFGANG WERNSDORFER, IOAN-MIHAI POP, Karlsruhe Institute of Technology, NICOLAS ROCH, NEEL — Josephson parametric amplifiers have become an essential element in cQED dispersive readout measurement schemes, enabling single-shot qubit readout. Over the last decade there was significant progress in the increase of their saturation power [1,2,3,4], which now reaches several thousand photons per μs. We demonstrate high saturation power in a Dimer Josephson Junction Array Amplifier [4] operating with a quantum efficiency of 60%. We use this parametric amplifier to perform dispersive readout of a fluxonium qubit with a superinductor made of granular aluminum [5]. We present quantum jump measurements acquired using up-to 100 circulating photons in the readout resonator, which allowed qubit state discrimination in tens of nanoseconds.


Towards autonomous digital feedback on a superconducting qubit  

ZIYI ZHAO (Presenter), ERIC ROSENTHAL, JILA and University of Colorado, Boulder, MAXIME MALNOU, NIST, Boulder, CHRISTIAN M. F. SCHNEIDER, University of Innsbruck, LEILA VALE, GENE C. HILTON, NIST, Boulder, GERHARD KIRCHMAIR, University of Innsbruck, JIANSONG GAO, NIST, Boulder, K. W. LEHNERT, JILA and University of Colorado, Boulder — Quantum error correction requires conditional operations predicated on measurement results. Such feedback schemes in superconducting qubit systems, however, can be hardware intensive. They may require dedicated control hardware at ambient temperature and consume precious high-bandwidth connections between temperature stages. Here we present preliminary data on the state preparation and stabilization of a superconducting qubit where we keep the measurement information at the base temperature stage of the cryostat, and then use it to conditionally \( \pi \) pulse a qubit. This scheme avoids the aforementioned problems and can ease the development of stabilized quantum networks within a scalable architecture.
**8:48AM R08.00005: Isolating a qubit from amplifier backaction by coordinated switching**

ERIC ROSENTHAL (Presenter), JILA and the University of Colorado, Boulder, CHRISTIAN M. F. SCHNEIDER, University of Innsbruck, MAXIME MALNOU, NIST, Boulder, ZIYI ZHAO, FELIX LEDITZKY, JILA and the University of Colorado, Boulder, BENJAMIN J. CHAPMAN, Physics and Applied Physics, Yale, XIZHENG MA, DANIEL A PALKEN, JILA and the University of Colorado, Boulder, LEILA R. VALE, GENE C. HILTON, NIST, Boulder, GERHARD KIRCHMAIR, University of Innsbruck, JIANSONG GAO, NIST, Boulder, GRAEME SMITH, K. W. LEHNERT, JILA and the University of Colorado, Boulder — We demonstrate a cQED qubit measurement scheme in which the qubit is isolated from amplifier backaction without ferrite circulators. We swap a readout signal from the qubit cavity to an ancillary cavity by temporarily coupling them. The state of the ancillary cavity is then amplified by parametrically pumping past bifurcation into one of two large amplitude states that are correlated with the qubit state. Isolation and efficiency are comparable to readout using a ferrite circulator, but are achieved using a chip-scale device compatible with the integration of superconducting qubits. Because the measurement result is contained in the digital state of a superconducting bifurcation amplifier, it is possible to use this scheme to create autonomous feedback loops at the cryostat base temperature. The integrated nature of this readout suggests an avenue toward the scalable measurement of larger quantum networks.

*This work is supported by the ARO under contract W911NF-14-1-0079 and the National Science Foundation under Grant No. 1125844. E.I.R. acknowledges support from the ARO QuaCGR fellowship.

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**9:00AM R08.00006: On-chip single-pump interferometric Josephson Isolator**  
BALEEGH ABDO (Presenter), OBLESH JINKA, NICHOLAS T BRONN, SALVATORE OLIVADESE, MARKUS BRINK, JERRY M. CHOW, IBM TJ Watson Research Center — Nonreciprocal microwave devices, such as circulators and isolators, play several critical roles in superconducting quantum processors. They route readout signals in a directional manner, protect the quantum system against noise coming from the output chain, and enable reflection measurements by separating input from output. However, the reliance of these devices, on magnetic materials and strong magnets for breaking reciprocity, makes them disadvantageous in scalable superconducting architectures. In this work, we realize and measure an on-chip Josephson isolator, which is formed by coupling two nondegenerate Josephson mixers in an interferometric scheme. Isolation is created, in the active device, by operating the two mixers in frequency conversion mode using balanced, same-frequency microwave pumps, whose phase difference is \( \pi/2 \). The applied pumps are generated using an on-chip quadrature hybrid, which equally splits the single pump feeding the device and imposes the required phase difference between the split drives.
9:12AM R08.00007: Novel Measurements for Annealing Capable Flux Qubits* WADE DEGOTTARDI (Presenter), DAVID J. CLARKE, SERGEY NOVIKOV, JAMES I BASHAM, JEFFREY GROVER, STEVEN M DISSELER, DAVID FERGUSON, Northrop Grumman - Mission Systems — Quantum Flux Parametron (QFP) based measurements have demonstrated the ability to implement high fidelity z-basis readout for high coherence capacitively shunted flux qubits (CSFQs) at the end of an anneal. This talk discusses alternative QFP readout procedures including: (i) at early times in the anneal, (ii) for other non z-loop currents, and (iii) for Josephson phase slip qubits (JPSQs). It is shown how the POVM (positive-operator valued measure) that characterizes the qubit measurement in these novel regimes can be derived from the final QFP POVM by modeling the dynamics of the coupled QFP-qubit system.

*This material is supported by the Intelligence Advanced Research Projects Activity (IARPA) through the Army Research Office (ARO) Contract No. W911NF-17-C-0050.

9:24AM R08.00008: Realizing large, tunable dispersive shifts with parametric couplings ZHIHAO XIAO (Presenter), University of Massachusetts Lowell, LEONARDO M RANZANI, LUKE GOVIA, Raytheon BBN Technologies, RAYMOND W SIMMONDS, JOSE AUMENTADO, National Institute of Standards and Technology Boulder, ARCHANA KAMAL, University of Massachusetts Lowell — In recent years, parametric couplings are being deployed in a variety of applications, ranging from parametric gates, state preparation to quantum annealing. Unlike their traditional applications such as parametric amplification, these new functionalities require much stronger parametric coupling strengths that can dominate qubit decay and measurement rates. The theoretical framework to capture the effect of such strong time-dependent couplings, however, remains rudimentary. In this work, we analyze the primary building block of such a platform --- a single qubit parametrically coupled to a single-mode resonator. We establish that even this simple system can support a rich structure in dispersive shifts, that can be rendered large and tunable by choosing suitable parametric coupling drive amplitudes and frequencies. In addition, this platform can enable enhanced cavity squeezing by multi-tone parametric pumping. Our scheme can be realized with state-of-the-art circuit-QED architecture, and we discuss our early experimental efforts to support this approach.
Remote entanglement via two mode squeezed light

XI CAO (Presenter), Physics and Astronomy, University of Pittsburgh, GANGQIANG LIU, Applied Physics, Yale University, TZUCHIAO CHIEN, CHAO ZHOU, PINLEI LU, MICHAEL JONATHAN HATRIDGE, Physics and Astronomy, University of Pittsburgh — Remotely entangling qubits which do not interact directly is very desirable for quantum information processing. One method for remote entanglement is to read out two qubits in parallel with their outputs entering the signal and idler mode of a phase-preserving amplifier. The amplifier squeezes away which-path information and can project the qubits into a Bell state. However, this measurement also produces an outcome-dependent phase kick on the qubits’ state. Thus, losses and inefficient amplification can prevent the generation of entangled states [1, 2]. However, we have recently demonstrated a new scheme which uses two-mode squeezed light (TMSL) in an interferometer formed by two phase-preserving amplifiers to measure a qubit. We find that the phase back-action of TMSL measurement alters the phase back-action relative to coherent readout, depending on the amplifiers’ relative phase. Here we present a two qubit, TMSL interferometric entangling readout. We will show how TMSL affects the back-action of the entangling readout and discuss the prospects for the use of TMSL to make the scheme more tolerant of hardware imperfections.


**Work supported by: ARO, LPS, NSF, and the Kauffman foundation**
9:48AM R08.00010: Fast high fidelity quantum non-demolition superconducting qubit readout* [Invited] RÉMY DASSONNEVILLE, Neel Institute, University Grenoble Alpes, CNRS, THOMAS RAMOS, Institute of Fundamental Physics, IFF-CSIC, VLADIMIR MILCHAKOV, LUCA PLANAT, ETIENNE DUMUR, FARSHAD FOROUGHI, JAVIER PUERTAS, SEBASTIEN LÉGER, KARTHIK SRIKANTH BHARADWAJ, JOVIAN DELAFORCE, CÉCILE NAUD, WIEBKE GUICHARD, Neel Institute, University Grenoble Alpes, CNRS, JUAN JOSE GARCIA-RIPOLL, Institute of Fundamental Physics, IFF-CSIC, NICOLAS ROCH, OLIVIER BUISSON (Presenter), Neel Institute, University Grenoble Alpes, CNRS — The most common technique of qubit readout in cQED relies on the transverse dispersive coupling between a qubit and a microwave cavity. However, despite important progresses, implementing fast high fidelity and QND readout remains a major challenge. Indeed, inferring the qubit state is limited by the trade-off between speed and accuracy due to Purcell effect and unwanted transitions induced by readout photons in the cavity. To overcome this, we propose and experimentally demonstrate a new readout scheme based on a transmon molecule inserted inside a 3D-cavity_[1,2]. The full system presents a transmon qubit mode coupled to a readout mode through an original non-pertubative cross-Kerr coupling. The readout mode, called polariton mode, results from the hybridization between the microwave cavity and the transmon molecule circuit. The direct cross-Kerr coupling is a key point of our readout scheme since it protects the qubit from Purcell effect. This first implementation, though perfectible, already enables a very efficient single-shot QND readout of the qubit in only 50ns, with a QND-ness of 99% and a fidelity of 97.4%.


*This work is supported by the French Agence Nationale de la Recherche (ANR-CE24-REQUIEM).

10:24AM R08.00011: Frequency-domain pulse engineering for fast qubit readout and resonator reset* RICCARDO BORGANI, MATS THOLEN, SHAN WILLIAMS JOLIN, DANIEL FORCHHEIMER, DAVID HAVILAND (Presenter), KTH Royal Inst of Tech — The state of a superconducting qubit is typically determined by measuring the dispersive shift $\chi$ of a superconducting resonator with coupling rate $\kappa$ to a transmission line. Large $\chi/\kappa$ ratio is beneficial for high-fidelity readout. While small $\kappa$ protects the qubit from the noisy environment, it has the big disadvantage of limiting the speed of measurement. In particular, photons linger in the resonator for a time of several $1/\kappa$, causing decoherence of the qubit and blocking subsequent measurement. Here we present a microwave pulse scheme which, regardless of the state of the qubit, populates the readout resonator, measures the state of the qubit, and empties the resonator, all in a time much faster than $1/\kappa$. The pulse is designed in the frequency domain by shaping its spectral content at the dressed-resonance frequencies. The pulse envelope is derived through inverse Fourier transform, rather than relying on brute-force numerical optimization. We evaluate the performance of the pulse scheme in different regimes of $\chi/\kappa$ through both simulation and experiment, and we comment on the theoretically achievable single-shot fidelity of the method.

*This work is supported by WACQT the Wallenberg Centre for Quantum Technology.
10:36AM R08.00012: High efficiency measurement of a superconducting qubit using a directional, phase-sensitive, parametric amplifier

FLORENT LECOCQ (Presenter), National Institute of Standards and Technology Boulder, LEONARDO M RANZANI, Raytheon BBN Technologies, GABRIEL PETERSON, SHLOMI KOTLER, KATARINA CICAK, X. Y. JIN, RAYMOND W SIMMONDS, JOHN TEUFEL, JOSE AUMENTADO, National Institute of Standards and Technology Boulder — The measurement of a superconducting quantum bit is often performed by encoding its state in a single quadrature of a microwave field. Ideal measurement efficiency of this observable could in principle be achieved by noiselessly amplifying the information-carrying quadrature, but in practice is limited by technical losses due to circulators, cables and connectors used in state-of-the-art amplification chains.

In this talk we will discuss how one can approach ideal measurement efficiency by directly connecting a 3D transmon to a non-reciprocal phase-sensitive amplifier [1]. After describing the setup and tuning of the amplifier, we will extract the measurement efficiency by comparing the qubit dephasing rate to the measurement rate.


10:48AM R08.00013: High fidelity dispersive qubit readout in circuit QED without using a Josephson Parametric Amplifier

SUMAN KUNDU (Presenter), KISHOR V SALUNKHE, ANIRBAN BHATTACHARJEE, SUMERU HAZRA, MEGHAN P. PATANKAR, R VIJAY, DCMP&MS, Tata Institute of Fundamental Research, Mumbai — In the cQED architecture, the Josephson parametric amplifier (JPA) enables high fidelity readout by providing minimal degradation of the signal-to-noise ratio (SNR) of the amplified readout signal. While the SNR can also be increased by increasing readout power and integration time, the fidelity typically gets limited due to unwanted transitions both within and outside the computational subspace. Here, we present and demonstrate an alternate design where qubit-cavity coupling does not rely on the dispersive approximation of the Jaynes-Cummings Hamiltonian. This multi-modal circuit is reminiscent of the quantronium qubit design but with two differences: the qubit is of the transmon type and the cavity is linear. The device is implemented in the 3D cQED architecture and we use a rectangular waveguide to couple the readout cavity to the measurement line. We achieve a readout fidelity of 97.8% for 800ns integration time with a histogram overlap error of only 0.3% without using a JPA. The best fidelity obtained with the JPA was 98.9% for a 300 ns integration time with an overlap error of less than 0.01%. We will conclude by discussing the variation of readout fidelity with measurement power and compare with a conventional transmon readout in cQED.
8:00AM R09.00001: Randomized benchmarking for qudit Clifford gates* BARRY SANDERS (Presenter), Institute for Quantum Science and Technology, University of Calgary, MAHNAZ JAFARZADEH, Physics Department, Urmia University, YADONG WU, Institute for Quantum Science and Technology, University of Calgary — We introduce unitary-gate randomized benchmarking (URB) for qudit gates by extending single- and multi-qubit URB to single- and multi-qudit gates. Specifically, we develop a qudit URB procedure that exploits unitary 2-designs. Furthermore, we show that our URB procedure is not simply extracted from the multi-qubit case by equating qudit URB to URB of the symmetric multi-qubit subspace. Our qudit URB is elucidated by using pseudocode, which facilitates incorporating into benchmarking applications.

*NSERC

8:12AM R09.00002: Quantum-Computing Architecture based on Large-Scale Multi-Dimensional Continuous-Variable Cluster States in a Scalable Photonic Platform* BO-HAN WU (Presenter), Physics, Univ of Arizona, RAFAEL ALEXANDER, Center for Quantum Information and Control, Univ of New Mexico, ZHESHEN ZHANG, Department of Materials Science and Engineering, Univ of Arizona — Quantum computing is a disruptive paradigm widely believed to be capable of solving classically intractable problems, but the route toward full-scale quantum computers is impeded by immense challenges associated with the scalability of the platform and the required fidelity of various components. One-way quantum computing is an appealing approach that shifts the burden from high-fidelity quantum gates and quantum memories to the generation of high-quality entangled resource states and high fidelity measurements. Here, we bridge two fields—Kerr microcombs and continuous-variable (CV) quantum information—to formulate a one-way quantum computing architecture based on programmable large-scale CV cluster states. The architecture accommodate hundreds of simultaneously addressable entangled optical modes multiplexed in frequency and an unlimited number of sequentially addressable entangled modes in time. One-, two-, three-dimensional CV cluster states can be deterministically produced, which allows for fault-tolerant one-way quantum computing with known error-correction strategies. This architecture opens a promising avenue for quantum computing at a large scale.

*Office of Naval Research Award No. N00014-19-1-2190, the National Science Foundation Award No. ECCS-1920742. and PHY-1630114.

8:24AM R09.00003: Proposed Universal Deutsch Gate Circuitry Using GaAs/InAs Quantum Dots PAUL BAILEY (Presenter), JEAN-FRANCOIS VAN HUELE, Brigham Young Univ - Provo — The Deutsch gate is a universal quantum logic gate, meaning that any quantum computing task can be completed using a combination of Deutsch gates. Although a proposal exists to build a Deutsch gate using Rydberg atoms [X-F Shi, Phys. Rev. Applied 9, 051001], to our knowledge no Deutsch gate has been experimentally realized so far. We propose to combine two GaAs/InAs quantum dots with photon polarization in a larger circuit comprised of linear optical elements to create a spin-spin-photon polarization three qubit Deutsch Gate similar to a proposal for a CNOT gate [Bouwmeester et al., Phys. Rev. Lett. 104, 160503]. We display the circuit and discuss the intricacies of designing this gate and reflect on the general feasibility of gate design.
Quantum-classical transition in analog quantum supremacy subject to Markovian decoherence*

RAZIEH MOHSENINIA (Presenter), Univ of Southern California, MILAD MARVIAN, Massachusetts Institute of Technology, DANIEL A LIDAR, Univ of Southern California — Instantaneous Quantum Polynomial time circuits are a promising way to demonstrate quantum supremacy. We study the robustness of quantum supremacy in an analog Hamiltonian version of such circuits in the presence of a Markovian environment whose noise operators commute with the system Hamiltonian. We find a transition from a regime of quantum supremacy to classical simulability that occurs at a finite critical decoherence rate, that depends on the system size.

*This work was supported in part by Oracle and by a DOE/HEP QuantISED program grant, Quantum Machine Learning and Quantum Computation Frameworks (QMLQCF) for HEP, award number DESC0019227.

Optimal recognition of exact free-fermion solutions for spin models*

ADRIAN CHAPMAN (Presenter), STEVEN FLAMMIA, Univ of Sydney — Finding exact solutions to spin models is a fundamental problem of many-body physics. A workhorse technique for many such exact solution methods is mapping to an effective description by noninteracting particles. The paradigmatic example of this method is the exact solution for the one dimensional XY model by mapping to free-fermions via the Jordan-Wigner transformation. We connect the general problem of recognizing models which can be exactly solved in this way to the graph-theoretic problem of recognizing line graphs, which has been solved optimally. Our solution method captures an entire class of spin models which are as exactly solvable as the Kitaev honeycomb model. We give an example of a previously unsolved spin model and demonstrate its exact solution by our method. We close by showing how these techniques can be used to design new fermion-to-qubit mappings.

*Centre for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia

Quantum Algorithms for Approximate Dynamic Programming

POOYA RONAGH (Presenter), University of Waterloo — We present a quantum algorithm for finding approximate solutions to dynamic programming problems using the multiplicative weight update method. Up to polylogarithmic factors, our algorithm provides a quadratic quantum advantage in terms of the number of states of a given dynamic programming problem, at the expense of the appearance of other polynomial factors representative of the number of actions of the dynamic programming problem, the maximum value of the instantaneous reward, and the time horizon of the problem. We also prove lower bounds for the query complexity of quantum algorithms and classical randomized algorithms for solving dynamic programming problems, and show that no greater-than-quadratic speedup in either the number of states or number of actions can be achieved for solving dynamic programming problems using quantum algorithms.
9:12AM R09.00007: A Novel Tensor Network Algorithm for Simulating Large Quantum Circuits*
JUSTIN REYES (Presenter), Univ of Central Florida, LEI ZHANG, STEFANOS KOURTIS, CLAUDIO CHAMON, ANDREI E RUCKENSTEIN, Physics, Boston University, EDUARDO R MUCCIOLO, Univ of Central Florida — Simulations of quantum circuits often involve an exponential number of resources, suffering from the so called "curse of dimensionality." Because of this, obtaining measurement information from states output by high-depth circuits is challenging. To overcome this limitation, we employ a novel tensor network methodology to compute expectation values that resembles the Keldysh formalism. This algorithm, which we term ICD (Iterative Contraction Decomposition), iteratively alternates between sequences of tensor contractions and global sweeps of tensor pair Schmidt decompositions. We demonstrate our algorithm's ability to determine measurement outcomes for random circuits of up to 40 qubits with circuit depths of 80 steps.

*NSF CCF-1844434

9:24AM R09.00008: Gate(s)-wise Optimization for Variational Quantum Eigensolvers*
LUCAS SLATTERY (Presenter), BENJAMIN VILLALONGA, BRYAN CLARK, University of Illinois at Urbana-Champaign — The variational quantum eigensolver (VQE) is a promising hybrid framework for solving chemistry and physics problems on noisy intermediate-scale quantum (NISQ) computers of the near future. VQE uses a NISQ device to prepare classically intractable parameterized quantum states. These states include ground states of chemistry and condensed matter models, as well as the solution to other optimization problems. A VQE method combines sampling from the NISQ device with a classical optimization routine to find target states. To optimize, most VQE algorithms use quantum circuits to measure gradients of a cost function in order to perform a gradient descent step. We provide and benchmark an alternative to gradient descent VQE methods with the potential for avoiding local minima and faster convergence. We demonstrate proof-of-concept results for local hamiltonians by optimizing one gate at a time.

*We acknowledge funding from DOE de-sc0020165
The resilience of quantum random access memory to generic noise*

CONNOR HANN (Presenter), GIDEON LEE, STEVEN GIRVIN, Yale University, LIANG JIANG, University of Chicago — Quantum random access memory (qRAM)—a memory which stores classical data but allows queries to be performed in superposition—is required for the implementation of numerous quantum algorithms. While naive implementations of qRAM are highly susceptible to decoherence and thus not scalable, it has been argued that the bucket brigade qRAM scheme [Phys. Rev. Lett. 100 160501 (2008)] possesses a remarkable resilience to noise. In this scheme, the infidelity of a memory call scales only logarithmically with the size of the memory. In prior analyses of the scheme, however, this favorable scaling followed directly from the use of restricted noise models, thus leaving open the question of whether experimental implementations would actually enjoy the purported scaling advantage. We prove that, quite surprisingly, the favorable scaling holds for general noise models (including depolarization) and hence should be achievable in realistically noisy devices. As a corollary, we show that the benefits of the bucket-brigade scheme persist even when quantum error correction is used, in which case the scheme offers improved resilience to logical errors and better hardware efficiency.

*Work supported by: ARO, AFOSR, DOE, NSF, and the Packard Foundation

QuSP: The Quantum Simulator Package*

MATTHEW JONES (Presenter), LINCOLN CARR, Colorado School of Mines — With the advent and recent popularity of quantum computing (QC) architectural design, there has never been greater focus on quantum simulators and how they might inform the associated design decisions. There are many libraries and tools that hope to bridge the gap between optimal design patterns and the intuition that informs those patterns, but there are very few platforms that streamline this iterative process. With the guidance of the Science Gateways Community Institute, and backed by OpenMPS, a highly generalizable matrix product state simulation toolkit, we will address the aforementioned gap with QuSP, the Quantum Simulator Package. By building a clean, hosted graphical interface for performing quantum simulator simulations, leveraging both the high performance computing resources of the Colorado School of Mines and XSEDE, we will bridge this gap. QuSP provides a guided user experience to defining a system, its evolution, and any metrics a user might want to track through that evolution.

*Funded by NSF
10:00AM R09.00011: Cost of Classical Strong Simulation of the T-Gate Magic State*  LUCAS KOCIA (Presenter), MOHAN SAROVAR, Sandia — The stabilizer rank of qubit T-gate magic state has been postulated to grow slowest with increasing number of qubits, suggesting that the T-gate is in this sense the most efficient state outside the Clifford subtheory that can be simulated by classical strong simulation that nevertheless extends this subtheory to quantum universality. Unfortunately, the T-gate magic state's stabilizer rank scaling is not formally known and has only been found numerically for up to seven qubits. We examine this problem from the perspective of the cost of strong classical simulation of discrete Wigner functions in systems with odd dimension and compare with the known results for qubits. To accomplish this, we develop and exploit relationships between the number of critical points of quantum states' Wigner functions in a periodized stationary phase approximation and spanning decompositions of stabilizer states that are closely related to the stabilizer rank. We report on the trends we observe.

*SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. Any subjective views or opinions that might be expressed in the abstract do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

10:12AM R09.00012: Alibaba Cloud Quantum Development Platform: Large-Scale Classical Simulation of Quantum Circuits  FANG ZHANG, CUPJIN HUANG, Alibaba Quantum Laboratory, MICHAEL NEWMAN, Departments of Physics and Electrical and Computer Engineering, Duke University, JUNJIE CAI, HUANJUN YU, ZHENGXIONG TIAN, BO YUAN, HAIHONG XU, JUNYIN WU, Alibaba Group, XUN GAO, JIANXIN CHEN (Presenter), MARIO SZEGEDY, YAOYUN SHI, Alibaba Quantum Laboratory — We report our work on the Alibaba Cloud Quantum Development Platform(AC-QDP). AC-QDP provides a set of tools for aiding the development of both quantum computing algorithms and quantum processors, and is powered by a large-scale classical simulator deployed on Alibaba Cloud. In this note, we report the computational experiments demonstrating the classical simulation capability of AC-QDP. We use as a benchmark the random quantum circuits designed for Google's Bristlecone QPU \cite{GRCS}. We simulate Bristlecone-70 circuits with depth 1+32+1 in 0.43 second per amplitude, using 1449 Alibaba Cloud Elastic Computing Service (ECS) instances, each with 88 Intel Xeon(Skylake) Platinum 8163 vCPU cores @ 2.5 GHz and 160 gigabytes of memory. By comparison, the previously best reported results for the same tasks are 104 and 135 seconds, using NASA's HPC Pleiades and Electra systems, respectively (\cite{arXiv:1811.09599}). Furthermore, we report simulations of Bristlecone-70 with depth 1+36+1 and depth 1+40+1 in 5.6 and 580.7 seconds per amplitude, respectively. To the best of our knowledge, these are the first successful simulations of instances at these depths.
10:24AM R09.00013: Alibaba Cloud Quantum Development Platform: Applications to Quantum Algorithm Design  
CUPJIN HUANG, MARIO SZEGEDY (Presenter), FANG ZHANG, JIANXIN CHEN, XUN GAO, YAOYUN SHI, Alibaba Quantum Laboratory —
We report our work on the Alibaba Cloud Quantum Development Platform (AC-QDP). The capability of AC-QDP’s computational engine was already reported in \cite{arXiv:1805.01450, arXiv:1907.11217}. In this follow-up article, we demonstrate with figures how AC-QDP helps in testing large-scale quantum algorithms (currently within the QAOA framework). We give new benchmark results on regular graphs. AC-QDP’s QAOA framework can simulate thousands of qubits for up to 4 layers. Then we discuss two interesting use cases we have implemented on the platform: 1. Optimal QAOA sequences for small-cycle free graphs; 2. Graph structure discovery.

10:36AM R09.00014: Quantum linear system solver based on time-optimal adiabatic quantum computing and quantum approximate optimization algorithm*  
DONG AN (Presenter), LIN LIN, University of California, Berkeley — The condition number dependence is a crucial aspect of quantum linear system solvers. We demonstrate that with an optimally tuned scheduling function, adiabatic quantum computing (AQC) can solve a quantum linear system problem with $O(\kappa/\varepsilon)$ runtime, where $\kappa$ is the condition number, and $\varepsilon$ is the target accuracy. This achieves at least quadratic speedup over the standard vanilla AQC and reaches the complexity lower bound with respect to $\kappa$. The success of the time-optimal AQC implies that the quantum approximate optimization algorithm (QAOA) can also achieve the $O(\kappa)$ complexity with respect to $\kappa$. Our method is applicable to general non-Hermitian matrices (possibly dense), but the efficiency can be improved when restricted to Hermitian matrices, and further to Hermitian positive definite matrices. Numerical results indicate that QAOA can yield the lowest runtime compared to the time-optimal AQC, vanilla AQC, and the recently proposed randomization method. The runtime of QAOA is observed numerically to be only $O(\kappa \text{*poly}(\log(1/\varepsilon)))$.

*This work was partially supported by the Department of Energy under Grant No. DE-SC0017867, the Quantum Algorithm Teams Program under Grant No. DE-AC02-05CH11231 (L.L.), and the Google Quantum Research Award (D. A. and L.L.).
10:48AM R09.00015: Quantum optimal algorithm for general polynomials  KEREN LI (Presenter), Peng Cheng Laboratory, PAN GAO, Tsinghua University — Gradient descent algorithms, which is a first-order iterative algorithm, is widely used for optimization problems. To obtain the local minimum of a objective function, one calculates the gradients at the current point in a d-dimension space and then move the function along the negative gradient. This procedure requires $O(poly(d))$ calculation operations, which hinders the performance of the algorithm in a high dimensional optimization situation. Here, by learning a framework of a quantum iterative optimization algorithm and introducing an adapted encoding scheme, we develop the quantum gradient operation for an in-homogenous polynomial objective function with a unit norm constraint. Under certain circumstances, the calculation operations required for the algorithm decreases and is linear with the $O(poly(log(d)))$. Besides, we experimentally demonstrate it on a 4-qubit Nuclear Magnetic Resonance(NMR) quantum system and show the feasibility in polynomial optimization. Since the potential value in high dimensional optimization problems, this algorithm is supposed to influence the interdisciplinary research including Quantum Information and Artificial Intelligence, such as Support Vector Machine, Logistic regression, (quantum) Neural network.

Thursday, March 5, 2020 8:00 AM - 9:36 AM

Session R15 DFD GSNP: Granular, Porous Media, & Multiphase Flows I

210/212 - Anthony Chieco, University of Pennsylvania

8:00AM R15.00001: Flow of emulsions in heterogeneous media*  MARINE LE BLAY (Presenter), DENIS BARTOLO, Univ. Lyon, ENS de Lyon, Univ. Claude Bernard, CNRS, Laboratoire de Physique, F-69342, Lyon, France — We elucidate the collective dynamics of particles hydrodynamically driven through disordered environments. We build on model microfluidic experiments where we track the individual dynamics of hundreds of thousands oil droplets advected by an aqueous fluid through random lattices of pinning sites. Increasing the driving flow, we identify a sharp transition between a creeping regime and a mobilization regime where a finite fraction of the droplets proceed through a sparse network of branched and reconnected rivers. This dynamical transition is a critical phenomenon characterised by diverging time and length scales at the onset of mobilization. We however demonstrate that criticality is not accompanied by the correlated motion of particles in avalanches events. Mobilization requires at most the coordinated motion of ten particles at a time, but these erratic rearrangements are geometrically correlated over system spanning scales along a smectic river network. We conclude by commenting on the similarities and profound differences with the plastic depinning transition of flux lines in super conductors, or grains in eroded sand beds.

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8:36AM R15.00002: Controlling capillary fingering using pore size gradients in disordered media  NANCY LU (Presenter), CHRISTOPHER BROWNE, DANIEL AMCHIN, Chemical and Biological Engineering, Princeton University, JANINE K NUNES, Mechanical and Aerospace Engineering, Princeton University, SUJIT DATTA, Chemical and Biological Engineering, Princeton University — Capillary fingering is a displacement process that can occur when a non-wetting fluid displaces a wetting fluid from a homogeneous disordered porous medium. Here, we investigate how this process is influenced by a pore size gradient. Using microfluidic experiments and computational pore-network models, we show that the non-wetting fluid displacement behavior depends sensitively on the direction and the magnitude of the gradient. The fluid displacement depends on the competition between a pore size gradient and pore-scale disorder; indeed, a sufficiently large gradient can completely suppress capillary fingering. By analyzing capillary forces at the pore scale, we identify a non-dimensional parameter that describes the physics underlying these diverse flow behaviors. Our results thus expand the understanding of flow in complex porous media and suggest a new way to control flow behavior via the introduction of pore size gradients.

8:48AM R15.00003: Fluid Flow Mechanisms in Shale Organic Nanopores  FELIPE PEREZ VALENCIA (Presenter), DEEPAK DEVEGOWDA, Univ of Oklahoma — From a fluid dynamics perspective, production of hydrocarbons from unconventional reservoirs represents a challenge because (1) the fluids are located in porous organic matter in shale rocks where the pore sizes range from a few to a couple hundred nanometers, (2) the permeability of shale rocks is on the order of nanodarcy (1 darcy ≈ 10^{-12} m^2), and (3) the behavior of the fluids and their interactions with the pore surface are poorly understood. In this work we use molecular dynamics simulations to create molecular models of organic matter (kerogen) that host a hydrocarbon mixture that is liquid at normal conditions of pressure and temperature. Our models account for the chemical functionality and pore geometry of kerogen and serve as rigid frameworks to study the mechanisms by which the different species of the mixture flow from organic pores to a microfracture.

Our simulations indicate that the two phases free- and adsorbed-fluid coexist in the pores, and the mechanisms by which the molecules of each phase flow are different. While the free phase can expand and diffuse, the strong interaction between adsorbed molecules and the pore surface gives rise to surface diffusion and retards or impedes the arrival of the longer, heavier and aromatic molecules to the microfracture.

9:00AM R15.00004: Colloidal transport in porous media: Pore-scale interplay of advection, deposition, and erosion  NAVID BIZMARK (Presenter), Princeton Institute for the Science and Technology of Materials, Princeton University, JOANNA SCHNEIDER, RODNEY PRIESTLEY, SUJIT DATTA, Chemical and Biological Engineering, Princeton University — There is significant interest in applying colloids to remediate contaminated soils or aquifers. However, the transport of such colloids to porous subsurface regions is complex due to the interplay of particle adsorption, surface erosion, and pore-space advection. Here, we use a transparent model porous medium to directly image in 3D the interplay between adsorption and erosion events at the pore scale. Analysis of these processes allows us to determine the net particle deposition rate and further to predict the macroscopic net particle deposition profile. These findings show how the pore-scale dynamics can be controlled for macroscopic aims in remediation practices.
9:12AM R15.00005: CFD-DEM Study of Anomalous Collapse of Interacting Bubbles into an Incipiently Fluidized Bed  AZIN PADASH (Presenter), CHRISTOPHER M BOYCE, Columbia University — Computational fluid dynamics – discrete element method (CFD-DEM) recreates the collapse phenomenon of the recent magnetic resonance imaging (MRI) study (Boyce et al., Phys. Rev. Fluids, 2019, 034303) in which one bubble collapses when two bubbles are injected side-by-side into an incipiently fluidized bed, and the other bubble does not collapse and reaches the surface of the bed. Our simulation results reveal the underlying physics behind the collapse phenomenon which was ambiguous in the 2D imaging plane of the experimental results. The 3D visualization of voidage field and gas velocity field from simulations demonstrates that bubble collapses and it does not move out of the imaging plane of the study. Also, our results confirm the hypothesis of the MRI study where there should be a slight difference in size of the bubbles, which causes the gas flow to channel more favorably to the larger bubble. Therefore, the smaller bubble does not receive enough gas flow to channel through it and support its roof which leads to its collapse.

**Keywords:** CFD-DEM; Fluidization; Bubbles; Collapse; Magnetic Resonance Imaging

9:24AM R15.00006: Colloid-Enhanced Mobilization of Immiscible Fluids in Porous Media  JOANNA SCHNEIDER (Presenter), Chemical and Biological Engineering, Princeton University, NAVID BIZMARK, Princeton Institute for the Science and Technology of Materials, Princeton University, RODNEY PRIESTLEY, SUJIT DATTA, Chemical and Biological Engineering, Princeton University — More than 50% of the United States receives its drinking water from porous groundwater aquifers that are susceptible to contamination from industrial processes. The persistence of these contaminants after their initial introduction requires specialized remediation techniques. Here, we show that injection of colloidal particles improves contaminant removal from a porous medium compared to ambient flow alone. Specifically, by tailoring colloidal properties and injection conditions, we find that particles deposit on the solid surfaces of the porous medium, enhancing the local fluid pressure and pushing out trapped non-aqueous contaminants. We also develop a model to describe how changing permeability impacts mobilization and compare the model’s predictions to experimental results. Importantly, this approach avoids the need for repeated pumping and treatment, representing a major advancement in simplicity and cost over current approaches.
R15.00007: Complex Conductivity in Saturated Porous Media: Role of Membrane Polarization  QIUZI LI (Presenter), LANG FENG, Corporate Strategic Research, ExxonMobil Research and Engineering, STEVE CAMERON, Retired, HARRY DECKMAN, DENIZ ERTAS, Corporate Strategic Research, ExxonMobil Research and Engineering — We quantitatively explain the origin of complex conductivity of a porous medium made of non-conductive grains, saturated with a binary electrolyte. The medium is assumed to possess a heterogeneous immobile charge density, and to interact with ions in the electrolyte only through electrostatic interactions. We establish a theoretical framework relating spectral complex conductivity in these systems to the geometry and intrinsic properties of the materials, and validate the results with experiments on model systems. We conclude that complex conductivity arises due to concentration (membrane) polarization, which is driven by spatial inhomogeneity in the ionic transferences, i.e., the proportion of current carried by the cation vs. the anion. We obtain quantitative agreement between experiment and theory, not just for characteristic frequencies and amplitudes, but for the entire spectral shape of the phase angle between electric field and current density. The amplitude, scaling of the characteristic frequency with feature size, and the spectral shape of the phase angle differ markedly from complex conductivity associated with dispersed electronic conductors.

Thursday, March 5, 2020 8:00 AM - 10:48 AM

Session R16 DQI: Superconducting Qubits: Gates, Couplers and Crosstalk I 201 - Chen Wang, UMass

8:00AM R16.00001: Two-qubit gate with a parity-violated superconducting qubit*  ATSUSHI NOGUCHI (Presenter), Univ of Tokyo, SHINO KONO, Center for Emergent Matter Science, RIKEN, SHUMPEI MASUDA, Tokyo Medical and Dental University, KENTARO HEYA, SAMUEL PIOTR WOLSKI, Univ of Tokyo, HIROKI TAKAHASHI, Osaka University, TAKANORI SUGIYAMA, ALTO OSADA, DANY LACHANCE-QUIRION, YASUNOBU NAKAMURA, Univ of Tokyo — The second-order nonlinearity has been intensively studied over the decades in nonlinear optics for applications such as squeezed light sources and optical frequency combs. Three-wave mixing, the elementary process induced by the second-order nonlinearity, is also a key concept in the latest development of quantum transducers and has also been utilized for high-fidelity quantum manipulations of trapped ions with a parametric coupling. As is well known, a parity violation is required for the second-order nonlinearity. Here we propose a parity-violated superconducting qubit, which enables us to achieve a strong parametric coupling with a neighboring qubit based on the second-order nonlinearity. The qubit consists of a capacitively-shunted SNAIL [1] circuit under a finite flux bias. We demonstrate fast two-qubit gates (CZ, SWAP, and iSWAP) combined with echo pulses to suppress the effect of a residual longitudinal coupling and evaluate the average gate fidelities using an interleaved randomized benchmarking technique.


*This work is partly supported by JST PRESTO (JPMJPR1429), JST ERATO (JPMJER1601), and MEXT Q-LEAP (JPMXS0118068682).
8:12AM R16.00002: Characterization and Tuneup of High-Fidelity Two-Qubit Operations on a Parametrically Driven Gate*  
CHRISTOPHER WARREN (Presenter), ANDREAS BENGTSSON, GIOVANNA TANCREDI, XIU GU, ANTON FRISK KOCKUM, PHILIP KRANTZ, PER DELSING, JONAS BYLANDER, Chalmers Univ of Tech — Maintaining the fidelity of single- and two-qubit gates is a necessary requirement for building a quantum computer, especially in the NISQ era where every gate is critical. At the ideal limit without coherent or systematic errors, the gate fidelity fluctuates as $T_1$ fluctuates. It is important to be able to characterize the timescales over which system parameters may fall out of calibration, and the worst-performance cases should be reported. Here we present our work towards characterizing these effects, and we compare schemes for automating the recalibration process on a device consisting of fixed-frequency transmon qubits with a tunable coupler. The coupler is parametrically driven to selectively perform an iSWAP or CZ gate. Our results indicate that we are primarily limited by incoherent errors with single-qubit gates performing with >99.9% fidelity and two-qubit gates with fidelities >99.0%.

*Knut and Alice Wallenberg Foundation, Swedish Research Council, EU Flagship on Quantum Technology

8:24AM R16.00003: Efficient cavity control with SNAP gates  
THOMAS FOESEL (Presenter), Max Planck Inst for Sci Light, STEFAN KRASTANOV, Massachusetts Institute of Technology, LIANG JIANG, University of Chicago, FLORIAN MARQUARDT, Max Planck Inst for Sci Light — Microwave cavities coupled to superconducting qubits have been demonstrated to be a promising platform for quantum information processing. A major challenge in this setup is to realize universal control over the cavity. A promising approach are selective number-dependent arbitrary phase (SNAP) gates combined with cavity displacements. Whereas it could be proven that this is a universal gate set, a central question remained open: how can a given target operation be realized efficiently with a sequence of these operations.

In this talk, we present a practical scheme to address this problem. We will compare our results to previously known techniques: for many experimentally relevant applications, we find that the sequence length can be reduced by a factor of around 10 or higher. We will also sketch the working principle of our method.
Demonstrating a Continuous Set of Two-qubit Gates for Near-term Quantum Algorithms  
BROOKS FOXEN (Presenter), AI Quantum, Google, BEN CHIARO, MATTHEW MCEWEN, University of California, Santa Barbara, JOHN M MARTINIS, AI Quantum, Google — Quantum algorithms offer a dramatic speedup for computational problems in machine learning, material science, and chemistry. However, any near-term realizations of these algorithms will need to be heavily optimized to fit within the finite resources offered by existing noisy quantum hardware. Here, taking advantage of the strong adjustable coupling of gmon qubits, we demonstrate a continuous two-qubit gate set that can provide a 3x reduction in circuit depth as compared to a standard gate decomposition. We implement two gate families: an iSWAP-like gate to attain an arbitrary swap angle, θ, and a CPHASE gate that generates an arbitrary conditional phase, Φ. Using one of each of these gates, we can perform an arbitrary two-qubit gate within the excitation-preserving subspace allowing for a complete implementation of the so-called Fermionic Simulation, or fSim, gate set. We benchmark the fidelity of the iSWAP-like and CPHASE gate families as well as 525 other fSim gates spread evenly across the entire fSim(θ, Φ) parameter space achieving purity-limited average two-qubit Pauli error of 3.8 \times 10^{-3} per fSim gate.

Experimental implementation of universal nonadiabatic geometric quantum gates with a superconducting circuit  
ZIYUE HUA (Presenter), YUAN XU, Tsinghua University, TAO CHEN, South China Normal University, XIAOXUAN PAN, XUEGANG LI, JIA XIU HAN, WEIZHOU CAI, YU WEI MA, HAIYAN WANG, YI PU SONG, Tsinghua University, ZHENG YUAN XUE, South China Normal University, LUYAN SUN, Tsinghua University — Using geometric phase to realize noise-resilient quantum computing is an important method to enhance control fidelity. In this work, we experimentally realize a universal nonadiabatic geometric quantum gate set in a superconducting qubit chain. We characterize the realized single- and two-qubit geometric gates with both quantum process tomography and randomized benchmarking methods. The measured average fidelities for single-qubit rotation gates and two-qubit controlled-Z gate are 0.9977 and 0.977, respectively. Besides, we also experimentally demonstrate the noise-resilient feature of the realized single-qubit geometric gates by comparing their performance with the conventional dynamic gates with different types of errors in the control field. Thus, our experiment proves a way to achieve high-fidelity geometric quantum gates for robust quantum computation.
9:00AM R16.00006: Bounds on cross-resonance gate fidelity in an extended parameter regime  EMILY PRITCHETT (Presenter), ABHINAV KANDALA, DAVID MCKAY, IBM Tj Watson Research Center — The cross-resonance (CR) interaction is the primary method for enabling two-qubit gates in systems with fixed-frequency transmons using only microwave control. Eliminating the need for tunable circuit elements reduces the system's susceptibility to low-frequency noise, but the cost is more complicated coherent dynamics during the gate [1,2,3,4], both between the targeted qubit pair and to qubits that are nominally idle (spectators). We bound the two-qubit CR gate fidelity as set by unitary dynamics, showing its sensitivity to the parameters governing the two-qubit interaction (coupling strength, relative energies, anharmonicities, and total gate time) and to parameters required to build larger devices (frequency allocation of neighboring qubits). As we reach the limit of fidelities achieved by control of our current devices, consideration of this larger parameter space will let us design devices with higher performance.


9:12AM R16.00007: Superconducting qubit gates based on accelerated adiabatic evolution*  FNU SETIAWAN (Presenter), PETER GROSZKOWSKI, University of Chicago, Pritzker School of Molecular Engineering, HUGO RIBEIRO, Max Planck Institute for the Science of Light, Erlangen, AASHISH CLERK, University of Chicago, Pritzker School of Molecular Engineering — Quantum gates based on adiabatic evolution are in principle desirable because of their intrinsic robustness against small errors or imperfections in the control pulses. In practice however, the requirement of extremely long evolution times makes them very susceptible to dissipation and noise, resulting in poor fidelities. Recently, protocols based on shortcuts to adiabaticity have been used to design accelerated version of adiabatic quantum gates [1,2]. These gates can be fast while still possessing some of the robustness properties of purely adiabatic gates. We perform detailed theoretical studies and simulations exploring the performance of such gates in realistic superconducting qubit platforms. This includes single qubit gates in protected qubit architectures such as fluxonium, as well as two-qubit gates in cavity-coupled transmon architectures [3].


*Research was sponsored by the Army Research Office and was accomplished under Grant Number W911NF-19-1-0328
Microwave-activated entangling gates in high coherence superconducting qubits  
LONG NGUYEN (Presenter), AARON SOMOROFF, QUENTIN FICHEUX, YEN-HSIANG LIN, IVAN PECHENEZHSKIY, University of Maryland, College Park, YINQI CHEN, KONSTANTIN NESTEROV, MAXIM G VAVILOV, University of Wisconsin-Madison, VLADIMIR MANUCHARYAN, University of Maryland, College Park — We report experimental progress on microwave-activated entangling gates with capacitively coupled fluxonium qubits. When biased at the flux sweet-spot, individual qubit transition has long coherence (the best device has $T_2 > 400$ us) [1]. A control-Z gate can be implemented by sending a short $2\pi$-pulse at the frequency near the $1\rightarrow 2$ transition of the target qubit [2]. The gate transition has higher frequency and larger matrix element than the qubit transition, resulting in fast gate and minimal spurious phase errors. Another microwave entangling gate, similar to the cross-resonance gate in transmon [3], can be applied to the computational subspace. We discuss qubits' design and fabrication, initialization, readout, and benchmarking of the gates.


Demonstration of entangling gate for all-to-all connected superconducting qubits*  
MARIE LU (Presenter), JEAN-LOUP VILLE, SYDNEY SCHREPPLER, University of California, Berkeley, FELIX MOTZOI, LUKAS F BUCHMANN, Physics, Aarhus University, IRFAN SIDDIQI, University of California, Berkeley — Exploring highly connected networks of qubits is invaluable for implementing various quantum codes and simulations. All-to-all connectivity allows for entangling qubits with reduced gate depth. In the ion community, the Mølmer-Sørensen gate is routinely used to entangle over a dozen qubits with high fidelity. We report on the observed fidelity for a Mølmer-Sørensen-like interaction through the use of shared coplanar waveguide (CPW) resonators to couple multiple superconducting qubits. This gate allows us to selectively entangle any subset of the qubits coupled to the shared resonator.

*This research was supported by the LPS HiPS program under ARO grant W911NF1810178 and the L’Oreal USA for Women in Science Fellowship.

Multi-qubit gate mediated by a shared microwave resonator: Error analysis*  
JEAN-LOUP VILLE (Presenter), MARIE LU, SYDNEY SCHREPPLER, University of California, Berkeley, FELIX MOTZOI, LUKAS F BUCHMANN, Aarhus University, IRFAN SIDDIQI, University of California, Berkeley — Using microwave dressing of superconducting qubits, it is possible to implement a multi-qubit gate via a shared resonator. The gate investigated here is analogous to the Mølmer-Sørensen gate commonly used for trapped-ion qubits, but using the photon mode of the resonator instead of the phonon mode of the ions. The gate requires the use of two-photon transitions induced by bi-chromatic fields. We discuss in this talk the different sources of errors currently limiting the fidelity of the gate, relative to the coherence of the driving fields and the lifetimes of the dressed qubits.

*This work was funded by the LPS HiPS program under ARO grant W911NF1810178 and L’Oréal USA For Women in Science Fellowship Program.
Fidelity Optimization of the Cross-resonance Gate on a Multi-qubit Quantum Processor

RAVI KAUSHIK NAIK (Presenter), BRADLEY MITCHELL, AKEL HASHIM, JOHN MARK KREIKEBAUM, IRFAN SIDDIQI, University of California, Berkeley — In this work, we benchmark the performance of the cross-resonance gate in a multi-qubit setting, and evaluate gate fidelity as a function of circuit and control parameters, such as qubit detuning, effective coupling rate, and control pulse shape. We use numerical techniques to efficiently optimize gate parameter configurations. Lastly, we monitor the error syndromes of calibrated gates to investigate their sensitivity to environmental drift. This work outlines systematic calibration and operation of cross-resonance gates with model-guided optimization for general algorithmic utilization in near-term quantum computers.

*This research was supported by the LPS HiPS program under ARO grant W911NF1810178.

10:12AM R16.00012: A continuously tunable coupler for switching off adjacent qubit coupling in a superconducting circuit

XUEGANG LI (Presenter), TIANQI CAI, ZHILING WANG, XIAOXUAN PAN, YUWEI MA, WEIZHOU CAI, JIAXIU HAN, XIYUE HAN, YUKAI WU, HONGYI ZHANG, YIPU SONG, LUMING DUAN, LUYAN SUN, Institute for Interdisciplinary Information Sciences, Tsinghua University — Controllable interaction between superconducting qubits is desirable for large-scale quantum computation and simulation. We experimentally realize a simply designed and flux-tunable coupler with continuous tunability that can turn off the adjacent qubit coupling in a superconducting circuit. Based on this coupler, we demonstrate a new scheme for a two-qubit controlled-Z gate: two Xmon qubits, originally far detuned, are first gradually brought into resonance while adjusting the coupler to keep the qubit-qubit coupling off; then the qubit-qubit coupling is turned on by the tunable coupler for the necessary interaction; finally the two qubits are brought out of resonance to the idle points while keeping the coupling off. This scheme not only efficiently suppresses the leakage out of the computational subspace but also allows for a large qubit-qubit interaction strength. We achieve an average controlled-Z gate fidelity of 98.3%, characterized via quantum process tomography and dominantly limited by the system decoherence.
10:24AM R16.00013: Cancellation of unwanted ZZ interactions by superconducting qubit engineering*  
RONI WINIK (Presenter), Research Laboratory of Electronics, Massachusetts Institute of Technology, CATHERINE LEROUX, AGUSTIN DI PAOLO, Département de Physique, Université de Sherbrooke, JOCHEN BRAUMUELLER, MORTEN KJAERGAARD, ANTTI VEPSALAINEN, Research Laboratory of Electronics, Massachusetts Institute of Technology, DAVID K KIM, JONILYN YODER, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, MIT Lincoln Laboratory, ALEXANDRE BLAIS, Département de Physique, Université de Sherbrooke, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, WILLIAM OLIVER, Research Laboratory of Electronics, Department of Electrical Engineering & Computer Science, Department of Physics, Massachusetts Institute of Technology and MIT Lincoln Lab — We present a method to cancel the unwanted always-on ZZ interaction in transmon based qubit architectures by qubit engineering. We employ a new engineered qubit, which operates as a weakly anharmonic oscillator and has anharmonicity comparable to the transmon qubit, but with a positive sign. We test this concept on the cross-resonance-gate architecture [1] and outline various strategies for optimal chip design. Based on that, we design a new architecture for a superconducting quantum processor that has an inherent suppression of the unwanted ZZ interactions. Our work addresses on one of the major challenges in a commonly used architecture for superconducting quantum processors, and it enables higher fidelity multiqubit gates.


*This research was funded in part by the ARO grant No. W911NF-18-1-0411; and by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

10:36AM R16.00014: Implementation of a conditional-phase gate by using in-situ tunable ZZ-interactions*  
JOHANNES HERRMANN (Presenter), MICHELE COLLODO, CHRISTIAN KRALGUND ANDERSEN, ANTS REMM, STEFANIA LAZAR, LIANGYU CHEN, NATHAN LACROIX, JEAN-CLAUDE BESSE, THEO WALTER, ANDREAS WALLRAFF, CHRISTOPHER EICHLER, Department of Physics, ETH Zurich — High fidelity two-qubit gates exhibiting low crosstalk are essential building blocks for gate-based quantum information processing. In superconducting circuits two-qubit gates are typically based either on RF-controlled interactions or on the in-situ tunability of qubit frequencies. Here, we present an alternative approach using a tunable ZZ-interaction between two-qubits, mediated by a flux-tunable coupler element. By adding a direct capacitive coupling path between the qubits, we are able to control the ZZ-coupling rate over three orders of magnitude. Using this coupling mechanism we implement a conditional-phase gate without relying on resonant exchange of excitations and characterize its performance in terms of gate fidelity, leakage and residual coupling in the idle configuration.

*We acknowledge support by the ODNI, IARPA, via grant W911NF-16-1-0071, by NCCR QSIT, the EU Flagship H2020-FETFLAG-2018-03 project 820363 OpenSuperQ and by ETH Zurich
8:00 AM R17.00001: Multiplexing quantum modules in computational and communication systems.* [Invited] KAE NEMOTO (Presenter), National Institute of Informatics — There are many advantages to processing quantum information in a distributed fashion. The technology required to connect multiple quantum computers together provides an ideal way to naturally scale up one's computational resources. Such a feature is now standard in the classical domain; however, quantum information systems fundamentally differ from their classical counterparts in several ways. It is these differences that bring unique advantages to the distributed quantum information processing realm. Distributed quantum information systems are decomposed into modules, the fundamental building block of such systems. Adding more modules significantly increases the computational resource. The modules are simple enough to be able fully characterizable and merge quantum communication and computation approaches together. They give an architecture free technology. In this talk, we focus on these unique features of distributed quantum information processing and give a few examples of how we can implement various protocols and architecture for quantum computation and communications with an NV-based quantum module. Further we illustrate the unique advantage quantum multiplexing enables.

*This work was partly supported by MEXT KAKENHI Grant number 15H05870, 19H00662 and MEXT Quantum Leap Flagship Program (MEXT Q-LEAP) Grant Number JPMXS0118069605.

8:36 AM R17.00002: Designing Scalable Quantum Network Architectures MARTIN SUCHARA (Presenter), JOAQUIN F CHUNG MIRANDA, RAJKUMAR KETTIMUTHU, Argonne National Laboratory, ALEXANDER KOLAR, Northwestern University, XIAOLIANG WU, Illinois Institute of Technology, TIAN ZHONG, University of Chicago — Simulation-driven design is an essential tool in the development of quantum communication networks. In the past few years experimental quantum network demonstrations moved from table-top experiments to metropolitan-scale deployments and long-distance repeater network prototypes. As the number of optical components in these experiments increases, simulations simplify experiment planning and allow comparisons of alternative network architectures. In this work we use simulations to quantify the performance of networks with quantum router and repeater nodes. Our simulator of quantum network communication, called SeQUeNCe, performs simulations at the individual photon level with picosecond resolution. Faithful evaluations are achieved by modeling interactions between the physical layer, control protocols, and applications. We implement simplified models of optical components and the control protocol stack. End-to-end performance is evaluated for quantum key distribution and quantum state teleportation applications, and correctness of our models is partially validated by comparing against prior experimental results.
Routing in a quantum network

WILLIAM MUNRO (Presenter), NTT Basic Research Labs, NICOLE LO PIPARO, MICHAEL HANKS, KAE NEMOTO, National Institute of Informatics, Tokyo, Japan — It is now well known that quantum physics offers novel ways for information communication. It is expected that these principles will lead to a quantum enabled internet supporting new communication, computation and metrologocial tasks. Given the global nature of such an internet, it is clear that quantum repeaters will play an essential role in both its development and abilities. As such the efficient routing of quantum (and classical) signals will be paramount.

We discuss how the different repeater generations naturally require different routing approaches: the lower ones favoring a circuit switched approach with static routing while the third generation are ideal for a packet switched approach with dynamic routing. We illustrate how dynamic routing significantly boosts the networks performance especially when multiple users want to communicate simultaneously while allowing multiple simultaneous routes to be used by a single user. It is important to characterize the performance of the various approaches and so we introduce various cost metrics associated with the resources used within the repeaters nodes to normalize our communication rates by. Our results show the performance of the network heavily depends on efficient classical communication and the network associated with that.

A novel approach towards designing and structuring Quantum Communication devices and Quantum information processing

ADITYA CHINCHOLE (Presenter), Electronics and Telecommunication, Yeshwantrao Chavan College of Engineering — A completely new approach to quantum computation and simulation has been devised. Looking into various methods like Trapped ion, quantum communication with microwave photons, space division multiplexing optical fibre and comparing these methods to know the best suitable technique for information processing. A modified quantum information processing system is also stated in this paper. Efficient and simple techniques are also studied in depth for optical fibre communication.
9:12AM R17.00005: Towards inter-city entanglement generation using solid state spins in diamond.* ARIAN STOLK (Presenter), Delft University of Technology, JACO MORITS, ERWIN VAN ZWET, RONALD HAGEN, AD VERLAAN, TNO, MATTHEW WEAVER, RONALD HANSON, Delft University of Technology — Large scale networks where entanglement is generated and exploited between nodes are of great interest for both practical applications as well as fundamental tests of nature[1]. The NV-centre in diamond provides an excellent platform for realizing such a network, with recent work demonstrating fast entanglement generation[2] and entanglement between the NV-centre qubit and a telecom photon [3]. In this talk I will show latest experimental progress towards generating entanglement between two Dutch cities via 30km of fibre. This experiment will be the first link in a metropolitan scale quantum network in the Netherlands, which will serve as a test bed for the development of the Quantum Internet.


*This work was supported by the Netherlands Organisation for Scientific Research (NWO) through a VICI grant, and the European Research Council through an ERC Consolidator Grant.

9:24AM R17.00006: Entanglement Certification in Witness Experiments with Arbitrary Noise BAS DIRKSE (Presenter), MATTEO POMPILI, RONALD HANSON, Delft University of Technology, MICHAEL WALTER, University of Amsterdam, STEPHANIE WEHNER, Delft University of Technology — Entanglement is a fundamental property of quantum mechanical systems and an essential resource for quantum network applications. Carefully certifying entanglement is therefore an important task that is often achieved using entanglement witness experiments. Given only finite trials, the statistical confidence is typically expressed as the number of observed standard deviations of witness violations. This method implicitly assumes that the noise is well-behaved so that the central limit theorem applies.

In this work, we derive a method to certify entanglement without putting any assumptions on the state at each trial. This allows for arbitrarily correlated noise. We quantify the confidence using the p-value, the probability of obtaining data as extreme as the observed experimental data with only separable states. We give a formal abstract model of witness experiments that takes into account imperfect measurement devices and random number generators. We provide a simple method for sound data collection and show how to compute an upper bound to the p-value from the observed measurement data and device characteristics. We illustrate the use of our method with detailed examples based on realistic simulation of NV centres. This method applies to any witness experiment in general.
A Quantum Internet will enable new applications that are provably impossible with classical communication alone. However, the optical fibers used to carry the quantum information are inherently lossy. To overcome the exponential losses over distance so-called quantum repeaters are needed to amplify the signal.

For the purpose of a scalability analysis we investigate the performance of different architectures using atomic-ensemble technology in a large repeater chain spanning hundreds of kilometers. We go on to determine hardware requirements needed to cross the theoretical bound on secret key rate generation through direct transmission. By including multi-pair emission, a main source of error for these types of architectures, into our simulation we go beyond current analytical modeling of perfect photon pair sources. This allows us to assess the potential of different component technologies, such as photon sources and quantum memories, and quantify what improvements are necessary to bridge long distances.

With our simulation we provide a crucial stepping stone towards a blueprint for a pan-European quantum internet.

*STW Netherlands, NWO VIDI grant, ERC Starting grant and NWO Zwaartekracht QSC. This project (QIA) has received funding from the European Union's Hori- zon 2020 research and innovation programme under grant agreement No 820445.
10:00AM R17.00009: Deterministic entanglement between non-interacting systems with linear optics*  LEIGH MARTIN (Presenter), Department of Physics, Harvard University, BIRGITTA K WHALEY, University of California, Berkeley — Measurement-based heralded entanglement schemes provide the primary method to entangle physically separated nodes in most quantum systems. However, the impossibility of performing a deterministic Bell measurement with linear optics bounds the success rate of these protocols to at most 50%. Here we show that the ability to perform feedback during the measurement process enables unit success probability in a single shot. Our primary feedback protocol, based on photon counting, retains the same robustness as the standard Barrett-Kok scheme, while doubling the success probability even in the presence of loss. Furthermore, it generalizes to creation of distributed $N$-particle Dicke states. In superconducting circuits, for which homodyne detectors are more readily available than photon counters, we give another protocol that can deterministically entangle remote qubits given realistic parameters. In constructing the latter protocol, we derive a general expression for locally optimal control that applies to any continuous feedback problem.

*The research is based upon work supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050.

10:12AM R17.00010: Protocols for creating and purifying GHZ states*  SEBASTIAN DE BONE (Presenter), Delft University of Technology, RUNSHENG OUYANG, Tsinghua University, KENNETH GOODENOUGH, DAVID ELKOUSS, Delft University of Technology — The distribution of high quality Greenberger-Horne-Zeilinger (GHZ) states is at the heart of many applications in quantum information and the upcoming quantum internet, ranging from extending the baseline of telescopes to secret sharing. They also play an important role in error-correction architectures for distributed quantum computation, where EPR pairs are leveraged to create an entangled network of quantum computers.

Here, we investigate the creation of GHZ states over quantum networks. In particular, we introduce an algorithm based on dynamical programming to optimize over a large class of protocols that create and purify GHZ states. The new protocols outperform previous proposals for relevant scenarios, by reducing the resources necessary for GHZ creation, thus bringing the aforementioned applications closer to reality.

*This work was supported by the Netherlands Organization for Scientific Research (NWO/OCW), as part of the Quantum Software Consortium program (project number 024.003.037 / 3368).
10:24AM R17.00011: Constraints on continuous variable entanglement swapping in the presence of photon loss  ALEX KWIATKOWSKI (Presenter), University of Colorado, Boulder, EZAD SHOJAEE, SCOTT GLANCY, EMANUEL H KNILL, National Institute of Standards and Technology — In many procedures for entanglement swapping in the continuous variable domain the entangling measurement is quadrature measurement of linear mixtures of the two modes sent by the two parties that wish to swap entanglement. In the presence of sufficient photon loss, which we model as a fictitious beamsplitter with the environment on each of the two modes, we show that such a measurement cannot be used to swap entanglement. We show analytically that if the modes sent by the two parties suffer losses that average between them to 50% or more, then any passive linear circuit followed by quadrature measurement has a separable POVM on those modes and therefore cannot be used to perform entanglement swapping. We will also discuss the case where the constraints on the measurement are relaxed to include arbitrary Gaussian resources.

10:36AM R17.00012: Quantum Control through Optical Nonlinearities for Error Corrected One-way Quantum Repeaters  STEFAN KRASTANOV (Presenter), MIKHEL HEUCK, Massachusetts Institute of Technology MIT, KURT JACOBS, Army Research Laboratory, PRINEHA NARANG, Harvard University, DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — The use of exclusively optical modes for quantum communication and quantum computing is intriguing due to its potential to work at room temperatures. However, restricting architectures to only optical modes (i.e. quantum harmonic oscillators with simple couplings), leaves very few knobs available for the control of such systems. We present how the couplings between multiple optical modes, mediated by material nonlinearities, enable the performance of error correction and logical operations for a number of small bosonic error correcting codes. This high level of control is achieved through designing arbitrary pulse shapes for the classical laser light used to trigger the resonant nonlinear interaction between multiple quantum modes. This would enable one-way quantum repeaters with error correction and is a necessary step for room-temperature quantum photonic information processing.
10:48AM R17.00013: Entanglement of a pair of quantum emitters under continuous fluorescence measurements* PHILIPPE LEWALLE (Presenter), CYRIL ELOUARD, SREENATH KIZHAKKUMPURATH MANIKANDAN, University of Rochester, XIAO-FENG QIAN, Stevens Institute of Technology, J H EBERLY, ANDREW N JORDAN, University of Rochester —
We examine the state and entanglement dynamics of two remote qubits, under continuous measurements of their spontaneous emission. Erasing information about which qubit emitted a particular contribution to the joint measurement signal is possible with both photodetection, and well-chosen quadrature measurements; in either case, measurements then effectively perform an entanglement swapping operation, taking entanglement created between each qubit and its emitted field mode, and generating correlations between the two remote qubits instead. We compare the quantum jump trajectories from photodetection with the diffusive quantum trajectories, which arise from quadrature measurements, demonstrating that they have equivalent average entanglement yield under ideal conditions. Outlook and next steps will be discussed.

*PL, CE, SKM, and ANJ acknowledge funding from NSF grant no. DMR-1809343, and US Army Research Office grant no. W911NF-18-10178. PL acknowledges support from the US Department of Education grant No. GR506598 as a GAANN fellow. XFQ and JHE acknowledge support from NSF grants PHY-1505189 and PHY-1539859.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R18 GSNP: Electron-Phonon Coupling and High-Temperature Superconductivity 205 - John Sous, Columbia Univ - Tag(s): Invited
8:00AM R18.00001: Reconsidering the electron-phonon problem and bounds on $T_c$ [Invited]
STEVEN KIVELSON (Presenter), Stanford Univ — We exploit the fact that the Holstein model of the electron-phonon problem can be treated without approximation using fermion-minus-sign-free determinant quantum Monte Carlo methods to establish results that can be compared quantitatively and unambiguously with approximate methods based on Migdal-Eliashberg (ME) theory. In the relevant limit in which the phonon frequencies are small compared to the Fermi energy (strong retardation), we find that ME theory is extremely accurate up to moderate values of the dimensionless electron-phonon coupling $\lambda$, and then breaks down relatively suddenly beyond a characteristic value, $\lambda^{*} \sim 1$, beyond which polaron physics is significant. One consequence of this is that – in contrast with earlier beliefs based on ME theory – the superconducting $T_c(\lambda)$ has its maximum value at $\lambda \approx \lambda^{*}$. This implies that there is an upper bound on $T_c$ from the electron phonon mechanism $T_c \leq A w_{\text{max}}$, where $w_{\text{max}}$ is the maximum phonon energy and we estimate that $A \approx 1/10$.

References

8:36AM R18.00002: Light bipolarons from strong Peierls electron-phonon coupling* [Invited]
MONA BERCIU (Presenter), Physics and Astronomy, University of British Columbia, JOHN SOUS, Physics, Columbia University, MONODEEP CHAKRABORTY, Centre for Theoretical Physics, Indian Institute of Technology, Kharagpur, ROMAN KREMS, Chemistry, University of British Columbia — It is widely accepted that phonon-mediated high-temperature superconductivity is impossible at ambient pressure, because of the very large effective masses of polarons and bipolarons at strong electron-phonon coupling. We challenge this by showing that strongly bound yet very light bipolarons appear for strong Peierls coupling. These bipolarons exhibit many unconventional properties; e.g., at strong coupling there are two low-energy bipolaron bands that are stable against strong Coulomb repulsion. Using numerical simulations and analytical arguments, we show that these properties result from the specific form of the phonon-mediated interaction, which is of “pair hopping” instead of regular density-density type. This unusual effective interaction is bound to have nontrivial consequences for the superconducting state expected to arise at finite carrier concentrations and should favor a large critical temperature.

*We acknowledge funding from the Stewart Blusson Quantum Matter Institute at the University of British Columbia and from the Natural Sciences and Engineering Research Council of Canada. We acknowledge access to the computing facilities of the DST-FIST (phase-II) project installed in the Department of Physics, Indian Institute of Technology (IIT), Kharagpur, India.
9:12AM R18.00003: Superconductivity in Ultra-Low Density Dirac Materials Driven by a Ferroelectric Quantum Critical Point* [Invited] JONATHAN RUHMAN (Presenter), Physics, Bar Ilan University, VLADYSLAV KOZII, Condensed Matter Physics, Berkeley, ZHEN BI, Massachusetts Institute of Technology MIT — According to standard lore, low-density materials such as semimetals should not become superconducting. They are characterized by a small Fermi energy, which is comparable to the Debye frequency and moreover, their density of states is extremely small. Nonetheless, superconductivity is ubiquitous in topological materials, including YPtBi, Bi$_2$Se$_3$, Bi, Cd$_3$As$_2$, PbTe and SnTe, which raise the question regarding the microscopic picture of pairing in these systems. In this talk, I will discuss the option of pairing mediated by ferroelectric fluctuations close to a quantum critical point in a Dirac semimetal. I will show that such fluctuations lead to pairing, even when the Fermi energy is smaller than any bosonic frequency in the problem and possibly, even at charge neutrality.

*I acknowledge funding from the Israeli Science Foundation under grant No. 967/19

9:48AM R18.00004: New Perspectives from Spectroscopy on the Bismuth Oxide Superconductors* [Invited] NICHOLAS PLUMB (Presenter), Swiss Light Source, Paul Scherrer Institute — Despite being known for decades, the perovskite bismuth oxide superconductors (max $T_c > 30$ K) were never experimentally probed to nearly the extent of more famous high-$T_c$ materials, such as cuprates and iron-based superconductors. This is a pity, because their phenomenology and underlying physics connect with a wide array of contemporary interests: not only unconventional/high-$T_c$ superconductivity, but also metal-insulator and insulator-superconductor transitions, (bi)polarons, CDWs/charge-order, disordered systems, and so on. Recently we have studied Ba$_{1-x}$K$_x$BiO$_3$ films using angle-resolved photoemission and resonant inelastic x-ray scattering. These experiments establish the unusual “bond disproportionated” nature of the parent compound and track its evolution into the superconducting doping region. The under- to optimally-doped region of the phase diagram is particularly fascinating. There spectra show a highly dispersive conduction band forming a well-defined Fermi surface, despite a total absence of sharp peaks that would typically accompany weakly interacting quasiparticles. We observe, moreover, two types of pseudogap-like spectral behaviors: The first extends over a broad energy scale and persists above room temperature; the other is set in a narrow region around $E_F$ and opens in a well-defined temperature range above $T_c$. I will discuss how these psuedogaps appear to be linked - namely that they represent the precipitation of ordered bipolaronic insulating regions out of a disordered polaronic liquid.

*This work is supported by the Swiss National Science Foundation under projects 200021_159678 and 200021_185037.
The nature of superconductivity in the dilute semiconductor SrTiO₃ has remained an open question for over half a century. Thin film heterostructures provide new opportunities to examine SrTiO₃ superconductivity using a newly developed method for engineering band alignments at oxide interfaces to access the electronic structure of Nb-doped SrTiO₃ using high-resolution tunneling spectroscopy. While we observe strong coupling to the highest-energy longitudinal optic phonon consistent with $\lambda \sim 1$, the superconducting gap is found to be in the weak-coupling limit of BCS theory, i.e. $\lambda_{BCS} \sim 0.1$. This discrepancy arises in the context of an unusual anti-adiabatic condition for superconductivity in SrTiO₃ (Fermi energy < Debye energy), which we find precisely bounds the superconducting dome.

This work was done in collaboration with Hyeok Yoon, Adrian Swartz, Hisashi Inoue, Yasuyuki Hikita, and Sri Raghu.

*This work was supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract No. DE-AC02-76SF00515; and by the Gordon and Betty Moore Foundations Emergent Phenomena in Quantum Systems Initiative through Grant GBMF4415.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R19 GMAG: Magnetic interactions at complex oxide interfaces
207 - Alexander Grutter, National Institute of Standards and Technology - Tag(s): Invited
Efficient bias-driven magnetization control by orbital selection at a La$_{0.67}$Sr$_{0.33}$MnO$_3$ interface* [Invited] LE DUC ANH (Presenter), TAKASHI YAMASHITA, NOBORU OKAMOTO, HIROKI YAMASAKI, DAISEI ARAKI, MUNETOSHI SEKI, HITOSHI TABATA, MASAAKI TANAKA, SHINOBU OHYA, Univ of Tokyo — Bias-driven magnetization control of a ferromagnet, which utilizes the ability of controlling the magnetic anisotropy (MA) with an electric field, is crucial for spintronic applications due to its low power consumption. However, it remains a challenge to induce a large change in the MA of ferromagnetic materials that can rotate the magnetization. In this work, using La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO)/SrTiO$_3$ (STO)/LSMO magnetic tunnel junctions (MTJs), we demonstrate that a drastic change in the MA of LSMO can be induced when the chemical potential ($E_F$) at the LSMO/STO interface is moved between bands with different orbital symmetries. By this new approach, we successfully realize a deterministic and magnetic-field-free 90°-magnetization switching of LSMO solely by applying a small electric field of 0.05 V/nm on the tunnel barrier, with a negligibly small current density of $\sim 10^{-2}$ A/cm$^2$.

The studied MTJs are grown on an STO (001) substrate by molecular beam epitaxy. We probe the orbital symmetry of the carriers and the MA of the LSMO layers at each bias $V$ by measuring the magnetic-field-direction dependence of the tunneling conductance and that of the tunneling magnetoresistance (TMR), respectively. Using this approach, we show that, with applying $V$, the MA of the LSMO switches from a two-fold symmetry to a four-fold symmetry by shifting $E_F$ from the $e_g$ band to the $t_{2g}$ band [1]. This change of MA is strong enough to rotate the magnetization direction from [110] to [1-10] without any assisting magnetic field. Our findings indicate that highly efficient magnetization control can be realized by designing materials so that the $E_F$ lies close to the band edges of different-symmetry orbitals [2].


*This work was supported by Grants-in-Aid for Scientific Research (No. 18H03860, 17H04922), the JST CREST Program (JPMJCR1777), and Spin-RNJ.
Spin-orbit coupling and local magnetism at a complex oxide interface

[Invited] VLAD PRIBIAG (Presenter), University of Minnesota — SrTiO$_3$-based thin-film heterostructures are a powerful platform for studying a wide array of electronic phases in two dimensions, at high carrier densities. This talk will discuss low-temperature electronic transport studies of NdTiO$_3$/SrTiO$_3$ interfaces, which reveal local ferromagnetic order and strong spin-orbit interaction. As the magnetic field angle is gradually tilted away from the sample normal, the data reveals an intriguing interplay between strong k-cubic Rashba-type spin-orbit coupling and a substantial magnetic exchange interaction from local magnetic regions. The resulting quantum corrections to the conduction are in excellent agreement with existing models and allow sensitive determination of the small magnetic moments (22 $\mu_B$ on average), their magnetic anisotropy and mutual coupling strength. This effect is expected to arise in other 2D magnetic materials systems and could provide a simple yet powerful tool for investigating local magnetism.


*This work was supported primarily by the Office of Naval Research under Award No. N00014-17-1-2884. Film growth and structural characterizations were funded by the U.S. Department of Energy through the University of Minnesota Center for Quantum Materials, under Grant No. DE-SC-0016371. Portions of this work were conducted in the Minnesota Nano Center, which is supported by the National Science Foundation through the National Nano Coordinated Infrastructure Network (NNCI) under Award No. ECCS-1542202. Sample structural characterization was carried out at the University of Minnesota Characterization Facility, which receives partial support from NSF through the MRSEC program under Award No. DMR-1420013.
Interfacial control of chiral magnetic interactions and Hall effect in iridate-manganite superlattices* [Invited] ELIZABETH SKOROPATA (Presenter), JOHN A NICHOLS, JONG MOK OK, Oak Ridge National Lab, RAJESH V CHOPDEKAR, Lawrence Berkeley National Laboratory, EUN SANG CHOI, National High Field Magnet Laboratory, ANKUR RASTOGI, CHANGHEE SOHN, XIANG GAO, THOMAS FARMER, RYAN DESAUTELS, Oak Ridge National Lab, YONGSEONG CHOI, DANIEL HASKEL, JOHN WILLIAM FREELAND, Argonne National Laboratory, SATOSHI OKAMOTO, MATTHEW BRAHLEK, HO NYUNG LEE, Oak Ridge National Lab — One of the most intriguing outcomes of symmetry breaking and spin-orbit interactions in magnetic systems is the possibility to create non-collinear and chiral spin textures. The Dzyaloshinskii-Moriya interaction (DMI) results from strong spin-orbit coupling and broken inversion symmetry to generate magnetization rotations with fixed chirality. The discovery of magnetic skyrmions originating from strong DMI in metal thin films has led to an explosion of efforts to manipulate magnetic phases originating from interfaces. I will describe our progress to understand interface-induced magnetism in epitaxial $3d/5d$ iridate/manganite superlattices. Our previous work on high-quality epitaxially stabilized SrMnO$_3$/SrIrO$_3$ superlattices revealed charge-transfer induced interfacial collinear ferromagnetism and an anomalous Hall effect [1,2]. In LaMnO$_3$/SrIrO$_3$ superlattices, we find a large additional topological Hall effect arising from the interaction of charge carriers with a noncoplanar chiral spin texture induced by interfacial DMI [3]. I will describe how the interfacial atomic layer stacking and symmetry enabled by the nonmagnetic A-sites determine the competition between collinear and chiral magnetic interactions originating from the oxide interface. These results will be compared with magnetometry measurements, soft and hard x-ray experiments, which provide a comparison of the bulk and interface electronic and magnetic properties. Our findings provide insight to the manipulation of chiral magnetism from atomic-scale control of DMI at oxide interfaces.


*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
Spin to charge conversion in the topological insulator HgTe and in STO-based two-dimensional electron gas* [Invited] JEAN-PHILLIPPE ATTANE (Presenter), Univ. Grenoble Alpes, CEA, IRIG, 38000 Grenoble (France) — While classical spintronics has traditionally relied on ferromagnetic metals as spin generators and spin detectors, a new approach called spin-orbitronics exploits the interplay between charge and spin currents enabled by the spin-orbit coupling in non-magnetic systems. However, the interconversion efficiency of the Hall effect is a bulk property that rarely exceeds ten percent, and does not take advantage of interfacial and low-dimensional effects otherwise ubiquitous in spintronics.

In this contribution, we first focus on strained mercury telluride, using spin pumping experiments at room temperature. We show that a HgCdTe barrier can be used to protect the HgTe topological surface states, leading to high conversion rates, with inverse Edelstein lengths up to 2.0±0.5 nm. These measurements, associated with the temperature dependence of the resistivity, suggest that these high conversion rates are due to the spin momentum locking property of HgTe surface states [1].

We then focus on the SrTiO3 (STO)-based 2D electron system, presenting experiments performed on NiFe/Al/STO heterostructures. We investigate the nature of the spin-to-charge conversion through a combination of spin pumping, magnetotransport, spectroscopy and gating experiments, finding a very highly efficient spin-to-charge conversion, with inverse Edelstein lengths beyond 20 nm. More importantly, we demonstrate that the conversion rate can be tuned in amplitude and rate by a gate voltage. We then discuss the amplitude of the effect and its gate dependence on the basis of the electronic structure of the 2DES and highlight the importance of a long scattering time to achieve efficient spin-to-charge interconversion.


*Support from the ANR SOspin, ANR OISO, ANR Toprise and LANEF (ANR-10-LABX51-01) is acknowledged,
The transition metal oxides exhibit a variety of interesting properties that are important for many practical applications, such as the dielectrics, magnetism, ferroelectricity, superconductivity, multiferroicity, etc. Such a rich plethora of functional properties primarily originate from the hybridized bands between the transition metal and the oxygen atoms. In artificially heterostructured oxide thin films, there exist the exciting new properties that are absent in the bulk materials, i.e. the emergent properties in oxide heterostructures. The understanding of the fundamental physics behind these emergent properties remains a huge challenge in condensed matter physics and attracts a lot of research interests in recent days. In this talk, I will introduce our recent advances in understanding the emergent magnetism in 2D oxide ferromagnets and a number of magnetic oxide heterostructures, from the symmetry aspects of the oxygen sublattice, including the octahedral rotations, tilts and the oxygen vacancies. Our study reveals the importance of the symmetry of the oxygen sublattice in shaping the emergent magnetism in low dimensional correlated oxide heterostructures.

*The National Key Research and Development Program of China (Grants No. 2016YFA0401004), the National Natural Science Foundation of China (Grants No. 51627901 and No. 11574287).
AYDOGAN OZCAN (Presenter), University of California, Los Angeles — Deep learning is a class of machine learning techniques that uses multi-layered artificial neural networks for automated analysis of signals or data. The name comes from the general structure of deep neural networks, which consist of several layers of artificial neurons, each performing a nonlinear operation, stacked over each other. Beyond its main stream applications such as the recognition and labeling of specific features in images, deep learning holds numerous opportunities for revolutionizing image formation, reconstruction and sensing fields. In fact, deep learning is mysteriously powerful and has been surprising optics researchers in what it can achieve for advancing optical microscopy, and introducing new image reconstruction and transformation methods. From physics-inspired optical designs and devices, we are moving toward data-driven designs that will holistically change both optical hardware and software of next generation microscopy and sensing, blending the two in new ways. Today, we sample an image and then act on it using a computer. Powered by deep learning, next generation optical microscopes and sensors will understand a scene or an object and accordingly decide on how and what to sample based on a given task – this will require a perfect marriage of deep learning with new optical microscopy hardware that is designed based on data. For such a thinking microscope, unsupervised learning would be the key to scale up its impact on various areas of science and engineering, where access to labeled image data might not be immediately available or very costly, difficult to acquire. In this presentation, I will provide an overview of some of our recent work on the use of deep neural networks in advancing computational microscopy and sensing systems, also covering their biomedical applications.

*NSF, HHMI and Koc Group are acknowledged for funding.
8:36AM R20.00002: Exploring Organic Ferroelectrics Using Data-driven Approaches*  
AYANA GHOSH (Presenter), Univ of Connecticut - Storrs, NICHOLAS LUBBERS, Computer, Computational and Statistical Sciences, Information Sciences, Los Alamos National Laboratory, SERGE M NAKHMANSON, Univ of Connecticut - Storrs, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory — Recent advances in the synthesis of polar molecular materials have produced practical alternatives to ferroelectric ceramics, opening up exciting new avenues for the incorporation of such compounds into modern electronic devices. However, in order to fully realize the prospects of polar polymer and molecular crystals for modern technological applications, it is paramount to acquire diverse datasets of potential organic ferroelectrics such that the mechanisms governing the emergence of ferroelectricity can be studied. Here we propose to use data-driven approaches to judiciously shortlist candidates from a wide range of chemical space with ferroelectric functionalities. First, this investigation will be governed by identification of chemical similarities between existing molecular compounds exhibiting similar ferroelectric behavior. Second, we investigate machine learning (ML) and deep neural network models for estimating charge transfer effects in organic chemistry. The dipole moment and ferroelectric properties estimated by ML can then be used to supplement the data-driven screening of possible organic ferroelectrics.

*This work was carried out under the auspices of the U.S. DOE NNSA (Contract No. 89233218CNA000001), and supported by the U.S. DOE LDRD Program.

8:48AM R20.00003: Deep Learning Model for Finding New Superconductors  
TOMOHIKO KONNO (Presenter), National Institute of Information and Communications Technology, HODAKA KUROKAWA, FUYUKI NABESHIMA, YUKI SAKISHITA, RYO OGAWA, University of Tokyo, IWAO HOSAKO, National Institute of Information and Communications Technology, ATSUTAKA MAEDA, University of Tokyo — It is very difficult for both theories and computational methods to predict the superconducting transition temperatures Tc of superconductors for strongly correlated systems, in which high-temperature superconductivity emerges. Exploration of new superconductors still relies on the experience and intuition of experts, and is largely a process of experimental trial and error. In one study, only 3% of the candidate materials showed superconductivity. Here we report an interdisciplinary attempt for finding new superconductors based on deep learning. We represented the periodic table in a way that allows a deep learning model to learn it. Although we used only the chemical composition of materials as information, we obtained an R2 value of 0.92 for predicting Tc for materials in a database of superconductors. We obtained three remarkable results. The deep learning method can predict superconductivity for a material with a precision of 62%, which shows the usefulness of the model; it found the recently discovered superconductor CaBi2, which is not in the superconductor database; and it found Fe-based high-temperature superconductors (discovered in 2008) from the training data before 2008. These results open the way for the discovery of new high-temperature superconductor families.
9:00AM R20.00004: Deep Learning for Energetic Materials: Predicting Material Properties from Electronic Structure using Convolutional Neural Networks*  ALEX CASEY (Presenter), Mechanical Engineering, Purdue University, BRIAN BARNES, Army Research Laboratory, ILIAS BILIONIS, STEVEN F. SON, Mechanical Engineering, Purdue University — Developing numerical descriptions of complex objects, like molecular structure, is a difficult task. The accuracy of a machine learned model depends on the input representation. Ideally, input descriptors encode the essential physics and chemistry that influence the target property. Thousands of molecular descriptors have been proposed and proper selection of features requires considerable domain expertise. In contrast, deep learning networks are capable of learning rich data representations. This provides a compelling motivation to use deep learning networks to learn molecular structure-property relations from 'raw' data. We develop a convolution neural network capable of directly parsing the 3D electronic structure of a molecule described by spatial point data for charge density and electrostatic potential concatenated into a 4D tensor. The model is jointly trained on over 20,000 molecules that are potentially energetic materials (explosives) to predict dipole moment, total electronic energy, Chapman-Jouguet (C-J) detonation velocity, C-J pressure, C-J temperature, crystal density, HOMO-LUMO gap, and solid phase heat of formation. This work demonstrates the first use of complete 3D electronic structure for machine learning of molecular properties.

*HPCMP
HPC Internship Program

9:12AM R20.00005: Optimization of Molecular Characteristic using Continuous Representation of Molecules by Variational Autoencoder with Discriminator  KYOSUKE SATO (Presenter), KENJI TSURUTA, Graduate School of Natural Science and Technology, Okayama University — Efficient molecular search contributes to an essential speedup of the development of organic devices and, in turn to the improvement of their characteristics. In the present study, we focus on the deep learning variational auto-encoder (VAE) model[1], where molecules represented by SMILES strings can be efficiently converted to multivariable continuous space. The VAE consists of two neural networks: an encoder and a decoder. The one-hot representation of SMILES is input to the encoder and mapped to the latent variable space. Here we further improve the output rate of valid SMILES of decoder by introducing a discriminator attached to the VAE stream. Adopting a molecular-mechanics method to calculate 3D structure from SMILES, we can optimize physical properties of the molecule by other simulation methods such as density-functional-theory calculations even when there is not enough data set. The range of physical property space covered by the SMILES representation is thereby expanded and the data-driven optimization using Kernel Ridge Regression method can be performed within the search space. In the presentation, we show the effectiveness of this method for optimizing a molecular HOMO-LUMO gap as an example.

An Initial Design-based Deep Learning Procedure for the Optimization of High Dimensional ReaxFF Parameters*  
MERT SENGUL (Presenter), Materials Science and Engineering, The Pennsylvania State University, YAO SONG, LINGLIN HE, YING HUNG, TIRTHANKAR DASGUPTA, Department of Statistics, Rutgers University, ADRI C.T. VAN DUIN, Mechanical Engineering, Pennsylvania State University — Atomistic level investigations are a significant part of today’s materials discovery research; however, most of the modeling methods that can describe chemical reactions are restricted to small molecular systems due to computational costs. The ReaxFF, an empirical interatomic potential, is capable of simulating reactions in larger molecular systems; however, the application of ReaxFF requires a significant preprocessing. One of the preprocessing steps is the optimization of functional parameters that are used to calculate interatomic interactions. This optimization process is complex due to high dimensionality. Here, we propose a deep learning (DL)-based procedure to be used in ReaxFF parameter optimization. The procedure is composed of three stages, which are: 1) data set creation; 2) DL model fitting and 3) local-minima detection. This DL procedure eliminates unfeasible regions in parameter space, which originate from the unphysical atomistic interactions, and constructs a more comprehensive understanding of a physically meaningful parameter landscape. The performance of the procedure will be evaluated by its application to molecular systems.

*The authors acknowledge funding support from U.S. National Science Foundation (Award No. DMR-1842922)

Feature Extraction Using Semi-Supervised Deep Learning.*  
MUAMMAR EL KHATIB (Presenter), WIBE A DE JONG, Computational Research Division, Lawrence Berkeley National Laboratory — Features are defined as measurable properties that characterize observed phenomena and represent a key part of machine learning (ML) algorithms. In materials sciences, ML has successfully accelerated atomistic simulations using man-engineered features for tasks such as energy or atomic forces predictions. These features fulfill physics constraints such as rotational and translational invariance, uniqueness and, locality (the sum of local contributions reconstructs a global quantity). However, these ML models are known to perform poorly when operating out of the training set regime because features are not representative of the underlying structure of the data. This could be improved if features are extracted with advanced hybrid architectures e.g. a variational autoencoder that is trained with physics constraints introduced with an external task and a loss function. We will explore how the use of semi-supervised learning techniques can be a powerful tool for the extraction of features for atomistic simulations. All results shown herein can be reproduced with ML4Chem: a free software package for machine learning in chemistry and materials sciences.

*The work is funded by Lawrence Berkeley National Laboratory through the Laboratory Directed Research and Development (LDRD) Program.
Unsupervised feature extraction in simple physical models through mutual information maximization

LEOPOLDO SARRA (Presenter), FLORIAN MARQUARDT, Max Planck Inst for Sci Light — When studying systems with many degrees of freedom, a typical problem is to find the correct low-dimensional variables to describe them on a higher level of abstraction. However, sometimes it is not clear how to choose meaningful quantities. By defining relevant features as low dimensional variables that preserve the largest mutual information with the original coordinates of the system, we set up an unsupervised learning technique to automatically extract those features. A variational bound allows to estimate mutual information through deep neural networks. We show example applications to statistical mechanics and classical dynamics.

Integration of Neural Network-Based Symbolic Regression in Deep Learning for Scientific Discovery*

SAMUEL KIM (Presenter), Electrical Engineering and Computer Science, Massachusetts Institute of Technology, PETER LU, Physics, Massachusetts Institute of Technology, MICHAEL GILBERT, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, SRIJON MUKHERJEE, LI JING, Physics, Massachusetts Institute of Technology, VLADIMIR ČEPERIĆ, University of Zagreb, MARIN SOLJACIC, Physics, Massachusetts Institute of Technology — Symbolic regression is a powerful technique that can discover the underlying analytical equations describing data, which can lead to explainable models and generalizability outside of the training data set. Here we use a neural network for symbolic regression based on the EQL network and integrate it into other deep learning architectures such that the whole system can be trained end-to-end through backpropagation. We demonstrate this system on an arithmetic task involving MNIST digits and on prediction of dynamical systems. The architecture is able to simultaneously extract meaningful latent variables and find the underlying equations that generalize extremely well outside of the training data set compared to a standard neural network approaches, paving the way for scientific discovery.

*This research is sponsored in part by the Army Research Office and under Cooperative Agreement Number W911NF-18-2-0048, by the Department of Defense through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program, by the MIT–SenseTime Alliance on Artificial Intelligence, and by the Defense Advanced Research Projects Agency (DARPA) under Agreement No. HR00111890042.
Rapid machine learning-based solutions of partial differential equations on complex domains. VIKAS DWIVEDI (Presenter), BALAJI SRINIVASAN, Indian Inst of Tech-Madras — Conventional methods like FEM (finite element method) and FVM (finite volume method) are mesh-based. However, if the computational domain consists of a complicated polygon with very short line segments, then it puts serious restrictions on mesh generation methods like triangulation. Recently, Berg et. al [1] have developed a deep unified ANN algorithm to solve PDEs on complex computational domains. Their method is based on an ansatz for the solution which requires deep neural networks and an unconstrained gradient-based optimization method such as gradient descent or a quasi-Newton method. In this paper, we present physics informed extreme learning machine (PIELM), a new machine-learning algorithm, which solves this problem with a simpler neural network architecture and an extremely fast learning routine. We demonstrate the efficacy of our method by solving the Poisson and biharmonic equation on complex 2D and 3D geometries such as the gyroid, which has important engineering applications.

Reference


Probabilistically-autoencoded horseshoe-disentangled multidomain item-response theory models* JOSHUA CHANG (Presenter), SHASHAANK VATTIKUTI, CARSON C CHOW, National Institutes of Health - NIH — Item response theory (IRT) is a non-linear generative probabilistic paradigm for using exams in order to quantify latent traits. In multidimensional IRT, one requires a factorization of the test items. For this task, linear factor analysis methods are often used, making IRT a posthoc model. We propose skipping the initial factor analysis by using a sparsity-promoting horseshoe prior to perform factorization directly within the IRT model so that all training occurs in a single self-consistent step. By binding the generative IRT model to a Bayesian neural network (forming a probabilistic autoencoder), one obtains a scoring algorithm consistent with the interpretable Bayesian model. In some IRT applications the black-box nature of a neural network scoring machine is desirable. Within this problem, we investigate the translation of some regularization principles common in Bayesian modeling to neural networks.

*NIH Intramural Research NIDDK
10:36AM R20.00012: Turbulence-generating networks ARMANDO GARCIA (Presenter), University of Texas, El Paso, RAO GUDIMETLA, Air Force Research Laboratory, JORGE MUNOZ, University of Texas, El Paso — The propagation of light through the atmosphere is often simulated with screens that impose a phase difference on an incoming wave. The screens are applied in series and have phase power spectral densities that are consistent with the strength of the turbulence to be simulated. We propose a new method to simulate the effect of turbulence on light propagation that uses mathematical graphs (networks) that are agnostic of spatial dimension or angle information. The intensity variation in the final screen is a measure of turbulence strength and we used several machine learning methods to adjust the probability distribution functions (PDF) of the weights of the edges of the networks to achieve the desired variations. We compare our results to the phase screen method for the case of the Kolmogorov spectrum using statistical measures such as the structure function. Finally, we explore avenues for improving the computational cost of producing turbulence-degraded images with this method as well as extending it to anisotropic turbulence.

10:48AM R20.00013: SignalTrain: Modeling Time-dependent Nonlinear Signal Processing Effects Using Deep Neural Networks WILLIAM MITCHELL (Presenter), SCOTT HAWLEY, Physics, Belmont University — The advent of increased consumer computing power and graphics processing unit (GPU) usage over the last decade has made possible machine learning approaches to modeling problems once thought impractical. This work expands on prior research published on modeling nonlinear time-dependent signal processing effects associated with music production by means of a deep neural network\(^1\). The presented results show the progress in accurately modeling these effects through architecture and optimization changes, increasing computational efficiency, lowering noise, and extending to a larger variety of nonlinear audio effects. Unique contributions of this effort include the ability to emulate the individual settings or “knobs” you would see on an analog piece of equipment, and with the production of commercially viable audio, i.e. 44.1kHz sampling rate at 16-bit resolution.


Thursday, March 5, 2020 8:00 AM - 10:36 AM

Session R21 GERA: Thermoelectric Materials 302
**8:00AM R21.00001: Computational Investigation of Ternary Na-V-VI$_2$ Chalcogenides and Their Thermoelectric Properties**

ISHAN KHARE (Presenter), Ottawa Hills High School, OH 43606, NATHAN J SZYMANSKI, Department of Materials Science and Engineering, UC Berkeley, RICHARD IRVING, Department of Physics and Astronomy, The University of Toledo — Ternary chalcogenides have been of recent investigation for applications such as solar cells and thermoelectrics. We have computed the structural, energetic, electronic, optical, and thermoelectric properties of nine ternary Na-V-VI$_2$ chalcogenides, NaAX$_2$, where A represents As, Sb, Bi and where X represents S, Se, Te, using first principles methods based on density functional theory and beyond. Optimized lattice parameters have been computed using the generalized gradient approximation (GGA). Phonon density of states computed at zero-temperature shows that only four of the nine compounds, NaAsS$_2$, NaAsTe$_2$, NaSbS$_2$, and NaSbSe$_2$, are dynamically stable. Our computations for these structures show that their electronic and optical properties are highly anisotropic. In addition, thermoelectric properties such as Seebeck coefficient (S) and power factor were computed using Boltzmann statistics. The compounds are predicted to have promising thermoelectric properties at 300 K, indicating that these materials are desirable for thermoelectric applications. Particularly, NaAsTe$_2$ is predicted to have S = 425 μV/K. Experimental verification is suggested.

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**8:12AM R21.00002: Enhanced thermoelectric efficiency in Bi$_2$Te$_3$ nanoplates and SnSe$_2$ films.**

JIHAN CHEN, INDU ARAVIND (Presenter), YU WANG, Univ of Southern California — We present a facile method to improve the thermoelectric efficiency of CVD grown 2D Bi$_2$Te$_3$ nanoplates through remediation of unintentional surface doping. The as-grown flakes of Bi$_2$Te$_3$ exposed to ambient conditions exhibit relatively small thermopowers. The high surface-to-volume ratio of these thin nanoplates makes them especially sensitive to surface doping, which is a common problem among nanomaterials in general. After surface passivation by deposition of 30nm of Al$_2$O$_3$ using ALD, the Seebeck coefficient of these flakes increases by a factor of 5X (from -34 to -169 μV/K). Here, the surface passivation can prevent the degradation of the thermoelectric properties caused by gas adsorption and surface oxidation processes, thus increasing the Bi$_2$Te$_3$ Seebeck coefficient.$^1$

We also report cross-plane thermoelectric measurements of SnSe and SnSe$_2$ films grown by the modulated element reactant (MER) approach. By performing post-growth annealing at a fixed Se partial pressure, a transition from SnSe-to-SnSe$_2$ is induced which results in a 16-fold increase (from -38.6 to -631μV/K) in the cross-plane Seebeck coefficient.$^2$


*DOE: DE-FG02-07ER46376, DE-FG02-07ER46377
NSF:1402906.
8:24AM R21.00003: High Thermoelectric Figure of Merit via Tunable Valley Convergence Coupled Low Thermal Conductivity in \(A^{II}B^{IV}C_{2}^{V}\) Chalcopyrites  MADHUBANTI MUKHERJEE (Presenter), GEORGE YUMNAM, ABHISHEK SINGH, Indian Institute of Science — Developing high performance thermoelectrics require designing strategy to obtain excellent electronic but poor phononic transport properties. Tetragonal chalcopyrites are of significant attention due to complex electronic structures affecting the transport properties. Conflicting requirements of achieving high Seebeck coefficient and electrical conductivity are simultaneously reached, by tuning crystal and electronic structures by isoelectronic substitution, leading to unprecedented enhancement in electronic transport properties of \(A^{II}B^{IV}C_{2}^{V}\) (\(II = \text{Be, Mg, Zn, and Cd}, \ IV = \text{Si, Ge, and Sn}; \ \text{and V = P and As}\)). Existing multiple valleys in conduction bands get converged by substitution of group IV dopants to offer enhanced powerfactors for n-type carriers. These substitutions improve convergence of valence bands having a direct correlation with tetragonal distortion (\(\eta\)) of these chalcopyrites. For small distortion in system (\(\eta\sim 1\)), complete convergence of bands is achieved, enhancing the p-type powerfactor. Excellent electronic transport and low thermal conductivity results in maximum ZT of 1.67 in CdGeAs\(_2\) for n-type doping. The approach developed to enhance the thermoelectric efficiency can be useful to design new thermoelectric materials.

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8:36AM R21.00004: Thermoelectric properties of n-type PbTe driven near ferroelectric phase transition by strain*  JIANG CAO (Presenter), School of Electronic and Optical Engineering, Nanjing University of Science and Technology, JOSE D. QUERALES-FLORES, DORDE DANGIC, Tyndall National Institute, STEPHEN B FAHY, University Colledge Cork, IVANA SAVIC, Tyndall National Institute — We recently showed that soft transverse optical (TO) phonons play the key role in high thermoelectric (TE) figure of merit (ZT) of PbTe: they strongly suppress its lattice thermal conductivity[1], but do not degrade its electronic transport properties[2]. In this work, using first principles calculations, we investigate how driving PbTe closer to the soft mode phase transition (PT) via strain affects the TE properties and ZT of n-type PbTe. We find that the lattice thermal conductivity decreases significantly when PbTe approaches the PT, which leads to considerable ZT enhancement. However, if PbTe is driven very close to the PT, the originally negligible electron-TO phonon scattering becomes the strongest scattering channel, due to an increased TO phonon amplitude and the electron-TO phonon scattering phase space. Such increased scattering strength rapidly degrades electrical transport and ZT very near the PT. We show how tuning the proximity to soft mode PT can increase the TE performance of PbTe and other materials with soft phonons that interact weakly with the electronic states relevant for transport.


*Science Foundation Ireland PI Award 15/IA/3160, and NSF of Jiangsu BK20180456.*
A high valley degeneracy of electronic bands in a material leads to its large efficiency of conversion between thermal and electrical energy, quantified by the thermoelectric figure of merit (ZT). Large ZT enhancements due to the alignment of the valence band maxima at L and Σ (or “valley convergence”) have been demonstrated in p-type PbTe and related materials [1], by tuning temperature and the doping concentration. However, it is still unclear why this strategy of improving ZT works well since the scattering processes between L and Σ valleys can deteriorate thermoelectric properties. Here, we introduce a first principle method to model electron-phonon scattering mechanisms in p-type PbTe [2]. The calculated room temperature thermoelectric parameters are in very good agreement with available experiments. Our model also allows accounting for the temperature dependence of the electronic band structure in thermoelectric transport calculations, which enables us to quantify the effect of L and Σ valley convergence at ~620 K [3] on the ZT values of p-type PbTe.


*Supported by Science Foundation Ireland under grant 15/IA/3160.
9:00AM R21.00006: Lessons from a thermoelectric transport trend study on half-Heusler alloys

KRISTIAN BERLAND (Presenter), Faculty of Science and Technology, Norwegian University of Life Sciences, OLE MARTIN LØVVIK, SINTEF — The thermoelectric properties of the 4-9-15 (Ti,Zr,Hf) (Co,Rh,Ir)(As,Sb,Bi) and 4-10-14 (Ti,Zr,Hf)(Ni,Pd,Pt)(Ge,Sn,Pb) series have been studied theoretically [J. App. Phys. 126, 145102 (2019)]. The electronic transport properties were calculated with density functional theory (DFT) and Boltzmann transport equations (BTE) at the hybrid functional level utilizing a recently developed k.p-based interpolation scheme [J. App. Phys 123, 205703 (2018)]. Phonon transport properties were calculated with the temperature-dependent effective potential (TDEP) method, including alloy and grain-boundary scattering.

Our trend study provides a number of key lessons:
1) Electronic band structures show much variation and there is, in particular, the potential for n-type Half Heusler with higher ZT.
2) The predicted thermoelectric properties are quite sensitive to the choice of exchange-correlation potential.
3) The thermal conductivity of a pure material is a poor indicator of the final thermal conductivity once other scattering mechanisms are included.
4) Sub-lattice alloying is generally more effective on the Z site than on the X site.

These findings provide valuable insights for more realistic high-thruput assessments of thermoelectric properties.

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9:12AM R21.00007: Solving the Thermoelectric Trade-Off Problem with Metallic Carbon Nanotubes

YOTA ICHINOSE (Presenter), AKARI YOSHIDA, KANAKO HORIUCHI, KENGO FUKUHARA, Tokyo Metropolitan Univ, NATSUMI KOMATSU, WEILU GAO, Rice University, YOHEI YOMOGIDA, Tokyo Metropolitan Univ, MANAHO MATSUBARA, TAKAHIRO YAMAMOTO, Tokyo University of Science, JUNICHIRO KONO, Rice University, KAZUHIRO YANAGI, Tokyo Metropolitan Univ — Semiconductors are generally considered far superior to metals as thermoelectric materials because of their much larger Seebeck coefficients $S$. However, a maximum value of $S$ in a semiconductor is normally accompanied by a minuscule electrical conductivity $\sigma$, and hence, the thermoelectric power factor $P = S^2\sigma$ remains small. An attempt to increase $\sigma$ by increasing the Fermi energy ($E_F$), on the other hand, decreases $S$. This trade-off between $S$ and $\sigma$ is a well-known dilemma in developing high-performance thermoelectric devices based on semiconductors. Here, we show using metallic carbon nanotubes (CNTs) with tunable $E_F$ solves this long-standing problem, demonstrating higher thermoelectric performance than semiconducting CNTs. We studied the $E_F$ dependence of $S$, $\sigma$, and $P$ in a series of CNT films with systematically varied metallic CNT contents. In metallic CNTs, both $S$ and $\sigma$ monotonically increased with $E_F$, continuously boosting $P$ with increasing $E_F$. Particularly, in an aligned metallic CNT film, the maximum $P$ was ~5 times larger than that in the high-purity (>99%) semiconducting CNT film. We attribute these superior thermoelectric properties of metallic CNTs to the simultaneously enhanced $S$ and $\sigma$ of one-dimensional conduction electrons near the first van Hove singularity.
9:24AM R21.00008: When Band Convergence is Not Beneficial for Thermoelectricity*
JUNSOO PARK (Presenter), Lawrence Berkeley National Laboratory, MAXWELL DYLLA, YI XIA, JEFF SNYDER, Northwestern University, ANUBHAV JAIN, Lawrence Berkeley National Laboratory — Band convergence is known to generally benefit thermoelectric performance for its capability to increase carrier concentration for given Fermi level, i.e., increase conductivity for given Seebeck coefficient. With explicit treatment of electron-phonon scattering, we show that this is not necessarily the case and the degree of attainability of the said benefit depends on the dominant scattering mechanism and the manner in which bands converge. Multi-band convergence at a single k-point under deformation scattering is less beneficial (if at all) than multi-pocket convergence under polar-optical scattering at distant k-points. In the former case, one band gains while the other band loses phase space, and the increasingly disparate pocket lifetimes and mobilities can lower the Seebeck coefficient and render higher power factor inaccessible. In the latter case, the convergence preserves the scattering behavior, thereby successfully leading to higher power factor. We establish these by performing state-of-the-art first-principles studies on CaMg2Sb2-CaZn2Sb2 Zintl alloy and full-Heusler Sr2SbAu.

*We thank the DOE Office of Basic Energy Sciences, Early Career Research Program. This work used resources of 1) NERSC and 2) TACC at the UT Austin through XSEDE.

9:36AM R21.00009: Potential barrier/well engineering for improving the power factor in nanostructured thermoelectric materials*  
NEOPHYTOS NEOPHYTOU (Presenter), SAMUEL FOSTER, VASSILIOS VARGIAMIDIS, Univ of Warwick — Energy filtering is one of the most successful ways to improve the Seebeck coefficient in nanostructured materials and superlattices. Despite the fact that nanostructuring emerges as the most promising method to reduce thermal conductivity and improve ZT, to-date, energy filtering has not been widely utilized because it did not achieve sufficient improvements in the thermoelectric power factor. In this work, we present a theoretical analysis of a novel concept for efficient design of the potential well/barrier region such that very large power factor improvements are achieved. The concept proposed combines aspects of: i) energy filtering from potential barriers with thermionically emitted carriers, ii) highly degenerate doping conditions but with non-uniform distribution of dopants, and iii) reduced energy relaxation of carriers after they passed the barriers and propagate into the wells. We employ simple analytical models, but verify the main design ‘ingredients’ with more advanced Non-Equilibrium Green's Function (NEGF) quantum transport simulations and semiclassical Monte Carlo simulations.

*This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 Research and Innovation Programme (Grant Agreement No. 678763).
9:48AM R21.00010: Tuning Thermoelectricity in Molecular Junctions via Quantum Interference*  RUIJIAO MIAO (Presenter), Energy Storage and Distributed Resources, Lawrence Berkeley National Lab — Studies of molecular junctions, created by trapping a single molecule or multiple molecules between metallic electrodes, not only provide fundamental knowledge of charge transport at the atomic scale, but also offer unique opportunities in developing molecule-based devices for energy conversion. It has been theoretically proposed that quantum interference effects can be employed to obtain impressive thermoelectric performance in molecular junctions. Toward this goal, we took advantage of the destructive interferences which arise in conjugated molecules to allow high-energy electrons to pass while blocking low-energy electrons. Specifically, we investigated this effect in oligo(phenylene ethynylene) (OPE) derivatives with a para-connected central phenyl ring (para-OPE3) and meta-connected central ring (meta-OPE3). Experiments on both single molecules and monolayers reveal a two-fold increase in thermopower in meta-OPE3 (~20 μV/K) junctions compared with para-OPE3 (~10 μV/K) junctions, which agrees with our initio modeling. Our results illustrate how enhancements in thermopower can be achieved in molecular junctions via quantum interferences.

*Office of Naval Research (N00014-16-1-2672, instrumentation)
Department of Energy (DE-SC0004871, scanning probe microscopy)

10:00AM R21.00011: Including the finite temperature atomistic evolution into thermoelectric theory*  JOHN VILLANOVA (Presenter), SALVADOR BARRAZA-LOPEZ, Univ of Arkansas-Fayetteville — Thermoelectric (TE) materials have enjoyed much attention because of their promise for energy savings and targeted low-power cooling. Bulk monochalcogenides (SnSe) are some of the most effective TE materials [1,2]. Phonon anharmonicity and softening modes play an important role in improved TE performance [3], but so far, theoretical approaches to computing TE properties do not account for such softening explicitly. To address this shortcoming, we use molecular dynamics data for two-dimensional SnSe as inputs for the electronic structure and phonon dispersions at finite temperature. We capture an increase in phonon velocity at the Γ-point and enhanced hole conductivity at the structural transition temperature, accounting for the change in structure and anharmonicity in predicting TE performance explicitly. These ideas enhance our understanding of TE materials, and the procedure is applicable to bulk systems as well.


*This work was supported by an Early Career Grant from the DOE (DE-SC0016139). Calculations were performed on Cori at NERSC (DE-AC02-05CH11231).
10:12AM R21.00012: Copper occupation and dynamics in Cu rich tetrahedrite; an NMR study* NADER GHASSEMI (Presenter), YEFAN TIAN, Texas A&M Univ, XU LU, Department of Applied Physics, Chongqing University, JOSEPH H. ROSS, Texas A&M Univ, YANCI YAN, XIAOYUAN ZHOU, Department of Applied Physics, Chongqing University — Thermoelectric materials can generate electricity from heat. Recently tetrahedrite with the chemical structure of Cu$_{12}$Sb$_4$S$_{13}$ emerged as the most promising thermoelectric material for mid-temperature applications. Here we report $^{63}$Cu NMR measurements for the Cu-rich phase of Cu$_{12+x}$Sb$_4$S$_{13}$ ($x \approx 2$) and compared to Cu$_{12}$Sb$_4$S$_{13}$. Based on NMR, T$_1$ and T$_2$ measurements, the results demonstrate Cu-ion hopping below room temperature with an activation energy of $\sim$150 meV for the Cu-rich phase, consistent with superionic behavior. The NMR results also demonstrate the effects of Cu-ion mobility in the Cu$_{12}$Sb$_4$S$_{13}$ phase, but with a larger activation barrier. We identify a small difference in NMR Knight shift for the metallic phase of Cu$_{12}$Sb$_4$S$_{13}$, compared to the Cu-rich phase, and when compared to DFT calculations the results indicate a mix of hyperfine contributions to the metallic shift.

*This work was supported by the Robert A. Welch Foundation, Grant No. A-1526.

10:24AM R21.00013: Heat is Work, and Work is Heat: a first-principles approach to find improved thermoelectrics* PHIL HASNIP (Presenter), GENADI NAYDENOV, MATT I. J. PROBERT, University of York — Thermoelectric materials have the potential to dramatically improve the energy efficiency of many devices and industrial processes by converting waste heat into electricity. An ideal thermoelectric material has high electrical conductivity and low thermal conductivity, requirements which are often in conflict. Simulating thermoelectric properties is extremely challenging: predicting electronic properties requires first-principles material modelling, yet thermal conductivity must be modelled on long lengthscales which are beyond direct first-principles modelling.

In this talk I will introduce the fundamental physics of thermoelectrics and how they may be modelled accurately, using \textit{ab initio} quantum mechanical simulations coupled with classical models. I will also show how this combination of modelling techniques is being used to explain the behaviour of current materials as well as predicting entirely new thermoelectrics, paving the way for a new generation of cheap, efficient thermoelectric devices.

*We acknowledge financial support from EPSRC (Grant Ref. EP/R025770/1). We are grateful for computational support from the UK national high performance computing service, ARCHER, for which access was obtained via the UKCP consortium and funded by EPSRC Grant Ref. EP/P022561/1.
8:00AM R22.00001: The strange case of Dr Jekyll and Mr Hyde: The two faces of singular models. [Invited] PAUL WIGGINS (Presenter), Physics, Bioengineering and Microbiology, University of Washington — Why does systems biology work in spite of a blizzard of poorly-defined parameters and yet the detection of the Higgs boson requires five-sigma? Both these statistical analyses involve singular models, defined by structural unidentifiability (i.e. the absence of a one-to-one map between parameters and distribution functions). This singular structure leads to profound changes in the phenomenology of inference. In this talk, we will explore the phenomenology of learning from two physical perspectives: First, we explore the correspondence between statistical physics and statistics and demonstrate that there is equivalence between predictive performance and heat capacity, which gives new physical insight into why learning has universal scaling as well as explaining how and why these universal rules fail in the context of singular models. Finally, we explore insights from the Riemannian geometry of the model parameter space to determine what face a singular model will show: anomalously high or low learning performance.

8:36AM R22.00002: Learning dynamical information from static protein and sequencing data PHILIP PEARCE (Presenter), Harvard Medical School, FRANCIS G WOODHOUSE, ADEN W FORROW, University of Oxford, ASHLEY KELLY, HALIM KUSUMAATMAJA, Durham University, JORN DUNKEL, Massachusetts Institute of Technology — Many complex processes, from protein folding to neuronal network dynamics, can be described as stochastic exploration of a high-dimensional energy landscape. While efficient algorithms for cluster detection in high-dimensional spaces have been developed over the last two decades, considerably less is known about the reliable inference of state transition dynamics in such settings. Here, we introduce a flexible and robust numerical framework to infer Markovian transition networks directly from time-independent data sampled from stationary equilibrium distributions. We demonstrate the practical potential of the inference scheme by reconstructing the network dynamics for several protein folding transitions, gene-regulatory network motifs and HIV evolution pathways. The predicted network topologies and relative transition time scales agree well with direct estimates from time-dependent molecular dynamics data, stochastic simulations and phylogenetic trees, respectively. Owing to its generic structure, the framework introduced here will be applicable to high-throughput RNA and protein sequencing datasets and future cryo-electron-microscopy data.
8:48AM R22.00003: Associative Memory of Structured Knowledge  JULIA STEINBERG (Presenter), HAIM SOMPOLINSKY, Harvard University — A long standing challenge in biological and artificial intelligence is to understand how new knowledge can be constructed from known building blocks in a way that is amenable for computation by neuronal circuits. While previous work has focused primarily on working memory tasks of structured data, here we focus on the task of storage and recall of structured knowledge in long term memory. Specifically, we ask how a Hopfield type network can store and retrieve episodic memories where each episode is a set of associations between events. We model each knowledge structure as a set of binary relations between events and cues (cues may represent e.g., temporal order, spatial location, role in semantic structure). We use a binarized version of holographic reduced representation (HRR) to map such structures to fixed length vectors. We then train a recurrent network to store these vectors as fixed points. By a combination of signal-to-noise analysis and numerical simulations we demonstrate that our model allows for an efficient storage and recall of these knowledge structures in a way that allows the full retrieval of the memorized structure and their building blocks from partial retrieving cues. Our work contributes to the understanding of neural computations of structured knowledge.

9:00AM R22.00004: Can model reduction replace expert intuition for modeling complex biological systems?*  CODY PETRIE (Presenter), DANE BJORK, MARK TRANSTRUM, Brigham Young Univ - Provo — One of the challenges to modeling biological systems is the overwhelming complexity. Mathematical models that account for all the known interactions would have an unwieldy number of components and parameters. Traditionally, real-world models have been based on expert intuition that judiciously relate only those components believed to be relevant to a behavior of interest. These models typically reflect intuition and physical insights that are difficult to rigorously justify or convey. Here, we consider whether recent advances in model reduction may be able to automatically construct comparable simplified models in a semi-automatic, data-driven way. We report on a comparative study of model reduction of the Wnt signaling pathway, comparing automatic methods with expert intuition. Automatic model reduction is done using the Manifold Boundary Approximation Method (MBAM), based on information geometry and "sloppy model" analysis. We find that MBAM leads to simplified models that closely resemble those proposed based on expert intuition. Our results suggest that data-driven methods of model reduction may be a viable alternative to expert-derived models, and can be used to extract comparable physical insights into the behavior of complex biological systems.

*NSF-1753357
9:12AM R22.00005: Limits on the suppression of molecular fluctuations and oscillation dephasing in stochastic reaction networks  JIAWEI YAN (Presenter), JOHAN PAULSSON, Harvard Medical School — Many efforts in synthetic biology have been dedicated to designing ultra-reliable gene networks, but so far there has been little theory capable of providing guidance on the experimental design, because small differences in rate functions or topology can sometimes change the dynamics drastically. Here we aim to identify general principles in stochastic reaction networks that apply regardless of parameters and the form of rate functions. First we studied the noise suppression in multi-component networks and asked if it is possible to design systems where the components control and mutually suppress the noise in each other. Specifically, we find that in any \( N \)-component system, regardless of how each component affects other's production rates, it is impossible to suppress fluctuations below the uncontrolled equivalents for all components. We next examined whether there exist similar design principles in oscillatory behaviours in stochastic reaction networks. We studied a broad class of feedback, allowing arbitrary time delay and control functions, and found that even when all the rest of the feedback loop is optimal for generating sustained oscillations, the information loss from one single reaction step can lead to severe constraints in the autocorrelation and power spectrum.

9:24AM R22.00006: Kalman-like Self-Tuned Sensitivity in Biophysical Sensing*  KABIR HUSAIN (Presenter), WEERAPAT PITTAYAKANCHIT, Department of Physics, University of Chicago, GOPAL PATTANAYAK, MICHAEL RUST, Department of Molecular Genetics and Cell Biology, University of Chicago, ARVIND MURUGAN, Department of Physics, University of Chicago — Living organisms need to be sensitive to a changing environment while also ignoring uninformative environmental fluctuations. Here, we argue that living cells can navigate these conflicting demands by dynamically tuning their environmental sensitivity. We analyze the circadian clock in *Synechococcus elongatus*, showing that clock-metabolism coupling can detect mismatch between clock predictions and the day-night light cycle, temporarily raise the clock's sensitivity to light changes, and thus re-entraining faster. We find analogous behavior in recent experiments on switching between slow and fast osmotic-stress-response pathways in yeast. In both cases, cells can raise their sensitivity to new external information in epochs of frequent challenging stress, much like a Kalman filter with adaptive gain in signal processing. Our work suggests a new class of experiments that probe the history dependence of environmental sensitivity in biophysical sensing mechanisms.

*KH thanks the JSMF for support via a postdoctoral fellowship. AM thanks the Simons foundation for support under the MMLS program.
Searching for the Relevant Properties of Binary Datasets: Is your Model Truly Pairwise?  
CLELIA DE MULATIER (Presenter), University of Pennsylvania, PAOLO PIETRO MAZZA, Institute for Theoretical Physics, University of Tübingen, MATTEO MARSILI, International Centre for Theoretical Physics — Uncovering the patterns hidden within noisy data is essential to science. Information theory provides a quantitative method to select the best of potential explanations for data, by optimizing the balance between goodness-of-fit and simplicity. Yet in practice finding “the” best model for a given dataset is impossible. A common practical issue is the huge number of potential models. But with a finite amount of data, the real limitation comes from the large degeneracy of models that perform nearly optimally. We illustrate this problem on examples of binary data using a heuristic procedure to perform an efficient search among all spin models with high order interactions. As good models tend to share a common sub-structure that is likely to capture relevant properties of the data, we focus our search on this structure rather than on finding the strictly best model. We show that minimally complex spin models are useful for this task. We obtain an analytic expression for their posterior probability, which makes them easy to fit and exactly comparable. We then show that working with equivalence classes of these models allows a) to find the spin basis in which the dependencies between basis variables are minimal and b) to quantify these dependencies and the relevance of each dimension.

Information efficiency of bacterial chemotaxis*  
HENRY MATTINGLY (Presenter), KEITA KAMINO, Yale University, XIAOWEI ZHANG, Peking University, BENJAMIN B MACHTA, THIERRY EMMONET, Yale University — Information transfer is central to the function of many biological systems. For example, the bacteria Escherichia coli climbs gradients of chemical attractants by modulating its rate of tumbling—randomly reorienting its swimming direction—when it senses time-changes in attractant concentration. But even in the absence of signal processing, the cell's tumble behavior is correlated with the signal it sees. The transfer entropy rate $I_{\phi \rightarrow M}$ from signal to tumble behavior removes these correlations and isolates the causal influence of the signal on the cell's tumble decisions. We show that climbing a gradient with drift speed $v_D$ requires an information rate of at least $I_{\phi \rightarrow M} = 12 \frac{D_r (v_D/v_0)^2}{v_0} (1-TB)$, where $D_r$ is the rate of rotational diffusion, $v_0$ is the run speed, and $TB$ is the fraction of time the cell is tumbling. To quantify E. coli cells' information rates, we measure, in single cells, signal transduction responses and fluctuations. Along with measurements of drift speeds, we determine how efficiently E. coli use information about the gradient during chemotaxis.

*HM*, KK*, and TE were funded by NIH R01 GM106189. HM was funded by NIH F32 GM131583. TE** and BM** were funded by Yale PEB. BM was funded by Simons Investigator Award 624156. *Equal contribution. **Corresponding.
10:00AM R22.00009: Decision-making at a T-junction by gradient-sensing agents  TANVI GANDHI, JINZI MAC HUANG (Presenter), ANTOINE AUBRET, DESMOND YAOCHENG LI, SOPHIE RAMANANARIVO, MASSIMO VERGASSOLA, JEREMIE PALACCI, University of California, San Diego — At the beginning of life, searching for food and evading hazards are two essential activities for microorganisms to survive, and the way they navigate is through chemotaxis. The optimal chemotaxis in complicated terrains determines the fate of living creatures, and natural selection ensures the existence of such an optimization. In our study, we investigate the navigation of inert particles in a network that has multiple junctions. In micro-networks manufactured through photolithography, a background gradient of salt is established as the signal of chemoattractant by placing a source and a sink of salt. Colloidal particles then follow this signal through diffusiophoresis and move towards the source. Through stochastic modeling, we show that particles prefer to exit each junction at the end with higher concentration gradient. This preference is further enhanced when the particle size is larger, which leads to a way to magnify small signals in a network so that the colloidal particles larger than a critical size can always move towards the source of salt through the shortest path. Ultimately, we compare the navigation schemes of inert particles and living organisms, aiming to understand biological chemotaxis and shed light on future manufacturing of navigable microswimmers.

10:12AM R22.00010: Trading bits in the readout of positional information*  MARIANNE BAUER (Presenter), WILLIAM S BIALEK, THOMAS GREGOR, Princeton University, MARIELA D PETKOVA, Harvard University, ERIC WIESCHAUS, Princeton University — Expression levels of gap genes, crucial for fly development, have been shown to be precise, matching the spatial precision in the expression of downstream genes. If the transcriptional machinery can read these gap expression levels only imprecisely, subsequent precision could not be reproduced. Yet, assuming that levels can be read with infinite precision is unrealistic. Reading expression levels with limited precision can be phrased mathematically by limiting the number of bits which are available for each measurement. The question of how to use these bits to capture the maximum positional information is an instance of the information bottleneck problem. We show that to capture ~90% of the available information, we need more bits than intuitively biologically reasonable. We can allow for an increased number of bits per measurement by having molecules bind to multiple sites. This is a generalization of the information bottleneck problem. We show that one can capture almost all the available information with multiple “low precision” encodings, which may correspond physically to multiple binding sites or even enhancers.

*Supported in part by the NSF CBPF (PHY-1734030), and Grant PHY-1607612; by AvH; by NIH Grants P50GM071508, R01GM077599, and R01GM097275; and by HHMI.
10:24AM R22.00011: Single-Molecule Conductance and Conformational Analysis with Engineered Nano-Junctions for Nucleic Acid Sequencing  LEE KORSHOJ, SEPIDEH AFSARI, ANUSREE CHATTERJEE, PRASHANT NAGPAL (Presenter), University of Colorado, Boulder — DNA sequencing on the single-molecule level can be used to study cellular heterogeneity and stochasticity with reduced time, cost, and complexity compared to traditional sequencing methods. However, sample noise and signature overlap due to varying nucleotide conformations prevent accurate sequencing results. We address these issues by engineering nano-junctions for conductance measurements on conformationally constrained single nucleotides within electrostatically bound DNA molecules on a self-assembled cysteamine monolayer. From STM break junctions with biochemical moieties in individual nucleobases, the unique conductance signature of each nucleobase is analyzed with machine learning algorithms [1]. Additionally, conformational variation, or smear, is quantified from the distance over which molecular junctions are maintained during each conductance measurement [2]. We demonstrate >93% accuracy for DNA nucleotide recognition with 20 repeat measurements. These results are a significant improvement over contemporary methods and show the potential for using simple surface modifications and existing biochemical moieties in nucleobases for single-molecule, nanoelectronic nucleotide identification.


Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R23 DBIO GSNP: Evolutionary and Ecological Dynamics III: Evolution 304 - Thierry Mora, Ecole Normale Superieure - Tag(s): Focus

8:00AM R23.00001: Evolutionary dynamics of immune repertoires* [Invited] THIERRY MORA (Presenter), Ecole Normale Superieure — Our adaptive immune system protects us against a wide variety of pathogens using a broad repertoire of specific receptors expressed by B and T cells, whose concentrations adapt to past experiences to encode immune memory. In this talk I will discuss how the diversity of receptors is generated and how it evolves and self-organises over time to protect us efficiently. I will present models of population dynamics as well as design principles of optimal memory encoding, and will relate them to high-throughput sequencing data. I will also discuss diversity measures and the power-law nature of the distribution of clone sizes observed in the repertoire.

*European Research Council Consolidator Grant n. 724208.
**8:36AM R23.00002: Evolutionary regain of lost network function**  
MIRNA KHEIR GOUDA, Laufer Center for Physical & Quantitative Biology, State Univ of NY - Stony Brook, MICHAEL MANHART, Institute of Integrative Biology, ETH Zurich, GABOR BALAZSI (Presenter), Laufer Center for Physical & Quantitative Biology, State Univ of NY - Stony Brook — Natural or synthetic genetic network modules can lose their function over long-term evolution if the function is costly. How populations can evolve to restore such broken function is poorly understood. To test the reversibility of evolutionary breakdown, we use a synthetic gene circuit (PF) integrated into yeast cells. In previous evolution experiments, mutations in a gene eliminated the fitness costs of PF activation, corrupting gene circuit function. Since PF activation also provides drug resistance, we grew such corrupted mutants in both drug and inducer, imposing selection to regain drug resistance and possibly PF function. We observe various adaptation scenarios with or without repairing lost gene circuit function. The data suggest interactions between intracellular gene network dynamics and evolutionary dynamics, with possible consequences for understanding the evolution of drug resistance and developing future synthetic biology applications.

*This work was supported by the NIH/NIGMS MIRA grant R35 GM122561 (GB), by the Laufer Center for Physical and Quantitative Biology (GB), and the Swiss National Science Foundation Ambizione grant PZ00P3_180147 (MM).*

**8:48AM R23.00003: Measuring mutations with droplet microfluidics**  
MIKE HENNESSEY-WESEN (Presenter), CALIN GUET, BJOERN HOF, Institute of Science and Technology Austria — Mutations are random errors in genetic material that create the diversity which underpins the development of all life. However, work done over recent years has suggested that certain mutations are not as random as once thought - several factors such as stress, chromosomal neighborhood, and transcription level have been implicated to affect genetic stability. Typically, quantitative measures of frequency and distribution of point mutations have either relied on fluctuation tests that make assumptions about the shape of mutation distributions, or on large volumes of data from multiple sources that can harbor unknown inconsistencies. We use a droplet-based, microfluidic platform to make real-time measurements of point mutations in bacteria under various conditions with high precision. We are able to alter various conditions of growth, such as heat/drug stress and transcriptional activity, and detect mutations without the use of a selective or metabolic screen, which makes our system a versatile tool for studying mutant occurrence. Our results offer a direct look into this often-simplified area of evolutionary dynamics.

*This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement No. 665385.*
9:00AM R23.00004: The Evolutionary Dynamics of Incubation Periods*

BERTRAND OTTINO-LOFFLER (Presenter), Condensed Matter Theory Group, Massachusetts Institute of Technology MIT, JACOB SCOTT, Translational Hematology and Oncology Research, Cleveland Clinic, STEVEN STROGATZ, Center for Applied Mathematics, Cornell University — The incubation period for typhoid, polio, measles, leukemia and many other diseases follows a right-skewed, approximately lognormal distribution. Although this pattern was discovered more than sixty years ago, it remains an open question to explain its ubiquity. Here, we propose an explanation based on evolutionary dynamics on graphs. For simple models of a mutant or pathogen invading a network-structured population of healthy cells, we show that skewed distributions of incubation periods emerge for a wide range of assumptions about invader fitness, competition dynamics, and network structure. The skewness stems from stochastic mechanisms associated with two classic problems in probability theory: the coupon collector and the random walk. Unlike previous explanations that rely crucially on heterogeneity, our results hold even for homogeneous populations. Thus, we predict that two equally healthy individuals subjected to equal doses of equally pathogenic agents may, by chance alone, show remarkably different time courses of disease.

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NIH Loan Repayment Grant

9:12AM R23.00005: Evolution of systems with power-law memory: Do we have to die?*

MARK EDELMAN (Presenter), Department of Physics, Yeshiva University — Various features of the development of individual living species are programmed. Is death also programmed and what can be the underlying mechanism providing the inevitability of death? The presented hypothesis is based on the similarity of human evolution to the evolution of discrete nonlinear systems with power-law memory. Caputo fractional logistic map is a discrete system with power-law memory and quadratic nonlinearity. In the area of parameters where the fixed point is unstable, its evolution starts as the evolution of a system with a stable fixed point but then this fixed point becomes unstable, suddenly breaks, and turns into a period two point. Under random perturbations the time spans of the evolution as a fixed point before the break (lifespans) obey the Gompertz-Makeham law, which is the observed distribution of the lifespans of living species. The reasons for modeling the evolution of humans by fractional systems are the observed power law in human memory and the viscoelastic nature of organ tissues of living species. Models with power-law memory may explain the observed decrease at very large ages of the rate of increase of the force of mortality and they imply limited lifespans.

*The author acknowledges support from the Joseph Alexander Foundation, Yeshiva University.
Spatial Expansions and Serial Bottlenecks Produce Different Topologies of Genealogical Trees

GABRIEL BIRZU (Presenter), Applied Physics, Stanford University, OSKAR HALLATSCHEK, Physics and Integrative Biology, University of California, Berkeley, KIRILL S KOROLEV, Physics, Boston University — What do the genealogies of expanding populations look like? While recent studies recognize the importance of genealogies for inferring and predicting evolutionary dynamics, very little is known about genealogies in expanding populations. Here, we show that range expansions can produce extremely different topologies of genealogical trees, which are very sensitive to the growth dynamics at the front. When growth is cooperative, genealogies are described by the Kingman coalescent—a backward-in-time analog to neutral evolution in which only pairwise mergers between lineages occur. Weakly cooperative and non-cooperative growth result in fundamentally different trees, with multiple lineages merging at the same time. We explain these results by deriving the distribution of the effective offspring number at the front, and show that the transition between the two topologies occurs when the variance of this distribution diverges. This divergence arises due to rare fluctuations of the front shape and position. Thus, evolutionary dynamics of range expansions cannot be approximated by a deterministic model of serial bottlenecks. Our results also show that range expansions provide a robust mechanism for non-Kingman genealogies, which previously have only been attributed to natural selection.

Early Multicellular Organisms Co-opt Cell-Level Characteristics into Group-Level Properties via the Principle of Maximum Entropy

THOMAS DAY (Presenter), DAVID B YANNI, SHANE JACOBEEEN, PETER YUNKER, Georgia Inst of Tech — In the earliest stages of the evolution of multicellularity, genetic changes occur at the individual cell level yet selection acts at the group level. New group level traits emerge when mutations affecting cell-level properties are co-opted into consistent group-level traits. However, it is unclear how readily coherent group-level properties emerge absent a regulatory developmental plan. It even seems likely that small fluctuations at the cellular level may elicit large fluctuations at the group level, destroying the chance for survival. Here we demonstrate that lab-evolved simple multicellular groups with permanent intercellular bonds follow the principle of maximum entropy. As a result, a large space of microstates (e.g. specific cell configurations) correspond to a smaller space of macrostates (e.g. cluster volume), thereby achieving robust, consistent macroscopic properties. We derive an equation of state that relates these macroscopic properties together and experimentally verify predictions from the equation of state, demonstrating that robust group-level properties readily emerge from individual cell traits. Finally, we speculate that the emergence of group-level properties is possible within any cluster with fixed bonds between mother and daughter cells.
Selection of mutants in a microbial population depends on multiple cellular traits. In serial-dilution evolution experiments, three key traits are the lag time when transitioning from starvation to growth, the exponential growth rate, and the yield (number of cells per unit resource). Here we investigate how these traits evolve in laboratory evolution experiments using a minimal model of population dynamics, where the only interaction between cells is competition for a single limiting resource. We find that the fixation probability of a beneficial mutation depends on a linear combination of its growth rate and lag time relative to its immediate ancestor, even under clonal interference. The relative selective pressure on growth rate and lag time is set by the dilution factor; a larger dilution factor favors the adaptation of growth rate over the adaptation of lag time. The model shows that yield, however, is under no direct selection.

*MM was supported by an F32 fellowship from the US 515 National Institutes of Health (GM116217) and an Ambizione grant from the Swiss National Science Foundation (PZ00P3 180147). AA thanks support from NSF 518 CAREER 1752024 and the Harvard Deans Competitive 519 Fund.

Physical constraints on epistasis

KABIR HUSAIN, ARVIND MURUGAN (Presenter), University of Chicago — Living systems evolve one mutation at a time, but a single mutation can alter the effect of subsequent mutations. The underlying mechanistic determinants of such epistasis are unclear. Here, we demonstrate that the physical dynamics of a biological system can generically constrain epistasis. We analyze models and experimental data on proteins and regulatory networks. In each, we find that if the long-time physical dynamics is dominated by a slow, collective mode, then the dimensionality of mutational effects is reduced. Consequently, epistatic coefficients for different combinations of mutations are no longer independent, even if individually strong. Such epistasis can be summarized as resulting from a global non-linearity applied to an underlying linear trait, i.e., as global epistasis. This constraint, in turn, reduces the ruggedness of the sequence-to-function map. By providing a generic mechanistic origin for experimentally observed global epistasis, our work suggests that slow collective physical modes can make biological systems evolvable.
10:12AM R23.00010: Emergence of heritability of higher-level traits in a major transition
ANTHONY BURNETTI (Presenter), Biological Sciences, GEORGIA TECH, SEYED ALIREZA ZAMANI DAHAJ, Physics, GEORGIA TECH, MATTHEW HERRON, WILLIAM RATCLIFF, Biological Sciences, GEORGIA TECH — Increases in biological complexity and the origins of life’s hierarchical organization are described by the “major transitions” framework. A crucial component of this paradigm is that after the transition in complexity or organization, adaptation occurs primarily at the level of the new, higher-level unit. For collective-level adaptations to occur, though, collective-level traits—properties of the group, such as collective size—must be heritable. Using the ‘snowflake yeast’ model system of early multicellularity, we investigated the biophysical basis of emergent multicellular traits. We genetically engineered four yeast genotypes to have different cellular aspect ratios, which prior work has shown affects cellular packing and the size of the multicellular group. We then measured the heritability of both the cellular trait (aspect ratio) and emergent multicellular trait (group size at fracture) and compared them to our theoretical predictions. Extrapolating from these results, we show mathematically that, for a wide range of functions relating the group traits to cellular traits, the emergent group-level traits will have higher heritability than their corresponding cell-level traits.

10:24AM R23.00011: Lineage Branching During Recovery from Simulated Mass Extinction*
DAWN KING, TYLER HANKE, SONYA BAHAR (Presenter), University of Missouri - St. Louis — How do population lineages diversify to fill new ecological niches? What governs the dynamics of population recovery from near-extinction? These questions are particularly urgent in our current age of climate-driven mass extinction. We investigate these questions using a computational model of evolutionary dynamics in which simulated organisms reproduce by bacterial fission or assortative mating on a two-dimensional phenotype space. This model has been shown to undergo a directed-percolation-like nonequilibrium phase transition from survival to extinction as system parameters such as maximum mutation size or death rate are varied. Here, we use methods from coalescent theory to show that population lineages undergo a structural change near the extinction-survival transition, with a sharp divergence in the time to most recent common ancestor (TMRCA). We also simulate mass extinctions, both in the neighborhood of the phase transition and in the survival regime, by either increasing the death rate of organisms, or increasing the parameter that controls their competition. We then analyze lineages, TMRCA, and other measures of population structure during successful and unsuccessful recoveries from mass extinction events.

*This research was supported by the James S. McDonnell Foundation.
The evolution of multicellular organisms on earth is one of the most transformative events in the history of life. Despite its importance, we know little about the process by which nascent microscopic multicellular organisms overcome substantial mechanical constraints and dramatically increase their size. We experimentally study this process with the snowflake yeast model system: baker's yeast (S. cerevisiae) with a single mutation in ACE2 gene allows mother and daughter cells to remain attached via uncut chitin bonds. These yeast clusters are composed of a few hundred cells and grow to a maximum diameter of 200 microns. After a year of artificial selection for larger multicellular size, five populations of snowflake yeast surprisingly evolved to grow to a diameter of 1 mm. In this work we show how small changes at the cell level trait lead to emergent properties in the microscopic level and helped to overcome tremendous mechanical constraints on their size.

10:48AM R23.00013: Evolution of hardwired behavioral strategies through competitive population dynamics  
TONG LIANG (Presenter), Department of Physics and Astronomy, Stony Brook University, BRADEN A. W. BRINKMAN, Department of Neurobiology and Behavior, Stony Brook University — Normative approaches are commonly used to predict an organism's hardwired behaviors by optimizing utility functions such as sensory information or reward, which are loosely interpreted as proxies for evolutionary fitness. However, the validity of the assumption that utility function optimization confers true evolutionary success has seldom been explored. Here we develop mechanistic evolutionary models to investigate whether normative principles can predict the most evolutionarily advantageous strategies. With mean-field approximations and agent-based stochastic simulations, we show that the most competitive strategies that emerged from these models in environments of randomly distributed resources conform well with normative predictions, but only when organisms are sparsely distributed and interactions are rare. These results suggest that normative approaches can predict the evolutionarily most competitive innate behavioral strategies, at least when the optimized utility is directly relevant for the organisms' survival and accounts for environmental constraints. This work bridges the gap between normative approaches and the underlying fundamental evolutionary dynamics.
The ability to determine the structure of a protein to near-atomic resolution using x-ray crystallography and NMR spectroscopy has been vital for advances in structural biology. However, it is unclear whether or not the structures obtained from these two methods are the same to within experimental uncertainties, or if these characterization methods influence the structures in some way. To address this important question, we compiled a dataset of paired high-resolution x-ray crystal structures and high-quality NMR structures to determine whether there are any systematic differences between the structures solved using the two experimental techniques. Backbone fluctuations of core Cα atoms reveal that core residues from x-ray crystal structures occupy smaller regions of configuration space than core residues in NMR structures. We also find that the core residues of NMR structures are more densely packed than core residues in x-ray crystal structures. We explain this result by preparing packings of amino-acid-shaped particles with thermalized packing-generation protocols, and find that packings with higher thermalization resemble cores in NMR structures, while in the limit of no thermalization we recover packings that resemble the cores of x-ray crystal structures. This result suggests that the differences between NMR and x-ray crystal structures are caused by the varying degree of thermal fluctuations in the two characterization methods. NMR solution structures are allowed to fluctuate more, which compacts the core, but allows for greater exploration of core configurations. In contrast, x-ray crystal structures occupy only well-defined, smaller regions of configuration space.

*NSF Grant No. PHY-1522467 (J.D.T. and C.S.O.)
Decoy Detection of Computational Protein Designs

ALEX GRIGAS (Presenter), ZHE MEI, JOHN TREADO, ZACHARY LEVINE, Yale University, LYNNE REGAN, University of Edinburgh, COREY SHANE O’HERN, Yale University — Decoy detection is one way to reframe protein folding, not in terms of folding a protein, but in terms of differentiating a well-folded protein from a poorly folded one. An effective decoy scoring metric would both improve prediction methods and indicate how prediction methods fail. The O’Hern group has been making progress in understanding protein structure by focusing on the core regions of proteins, which are inaccessible to solvent. Core structure is uniquely specified by purely repulsive atomic interactions, as hard-sphere interactions are able to predict core structure. In this work, we apply this framework to the decoy detection problem and find that state-of-the-art protein predictions in the CASP11, 12 and 13 competitions often have core regions that are overpacked, due to overlapping residues. Additionally, cores in the predicted protein structures are often too small and too solvent-exposed, suggesting that the prediction methods do not properly capture hydrophobic collapse. Finally, by scoring CASP predictions based on its core structure, we can effectively distinguish between high- and low-quality computational protein designs.

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NSF Grant No. PHY-1522467

Low-Force Elasticity Reveals Complex Structure of an Intrinsically Disordered Protein

HOANG TRUONG (Presenter), IAN L MORGAN, OMAR SALEH, University of California, Santa Barbara — Intrinsically disordered proteins (IDPs) do not possess a well-defined three-dimensional structure, which presents a challenge to investigating their conformations. To overcome this challenge, we explore low-force polymeric elasticity as a means to quantify structural properties. Here, using a high-resolution single-molecule magnetic tweezer, we stretch a polypeptide construct derived from the neurofilament tail domains and study its conformations. At low forces, the construct behaves as an ideal coil instead of a self-avoiding coil. This is surprising given the IDP’s high net charge, suggesting the presence of weak long-range attractive interactions. In addition, the measured persistence length is longer than expected for a random polypeptide chain. This result suggests the IDP has residual structure, which stiffen the chain at low force. We further probe the response of long-range attraction and chain stiffening to changes in salts and denaturants. Our data reveals a rich elastic behavior and complex structure in a nominally disordered chain.

This work is supported by the National Science Foundation under grant number 1715627.
9:00AM R24.00004: ProSPr: Protein Structure Prediction via Interatomic Distances  
WENDY BILLINGS (Presenter), BRYCE E HEDELIUS, TODD MILLECAM, DAVID WINGATE, DENNIS DELLA CORTE, Brigham Young Univ - Provo — Substantial progress has been made in the past several years towards the accurate prediction of protein tertiary structures from primary sequence, aided greatly by the integration of machine learning. Current success is based on two-stage protocols: first, the training of a deep convolutional neural network (CNN) to predict macromolecular structure restraints, and second, the use of these restraints to construct a folded three-dimensional structure of the target protein. Such a two-stage folding protocol was used by DeepMind in the recent Critical Assessment of Structure Prediction (CASP13), which outperformed all established groups. However, DeepMind has not expressed a plan to publish the code of their AlphaFold protocol. Here we present ProSPr, a network representing the first part of the AlphaFold pipeline for predicting interatomic distances, and demonstrate its abilities in the contact prediction task relative to other state-of-the-art methods. We also investigate and report on the roles of certain input features in prediction quality. ProSPr is made freely available to the scientific community both as source code and a Docker container, which we anticipate will encourage the development of better techniques for assembling protein structures from restraints.

9:12AM R24.00005: Landscapes, Nonlinearity, and Biomolecular Energy Redistribution  
JUSTIN ELENEWSKI (Presenter), National Institute of Standards and Technology, KIRILL VELIZHANIN, Los Alamos National Laboratory, MICHAEL ZWOLAK, National Institute of Standards and Technology — Although selective energy redistribution is critical to the function of numerous biomolecules and functional nanomaterials, the processes mediating these dynamics remain a poorly understood facet of nonequilibrium thermodynamics. In this talk, I will discuss how topological features, nonlinearities, and energy landscape architecture can collude to define biomolecular heat propagation [1]. Our exhaustive all-atom simulations and novel local-in-time and space analysis - which is equally applicable to both theory and experiment - permit the multiscale dissection of energy migration in biomolecules. Unlike transport through small-molecule systems, we find that nonlinearity dominates over coherent processes at even at short length- and time-scales. Leveraging these observations, I will demonstrate how vibrational energy transport can probe otherwise inaccessible aspects of macromolecular dynamics and the interactions that underlie biological function.

Understanding the native fluctuations of protein cores

ZHE MEI (Presenter), JOHN TREADO, ZACHARY LEVINE, Yale University, LYNNE REGAN, University of Edinburgh, COREY SHANE O’HERN, Yale University — Understanding how thermal fluctuations affect protein structure is essential for characterizing the energy landscape of proteins, as well as determining the response to amino acid mutations. Protein structures obtained from liquid-state NMR, unlike those from x-ray crystallography, provide a number of model structures that satisfy the experimental constraints. Using a database of high-quality, paired NMR and x-ray crystal structures, we have shown that there are important differences between NMR structures and those solved by x-ray crystallography including differences in the root-mean-square deviations of the core C\textalpha atomic positions, identities of the core amino acids, and packing fractions of core residues. In this work, we carry out all-atom molecular dynamics simulations to study the fluctuating conformational dynamics of wildtype globular proteins, as well as mutants, in aqueous solvent at room temperature. We study the fluctuating conformations using several metrics including the radius of gyration \(R_g\), packing fraction, and \(C_{\alpha}\) atomic positions. We find that most often the MD simulations sample conformations that are representative of the NMR and x-ray conformations, but \(~40\%\) of the sampled structures are not consistent with the experimental structures, with larger \(R_g\) and lower packing fractions.

*The Raymond and Beverly Sackler Institute for Biological, Physical, and Engineering Sciences (Z.M.)

Steric Equation of State for Monoclonal Antibodies from Low to High Concentrations

HASSAN SHAHFAR (Presenter), Physics and Astronomy, University of Delaware, CHRISTOPHER J ROBERTS, Chemical and Biomolecular Engineering, University of Delaware — Steric interactions potentially play a significant role in packing behavior of proteins as one considers increasing concentrations, particularly for monoclonal antibodies (MAbs) due to their extended, anisotropic, and flexible structure. Steric contributions to the equation of state are key to balancing attractive contributions in crowded environments that result in phase separation. Steric protein-protein interactions are sensitive to the size and shape of proteins and can be considered as the minimal level of interactions to be captured in coarse-grained models. To date, all atom simulation was used to calculate only the role of steric only behavior of monoclonal antibodies on the second osmotic virial coefficients. A biased Monte Carlo algorithm (Mayer sampling) used to calculate the steric interactions up to the fifth virial coefficient using all atom simulations for representative MAb structures. The results are compared with different levels of coarse grained models to assess the accuracy of predictions of lower resolution models. The results show that, upon increasing concentration to approx. 10 volume percent, the deviation of the predictions of coarse grained models is pronounced, but can be mitigated by the choice of model.
10:12AM R24.00008: Origins of Critical Phenomena in the Folding Phase Diagram of Proteins* ANDREI GASIC (Presenter), MARGARET CHEUNG, Department of Physics, University of Houston; Center for Theoretical Biological Physics, Rice University — Proteins are folded polymers that are able to respond to slight environmental perturbations to preformation their biological function while also keeping a quasi-unique conformation. Such properties may be exhibited by a physical system near a critical point. Recent experimental and computational findings demonstrate that protein folding transitions in the temperature ($T$), pressure ($P$), and crowding volume-fraction ($\phi$) phase diagram have signatures of criticality, where distinct folding phases merge [A. G. Gasic et al., Phys. Rev. X (2019)]. Here we investigate the origin of this critical behavior using insight from polymer physics. Based on our theory, we show that the separation of $T$ between the folding and collapse transition temperatures ($T_F$ and $T_\Theta$, respectively) lead to a critical transition. We derive the relationship for the correlation length and show divergence approaching the critical regime. Structure-based model simulations of a protein in a crowded environment are used to validate our predictions. Our study illustrates the importance of the crowded cellular environment for a protein biological function.

*This work is funded by the NSF through MCB:1412532, PHY:1427654, and OAC:1531814. AGG is supported by a fellowship on the Houston Area Biophysics Program: T32 GM008280.

10:24AM R24.00009: Dissimilar ligands bind in a similar fashion: guiding the ligand binding mode prediction* XIANJIN XU, XIAOQIN ZOU (Presenter), Univ of Missouri - Columbia — The Molecular Similarity Principle have achieved great successes in the field of drug design/discovery. Existing studies focus on similar ligands, while the behavior of dissimilar ligands remains hidden in darkness. In this study, a strategy was introduced for comparing the binding modes of ligands with different molecular structures for the first time. Our systematic analysis on a newly constructed dataset of protein-ligand complexes showed that ligands with similar structures tend to share a similar binding mode, which is consistent with the molecular similarity principle. More importantly, the results revealed that dissimilar ligands can also bind in a similar fashion. This finding would open a new avenue for rational drug design. Furthermore, a template-guided method was introduced for predicting protein-ligand complex structures. Encouragingly, even with the use of dissimilar ligands as templates, our method significantly outperformed bound docking of the molecular docking method.

*NIH R01GM109980 (PI: XZ), NIH R01HL126774 and NIH R01HL142301 (PI: Jianmin Cui).
An escape rate analysis for pulling experiments based on energy landscapes in two reaction coordinates

Sudeep Adhikari (Presenter), Kevin Stuart David Beach, Univ of Mississippi — The structural dynamics of biopolymers such as proteins are described in the context of their conformational energy landscapes. In optical-tweezer pulling experiments, features of the energy landscapes are extracted from the observed distribution of the critical force at which the polymer unfolds, and typically the analysis is based on a one-dimensional (1D) reaction coordinate, the extension. But a 1D analysis is inadequate when various possible folded configurations are degenerate in the end-to-end length. We present an analytical framework for the well escape rate in the context of an effective 2D landscape. We test our analysis against simulated pulling experiments and verify our ability to extract meaningful well parameters.

Thursday, March 5, 2020 8:00 AM - 10:48 AM

Session R25 GSNP DSOFT: Active Matter

8:00AM R25.00001: Propagating Activity Fronts in Columns of Fire Ants* Caleb Anderson (Presenter), Alberto Fernandez-Nieves, Guillermo Goldsztein, Georgia Inst of Tech — For the past three decades, the study of active matter has revealed rich physics and universal behaviors, such as collective motion, across a wide variety of biological and synthetic systems with seemingly disparate particle interactions. Here we present our surprise observation and measurements of stable activity fronts propagating through two-dimensional columns of thousands of fire ants. We then propose both computational and analytical models to explain the origin of these macroscopic non-linear fronts from simplified pairwise interactions between ants. Finally, we finish by comparing these fronts to other instances of collective motion observed in active systems.

*FLAMEL, NSF IGERT program

8:12AM R25.00002: Self- and air-driven fluidization of black soldier fly larvae Olga Shishkov (Presenter), David Hu, Daniel I Goldman, Georgia Inst of Tech — Active systems can be driven via internal activity of individual elements or via external mechanical forcing. Here we study a living system in which both internal and external activity can be varied. In laboratory experiments, we confine thousands of ~10 mm long black soldier fly larvae in an air fluidized bed (~4 larva lengths in diameter, 10 in height) and study the collective and individual dynamics. When larvae are not externally fluidized, due to their internal activity they self-pack and the height of the column of larvae decreases over time to a steady state value. In steady state, larval motion is distributed heterogeneously and transiently, with regions of motion and clustering appearing and disappearing throughout the bed volume. These dynamics can be altered by gentle flow of air to the bed: like fluidized beds of inactive (non-living) particles, steady-state larval collective volume (column height) increases with increasing air flow, and the persistence of the transient regions change. Further, external fluidization has the same effect as the addition of food, where activity also causes large-scale mixing.
8:24AM R25.00003: Stochastic thermodynamics for self-propelled particles* GRZEGORZ SZAMEL (Presenter), Colorado State University — We present a generalization of stochastic thermodynamics to systems of active particles, which move under the combined influence of stochastic internal self-propulsions (activity) and a heat bath. The generalization relies upon a formal similarity of an active system and a system consisting of two subsystems interacting with different heat reservoirs and coupled by a non-symmetric interaction. The resulting thermodynamic description closely follows the standard stochastic thermodynamics. In particular, total entropy production, $\Delta s_{\text{tot}}$, can be decomposed into housekeeping, $\Delta s_{\text{hk}}$, and excess, $\Delta s_{\text{ex}}$, parts. Both $\Delta s_{\text{tot}}$ and $\Delta s_{\text{hk}}$ satisfy fluctuation theorems. The average rate of the steady-state housekeeping entropy production can be related to the violation of the fluctuation-dissipation theorem via a Harada-Sasa relation. The excess entropy production enters into a Hatano-Sasa-like relation, which leads to a generalized Clausius inequality involving the change of the system's entropy and the excess entropy production.

*I gratefully acknowledge the support of NSF Grant No. CHE 1800282.

8:36AM R25.00004: Odd viscosity in active materials: microscopic origin and 3D effects* TOMER MARKOVICH (Presenter), Center for Theoretical Biological Physics, Rice University, TOM LUBENSKY, Physics and Astronomy, University of Pennsylvania — Active materials are composed of many components that convert energy from the environment into directed mechanical motion, thus locally breaking time reversal symmetry (TRS). Examples of active materials go beyond living systems such as bacteria and is also realized in e.g. colloidal rollers. A striking phenomenon of breaking TRS is the possible appearance of odd viscosity. Onsager reciprocal relations require that when TRS holds the viscosity tensor is symmetric for exchanging its first and last pair of indices. However, when TRS is broken, Onsager relations predict an odd viscosity that is both odd under TRS and under the change of indices. Such odd viscosity is non-dissipative and should thus be derivable from a Hamiltonian theory. Active materials innately break TRS, which led to recent studies of odd viscosity in 2D active materials. In this talk I will present a novel microscopic Hamiltonian theory for odd viscosity, valid also in 3D. Our theory give rise to intriguing 3D effects such as generalization of Bernoulli's principle, propagation of bulk waves, and a few types of unidirectional surface waves. We further predict that odd viscosity should emerge in actomyosin gels and bacterial suspensions.

*This work was supported by the CTBP and sponsored by the NSF (PHY-1427654).
Quincke Oscillation of Colloids at Planar Electrodes* ZHENGYAN ZHANG (Presenter), YONG DOU, KYLE BISHOP, Columbia Univ — Dielectric particles immersed in a weakly conducting liquid are known to exhibit spontaneous rotational motion under uniform DC electric fields above a critical magnitude. So-called Quincke rotation near a planar substrate leads to particle translation and provides a useful experimental model for studying the collective dynamics of active colloids. Here, we show that individual Quincke rollers at planar electrodes can also exhibit oscillatory dynamics, whereby particles move back and forth about a stationary location. The transition from steady rolling to oscillatory motion occurs at a critical field three times larger than that required for rolling. In contrast to previous reports of oscillatory Quincke dynamics based on inertial effects, our observations of micron-scale particles are characterized by low Reynolds numbers (Re \(\sim\) 0.01) and therefore negligible inertia. We propose a plausible explanation for Quincke oscillations using the leaky-dielectric model and accounting for electric (and hydrodynamic) interactions of the particle with the conductive substrate.

*We gratefully acknowledge funding from the CBES(Center for Bio-Inspired Energy Science) and Department of Energy.

Capturing the local entropy production of an active Brownian particles system by compression* BUMING GUO (Presenter), Center for Soft Matter Research, New York University, STEFANO MARTINIANI, Department of Chemical Engineering and Materials Science, University of Minnesota, PAUL M CHAIKIN, Center for Soft Matter Research, New York University, DOV LEVINE, Department of Physics, Technion - IIT — The entropy production of a stationary process is known to be the Kullback-Leibler divergence (KLD), or relative entropy, between the probability of observing a trajectory with time running forward and its time reversal, which quantitatively characterizes the time-reversal asymmetry and features the nonequilibrium nature of the system. Here we use a compression based Ziv-Merhav method and other techniques to estimate KLD and time reversal symmetry to define a natural spatial decomposition of entropy production by applying the algorithms on discrete time series of state evolution in local block regions. As an example, we will discuss how local entropy production is captured with this method in a phase-separated system of active Brownian particles.

*National Science Foundation Physics of Living Systems Grant No. 1504867
9:12AM R25.00007: Superdiffusion and hydrodynamic phase separation in a uniaxial active suspension* LOKRSHI DADHICHI (Presenter), TIFR Centre for Interdisciplinary Sciences, K VIJAY KUMAR, TIFR-ICTS, J K BHATTACHARJEE, Indian Association for the Cultivation of Science, SRIRAM RAMASWAMY, Physical Science, Indian Institute of Science — We examine, analytically and to some extent numerically, the dynamics of the concentration field in an active suspension with permanent uniaxial anisotropy. We show that in the homogeneous phase the advection of fluctuations in the concentration, by the active flow they themselves generate, leads to a superdiffusive dynamic exponent $z = d/2$ for dimension $d < 4$. We uncover a novel flow-induced contribution to active-particle currents that can lead to a negative effective diffusivity on a cone of directions, and hence to a purely hydrodynamic mechanism for phase separation. We suggest experimental tests of our predictions.

*SR was supported by the SERB (India) and the Tata Education and Development Trust.

9:24AM R25.00008: Chemistry-Induced Mobility in Catalytic Chemical Reactions HUAN WANG (Presenter), MYEONGGON PARK, TSVI TLUSTY, STEVE GRANICK, Institute for Basic Science — With a standard pulse-field gradient nuclear magnetic resonance based diffusion ordered spectroscopy (DOSY), we measure chemical-shift specific molecular diffusivity simultaneously with reaction kinetics in situ as reaction progresses. In simple exothermic, catalysed chemical reactions, we observe unexpected solvent enhanced diffusion, both in water and in organic solvents, to be tightly correlated with molecular catalytic cycles. Scaling analysis suggests the critical role of hydrodynamic coupling at nanoscale among “force-dipole-like” chemical reaction centers. The observation of chemistry-induced mobility challenges the simple “passive” picture of chemical reaction, suggesting rich energy dissipation pathways that eventually lead to collective consequences, for example, a counterintuitive antichemotaxis flux, revealed from a gradient microfluidic chip measurement.
9:36AM R25.00009: Spontaneous locomotion of nano-catalysed BZ droplets  
D JAYA PRASANNA KUMAR, KABEER JASUJA, PRATYUSH DAYAL (Presenter), Indian Inst of Tech Gandhinagar
— The motion in living systems by chemo-mechanical transduction has inspired the scientists to design and develop self-moving biomimetic systems. Here, we harness self-oscillating Belousov-Zhabotinsky (BZ) reaction, synergized by graphene-based catalytic mats to demonstrate the spontaneous motion of the BZ reaction droplet in oil-surfactant medium. Specifically, we synthesize graphene-based catalytic mats by decorating Ru nanoparticles (NP) on graphene nanosheets, thereby creating 0D-2D heterostructures; subsequently, use these mats to catalyze BZ reaction within a droplet. Our results demonstrate spontaneous locomotion of BZ droplets due to Marangoni flow facilitated by the interaction between BZ reaction intermediates and the surfactant in the surrounding oil. We further show that the velocity of droplet motion depends upon the conductivity of the catalytic mats. In particular, we observe highest droplet velocities when RuNP decorated graphene sheets are used to catalyze the BZ reaction. In addition, we witnessed some interesting behaviours when multiple BZ droplets interact within the oil-surfactant medium. Our findings can be used to design self-moving synthetic systems to control their behavior through the use of 0D-2D hybrid nanomaterials.

*DST-SERB (EMR/2016/007778) and IITGn

NGUYEN T NGUYEN (Presenter), SPENCER SMITH, Mt Holyoke Coll
— A general feature of active matter systems is that they consume energy on the small scale and coherent flows emerge on the large scale. Whether the units comprising these systems are bacteria, birds, or the microtubules of active nematics, coherence arises due to local interactions. In a now classic model, the Vicsek model, coherence, as measured by an order parameter, undergoes a phase transition with the changing importance of local interactions. We revisit this result from the perspective of mixing and fluid advection. In particular, we use a measure of dynamic disorder, the topological entropy, which captures the complexity of how the trajectories of these active agents wind about one another. We are able to calculate this mixing measure, and probe the thermodynamic limit of larger ensembles of agents, thanks to a new algorithm, which combines ideas from low dimensional topology and computational geometry. We will show some interesting results in how this disorder parameter behaves as we change the importance of local interactions.
10:00AM R25.00011: Anomalous topological active matter*   KAZUKI SONE (Presenter), YUTO ASHIDA, Department of Applied Physics, Univ of Tokyo — Systems with topologically nontrivial band structures, which are at the center of the modern condensed matter physics, exhibit unidirectional modes that propagate along the edge of a sample and are immune to disorder. Here, we show that the topological edge modes can ubiquitously emerge in active matter, the collection of self-propelled particles, under influences of spatially periodic structures [1]. Topological edge modes have been found in some active systems by constructing the counterparts of quantum Hall effect. However, to realize the effective external magnetic field, they introduce intricate structures, which can be the bottleneck for an experimental realization. We conclude that, without those intricate structures, it is hard to construct an active-matter counterpart of quantum Hall effect. Instead, by constructing the analogy with quantum anomalous Hall effect, our theoretical proposal eliminates the bottleneck for realizing topological active matter and broadens its applicability. We also discuss its relevance to ongoing experiments in biological systems.


*This work is supported by JSPS through Program for Leading Graduate Schools (ALPS) and Grant No. JP16J03613 and JP19K23424.

10:12AM R25.00012: Homotopy analysis method for Non-Markovian processes in active matter   LEONARDO APAZA PILCO (Presenter), MARIO SANDOVAL-ESPINOZA, Physics, Metropolitan Autonomous University — We solve the Fokker-Planck (FP) equation for active non-Markovian and quasi-Markovian processes using the homotopy analysis method, and provide analytical expressions for classic mean values as a series in time. For non-Markovian processes we show that the solution is equivalent to a Dyson series in the Fokker-Planck operator. As an example, the active particles case with color noise in an arbitrary potential is solved. Our analytical results were compared to Brownian dynamics simulations showing a good agreement.

10:24AM R25.00013: Computational study of autonomous mechanical oscillations in a colloidal network crosslinked via clock proteins*   LAUREN MELCHER (Presenter), Rochester Institute of Technology, ELISABETH RENNERT, University of Chicago, JENNIFER L ROSS, Syracuse University, MICHAEL RUST, University of Chicago, RAE M ROBERTSON-ANDERSON, University of San Diego, MOUMITA DAS, Rochester Institute of Technology — We investigate a colloidal network as a model system that can dynamically switch between crosslinked and unlinked states when connected via crosslinkers made of clock proteins such as the bacterial circadian oscillator proteins KaiABC. We study this system using Brownian Dynamics simulations and obtain collective properties, such as the degree of order in the system, size of connected clusters, and the mechanical rigidity of the system as a function of time for different volume fractions of colloids, interaction strengths, and crosslinking kinetics. Using experimental parameters for polystyrene spheres and biotinylated KaiABC crosslinkers, we predict the behavior of real systems. Our results can provide insights into the design of self-sustaining soft materials that can autonomously transition between solid-like and fluid-like states, and how the properties of such materials can be tuned.

*This work was funded by a W.M. Keck Foundation Research Grant.
**10:36AM R25.00014: Scalar activity induced phase separation and liquid–solid transition in a Lennard-Jones system**  
* CHANDAN DASGUPTA (Presenter), S SIVA NASARAYYA CHARI, PRABAL K MAITI, Indian Institute of Science - Dept of Physics — Molecular dynamics simulations are used to investigate the effects of scalar activity in a three-dimensional system of Lennard-Jones particles at state points spanning from the gas to the liquid regime. Scalar activity is introduced by increasing the temperature of half of the particles (labeled 'hot') while keeping the temperature of the other half (labeled 'cold') constant at a low value. The ratio of the temperatures of the two subsystems is considered to be a measure of scalar activity. We observe that the two species tend to phase separate at sufficiently high temperature ratio. The degree of phase separation is quantified by a suitably defined order parameter and the entropy production in the process of phase separation is determined by employing the two-phase thermodynamics (2PT) method. We observe that the degree of phase separation and the entropy production increase with the density of the system. The mean number of clusters and the mean size of the largest cluster are determined as functions of the density and the temperature ratio. A calculation of bond orientation order parameters reveals that the largest cluster develops solid-like order consisting of both FCC and HCP packings.

*This work was supported by the Department of Science and Technology, India.

**Thursday, March 5, 2020 8:00 AM - 10:48 AM**

**Session R26 DBIO DPOLY GSNP: Physics of Genome Organization: From DNA to Chromatin: I**  
403 - Alexandre Morozov, Rutgers University, New Brunswick - Tag(s): Focus

**8:00AM R26.00001: Strategies transcription factors use to gain access to nucleosomal DNA**  
* [Invited] MICHAEL POIRIER (Presenter), Ohio State Univ - Columbus — The physical organization of all eukaryotic genomes is evolutionarily conserved. Histone protein octamers repeatedly wrap genomic DNA into nucleosomes to form long chromatin fibers. Nucleosomes and chromatin function to control accessibility of transcription factors to their DNA target sites, while transcription factors target DNA sites to active transcription by “opening up” chromatin. However, the dynamic interplay between transcription factor binding and nucleosome/chromatin DNA compaction is poorly understood at the mechanistic level. I will discuss proposed strategies for how transcription factors bind to their sites within compact chromatin, and the differences between activating and pioneering transcription factors. I will then present our recent single molecule studies on how nucleosomes have profoundly different impacts on the DNA binding and dissociation dynamics of these two types of transcription factors. Our finds provide a potential way to define the functional differences between activating and pioneering transcription factors.

*This work was funded by NIH grants: GM121966, GM121858 and GM131626.
8:36AM R26.00002: Theory and modeling of active nucleosome repositioning* ZHONGLING JIANG (Presenter), BIN ZHANG, Massachusetts Institute of Technology MIT — Nucleosome positioning controls the accessible regions of chromatin and plays essential roles in DNA-templated processes. Its establishment in vivo is significantly influenced by ATP driven remodeling enzymes and transcription, which involves remodeler recruitment. On one hand, the non-equilibrium nature of remodelers has hindered the development of a unified theoretical framework for nucleosome positioning. On the other hand, explicit models are lacking in explaining the impact of transcription levels on nucleosome positioning since the complicated transcription process. For remodeling enzymes, we use a perturbation theory to show that the effect of these enzymes can be well approximated by effective equilibrium models with rescaled temperatures and interactions. Our theory provides an intuitive understanding for the impact of remodelers. By combining remodelers and RNAP II, we developed a transcription model, which illustrates opposite trends of nucleosome positioning patterns changing with transcription levels in yeasts and higher animals. This explanation qualitatively reproduces the experimental nucleosome positioning patterns.

*This work was supported by the National Institutes of Health (Grant 1R35GM133580-01) and the Amy Lin Shen Fellowship.

8:48AM R26.00003: Centromeres and Telomeres as Rheological Probes of the Human Nucleus* ALEXIS CLAVIJO (Presenter), STEVEN IONOV, ALEXANDRA ZIDOVSKA, Physics, New York Univ NYU — The nucleus of eukaryotic cells stores genetic information in chromatin, the functional form of DNA in cells. Chromatin loci have been observed to exhibit anomalous motion that is often ascribed to the viscoelastic nature of the chromatin, transient interactions of DNA-associated proteins and/or physical obstructions [1,2]. However, a direct link between motion of a chromatin locus and the rheology of its local environment is missing. In this work, we investigate dynamics of specific genomic loci, centromeres and telomeres, the centers and ends of the linear interphase chromosomes, respectively, in the context of their local rheological environment. Using simultaneous two-color spinning disc confocal microscopy combined with recently developed machine-learning-assisted tracking algorithms [3], we monitor the motion of telomeres and centromeres in live human cells and extract the rheological properties of their surrounding environment, mapping the chromatin rheology across the cell nucleus.


*This work was supported by the National Institutes of Health Grant R00-GM104152 and by the National Science Foundation Grants CAREER PHY-1554880 and CMMI-1762506.
9:00AM R26.00004: Knot dynamics of a DNA strand pushed inside a nanochannel  JAN ROTHÖRL (Presenter), PETER VIRNAU, Institute for Physics, Johannes Gutenberg University, ANIKET BHATTACHARYA, Univ of Central Florida — We investigate knot formation for a model DNA polymer pushed inside a square nanochannel whose width is much shorter compared to the contour length of the chain using Brownian dynamics simulation. We characterize different kind of knots formed, and monitor their evolution as the DNA is pushed inside the channel towards a steady state distribution. We repeat the calculations for several chain persistence lengths to understand how knots affect the DNA dynamics inside a nanochannel.

9:12AM R26.00005: Error-speed correlations in biopolymer synthesis  SIMONE PIGOLOTTI (Presenter), DAVIDE CHIUCHIU, Okinawa Institute of Science and Technology, YUHAI TU, BM T.J. Watson Research Center — Synthesis of biopolymers such as DNA, RNA, and proteins are biophysical processes aided by enzymes. Performance of these enzymes is usually characterized in terms of their average error rate and speed. However, because of thermal fluctuations in these single-molecule processes, both error and speed are inherently stochastic quantities. We study fluctuations of error and speed in biopolymer synthesis and show that they are in general correlated. This means that, under equal conditions, polymers that are synthesized faster due to a fluctuation tend to have either better or worse errors than the average. The error-correction mechanism implemented by the enzyme determines which of the two cases holds. For example, discrimination in the forward reaction rates tends to grant smaller errors to polymers with faster synthesis. The opposite occurs for discrimination in monomer rejection rates. Our results provide an experimentally feasible way to identify error-correction mechanisms by measuring the error-speed correlations.

9:24AM R26.00006: Noninvasive Measurement of Interphase Chromatin Rheology In Vivo*  IRAJ ESHGHI (Presenter), JONAH EATON, ALEXANDRA ZIDOVSKA, New York Univ NYU — Material properties of the genome are critical for its proper function and organization inside the cell nucleus. Chromatin, the functional form of DNA in cells, consists of DNA and associated proteins, forming long linear fibers in the interphase nucleus of eukaryotic cells. Traditionally, rheology of cellular components has been studied by tracking microparticles injected inside the cell [1]. Recently, we developed an injection-free noninvasive approach to study chromatin rheology using nuclear organelles as native probes [2]. Here, we show an alternative noninvasive experimental strategy using intrinsic dynamics to measure chromatin rheology across a large range of timescales, and elucidate the viscoelastic nature of chromatin in live cells. The measured rheology is captured by a surprisingly simple model whose few parameters have clear physical interpretations for this complex active material.


*This work was supported by the National Institutes of Health Grant R00-GM104152, the National Science Foundation (NSF) Grants CAREER PHY-1554880 and CMMI-1762506, New York University (NYU) MRSEC NSF Grant DMR-1420073 and NYU Whitehead Fellowship for Junior Faculty in Biomedical and Biological Sciences (to AZ).
Variability in gene expression ensures that cells with the same genotype always exhibit different phenotypes. Transcription bursting, or the random interruptions in the production of messenger RNA molecules, is one probable cause of this ubiquitous variability. Yet, the molecular mechanisms behind the bursting behavior remain unclear. Recent studies suggest that DNA supercoiling, which occurs during transcription, might be directly related to the bursting behavior. Stimulated by these observations, we developed a stochastic mechano-chemical model of supercoiling-induced transcriptional bursting. Using thermodynamically consistent coupling between mechanical and chemical processes, dynamic properties of transcription are explicitly evaluated. Theoretical analysis shows that the transcription bursting is observed when both supercoiling and the mechanical stress-release due to an enzyme gyrase are present in the system. A comparison with experimental data on bacteria allowed us to evaluate the energetic cost of supercoiling during transcription. We find that a relatively weak mechano-chemical coupling allows transcription to be regulated most effectively.

*Welch Foundation (C-1559), NSF (CHE-1664218), Center for Theoretical Biological Physics sponsored by NSF (PHY-1427654)

Chromosomal regions are known to adopt stable, heritable states which result in bistable gene expression without changes to the underlying DNA sequence. Such epigenetic control is a consequence of covalent modifications of histones. We introduced a (0+1)-dimensional kinetic model, wherein modified nucleosomes recruit enzymes that similarly modify neighbouring nucleosomes, to investigate the stability and heritability of the states. To make the model analytically tractable, we used the Doi-Peliti formalism, a second quantized description of the underlying master equation of a stochastic process such as the epigenetic problem at hand, that makes it amenable to attack via path integral methods such as semi-classical approximations, perturbation theory and renormalization group. Our model exhibits bistability, and using minimum action methods we can compute escape paths and probabilities between the two stable states. We are now coupling the model with a gene switch to quantify the developmental landscape of cell differentiation.

*This work has been supported by the Lester Wolfe Fellowship.
10:00AM R26.00009: Pulling a DNA through a Double-Nanopore system: A Brownian Dynamics Study  
PETER SMUCZ (Presenter), SWARNADEEP SETH, ANIKET BHATTACHARYA, Univ of Central Florida — We study translocation of a model DNA polymer captured in a double nanopore (DNP) system using Brownian dynamics (BD). We consider two different configurations as reported in recent experimental studies. In the first case, the direction of translocation is parallel to the vector connecting the two pores (X. Liu et al., Small 2019, 1901704). In the second case, the direction of translocation is perpendicular to the vector connecting the two pores (S. Pud et al., Nano Lett. 2016, 16, 8021-8028). In the former case we demonstrate that in the absence of a time dependent feedback mechanism, the velocity of the segment in between the pores is not constant, which hinders the mapping of the data from the time domain into genomic length. In the second case, we investigate parameters for optimal translocation of the chain through the DNP system. We consider limiting cases, where the distance between the pores is much shorter than the contour length of the chain, and show that one can use scaling results for single nanopore translocation to interpret results for the DNP translocation.

10:12AM R26.00010: Loop extrusion in chromatin: A question of time!*  
AJOY MAJI (Presenter), Physics, Indian Institute of Technology Bombay, RANJITH PADINHATEERI, Biosciences and Bioengineering, Indian Institute of Technology Bombay, MITHUN KUMAR MITRA, Physics, Indian Institute of Technology Bombay — One important question in the context of the 3D organization of chromosomes is the mechanism of formation of large loops between distant base pairs. Recent experiments suggest that the formation of loops might be mediated by Loop Extrusion Factors like cohesin. Experiments of cohesin have shown that cohesins walk diffusively on the DNA and nucleosomes act as obstacles to the diffusion, lowering the permeability and hence lowering the effective diffusion constant. An estimation of the times required to form the loops of typical sizes seen in Hi-C experiments using these low effective diffusion constants leads to times that are unphysically large. The puzzle then is the following, how does a cohesin molecule diffusing on the DNA backbone achieve speeds necessary to form the large loops seen in experiments? We propose a simple physical answer to this puzzle and show how a naive obstacle view of nucleosomes can be misleading.

*Ajoy Maji acknowledges fellowship given by IIT Bombay in Teaching Assistant category
**10:24AM R26.00011: Structural and Dynamical Signatures of Local DNA Damage in Live Cells**

JONAH EATON (Presenter), ALEXANDRA ZIDOVSKA, New York Univ NYU — The dynamic organization of chromatin inside the cell nucleus plays a key role in gene regulation and maintaining genome integrity. While the static folded state of the genome has been studied before, the dynamical signatures of processes such as transcription or DNA repair are unknown. We investigate the interphase chromatin dynamics in human cells in response to local damage, DNA double strand breaks (DSBs), by monitoring the DSB dynamics and the compaction of the surrounding chromatin in live cells. We find DSBs to possess a unique chromatin compaction profile, while being more mobile when located in the nuclear interior as opposed to the periphery. We show that DSB motion is subdiffusive, ATP-dependent, and exhibits unique dynamical signatures compared to undamaged chromatin. We find that DSB mobility follows a universal relationship based on the local environment suggesting that the repair processes are robust and likely deterministic. Such knowledge may help in detection of DNA damage in live cells and aid our biophysical understanding of genome integrity in health and disease [Eaton & Zidovska, Biophys. J., 2019].

*This work was supported by the National Institutes of Health Grant R00-GM104152 and by the National Science Foundation Grants CAREER PHY-1554880 and CMMI-1762506.

**10:36AM R26.00012: Extracting the degree of order in the bacterial chromosome using statistical physics**

JORIS MESSELINK (Presenter), Arnold Sommerfeld Center for Theoretical Physics, Ludwig Maximilian University of Munich, JACQUELINE JANSSEN, Max Planck Institute for the Physics of Complex Systems, Dresden, MURIEL VAN TEESELING, MARTIN THANBICHLER, Faculty of Biology, Philipps University Marburg, CHASE BROEDERSZ, Arnold Sommerfeld Center for Theoretical Physics, Ludwig Maximilian University of Munich — Elucidating the three-dimensional spatial organization of the bacterial chromosome is essential to understand how genomic processes are spatially regulated inside the cell. Recent Hi-C chromosome conformation capture experiments provide contact frequency maps of the chromosome. These experiments reveal structural organization beyond that of an amorphous polymer. However, despite such experimental advances, the degree of spatial organization of the bacterial chromosome remains unclear. To investigate this, we develop a maximum entropy approach to extract the three-dimensional structure of the bacterial chromosome from such data. Using this approach, we obtain a coarse-grained model for the full distribution of chromosome configurations for the bacterium *C. crescentus*. We validate the predictive power of our model by experiments on the localization of chromosomal loci in the cell. Our model reveals novel features of spatial chromosome organization on various length scales. Our approach is not organism-specific, and opens up a new way of analyzing spatial chromosome organization.

*Graduate school for Quantitative Biosciences Munich (QBM)
TRR174: Spatiotemporal dynamics of bacterial cells
R26.00013: Direct Quantification of Gene Regulation by Transcription-Factor Binding at an Endogenous Gene Locus  
JINGYAO WANG, School of Life Sciences and Biotechnology, Shanghai Jiao Tong University, YIJING DONG, HUIHAN BAO, XINTAO YAO, School of Physics and Astronomy, Shanghai Jiao Tong University, ANNA MARIE SOKAC, School of Molecular & Cellular Biology, University of Illinois at Urbana-Champaign, IDO GOLDING, Department of Physics, University of Illinois at Urbana-Champaign, HENG XU (Presenter), School of Physics and Astronomy, Shanghai Jiao Tong University — Gene activity is controlled by the binding of transcription factors (TFs) to the regulatory sequence of the gene, yet a direct in situ mapping from TF binding to mRNA production of a single gene remains elusive, due to the difficulty of capturing individual TF binding events of a specific gene from the ocean of TF signal in cell nucleus. Here we combine single-molecule fluorescent imaging of protein, mRNA, and gene loci to detect and quantify distinct binding configurations of multiple TFs and epigenetically modified histones, as well as the resulting nascent mRNAs at endogenous hunchback (hb) gene loci in early Drosophila embryos. Using stochastic theoretical analysis, we show that TF binding follows nonequilibrium multi-state kinetics, breaking the law of mass action. hb transcription activation is a multi-step process initiated by transient binding of the Bicoid transcription factor. Unlike TF binding at hb, the histone signal is deprived at active gene loci, indicating that nucleosome unwinding is necessary for gene activation. Our method provides a general framework to decipher the dynamics of complex gene regulatory networks in situ.

Thursday, March 5, 2020 8:00 AM - 10:36 AM

Session R27 FIAP: Thermal and Ballistic Transport in Semiconductors

8:00AM R27.00001: Non-degenerate heavy electrons and Planckian limit to scattering in doped strontium titanate*  
CLEMENT COLLIGNON (Presenter), BENOIT FAUQUE, JEIP, College de France, KAMRAN BEHNIA, LPEM, ESPCI — The metallicity of lightly doped SrTiO$_3$ is strange. The combination of the effective mass extracted from quantum oscillations and the amplitude of room-temperature mobility implies a mean-free-path (mfp) below the Mott Ioffe Regel (MIR) limit and a scattering time shorter than the Planckian time ($\tau_P$=h/2πkB$T$). Here, we present a study of electric resistivity and thermoelectric power above room temperature pointing to a possible exit out of this maze. According to our data, resistivity is metallic and does not saturate up to 900 K. In the non-degenerate regime, the Seebeck coefficient is set by the ratio of the de Broglie wavelength, $\lambda_{dB}$, to the interelectron distance, $n^{-1/3}$. We demonstrate that the temperature dependence of the shrinking $\lambda_{dB}$ (before its saturation to a length twice the lattice parameter) points to a continuous change in the effective mass of charge carriers. Combining the latter with mobility keeps the mfp above the MIR limit and the scattering time longer than $\tau_P$. Our results imply the existence of a hitherto unknown case of non-degenerate metallicity driven by temperature-induced mass amplification.

*This work is supported by Agence Nationale de la Recherche through the QUANTUM LIMIT project, by Fonds-ESPCI-Paris and by JEIP-Collège de France.
Energetics of solid-state metathesis reactions in nanostructured thermoelectric systems*  

XIA HUA (Presenter), JEFF W DOAK, CHRISTOPHER MARK WOLVERTON, Northwestern University — Thermoelectric systems with large compositions of AB (e.g. SnTe) and much smaller compositions of A′B′ (e.g. CdS, ZnS) are promising candidates since the second-phase nanostructures scatter phonons, reducing lattice thermal conductivity and increasing ZT. In this work, we use high-throughput density functional theory (DFT) calculations to evaluate the metathesis reactions (AB+A′B′↔A′B+AB′) of 1638 quaternary phase systems (A,A')(B,B′) in order to understand the behaviors and predict potential nanostructured thermoelectrics. We include systems most relevant for rocksalt-based thermoelectrics: group II, IIb, and IV cations, and group VI anions. In addition, we include group III cations and group V anions as possible secondary phases. We find that the metathesis reactions exhibit well-defined trends, which can be explained within the context of hard-soft acid-base theory (HSAB). Deviations from these trends are examined in more detail and finite temperature effects are investigated for select systems.

*The authors acknowledge financial support received from the US Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, under Award No. DE-SC0014520

The thermoshape voltage induced by quantum shape effects  

ALTUG SISMAN, Uppsala University, ALHUN AYDIN (Presenter), Istanbul Tech Univ, JONAS FRANSSON, Uppsala University — We propose here a new effect for the conversion of heat energy into electricity with nanostructures. We recently used size-invariant shape transformation to completely separate quantum size and shape effects from each other, which allows one to focus on purely quantum shape effects. In this work, we first present the existence of the quantum shape effects on thermoelectric transport properties of GaAs nanostructures at ballistic regime. Then we consider a junction composed of the same material having exactly the same geometric sizes, but distinct shapes. We show that an electric voltage is induced under a temperature gradient in such a junction because of the quantum shape effects on Seebeck coefficients. This cross effect is called the thermoshape effect. Our calculations based on Landauer formalism predict that the thermoshape voltage is persistent and in the order of mV/K for non-degenerate GaAs semiconductors. Our study explicitly suggests how important the effect of overall geometry is in nanoscale thermoelectric materials, and can be utilized even if all sizes are the same. A thermoshape junction not only represents a viable setup for the macroscopic manifestation of quantum shape effects, but also constitutes their first possible device application.
Observation of anomalous Shapiro steps in ballistic Josephson junctions of InAs nanowires

KENTO UEDA (Presenter), Univ of Tokyo, SADASHIGE MATSUO, RIKEN, HIROSHI KAMATA, YUUSUKE TAKESHIKE, YOSUKE SATO, SHOJI BABA, Univ of Tokyo, LARS SAMUELSON, Lund University, KAN LI, Peking University, SOREN JEPPESEN, Lund University, HONGQI XU, Peking University, SEIGO TARUCHA, RIKEN — Advances in semiconductor technology provide the high electric controllability and long mean free path in various kinds of nanostructure. Especially proximity-induced superconductivity in semiconductor nanowire (NW)-superconductor junctions provides intriguing platforms to study exotic superconducting phenomena occurring in the ballistic transport regime.

For example, the quantized conductance due to Majorana Fermions (MFs) [1], and high-efficient Cooper pair splitting [2] have been observed in a superconducting junction of a single NW, and double NW, respectively.

Here we report on observation of anomalous Shapiro steps measured in Josephson junctions (JJ) of InAs NWs. The Shapiro steps appear on not only integer multiples of hf/2e but also the half-integer multiples. We attribute these anomalous steps to the skewed current-phase relation (CPR) expected in the ballistic JJ. Our results contribute to establish the relationship between the CPR and Shapiro step anomalies, which is also important for study of MFs.


Ballistic transport in black phosphorus transistors*

XUEFEI LI (Presenter), Huazhong University of Science & Technology — As a strong candidate for future electronics, atomically thin black phosphorus (BP) has attracted great attention in recent years due to its tunable bandgap and high mobility. Here we show that the transport properties of BP device under high electric field can be improved greatly by the interface engineering of high-quality HfLaO dielectrics and transport orientation. By designing the device channels along the lower effective mass armchair direction, a record high drive current up to 1.2 mA/μm at 300 K and 1.6 mA/μm at 20 K can be achieved in a 100 nm back-gated BP transistor, surpassing any two-dimensional semiconductor transistors reported to date. The highest hole saturation velocity of $1.5 \times 10^7$ cm/s is also achieved at room temperature. Ballistic transport shows a record high 36% and 79% ballistic efficiency at room temperature and 20 K, respectively, which are also further verified by theoretical simulations.

*This work was supported by the National Natural Science Foundation of China (grant nos. 61574066, 618744162, and 61522402), the Strategic Priority Research Program of Chinese Academy of Sciences under grant no. XDB30000000 and, in part, by the Fundamental Research Funds for the Central Universities under grant 2018KFYYXJJ069 and 2019kfyXKJC014.
9:00AM R27.00006: Quantum Technologies using Ge and GeSn on Si. YILMAZ GUL (Presenter), STUART NICHOLAS HOLMES, London Center for Nanotechnology, MAKSYM MYRONOV, Physics, University of Warwick, MICHAEL PEPPER, London Center for Nanotechnology — Large scale fabrication using Complementary Metal Oxide Semiconductor compatible technology of semiconductor nanostructures that operate on the principles of quantum transport is an exciting possibility now due to the development of ultra-high mobility hole gases in epitaxial germanium grown on standard silicon substrates. We present here a ballistic transport study of patterned surface gates on strained Ge quantum wells with SiGe barriers, which confirms the quantum characteristics of the Ge heavy hole valence band structure in 1-dimension. We also present transport properties of light holes in GeSn quantum well structures grown on standard Si (001) substrate. Furthermore we present the current and future measurements taking place using Ge, including spin focusing and majorana fermion studies using superconducting junctions on Ge layers. The experimental results shown here suggests a new area of experimentation in quasi 1D systems, particularly direct measurement of the charge, with implications for possible schemes of topological quantum information processing.

9:12AM R27.00007: Thermal transistor and thermometer based on coupled quantum dot and point contact*. JING YANG ( Presenter), CYRIL ELOUARD, University of Rochester, JANINE SPLETTSTOESSER, Chalmers University of Technology, BJÖRN SOTHMANN, Universität Duisburg-Essen and CENIDE, RAFAEL SÁNCHEZ, Universidad Autónoma de Madrid, ANDREW N JORDAN, University of Rochester — We propose a three-terminal setup consisting of a Coulomb coupled quantum dot quantum point contact. The source and drain reservoirs are connected to the QPC while the base reservoir is tunnel coupled to the Coulomb blockade quantum dot, which can contain at most one electron. We show that the setup can work as a nanoscale thermal transistor to control the electric or heat current flow in the quantum point contact. Alternatively, by detecting the electric current in the quantum point contact, the setup can also act as the nanoscale thermometer. We calculate the sensitivity and power gain for the transistor and the sensitivity for the thermometer respectively. We derive the operating condition maximizing their respective sensitivities. We show that the resolution in previous experiments on temperature sensing can be further improved if it is tuned to the optimal regime we derived here.

*This research was supported in part by the National Science Foundation under Grant No. NSF PHY-1748958 (KITP program QTHERMO18). We thank the KITP for hosting the program Thermodynamics of Quantum Systems: Measurement, engines, and control, where this work was initiated. We thank the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award No. DE-SC-467 0017890.
9:24AM R27.00008: Hopping conduction characterization in amorphous semiconductors and cross-linked metal nanoparticles*  BRIANNA WESTERN (Presenter), MICHAEL HARCROW, ATHANASIOS J SYLLAIOS, VINCENT LOPES, CHRISTOPHER LITTLER, University of North Texas, ZHI-GANG YU, RAY GUNAWIDJAJA, Washington State Univ — In amorphous semiconductors, e.g. a-Si, conduction occurs via charge carrier hopping between localized states. The key figures of merit in characterization, particularly in microbolometer applications, include the temperature dependence of conductivity, summarized by the temperature coefficient of resistance (TCR), and electrical noise, which are controlled in the hopping regime by the hopping conduction parameters. For next-generation bolometer material, cross-linked metal nanoparticles (CLMPs) conduction occurs via electron hopping between adjacent nanoparticles, and the conductivity exhibits Arrhenius temperature-dependent behavior. In these systems, TCR and noise are theorized to be controlled by nanoparticle diameter and separation distance between adjacent nanoparticles, respectively. Diameter and separation distance in CLMPs are independent of each other, with the separation distance being controlled by organic ligands bonded to the nanoparticle surface. This work examines the effect of different organic ligands on electrical conductivity and TCR in CLMPs.

*This work is supported by ARO Contract W911NF-17-1-0511, Dr. Michael D. Gerhold, Program Manager 
Characterization, Modeling, and Optimization of Cross-Linked Metal Particles for Microbolometers

9:36AM R27.00009: Non-equilibrium nature of non-linear optical response: Application to the bulk photo voltaic effect  TAMOGHNA BARIK (Presenter), JAY SAU, University of Maryland, College Park — The bulk photo-voltaic effect (BPVE) is an example of non-linear optical response that leads to a DC current in non-centrosymmetric materials which is relevant to photo-voltaic applications. We theoretically study this effect in the presence of electron-phonon interactions. Using the response function formalism, we show that the non-linear optical response, in general, contains correlator of three operators which are not ordered in time. This out of time-ordered correlator (OTOC) for an interacting system cannot be calculated using equilibrium field theory. Using a semiclassical approach instead, we show that BPVE can be attributed to the dipole moment of generated electron hole pairs. We confirm the validity of semiclassical result for the non-linear DC response from a quantum master equation approach. From this formalism we also find that the electron-phonon coupling strength has a strong implicit effect on the scaling dependence of the non-linear DC response on the optical field. Most interestingly, the semiclassical treatment shows that the non-linear DC response for spatially inhomogeneous excitation profiles is strongly non-local and must involve the aforementioned OTOC that cannot be computed by equilibrium field theory.

9:48AM R27.00010: Measurement of Hall conductivity near the metal insulator transition by torque magnetometry*  
SAMUEL MUMFORD (Presenter), TIFFANY PAUL, Physics, Stanford University, SEUNG HWAN LEE, AMIR YACOBY, Physics, Harvard University, AHARON KAPITULNIK, Physics, Stanford University — We study Hall conductivity near the disorder-induced metal-insulator transition and present the first measurements of Hall conductivity utilizing a torque magnetometry method. A Corbino disk exhibits a magnetic dipole moment proportional to Hall conductivity when voltage is applied across a test material. This magnetic dipole moment can be measured through torque magnetometry. The symmetry of this contactless technique allows us to measure the Hall conductivity of insulating materials and materials near the metal-insulator transition such as sputtered indium tin oxide. We have measured the Hall conductivity of indium tin oxide with a ratio of transverse to longitudinal resistivity of 1E-4 and can now measure Hall conductivity independently of longitudinal resistance.

*This work was funded by the Army Research Office grant W911NF1710588, and by the Gordon and Betty Moore Foundation through Emergent Phenomena in Quantum Systems (EPiQS) Initiative Grant GBMF4529.

10:00AM R27.00011: Kinetic Inductance in Ballistic Transport Jashan Singhal¹ and Debdeep Jena¹,²,³  
¹ School of Electrical and Computer Engineering, Cornell University ² Department of Materials Science and Engineering, Cornell University ³ Kavli Institute at Cornell for Nanoscale Science, Cornell  
JASHAN SINGHAL (Presenter), DEBDEEP JENA, School of Electrical and Computer Engineering, Cornell University — Electron transport in nanoscale semiconductors approaches the ballistic limit. Without scattering, the kinetic inductance (KI) of carriers becomes considerably large [1,2]. What are the consequences in devices and circuits? We investigate the generalized kinetic inductance in a d-dimensional conductor with various band-structures (e.g. parabolic and conical) in the ballistic limit. The KI per unit length is evaluated as a function of carrier density and temperature at low bias voltages. The KI is found to very weakly depend on V, and strongly on the electron density. An increase in KI at low density is expected because more velocity is needed to maintain the same current. The ballistic model predicts that even without considering phonon scattering, the KI decreases at high temperature. Because of the Fermionic nature of electrons, their collective excitation exhibits a Newtonian inertia, which decreases with an increase in temperature. The quantum mechanical ballistic KI is compared to the standard ‘classical’ inductance, and its importance is classified for various carrier densities, and dimensions.

² C. Rutherglen and P. Burke, Small 5.8 (Apr. 2009), pp. 884-906
10:12AM R27.00012: Novel computational approach for electron-transport from first-principles*  
ALEX GANOSE (Presenter), JUNSOO PARK, ANUBHAV JAIN, Lawrence Berkeley National Laboratory — Accurate calculation of transport properties has so far proved challenging due to the difficulty of computing carrier relaxation times. Methods which explicitly include electron-phonon interactions, such as Electron-Phonon Wannier (EPW), yield high-quality predictions but are incredibly computationally expensive and therefore limited to systems with few electrons. Conversely, using the constant relaxation time approximation (CRTA), predictions are obtained quickly but can be unreliable.

We have developed a new framework for calculating the electronic transport properties of solid-state materials from first-principles. With performance close to that of EPW at a fraction of the computational cost, the technique is both accurate and amenable to high-throughput calculations. We demonstrate the speed and performance of the package by screening the Materials Project database for novel thermoelectric materials.

*We acknowledge support from the US Department of Energy, Office of Basic Energy Sciences, Early Career Research Program (ECRP). Computing resources were provided by the National Energy Research Scientific Computing Center (NERSC), a DOE Office of Science User Facility supported by the Office of Science of the US Department of Energy under contract no. DE-AC02-05CH11231.

10:24AM R27.00013: A model of dephasing in shift current processes*  
BENJAMIN FREGOSO (Presenter), Kent State Univ - Kent — The shift current is a second order nonlinear effect in the optical field thought to be the dominant transport mechanism in many ferroelectric materials and to carry information about the topology of the Bloch wave functions. The shift current requires quantum coherence in the solid. We construct a simple model of electrons coupled to a chain of one-dimensional ions lacking inversion symmetry. We analyze the thermalization of electrons within the model at high and low excitations frequencies (close to the band edge). The model allows the study of decoherence in shift current process beyond the classical transport regime.

*NERSC-DOE DE-AC02-05CH11231
8:00AM R28.00001: Following a Theoretical Roadmap to Low Nucleation Barriers for CO₂

**Nucleation in Polyol** [Invited] JULIA A KORNFIELD (Presenter), Caltech — The quest for insulation with thermal conductivity as low as stagnant air motivates production of ultra-low density foams with cells as small as 1μm across, requiring the controlled nucleation and growth of \(10^{10}\) bubbles/(cm³ mother liquid). In relation to polyurethane foam, we seek high nucleation density guided by predictions from density functional theory (DFT) with the string method for the activation barriers. Predicted composition profiles across the interface suggest that cyclopentane (C5), a physical blowing agent, promotes CO2/polyol nucleation in multiple ways: C5 increases the density of the CO₂-rich nucleus, and C5 preferentially concentrates at the interface---both tend to reduce the interfacial tension. To test theoretical predictions, we validated the thermodynamic properties of binary (CO₂/polyol) and ternary (CO₂/C5/polyol) systems. Experimental results for binary systems quantify the reduction of interfacial tension near the critical point and accord with predictions. In ternary systems, theory directed our attention to a range of composition and pressure in which three-phase coexistence may occur and preliminary results support the theoretical predictions. Then we investigated nucleation kinetics using a high-pressure microfluidic apparatus. Initial results obtained using optical microscopy will be presented, laying the foundation for future scattering measurements to quantify the number and size of incipient bubbles. This work was conducted in collaboration with Dow, including T Fitzgibbons, WJ Zhou, HK Chao, J Griffith, B Winniford, S Horsch and V Ginzburg; E DiMaio at Uni Naples and A Ylitalo, ZG Wang and RC Flagan at Caltech.

*This research is funded by Dow.

8:36AM R28.00002: Polymer Foams for Building Insulation (STYROFOAM and beyond) [Invited]

STEPHANE COSTEUX (Presenter), Safety & Construction, DuPont — Thermoplastic foams have been used in buildings for over 75 years, since the initial introduction of STYROFOAM™ extruded polystyrene foam. Although significant progress has been made to improve the product performance, durability and sustainability, the process itself has remained relatively unchanged, and the levers used to control foam structure – and thus performance - still rely on empiricism. An examination of mechanisms involved in the foaming process of thermoplastic polymers points to the difficulty of predicting cell nucleation density, as well as the quantitative influence of cells interactions during expansion and stabilization. These limitations are particularly apparent now that the foam community has turned its attention to nanocellular foams, which are expected to demonstrate superior properties but are very difficult produce by known commercial processes.

[ STYROFOAM™ is a trademark of DuPont Inc. ]
9:12AM R28.00003: Polyurethane Application Innovation: Translating Chemistry to Materials to Solve Real-World Problems [Invited]  WILLIAM KOONCE (Presenter), Dow Chemical — Polyurethane materials have grown rapidly in recent years and now touch most facets of modern life from comfortable sleep to energy efficiency and transportation among others. Polyurethane chemistry provides high versatility in application processes with conversion from low viscosity liquids to polymeric solids in seconds. This processing versatility enables generation of varied foam structures, filling of complex geometries, and coating of diverse substrates. Beyond processing, polyurethane polymers can be designed to deliver a range of structures and resulting properties from hard to soft, viscoelastic to elastic, hydrophobic to hydrophilic. Examples of using these versatile processing and material properties to solve real world problems will be shared.

9:48AM R28.00004: Modeling Nucleation in Polymeric Foams using Self-Consistent Field Theory* [Invited]  RUSSELL B THOMPSON (Presenter), University of Waterloo — Self-consistent field theory is a method in statistical mechanics that is effective for the study of inhomogeneous polymer structures, typically block copolymer self-assembly. Self-consistent field theory can also be used to understand some aspects of nucleation in polymer foaming, especially for nano-cellular foams. An introduction to this approach, including its advantages and disadvantages, will be given. Implications for the validity of classical nucleation theory and nucleation barriers from this perspective will be discussed, as will some new predictions related to heterogeneous nucleation.

*NSERC

10:24AM R28.00005: Fluid dynamics of bubbly drinks [Invited]  ROBERTO ZENIT (Presenter), School of Engineering, Brown University — Most people find bubbly drinks to be attractive and refreshing. With the excuse of trying to answer why, we explore the physics involved in this particular kind of two-phase, mass-transfer-driven flows. Discussion and analysis of the processes of bubble formation, ascension, accumulation and bursting are presented. Links to other relevant flow phenomena are presented in each case.

Thursday, March 5, 2020 8:00 AM - 10:24 AM

Session R29 DSOFT DBIO GSNP DPOLY: Active Matter and Liquid Crystals in Biological Systems II  501 - Kimberly Weirich, University of Chicago - Tag(s): Focus
8:00AM R29.00001: Defect Ordering and Patterning in Active Nematics*  
SURAJ SHANKAR  
(Presenter), Physics, Harvard University, M CRISTINA MARCHETTI, Physics, University of California, Santa Barbara — Active nematics combine liquid crystalline orientational order with internal active driving to generate novel dynamical states involving complex spatio-temporal flows along with spontaneous defect pair creation and proliferation. Topological defects acquire self-propulsion due to activity and play a prominent role in driving large scale flows in two-dimensional active nematics. By focusing on defects as the relevant excitations, we develop a hydrodynamic theory of active defects incorporating both defect motility and active torques that align defect orientations. Our model predicts a defect ordered polar flock at high activity and uncovers the underlying physical mechanism for defect ordering. Extending our framework to include spatially inhomogeneous activity, we show how activity gradients act as "electric fields" that can sort defects based on their topological charge. Our continuum model hence offers a useful and versatile approach to quantify the patterning of defects and flow in active nematics by the spatial control of activity.

*This work was supported by the NSF grants DMR-1609208, at KITP under PHY-1748958, and at the Aspen Center for Physics under PHY-1607611.

8:12AM R29.00002: Ordering and Correlations of Active Nematic Defects in 2D Flat Space  
JYOTHISHRAJ NAMBISAN  
(Presenter), Georgia Institute of Technology, DANIEL PEARCE, University of Geneva, PERRY W ELLIS, Harvard University, LUCA GIOMI, Leiden University, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Topological defects are regions in an ordered material where the characteristic order is undefined. These defects are of significant interest in understanding the dynamics of active nematics, which are intrinsically out of equilibrium. One of the aims of our work is to address the orientation of defects in curved geometries. However, in this talk, I will discuss our results in flat space. We first explain how we prepare and image the system and how we identify defects using image analysis techniques. We focus on their orientation calculated directly from the divergence of the nematic tensor order parameter. We then use the defect positions and orientations to define relevant order parameters – polar and nematic order for the +1/2 defects, and a 3-fold bond angle order for the -1/2 defects. These quantities give us insights on the average orientational ordering of our system of defects. We then proceed to look at orientational correlations, and present insights into the configurations adopted by the defects as a function of the inter-defect spacing. Remarkably, we find that the local orientational order persists irrespective of the defect density.

8:24AM R29.00003: Defect order in active nematics  
ZHITAO CHEN  
(Presenter), MARK J BOWICK, M CRISTINA MARCHETTI, University of California, Santa Barbara — Using a recently derived model of active defects as quasi-particles, some of us have reported emergent states where +1/2 defects in active nematics organize in structures with large scale polar order. While ordered states of +1/2 defects have been obtained in both experiments and simulations of active nematic hydrodynamics, both polar and nematic alignment of the +1/2 defects have been seen depending on whether active flows are dissipated by friction with a substrate or by viscous stresses. In this talk, we will discuss the interplay between elastic and active torques, active flows and frictional dissipation in controlling defect patterns in these active liquid crystals.
8:36AM R29.00004: Dynamical Behavior of Defects in Circularly Patterned Active Nematics
ALI MOZAFFARI (Presenter), RUI ZHANG, University of Chicago, ANDREY SOKOLOV, ALEXEY SNEZHKO, Argonne National Laboratory, JUAN DE PABLO, University of Chicago — Active nematics represent a new class of non-equilibrium systems that combine orientational ordering with active stresses applied to elongated particles. Continuum simulations of the active nematic are employed to explain how the interplay of activity-fueled energy injection to the system and frictional damping forces impact the dynamics of topologically imposed self-propelling +1/2 defects. We show that by patterning the activity by imposing active stresses in circular domains near the center of confinement, it is possible to regulate the motion of defects. A phase diagram of the dynamical response of defects based on activity strength and hydrodynamic friction is developed, revealing a wealth of new phenomena. Our results disclose that defects synchronize their dynamics to minimize the elastic distortion energy while being driven out of equilibrium by active stresses. A phase diagram is presented that displays a rich dynamical behavior, including immobile defects, steady rotation, bouncing defects, cruising defects, and a synchronized dancing state.

8:48AM R29.00005: Photo-Patterning DNA Structures with Topological Defects and Arbitrary Patterns through Multiple Length Scales CHENHUI PENG (Presenter), JINGHUA JIANG, NETRA DHAKAL, Physics and Materials Science, The University of Memphis — DNA is the building block for all living organisms, hence controlling supramolecular self-assembly of DNA structures is important not only for better understanding its biological properties, but also sheds light to designing new functional materials for biological engineering and material science applications. However, it is still challenging to control the DNA molecular self-assembly structures in the predesigned manner across multiple length scales. In this work, we demonstrate that the orientational order of DNA molecules can be precisely controlled by using photo-patterning technique. This technique imprints various spatially varying patterns into a layer of liquid crystalline polymer which will be further used to control the DNA structures. It is demonstrated that DNA orientations can be patterned with two dimensional lattice of topological defects and arbitrary patterns through length scale from micrometers to millimeters. The resulting programmable and predesigned DNA self-assembly structures will open opportunities in advanced materials and devices for optical and biological applications.
9:00AM R29.00006: Cells as liquid crystals, and what happens when they can't align [Invited]
KIRSTEN ENDRESEN, MINSU KIM, FRANCESCA SERRA (Presenter), Johns Hopkins University — The organization of cells in tissues is crucial in determining their properties and functionalities. From the embryonic organization to mature tissues, cells are often arranged in well-determined patterns, which control the mechanical properties of the tissue and the ability to sense the environment. Many cell types have a characteristic anisotropic shape, and show an intrinsic ability to align with their neighbors. This behavior is analog to nematic liquid crystals (LCs). One special feature of LCs is the presence of topological defects, regions where the nematic order is lost and where stresses are concentrated in small regions. Monolayers of cells show alignment defects analog to LC topological defects. There is increasing evidence that such defects have a biological role, and their importance has been discussed in processes such as cell apoptosis, formation of 3D protrusions, growth of tumors stroma and cell migrations from tumors.
To better understand the role of these disordered regions in tissues, we induce topological defects in cell monolayers and study the cells behavior. Our goal is to connect biological properties of cells to the LC properties of the monolayers that the cells can form. We use topography to investigate the behavior of cells near induced topological defects, each characterized by their topological charge. Using shallow patterned grooves, we can impose defects with various charges without totally constraining the cells, and we study the cells’ behavior. Our data show a very different behavior of fibroblasts 3T6 and epithelial cells EpH-4 near topological defects with azimuthal or hyperbolic orientation of cells (+1 and -1 topological charge respectively), both in the ability to align and in the distribution of cell density within the monolayers. Finally, the behavior of cells near defects can provide a unique way to determine the size of the defect core.

9:36AM R29.00007: Quantifying orientational interactions among defects in active nematics*
SUPAVIT POKAWANVIT (Presenter), ZHIHONG YOU, M CRISTINA MARCHETTI, MARK J BOWICK, University of California, Santa Barbara — In passive two-dimensional systems, from superfluid films to nematic layers, topological defects play a key role in controlling continuous order-disorder transitions. Inspired by this, some of us have recently derived an effective description of the dynamics of topological defects in 2D active nematics as quasiparticles, where the unbound defects are modeled as a gas of self-propelled (+1/2) and passive (-1/2) particles with Coulomb interactions and aligning torques. We have now tested this model against defect trajectories obtained from numerical simulations of 2D active nematic hydrodynamics. Specifically, we demonstrate that the polar +1/2 defects interact via torques that tend to align the defect polarization with the elastic force they experience from other defects, as in previously studied models of flocking.

*This work was supported by NSF Grants No. PHY-1748958 (MJB) and DMR-1609208 and DMR-1938187 (MCM).
9:48AM R29.00008: Effect of active enzyme diffusion on mesoscale particles

BAHAR ROUHVAND (Presenter), Univ of Mass - Amherst, JENNIFER L ROSS, Physics, University of Syracuse —

Most of the phenomena in a living matter occur far from equilibrium and, therefore, cannot be treated within the framework of classical equilibrium thermodynamics. The elements of active matter, self-propelled particles, can be used to power active baths that can be rectified to recover work from noisy, non-equilibrium systems. Prior work has used bacteria or colloidal active matter to serve as active baths that can turn rotors or be rectified. However, the large size of bacteria creates a lower limit on the size of a material powered by a bacterial active bath. Cell biological studies have implied that metabolism enzymes serve to mix the viscous and complex fluid of the cytoplasm. Using these ideas our prior expertise in studying enzymes, we will focus on how enzyme baths can power the fluctuation spectrum of nano particles, and their effect on the diffusivity and fluctuations of larger particles such as passive proteins, quantum dots, and colloidal particles. Activity of passive elements will be analyzed through single particle tracking and differential dynamic microscopy.

10:00AM R29.00009: Collective trapping of flocking particles by asymmetric obstacles*

JUAN ARAGONES (Presenter), RAUL MARTINEZ, Univ Autonoma de Madrid, FRANCISCO ALARCON, Departamento de ingenieria fisica, Universidad de Guanajuato, CHANTAL VALERIANI, Departamento de Estructura de la Materia, Fisica Termica y Electronica, Universidad Complutense de Madrid — Anisotropic obstacles not only are capable to induce ratchet effects on suspensions of run-and-tumbling particles, but also affect the collective behaviour of active aligning particles, such as Vicsek particles [1, 2]. In this talk, I will show that flocking particles which follow the Vicsek model aligning rules experience a collective trapping in the presence of a wall of funnels made of chevrons, concentrating at the opposite side of a wall of funnels than run-and-tumbling particles. We study the dynamics of this collective self-trapping behaviour and identify two regimes, one static and other dynamical in which particles are effectively trapped by constantly escaping and getting into the channels. Exploiting these two regimes, we engineer a system showing two perpendicular flows of Vicsek particles.


*The project that gave rise to these results received the support of a fellowship from "la Caixa" Foundation (ID 100010434). The fellowship code is LCF/BQ/LI18/11630021.
10:12AM R29.00010: Polar flocking of active clusters  PAUL DOMMERSNES (Presenter), JON OTTO FOSSUM, Department of Physics, Norwegian University of Science and Technology — Biological active matter, such as populations of cells and animals, often change between different flocking regimes. One example is shoaling, milling and schooling transitions in fish. Synthetic active matter consist of self-propelled inanimate units and can emulate the flocking behavior of biological active matter. Here we report on a system of electro-propelled rolling granular beads with tuneable interactions. Many active matter regimes is realized in the same experiment as a function of the electric field: including active crystals and clusters with long range polar order, a stripe phase of clusters, and polar liquid flocks. Remarkably, the crystal to liquid transition occurs at a different velocity threshold than the local to global polar order transition. The stripe phase is reminiscent of those seen in quasi two-dimensional matter with competing interactions. The experimental system offers a physical model for flocking transitions in biological active matter, and can also open new routes for controlling self-assembly in soft matter technologies.

R29.00011: Flocking and clustering of self-propelled disks with active reorientation  TING ZHENG (Presenter), School of Physics, Southeast University, LU CHEN, Beijing Computational Science Res Ctr, ZHANCHUN TU, Beijing Normal University, XIANG CHENG, University of Minnesota, XINLIANG XU, Beijing Computational Science Res Ctr — In this talk we present a numerical investigation of self-propelled disks that integrates a behavior of active reorientation in analogy to collision avoidance in animal herds. The results of our simulations show rich phase dynamics including a flocking state, and a clustering state as a result of the mobility-induced phase separation. With a systematic exploration, our study reveals the unexpected link between the two collective behaviors. This study illustrated the importance of active reorientation on the emergent behaviors of self-propelled particles relevant to many natural and engineered active systems.

Thursday, March 5, 2020 8:00 AM - 10:48 AM

Session R30 DSOFT DPOLY GSNP DBIO: Visualizing Forces in Soft Materials via Photoelastic and Other Optical Techniques 502 - Karen Daniels, North Carolina State University - Tag(s): Focus
8:00AM R30.00001: Stress and velocity fluctuations in photoelastic granular avalanches*
NATHALIE VRIEND (Presenter), BP Institute, Univ of Cambridge, AMALIA THOMAS, DAMTP, Univ. of Cambridge, KAREN DANIELS, Department of Physics, NCSU — We study granular avalanches using a custom-built narrow chute where we release 2D photoelastic disks down an incline. Using high-speed imagery, we are able to obtain position and velocity data from particle tracking, and the full stress tensor, including normal and shear stress components, from the photoelastic response of interacting particles. Even though the avalanche is steady-state in time and space, minute fluctuations in velocity and forces away from the mean directly influence the rheology and fluidity.

In this study, we analyze the correlation between velocity fluctuations and stress fluctuations in both the quasi-steady layer (close to the rough base) and the flowing layer (near the free surface). We correlate the fluctuations with direct measurements of the measured non-local properties within this photoelastic avalanche.

*This work is funded by IFPRI, Royal Society Dorothy Hodgkin Fellowship DH120121, Royal Society Research Grant RG130403, and the Cambridge International Trust.

8:12AM R30.00002: Photoelastic Analysis of Cohesive Granular Aggregates CARTER PATTERSON (Presenter), Haverford College, JONATHAN KOLLMER, Universität Duisburg-Essen, THEODORE ANTHONY BRZINSKI, Haverford College — Photoelasticimetry facilitates the non-invasive measurement of individual contact forces in granular materials. This gives us greater insight into the spatially heterogeneous structure of force transmission characteristic of amorphous granular solids. To our knowledge, photoelasticimetry has been used exclusively to measure contact force networks in aggregates of repulsive particles. We present photoelasticimetric force measurements of systems of particles which exhibit attractive interparticle forces, and contrast the structure of force networks in these systems with the networks in purely repulsive aggregates.
8:24AM R30.00003: Optical characterization of underwater contact mechanics  MENGYUE SUN (Presenter), SUKHMANJOT KAUR, Univ of Akron — For survival in extreme environments, organisms have evolved adhesive mechanisms and materials. While chemistry of underwater bio-adhesion is a source of valuable insight, the mechanics by which surfaces expel water and come in contact underlies critical understanding of natural solutions and evaluating biomimetic analogs. Hydrophobicity of an adhesive surface has been shown to be crucial in removing water from a hydrophilic substrate, but the resulting contact is typically heterogeneous, with patches of unevacuated water. Here, we present a simple, FTIR-based imaging technique to spatially resolve and quantify thickness of nanoscopic puddles formed between two solids in contact under water. The technique is validated by comparing measured air gap thickness of a glass lens in contact with glass prism with Hertzian contact theory, and then applied to characterize the drainage and formation of patches of water as a soft PDMS lens approaches a glass surface at varying speeds. The work paves the way for better characterization of interfaces in contact under water and can find application in adhesive development, biological study and tribology.


8:36AM R30.00004: Worms in Jell-O: Using photoelastic stress analysis to measure burrowing forces* [Invited]  KELLY DORGAN (Presenter), Dauphin Island Sea Lab — Muddy marine sediments are elastic materials through which worms and other animals extend burrows by fracture. Gelatin has similar fracture properties to muds, and worms burrow readily through this transparent analog. Polarized light shows that the water-filled burrow has an elongated, tongue-depressor-shaped crack. Photoelastic stress analysis was used to measure forces applied by worms burrowing in gelatin. These results, combined with modeling, show that stress intensity factors at the crack tip reach the fracture toughness, validating the method of burrow extension by fracture. Additionally, these measured forces and understanding of the mechanics of burrowing allowed for quantification of the energetic cost of burrowing, which is much lower than previously thought. Stress visualization in gelatin has also been used to test instruments to measure fracture toughness and stiffness of marine sediments. These properties govern burrowing behaviors and may be important metrics to quantify the ecosystem engineering impacts of animals living in sediments.

*This work was supported by the Office of Naval Research Young Investigator Program Award N00014-17-1-2625 and Code 322 Award N00014-18-1-2806.
9:12AM R30.00005: Exploiting photoelasticity to characterize dynamics of polymer networks  CAROLINE SZCZEPANSKI (Presenter), Michigan State Univ, KELSEY-ANN NATASHA LESLIE, ROBERT DOANE-SOLOMON, SRI SHTI ARORA, MICHELLE R DRISCOLL, Northwestern University — The development of internal stresses within polymer networks is a major factor to consider when utilizing this class of soft materials, particularly when compared to their linear analogues. As an example, internal stresses that develop during network polymerizations often lead to macroscopic failures such as delamination or cracking when networks are constrained at one or multiple interfaces. To better understand and mitigate stress behavior, macroscopic mechanical characterization techniques (e.g. tensile testing, rheometry) have typically been employed. However, these methods provide little to no insight as to the dynamics of stress evolution on a local level, nor how internal stresses evolve in response to environmental changes. In this work, we exploit the photoelastic behavior of polymer networks to characterize internal stresses that develop during swelling and subsequent rupture of hydrogels. Compared to the majority of studies into mechanics of hydrogels, which typically characterize materials in one of two separate states (dry or swollen), this approach enables a non-invasive, real-time assessment of internal stress development during swelling. We discuss how this approach can better inform soft materials developed for dynamic environments.

9:24AM R30.00006: The local mechanics of macroscopic heterogeneous photoelastic polymer networks  JOHANNES N.M. BOOTS (Presenter), JORIK SCHAAP, JOSHUA DIJKSMAN, JASPER VAN DER GUCHT, THOMAS KODGER, Wageningen University — Stress localization and fracture within networks are common observations but predicting failure relies on a complex interplay between each connected component or beam. Simulations on model networks have shown intriguing connections between connectivity and stress. But do these results translate into physical experiments? To explore this, we produce macroscopic (~cm), heterogeneous (removing beams or varying beam thickness), 2D networks by using a 3D printed mold that is cast first with a silicone rubber, and then with a highly responsive photoelastic resin. Upon straining these networks to failure, each beam experiences a local stress resulting in a proportional photoelastic signal which is captured with a camera while measuring the bulk force with a capacitive load cell. This signal is compared to a previously measured force-intensity calibration curve from a single beam. Concomitantly, a second camera captures brightfield images, used to calculate the local strain. This local stress/stRAIN information in programmable heterogenous networks is used as input for spring network simulations. We will present the comparisons between simulations/experiments and explore the underlying mechanics of a polymer network in both the linear and non-linear regime just before network failure.
9:36AM R30.00007: Direct force measurement of microscopic droplets pulled along soft surfaces*  HAMZA KHATTAK (Presenter), KARI DALNOKI-VERESS, McMaster Univ — Recently, there has been growing interest in understanding the interactions of liquid droplets with soft materials. In these systems, forces exerted by a droplet can deform the material it contacts. This property leads to a plethora of unique physical phenomena with applications in fields ranging from water collection to surface sensing. We explore droplet dynamics on soft materials using a micropipette-based technique to simultaneously image, and measure the forces on, a microscopic droplet dragged along a soft interface. By changing the thickness of the soft material, we can control the compliance independent of surface chemistry. We show that material stiffness is a key parameter in droplet dynamics.

*Financial support was provided by the National Sciences and Engineering Research Council of Canada (NSERC).

9:48AM R30.00008: Experimental Studies on Slow Impacts and Interaction with Regolith Covered Surfaces in Low Gravity* [Invited]  JONATHAN KOLLMER (Presenter), Experimental Astrophysics, Universität Duisburg-Essen — Splashes from slow impacts into granular materials play an important role in the sculpting of asteroid surfaces and for the structures formed in wind blown sands. This talk I will give an overview of some recent experiments that explore ejecta generation and material redistribution from slow impacts into a granular bed under realistic space conditions. Most prominently an experiment which shows that ejecta created by slow impacts will stay close to the impact site under conditions realistic for a small asteroid, which has implications for observed size sorting effects. However this experiment also found that ejecta will not always be created directly at the impact site. By using photoelastic materials it was possible to identify that subsurface buckling introduced by the impact is responsible for this effect. Also, using similar techniques, it is possible investiage the ejecta creation process when mechanically interacting with planetary surfaces, e.g. landing or sampling, with the goal to identify an interaction design that will minimize ejecta creation.

*The author is supported by the DLR Space Administration with funds provided by the Federal Ministry for Economic Affairs and Energy (BMWi) under grant number 50WM1943.
10:24AM R30.00009: Optical spatio-temporal control of active matter systems in 2-D.*
NESRIN SENBIL (Presenter), Brandeis Univ, LINNEA LEMMA, ZVONIMIR DOGIC, University of California Santa Barbara, SETH FRADEN, Brandeis Univ — Active matter systems consist of self-driven units which convert chemical energy into mechanical energy and organize themselves into various patterns. Their pattern and flow properties exhibit non-equilibrium properties. In our experiments, we investigate the pattern formation of microtubule, kinesin motor kinesin motor proteins in 2-D fluid/fluid interfaces. The kinesin motor proteins are engineered in a way that light induces reversible linkage between them. Thus, under the exposure to the light (blue light centered at wavelength 460nm) the end groups of kinesin motor proteins bind and create the sliding motion between the microtubule bundles. Due to topological constraints, bundles create + ½ (motile) and - ½ (non-motile) defects. Using various light patterns, we confine the sample both in space and time. Illuminated regions exhibit strong bundling where the flow patterns and speed of the + ½ defects depend on the power and the design of the light pattern. Our goal is to control the defect velocity and their direction to guide them towards a certain destination.

*We acknowledge support from the NSF MRSEC DMR-1420382.

10:36AM R30.00010: Dynamical Inference of Forces Using Three-dimensional Tomographic Imaging of Dusty Plasmas* WENTAO YU (Presenter), GUGA GOGIA, JOSHUA MENDEZ, BRADY WU, JUSTIN BURTON, Physics, Emory University — Charged, micron-sized particles can be suspended in a in a low-pressure plasma through a balance of gravitational and electrostatic forces. Known as a dusty plasma, the particles are also subject to a screened, Coulomb repulsion, in addition to a number of kinetic and hydrodynamic drag forces from the ambient environment, leading to a rich array of nonequilibrium collective behavior. Using a new, high-speed, three-dimensional imaging technique based on laser-sheet tomography, we are able to track the dynamics of up to 50 individual particles over tens of seconds. In small systems with 2-3 particles, normal-mode decomposition provides a quantitative estimate of the equilibrium charge of the particles, the Debye length in the plasma, and the local electric field. For larger systems with many particles, the data also allows us compute the average pairwise forces between particles as a function of separation. The method is robust to noise in the data, and can be applied to other many-body systems with complex interactions.

*This work was supported by the National Science Foundation DMR Grant No. 1455086.

Thursday, March 5, 2020 8:00 AM - 10:36 AM

Session R31 DSOFT: Membranes, Micelles, and Vesicles 503 - Joseph Zasadzinski, University of Minnesota
8:00AM R31.00001: A super-swelled lamellar lipid system*  JACOB RUEBEN (Presenter), DYLAN STEER, CECILIA LEAL, University of Illinois at Urbana-Champaign — Lipid bilayers are an integral structure found in myriad biological systems. Sometimes lipid bilayers stack to make a lamellar phase, in which bilayers are separated by water layers with thicknesses determined by intermolecular interactions such as undulation repulsion, attractive van der Waals forces, and in the case of charged lipids, double layer forces. Water layers in charged lipid systems have demonstrated swelling abilities up to 30 nm, but soft (low bending rigidity) bilayers usually lose periodicity approaching these values due to higher undulation force effects [1]. Here we report a simple lipid system of low-bending-rigidity lipid doped with small amounts of charged lipid that forms a previously undocumented super-swelled lamellar phase with layer spacings upwards of 80 nm at low dilution. These results differ from previous studies into similar systems, and defy currently held theories of maximum lamellar spacings for soft membranes. The formulated lipid systems were characterized with confocal fluorescence microscopy, cryogenic TEM, and ultra-small angle X-ray scattering.


*Funded by the NIH under grant no. 1DP2EB024377-01

8:12AM R31.00002: Characterization of phospholipid monolayer viscoelasticity using microbubble acoustic radiation force*  AWANEESH UPADHYAY (Presenter), University of Colorado, Boulder, OUTI SUPPONEN, Mechanical Engineering, McGill University, FRANCESCO GUIDI, Information Engineering, University of Florence, HENDRIK VOS, Biomedical Engineering Thorax Center, Erasmus MC Rotterdam, PERO TORTOLI, Information Engineering, University of Florence, MARK BORDEN, University of Colorado, Boulder — Lipid monolayers (LM) stabilize the gas/water interface of the lung, ear and eye, and serve as model membrane for understanding the properties of bilayer leaflets. However, the nature of viscoelasticity of gel-phase LM for dilatational deformations remains poorly characterized. Microbubbles offer a novel experimental platform to study LM viscoelasticity, and their behavior is directly relevant to medical ultrasonics applications. The acoustic radiation force acting on a microbubble (MB) is maximal at the resonance frequency, which depends on its size and the LM shell viscoelastic properties. Here, we demonstrate a method using multi-gate spectral Doppler with an open source ultrasound scanner to measure the acoustic radiation force displacements of individual resonant MBs as we scan a frequency range between 3 and 7 MHz. The LM shell viscoelastic properties are determined by fitting the measured displacements to a modified Rayleigh-Plesset equation with Sarkar shell terms. Our results show the effects of lipid composition and temperature. These results provide mechanistic insights into LM dilatational viscoelasticity and illustrate rational design principles to engineer MBs for ultrasound imaging and therapy.

*M.B. acknowledges the funding provided by NIH grant R01CA195051.
8:24AM R31.00003: Tuning the microstructure of phospholipid monolayers using substrate curvature*  JOSEPH BARAKAT (Presenter), TODD M SQUIRES, University of California, Santa Barbara — Two-dimensional monolayers and bilayers of phospholipids exhibit a heterogeneous microstructure, which is essential for fluidity, mechanical stability, and spatial localization of proteins, cholesterol, and signaling molecules. There is a growing body of evidence that lipid morphology is influenced by the curvature of the underlying template. Although this geometric dependence remains poorly understood, it becomes extremely relevant to the study of monolayers (e.g., in lung alveoli and microemulsions) and bilayers (in cells, organelles, and vesicles) with radii of curvature on the order of 10-100 microns. In this work, I will discuss how continuum-level theory can predict the effect of curvature on the phase behavior of lipid monolayers, using planar and spherical geometries as model templates. First, I will demonstrate that curvature decreases the expected radius of condensed domains due to the attenuation of dipolar repulsions. Second, I will show that curvature stabilizes circular domains (“droplets”) from elliptic distortions into elongated structures (“stripes”). The transition between these states is determined by the substrate curvature and condensed-phase area fraction, which parametrize the phase space of lipid morphologies on curved templates.

*NIH NHLBI R01-HL135065

8:36AM R31.00004: Molecular dynamics study on encapsulation of ibuprofen and indomethacin in Triton X-100 micelles  HRACHYA ISHKHANYAN (Presenter), Department of Physics, King's College London, DAVE BARLOW, Institute of Pharmaceutical Science, King's College London, CHRISTIAN D. LORENZ, Department of Physics, King's College London — Surfactants are widely used in biological applications including the extraction of proteins from cell membranes, the enhancement of the permeability of cell membranes\(^1\) and the encapsulation of poorly soluble drug molecules\(^2\). In this study, drug encapsulation capabilities of a non-ionic surfactant Triton X-100 were studied using molecular dynamics (MD) simulations. An all-atomic simulation has been performed in an aqueous solution of pre-assembled surfactants and drug molecules using the CHARMM force-field. The micelle becomes saturated with ibuprofen molecules after approximately around 50% of them are encapsulated within 50ns. Whereas the micelle does not get saturated with indomethacin until approximately 70% of the available molecules are encapsulated. Furthermore, the simulation shows that in the presence of drug molecules the semi-spherical micelle becomes increasingly rod-like in shape. More analysis shows that the volume as well as the surface area of the micelle expand significantly in the presence of indomethacin, and are fairly the same in the presence of ibuprofen.

8:48AM R31.00005: Faceted Shapes of Cooled Emulsion Droplets of CTAB and Hexadecane*
ABDULLAH HASHIM (Presenter), SUBAS DHAKAL, Department of Physics, Le Moyne College — Recent experiments [Denkov et al., Nature 528 (2015) 392] have shown that the emulsion droplets resulting from the spontaneous self-assembly of cetyltrimethylammonium bromide (CTAB) surfactants with alkanes of similar carbon chain length such as Hexadecane in water “self-shape” into regular polyhedral, platelets, and rods on cooling. To understand the mechanism of the faceting of those emulsion droplets, we performed the coarse-grained (CG) molecular dynamics simulation of aqueous solutions of CTAB and Hexadecane using the Martini force field in GROMACS. In 1 (CTAB): 1(Hexadecane) solutions, we find that the average droplet size scales as $c^{0.4}$ with the concentration of Hexadecane (C). A variety of polyhedral shapes of the emulsion droplets observed at low temperatures in simulations will be compared with those of the experiments. The mechanism for faceting of the droplets will be discussed.

*This work used the computational resources provided by Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation Grant Number OCI-1053575.

9:00AM R31.00006: Pore Formation: How Cubic Lipid-siRNA Constructs Escape the Endosome*
LINING ZHENG (Presenter), CECILIA LEAL, University of Illinois at Urbana-Champaign — Small interfering RNA (siRNA) silences gene expression and has shown great potential in medical applications. However, intracellular delivery of siRNA remains a great challenge. Lipid nanoparticles have been one of the most successful siRNA carriers to date, but their delivery efficiency is limited due to low endosomal release. We have shown that cubic structured lipid nanoparticles (cubosomes) loaded with siRNA - cuboplexes, show greater siRNA knockdown compared to traditional lamellar structured liposomes. In this work, we aim to elucidate the reason behind this difference in delivery efficiency. We will show confocal microscopy (CF), flow cytometry and live cell imaging data demonstrating higher cellular uptake of cubosomes compared to liposomes. CF, fluorescent based fusion assays, cryogenic transmission electron microscopy and dynamic light scattering measurements indicate that compared to liposomes, cubosomes are more prone to fuse and form aggregates with endosomes, which implies a stronger pore forming capability that leads to siRNA escape. These results support our suggestion that cubosomes can lower the free energy required to promote endosome pore formation and establish a topologically active delivery mechanism.

*This work is supported by the NIH (1DP2EB024377-01).
Osmotic Shrinking of Vesicles Embedded in Hydrogels  NATASHA RIGBY (Presenter), MARGARITA STAYKOVA, Durham University — Lipid vesicles can be dispersed in various gel matrices as an encapsulation technology and as a model system for cells supported by an extracellular matrix.

By using confocal fluorescence microscopy on Giant Unilamellar Vesicles (GUVs) embedded in an agarose hydrogel matrix, we can observe changes in the liposome shape under hyperosmotic shocks.

Compared to free floating vesicles, gel-supported vesicles show irregular shapes during shrinkage. The results from our simple model system are reminiscent of plant cell plasmolysis.

We propose that the observed membrane shapes are caused by a non-specific adhesion between the membrane lipids and the agarose gel matrix. By varying the membrane-gel contact (chemical or physical), the strength of the gel and the osmotic shock, we want to explore the analogy between our system and biological systems, and use the effects to create functional hydrogels.

Mechanically mediated interactions between solid domains in composite vesicles*  HAO WU (Presenter), MARIA SANTORE, GREGORY GRASON, Univ of Mass - Amherst — We explore the structure and interactions of fluid/solid composite vesicles using continuum models compared with experimental studies of phase-separated two-component vesicles. In contrast to well-known fluid-fluid phase-separated domain structure, we show that shear rigidity of solid phospholipid domains coexisting with a fluid phase produces qualitatively new collective behaviors in composite vesicles. Beyond simply an enhanced bending stiffness, shear rigidity of the solid domains tends to expel Gaussian curvature into the fluid membrane phase, an effect which generically competes with the global spherical topology of the vesicle. We show that fluid membrane elasticity leads to bending-mediated interactions between solid domains, controlled by their size and the vesicle area-to-volume ratio. For sufficiently tensed vesicles we find that fluid phase bending induces a depletion-like attraction between solid domains of sufficiently large size, driven by tendency to consolidate elastic high-bending “hinges” that flank the solid domains at high pressure. This result suggests a qualitatively new picture of large solid domains as “2D colloids” dispersed in a fluid background, whose effective interactions are tunable through global vesicle properties.

*DOE BES, Award No. DE-SC0017870
Biomimetic Lung Surfactant Nanodrops for Acoustic Droplet Vaporization

ACLE N THOMAS, MARK BORDEN (Presenter), University of Colorado, Boulder — Acoustic droplet vaporization (ADV) involves the liquid-to-gas phase conversion of a superheated emulsion droplet by ultrasound to form an echogenic bubble. This technology may be useful for medical ultrasound, as nanodroplets small enough to leak through endothelial fenestrations may be converted to echogenic microbubbles for extravascular ultrasound imaging of inflamed and angiogenic vasculature. Additionally, droplets may be transformed to acoustically pulsating microbubbles to enhance ultrasound-guided drug delivery. However, surfactant coverage on the droplet often fails to stabilize the expanding interface during ADV, resulting in transitory microbubbles with limited utility. Here we show that interfacial melting and spreading by lung surfactant during surface dilation can be harnessed to increase the echogenicity and stability of post-ADV microbubbles. Lung surfactant, whose composition in the mammalian lung has been honed over millions of years of evolution, has thus proven to be a superior coating material for ADV droplets, and its biomimicry will be an important step toward clinical translation of ADV in ultrasound imaging and therapy.

Microsecond Coarse-Grained MD Simulations of Beta-Amyloid Fibrils Binding to Phase Separated Lipid Raft Domains Reveal Diverse Membrane-bounded Conformations and Binding Kinetics of Protein Depending on the Fibril size and Lipid Domain Structure

KWAN CHENG (Presenter), Physics, Trinity University, SARA CHENG, Physics, UT Austin, YIYI CAO, Physics, Trinity University, M ROUZBEHANI, Neuroscience, Trinity University, RONALD J DAVENPORT-DENDY, A URBY, S SPURLOCK, Physics, Trinity University — An early event associated with several protein aggregation diseases is the binding of amyloidogenic fibrils to cell membranes. At present, the binding conformation and kinetics of these fibrils on structurally heterogeneous and dynamic cholesterol-enriched raft domains remain elusive. We have constructed 4 coarse-grained (CG) beta-amyloid fibrils, ranging from dimer to pentamer, and 5 phase-separated CG lipid rafts, containing phospholipid and cholesterol or tail- or headgroup modified cholesterol. Using CG-MD simulations, the binding conformation, kinetics and interaction energetics of each fibril from solution to the rafts were studied. Within 20 μs, all fibrils bound to the raft surface and formed stable fibril/raft complexes at the liquid-ordered and -disordered phase boundary. The dimer fibrils bound to the raft exclusively via its hydrophobic C-terminal (C-state). Other than the C-state, the larger fibrils bound to the rafts via the hydrophilic N-terminal (N-state) and termini (T-state) with weaker binding energies. Interestingly, a transmembrane inserted state (I-state) of a trimer fibril was found for the raft containing tailgroup modified cholesterol. Our study indicates diverse conformations, kinetics and energetics of fibril/raft interactions in cells.

*NSF OAC-153159
An implicit lipid model to simulate reaction-diffusion of proteins binding to membrane surface  

YIBEN FU (Presenter), Johns Hopkins University — Localization of proteins to a membrane surface is an essential step in a broad range of biological processes such as signaling, virion formation, and clathrin-mediated endocytosis. The strength and specificity of proteins binding to a membrane depend on the lipid composition. Single-particle reaction-diffusion method is a powerful tool for capturing lipid-specific binding to membrane by treating lipids explicitly as individual diffusable binding sites. However, modeling lipid particles is computationally expensive. Here we present an algorithm for reversible binding of proteins to continuum surfaces with implicit lipids, providing dramatic speed-ups to many body simulations. The kinetics show excellent agreement between our method and the full explicit lipid model. Crucially, we demonstrate our method’s application to membranes of arbitrary curvature and topology, modeled via a subdivision limit surface. We also utilize this method to describe experimental data of membrane binding and the feedback from the curvature generation. Our method will enable efficient cell-scale simulations involving proteins localizing to realistic membrane models, which is a critical step for predictive modeling and quantification of \textit{in vitro} and \textit{in vivo} dynamics.

Relationship among Phase Behavior, Micellar Structure and Thin Film Drainage in Aqueous Surfactant Solutions  

SHANG GAO (Presenter), Chemical and Biomolecular Engineering, University of California, Los Angeles, CHRSTIAN OCHOA, VIVEK SHARMA, Chemical Engineering, University of Illinois at Chicago, SAMANVAYA SRIVASTAVA, Chemical and Biomolecular Engineering, University of California, Los Angeles — Sodium naphthenates (NaNs) are petrochemical anionic surfactants that stabilize petroleum emulsions and foams and pose significant environmental challenges when released into water bodies. Relatively little is known about the phase behavior and self-assembly (including micelle formation) as well as thin film drainage kinetics of aqueous NaN self-assemblies, impeding the development of strategies for NaN sequestration and petroleum foams and emulsions destabilization.

In this presentation, we will discuss experimental methodologies to elucidate surfactant phase behavior and self-assembly microstructure through a combination of small-angle X-ray scattering and cryoelectron microscopy. First, we will explicate the influence of surfactant and salt concentrations on micellar micromorphology of aqueous solutions of sodium dodecyl sulfate (SDS), a model, well-researched system. These trends will be compared with nanoscopic topography of draining SDS foam films, highlighting the striking similarity between intermicellar separations in bulk solutions and stratification step sizes in thin films. Next, phase behavior and microstructure of aqueous NaN self assemblies will be discussed, again highlighting the role of intermicellar correlations in dictating drainage of thin liquid films.
Alkylbenzene sulfonates are one of the most important synthetic surfactant families, considering their wide applicability, cost-effectiveness, and overall consumption levels. Nevertheless, their low salt tolerance (especially divalent ion contents) prevented wider applications such as enhanced oil recovery in high salinity reservoirs. Here, using experiments and atomistic molecular dynamics simulations, we demonstrated that the high salinity colloidal stability of alkylbenzene sulfonates can be dramatically increased by mixing with zwitterionic co-surfactants in oil-swollen micelles. By mixing with co-surfactants we had two important observations: (1) The polydispersity of surfactant mixture oil-swollen micelles were largely decreased due to the less rigid oil/water interfaces with mixed surfactants, which formed fewer but larger uniform micelles. (2) Strong dehydration of sulfonates due to the shielding from protruding more extended zwitterionic co-surfactants at the oil/water interfaces. Both observed molecular assembly characteristics triggered by the co-surfactants effectively reduced the total exposure of sulfonates to the water phase which may form divalent ion bridging and large aggregates, thus increasing the high salinity colloidal stability.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R32 DPOLY DSOFT DCP DMP: Molecular and Polymer Glass Structure

8:00AM R32.00001: On the Allowable or Forbidden Nature of Vapor-Deposited Glasses*
MATHIEU BAUCHY (Presenter), University of California, Los Angeles — Vapor deposition can yield glasses that are more stable than those obtained by the traditional melt-quenching route. However, it remains unclear whether vapor-deposited glasses are "allowable" or "forbidden," that is, if they are equivalent to glasses formed by cooling extremely slowly a liquid or if they differ in nature from melt-quenched glasses. Here, based on reactive molecular dynamics simulation (MD) of silica glasses, we show that, under certain conditions, vapor-deposited glasses can indeed be more stable than melt-quenched glasses. Importantly, we demonstrate that the allowable or forbidden nature of vapor-deposited glasses depends on the temperature of the substrate and, in turn, is found to be encoded in their medium-range order structure.

*This work was supported by the National Science Foundation under Grant No. 1928538.
8:12AM R32.00002: Stable polystyrene glass films through PVD and UV radiation  JUNJIE YIN (Presenter), ADAM RAEGEN, JAMES A FORREST, University of Waterloo — Stable glasses have proved to be an extraordinary type of material with enhanced density and exceptional kinetic stability compared to normal glasses. So far stable glasses prepared through physical vapor deposition (PVD) have been generally limited to organic small molecules such as indomethacin. We have recently employed PVD to make stable oligomeric glasses. In this study, we extend our capacity to make high molecular weight polystyrene stable glass by using oligomeric stable glass as a starting point. We do this by crosslinking the stable oligomeric glasses by dehydrogenation reaction under ultraviolet (UV) radiation. Depending on the degree of crosslinking, the resulting stable glass can have significantly higher molecular weight and kinetic stability. The sample molecular weight distribution is characterized by MALDI (matrix-assisted laser desorption/ionization), and the stable glass properties are characterized by ellipsometry.

8:24AM R32.00003: Physical vapor deposition of a polyamorphic system  BENJAMIN KASTING (Presenter), MADELEINE BEASLEY, MEGAN TRACY, MARK EDIGER, University of Wisconsin - Madison — In a few recently investigated systems, physical vapor deposition (PVD) has been shown to produce glasses that transform into liquids with properties that differ from the liquid produced by melting the crystal. Here we use PVD to investigate triphenyl phosphite (TPP), a known polyamorphic system where the second amorphous state (glacial phase) can be obtained by annealing the ordinary liquid (liquid 1) for hours slightly above its glass transition temperature (205 K). The properties of PVD glasses of TPP and the liquids formed from these glasses are studied by alternating current nanocalorimetry and interdigitated electrode dielectric spectroscopy. Deposition between 0.75 and 0.95 T_g results in glasses with very high kinetic stability. Independent of substrate temperature, the liquid that results from transforming the deposited glasses displays the properties of liquid 1, the ordinary liquid. Interestingly, films deposited above T_g also grow as liquid 1 even at temperatures previously used to transform liquid 1 into the glacial phase. The PVD mechanism allows the bulk of the film to inherit the structure at the free surface. These results suggest the preferred surface structure of TPP is similar to the structure of liquid 1, irrespective of deposition temperature.

8:36AM R32.00004: Physical properties of ultrastable computer-generated glasses  [Invited] LUDOVIC BERTHIER (Presenter), University of Montpellier — Computer simulations give unique insights into the microscopic behavior of amorphous materials. It became recently possible to generate ultrastable glass configurations using a simple Monte Carlo algorithm for a broad variety of model glass-formers. In this talk, we show that this discovery has allowed a deeper understanding of the rheological, thermodynamic and thermal properties of amorphous solids. We discuss in particular recent work regarding the brittle yielding of glassy materials, the Kauzmann transition, and low-temperature excitations of amorphous solids.
9:12AM R32.00005: Effects of internal degrees of freedom on simulated vapor deposited glass films
ALEX MOORE (Presenter), PATRICK WALSH, ZAHRA FAKHRAAI, ROBERT RIGGLEMAN, University of Pennsylvania — Recently, amorphous films of small molecules formed via physical vapor deposition (PVD) have been shown to exhibit remarkable thermodynamic and kinetic properties, equivalent to those that have been aged on the order of hundreds of years. Previous results suggest that the stability differences observed in these PVD glasses are the result of enhanced mobility near the free surface, such that molecules are allowed to sample a greater number of configurations before being trapped by subsequent deposited layers. However, much remains to be learned about the effects of properties like molecular shape and rotational freedom on the stability and morphology of these PVD amorphous packings. By using molecular dynamics simulations to mimic the PVD process of coarse-grained small molecules, we can make fine-tuned changes to these properties and then closely observe changes in films, both during and after the deposition process. Notably, we can then potentially make a connection between changes in internal degrees of freedom and the corresponding molecular entropy and changes in PVD film properties. Thus far, we suggest that molecules exhibiting greater entropy in their supercooled liquid state create more stable PVD glass films.

*This project is supported by the NSF DMREF-1628407.

9:24AM R32.00006: Anisotropy of extremely monodisperse polymer stable glass thin films
ADAM RAEGEN (Presenter), JUNJIE YIN, QI ZHOU, JAMES A FORREST, Physics and Astronomy, University of Waterloo — In the twelve years since their introduction, ultrastable molecular glasses have become a topic of great interest. Thin films prepared by vapour deposition at substrate temperatures slightly below T_g can exhibit increased densities and stabilities similar to those expected for isotropic glassy films aged hundreds or thousands of years. However, these ultrastable glasses may not truly present the same state as aged glasses. In many ultrastable glasses, the samples display anisotropy, unless steps are taken to make films only in a narrow range of production parameters such as substrate temperature and deposition rate. Simulations have suggested (Lin et. al. J. Chem. Phys. 140, 204504 (2014)) that evaporated oligomeric samples may provide a way to avoid this anisotropy and produce truly isotropic stable glass. In this case, the length of oligomeric samples can greatly influence anisotropy. Using our recently demonstrated technique for making polymer stable glasses, we present an experimental study of extremely monodisperse, ultrastable polymeric/oligomeric thin films. We use spectroscopic ellipsometry to measure birefringence caused by anisotropy in such samples as a function of the stability (fictive temperature) and the oligomeric size.
9:36AM R32.00007: Stability dependence of local elastic inhomogeneities of amorphous solids*  ALIREZA SHAKERPOOR (Presenter), ELIJAH FLENNER, GRZEGORZ SZAMEL, Colorado State University — There is a rich history of studies that suggest the vibrational and thermal anomalies in amorphous solids are linked to the local fluctuations in the elastic matrix of the amorphous medium. More recently numerical and experimental studies have shown a correlation between the vibrational properties and the stability of the medium. In this work, we studied the interplay between the stability and the fluctuations in the local elastic constants for a wide range of stabilities. We found that the variance of the local elastic constants becomes smaller with increasing stability. We also investigated the spatial correlations of the local elastic constants and determined that these constants have only very short range correlations.

*NSF DMR-1608086
NSF CHE-1800282

9:48AM R32.00008: Strong elasticity anisotropy in molecular glasses*  ZUYUAN WANG (Presenter), YU CANG, GEORGE FYTAS, Max Planck Institute for Polymer Research, CAMILLE BISHOP, MARK EDIGER, Department of Chemistry, University of Wisconsin-Madison — Although glass is often considered isotropic, anisotropic glasses can be prepared by physical vapor deposition of rod-shaped organic molecules. Those glasses feature tunable molecular orientations and anisotropic properties that are beneficial for applications such as organic semiconductors. While the deposition-condition-dependent molecular orientation and the associated optical birefringence of molecular glasses have been investigated, little is known about their mechanical anisotropy, which, however, is needed for understanding their strength upon mechanical loading in packaging and application. In this work, we use micro-Brillouin light spectroscopy to determine the elastic stiffness tensors of three glass films of itraconazole vapor-deposited at substrate temperatures \((T_{\text{sub}})\) of 330, 315, and 290 K, respectively. The five independent elastic constants in each tensor demonstrate the strong influence of the molecular orientation on the elastic anisotropy. The in- and out-of-plane Young’s moduli of the high \(T_{\text{sub}}\) sample, which features a vertical molecular orientation, exhibit a record high anisotropy ratio of 2.1 among molecular systems.

*ERC AdG SmartPhon (#694977), University of Wisconsin MRSEC.
10:00AM R32.00009: High Stability of Ultrathin Vapor Deposited Molecular Glasses  *  YI JIN (Presenter), YUE ZHANG, SARAH WOLF, AIXI ZHANG, SHIVAJEE GOVIND, CONNOR N WOODS, SUBARNA SAMANTA, Department of Chemistry, University of Pennsylvania, MIKHAIL ZHERNENKOV, GUILLAUME FREYCHET, National Synchrotron Light Source II, Brookhaven National Laboratory, ZAHRA FAKHRAAI, Department of Chemistry, University of Pennsylvania — Previous studies demonstrate that a mobility gradient exists within organic glass films, where molecules at or close to the free surface are more mobile than those in the bulk. The stability of glasses formed via vapor deposition relies on the equilibration of as-deposited molecules at the surface. An ultrathin stable glass (SG) film (~50 nm) has a higher proportion of molecules affected by the free surface dynamics, therefore likely has enhanced stability compared to a bulk SG (>200 nm). Here, we show that ultrathin SG films of TPD (N,N'-diphenyl-N,N'-bis(3-methylphenyl)-1,1'-biphenyl-4,4'-diamine) have higher stability, indicated by a higher density increase and a lower fictive temperature than bulk SG films of TPD. Surprisingly, at optimal deposition conditions, density increases higher than the limiting super-cooled liquid states are achieved. Anisotropy indicated by synchrotron scattering measurements suggest a possibility that there exists an amorphous as-deposited state of the molecule, volumetrically denser than its supercooled liquid counterpart, that is more isotropic than bulk SG. The potential origins of this phenomenon will be discussed in this presentation.

*NSF-DMREF DMR-1628407
NSF-MRSEC DMR-1720530

10:12AM R32.00010: Over what length-scale can the substrate perturb the structure of a vapor-deposited organic glass?  *  KUSHAL BAGCHI (Presenter), University of Wisconsin - Madison, CHUTING DENG, University of Chicago, CAMILLE BISHOP, YUHUI LI, University of Wisconsin - Madison, NICHOLAS JACKSON, University of Chicago, MICHAEL TONEY, SLAC National Accelerator Laboratory, LIAN YU, University of Wisconsin - Madison, JUAN DE PABLO, University of Chicago, MARK EDIGER, University of Wisconsin - Madison — Ultrathin (<30 nm) vapor-deposited layers are often utilized in OLED (organic light emitting diodes) devices. However, the vast majority of structural studies of vapor-deposited glasses have focused on films that are 100 nm or thicker. As a result these studies have not been sensitive to glass structure at the buried interface, which is of significance for OLED performance. Here we study, with grazing incidence x-ray scattering, the structure of vapor-deposited glasses of molecular glass former DSA-Ph as a function of film thickness. We span a thickness range of 10-600 nm. For films deposited on a Si/SiO₂ substrate at ~ 0.8 Tg, we estimate that the region near the buried interface with qualitatively different packing is less than 4 nm. A coarse-grained Lennard-Jones model of DSA-Ph qualitatively reproduces the short interfacial length-scale observed experimentally, implying our results are broadly applicable to molecular glasses that form continuous films on deposition.

*This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, Award DE-SC000216.
Molecular Orientation Depth Profiles from Resonant Soft X-ray Reflectivity

JACOB THELEN (Presenter) National Institute of Standards and Technology, KUSHAL BAGCHI, CAMILLE BISHOP, Chemistry, University of Wisconsin - Madison, SUBHRANGSU MUKHERJEE, ELIOT H GANN, R. JOSEPH KLINE, National Institute of Standards and Technology, MARK EDIGER, Chemistry, University of Wisconsin - Madison, DEAN DELONGCHAMP, National Institute of Standards and Technology — Orientation within amorphous molecular glass films can impart unique optoelectronic properties that provide enhanced performance in devices such as organic light emitting diodes (OLEDs). Bulk molecular orientation in vapor-deposited glass films can be tuned through processing conditions; however, little is known about the molecular orientation at the film surface or at the buried interface(s), where anisotropic optoelectronic properties can have a large impact on device performance. We use vapor-deposited films of tris(4-carbazoyl-9-ylphenyl)amine (TCTA) as a model system to develop soft X-ray techniques to extract molecular orientation from organic thin films. Variable incident-angle near edge X-ray absorption fine structure (NEXAFS) spectroscopy is used to probe the average molecular orientation within the top few nanometers of the TCTA films, as well as to determine the energy-dependence of orientation sensitivity for TCTA. Informed by the NEXAFS spectra, polarized resonant soft X-ray reflectivity (pRSoXR) measurements are performed at selected X-ray energies to probe molecular orientation through the depth of the film. Using the combined NEXAFS and pRSoXR data, we demonstrate a methodology to extract molecular orientation depth profiles with (sub)nanometer-level resolution.

Molecular dynamics simulation for investigation of Boson peak in a polymer system

AKIRA KOYAMA (Presenter), Department of General Education, National Institute of Technology, Toyota College, KOJI FUKAO, Department of Physical Sciences, Ritsumeikan University, TAKASHI YAMAMOTO, Graduate School of Science and Engineering, Yamaguchi University — We performed a molecular dynamics simulation to investigate Boson peak (BP) in a united atom polyethylene system. We computed vibrational density of states (DOS), dynamic structure factor (DSF) and wave-vector-dependent dynamic susceptibility (WDS) in a wide range of the angular frequency $\omega$ and the wave vector $q$. The BP was successfully observed in the profiles of DOS and DSF at the temperatures near and below the glass transition point. We determined the peak position of the BP ($\omega_{BP}/2\pi=0.25$ THz) from the fitting results of DOS; the peak position does not change with changing temperature. The BP was also recognized as an isolated peak on the 3D graph of DSF; the peak position along the $q$ axis ($q_{BP}$) on the line of $\omega=\omega_{BP}$ shifts toward high $q$ with decreasing temperature $T$, where $q_{BP} \sim T^{-0.5}$.

Using a simple harmonic oscillation model, we estimated the number of monomers $n_{BP}$ giving rise to the BP; $n_{BP}=3.2$. In the 3D graph of the real part of WDS, 2 distinct steps intersect on the line of $\omega=\omega_{BP}$; and in that of the imaginary part, a ridge laying diagonally from high $q$ and $\omega$ region to low $q$ and $\omega$ region terminates on the same line. From these results, we conclude that the BP in this simulation originates from the localized oscillation of the monomer groups consisting of 3.2 monomers.
10:48AM R32.00013: The effect of molecular architecture on the physical properties of supercooled liquids studied by MD simulations. Density scaling and its relation to the equation of state

KAJETAN KOPERWAS (Presenter), GRZYBOWSKI ANDRZEJ, MARIAN PALUCH, Institute of Physics, University of Silesia in Katowice — Theoretical concepts in condensed matter physics are typically verified and also developed by exploiting computer simulations mostly in simple models. However, the simplicity of the simple-liquids makes that predictions based on the mentioned model systems are often at odds with measurement results obtained for real materials. One of the examples is an intriguing problem within the density scaling idea (which has attracted attention in recent decades due to its hallmarks of universality), i.e., the fact that difference between density scaling exponent and exponent of the equation of state is observed for real materials, whereas it has not been reported for the model system. Given this problem into account, we project new model systems, which in contrast to the simple-liquids exhibit structural anisotropy, and we examine the effect of molecular anisotropy on the dynamic and thermodynamic properties of the material. We identify the applicable range of intermolecular interactions for a given physical process, and then we explain the reason for observed differences between the behavior of the model and real systems [J.Chem.Phys.150,014501(2019)].

*We are grateful for the support by National Science Centre within the framework of the Maestro10 project (grant no UMO-2018/30/A/ST3/00323).

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R33 DPOLY DSOFT DBIO: Chirality in Polymers and Soft Matter: From Molecular to Hierarchical Scales

505 - Gerd Schroeder-Turk, Murdoch Univ - Tag(s): Focus
Spontaneous Appearance of Chiral Structures from Lyotropic Liquid Crystals in Confinement

MOHAN SRINIVASARAO (Presenter), Georgia Inst of Tech, KARTHIK NAYANI, Chemical and Biomolecular Engineering, Cornell University, RUI CHANG, Georgia Inst of Tech, JINXIN FU, Materials Science and Engineering, Georgia Institute of Technology, JUNG O PARK, Georgia Inst of Tech — Optical activity, a consequence of reflection-symmetry breaking, since the time of its discovery by Biot in the early 1800s, has captivated the imagination of scientists. Since Pasteur's time, the appearance of macroscopic chirality during crystallization from both chiral and achiral molecules has frequently been observed. Crystallization apart, optical activity resulting from achiral units has been observed in liquid crystals, and polymeric materials, without a molecular chiral center.

In this talk, I intend to discuss the appearance of chiral structures from a class of liquid crystals, the so-called lyotropic liquid crystals. In particular, in recent years there has been significant research conducted on a class materials known as Lyotropic Chromonic Liquid Crystals (LCLCs). LCLCs consist of many dyes, drugs, nucleic acids, antibiotics, carcinogens and anti-cancer agents. I will explore the spontaneous emergence of chiral structures from achiral lyotropic chromonic liquid crystals as well as polymeric lyotropic systems, when confined to cylindrical capillaries with various boundary conditions, as well as in capillaries with rectangular and square cross-sections.

Threading the Spindle: A Geometric Study of Chiral Liquid Crystal Polymer Microparticles

HELEN ANSELL (Presenter), DAE SEOK KIM, RANDALL D KAMIEN, ELENI KATIFORI, University of Pennsylvania, TERESA LOPEZ-LEON, ESPCI Paris — Polymeric particles are strong candidates for designing artificial materials capable of emulating the complex twisting-based functionality observed in biological systems. In this study we investigate the swelling behavior of chiral twisted spindle-shaped polymer microparticles, which are formed due to the anisotropic contraction of spherical bipolar polymer liquid crystalline microparticles during deswelling. We observe a relationship between the aspect ratio of the spindle shape and the corresponding twist angle of the polymer at the surface. We find that there are two regions in the deswelling process: shrinking without twisting followed by shrinking due to twisting. We propose a geometric model to interpret these two behaviors as well as describing the observed spiral patterns on the surface.

8:48AM R33.00003: Chiral nematic liquid crystals in cylinders: Layering transition and conservation of layer structure* JONGHEE EUN, SUNG-JO KIM, JOONWOO JEONG (Presenter), Physics, Ulsan Natl Inst of Sci & Tech — Chiral nematic lyotropic chromonic liquid crystals (LCLCs) confined in a cylindrical cavity exhibit layering transition and intriguing topological defects. With a planar degenerate anchoring at the cavity wall, the chiral LCLCs have the double-twist (DT) director configuration. To our interest, as we increase the chiral dopant concentration, the degree of twist in the DT configuration increases discontinuously. This "step-like" layering transition occurs because there exist local minima in the elastic free energy landscape; depending on the dopant concentration, one of the minima becomes the ground state. Consequently, meta-stable domains with different twist angles can coexist with dislocation-like defects between them. Lastly, we learn that the meta-stable domains are topologically protected because of the layer number conservation.

*The authors acknowledge the support from the Korean National Research Foundation through NRF-2018R1C1B6002811 and IBS-R020-D1.

9:00AM R33.00004: Truth about the origin of twist - a circular argument* ELISABETTA MATSUMOTO (Presenter), Georgia Inst of Tech, ALIREZA DASTAN, DOUG J CLEAVER, Materials and Engineering Research Institute, Sheffield Hallam University — We examine emergent twist by applying both simulation and molecular theory to chromonic amphiphiles. Specifically, we study intrinsically achiral particles: amphiphilic discotics in a solvent of spheres. While these systems exhibit a veritable zoo of hierarchical, chiral self-assembled structures, we restrict ourselves here to a set of parameterizations that lead to twisted bilayer structures. Here, we return to the elephant in the room – what causes and controls the supramolecular twist that develops in these systems? In considering this, we demonstrate that, while chirality is manifested at several levels in the twisted bilayers formed by amphiphilic chromonics, it originates from spontaneously-chiral preferred packing at a molecular level.

While this structural chirality sets the underlying template for the twist, stresses from the growth dynamics yield topological defects. There is surprisingly little sensitivity to molecular-level properties (unless they render the bilayer unstable with respect to an alternative aggregate). Thus, the emergence of a supramolecular pitch in these systems is demonstrated to be a many-body but molecular-scale process, founded on the stabilization of a packing-optimising chiral complex.

*EAM: DMR-1847172
AD and DJC: Unilever
9:12AM R33.00005: Thermoresponsive Colloidal Chains Collapse to Form Helices*  BIPUL BISWAS, KP FAYIS, SURESH BHAT, Polym Sci Engg, Natl Chem Lab, GURUSWAMY KUMARASWAMY (Presenter), Indian Inst of Tech-Bombay — Colloids linked to form linear chains represent model systems for polymers. Chains are prepared using fluorescent micron sized colloidal polystyrene beads that are coated with 100 nm thermoresponsive PNIPAM microgels. Microgel-coated PS beads are lined up in an AC electric field and are crosslinked through amine groups in the microgels, to form thermoresponsive colloidal chains. Here, we demonstrate that these chains exhibit thermally-induced reversible transitions. Interestingly, we show that chains characterized by intermediate flexibility spontaneously organize into helices on heating. In contrast, stiffer chains exhibit a modest decrease in size, without a qualitative change in shape. More flexible chains exhibit a dramatic decrease in size but do not form an ordered helical structure. Thus, in chains where there is no directional specificity to the interactions between monomeric beads, we obtain helical structures when chains with intermediate flexibility collapse. Our work suggests that a purely mechanical instability for semiflexible filaments can drive helix formation, without the need to invoke any directional interactions.

*DST (Chemical Engineering)

9:24AM R33.00006: Skyrmion formation and organization on a shell*  VIVIANA PALACIO-BETANCUR (Presenter), University of Chicago, GUILLAUME DUREY, Laboratoire Gulliver, ESPCI Paris, ALEXANDER COHEN, University of Chicago, MONIROSADAT SADATI, Chemical Engineering, University of South Carolina, TERESA LÓPEZ LEÓN, Laboratoire Gulliver, ESPCI Paris, JUAN P. HERNANDEZ-ORTIZ, Departamento de Materiales y Minerales, Universidad Nacional de Colombia, Sede Medellin, JUAN DE PABLO, University of Chicago — Blue phases (BPs) arise spontaneously in chiral liquid crystals (ChLCs) as the result of minimizing the global free energy, by forming networks of defects with specific cubic symmetry. Confining cuboidal phases to a channel smaller than the molecular pitch results in frustrating the full development of a BP cell, creating skyrmions that pack with hexagonal order. Beyond confinement in a channel, here, we consider the effect of curvature by confining a ChLC in spherical shells. The equilibrium configurations are obtained following a theoretically-informed Monte Carlo relaxation and a Ginzburg-Landau relaxation of the free energy functional, described within the Landau-de Gennes formalism, and solved numerically through finite element discretization. By considering homeotropic and planar anchoring, we stabilize half and full skyrmions. When stabilized in a shell, the hexagonal packing becomes imperfect, to accommodate for the closed surface, resulting in the creation of 5-7 pairs of skyrmions on the surface of the shell. The control over the formation and packing of the skyrmions offers opportunities for pattern design and engineering 2D ordered nanoparticle assemblies.

*Fulbright commision in Colombia and Colciencias - PhD Schollarship program.
9:36AM R33.00007: Peculiar Phase Morphologies from Twisting of Self-Assembled Ribbons in Chiral Block Copolymers KAI-CHIEH YANG (Presenter), RONG-MING HO, Natl Tsing Hua Univ — The chirality effects on BCP self-assembly gives rise to the formation of helical phase (H*) from the self-assembly of polylactide-based chiral block copolymers (BCPs*) with achiral segment-rich fraction. The formation of the helical cylinder is attributed to the packing of helical chains with which twisted cylinder microdomain can be formed from twisting and shifting. By contrast, twisted ribbon with a bilayer-like lamellar texture can be formed in self-assembled polylactide-based BCPs* with chiral segment-rich fraction from twisting and bending. Those twisted ribbons can be further developed to give peculiar phase morphologies in bulk through scrolling, giving a roll cake and concentric lamellar textures. We speculate that those helical and twisted textures are built from the chiral interface of chiral and achiral segments as proposed by the tilted chiral lipid bilayer (TCLB) theory and also the mesochiral assembly of the helical chains predicted by the orientational self-consistent field theory (oSCFT). With the homochiral evolution from helical conformation to hierarchical superstructure via inter-chain chiral interactions, it is appealing to control the handedness of the forming morphologies from BCPs*.

9:48AM R33.00008: Folding of chiral colloidal membranes* [Invited] PRERNA SHARMA (Presenter), LACHIT SAIKIA, AYANTIKA KHANRA, Indian Institute of Science - Dept of Physics, ZVONIMIR DOGIC, Physics, University of California Santa Barbara — Rod-like viruses self-assemble into one rod-length thick liquid-like monolayers in presence of depletion attraction induced by non-adsorbing polymers. The global constraint of 2-D geometry of these colloidal membranes is incompatible with local chiral interactions of the rods. Consequently, competition between these opposing tendencies leads to a variety of polymorphic transitions. We illustrate this through phenomena that cause flat colloidal membranes to transform into 3-D structures. Crystallization of colloidal membranes proceeds through the usual nucleation and growth pathway. However, the growing crystalline domains spontaneously wrinkle to satisfy local chiral interactions and on completion of the growth lead to macroscopic buckling of the membrane. In contrast, fluid colloidal membranes can be folded by simply doping them with shorter rods of same chirality. These uniformly mixed bi-disperse membranes become unstable and deform into saddle shapes. The origin of this instability lies in enhancement of Gaussian modulus of the monolayer membranes due to doping. At high doping ratio, membranes fold into higher order structures of increasing complexity. These include unduloids, tri-unduloids, unduloid-enneper surfaces as well as system spanning plumber's nightmare-like phases. Taken together, these results show how chirality may have similar implications for conventional lipid bilayers which are rich in chiral molecules like cholesterol.

*This work is supported by DST-SERB.
Self-assembly of chiral networks in achiral block copolymer systems using coarse-grained simulations*  

NATALIE BUCHANAN, KRYSLA BROWKA, LIANNA KETCHAM, HILLARY LE, POORNIMA PADMANABHAN (Presenter), Rochester Institute of Technology — Ordered network materials, such as the double gyroid, are comprised of two interwoven networks embedded in a matrix and can be formed via the self-assembly of block copolymers. By selecting the interaction parameters that promote elongated conformations, an alternating gyroid morphology can be formed, thereby breaking network symmetry and resulting in a structurally chiral morphology. In this talk, we investigate the self-assembly of model achiral block copolymers into alternating gyroid morphologies using coarse-grained molecular simulation. We show that effective chirality can further be tuned by co-assembling with a suitable species to grow one network and shrink the other. Insights into stability are obtained by measuring polymer end-to-end distances and network topology.

*Gleason Fund

Amino Acids as RNA-Folding Chaperones: Single Molecule Experiments Reveal Chiral Sensitivity  

DAVID NICHOLSON (Presenter), DAVID JOHN NESBITT, University of Colorado, Boulder — Early RNA-based life may have relied on amino acids to promote correct folding in RNA molecules, i.e. to act as RNA-folding chaperones. Chiral specificity in this interaction could have driven evolutionary mechanisms to favor a single chirality of amino acid, which may explain the origin of amino acid homochirality. To probe how chirality determines an amino acid’s influence on RNA folding dynamics, we have performed single molecule spectroscopy on a ubiquitous RNA tertiary motif, the tetraloop-tetraloop receptor (TL-TLR). Our kinetic measurements show that TL-TLR folding is sensitive to many amino acids, but only one amino acid, arginine, is observed to have a chirally-specific effect. The kinetic and thermodynamic features of this chiral interaction are presented, and with the help of all-atom molecular dynamics simulations, we propose a mechanistic interpretation of these results based on nonspecific arginine-RNA interactions.
The interplay between polymer–solvent interaction and interactions that impose secondary structures determines polymer chain conformation in dilute solution. Polypeptoids–poly(N-substituted glycines) can form helical secondary structures primarily driven by steric interactions from chiral, bulky side chains, while a racemic mixture of the same side chains results in unstructured coil chains. Small-angle neutron scattering (SANS) reveals that the helical polypeptoids are locally stiffer but overall flexible. However, the radii of gyration ($R_g$) of both helical and coil polypeptoids do not increase with improved solvent quality ($A_2$), and the chain expansion deviates from the universal swelling of polymer chains in dilute solution. Potential effects from solvents disrupting the steric interactions of chiral side chains are excluded by comparing to another chemically analogous coil polypeptoid devoid of side chain chirality. The results indicate that chain conformation change of these polypeptoids cannot be simply captured by excluded volume interactions, nor the steric interactions imposing the helical secondary structure. It is likely that the specific interactions between polypeptoid segments dominate the chain shape as opposed to polypeptoid–solvent interactions.

*NSF 1608297

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R34 DPOLY DSOFT: Processing-Dependent Nanoscale Structures in Polymers and Predictive Methods 506 - Michael Hore, Case Western Reserve University - Tag(s): Focus
8:00AM R34.00001: Solvent-Non-Solvent Rapid Injection for the Preparation of Hierarchically Ordered Hydrogels  ROBERT HICKEY (Presenter), Pennsylvania State University — Non-solvent-induced phase separation is a non-equilibrium method used heavily in industry for fabricating separation membranes. The resulting microstructure forms when a homopolymer initially in a good solvent is immersed into a poor solvent, inducing polymer phase separation and forming a microporous membrane consisting of polymer-rich and non-solvent-rich regions. We recently showed that non-solvent-induced phase separation methods will produce hierarchically ordered physically crosslinked hydrogels when amphiphilic triblock copolymers are used instead of homopolymers. In our system, when triblock copolymers comprising of a hydrophobic-hydrophilic-hydrophobic chain sequence initially in a common solvent will rapidly self-assemble at the nano and microscale when injected into water. We have developed a universal and quantitative method for producing physically crosslinked hydrogels exhibiting tunable mechanical properties superior to typical physically crosslinked triblock copolymer hydrogels, and interesting structural color properties. At a fundamental level, the rapid injection process described here encompasses two self-assembly processes (microphase and macrophase separation), further increasing the tunable parameters for controlling material structure and property.

8:12AM R34.00002: WITHDRAWN ABSTRACT  —

8:24AM R34.00003: Understanding and controlling metal oxide growth within block copolymers  NETA SHOMRAT, INBAL WEISBORD (Presenter), ROTEM AZOULAY, BARUN BARICK, ASSAF SIMON, TAMAR SEGAL-PERETZ, Technion - Israel Institute of Technology — In recent years, sequential infiltration synthesis (SIS) has emerged as a novel technique for growth of inorganic materials within block copolymers (BCP) and templating inorganic nanostructures from BCP due to SIS high growth rate and selectivity within polar BCP domains. However, to utilize SIS in a variety of BCP and in multiple length scales, there is high need for a full description of SIS mechanism.

Here we investigate the principles that govern SIS growth in homopolymers and block copolymers using cominnation of in situ growth characterization, 3D TEM tomography, and quantum mechanical calculations. We probe the diffusion and growth within the polymers and show its relationship to the polymer chemistry, precursor chemistry, and SIS process parameters. From this data, SIS model was constructed that enabled us to fabricate new BCP-templated nanostructures, including porous particles, heterostructure nanorod array and multi-layer membranes.
Process-directed self-assembly: Do we understand the collective short-time dynamics in multicomponent polymer melts?

MARCUS MUELLER (Presenter), University of Gottingen — Process-directed self-assembly refers to processes that reproducibly trap the kinetics of structure formation that ensues after a sudden change (“quench”) of the thermodynamic state into a desired, (meta)stable target state. This strategy benefits from specific advantages of copolymer systems, such as the rather comprehensive knowledge of equilibrium properties and the timescale separation between the quench of thermodynamic state variables, the spontaneous relaxation of the system towards the “nearest” metastable state, and the thermally activated escape from the metastable target state. Typically the relaxation from the unstable state occurs on a time scale that is comparable to the single-chain relaxation time. This short-time kinetics of structure evolution templates the morphology at later stages but poses challenges for a theoretical description. Examining simple, prototypical examples, we highlight the role of internal modes and indicate how dynamic SCFT can be generalized to include the consequences of the subdiffusive single-chain dynamics for the collective kinetics on times comparable to the Rouse-relaxation time.

Financial support has been provided by the Deutsche Forschungsgemeinschaft (DFG) und grant Mu1674/16.

Nonsolvent Induced Phase Separation in Polymer Droplets

DOUGLAS TREE (Presenter), RAMI ALHASAN, DAKOTA BANKS, TANNER WILCOXSON, Brigham Young Univ - Provo — Nonsolvent induced phase separation (NIPS) occurs when a polymer solution is brought into contact with a miscible nonsolvent, leading to the precipitation of a polymer-rich phase. Because of its simplicity, NIPS processes are widely used to generate a variety of microstructures in polymer materials such as membranes and micro/nanoparticles. Despite its prevalence, predicting and controlling the microstructure generated by NIPS remains a difficult challenge, owing to the complex interactions between the diffusive transport, hydrodynamics and phase-separation kinetics in the process. In our approach, we use simulations of a phase-field model of a polymer solution to examine the effect of mass transfer, hydrodynamics and geometry on the formation of microstructure. In particular, we study the NIPS process in polymer droplets, where we examine the effect of droplet size, shape, and composition on the resulting microstructure. We also examine the impact of finite solvent/nonsolvent miscibility on the kinetics and microstructure of the phase separation.

*We acknowledge funding from the Board of Trustees at Brigham Young University as well as computational resources from the Brigham Young University Office of Research Computing.
9:00AM R34.00006: Arrested mobility and thermal fluctuation effects on the mass transfer induced phase separation of ternary polymer solutions*  JAN ULRIC GARCIA (Presenter), University of California, Santa Barbara, DOUGLAS TREE, Brigham Young University, TATSUHIRO IWAMA, Asahi Kasei Corporation, KRIS T DELANEY, GLENN H FREDRICKSON, University of California, Santa Barbara — Many polymer membranes are made by immersion of a polymer solution film in a nonsolvent bath: the mass transfer exchange between the nonsolvent from the bath and the solvent in the film induces phase separation of the film into a polymer-rich phase that becomes the membrane matrix and a polymer-poor phase that becomes the membrane pores. Microstructure formation of these membranes is still not fully understood due to the nature of the physical processes involved: the mass transfer induced phase separation, the coarsening of domains, and the vitrification of the polymer-rich phase that arrests membrane microstructure. In this work, we use phase-field models of the ternary polymer-nonsolvent-solvent system to solve the coupled convection-diffusion and momentum equations that describe membrane formation. We model the glass transition using contrasts in the viscosity and mobility of the polymer-rich and polymer-poor phases. We report how glassy dynamics, and the inclusion of thermal fluctuations, contribute to microstructure formation.

*We acknowledge support from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-1720256) and NSF CNS-1725797. We also thank Asahi Kasei Corp for support.

9:12AM R34.00007: Precision polymer nanoparticles* [Invited]  RACHEL O’REILLY (Presenter), Chemistry, University of Birmingham — Polymerization-induced self-assembly (PISA) is a versatile method to prepare nanoparticles of various morphology. Traditionally, nanoparticles are prepared via self-assembly of pre-formed polymers in H2O. Rigorous optimization is often required in these systems, involving iterative cycles of polymer synthesis, self-assembly, and evaluation of the self-assembled morphologies. PISA offers an elegant solution to the tedious procedures of conventional self-assembly by forming the particles in situ as the polymerization progresses. PISA involves chain-extension of a hydrophilic macroinitiator (or macro-chain-transfer agent) with monomers that are miscible with water, but form a hydrophobic, immiscible polymer, driving self-assembly. PISA can be conducted at high solids contents under a wide variety of reaction conditions (i.e., low or high temperature, variable solvent mixtures, or in the presence of drugs or biomacromolecules). However, monomers which can be utilized in PISA are often difficult to identify from their chemical structures alone, and experiments are often necessary to determine their usefulness in PISA. We have been developing synthetic methods and developing predictive tools to expand the scope of PISA and also show its application in the design of functional materials.

*ERC (grant number 615142) is thanked for funding.
**9:48AM R34.00008: Molecular Modeling of Poly(methylmethacrylate-block-acrylonitrile) as Precursors of Porous Carbon Fibers**

XI RYAN HAO (Presenter), JOEL M. SERRANO, TIANYU LIU, ASSAD ULLAH KHAN, BRANDON BOTSET, BENJAMIN J. STOVALL, ZHEN XU, DONG GUO, KE CAO, GUOLIANG LIU, SHENGFENG CHENG, Virginia Tech — Porous carbon fibers (PCFs) based on block copolymers exhibit well-controlled hierarchical porous structures and high specific interfacial areas, which lead to excellent electrochemical properties. Understanding the conformation and morphology of polymer precursors before conversion is crucial for designing and optimizing PCFs. To expedite materials discovery, we perform molecular dynamic simulations for a series of poly(methylmethacrylate-block-acrylonitrile) (PMMA-b-PAN) with various block molecular weights and develop a model to characterize the morphology and compute the interfacial area of PMMA-b-PAN melts. We build both laminar and disordered phase of PMMA-b-PAN melts with an atomistic model of the polymer. For the disordered melts, our results show that the interfacial area is maximized when the volume fraction of either block is close to 50%, consistent with experimental results. The stability of the laminar phase is probed by performing thermal annealing on the systems and the conversion to a disordered phase is realized by introducing extra attractions between PAN blocks, which mimic the cross-linking reactions of PAN blocks in experiments. Our models pave the way of optimizing PCFs by designing PMMA-b-PAN precursors in silico.

*Supported by AFOSR (FA9550-17-1-0112).

**10:00AM R34.00009: Phase diagram for diblock copolymer melts from Langevin field-theoretic simulations**

TOM BEARDSLEY (Presenter), MARK W MATSEN, University of Waterloo — Field-theoretic simulations (FTS) provide fluctuation corrections to self-consistent field theory (SCFT) by simulating its field-theoretic Hamiltonian rather than applying the saddle-point approximation. Here, we apply Langevin FTS (L-FTS) to AB diblock copolymer melts, where the composition field fluctuates via Langevin dynamics but the saddle-point approximation is still applied to the pressure field that enforces incompressibility. The method is demonstrated to be one or two orders of magnitude faster than previous Monte Carlo simulations (MC-FTS), permitting the rapid formation of spontaneously ordered configurations and the accurate determination of their order-disorder transitions. The results are used to construct a phase diagram for diblock copolymer melts of high invariant polymerization index, N = 10^4.

*This work was supported by NSERC of Canada and computer resources were provided by Compute Canada.
Entanglements in block copolymers self-assembled into lamellae morphology

NICOLAS GARCIA (Presenter), Institut Laue-Langevin, 71 Avenue des Martyrs, 38042 Grenoble, France, JEAN-LOUIS BARRAT, Université Grenoble Alpes, Liphy, CNRS, France — Understand the viscoelastic behavior of polymers is of fundamental interest but also is relevant to consider their technological applications. It is well-known that the mechanical properties of polymers depend fundamentally on the molecular chain weight. The main effect of increasing weight is the arise of entanglements.

Entanglements in homopolymer systems have been studied through simulations and experiments and supported by theories. However, little is known about those topological constraints on multi-component systems, like the block copolymers (BCPs).

In this work, we investigate the viscoelastic properties of BCPs when segregating in a lamellar morphology. We found the entanglements are not distributed homogeneously in the space but instead follow the underlying pattern of the segregated domains. Moreover, the interface separating nearby domains induces a surface effect, decreasing the number of entanglement. On the other hand, in the center of the lamellae domain, the monomer density slightly increases due to the impact of the attractive potential, whose main consequence is an increment of the number of entanglements. Both results are locals, compete with each other, and depend on the segregation regime, being more extended in space in the regime of strong segregation.

Systematic construction of the dynamic density functional theory for inhomogeneous polymer systems

SRITEJA MANTHA (Presenter), FRIEDERIKE SCHMID, Johannes-Gutenberg Univ — Time scales predicted by the dynamic density functional theory (DDFT) for an inhomogeneous polymer system are far from accurate. One of the main reasons for this is, approximate local and non-local schemes employed to compute the mobility coefficient, $\Lambda_{\alpha\beta}(r,r')$. In the DDFT calculations, $\Lambda_{\alpha\beta}(r,r')$, relates the thermodynamic driving force due to the monomer $\beta$ at $r'$ to the current of the monomer $\alpha$ at $r$. In this talk, we will put forward a physically motivated approach to compute the $\Lambda_{\alpha\beta}(r,r')$ with the objective to improve the DDFT predictions. We compute the $\Lambda_{\alpha\beta}(r,r')$ from the relaxation time of the single chain dynamic structure factor. We find that the $\Lambda_{\alpha\beta}(r,r')$ obtained from such an approach captures both the global dynamics and the effective local rearrangements of the chain at relevant length scales. Using this scheme, we conduct DDFT calculations to study two related problems. One is the formation of the lamellar morphology in a symmetric diblock copolymer system starting from a homogeneously dispersed state, and the other is the relaxation of the lamellar morphology into a homogeneously dispersed state. We show that the DDFT predictions for the above problems are in reasonably good agreement with the corresponding fine-grained simulations.

*SFB TRR 146 (Grant No. 233630050)
10:36AM R34.00012: Spectrally-Accurate Linear-Scaling Self Consistent Field Theory and Applications*  DANIEL VIGIL (Presenter), CARLOS J GARCIA-CERVERA, KRIS T DELANEY, GLENN H FREDICKSON, University of California, Santa Barbara — We present a new algorithm for numerical polymer self-consistent field theory (SCFT) that has spectral accuracy in the contour dimension while maintaining near-linear computational cost scaling with number of contour sample points, which no other reported algorithm achieves. The new algorithm is enabled by using a coherent states (CS) model of the polymer field theory, which replaces the chain propagator objects from auxiliary field (AF) models with fields that generate chain statistics. We also show that the newly reported algorithm is compatible with a variety of AF algorithms, but can replace their propagator algorithms with our linear-scaling spectrally accurate algorithm. Applications enabled by this new algorithm are presented.

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10:48AM R34.00013: Open-source SCFT on graphics processing units  GUO KANG CHEONG (Presenter), ANSHUL CHAWLA, DAVID CLARK MORSE, KEVIN D DORFMAN, University of Minnesota — Self-consistent field theory provides an effective framework for materials discovery, allowing one to target particular morphologies by rapid examination of their phase space. We present a GPU-accelerated self-consistent field solver parallel to the open-source Polymer Self-Consistent Field (PSCF) codebase. The codebase is built from the ground up to utilize highly efficient GPU-acceleration yet remains backwards-compatible with PSCF. Our testing shows up to 60x acceleration in computing time for the largest problems. Improvement in open-source tools enables new opportunities by the community to pursue various problems of interest such as the inverse design of the bulk phases. Increasingly, speed becomes vital in such problems especially in an era of data and machine learning where the manipulation of large data sets is key to the understanding of fundamental polymer physics.
**8:00AM R35.00001: How to Define Electric Potential in a Polarized Polymer Electrolyte Why is it Important?** [Invited] NITASH BALSARA (Presenter), University of California, Berkeley — Polymer electrolytes comprise mobile ionic species, usually both cations and anions, but are electronic insulators. The definition of electric potential is not trivial as the case of the metallic current collectors wherein the presence of excess electronic charge can readily be sensed by a voltmeter. Newman's concentrated theory is built on potential measured using an electrode that undergoes a reversible electrochemical reaction. We apply this theory to polymer electrolytes that are examined under a constant direct current (dc). The concentration gradients in the electrolyte can be calculated without invoking the potential. For practical applications, however, it is important to know if the potential drop necessary to drive the current is within the range afforded by the chosen electrodes. We have worked through these relationship for homopolymer electrolytes. We are currently working on establishing these relationships in block copolymer electrolytes. We hope to present these results at the meeting.

*BMR Program of DOE*

**8:36AM R35.00002: The impact of chemical modification on charge injection at metal/polyolefin interfaces** YIYUAN WANG (Presenter), Departments of Materials and Physics, and the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, UK, MIKAEL UNGE, ABB Corporate Research, 72178 Västerås, Sweden, SARI J. LAIHONEN, Power Grid Research, 72178 Västerås, Sweden, ARASH A MOSTOFI, Departments of Materials and Physics, and the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, UK — The process of charge injection at metal/polymer interfaces is crucial to many areas of research and technology, such as organic light emitting and harvesting devices, high-voltage capacitors and cables. In this work, we study charge injection at metal/polymer interfaces for two polymers commonly used in high-voltage applications, namely polyethylene (PE) and polypropylene (PP). Using first-principles electronic structure methods, we compute charge injection barriers at model aluminium/PE and aluminium/PP interfaces. We show that the introduction of polar chemical groups (e.g., -COOH, -CH2Cl, and -CHO) in the polymer chains at the interface can tune the intrinsic charge injection barrier significantly. We take into account of thermal disorder by averaging over a large ensemble of interface structures obtained from first-principles molecular dynamics trajectories. Our results suggest the possibility of rational design of metal/polymer interfaces via localised chemical modification.
Field-theoretic study of salt-induced order and disorder in a polarizable diblock copolymer

DOUGLAS GRZETIC (Presenter), KRIS T DELANEY, GLENN H FREDRICKSON, University of California, Santa Barbara — We study a salt-doped polarizable symmetric diblock copolymer using a recently-developed field theory that self-consistently embeds dielectric response, ion solvation and van der Waals (vdW) attractions via the attachment of classical Drude oscillators and/or fixed dipoles to the constituent fluid elements. This field theory can be directly simulated via the complex Langevin sampling technique, requiring no approximations beyond the phenomenology of the underlying coarse-grained model. We measure the shift in the order-disorder transition with salt-loading in our simulations and observe rich non-monotonic behavior in which ion solvation competes with dilution and charge screening effects to determine whether the ordered or disordered phase is stabilized. At low salt concentrations, the salt behaves as a selective solvent, localizing into the high-dielectric domains and stabilizing the ordered phase. At high salt concentrations, however, the salt localization vanishes due to charge screening effects, and the salt behaves as a nonselective solvent that screens vdW attractions and stabilizes the disordered phase. Our results raise questions regarding the conditions under which it is appropriate to ignore the screening effect of the ion cloud in theories of salt-doped polymers.

Nanostructure and Local Dynamic Effects on Ionic Conductivity of Polymer-Grafted Nanoparticles in Ionic Liquids*

SIQI LIU (Presenter), Stevens Inst of Tech, MADHUSUDAN TYAGI, Neutron-Condensed Matter Science Group, National Institute of Standards and Technology, PINAR AKCORA, Stevens Inst of Tech — In this talk, I will present our recent results about structures and dynamics of poly(methyl methacrylate) (PMMA)-grafted iron oxide nanoparticles in (1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide) (HMIM-TFSI) / solvent mixtures. The dynamics of HMIM$^+$ cation is measured with QENS experiments and conductivity of grafted particles in HMIM-TFSI is obtained from impedance spectroscopy. Higher diffusivity and conductivity were achieved when grafted particles are dispersed in HMIM-TFSI/acetonitrile mixture than in methanol. These results reveal that acetonitrile solvates HMIM-TFSI and better dispersion of grafted particles leads to better mixing between PMMA and TFSI$^-$ anions. The ion-dipole interactions between TFSI$^-$ and PMMA self-dissociate HMIM-TFSI, thereby increase the number of free cation carriers. The dynamic measurements combined with conductivity results suggest that grafted particles dispersion and conductivity increases with the solvation and with the interactions between high graft density PMMA and TFSI$^-$. Particles form strings in methanol and yield lower conductivity. In conclusion, both solvation and solubility of grafted particles in ionic liquid/solvent mixtures determine the mobility of ions in well-defined particle dispersions.

*NSF DMR grand # 1807802
9:12AM R35.00005: Capacitance of films containing polymerized ionic liquids

RAJEEV KUMAR (Presenter), VERA BOCHAROVA, JYOTI P MAHALIK, Oak Ridge National Laboratory, Oak Ridge, TN 37831, KEVIN SILMORE, Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 — Electrode-polymer interfaces, which encompass adsorbed layers of polymers, dictate many of the properties of thin films such as capacitance, electric field experienced by polymers and charge transport. To develop an understanding of electric field-induced transformations of electrode-polymer interfaces, we have studied electrified interfaces of an imidazolium based polymerized ionic liquid (PolyIL) using combinations of broadband dielectric spectroscopy (BDS), specular neutron reflectivity and simulations based on the Rayleigh dissipation function formalism. We demonstrated that the Rayleigh dissipation function formalism provides key insights into charge storage, which include information about capacitance of interface, thicknesses of absorbed and diffuse layers. Overall, the camel-shaped dependence of the capacitance on applied voltage was obtained which originated from responses of absorbed layer to applied voltages. Furthermore, the diffuse layer contribution to the capacitance should decrease with applied voltage \( V \) as \( V^{-1/2} \), which is a direct consequence of local incompressibility/crowded nature of the PolyIL melts.

9:24AM R35.00006: Comparing Stockmayer Fluid Simulation and Experiment: Ion Solvation with Permanent Dipoles

CAMERON SHOCK (Presenter), ISSEI NAKAMURA, Michigan Technological Univ, AMALIE FRISCHKNECHT, MARK STEVENS, Sandia National Laboratories — The solvation of ions in polymer membranes has been studied over many decades. Nevertheless, understanding of the solvation mechanism involves various computational challenges. This is primarily because molecular simulations for ion solvation that can simultaneously consider both atomic and molecular length scales are still significantly limited, even in cases of non-polymeric solvents. In this study, we developed a coarse-grained Stockmayer fluid simulation to address this issue, treating solvent molecules as soft-core spheres with permanent dipole moments. In this talk, we validate our model concept by considering monovalent and divalent ions dissolved in various non-polymeric solvents, such as water and methanol. Despite model simplicity, the results of our simulations show striking agreement when compared with experimental data for the free energy and enthalpy of ion solvation. We will also discuss that the primary contribution to the solvation energy arises mainly from the first and possibly second solvation shells near the ions.

*Research Excellence Fund of Michigan Technological University
Enhancing the Dielectric Breakdown Strength of Solid-State Polymer Capacitors by Chain End Manipulations

MANINDERJEET SINGH, WENJIE WU, Univ of Houston, MEI DONG, DAVID TRAN, KAREN L WOOLEY, Texas A&M University, NIHAR PRADHAN, Jackson State University, DHARMARAJ RAGHAVAN, Howard University, ALAMGIR KARIM (Presenter), Univ of Houston

— The need for high power density, flexible and light weight energy storage devices requires the use of polymer film-based dielectric capacitors. Theoretically, it has been shown that chain ends contribute adversely to electrical breakdown, resulting in low energy density in polymer capacitors. In this work, we enhanced the energy density of polymer capacitor by using well-ordered high molecular weight block copolymer (BCP), in which the chain ends are segregated to narrow zones. Cyclic homopolymers (no chain ends) and linear homopolymers having chemistry-controlled chain ends also show enhanced breakdown strength, resulting in higher energy density as compared to the linear counterparts. These novel insights into manipulating chain end distribution such as in BCPs and with molecular topology to increase the energy density of polymers will be helpful for fulfilling next-generation energy demands.

The authors would like to acknowledge NSF HBCU-UP EiR NSF DMR # 1900692 and NSF DMR# 1905960 grants for funding this research.

Dendrimer Approach toward High Permittivity Polymer Dielectrics for Electrical Energy Storage

BEIBEI CHEN (Presenter), SAMANTHA DAYMON, Univ of Southern Mississippi, OLUWAPELUMI KAREEM, MCKENNA REDDING, Tulane University, BRIAN OLSON, Univ of Southern Mississippi, MOHAMED K. HASSAN, Qatar University, SCOTT M GRAYSON, Tulane University, SERGEI NAZARENKO, Univ of Southern Mississippi

— Polymers which display high dielectric permittivity (DP) and low dissipation factor (DF) are important in the area of energy storage using film capacitors. Unfortunately, most polymers, even polar, exhibit fairly low DP, 2-4. It has been shown in this study that well dried films prepared from second generation dendrimer (D2) (T_g ~ 50°C) synthesized using 2,2-bis(hydroxymethyl)propionic acid monomer (bis-MPA) demonstrate at room temperature a fairly high DP = 10.5 and low DF = 0.014 in the kHz range of frequencies. The dipole relaxation mechanism, which contributes to this unusual dielectric response was found to be linked to numerous hydroxyl groups situated in the periphery of dendrimer molecules. WAXS and computer molecular dynamics (MD) simulation all indicated that these highly mobile hydroxyl groups in bis-MPA D2 glassy films exhibit a very high level of dipole-dipole (OH-OH) correlation mediated by H-bonding. In fact, terminal hydroxyls readily form H-bonded ‘chain-like’ clusters of different lengths which can range from single H-bond associations to clusters containing tens of hydroxyls. This behavior explains why D2 exhibits a high dielectric constant.

This work was supported by National Science Foundation.
High κ polymers of intrinsic microporosity: A new class of high-temperature and low-loss dielectrics for microelectronic applications

**LEI ZHU (Presenter), ZHONGBO ZHANG, MAN HIN KWOK, Case Western Reserve University** — High performance polymer dielectrics is a key component for power and printable electronics. In this work, organo-soluble polymers of intrinsic microporosity (PIMs) are reported for the first time to show desirable dielectric properties with high permittivity (or κ), high temperature capability, and low dielectric loss. Due to the polar sulfonyl side groups and rigid contorted polymer backbone, sulfonylated PIM (SO2-PIM) exhibited an optimized balance between relatively high κ and low dielectric loss in a broad temperature window (up to 200 °C). For examples, its discharged energy density reached as high as 17 J cm⁻³ with κ = 6.0. The discharge efficiencies were 94% at 150 °C/300 MV m⁻¹ and 88% at 200 °C/200 MV m⁻¹. Furthermore, its application as high-κ gate dielectrics in field effect transistors (FETs) is demonstrated. With the bilayer SO2-PIM/SiO2 gate dielectric, the InSe FETs exhibited a significantly improved electron mobility in the range of 200-400 cm² V⁻¹ s⁻¹, much higher than 40 cm² V⁻¹ s⁻¹ for the bare SiO2-gated InSe FET. This study indicates that highly dipolar PIMs with rigid polymer backbone and large free volume are promising as high performance, next generation polymer dielectrics.

*This work is supported by National Science Foundation (DMR-1708990).

Phase equilibria in P(TrFE-VDF): conformation and chirality

**BING ZHANG (Presenter), WENCHANG LU, Department of Physics, North Carolina State University, YANG LIU, WENHAN XU, AZIGULI HAIBIBU, ZHUBING HAN, QING WANG, Department of Materials Science and Engineering, The Pennsylvania State University, JERRY BERNHOLC, Department of Physics, North Carolina State University** — Ferro- and piezo-electric materials near a phase boundary usually possess enhanced dielectric or piezoelectric properties. We have discovered a morphotropic phase boundary (MPB) in P(VDF-TrFE) polymers [1], the first for any organic material. We show that the MPB forms due to intrachain rather than interchain conformation competition between the planar all-trans and 3/1-helical conformations in single P(VDF-TrFE) chains [2]. Our ab-initio calculations reveal low energy barrier electric dipole moment rotations between the nearly energetically degenerate chain conformations, which result in the piezoelectric enhancement near MPB. In particular, chirality plays a crucial role in the formation of a helical conformation and the relative stability of chain conformations strongly depends on the spatial arrangement of chirality centers. Our results explain the experimental data and the near degeneracy of multiple phases in the P(VDF-TrFE) material. They also provide a guideline for designing new polymers with MPB from a molecular point of view.

10:24AM R35.00011: Ionic and Local Electric Polarization Effects in Polymers [Invited]
GEORGE FLOUDAS (Presenter), Dept. of Physics, University of Ioannina & MPIP — The fundamental role of electric polarization in polymer physics is discussed via two examples. The first discusses purely ionic polarization effects in single ion conductors that are based on polymerized ionic liquids (PILs) (collaboration with the group of Ulli Scherf, Wuppertal). We employ a series of PILs with a polythiophene backbone bearing imidazolium salts with butyl, hexyl, octyl, and decyl side groups and several counteranions. PILs bearing the polythiophene backbone are unique as they can simultaneously conduct electronic charge and ions at nanometer length scales. Dielectric spectroscopy measurements performed as a function of temperature and pressure revealed that ionic conductivity is controlled by the balance between ion diffusion and ion complexation. The former is favored by the small ion size, the presence of ion channels and the decoupling from the backbone dynamics. On the other hand, ion complexation is controlled by ion size, the dielectric constant and charge delocalization. We propose a stick and jump model for ion motion in PILs.

The second example explores the local electric polarization effects in polymer blends (collaboration with M. Kappl, H.-J. Butt, Mainz). The design of multi-component materials for nanotechnology requires knowledge of the local composition. Hence, it is essential to develop techniques that can probe the local composition at the nanoscale. Local dielectric spectroscopy (LDS) is based on the electrostatic interaction between a conductive atomic force microscopy (AFM) probe in close proximity with the sample supported by a flat conductive substrate. Here, LDS is employed to analyze the dynamic heterogeneity in miscible blends as a function of film thickness. In thin films, phase segregation occurs and the kinetics of phase demixing was studied using as a probe the change in local composition. These results open new possibilities for studying interdiffusion and adhesion at polymer-polymer interfaces.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R36 DBIO: Physics of Organelles 601/603 - Elena Koslover, University of California, San Diego - Tag(s): Invited

8:00AM R36.00001: Is the endoplasmic reticulum an obstacle to intracellular diffusion? [Invited]  GREG HUBER (Presenter), Chan Zuckerberg Biohub — Intracellular spaces are tightly packed and the biggest potential obstacle in the crowded interior of a eukaryotic cell is the endoplasmic reticulum (ER), whose total membrane area can be 20-30 times that of the cell’s plasma membrane. Much of this area is in parallel sheets, however the sheet-like ER has also been found to be riddled with spiral dislocations, known as ‘Terasaki ramps’, in the vicinity of which the sheets’ doubled bilayer membranes can be approximately modeled by helicoids. We analyze diffusion on a surface with locally helicoidal topological dislocations, and use the results to argue that the Terasaki ramps facilitate an efficient transport of water-soluble molecules both within the lumen of the endoplasmic reticulum, and in the adjacent cytoplasmic space. (This is joint work with Michael Wilkinson.)
The interior of eukaryotic cells is highly compartmentalized by a variety of organelle structures. A particularly prominent organelle is the endoplasmic reticulum (ER) that feeds virtually all secretory processes of a cell (amongst other duties). Large portions of the ER are organized as a vast dynamic network of membrane tubules that are connected by three-way junctions. Dispersed on this network are numerous membrane domains, so-called ER exit sites (ERES), at which nascent proteins leave the ER via transport vesicles to get transported along the cell's secretory pathway.

Using time-resolved imaging, we have analyzed the dynamics of ER junctions and of ERES domains as well as the self-organization of ERES on the ER network. As a result, we observed that both, ER junctions and ERES, show a marked subdiffusion with signatures of an anti-persistent fractional Brownian motion and a strong dependence on the cytoskeleton's integrity: ER junctions move like monomer units of (semi)flexible polymers with the overall dynamics of the ER network being governed by fractons due to the network's self-similar geometry. Moreover, active cytoskeleton-associated processes endow the subdiffusion of ER junctions with a distinct nonequilibrium character. In contrast, ERES rather are mobile domains that perform a quasi-one-dimensional random walk on the shivering ER backbone. Moreover, ERES show a self-organization that is reminiscent of two-dimensional droplet formation where coarsening is hindered by geometric and topological constraints imposed by ER junctions. In line with this view, a substantial coarsening of ERES to fewer but larger domains is observed upon lifting the hindrance via an RNAi-induced reduction of ER junctions.

*Financial support by the VolkswagenStiftung (Az. 92738) and by the Elite Network of Bavaria (Study Program Biological Physics) is gratefully acknowledged.
9:12AM R36.00003: Fundamental limits to organelle biogenesis control in *Saccharomyces cerevisiae* [Invited]  KIANDOKHT PANJTAN AMIRI, ASA KALISH, SHANKAR MUKHERJI (Presenter), Washington University, St. Louis — Among the most important processes in the self-assembly of the eukaryotic cell is the synthesis of its organelles, specialized biochemical compartments that house processes crucial to cellular physiology. Two critical properties closely linked with organelle function are their copy numbers and sizes. Numerous molecular factors that regulate the numbers and sizes of a diverse array of organelles, including the Golgi, mitochondria, peroxisomes and lipid droplets among others, have been identified. However, our understanding of the quantitative principles governing organelle number and size control remains incomplete. Here, we combine experimental data from the single-celled eukaryote *Saccharomyces cerevisiae* and mathematical theory to show that cells tolerate substantial fluctuations in organelle number while robustly controlling fluctuations in organelle sizes. In particular, our framework suggests that organelle size increases in random bursts from a limited pool of building blocks, which in turn imposes an asymmetry in optimal organelle number and size control. Burst like growth is a potentially general mechanism by which the cell efficiently assembles subcellular structures from its finite resources.

9:48AM R36.00004: Decoding the variance in intracellular organization of the undifferentiated hiPS cell [Invited]  MATHEUS VIANA (Presenter), SUSANNE RAFELSKI, Allen Institute for Cell Science — The Allen Institute for Cell Science is developing a state space of structural signatures of the undifferentiated human induced pluripotent stem cell (hiPSC) to understand how cells organize and transition between states (cellular morphogenesis). To do this we take advantage of the ~35 endogenous fluorescently tagged hiPSC lines in the Allen Cell Collection (www.allencell.org), each expressing a monoallelic EGFP-tagged protein representing a particular organelle. We develop image-based assays and segmentations for quantitative analyses, taking advantage of thousands of replicate high-resolution 3D images for each structure. We are investigating biological sources of cellular variation in a high-dimensional space that represents integrated intracellular organization. We applied the Allen Cell Structure Segmenter to images of lamin B1-tagged cells to extract nuclear shapes, which we then fit using spherical harmonics. We performed principal component analysis on the fitting coefficients and we found the first five components explain 85% of the total variance. Each of these components was mapped into a mode corresponding to a distinct biological source of variation. The first mode represented nuclear volume, which increases throughout interphase at timescales of hours. The second mode represented how flat (vs. round) a nucleus appeared in the apical-basal axis (Z-direction), which was linked to changes in colony cell packing dynamics consistent with a timescale of several days for cell packing within colonies. The remaining modes represented how elongated a nucleus appeared in the XY plane and how tilted the nucleus appeared along the major and minor axis. We found these modes to be caused by interactions with neighboring cells occurring at timescales of minutes. We are now applying these analyses to develop biophysical models of nuclear shape. Our framework will be extended to cell shape and key intracellular structures in an integrative fashion.
10:24AM R36.00005: Modelling membrane-bound cellular organelles with non-equilibrium dynamics [Invited]  PIERRE SENS (Presenter), Insitut Curie / CNRS, JEAN-PATRICK VREL, Institut Curie, QUENTIN VAGNE, MPI-CBG — Membrane-bound cellular organelles perform many essential functions, among which the sorting and biochemical maturation of cellular components. Organelles along the secretory and endocytic pathways are strongly out-of-equilibrium structures, which display large stochastic fluctuations of composition and shape resulting from inter-organelle exchange and enzymatic reactions. Understanding how the different molecular mechanisms controlling these processes are orchestrated to yield robust fluxes of matter and to direct particular components to particular locations within the cell is an outstanding problem of great interest for cell biologist, but also for physicists.

In this talk, I will discuss a conceptual model of organelle biogenesis and maintenance that include vesicular exchange (budding, transport, and fusion) and biochemical maturation, i.e. the change of identity of an organelle over time (early to late endosomes, cis to trans Golgi cisternae...). I will show how the non-equilibrium steady-state of an organelle or a network of organelles may be varied in a controlled manner by modifying a limited number of coarse-grained parameters (essentially, the budding, fusion and maturation rates) and discuss the relevance of these results for the structure of the Golgi apparatus.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R37 GPC: Predictability of the Climate System 605 - William Collins,
Lawrence Berkeley National Laboratory - Tag(s): Invited, Undergrad Friendly

8:00AM R37.00001: Data Assimilation and Uncertainty Quantification in the Geosciences*
[Invited]  JUAN RESTREPO (Presenter), Mathematics, Oregon State University — Data assimilation is the name commonly given to the estimation process that generates moments of probability density functions of time dependent processes modeled by physics, and observations. The inherent uncertainties of model and data are taken into account using a Bayesian framework. Data assimilation is presently used in applications as diverse as weather forecasting and spacecraft navigation. I will appeal to familiar statistical physics to present the general methodology. I will briefly describe a couple of computational implementations of the method summarize some of the key research challenges that arise in their application. I will also describe some novel applications of the methodology, potentially useful in tracking targets, hurricanes, and ongoing research in the application of stochastic parametrization and machine learning for the purpose of dimension reduction.

*National Science Foundation NSF/OCE no. 1434198 and Pacific Earthquake Engineering Research Center (PEER) research grant no. 1123-NCTRYH supported this research
8:36AM R37.00002: Climate Change and Climate Variability: A Unified Framework* [Invited]
MICHAEL GHIL (Presenter), Ecole Normale Supérieure, Paris and University of California, Los Angeles —
The “death of stationarity” poses a substantial challenge to climate predictability and to the climate sciences in general. This challenge is addressed herein by formulating the problems of change in the climate's intrinsic variability within the framework of the theory of nonautonomous and random dynamical systems (NDS and RDS) with time-dependent forcing. A key role in this theory is played by the pullback attractors (PBAs) that replace the strange attractors of the more familiar theory of autonomous dynamical systems, in which there is no explicit time dependence of either forcing or coefficients.
The concepts and methods of the NDS and RDS approach will be introduced and will be illustrated using a stochastically perturbed version of the Lorenz (1963) convection model. This illustration will be followed by applications to models of the wind-driven ocean circulation and the El Niño–Southern Oscillation (ENSO). One finds that two local PBAs, a quiescent and a chaotic one, coexist within the wind-driven ocean model's decadally modulated global PBA, whereas a critical transition between two types of chaotic behavior occurs in the seasonally forced ENSO model.
Implications for the climate sciences in the era of anthropogenic change will be discussed.
Reference

*The Tipping Points in the Earth System (TiPES) project is supported by the European Union's Horizon 2020 research and innovation program under grant agreement No. 820970.

9:12AM R37.00003: Quantifying uncertainty in climate predictability using perturbed physics ensembles and climate model emulation [Invited] KATHERINE DAGON (Presenter), National Center for Atmospheric Research, BENJAMIN SANDERSON, ROSIE FISHER, CERFACS, DAVID LAWRENCE, National Center for Atmospheric Research — Climate models are essential tools for understanding and predicting Earth system processes and feedbacks, but uncertainties in their future projections remain challenging to characterize. Improvements in physical process realism and the representation of human influence arguably make models more comparable to reality, but also increase the degrees of freedom in model configuration leading to parametric and structural uncertainties in projections. Perturbed physics ensembles sample the uncertainty space through different choices of parameter settings. Climate model emulators can be a computationally efficient method of producing large ensembles of climate model output, in order to study different sources of uncertainty. In this work we use a machine learning algorithm to build an emulator for the land surface component of a climate model. Using a perturbed physics ensemble of model simulations, we train the emulator to predict model output given a set of parameter values as input. We optimize parameter values by comparing emulated model output with observations across multiple relevant metrics, including global carbon and water flux benchmarks. We also account for structural and observational uncertainty through a novel Bayesian calibration approach. By sampling the resulting posterior distributions and running future climate simulations, we can then estimate the contribution of land model parameter uncertainty in future projections of climate change.
9:48AM R37.00004: Earth System Modeling 2.0: Toward Data-Informed Climate Models With Quantified Uncertainties* [Invited] TAPIO SCHNEIDER (Presenter), Caltech — While climate change is certain, precisely how climate will change is less clear. But breakthroughs in the accuracy of climate projections and in the quantification of their uncertainties are now within reach, thanks to advances in the computational and data sciences and in the availability of Earth observations from space and from the ground. To achieve a leap in accuracy of climate projections, we are developing a new Earth system modeling platform. It will fuse an Earth system model (ESM) with global observations and targeted local high-resolution simulations of clouds and other elements of the Earth system. The ESM is being developed by the Climate Modeling Alliance (CliMA), which encompasses Caltech, MIT, and the Naval Postgraduate School. CliMA will capitalize on advances in data assimilation and machine learning to develop an ESM that automatically learns from diverse data sources, be they observations from space or data generated computationally in high-resolution simulations. It will also engineer the ESM from the outset to be performant on emerging computing architectures, including heterogeneous architectures that combine traditional CPUs with hardware accelerators such as graphical processing units (GPUs). This talk will cover key new concepts in the ESM, including turbulence, convection, and cloud parameterizations and fast and efficient algorithms for assimilating data and quantifying uncertainties.

*Eric and Wendy Schmidt (by recommendation of Schmidt Futures); Earthrise Alliance; National Science Foundation; Paul G. Allen Family Foundation; Charles Trimble.
Bayesian Inference for Climate prediction — Bayesian Inference in the geosciences is called data assimilation. It studies how to best combine information from complex numerical models with information from observations of the system at hand, given limited computational resources. This requires knowledge of the physics, numerical modeling including computer architecture, quantification of deficiencies in the numerical models, characteristics of observation errors, and Bayesian inference for very high dimensional highly nonlinear systems.

An important characteristic of the climate system is that the different Earth system components (e.g. atmosphere, ocean, land surface and icecaps) have vastly different internal time scales. The main work horse for weather prediction, a (variational) smoother in which observations over a time window of 6-12 hours are used to find the best starting point for predictions, is problematic because the optimal time window length is substantially different for the different components. Even after 20 years of intensive research no satisfying smoother solution has been found. This suggests to use a filter solution without an assimilation window, but the main workhorse there, the Ensemble Kalman Filter, suffers from too small ensemble sizes to accommodate the large number of observations (even when so-called localization is applied).

Another issue is that with its many feedbacks the climate system is highly nonlinear, while the standard methods for weather predictions are only optimal for linear, and perhaps weakly nonlinear systems. Furthermore, system updates are typically too abrupt and need to be added incrementally during the prediction.

We will discuss potential solutions based on existing techniques, and alternative ideas based on so-called particle flows. The latter are fully nonlinear while combining the strong points of smoothers and filters mentioned above, and have the potential to make substantial strides forwards towards better climate prediction.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R38 DQI: DQI Invited Session: Quantum State Preparation and Measurement (SPAM) in Semiconductor Qubits — Exchange-only triple-quantum-dot spin qubits are a promising approach to scalable quantum information processing. In such systems, state preparation is generally performed by biasing the device to exchange electrons with a cold electron reservoir, while measurement is realized by spin-to-charge conversion and detection with a nearby electrometer. In this talk I will discuss implementation of these techniques in isotopically-enriched Si/SiGe triple dots using a direct dot-sensor electrometer with a cryogenic HEMT amplifier. I will examine the non-idealities in these operations, and explain how those factors can be hidden or revealed by choice of metric, showing data which exhibits SPAM infidelity in the low parts-per-thousand level. Further, I’ll detail a budget for what performance is expected, given properties of the device and instrumentation.
9:12AM R38.00003: Quantum non-demolition measurement of an electron spin qubit*
[Invited] JUN YONEDA (Presenter), CEMS, RIKEN — While single-shot spin detection of electron spin qubits in semiconductor quantum dots is now a laboratory routine, the need for quantum error correction in a large-scale system demands a quantum non-demolition (QND) implementation. The QND spin readout imposes minimal disturbance to the probed spin polarization and can therefore be repeated to extinguish measurement errors. Furthermore, it also works as a high-fidelity state preparation device. However, its realization is challenging as it involves exquisite exposure of the system to the external readout circuitry while maintaining the qubit coherence and integrity. In this talk, we show that an electron spin qubit in quantum dots can be measured in a highly non-demolition manner by probing a neighboring electron spin qubit Ising-coupled to the qubit spin. The high QND fidelity enables enhancement of the measurement fidelity of a single electron spin state by repeating the readout process several dozens of times. We describe the analysis method based on statistical inference, which is crucial to achieve the optimal performance in the presence of the qubit relaxation. We will further discuss how such QND measurements can improve the fidelity of measurement-based state preparation in addition to the measurement fidelity.

*This research is supported financially by CREST, JST (JPMJCR15N2 and JPMJCR1675) and Q-LEAP project initiated by MEXT (JPMXS0118069228).

9:48AM R38.00004: David Reilly Invited Talk [Invited] —

10:24AM R38.00005: M Fernando Gonzalez-Zalba Invited Talk [Invited] —

Thursday, March 5, 2020 8:00 AM - 10:48 AM

Session R39 DCOMP GDS DMP: Machine Learning for Quantum Matter

III 703 - Annabelle Bohrdt, Tech Univ Muenchen - Tag(s): Focus
8:00AM R39.00001: Frustrated magnets and fermions with Neural Network Quantum States* [Invited] KENNY JING CHOO (Presenter), Univ of Zurich, ANTONIO MEZZACAPO, IBM T.J. Watson Research Center, TITUS NEUPERT, Univ of Zurich, GIUSEPPE CARLEO, Flatiron Institute — Neural-Network quantum states (NQS) have been recently proposed as a method to solve challenging interacting quantum problems. During this talk, I will discuss the application of NQS to two problems. First, we use a deep convolutional network to find the ground state of the frustrated J1-J2 model on the square lattice. While early representations of many-body quantum states in terms of neural networks are usually based on shallow architectures such as the restricted Boltzmann machine, the benefits of deeper architectures are emerging in the latest research. Here, we show that these deep convolutional NQS can achieve results that are competitive with other state of the art variational methods developed in the past decade. Second, we present an extension of NQS to model interacting fermionic problems. Borrowing techniques from quantum simulation, we directly map fermionic degrees of freedom to spin ones, and then use NQS to perform electronic structure calculations. On small test molecules, we achieve energies below chemical accuracy, and frequently improves upon coupled cluster methods.

*The Flatiron Institute is supported by the Simons Foundation. A.M. acknowledges support from the IBM Research Frontiers Institute. KC was supported by the European Unions Horizon 2020 research and innovation program (ERC-StGNeupert-757867-PARATOP).

8:36AM R39.00002: Learning the Ground State Wavefunction of Periodic Systems Using Recurrent Neural Networks* CHRISTOPHER ROTH (Presenter), ALLAN MACDONALD, University of Texas at Austin — Modeling quantum many-body systems is enormously challenging due to the exponential scaling of Hilbert dimension with system size. Finding an Ansatz that efficiently compresses the wavefunction is key to simulating large systems. Here, we present an approach for simulating periodic quantum systems using long short term memory networks (LSTMs), whose recurrent structure is able to efficiently capture invariance to discrete translations in the bulk. We perform Variational Monte Carlo using an autoregressive Ansatz, where the probability amplitude associated with an electron having a particular quantum number is conditioned on the quantum numbers of the electrons behind it. These amplitudes and phases are iteratively generated by an LSTM, which is trained to minimize the energy using stochastic gradient descent. We show that such a formulation can be used to find the ground state of the 1D Hubbard and J1-J2 Heisenberg models for several hundred electrons. Furthermore, we can learn about the bulk by "growing" the sample; iteratively training the solution on progressively larger systems until the edge effects become negligible. We argue that such a scheme can be generalized more naturally to higher dimensions than Density Matrix Renormalization Group.

*DOE grant DE- FG02-02ER45958
**8:48AM R39.00003: Calculating Renyi Entropies with Neural Autoregressive Quantum States**
ZHAOYOU WANG (Presenter), EMILY J DAVIS, Stanford Univ — Entanglement entropy is an essential metric for characterizing quantum many-body systems, but its numerical evaluation for neural network representations of quantum states has so far been inefficient and only demonstrated for the restricted Boltzmann machine architecture. We estimate generalized Renyi entropies $S_n$ of an autoregressive neural quantum state using quantum Monte Carlo methods. A naive “direct sampling” approach performs well for small Renyi order $n$ but fails for larger orders when benchmarked on a 1D Heisenberg model. We therefore propose an improved “conditional sampling” method exploiting the autoregressive structure of the network ansatz, which outperforms direct sampling in both 1D and 2D Heisenberg models. Conditional sampling facilities calculations of high-order Renyi entropies up to at least $n > 30$, which allows for a polynomial approximation of the von Neumann entropy as well as extraction of the largest eigenvalue of the reduced density matrix, and thus the single copy entanglement. By demonstrating good convergence even up to high Renyi order, our methods elucidate the potential of neural network quantum states in quantum Monte Carlo studies of entanglement entropy for many-body systems.

**9:00AM R39.00004: Probabilistic Simulation of Quantum Circuits with the Transformer**
JUAN CARRASQUILLA, Vector Institute, DI LUO (Presenter), University of Illinois at Urbana-Champaign, FELIPE PEREZ, Layer6 AI, BRYAN CLARK, University of Illinois at Urbana-Champaign, ASHLEY MILSTED, Perimeter Institute for Theoretical Physics, MAKSIMS VOLKOVS, Layer6 AI, MARIO AOLITA, Universidade Federal do Rio de Janeiro — In this work, we present an exact probabilistic formulation of quantum dynamics through positive value-operator measurements (POVM). In this formulation, unitary dynamics and quantum channels are represented by quasi-stochastic matrices acting on true probability distributions which specify the quantum state univocally. The probability distribution representation of the quantum state opens up the possibility of bridging the state-of-the-art techniques from machine learning into the simulation of quantum mechanics. Using the POVM formalism, we have developed a practical algorithm for the probabilistic simulation of quantum circuits with the Transformer, a powerful ansatz responsible for the most recent breakthroughs in the natural language processing research. The method is applied to state preparation of GHZ state and Linear Graph state up to 60 qubits, as well as variational quantum circuit preparation of the ground state of the Transverse Field Ising Model.

*This research is supported by the National Science Foundation under Grant No. NSF PHY-1748958, and has support from the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Canada CIFAR AI chair program.
9:12AM R39.00005: Variational optimization in the AI era [Invited] BRYAN CLARK (Presenter), DMITRII KOCHKOV, DI LUO, University of Illinois at Urbana-Champaign — The variational method has been a cornerstone approach to tackling the quantum many-body problem since the beginnings of quantum mechanics. Throughout this history, wave-functions have grown in number of parameters and generality. The eventual conclusion to this arc is to consider the variational space of all computer programs. Using tools and inspiration from AI, we have developed an approach to represent this class (computational graph states); a novel way to optimize tens of thousands of parameters within this space (supervised wave-function optimization); and multiple novel variational ansatz (neural net backflow, etc). We will describe these advancements and our effort to push forward, in the age of AI, the variational approach to the quantum many body problem.

9:48AM R39.00006: Deep neural network solution of the electronic Schrödinger equation JAN HERMANN (Presenter), ZENO SCHÄTZLE, FRANK NOE, Free University of Berlin — The electronic Schrödinger equation describes fundamental properties of molecules and materials, but cannot be solved exactly for larger systems than a hydrogen atom. Quantum Monte Carlo is an apt approach for high-quality approximations, because its accuracy is limited in principle only by the flexibility of the used wave-function ansatz, but traditional trial wave functions are too rigid to take full advantage of this potential. Here, we greatly increase the flexibility of existing ansatzes by incorporating deep neural networks, which are known as superb universal function approximators. Our architecture, dubbed PauliNet, is built around the Hartree–Fock solution as a baseline, includes analytical cusp conditions, and uses the Jastrow-factor and backflow constructions as entry points for graph-convolutional neural networks, which ensure the exact permutational antisymmetry. We demonstrate that PauliNet outperforms comparable state-of-the-art trial wave functions on atoms, small molecules, and a strongly correlated model system. Our approach opens a new path towards highly accurate and systematically improvable electronic structure methods with explicit access to the corresponding wave function and hence a variety of electronic properties.
10:00AM R39.00007: Ab-Initio Solution of the Many-Electron Schrödinger Equation with Deep Neural Networks  JAMES SPENCER (Presenter), DAVID PFAU, ALEX MATTHEWS, DeepMind, W MATTHEW C FOULKES, Physics, Imperial College London — Calculating analytic solutions to the Schrödinger equation is impossible except in a small number of special cases. Approximate solutions typically impose a fixed functional form on the wavefunction. Neural networks have shown impressive power as accurate practical function approximators\(^1\) and have been recently used in bosonic\(^2\) and lattice systems\(^3\). We show that deep neural networks can learn the ground state wavefunction of chemical systems given only the positions and charges of the nuclei using a combination of variational Monte Carlo (VMC) and optimisation methods from machine learning\(^4\). The neural network Ansatz, FermiNet, is compact yet flexible and gives more accurate energies than conventional Ansätze. We obtain ground state energies, ionisation potentials and electron affinities to within chemical accuracy on a variety of atoms and small molecules and outperform VMC using conventional Slater-Jastrow wavefunctions.


DP and JS contributed equally to this work.

10:12AM R39.00008: Towards neural network quantum states with nonabelian symmetries*  TOM VIEIJRA (Presenter), CORNEEL CASERT, JANNES NYS, Department of Physics and Astronomy, Ghent University, WESLEY DE NEVE, Center for Biotech Data Science, Ghent University Global Campus, JUTHO HAEGERMAN, JAN RYCKEBUSCH, FRANK VERSTRAETE, Department of Physics and Astronomy, Ghent University — Although artificial neural networks have recently been proven to provide a promising new framework for constructing quantum many-body wave functions, the parameterization of a quantum wavefunction with nonabelian symmetries in terms of a Boltzmann machine inherently leads to biased results due to the basis dependence. We demonstrate that this problem can be overcome by sampling in the basis of irreducible representations instead of spins, for which the corresponding ansatz respects the nonabelian symmetries of the system. We will show that this representation is connected to symmetric tensor network states.

We apply our methodology to find the ground states of the one-dimensional antiferromagnetic Heisenberg (AFH) model with spin-half and spin-1 degrees of freedom. The proposed ansatz can target excited states, which is illustrated by calculating the energy gap of the AFH model.

Implementing non-abelian symmetries in variational quantum states is an important step towards solving frustrated quantum systems. We demonstrate recent results using our ansatz on the frustrated J1-J2 model.

*This work was supported by Ghent University, Research Foundation Flanders (FWO-Flanders), and ERC Grants QUTE (No.647905) and ERQUAF (No.715861).
10:24AM R39.00009: Designing neural networks for stationary states in open quantum many-body systems*  NOBUYUKI YOSHIOKA (Presenter), RYUSUKE HAMAZAKI, Department of Physics, University of Tokyo — We propose a new variational scheme based on the neural-network quantum states to simulate the stationary states of open quantum many-body systems [1]. Using the high expressive power of the variational ansatz described by the restricted Boltzmann machines [2], which we dub as the neural stationary state ansatz, we compute the stationary states of quantum dynamics obeying the homogeneous Markovian quantum master equations. The mapping of the stationary-state search problem into finding a zero-energy ground state of an appropriate Hermitian operator allows us to apply the conventional variational Monte Carlo method for the optimization. Our method is shown to simulate various spin systems efficiently, i.e., the transverse-field Ising models in both one and two dimensions and the XYZ model in one dimension.


*JSPS KAKENHI Grant Numbers JP17J00743 (N. Y.) and JP17J03189 (R. H.) and financial support from Institute for Physics of Intelligence, University of Tokyo.

10:36AM R39.00010: Deep Learning-Enhanced Variational Monte Carlo Method for Quantum Many-Body Physics  LI YANG (Presenter), Google Research, ZHAOQI LENG, Princeton University, LI LI, Google Research, ANKIT PATEL, Rice University, WENJUN HU, University of Tennessee, HAN PU, Rice University — Artificial neural networks have been successfully incorporated into variational Monte Carlo method (VMC) to study quantum many-body systems. However, there have been few systematic studies of exploring quantum many-body physics using deep neural networks (DNNs), despite of the tremendous success enjoyed by DNNs in many other areas in recent years. One main challenge of implementing DNN in VMC is the inefficiency of optimizing such networks with large number of parameters. We introduce an importance sampling gradient optimization (ISGO) algorithm (arXiv:1905.10730), which significantly improves the computational speed of training DNN in VMC. We design an efficient convolutional DNN architecture to compute the ground state of a one-dimensional (1D) SU(N) spin chain. Our numerical results of the ground-state energies with up to 16 layers of DNN show excellent agreement with the Bethe-Ansatz exact solution. Furthermore, we also calculate the loop correlation function using the wave function obtained. Our work demonstrates the feasibility and advantages of applying DNNs to numerical quantum many-body calculations.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R40 DCOMP DAMOP DCMP: Precision many-body physics VI: Novel methods and algorithms  705 - Olga Goulko, Boise State University - Tag(s): Focus
8:00AM R40.00001: DMRG Approach to Optimizing Two-Dimensional Tensor Networks
[Invited] KATHARINE HYATT (Presenter), MILES STOUDENMIRE, Simons Foundation — Tensor network algorithms have been remarkably successful solving a variety of problems in quantum many-body physics. However, algorithms to optimize two-dimensional tensor networks known as PEPS lack many of the aspects that make the seminal density matrix renormalization group (DMRG) algorithm so powerful for optimizing one-dimensional tensor networks known as matrix product states. We implement a framework for optimizing two-dimensional PEPS tensor networks which includes all of steps that make DMRG so successful for optimizing one-dimension tensor networks. We present results for several 2D spin models and discuss possible extensions and applications.

8:36AM R40.00002: Diagrammatic Monte Carlo for the Hubbard Model: Recent developments* [Invited] MICHEL FERRERO (Presenter), FEDOR SIMKOVIC, Ecole Polytechnique, RICCARDO ROSSI, CCQ, Flatiron Institute — In this talk, I will present recent developments of the diagrammatic Monte Carlo method applied to the Hubbard model. Diagrammatic Monte Carlo methods are based on the construction of a perturbation series for physical observables. They face two main challenges: The first challenge is the accurate stochastic computation of the series coefficients that suffers from the fermionic sign problem. The second difficulty is the resummation of the series whose success depends on the structure of the physical observable expressed in the complex plane of the expansion parameter, e.g. the onsite repulsion U in the Hubbard model. I will discuss how these two issues can be addressed and, in particular, how the freedom to choose the non-interacting starting point of the theory can be used to construct more efficient perturbation series. I will illustrate these developments with calculations performed in different regimes of the Hubbard model.

*We acknowledge support from the Simons Foundation within the Many-Electron Collaboration program.

9:12AM R40.00003: Differentiable Programming Tensor Networks HAI-JUN LIAO (Presenter), JIN-GUO LIU, LEI WANG, TAO XIANG, Institute of Physics, The Chinese Academy of Sciences — Differentiable programming is a fresh programming paradigm which composes parameterized algorithmic components and trains them using automatic differentiation (AD). We present theory and practice of programming tensor network algorithms in a fully differentiable way. By formulating the tensor network algorithm as a computation graph, one can compute higher order derivatives of the program accurately and efficiently using AD. We present essential techniques to differentiate through the tensor networks contractions, including stable AD for tensor decomposition and efficient backpropagation through fixed point iterations. As a demonstration, we compute the specific heat of the Ising model directly by taking the second order derivative of the free energy obtained in the tensor renormalization group calculation. Next, we perform gradient based variational optimization of infinite projected entangled pair states for quantum antiferromagnetic Heisenberg model and obtain start-of-the-art variational energy and magnetization with moderate efforts. Differentiable programming removes laborious human efforts in deriving and implementing analytical gradients for tensor network programs, which opens the door to more innovations in tensor network algorithms and applications.
Simulating open quantum many-body systems using matrix product state purifications* YIKANG ZHANG (Presenter), XIN ZHANG, THOMAS BARTHEL, Duke University — Although we usually try to isolate quantum systems in the lab as effectively as possible, some degree of external noise and interaction with the environment is inevitable. This generally leads to decoherence, dissipation, and can alter the critical behavior in many-body systems. One can also try to engineer the environment coupling to achieve new physical phenomena. We consider Markovian systems, evolving according to Lindblad master equations. We introduce a new algorithm based on matrix product state purifications to simulate open many-body systems. This resolves a fundamental problem in simulations using matrix product density operators (MPDO) which generally lose positivity in truncations, leading to nonphysical states. We test and demonstrate our algorithm for spin chains and fermionic systems, comparing to exact diagonalization, analytical solutions, and MPDO simulations.

*T.B. acknowledges supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0019449.

Compressing Infinite Matrix Product Operators with an Application To Twisted Bilayer Graphene* DANIEL PARKER (Presenter), XIANGYU CAO, TOMOHIRO SOEJIMA, MICHAEL ZALETEL, University of California, Berkeley — We present a new method for compressing matrix product operators (MPOs) which represent sums of local terms, such as Hamiltonians. Just as with area law states, such local operators may be fully specified with a small amount of information per site. Standard matrix product state (MPS) tools are ill-suited to this case, due to extensive Schmidt values that coexist with intensive ones, and Jordan blocks in the transfer matrix. We ameliorate these issues by introducing an "almost Schmidt decomposition" that respects locality. Our method is "ε-close" to the accuracy of MPS-based methods for finite MPOs, and extends seamlessly to the thermodynamic limit, where MPS techniques are inapplicable. As an application, we compress the Hamiltonian for a model of twisted bilayer graphene --- whose naive bond dimension is tens of thousands --- down to a size where its ground state may be computed.

This talk is based on arXiv: 1909.06341.

*We acknowledgesupport from the NSF Graduate Research FellowshipProgram NSF DGE 1752814 (DP), ERC synergy GrantUQUAM and DOE grant DE-SC001938 (XC). MZ was supported by the DOE, office of Basic Energy Sciences under contract no. DEAC02-05-CH11231.
We present a quantum electronic embedding method derived from the exact factorization approach to calculate static properties of a many-electron system. The method is exact in principle but the practical power lies in utilizing input from a low-level calculation on the entire system in a high-level method computed on a small fragment, as in other embedding methods. Here, the exact factorization approach defines an embedding Hamiltonian on the fragment. Various Hubbard models demonstrate that remarkably accurate ground-state energies are obtained over the full range of weak to strongly correlated systems.

*Financial support from the U.S. National Science Foundation CHE-1940333 and the Department of Energy Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences under Award DE-SC0020044 are gratefully acknowledged.
10:00AM R40.00007: Putting modern many-body methods to the test: the two-dimensional Hubbard model at weak coupling

THOMAS SCHAEFER (Presenter), CPHT, École Polytechnique, NILS WENTZELL, Center for Computational Quantum Physics (CCQ), Flatiron Institute, FEDOR SIMKOVIC, CPHT, École Polytechnique, YUAN-YAO HE, Center for Computational Quantum Physics (CCQ), Flatiron Institute, CORNELIA HILLE, Institute for Theoretical Physics, Universität Tübingen, CHRISTIAN ECKHARDT, Institute of Solid State Physics, TU Wien, BEHNAM ARZHANG, Department of Physics and Physical Oceanography, Memorial University of Newfoundland, VIKTOR HARKOV, Institute of Theoretical Physics, Universität Hamburg, FRANÇOIS-MARIE LE RÉGENT, ALFRED KIRSCH, CPHT, École Polytechnique, YAN WANG, Département de Physique and Centre de Recherche en Physique du Solide, Université de Sherbrooke, AARAM J. KIM, EVGENY KOZIK, Department of Physics, King's College London, EVGENY STEPanOV, Institute of Theoretical Physics, Universität Hamburg, ANNA KAUCH, Institute of Solid State Physics, TU Wien, SABINE ANDERGASSEN, Institute for Theoretical Physics, Universität Tübingen, JAMES LEBlANC, Department of Physics and Physical Oceanography, Memorial University of Newfoundland, SHIWEI ZHANG, Center for Computational Quantum Physics (CCQ), Flatiron Institute, ANDRE-MARIE TREMBLAY, Département de Physique and Centre de Recherche en Physique du Solide, Université de Sherbrooke, MICHEL FERRERO, CPHT, École Polytechnique, OLIVIER PARCOLLET, ANTOINE GEORGES, Center for Computational Quantum Physics (CCQ), Flatiron Institute — We provide a detailed synopsis and comparison of a comprehensive set of state-of-the-art many-body techniques for the weak-coupling regime of the two-dimensional half-filled Hubbard model on a square lattice. We put each of these methods to the test, for both one- and two-particle observables, in relation to the salient physical crossovers of this model: upon cooling from the high-temperature incoherent regime, coherent quasiparticles are formed below $T_{QP}$. At lower $T$, magnetic correlations stemming from the antiferromagnetically ordered phase at $T=0$ are gradually enhanced, resulting in the opening of an electronic (pseudo-)gap at $T^{*}$. By covering the range of modern many-body techniques available today, from numerically exact benchmark methods (determinantal and diagrammatic QMC [CDet]), over (dynamical) mean field theory (RPA, DMFT) and its cluster (DCA) and vertex based extensions (DΓA, TRILEX, DF, DB) to well-known approximations like parquet approximation (PA), the two-particle-self-consistent approach (TPSC) and the functional renormalization group (fRG), the realm of their applicability is put into perspective and a reference and agenda for future improvements is provided.

*Erwin-Schrödinger Fellowship J 4266 - "SuMo" (FWF), Grant No. 319286 "QMAC" (ERC), The Simons Foundation
10:12AM R40.00008: A time-dependent tunneling approach to RIXS and other core-hole spectroscopies* ADRIAN FEIGUIN (Presenter), KRISSIA ZAWADZKI, Northeastern University, ALBERTO NOCERA, Stewart Blusson Quantum Matter Institute, University of British Columbia — We introduce a numerical approach to calculate the Resonant Inelastic X-Ray Scattering (RIXS) in strongly correlated systems. Since accounting for intermediate processes involved in RIXS requires the knowledge of all eigenstates of the Hamiltonian, these computations have remained very challenging. We recast the calculation as a tunneling problem that can be readily solved by means of the time-dependent DMRG method and does not require a full knowledge of the excitations. This powerful formulation overcomes all the hurdles imposed by other techniques that rely on explicitly obtaining dynamical spectral functions. Results for the Hubbard model are achieved with minimal effort on large systems using a fraction of the states -- and simulation time-- required by the dynamical DMRG formulation. These ideas can be readily applied without modification away from equilibrium.

*AEF is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, grant No. DE-SC0014407, KZ by a Faculty of the Future fellowship, Schlumberger Foundation, AN by the Canada First Research Excellence Fund.

10:24AM R40.00009: A time and momentum resolved tunneling spectroscopy approach to non-equilibrium phenomena in correlated systems* KRISSIA ZAWADZKI (Presenter), ADRIAN FEIGUIN, Northeastern University — We introduce a numerical method to calculate the spectral density of correlated systems using a tunneling approach efficiently implemented through the time-dependent Density Matrix Renormalization-Group (tDMRG). By using an extended probe, which is basically a copy of the system of interest, we are able to extract the time-resolved spectrum with the momentum information of the excitations. We illustrate our ideas by calculating the time-resolved spectrum of a Mott-insulating extended Hubbard chain after a sudden quench. Our results demonstrate that the system realizes a non-thermal state that contains an admixture of spin and charge density excitations, with corresponding signatures recognizable as in-gap subbands. In particular, we identify a band of excitons and one of stable anti-bound states at high energies that gains enhanced visibility after the pump. We do not appreciate noticeable relaxation within the time-scales considered, which is attributed to the lack of decay channels due to spin-charge separation.

*KZ is supported by a Faculty of the Future fellowship of the Schlumberger Foundation. AEF acknowledges the U.S. Department of Energy, Office of Basic Energy Sciences for support under grant No. DE-SC0014407.
The effect of electron-phonon coupling on Dirac fermions raises interesting questions concerning charge-density wave (CDW) formation in a semi-metal, which have recently been explored on a honeycomb lattice \[1,2\]. Here, we use the unbiased determinant Quantum Monte Carlo (DQMC) method to study the Holstein model on a half-filled staggered-flux square lattice, and compare with the results on the honeycomb lattice. Our work analyzes a range of phonon frequencies, \(0.1 \leq \omega \leq 2.0\). We find that interactions give rise to charge-density wave order but only above a finite coupling strength \(\lambda_{\text{crit}}\). The transition temperature is evaluated and presented in a \(T_c - \lambda\) phase diagram. An accompanying mean-field theory (MFT) calculation also reveals the existence of quantum phase transition, although at a smaller critical coupling strength than found in DQMC.


*This work was supported by the Department of Energy, grant DE-SC0014671.

The effect of disorder on the phase diagrams of hard-core lattice bosons with cavity-mediated long-range and nearest-neighbor interactions

We use quantum Monte Carlo simulations with the worm algorithm to study the phase diagram of a two-dimensional Bose-Hubbard model with cavity-mediated long-range interactions and uncorrelated disorder in the hard-core limit. Our study shows the system is in a supersolid phase at weak disorder and a disordered solid phase at stronger disorder. Due to long-range interactions, a large region of metastable states exists in both clean and disordered systems. By comparing the phase diagrams for both clean and disordered systems, we find that disorder suppresses metastable states and superfluidity. We compare these results with the phase diagram of the extended Bose-Hubbard model with nearest-neighbor interactions. Here, the supersolid phase does not exist even at weak disorder. We identify two kinds of glassy phases: a Bose glass phase and a disordered solid phase. The glassy phases intervene between the density-wave and superfluid phases as the Griffiths phase of the Bose-Hubbard model. The disordered solid phase intervenes between the density-wave and Bose glass phases since both have a finite structure factor.
8:00AM R41.00001: Magnetic textures with particle properties beyond skyrmions: chiral bobbers, globules, and hopfions [Invited]  NIKOLAI S. KISELEV (Presenter), Institute for Advanced Simulation, Forschungszentrum Julich GmbH — Magnetic crystals with competing interactions allow the existence of localized magnetic textures possessing a lot of similarities to ordinary particles meaning that they can move and interact with each other: attract, repel, or mutually annihilate. In my presentation, I discuss a wide variety of different types of such textures existing in magnetic crystals.

First, I will discuss the chiral magnets where the competition between the Heisenberg exchange and the Dzyaloshinsky-Moriya interactions leads to the emergence of magnetic skyrmions (Sk). Recently we have shown that besides ordinary Sk [1], the micromagnetic functional for chiral magnets admits an infinite number of solutions with different topological charges, energies, static, and dynamical properties [2].

We have shown theoretically [3] and experimentally [4] that in 3D crystals of isotropic chiral magnets besides Sk tubes (SkTs) penetrating through the whole sample, there are also other types of solutions, so-called hybrid solitons (HSs) [3]. HSs are topologically trivial objects, which can be thought of as a SkT with one end – chiral bobber [3,4] or two ends – magnetic globule [5], where the ends are magnetic singularities – Bloch points.

In the final part, I will discuss true 3D to topological magnetic solitons or magnetic hopfions [6,7]. The magnetic hopfions can be thought of as SkTs with closed ends. Such closed tubes, in general, have the shape of complex mathematical knots. I present the micromagnetic functional [8] and magnetic interactions allowing the stability of these objects and discuss the static and dynamic properties of these objects.

**8:36AM R41.00002: Magnetic structures in 1D spin chains with long-range RKKY and Dzyaloshinskii-Moriya interactions**  
EDSON VERNEK (Presenter), OSCAR AVALOS-OVANDO, SERGIO E ULLOA, Physics and Astronomy, Ohio University — Magnetic order in 1D magnetic chains has gained considerable interest in recent years. Absent in one dimensional systems with only short-range interaction (SRI), magnetic order is still possible if long-range interaction (LRI) is present, without violating the celebrated Mermin-Wagner theorem. Indeed, interesting quantum phase transitions have been investigated in a Heisenberg chain with LRI [1]. We investigate the role of spin-orbit effects by considering spin-1/2 chains in the presence of both RKKY and Dzyaloshinskii-Moriya (DM) LRIs. Our results show an interestingly rich phase diagram in which the system transitions from collinear to transverse magnetic correlated order as the ratio between RKKY and DM coupling strength changes. We analyze the new ground states and explore their possible physical implementation in different systems.


**8:48AM R41.00003: Magnetic field induced spin liquids and quantum phase transitions in spin orbit coupled quantum magnets.**  
MINSEONG LEE (Presenter), VIVIEN ZAPF, Los Alamos National Laboratory, HAIDONG ZHOU, Physics and Astronomy, University of Tennessee — When an external magnetic field suppressed the magnetic ordering in spin-orbit coupled system, a new magnetic phase is often observed. For example, controversial theoretical and experimental results propose spin liquid behavior above in-plane 7 T where antiferromagnetic order is suppressed in a-RuCl3. Theoretical studies also show that out-of-plane magnetic field can induce spin liquid phase in this system as well. In this work, we present the analysis of inelastic neutron scattering data of a-RuCl3 and extracted g-factor and the $\Gamma/J$ using linear spin wave theory. In addition, we present the out-of-plane pulsed field data of a-RuCl3 to study a new phases predicted by theoretical studies by drawing the full field vs temperature phase diagram. We also explore the how the magnetic field breaks the orbital assisted spin dimerized phase in one dimensional spin chains, and new magnetic phases are induced to discuss the role of the orbital degrees of freedom in rescale the Hund coupling and on-site interorbital Coulomb interactions in spin-orbit coupled systems.
9:00AM R41.00004: Exchange Coupling Torque in Ferrimagnetic Bi-layer Systems at the Angular Momentum Compensation Temperature*  
ROBIN BLÄSING (Presenter), TIANPING MA, Max Planck Institute of Microstructure Physics, SEE-HUN YANG, CHIRAG GARG, IBM Almaden Res Ctr, STUART PARKIN, Max Planck Institute of Microstructure Physics — Within the last decade, the efficiency of current-induced motion of magnetic domain walls (DWs) has been enhanced tremendously by utilizing the exchange coupling torque (ECT) in synthetic antiferromagnets. In this talk we show that this mechanism also applies to ferrimagnetic layers consisting of a transition metal layer and a rare earth metal layer which couple antiferromagnetically. The motion is most efficient when the angular momenta of both layers compensate each other and the ECT is maximized. Additionally, we demonstrate that at angular momentum compensation a magnetic field, which is applied along the effective Dzyaloshinskii-Moriya interaction field, has no influence on the DW velocity. By changing the temperature of a Co/Gd ferrimagnetic bi-layer, we can to tune the ratio of angular momenta of Co and Gd and identify the angular momentum compensation temperature $T_A$. Since the device temperature is significantly increased by the current pulses, taking into account Joule heating is of major importance. The presented findings can be used for the development of novel storage devices and improving their efficiency.

*This work was funded by the European Research Council under the European Union's Horizon 2020 research and innovation programme (grant agreement No 670166).

9:12AM R41.00005: Spontaneous rotation of ferrimagnetism driven by antiferromagnetic spin canting*  
ANURADHA VIBHAKAR (Presenter), University of Oxford, DMITRY KHALYAVIN, PASCAL MANUEL, ISIS facility, Rutherford Appleton Laboratory, ALEXEI BELIK, National Institute for Materials Science, ROGER JOHNSON, University College London — Spin-reorientation phase transitions that involve the rotation of a crystal's magnetisation have been well characterised in distorted perovskite oxides such as the orthoferrites. In these systems spin reorientation occurs due to competing rare earth and transition metal anisotropies coupled via $f - d$ exchange. Here, we demonstrate an alternative paradigm for spin reorientation in distorted perovskites. We show that the $R_2CuMnMn_4O_{12}$ ($R = Y$ or Dy) triple A-site columnar ordered quadruple perovskites have three ordered magnetic phases and up to two spin reorientation phase transitions. Unlike the spin reorientation phenomena in other distorted perovskites, these transitions are independent of rare earth magnetism, but are instead driven by an instability towards AFM spin canting originating in frustrated Heisenberg exchange interactions, and the competition between Dzyaloshinskii-Moriya and single-ion anisotropies.

*We acknowledge financial support from the Royal Society, EPSRC Grant No. EP/M020517/1, entitled Oxford Quantum Materials Platform Grant, JSPS KAKENHI Grant No. JP16H04501, a research grant from Nippon Sheet Glass Foundation for Materials Science and Engineering, and Innovative Science and Technology Initiative for Security, ATLA, Japan.
9:24AM R41.00006: Using structural phase transitions to enhance the coercivity of ferromagnetic films  
RYAN NEED (Presenter), Materials Science and Engineering, University of Florida, JOSHUA P LAUZIER, LOGAN SUTTON, Physics, Colorado State University, BRIAN JAMES KIRBY, National Institute of Standards and Technology, JOSE DE LA VENTA, Physics, Colorado State University — Heat-assisted magnetic recording (HAMR) is a promising magnetic information storage technology that uses a heating step to lower the coercivity of the recording media and decrease the energy of each writing operation. However, HAMR currently requires temperature increases of several hundred Kelvin, which can cause heat spreading and limit recording rates. Here, we describe a mechanism for tuning the coercivity of ferromagnetic films over small temperature ranges by coupling them to a layer that undergoes a structural phase transition. The method is demonstrated in Ni/FeRh bilayers where Ni layers were deposited either above or below the FeRh metamagnetic transition at 370 K. When the Ni layer is grown at high temperatures, the 1% FeRh lattice expansion alters the Ni’s crystallographic texture and leads to a 500% increase in coercivity upon cooling through the FeRh’s metamagnetic transition. Analysis suggests this effect is due to domain wall pinning across grain boundaries with different orientations and strain states. Our work highlights a means to increase the thermal coercivity response of ferromagnetic materials through structural coupling to underlying films, which could enable simplified heatsink designs and expand the selection of materials compatible with HAMR.

9:36AM R41.00007: Parity-Time Symmetric Spintronics and Spin Cavitronics*  
YUNSHAN CAO, HUANHUAN YANG, CHEN WANG, TIANLIN YU (Presenter), PENG YAN, University of Electronic Science and Technology of China — Non-Hermitian Hamiltonian obeying parity-time (PT) symmetry can exhibit real spectra and a spontaneous symmetry breaking accompanied by a real-to-complex spectral phase transition at the ‘exceptional point (EP)’. Here, we predict that a ferromagnet with gain (loss) is equivalent to an antiferromagnet with an equal amount of loss (gain), and show a ferromagnet to antiferromagnet phase transition in PT-symmetric magnetic bilayers when the balanced gain-loss parameter exceeds a critical value. We then generate the idea to a spin cavitronic device that allows the strong coupling between photons and magnons. We demonstrate a “Z”-shape transmission spectrum in the exact PT phase. The spectrum evolves to a step function when the polariton touches the third-order exceptional point. The estimated magnetic sensitivity can approach $10^{-15}$ T Hz$^{-1/2}$ around the third-order EP. Our work paves the way for investigating the parity-time symmetry in spintronics and spin cavitronics, and for designing ultrasensitive magnetometers.

* This work was supported by the National Natural Science Foundation of China (Grants No. 11704060 and No.11604041).
9:48AM R41.00008: Ultrafast Control of Charge Density and Spin Density waves in Chromium   LOUIS PONET (Presenter), Istituto Italiano di Tecnologia, OLEG GOROBTSOV, ANDREJ SINGER, Cornell University, SERGEY ARTYUKHIN, Istituto Italiano di Tecnologia — Experimental advances in ultrafast physics have allowed to monitor structural and electronic processes and even phase transitions on their natural timescales. Here we model recent experiments on ultrafast control of spin density wave phase in elemental Chromium with a sequence of optical pulses. The strain wave and CDW, induced by the spin density modulation via exchange striction, are monitored using x-ray diffraction. Results show order parameter oscillations and a partial melting of the SDW in response to optical pulses. Interestingly, depending on the exact delay between two sequential optical pulses, one can increase or decrease the oscillation amplitude, allowing for optimal control. We use Landau theory and heat transfer equations to describe the dynamics of the interacting charge and spin density waves. All details of the experiment are replicated to a high degree by the model.

10:00AM R41.00009: Realizing corner states in artificial crystals based on topological spin textures*   PENG YAN (Presenter), ZHIXIONG LI, YUNSHAN CAO, University of Electronic Science and Technology of China, XIANG RONG WANG, Physics, The Hong Kong University of Science and Technology — The recent discovery of higher-order topological insulators (HOTIs) has significantly extended our understanding of topological phases of matter. Here, we predict that second-order corner states can emerge in the dipolar-coupled dynamics of topological spin textures in two-dimensional artificial crystals. Taking a breathing honeycomb lattice of magnetic vortices as an example, we derive the full phase diagram of collective vortex gyrations and identify three types of corner states that have not been discovered before. We show that the topological "zero-energy" corner modes are protected by a generalized chiral symmetry in the sexpartite lattice, leading to particular robustness against disorder and defects, although the conventional chiral symmetry of bipartite lattices is absent. We propose the use of the quantized Z_6 Berry phase to characterize the nontrivial topology. Full micromagnetic simulations confirm the theoretical predictions with good agreement. Our findings open up a promising route for realizing higher-order topologically protected corner states in magnetic systems and finally achieving topological spintronic memory and computing.

*National Natural Science Foundation of China (NSFC) (Grants No. 11604041, 11704060, and 11904048)
10:12AM R41.00010: 3D Topological solitons in chiral magnets  ROBERT VOINESCU (Presenter), IVAN I SMALYUKH, JUNG-SHEN TAI, University of Colorado, Boulder — Three dimensional knotted solitons are continuous field configurations classified by a Hopf topological invariant. These quasi-particles are known to arise in many laboratory systems and more exotic settings ranging from theories in particle physics to cosmology. By exploiting the external magnetic field and crystalline anisotropy couplings in a micromagnetic hamiltonian we numerically model a new class of 3D topological solitons embedded in a helical background. We determine the parameter region of stability afforded by the non-trivial twisting and windings present in our particle-like excitation. Furthermore, we analyze individual topological solitons and an ensemble of such in the bulk with multiparticle simulations to determine their interaction and self-assembly properties. Finally, we discuss how such topological excitations may find uses in racetrack magnetic memory devices and spintronics applications.

10:24AM R41.00011: Unprecedented Electronic Structure, Magnetism, and Anisotropy in Rare Earth Intermetallics  DURGA PAUDYAL (Presenter), RENU CHOUDHARY, Ames Lab, RALPH SKOMSKI, University of Nebraska — We investigate magnetic rare earth intermetallics with quantum properties. Many quantum features of rare earth intermetallics are consistent with the past research, but some of the findings are seemingly contradictory. The disagreement is not caused by numerical errors or accidental mistakes but reflects how the many-electron nature of the rare-earth 4f electrons is interpreted by crystal-field and local spin density approximation with onsite electron correlation and spin orbit coupling theories [Das et. al, PRB 100, 024419 (2019)]. The two-sublattice crystal-field theory describes a broad variety of physical properties exhibited by rare earth transition metals, such as the temperature dependence of magnetization and anisotropy, but it is not a first-principles approach. By contrast, our first-principles approach yields a substantial orbital-moment quenching, which violates Hund's rules and is contradictory to conventional knowledge accumulated over decades of rare-earth research. Rationalizing the orbital-moment quenching in terms of the dependence of the 4f charge distribution on the magnetization angle, we argue that medium- and long-run future research will be necessary to reconcile experiment, sublattice models, and first-principle calculations in rare earth intermetallics.
10:36AM R41.00012: Nanoscale Spatial Dependence of Photoinduced Structural Phase Transition in FeRh*  YOUNGJUN AHN (Presenter), Department of Materials Science and Engineering, University of Wisconsin - Madison, MATHEW J. CHERUKARA, Center for Nanoscale Materials, Argonne National Laboratory, ZHONGHOU CAI, DONALD A WALKO, Advanced Photon Source, Argonne National Laboratory, MICHAEL BARTLEIN, TAO ZHOU, Center for Nanoscale Materials, Argonne National Laboratory, JAN-ULRICH THIELE, Seagate Technology, ERIC FULLERTON, Center for Magnetic Recording Research, University of California at San Diego, MARTIN HOLT, Center for Nanoscale Materials, Argonne National Laboratory, PAUL G. EVANS, Department of Materials Science and Engineering, University of Wisconsin - Madison, HAIDAN WEN, Advanced Photon Source, Argonne National Laboratory — Simultaneous temporal and spatial characterization of materials with high resolution provides multidimensional data essential for a deeper understanding of nanoscale heterogeneities that arise from complex interactions during solid-solid phase transitions. Time-resolved hard x-ray microscopy has unique capabilities to provide a direct structural probe. Here, using newly developed x-ray diffraction microscopy with unprecedented 100 ps and 30 nm resolution at the Advanced Photon Source, we have observed the nanoscale dependence of the structural relaxation dynamics following ultrafast laser excitation of an FeRh thin film. The spatial dependence is linked to variations in spatially inhomogeneous strain, resulting in different thresholds for driving the antiferromagnetic-ferromagnetic phase transition. In addition, we have found the spatially different degree of the broadening of transition in temperature near nano-island regions. The observed relationship between lattice parameter and transition threshold gives new insight on the photoinduced phase transition at the nanoscale and has important implications in heat-assisted magnetic recording.

*This work is supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:48AM R41.00013: Electric-field control of the interlayer exchange coupling*  SHEHRIN SAYED (Presenter), CHENG-HSIANG HSU, NIKLAS ROSCHEWSKY, EECS, University of California, Berkeley, SEE-HUN YANG, IBM Research, Almaden, SAYEEF SALAHUDDIN, EECS, University of California, Berkeley — Magnetization switching with electric-field is of great current interest to achieve high density and low energy non-volatile memory devices. We propose a new mechanism for electric-field controlled magnetization switching, assisted solely by the interlayer exchange coupling (IEC) between the fixed and the free magnets. Using non-equilibrium Green's function (NEGF) method, we show that the resonant tunneling mechanism can tune the IEC with an electric-field, which in turn can switch the free magnet to have either a parallel or antiparallel configuration with respect to the fixed magnet, depending on the sign of the IEC. Such bi-directional switching can be achieved with the same voltage polarity but different magnitudes. Due to the 'conservative' nature of the exerted torque by IEC, the switching threshold is decoupled from the speed, while the conventional spin-torque devices exhibit a trade-off due to the 'non-conservative' nature of the exerted torque.

*This work was in part supported by ASCENT, one of six centers in JUMP, a SRC program sponsored by DARPA and in part by the Center for Energy Efficient Electronics Science (E3S), NSF Award 0939514.
8:00AM R42.00001: Manipulation of magnetic coupling and magnon transport in magnetic insulator-ferromagnetic metal hybrid structures [Invited]  YABIN FAN (Presenter), Massachusetts Institute of Technology MIT, PATRICK QUARTERMAN, National Institute of Standards and Technology, JOSEPH FINLEY, Massachusetts Institute of Technology MIT, ALEXANDER GRUTTER, National Institute of Standards and Technology, LUQIAO LIU, Massachusetts Institute of Technology MIT — Magnetic insulators and ferromagnetic metals are widely used in spintronic structures for the generation of magnon spin current, control of magnetization states, and for detecting magnon spins. Most of the previous spintronic structures are based primarily on either magnetic insulators or ferromagnetic metals, and the heterostructures that integrate both have not been fully explored while they may exhibit new magnetic coupling and magnon transport properties. Here, we introduce a Pt/yttrium iron garnet (YIG)/permalloy(Py) hybrid structure grown on Si substrate, where YIG is a ferrimagnetic insulator and Py is a ferromagnetic metal. Surprisingly, the YIG and the Py layers show antiferromagnetic coupling when external field is small, and the two layers align to the same direction only when in-plane field is large enough, as evidenced by both vibrating-sample magnetometry and polarized neutron reflectometry measurements. More importantly, the parallel and antiparallel magnetization configurations in this YIG/Py structure could be utilized to control magnon spin current in spin-pumping and spin Seebeck experiments. With easy access to grow by magnetron sputtering, fully controllable magnetization configuration, and efficient control of magnon spin current, the Pt/YIG/Py hybrid structure could potentially find applications in spin logic devices that are fabricated on a Si chip.
8:36AM R42.00002: Xe-PFIB microstructuring of Yttrium Iron Garnet films for quantum magnonic applications  DMYTRO BOZHKO (Presenter), Department of Physics, University of Colorado at Colorado Springs, PAUL BAITY, SERGEY DANILIN, RAIR MACEDO, VALENTINO SEFERAI, UMBERTO NASTI, ALESSANDRO CASABURI, James Watt School of Engineering, University of Glasgow, WILLIAM SMITH, STEPHEN MCVITIE, School of Physics and Astronomy, University of Glasgow, ROBERT HADFIELD, MARTIN WEIDES, James Watt School of Engineering, University of Glasgow — Recently, the growing interest in quantum magnonics triggered intensive investigation of magnetic materials in the quantum limit. One of the main challenges in this area is to achieve long magnon lifetimes at cryogenic temperatures. Among all currently known magnetic materials, single-crystal Yttrium Iron Garnet (YIG, Y₃Fe₅O₁₂) possesses the lowest damping due to low spin-orbit coupling. Thin YIG films are, however, grown on GGG (Gd₃Ga₅O₁₂) substrates, which induce high magnetic damping at low temperatures [1]. Here we report on using Xenon Plasma Focused Ion Beam (Xe-PFIB) technique to prepare high-quality microstructured YIG films detached from GGG substrates. This technique allows production of relatively large (50 x 50 x 20 µm³) structures in a reasonable time of a few hours. The magnetic properties of these samples were evaluated using broadband ferromagnetic resonance spectroscopy in a wide temperature range (down to 80mK). Additional investigations were done by means of wavevector-resolved Brillouin light scattering spectroscopy. Through these techniques, we evaluate the effects of Xe-PFIB structuring on the magnetic damping. We believe that our findings will pave the way to efficient implementation of YIG elements into hybrid quantum circuits.

8:48AM R42.00003: Py-Cu Graded-Index Magnonic Waveguides*  KRISTEN REPA (Presenter), CELIA MERCOVICH, CASEY MILLER, Rochester Institute of Technology — Spin waves (magnons) have many optical analogies, including the law of reflection, which allows total internal reflection (akin to a fiber optic cable). For this reason, we’re working to create a magnonic waveguide made from Py-Cu multilayered films. We grow films via sputter deposition with a 10 nm core of Py₀.₈Cu₀.₂ that is symmetrically bound by 10 nm of Cu and 10 nm of Py₀.₆Cu₀.₄. Py-Cu alloys are attractive for this study because we can easily tune magnetic properties by changing the Cu content of each layer (Tₐ decreases as Cu content increases). We measure samples using ferromagnetic resonance (FMR) with frequencies from 3-20 GHz and fit results to the Kittel equation. We extract values for the Gilbert damping parameter and inhomogeneous broadening, which informs us of how magnons propagate through each multilayer film. Ideally, if we reverse the magnetic layers, instead of seeing total internal reflection, we should observe a complete spin absorber.

*This work is supported by NSF Grant #1609066
Non-linear spin torque, pumping and cooling in superconductor/ferromagnet systems

RISTO OJAJÄRVI (Presenter), Department of Physics and Nanoscience Center, University of Jyväskylä, JUUSO MANNINEN, Department of Applied Physics, Low Temperature Laboratory, Aalto University, PAULI VIRTANEN, TERO T HEIKKILÄ, Department of Physics and Nanoscience Center, University of Jyväskylä — We study the effects of the coupling between magnetization dynamics and the electronic degrees of freedom in a heterostructure of a metallic nanomagnet with dynamic magnetization coupled with a superconductor containing a steady spin-splitting field. We predict how this system exhibits a non-linear spin torque, which can be driven either with a temperature difference or a voltage across the interface. We generalize this notion to arbitrary magnetization precession by deriving a Keldysh action for the interface, describing the coupled charge, heat and spin transport in the presence of a precessing magnetization. We characterize the effect of superconductivity on the precession damping and the anti-damping torques. We also predict the full non-linear characteristic of the Onsager counterparts of the torque, showing up via pumped charge and heat currents. For the latter, we predict a spin-pumping cooling effect, where the magnetization dynamics can cool either the nanomagnet or the superconductor.

This work was supported by the Academy of Finland project number 317118, the European Union Horizon 2020 research and innovation programme under grant agreement No.~800923 (SUPERTED), and Jenny and Antti Wihuri Foundation.

Acoustic Ferromagnetic Resonance Assisted Spin-Torque Switching of Perpendicular MTJs

WALID AL MISBA (Presenter), MD MAHADI RAJIB, DHRITIMAN BHATTACHARYA, JAYASIMHA ATULASIMHA, Virginia Commonwealth Univ — Resonant Surface Acoustic Wave (SAW) assisted Spin Transfer Torque (STT) can drive the magnetization of a perpendicular magnetic tunnel junction (p-MTJ) and write bits with an order of magnitude lower energy dissipation compared to the conventional STT current approach [1]. Simulations show that such acoustically driven ferromagnetic resonance (FMR) results in the magnetization precessing in a cone with large deflections relative to the perpendicular direction. The larger the precession angle, the lower the STT current required for switching the magnetization. While our prior simulations [1] of such magnetization dynamics were based on macro-spin assumptions, here we will perform micromagnetic simulations to study incoherent switching in the presence of room temperature thermal noise as well as incorporate realistic effects such as material inhomogeneity, grains, surface roughness and lithographic imperfections. The ramification of such incoherency in magnetization dynamics on the switching error will be discussed. Preliminary experimental work will also be presented.

Reference:

NSF SHF Small Grant No. #CCF-1815033
9:24AM R42.00006: Transport and Magnetic Properties of Amorphous Fe:Dy Oxide Films.
SARA BEY (Presenter), OLIVIA DENTON, TATIANA ALLEN, Univ of Tennessee, Chattanooga, KRISHNA KOIRALA, University of Tennessee, WILLIAM ROES, Tennessee Valley Association, GERD DUSCHER, RAMKI KALYANARAMAN, University of Tennessee — Novel amorphous FeDy-Oxide thin films, deposited by e-beam evaporation, show room-temperature magnetism, as well as high electrical conductivity, carrier mobility, and optical transparency that is very promising for a multitude of applications. We have systematically studied transport, optical and magnetic properties of a large set of films deposited on Quartz and SiO2/Si substrates at different oxygen partial pressures [10-6,10-8,10-9 Torr]. Atomic ratios of Fe to Dy in the films (confirmed by EDS) varied from 0.3 to 6, but all samples had resistivity less than 2.5E-03 Ohm*cm. Optical bandgap of as prepared films was 2.4±0.1 eV. The films showed high ordinary Hall mobility (~10 cm2/V-s) which is among the highest for amorphous oxides, as well as anomalous Hall mobility (~102 cm2/V-s). At low temperatures there was two step magnetization that suggests coexistence of two magnetic phases below H=0.08 T and ferromagnetic phase at higher fields. Select films were taken through cyclic annealing (300-700K) which, after 3 cycles, resulted in still amorphous, thermally stable homogeneous FeDyO material. These results will motivate further investigation into the fundamental mechanisms responsible for these properties and how they might be tuned for integration in devices.

9:36AM R42.00007: Nonlinear Optical Imaging of Current Induced Spin Switching in Antiferromagnetic Materials* JOONGWON LEE (Presenter), YONGJIAN TANG, ANTONIO B MEI, OKAN KOKSAL, DARRELL SCHLOM, DANIEL RALPH, FARHAN RANA, Cornell University — Electrical switching of the Neel order in Antiferromagnetic (AF) materials via spin transfer (STT) has attracted considerable attention [1,2]. Experiments have shown that AF switching is non-uniform, influenced by magneto-elastic coupling, and the efficacy of STT in inducing AF switching has also been questioned [3]. In this paper, we show that scanning optical second harmonic generation (SHG) can be used to image and identify magnetic domains in inversion symmetric AF materials. Using this technique, we image magnetic domains in nanometer thick epitaxial AF layers. We show that the SHG technique can image even when AF materials are covered with metallic spin Hall layers such as Pt. We use scanning SHG to study electrical switching in NiO/Pt devices. Our results show that AF switching is non-uniform across our 100 sq-micron devices. We observe regions that show AF switching in agreement with the STT predictions and regions where magnetoelastic effects seem to dominate, and we also see regions which exhibit no evidence of switching. The contributions of various effects will be discussed. [1] Phys. Rev. Lett. 120, 207204 (2018). [2] Scientific Reports 8, 14167 (2018). [3] arXiv:1907.00314 (2019).

*The research was funded by NSF DMR-1120296.
AURELIEN MANCHON (Presenter), Physics Department, Aix-Marseille University, SUMIT GHOSH, ADEL ABBOUT, GUILHEM MANCHON, AHEMD HAJIR, ABDULKARIM HARIRI, King Abdullah Univ of Sci & Tech (KAUST) — Magnetic materials lacking inversion symmetry constitute a unique platform for the exploration and control of magnetism [1]. In these systems, typically multilayers of transition metal ferromagnets and heavy metals (W, Pt, Bi$_2$Se$_3$ etc.), interfacial spin-orbit coupling promotes a wealth of physical phenomena, among which the emergence of magnetic skyrmions – topological magnetic textures –, spin-orbit torques– an efficient means to electrically control magnetization dynamics –, as well as chiral magnetic damping – energy dissipation that depends on the texture chirality. While most of the initial theoretical progress has been achieved using minimal models (e.g., the Rashba two-dimensional gas), we have recently developed a multiorbital tight-binding model of such heterostructures that enables us to model these various phenomena on equal footing and in a transparent manner [2,3]. Based on the results of this model, I will address various aspects of the interplay between spin transport and magnetism mediated by spin-orbit coupling. I will first discuss the orbital nature of interfacial spin-orbit coupling in multilayers and examine how it facilitates the onset of chiral magnetic textures. I will then present the physics of spin-orbit torques, and inspect their relation to chiral magnetic properties such as Dzyaloshinskii-Moriya interaction and chiral magnetic damping. Finally, I will discuss the current-driven dynamics of magnetic skyrmions and propose various strategies to enhance their mobility, exploiting topological spin currents flowing through the texture [4].


*AM acknowledges support from King Abdullah University of Science and Technology and AMIDEX foundation at Aix-Marseille University.
Magnetotransport properties of granular oxide-segregated CoPtCr films for applications in future magnetic memory technology*  

MORGAN WILLIAMSON, MAXIM TSOI (Presenter), University of Texas at Austin, PIN-WEI HUANG, GANPING A JU, CHENG CW WANG, Fremont Research Center, Seagate Technology — Magnetotransport properties of granular oxide-segregated CoPtCr films were studied on both macroscopic and microscopic length scales by performing bulk and point-contact magnetoresistance measurements, respectively. Such a perpendicular magnetic medium is used in state-of-the-art hard disc drives and if combined with magnetoresistive phenomena (for read/write operations) may lead to a novel concept for magnetic recording with high areal density. While the bulk measurements on the films showed only small variations in dc resistance as a function of applied magnetic field (magnetoresistance of less than 0.02 %), the point-contact measurements revealed giant-magnetoresistance-like changes in resistance with up to 50,000 % ratios. The observed magnetoresistive effect could be attributed to a tunnel magnetoresistance between CoPtCr grains with different coercivity. The tunneling picture of electronic transport in our granular medium was confirmed by the observation of tunneling-like current-voltage characteristics and bias dependence of magnetoresistance; both the point-contact resistance and magnetoresistance were found to decrease with the applied dc bias.

*This work was supported in part by SRA No. UTA18-000691 between the University of Texas at Austin and Seagate Technology.

The spontaneous electrical and spin Hall effect in a collinear antiferromagnet*  

GEN YIN (Presenter), Department of Electrical and Computer Engineering, University of California, Los Angeles, JIE-XIANG YU, Department of Physics, University of Florida, ROGER LAKE, Department of Electrical and Computer Engineering, University of California, Riverside, JIADONG ZANG, Department of Physics and Astronomy, University of New Hampshire, KANG L. WANG, Department of Electrical and Computer Engineering, University of California, Los Angeles — In collinear antiferromagnets, since the combined operation of time reversal and a half-unit-cell translation is symmetric for the magnetic lattice, a spontaneous Hall effect is usually absent. Here, we show that in a collinear antiferromagnet, MnTe, the non-magnetic atomic structure breaks such symmetry, therefore allows a spontaneous Hall effect, which is known as planar Hall effect. Such spontaneous Hall effect does not result from the intrinsic Berry curvature. Instead, it comes from the extrinsic scattering centers with either positive or negative polarized spins along the easy axis of the Neel vector. This behavior is intriguing since it is by now the most convenient method to read-out (and potentially to write) the information encoded in antiferromagnets for high-speed device applications. Such zero-field planar Hall effect has already been observed in experiments. Our calculation shows that the spontaneous Hall effect and spin Hall effect can be up to 30%, suggesting a vast space to improve the performance for device applications.

*This work is supported by (1) Spins and Heat in Nanoscale Electronic Systems, an EFRC funded by the U.S. DOE, Office of Science, Basic Energy Sciences (No. SC0012670); (2) NSF (DMR-1411085), and (3) the ARO contract No. W911NF-15-1-10561
8:00AM R43.00001: Creating Novel Magnetic Compounds with Complementary Experimental and Computational Methods* [Invited] BALAMURUGAN BALASUBRAMANIAN, DAVID SELLMYER (Presenter), Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska — New materials discovery has governed the development of science and technology for decades. In particular, the search for new magnetic compounds is important to satisfy ever-increasing demand for magnets with a wide range of applications including spintronics, data storage, hybrid vehicles, and wind turbines. This requires efficient computational and experimental approaches for high throughput and efficiency [1]. When increasingly powerful computational techniques are combined with special fabrication methods far from equilibrium, the search also can uncover new metastable magnetic compounds [2-6]. This talk will focus on the development of novel magnetic compounds with high magnetocrystalline anisotropy, magnetization, and Curie temperature by combining experiments, an adaptive genetic algorithm search, and electronic-structure calculations. Magnetism of novel compounds such as Fe$_{3+x}$Co$_{3-x}$Ti$_2$, Co$_3$N, Fe$_2$CoC, and Co$_3$Si will be discussed in terms of intrinsic atomic-scale and extrinsic nanoscale effects. This research is done in collaboration with D.J. Sellmyer, C.Z. Wang, K.M. Ho, X. Xu, and J. R. Chelikowsky.

References

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8:36AM R43.00002: A high throughput workflow for magnetic ferroelectrics from first-principles

STEPHANIE MACK (Presenter), University of California, Berkeley, TESS E SMIDT, SINÉAD GRIFFIN, JEFFREY B NEATON, Lawrence Berkeley National Laboratory — Multiferroics, which combine ferroelectricity and magnetism, are of great interest for a variety of electronics applications. Although discovery of new multiferroics based on chemically manipulating known structural motifs has yielded new candidates, there are still relatively few known multiferroics with highly tunable electric and magnetic orders at room temperature. Using symmetry constraints based on Landau theory of phase transitions, and on the identification of both a polar and nonpolar reference structure, and first-principles density functional theory calculations using the Materials Project database, we develop a high throughput workflow to predict the ground state magnetic ordering and spontaneous polarization of new multiferroic candidate materials. Comparison to known multiferroics will be discussed, and we will classify the most promising candidate materials to aid future synthesis efforts. This work is supported by the Department of Energy through the Materials Project FWP at Berkeley Lab. Computational resources provided by NERSC.

8:48AM R43.00003: Generating a database of predicted ground-state magnetic orderings of inorganic crystalline materials suitable for high-throughput screening applications

MATTHEW HORTON (Presenter), KRISTIN PERSSON, Lawrence Berkeley National Laboratory — Bridging the gap from toy model to synthesizable material and ultimately to working device is of crucial importance when investigating exotic magnetic phenomena. Since 2011, The Materials Project has offered an open-access database of inorganic crystalline materials and their associated properties as calculated by Density Functional Theory. However, to date, the magnetic ordering of these materials has not been explored in a systematic way.

We have developed a workflow suitable for high-throughput use, benchmarked to experiment, to predict the ground-state magnetic ordering for ferromagnetic, antiferromagnetic and ferrimagnetic materials with collinear spin even in the case of multiple magnetic sub-lattices and complex orderings[1]. This workflow has been applied to create a large database of predicted ground states for transition metal oxides which can be searched across a variety of axes including magnetic lattice type.

We share an example of screening this database for discovery of new materials for magnetocaloric applications.

TANUSRI SAHA-DASGUPTA (Presenter), ANITA HALDER, S N Bose Natl Ctr Basic Sci, AISHWARYO GHOSH, Presidency University — In the present study, we use a combination of computational tools; machine learning technique for screening of stable candidates, evolutionary algorithm for crystal structure determination, and first-principles calculations for characterization of electronic and magnetic states, to make predictions on a set of new magnetic double-perovskites of composition $A_2BB'O_6$. Out of 412 scanned candidates composition with 3$d$ and 4$d$ or 5$d$ transition metals at B and B' sites, 33 compounds are found to form in stable double-perovskite structure, 25 of which are further considered for characterization of their crystal structure and properties. This exercise provides 21 new double-perovskites of varying magnetic and electronic properties, which range from ferromagnetic half-metals to ferri- and antiferro-magnetic insulators to ferromagnetic metals and rare example of antiferromagnetic metals. Our computational study is expected to help in discovering new magnetic double perovskites.

*The authors acknowledge funding from Department of Science and Technology, India.
Defects and impurities play an important role in determining the properties of materials and must be carefully considered as part of materials design and synthesis. This applies to semiconductors and materials used for energy generation and storage. Defects can act as electron donors or acceptors, implying that their concentrations can be tuned by introducing oppositely charged species. These dopants must be carefully chosen to avoid undesirable side effects, such as autocompensation or, in the case of ionic conductors, high mobile carrier binding energies.

We discuss how first-principles calculations can address these considerations for two promising solid-state hydrogen electrolyte materials. The alkaline-earth zirconates (AeZrO$_3$; Ae = Sr, Ca, Ba) are solid-state hydrogen conductors in which protons move interstitially. Oxygen vacancies, which act as donors, act as precursors to proton incorporation. To maximize oxygen vacancy concentrations, acceptor dopants are introduced. We identify the alkali metal dopants that are most ideal for incorporating oxygen vacancies, while avoiding harmful compensation effects.\(^1\) The alkaline-earth hydrides (AeH$_2$) conduct hydrogen via a vacancy-mediated mechanism. Optimizing the vacancy concentration again requires the introduction of acceptor dopants, and alkali metal dopants are most effective to this end. We estimate an increase in ionic conductivity by roughly two orders of magnitude in the case of BaH$_2$ doped with potassium.\(^2\) We discuss implications of our results for studies of other novel hydrogen-conducting materials and, in general, how to use defect engineering to optimize material performance.


*Work performed in collaboration with Leigh Weston and Chris G. Van de Walle and supported by DOE and NSF.
9:48AM R43.00006: Atomistic Kinematics of Carbon Diffusion and Clustering in BCC Fe with Point Defects*  
TIEN QUANG NGUYEN (Presenter), Institute for NanoScience Design, Osaka University, 
KAZUNORI SATO, Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, 
YOJI SHIBUTANI, Division of Mechanical Engineering, Graduate School of Engineering, Osaka University — Carbon diffusion and clustering in iron are important phenomena as they closely link to processes of production of steels such as cementite formation, phase transition, and so on. Here, we studied these phenomena using multi-scale approach. First, the stability of carbon and its interaction with point defect were examined via total energy optimization using our own newly developed Fe-C potential. Then, the diffusion mechanisms for carbon interstitials were analyzed. By using kinetic Monte Carlo (kMC) simulations, diffusion coefficients of carbon depending on temperature were estimated to clarify the influence of vacancy on the diffusion and clustering processes. We found that in perfect lattice, carbon atoms tend to form stable C-C pairs, while the presence of vacancies leads to the formation of larger vacancy-carbon (VC_n) clusters with VC_2 as the most stable structure. In addition, due to the presence of vacancies, the diffusion paths of carbon are strongly modified. The kMC simulations show that diffusion coefficient is decreased as vacancy content increases. Therefore, it is suggested that vacancies may play an important role in the clustering process of carbon.

*Building of Consortia for the Development of Human Resources in Science and Technology (MEXT, Japan)

10:00AM R43.00007: First-principles Study of Large Seebeck Coefficients in Fe-doped Si-Ge Alloys*  
RYO YAMADA ( Presenter), Division of Materials and Manufacturing Science, Osaka University, 
AKIRA MASAGO, Center for spintronics research network (CSRN), Osaka University, 
TETSUYA FUKUSHIMA, Institute for Solid State Physics, University of Tokyo, 
HIKARI SHINYA, Research Institute of Electrical Communication, Tohoku University, 
TIEN QUANG NGUYEN, Institute for NanoScience Design, Osaka University, 
KAZUNORI SATO, Division of Materials and Manufacturing Science, Osaka University — Si-Ge alloys are one of the cheapest nontoxic thermoelectric materials utilized at high temperatures, but their dimensionless figure of merit, $ZT$, is relatively small. To improve their low $ZT$ values, there are some attempts to modify an electronic band structure by doping Fe, and it has been reported that a high $ZT$ value, $ZT>1.88$ (at $T=873K$), as well as a large Seebeck coefficient, $|S|>517\mu V/K$ (at $T=673K$), were produced in the nanostructured Si$_{0.55}$Ge$_{0.35}$P$_{0.10}$Fe$_{0.01}$ sample [1]. It is believed that they originate from a strong peak at the edge of the conduction band generated by the Fe-doping (a so-called impurity state). However, an occurrence of the impurity state in the Fe-doped Si-Ge system has not been confirmed yet. In this work, therefore, the impurity state in the Fe-doped Si-Ge alloys is calculated from an electronic band structure calculation, and the reported large Seebeck coefficient is reproduced with the use of the linear response theory. Using a special quasi-random structure with a hybrid functional (HSE06), the impurity state was successfully produced, and computed Seebeck coefficients showed good agreement with the experimental data.


*This work was partly supported by JST CREST (JPMJCR1812).
10:12AM R43.00008: Assessing Aqueous Stability of Nonequilibrium Nickel Chromium Oxides from First Principles*  KATHLEEN MULLIN (Presenter), MICHAEL WATERS, JAMES RONDINELLI, Northwestern University — Ni-Cr alloys are used in high temperature applications where corrosion resistance is critical to performance. It has generally been thought that this corrosion resistance comes from a passive film made of NiO with the rock salt crystal structure and Cr$_2$O$_3$ with the corundum crystal structure. Recently, however, new data shows that valence-precise compositions and bulk equilibrium structures do not necessarily form in the ultrathin limit[1]. Specifically, Ni-Cr alloys form nonequilibrium phases through a solute capture process, whereby Ni-Cr oxide in the rock salt structure with unexpectedly large solubility of Cr on the Ni lattice occurs (and likewise for Ni in the corundum lattice). In order to better understand the formation of this nonequilibrium oxide, we use ab-initio Density Function Theory calculations to parameterize a cluster expansion model of the Ni-Cr-O system as a function of Cr and Ni content. Next, we use energies of formation derived from the cluster-expansion for use in electrochemical Pourbaix diagrams to understand the impact of the nonequilibrium compositions on the stability of the oxide in aqueous environments.


*This work was supported by ONR MURI Grant No. N000014-16-12280.

10:24AM R43.00009: Influence of cation site disorder in ZnGeN$_2$ on electronic properties  JACOB CORDELL (Presenter), NREL/Colorado School of Mines, JIE PAN, National Renewable Energy Laboratory, CELESTE MELAMED, NREL/Colorado School of Mines, GARRITT TUCKER, Mechanical Engineering, Colorado School of Mines, ADELE TAMBOLI, STEPHAN LANY, National Renewable Energy Laboratory — Cation disorder-dependent II-IV-V$_2$ materials show promise for tuning band gaps with lattice parameters matched to their analogue III-V semiconductors for use in energy-relevant devices such as LEDs and PV. Disorder-synthesis-property relationships for these materials are not well understood, but new computational techniques can provide information complementary to experimental investigations and reveal the underlying physics of these materials. Using a combination of first principles, cluster expansion, and Monte Carlo methods, we investigated cation disorder in ZnGeN$_2$ and its effect on electronic structure as a function of effective temperature. We identify an order-disorder transition at an effective temperature of 2500K (achievable using nonequilibrium synthesis), where the local environment of nitrogen changes from exclusively 2:2 Zn:Ge coordination to the inclusion of higher energy motifs. Since ordering is a complex effect with implications on multiple length scales, metrics for assessing ordering based on cation site occupancy are compared for disordered structures at effective temperatures above this transition. This study provides insight into the synthesis-property relationship for ZnGeN$_2$ and provides a point of comparison with other ternary semiconductor systems.
Perfect short-range ordered alloy with line-compound-like properties in the ZnSnN$_2$:ZnO system*  

**STEPHAN LANY** (Presenter), **JIE PAN**, National Renewable Energy Laboratory, **JACOB CORDELL**, **GARRITT TUCKER**, Colorado School of Mines, **ANDRIY ZAKUTAYEV**, **ADELE TAMBOLI**, National Renewable Energy Laboratory — Inorganic crystalline materials are either line compounds or solid solutions, and computational materials discovery has so far focused primarily on the former. We here present a new condensed-matter phase which is a disordered solid solution but offers many ordered line-compound features. The emergent physical phenomena are rooted in the perfect short-range order. We model the dual-sublattice mixed semiconductor alloy (ZnSnN$_2$)$_{1-x}$(ZnO)$_{2x}$ using first-principles calculations, Monte-Carlo simulations with a model Hamiltonian, and an extension of the regular solution model by incorporating short-range order. We demonstrate that this unique solid solution, occurring at a “magic” composition, can provide an electronically pristine character without disorder-induced charge localization and, therefore, a superior carrier transport similar to ordered phases. Interestingly, this phase shows singularities that are absent in the conventional solid-solution models, such as the regular solution and band-gap bowing model. Thermodynamically, this alloy phase has a sharply reduced enthalpy at its composition (like a line compound), but it still requires the entropy from long-range disorder to be stabilized at experimentally accessible temperatures.

*DOE-SC-BES

The design of disordered three-dimensional auxetic networks*  

**MENG SHEN** (Presenter), **MARCOS REYES-MARTINEZ**, **EDWIN P CHAN**, **CHRISTOPHER SOLES**, **NIST**, **NIDHI PASHINE**, **SIDNEY ROBERT NAGEL**, **HEINRICH M. JAEGER**, **JUAN DE PABLO**, University of Chicago — Auxetic materials are characterized by a negative Poisson's ratio. They have attracted a lot of attention from both the scientific and engineering communities because of a variety of potential applications, such as impact mitigation, indentation resistance and biocompatibility. The design of auxetic materials is usually realized in lattice-based periodic structures in an Edisonian way. Disordered networks have the potential for the design of tunable isotropic auxetic metamaterials. However, the design of disordered three-dimensional auxetic networks has been challenging due to lack of a universal design principle. Here we propose computational strategies for the systematic design of disordered three-dimensional auxetic networks. Our designs are validated by experimental measurement of 3D-printed networks. This work builds a powerful computational framework to manipulate the auxetic properties.

*NSF, ChIMaD

Thursday, March 5, 2020 8:00 AM - 10:36 AM

Session R44 DCOMP DMP: Electrons, Phonons, Electron Phonon Scattering, and Phononics IV  

704 - Ludger Wirtz, University of Luxembourg Limpertsberg - Tag(s): Focus
8:00AM R44.00001: Phonon anharmonicity and structural transitions – neutron scattering and first-principles simulations* [Invited] OLIVIER DELAIRE (Presenter), Duke University — Using a combination of inelastic neutron/x-ray scattering and first-principles simulations, we investigate anharmonic effects on phonons across phase transitions. This presentation will focus on transitions potentially associated with soft mode condensation. In particular, we will highlight results on phonons in SnS and SnSe across the high-temperature Pnma-Cmcm transition, in VO2 across the rutile-M1 transition, and NbNiTe2 across its subtle structural orthorhombic-monoclinic transition at 373K. The effects of phonon anharmonicity on thermal transport and thermodynamics will be discussed.

*Funding from the US DOE, Basic Energy Sciences, Materials Sciences and Engineering Division.

8:36AM R44.00002: Ab initio study of electron and hole transport in a naphthalene crystal including polaron effects BENJAMIN CHANG (Presenter), JIN-JIAN ZHOU, NIEN-EN LEE, MARCO BERNARDI, Department of Applied Physics and Materials Science, California Institute of Technology — Organic semiconductors have broad applications in electronics, but their transport properties are notoriously difficult to predict due to their complex structure, strong electron-phonon (e-ph) interactions and localized charge carriers (polarons). We recently showed [1] calculations of the hole mobility in naphthalene, assuming band-like transport and using lowest-order ab initio e-ph interactions within the Boltzmann equation approach. Although our calculations provided hole mobilities in agreement with experiment, several open questions remain, such as improving the accuracy of the method and extending it to charge transport in the polaron regime. In this work, we employ our recently developed finite-temperature cumulant-expansion method [2] to compute the electron spectral functions, and from them the mobility, in a naphthalene crystal. Our method can correctly include strong e-ph interactions and polaron effects. We will discuss the carrier spectral functions and mobilities as a function of temperature in naphthalene, comparing the results with experiments and lowest-order theory. The applicability of our method to a range of organic crystals will be discussed.

Towards ultrafast control of dielectric response through nonlinear lattice excitation

GURU KHALSA (Presenter), NICOLE A BENEDEK, JEFFREY A. MOSES, Cornell University — The development of intense laser sources in the infrared has created an opportunity for unprecedented ultrafast selective control of crystal structure. Striking changes in material properties have been achieved by the optical nonlinear phononics effect - where large amplitude infrared (IR) phonons drive Raman active phonons through nonlinear lattice coupling. [Rep. Prog. Phys. 79, 064503 (2016)] Excitation of IR phonons with light is conventionally described by coupling of the infrared electric field to a linear dipole induced by the IR phonon. When IR phonons are excited to large amplitude, when multiple optical phonons are displaced simultaneously, or when multiple laser sources are used concurrently, the conventional linear description of the crystal's dipole may be insufficient.

Using theory and first-principles calculations, we explore the implications of the nonlinear dipole moment to optical experiments. When considered in concert with nonlinear lattice coupling, we find sizable polarization dependent dielectric changes can span a broad frequency range, including frequencies far above the IR resonance. In addition to changes in the optical response, the nonlinear dipole moment provides an additional strategy for ultrafast structural control.

*NSF: DMR-1719875, DMR-1550347

Theoretical Study of Pressure-Induced Superconductivity in Palladium Chalcogenides

OLIVIER GINGRAS, FELIX ANTOINE GOUDREAULT, MICHEL COTE (Presenter), Universite de Montreal — The pressure-induced superconductivity observed in palladium chalcogenides is not fully understood. Although insulating at ambient conditions, increasing isotropic pressure in PdSe$_2$ and PdS$_2$ leads to metallic phases, followed by structural transitions. These materials eventually become superconductors at higher pressure. In PdSe$_2$, the critical temperature is directly correlated with the bonding strength of Se-Se dumbbells, suggesting phonon mediated superconductivity[1]. However, the opposite is observed in PdS$_2$[2]. In order to understand the pairing mechanism in these emerging superconducting materials, we investigate the different transition temperatures using first-principles density functional theory and test the phonon mediated pairing hypothesis by calculating the superconducting dome.


*NSERC Grants No. RGPIN-2016-06666, Calcul Québec, Calcul Canada.
9:12AM R44.00005: Renormalization of magnetic interactions due to thermal disorder from first principles  MATTHEW HEINE (Presenter), Department of Physics, Boston College, OLLE HELLMAN, Department of Physics, Chemistry and Biology (IFM), Linkoping University, DAVID BROIDO, Department of Physics, Boston College — In magnetic materials, temperature dependent magnetic properties can be investigated using a Heisenberg Hamiltonian. In such a picture, raising T increases disorder in local magnetic moment orientations, the interaction of which are governed by a constant exchange parameter, J. In a more complete picture, however, such increase in moment disorder may affect the strength of the moment interactions, thereby renormalizing J as a function of T, J(T). Moreover, raising T also increases lattice disorder, which may also renormalize the interaction J(T) via spin-lattice coupling thus affecting physical quantities such as M(T) and phonon frequencies. In this study, we extend the Temperature Dependent Effective Potential (TDEP) framework to calculate such renormalized J(T) from first principles. Density Functional Theory (DFT) is employed using constrained noncollinear magnetic moments. We calculate J(T), M(T) and phonons for the test case of bcc Fe and find good agreement with experiment. We also find the lattice disorder to significantly renormalize J in the vicinity of the Curie Temperature.

9:24AM R44.00006: Emergence of Superconductivity Around Polar Quantum Critical Point in Doped Ferroelectrics*  JIAJI MA (Presenter), New York University Shanghai, RUIHAN YANG, Donald Bren School of Information and Computer Science, University of California Irvine, HANGHUI CHEN, New York University Shanghai — We combine first-principles calculations and Eliashberg equation to demonstrate that with itinerant electrons inducing a polar-to-centrosymmetric quantum critical point (pQCP) in doped ferroelectrics, softened zone-center polar phonon modes strongly couple to itinerant electrons, which enhances electron-phonon coupling around pQCP. By considering a prototypical ferroelectric material BaTiO3, we find that around its pQCP, electron-phonon coupling is increased to about 0.5, sufficiently large to induce phonon-mediated superconductivity with an optimal transition temperature of about 1 K. However, different from superconducting dome associated with other structural quantum critical points, around pQCP the superconducting transition temperature of doped BaTiO3 is enhanced much more substantially in the polar phase than in the cubic phase.

*This project was supported by NSFC (Grant No. 11774236), Shanghai Pujiang Talents Program (Grant No. 17PJ1407300), Seed Grant of NYU-ECNU Research Institute of Physics, and SRPP of NYU Shanghai.
9:36AM R44.00007: Electron-phonon interactions and photoemission kink in cuprates: A GW perturbation theory study* ZHENGLU LI (Presenter), MENG WU, YANG-HAO CHAN, STEVEN LOUIE, Lawrence Berkeley National Laboratory and University of California at Berkeley — The nexus of electron-phonon (e-ph) and many-electron interactions plays an important role in shaping the electron spectral function. We present first-principles calculations of the observed photoemission kink in cuprates using our recently developed method for e-ph coupling, the GW perturbation theory (GWPT) [1]. In this approach, the e-ph coupling is calculated using linear-response theory within the ab initio GW method, combined with Wannier interpolation technique. We find that self-energy effects significantly renormalize the e-ph interactions in the cuprates, giving rise to dramatic changes in the strength of the photoemission kink as compared with results from standard density-functional perturbation theory.


*This work was supported by the Theory of Materials Program and by the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) at the Lawrence Berkeley National Laboratory funded by the U.S. Department of Energy, Office of Basic Energy Sciences under Contract No. DE-AC02-05CH11231, and by the National Science Foundation. Computational resources have been provided by NERSC and XSEDE.

9:48AM R44.00008: First-principles study of vibrational properties of lithium niobate MONA ASADI NAMIN (Presenter), STEVEN LEWIS, University of Georgia — We present first-principles calculations of the well-known non-linear optical material LiNbO₃. Starting from the ground state properties, e.g. band structure of the stoichiometric system, we use density functional perturbation theory to find the vibrational modes. Since LiNbO₃ is a polar ferroelectric material that involves long range interactions, we use the Ewald summation to add the coulombic interaction to the dynamical matrix formalism. The transverse and longitudinal modes are in good agreement with the other ab-initio calculations, as well as the spectroscopic measurements. In addition, we calculate the relative stability of various intrinsic and extrinsic defects in this material and study their effect on the electronic, optical, and vibrational properties of this system. Achieving desirable defect properties is essential for improving the photorefractive response of LiNbO₃.

10:00AM R44.00009: BaTiO₃ as electric field controllable reservoir of phonon angular momentum* KEVIN MOSENI (Presenter), SINISA COH, Materials Science and Engineering, University of California, Riverside — We studied the angular momentum of phonons (PAM) in BaTiO₃ from first principles. We find that the PAM is four times larger in directions perpendicular to polarization than parallel. Furthermore, PAM is strongly non-linear as a function of BaTiO₃ tetragonality. We assign these observations to specific interatomic force constants in the material. Finally, we suggest experiments using BaTiO₃ as an electric field controllable phonon angular momentum reservoir.

*This work was supported by grant NSF DMR-1848074.
10:12AM R44.00010: Lattice Dynamics and Electron Transport in α-Ga$_2$O$_3$  ANKIT SHARMA
(Presenter), Electrical Engineering, University at Buffalo, MAHITOSH BISWAS, ELAHEH AHMADI, EECS, University of Michigan, UTTAM SINGISETTI, Electrical Engineering, University at Buffalo — Ga$_2$O$_3$ is an important wide bandgap material with applications ranging from power to RF electronics. It occurs in 5 polymorphs α, β, γ, δ and ε. β-Ga$_2$O$_3$ is extensively studied as it is thermodynamically a more stable phase & availability of bulk crystals. However, α-Ga$_2$O$_3$ has higher bandgap than β-phase, so better performance is expected for power applications. Although few reports exist on α-Ga$_2$O$_3$, it has not gained much traction as it is thermodynamically semi-stable making its synthesis challenging until recently where single crystalline α-Ga$_2$O$_3$ thin films were successfully grown. This opens a wide array of fields in device synthesis using α-phase (R3-c) which has a structure like corundum and thus can be potentially alloyed with materials like Cr$_2$O$_3$ and Fe$_2$O$_3$, with possibilities for magnetoelectric applications. We will present a detailed study of the lattice dynamics, electronic structure and low field electron transport properties in α-Ga$_2$O$_3$. Calculated Raman spectra is compared with experiments. The electron-phonon matrixelements are calculated under the DFT, DFPT and Wannier function formalism. We will also analyze the effects of temperature and doping on the mobility using the Boltzmann transport eqn. Emphasis will be laid on identifying the dominant scattering mechanism.

10:24AM R44.00011: Superconductivity of Liquids*  HUIYING LIU, YING YUAN, DONGHAO LIU, XIN-ZHENG LI, JUNREN SHI (Presenter), Peking Univ —
We develop a non-perturbative approach for calculating the superconducting transition temperatures ($T_c$'s) of liquids. The electron-electron scattering amplitude induced by electron-phonon coupling (EPC), from which an effective pairing interaction can be inferred, is related to the fluctuation of the $T$-matrix of electron scattering induced by ions. By applying the relation, EPC parameters can be extracted from a path-integral molecular dynamics simulation. For determining $T_c$, the linearized Eliashberg equations are re-established non-perturbatively. We apply the approach to estimate $T_c$'s of metallic hydrogen liquids. It indicates that metallic hydrogen liquids in the pressure regime from 0.5 to 1.5 TPa have $T_c$'s well above their melting temperatures, therefore are superconducting liquids.


*This work is supported by National Basic Research Program of China (973 Program) Grant No. 2015CB921101, 2016YFA0300900, and National Natural Science Foundation of China Grant No. 11325416, 11774003.
Coupling many-body-perturbation-theory calculations of electron-electron and electron-phonon coupling

HAN YANG (Presenter), Department of Chemistry, University of Chicago, MARCO GOVONI, Materials Science Division and Center for Molecular Engineering, Argonne National Laboratory, GIULIA GALLI, Pritzker School of Molecular Engineering, University of Chicago — Recently a method [1] was proposed to couple the calculations of $G_0W_0$ quasiparticle energies and electron-phonon scattering in molecules and nanostructures by using the spectral decomposition of dielectric matrices [2]. Here we generalize this approach to solids. Our implementation in the WEST [3] code (www.west-code.org) does not require summation over conduction bands or any self-consistent density-functional-perturbation-theory calculations. We validate our framework by computing phonon frequencies and electron-phonon lifetimes of several semiconductors and insulators, and we discuss the accuracy and efficiency of the method relative to existing techniques.


*This work was supported by the Midwest Integrated Center for Computational Materials (MICCoM), as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division through Argonne National Laboratory, under contract number DE-AC02-06CH11357.

Thursday, March 5, 2020 8:00 AM - 10:36 AM

Session R45 DCOMP GSNP: Computational Methods for Statistical Mechanics: Advances and Applications I 706 - Markus Eisenbach, Oak Ridge National Lab - Tag(s): Focus
Self-avoiding walks are simply defined as walks on a lattice that avoid themselves, and provide the simplest model of a polymer that captures universal features such as the Flory exponent $\nu$ which characterises the size of a polymer. In recent years, high precision Monte Carlo simulations of self-avoiding walks with many millions of steps have been realised through the use of a radically efficient implementation of the pivot algorithm via a hierarchical data structure. This data structure allows for global updates of the system to be performed in the same CPU time as local updates.

I will describe the key geometric intuition behind this implementation, and outline its application to the calculation of various quantities for self-avoiding walks, such as the critical exponents $\nu = 0.58759700(40)$ [1] and $\gamma = 1.15695300(95)$ [2] for three-dimensional walks, and the study of logarithmic corrections for four-dimensional walks [3].

Finally, I will discuss some recent extensions of the method to dense polymer systems and to continuum models of polymers, and will speculate on possible future applications of fast global Monte Carlo moves to other models in statistical physics.


*Support from the Australian Research Council under the Future Fellowship scheme (Project Number FT130100972) and Discovery scheme (Project Number DP140101110) is gratefully acknowledged.
**8:36AM R45.00002: Smart random walks for accelerated Monte Carlo simulations**

YING WAI LI (Presenter), Los Alamos National Laboratory, ALFRED C.K. FARRIS, Emory University, MARKUS EISENBACH, Oak Ridge National Lab — Monte Carlo simulations are robust methods to study statistical physics. However, the unpredictable convergence time and the ease of being trapped in local minima have plagued the efficiency of both traditional and modern Monte Carlo algorithms. We propose strategies to mitigate these problems. We highlight two recent algorithmic developments: the histogram-free multicanonical method for obtaining the density of states for physical systems [1], and a global update scheme that adjusts the sampling weights across the phase space simultaneously. Combining these two methods, we have observed speedups ranging from 1-3 orders of magnitude compared to existing flat-histogram methods such as Wang-Landau sampling and multicanonical sampling, depending on the problem of interest. These methods are implemented and publicly available in an open-source Monte Carlo software suite, the Oak-ridge Wang-Landau (OWL) code [2].


*We acknowledge the support of the U.S. Department of Energy through the Los Alamos National Laboratory (LANL)'s Laboratory-Directed Research and Development (LDRD) Program for this work.

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**8:48AM R45.00003: Replica-Exchange Wang-Landau Simulations of Lattice Peptide Aggregation**

MATTHEW WILSON (Presenter), GUANGJIE SHI, University of Georgia, THOMAS WUEST, Scientific IT Services, ETH Zurich, DAVID P LANDAU, University of Georgia, FRIEDERIKE SCHMID, Institute of Physics, Johannes Gutenberg University — The computational study of interacting biomolecules is a challenging endeavor due to the large range of time and length scales associated with the relevant physical transitions. In order to analyze the general, qualitative statistical physics of such systems as they transition from dissolved to aggregated crystalline states, we use the H0P lattice protein model\(^1,2\) simulated on simple cubic and face centered cubic lattices. Utilizing the parallel Replica-Exchange Wang-Landau\(^3\) Monte Carlo algorithm, the energy states and density of states are calculated for multiple interacting H0P peptides. Thermodynamic quantities are studied for short (< 20 residues) model peptides at a range of concentrations and temperatures as structures such as disordered oligomers, amyloid fibrils, and aggregates are formed. Additional structural observables such as the cluster size distribution are calculated in a post-simulation production run, and used to further elucidate the physical behavior during transitions.

9:00AM R45.00004: A Combinatorial Perspective on Ising Model Hysteresis  YULING GUAN (Presenter), ANG LI, STEPHAN WOLFGANG HAAS, SATISH KUMAR THITTAMARANAHALLI, SVEN KOENIG, Univ of Southern California — In this work, we apply combinatorial methods used extensively in Artificial Intelligence (AI) to understand Ising model hysteresis. Our approach is based on efficiently generating the top K solutions of the Ising model and its generalization in AI, called the Weighted Constraint Satisfaction Problem (WCSP). We discuss how the WCSP model with a memory effect can be used to study hysteresis combinatorially; and in this context, we also discuss how the memory effect is related to an effective temperature parameter. Turning to more complex variants of the Ising model, we show that the introduction of long-range dipole interactions leads to variations of the hysteresis curves and the introduction of three-spin interactions leads to the emergence of meta-stable plateau states. We also show how to apply the Discrete Fourier Transform for the analysis of such phase transitions in the Ising model induced by three-spin interactions.

9:12AM R45.00005: Steering a solute between coexisting solvation states: calculation of free energy differences in the adaptive resolution method* MAZIAR HEIDARI, ROBINSON CORTES HUERTO (Presenter), Max Planck Inst, RAFFAELLO POTESTIO, Physics Department, University of Trento, KURT KREMER, Max Planck Inst — In the adaptive resolution method, it is possible to represent molecules with atomistic resolution in a simulation subregion and as ideal gas particles in a large reservoir. To enforce a uniform density profile across the simulation box, an external potential is applied and identified with the system's excess chemical potential. Indeed, atomistic and ideal gas images coexist at a constant temperature, volume, and chemical potential. In this context, we present a method to calculate solvation free energies (SFEs) [1]. The idea is to steer the solute between coexisting solvation states, represented by incorporating solvent and ideal gas at a constant chemical potential. At finite pulling speeds, the applied work gives SFEs via non-equilibrium relations, whereas at infinitely slow pulling, the calculation is equivalent to a thermodynamic integration. Results for small molecules well agree with literature data and pave the way to systematic studies of arbitrarily large and complex molecules.


*This work was supported by the Deutsche Forschungsgemeinschaft Project No. 233630050 TRR 146 and the European Research Council under the European Union’s Seventh Framework Programme (No. FP7/2007-2013)/ERC Grant Agreement No. 340906-MOLPROCOMP.
ALFRED FARRIS (Presenter), Oxford College of Emory University, DANIEL T SEATON, Open Learning, Massachusetts Institute of Technology, DAVID P LANDAU, University of Georgia — Using Wang-Landau sampling [1], we compare and contrast folding behavior in coarse-grained models for Crambin -- a 46 amino acid protein. We investigate Crambin in the context of the hydrophobic polar (HP) lattice model [2] and the semi-flexible H0P lattice model [3] -- an extension to the HP model in which an additional monomer type and an interaction accounting for chain-stiffness are included. We also examine folding behavior in the analogous continuum models, with potentials designed specifically to mimic the lattice models. Through analysis of thermodynamic and structural behavior, we paint a clear picture of the folding process in all cases, and gain an understanding of the effects of certain interactions on the folding process, as well as how lattice constraints impact the folding process. As the complexity of the model interactions increases, the two major transitions observed in nature -- the coil-globule collapse and the folding transition, split into multi-step processes, wherein the level of model coarse-graining has a significant impact on the details of the folding.


9:36AM R45.00007: The self-consistent multi scale simulation of complex fluids*  
HIDEKI KOBAYASHI (Presenter), Department of Chemistry, University of Cambridge, PAUL ROHRBACH, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, ROBERT SCHEICHL, Institute for Applied Mathematics and Interdisciplinary Center for Scientific Computing (IWR), University of Heidelberg, NIGEL B. WILDING, School of Physics, University of Bristol, ROBERT L JACK, Department of Applied Mathematics and Theoretical Physics, University of Cambridge — We present a method that uses self-consistent simulation of coarse grained and fine-grained models, in order to analyse properties of physical systems. The method uses the coarse-grained model to obtain a first estimate of the quantity of interest, before computing a correction by analysing properties of the fine system.

We illustrate the method by applying it to the Asakura-Oosawa (AO) model of colloid-polymer mixtures. We show that the liquid-vapour critical point in that system is affected by three-body interactions which are neglected in the corresponding coarse-grained model. We analyse the size of this effect and the nature of the three-body and higher interactions. Additionally, we apply our methodology to the binary hard-sphere mixture to demonstrate the existence of the liquid-vapour critical point.

*This work was supported by the Leverhulme Trust through research project grant number RPG-2017-203.
9:48AM R45.00008: Equilibrium density calculation of generalized Muttalib-Borodin ensembles. SWAPNIL YADAV (Presenter), KAZI ALAM, KHANDKER A MUTTALIB, University of Florida, DONG WANG, Mathematics, National University of Singapore — The Muttalib-Borodin (MB) random matrix ensemble, which has an additional interaction, was introduced as a solvable toy model for quasi one-dimensional (1D) disordered conductors. We generalize the MB random matrix ensemble with a disorder dependent parameter $\gamma$ which characterizes the strength of the additional interaction term. This generalization can be considered as a simple toy model which captures the essential features of a quasi 1D to 3D generalization of disordered conductors and we call it the $\gamma$-ensembles. Our results suggest that the $\gamma$-ensembles can be mapped on to an MB ensemble by replacing the single particle confining potential with a $\gamma$-dependent effective confining potential. We numerically solve the Riemann-Hilbert (RH) problem associated with the equilibrium density of $\gamma$-ensembles for a range of $\gamma$ between 0 and 1. We also study some interesting limits of the parameters of the $\gamma$-ensembles, where the equilibrium density for a generalized form of the $\beta$-ensembles can be explored.

10:00AM R45.00009: Enhanced sampling of cylindrical microphase separation via shell-averaged bond-orientational order parameter* MIN YOUNG HA (Presenter), BUMJOON SEO, WON BO LEE, Seoul Natl Univ — The formation of a hexagonal phase from the disordered phase is one of the typical order-disorder transitions (ODT) observed in asymmetric diblock copolymer systems. In order to drive this transition in a particle-based simulation, we introduce a shell-based bond-orientational order parameter that selectively responds to the mesoscopic order of the hexagonal cylinder phase. From metadynamics simulations in a bond-free particle model system, the characteristic pathway involved with the underlying free energy surface is deduced for the disordered-to-hexagonal transition. It is shown consecutively that the transition pathway and the metastable state are reproduced in dissipative particle dynamics simulations for the corresponding transition in bulk asymmetric block copolymer melt system. These agreements suggest that efficient strategies for enhanced sampling with particle-based simulations of block copolymer systems can be devised using coarse-grained pictures of the mesoscopic order.

*This research was supported by the National Research Foundation of Korea(NRF) grant funded by the Korean Government through the Ministry of Science, ICT and Future Planning (MSIP) (NRF-2015R1A5A1036133, 2019R1A2C1085081)
Probing predictions due to the nonlocal interface Hamiltonian: Monte Carlo simulations of interfacial fluctuations in Ising films*  
LIJUN PANG (Presenter), Georgia Gwinnett College, DAVID P LANDAU, University of Georgia, KURT BINDER, Johannes Gutenberg University Mainz — Extensive Monte Carlo simulations have been performed on an Ising ferromagnet under conditions that would lead to complete wetting in a semi-infinite system. We studied an $L \times L \times D$ slab geometry with oppositely directed surface fields so that a single interface is formed and can undergo a localization-delocalization transition. Under the chosen conditions the interface position is, on average, in the middle of the slab, and its fluctuations allow a sensitive test of predictions that the effective interactions between the interface and the confining surfaces are nonlocal. The decay of distance dependent correlation functions are measured within the surface, in the middle of the slab, and between middle and the surface for slabs of varying thickness $D$. From Fourier transforms of these correlation functions a non-linear correlation length is extracted, and its behavior is found to confirm theoretical predictions for $D>6$ lattice spacings.

*Alexander von Humboldt Foundation and the Graduiertenschule Materials Science in Mainz

Integer lattice gases, Molecular Dynamics Lattice Gas and an alternative derivation of the lattice Boltzmann method  
ALEXANDER WAGNER (Presenter), NOAH SEEKINS, REZA PARSA, ALEKSANDRA PACHALIEVA, North Dakota State Univ — We report on recent progress in two related areas:

1) that lattice Boltzmann methods can be derived rigorously from Molecular Dynamics simulations through a coarse graining approach (MDLG) that maps Molecular Dynamics onto an integer lattice gas. This gives insights into the surprisingly large correct fluctuations for non-ideal gases and fluids as well as the physical meaning of over-relaxation in lattice Boltzmann.

2) the efficient implementation of integer lattice gases that can be considerably more efficient than the equivalent lattice Boltzmann implementation.
R45.00012: Machine-learning approach to real-space renormalization of the 2D Potts model

*CHAK MING CHAN (Presenter), LIANG TIAN, LEI-HAN TANG, Hong Kong Baptist Univ — The ordering transition of the q-state Potts model on a square lattice changes from continuous to first-order at q=4. This changeover has been analyzed in real-space renormalization group (RSRG) studies[1] but a clear physical picture is lacking. We have previously conjectured that the weak first order transition at q>4 is related to the four-color theorem in graph theory[2]. Here we implement a recently proposed deep-learning scheme that maps configurations at successive scales to each other[3]. Parameters of the mapping are learned by maximizing mutual information. We take into account symmetry properties of the model and analyze the resulting RG flow to extract critical exponents and other properties. The emergence of "mosaic domains" which represent dilution of the original Potts model under the RG transformation will be discussed[4].


*LHT is supported in part by the Research Grants Council of the Hong Kong Special Administrative Region (HKSAR) under Grant No. 12324716.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R46 GMAG DMP: Triangular Lattice II

8:00AM R46.00001: Characterizing the Spin-½ Heisenberg model on the triangular lattice through the Dynamical Spin Structure

TA TANG (Presenter), THOMAS DEVEREAUX, Stanford Univ, BRIAN MORITZ, SLAC, YI-FAN JIANG, Stanford Univ — The ground state phase of the spin-1/2 Heisenberg model on the triangular lattice with nearest-neighbor exchange $J_1$ can be frustrated by the next nearest neighbor coupling $J_2$ and turns into a stripe phase for large $J_2$. While both small and large values of $J_2/J_1$ lead to magnetically ordered phases, a spin liquid phase with short correlation length can be established at intermediate values. However, the nature of this spin liquid phase remains under debate, with finite size DMRG calculations suggesting a gapped $Z_2$ spin liquid phase, but also showing possible gapless spinon excitations. Here, we use exact diagonalization on a series of finite-size clusters to analyze the character of the ground state and lowest-lying the excited states of the model for various values of $J_2$. We further characterize the evolution of the model as a function of $J_2$ by analyzing the dynamical spin structure factor $S(q,w)$ to provide key information on the changes of the underlying magnetic structure.
Generalized SU(3) Spin Wave Theory on Effective S=1 Triangular Lattice Magnet FeI₂

HAO ZHANG (Presenter), SHANG-SHUN ZHANG, Department of Physics and Astronomy, University of Tennessee, XIAOJIAN BAI, ZHILING DUN, School of Physics, Georgia Institute of Technology, MATTHEW STONE, ALEXANDER KOLESNIKOV, FENG YE, Neutron Scattering Division, Oak Ridge National Laboratory, MARTIN MOURIGAL, School of Physics, Georgia Institute of Technology, CRISTIAN BATISTA, Department of Physics and Astronomy, University of Tennessee — Magnetic and quadrupolar excitations can coexist in magnetically ordered S=1 spin systems because the local Hilbert space has dimension three. By using a generalized SU(3) spin wave theory (GSWT), we uncover the hybridized nature of the low-energy modes revealed by inelastic neutron scattering (INS) measurements of the effective S=1 triangular antiferromagnet FeI₂. Band crossing between dipolar and quadrupolar modes enables a large hybridization between them that is induced by symmetric exchange anisotropy. Because of this hybridization, modes with dominant quadrupolar character can be observed with INS. These modes can also be obtained from a generalized Landau-Lifshitz dynamics of SU(3) spins (3 dipolar + 5 quadrupolar components), which turns out to be the adequate dynamics for describing the low-temperature dynamical properties of FeI₂.

Magnetic Excitations of the Frustrated Triangular Ising Magnet FeI₂*

XIAOJIAN BAI (Presenter), School of Physics, Georgia Institute of Technology, SHANG-SHUN ZHANG, Department of Physics and Astronomy, University of Tennessee, Knoxville, ZHILING DUN, School of Physics, Georgia Institute of Technology, HAO ZHANG, Department of Physics and Astronomy, University of Tennessee, Knoxville, WILLIAM ADAM PHELAN, Department of Chemistry, Johns Hopkins University, HAIDONG ZHOU, Department of Physics and Astronomy, University of Tennessee, Knoxville, MATTHEW STONE, ALEXANDER KOLESNIKOV, FENG YE, Neutron Scattering Division, Oak Ridge National Laboratory, CRISTIAN BATISTA, Department of Physics and Astronomy, University of Tennessee, Knoxville, MARTIN MOURIGAL, School of Physics, Georgia Institute of Technology — We present a detailed investigation of the spin dynamics in single-crystals of the layered spin-one triangular-lattice compound FeI₂. Previous thermo-magnetic measurements revealed a strong Ising single-ion anisotropy for the Fe²⁺ ions in FeI₂ and a magnetically long-range ordered state below 9.3K, which can be understood from the competition between nearest neighbor ferromagnetic interactions and a complex set of further-neighbor interactions. Early neutron scattering, far-infrared and ESR measurements, revealed the emergence of a two-magnon bound state (TMBS) as the lowest energy mode from this ordered state. The TMBS carries an apparent g-factor that is doubled compared to that of single magnon excitations, which can be explained by a change of 2 units in spin angular momentum, at odds with the dipole selection rule. We revisit the spin excitations of FeI₂ using modern neutron-scattering instrumentation and map out the magnetic structure, diffuse scattering and low-energy magnetic excitation spectrum. We extract a model Hamiltonian for FeI₂ and elucidate a novel hybridization mechanism that quantitatively explains current and previous spectroscopic experiments on this enigmatic compound.

*The work at Georgia Tech was sponsored by the Department of Energy under DE-SC-0018660.
8:36AM R46.00004: Anisotropic-exchange magnets: triangular lattice and all* [Invited]
ALEXANDER CHERNYSHEV (Presenter), University of California, Irvine — I will describe our efforts to understand the phase diagram of a model that combines paradigmatic geometrical frustration of spins on a triangular lattice with strong spin-orbit-induced interactions. This model is relevant to a growing family of rare-earth-based magnets and other related materials and our work sets up a consistent interpretation of the current and future experiments in them. I will also attempt to review our recent incursion to the honeycomb-lattice territory and attempts to shed light on the properties of the Kitaev materials such as α-RuCl₃.

*Funded by the DoE, Award No. DE-FG02-04ER46174

9:12AM R46.00005: Interplay between magnetic structures, domain physics, and transport properties in a family of triangular layered materials  
CHUNXIAO LIU (Presenter), University of California, Santa Barbara, LEON BALENTS, Kavli Institute for Theoretical Physics — The triangular layered magnet PdCrO₂ has attracted interest due to the interplay between its antiferromagnetic order and high in-plane conductivity, widely believed to be the key to understanding an unconventional anomalous Hall effect (AHE) in the material. More recent experiments reveal that the domain physics in the material may also play an important role on its electronic transport. Motivated by these experimental findings, we study the interplay between magnetic structures, domain physics, and transport properties of a layered triangular lattice with alternating layers of hopping electrons and localized spins. We analyze the possible magnetic orders of the most general symmetry allowed spin Hamiltonian at nearest neighbor level. Assuming appropriate intralayer exchange parameters and treating the interlayer exchange perturbatively, we show that threefold rotation symmetry breaking domains can emerge, in accordance with the experiments. We further show that, under certain conditions the Kondo lattice Hamiltonian possesses a particular symmetry that forbids contribution from the electron band topology to the Hall conductance. Finally we study various other effects including magnetic breakdown and spin-orbit coupling and comment on their contribution to the unconventional AHE.
9:24AM R46.00006: Triangular antiferromagnet NiGa2S4: a low-dimensional analog of the pyrochlores*  
HAOYU WANG (Presenter), OLEG TCHERNYSHYOV, Johns Hopkins University — NiGa2S4 is a frustrated magnet on a triangular lattice with a strong antiferromagnetic third-neighbor exchange J3 and a weak ferromagnet first-neighbor exchange J1. Although the system has been studied for more than a decade [1], its behavior, particularly the lack of long-range order, remains enigmatic. Exotic scenarios have been proposed for its explanation, including the formation of a quadrupolar spin order that cannot be seen by the usual probes like neutrons [2]. We propose a different scenario based on a simple observation: the 4-sublattice structure resulting from a strong J3 makes the system similar to a pyrochlore antiferromagnet. The geometrical frustration of the pyrochlore antiferromagnet can be relieved by a lattice distortion [3]. A similar tendency may exist in NiGa2S4. The spin-Peierls phase transition may be preempted by structural disorder involving random strains.


*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331

9:36AM R46.00007: Complex magnetic behavior of the Co2+ triangular (saw-tooth) 1D chains in CsCo2(MoO4)2(OH)*  
DUMINDA SANJEEWA (Presenter), VASILE O GARLEA, JIE XING, ATHENA S. SEFAT, Oak Ridge National Lab — Low-dimensional magnetic materials have drawn continued attention in condensed-matter physics for their electronic and magnetic anisotropic properties. In particular, the oxyanion-based systems, with transition-metal (M) oxide sublattices that are magnetically isolated by closed-shell nonmagnetic oxyanions (SiO4−4, PO3−4, AsO3−4), show great potential for diverse magnetic phenomena. We synthesize CsCo2(MoO4)2(OH) single crystals, find the crystal structure, and characterize thermodynamic properties. CsCo2(MoO4)2(OH) belongs to a rare class of compounds named delta-chain (or sawtooth) type structure, with corner-sharing isosceles triangles whose vertices consist of one Co(1) and two Co(2) atoms. The magnetic susceptibility result reveals long-range ordering below 5 K with a strong anisotropy. The isothermal magnetization data shown a stepwise magnetization when the magnetic field is along the Co-O-Co (saw-tooth chain) direction, with two metamagnetic transitions at 0.3 kOe and 40 kOe. The magnetic structure consists of ferrimagnetic chains which are antiferromagnetically coupled with each other, seen in neutron diffraction.

*Work at ORNL was supported by U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Science and Engineering Division.
**9:48AM R46.00008: Synthesis and Characterization of Rare-Earth Based Triangular Antiferromagnet Borates**  MATTHEW ENNIS (Presenter), RABINDRANATH BAG, SACHITH DISSANAYAKE, ZHENZHONG SHI, Department of Physics, Duke University, ALEXANDER KOLESNIKOV, Neutron Scattering Division, Oak Ridge National Lab, JOSE RODRIGUEZ-RIVERA, HUI WU, CRAIG BROWN, Center for Neutron Research, National Institute of Standards and Technology, DAVID E GRAF, National High Magnetic Field Laboratory and Department of Physics, Florida State University, SARA HARAVIFARD, Department of Physics and Department of Mechanical Engineering & Materials Science, Duke University — Recently, triangular antiferromagnetic materials have attracted attention because competing interactions on the lattice can give rise to exotic phenomena, such as Quantum Spin Liquids. We have initiated systematic efforts to synthesize single crystal samples of a family of rare-earth based triangular antiferromagnet borates. We have used x-ray diffraction as well as thermal and magnetic measurements to characterize these compounds. Additionally we have carried out neutron scattering experiments to probe the static and dynamic properties of these systems. In this talk, we will present the results of our experimental efforts.

**10:00AM R46.00009: Magnetic short-range correlations and Kosterlitz-Thouless transitions in TmMgGaO4**  MARCUS DAUM (Presenter), ZHILING DUN, Georgia Inst of Tech, HAIDONG ZHOU, University of Tennesse, Knoxville, MARTIN MOURIGAL, Georgia Inst of Tech — Transverse Ising model on a triangular lattice is known to host two Kosterlitz-Thouless (KT) transitions at low temperatures. Triangular lattice antiferromagnet TmMgGaO4 is a promising candidate to realize such physics due to the interplay between geometric frustration, spin orbit coupling, and crystal electric fields. In TmMgGaO4 short-range magnetic correlations are observed over a broad temperature range. However, the nature of this short-range magnetic order is under debate. Recent numerical work has predicted a Kosterlitz-Thouless transition at 4 K, which however lacks any experimental evidence thus far. Using AC susceptibility and neutron scattering measurements, we unveil this transition and discuss its implications in understanding the rich physics of TmMgGaO4.

*The work at Georgia Tech was sponsored by the National Science Foundation under NSF-DMR-1750186*
10:12AM R46.00010: Studying the Dynamic Magnetic Properties of the Triangular Antiferromagnet YbZnGaO4 in Applied Field  WILLIAM STEINHARDT (Presenter), SACHITH DISSANAYAKE, ZHENZHONG SHI, Department of Physics, Duke University, NICHOLAS BUTCH, Center for Neutron Research, National Institute of Standards and Technology, DAVID E GRAF, National High Magnetic Field Lab, Florida State University, ANDREY PODLESNYAK, YAOHUA LIU, Neutron Scattering Division, Oak Ridge National Laboratory, YANG ZHAO, GUANGYONG XU, JEFFREY LYNN, Center for Neutron Research, National Institute of Standards and Technology, CASEY MARJERRISON, Department of Physics, Duke University, SARA HARAVIFARD, Department of Physics, Department of Mechanical Engineering & Materials Science, Duke University — In the last few years Yb-based triangular antiferromagnets emerged as promising quantum spin liquid candidates, and subsequently their ground states have been the subject of ardent debates. Though many experimental and theoretical studies have been devoted to investigating the magnetic properties of these systems at very low temperatures, and exploring a range of possible explanations for the observed spin liquid-like phenomena, a definitive description remains elusive mainly due to thermal fluctuations and chemical disorder. In this talk we discuss neutron scattering experiments in applied magnetic field to probe features of the “partially magnetized” state in YbZnGaO4, which generated great excitement in YbMgGaO4 as a possible signature in support of spinon Fermi surface hypothesis [1].


10:24AM R46.00011: A quantitative study of short-range correlations in triangular Ising antiferromagnet TmMgGaO4 via magnetic pair distribution function analysis  RAJU BARAL (Presenter), BENJAMIN FRANDSEN, Department of Physics and Astronomy, Brigham Young University, HENRY EDWARD FISCHER, Institut Laue-Langevin, QING HUANG, HAIDONG ZHOU, Department of Physics & Astronomy, University of Tennessee, MARCUS DAUM, ZHILING DUN, MARTIN MOURIGAL, School of Physics, Georgia Institute of Technology — Interacting Ising spins decorating a triangular lattice are expected to show rich magnetic behavior, including a possible Kosterlitz-Thouless (KT) transition at low temperature. Recently, TmMgGaO4 has been found to exhibit a perfect triangular lattice of Ising-like Tm$^{3+}$ magnetic moments, providing a promising platform for investigating potential KT physics in a solid-state magnetic system. Initial studies have revealed significant diffuse magnetic scattering at low temperature, indicating the presence of short-range magnetic correlations that may hold the key to understanding the magnetic ground state of this system. Here, we utilize the magnetic pair distribution function (mPDF) technique to probe these correlations in real space via Fourier transformation of the diffuse scattering pattern. We present a magnetic model that reproduces the observed mPDF pattern with quantitative accuracy and discuss the significance of these results in the context of existing work on TmMgGaO4.
10:36AM R46.00012: Chiral correlation in triangular lattice Hubbard model*  BIN-BIN CHEN
(Presenter), Ludwig Maximilian University of Munich, WEI LI, Department of Physics, Beihang University, ANDREAS WEICHSELBAUM, Brookhaven National Laboratory — The fermionic triangular lattice Hubbard (TLH) model constitutes a playground for intriguing emergent quantum phenomena and novel exotic states in strongly correlated system. In a recent paper [1], by using mixed real- and momentum-space basis in iDMRG, a chiral spin liquid is found for intermediate onsite Coulomb interaction U between the small-U metallic phase and large-U three-sublattice magnetic phase, against the conclusion in ref. [2].
In this talk, I will focus on finite-size DMRG simulations of the TLH for system sizes that go clearly beyond [2] while also exploiting SU(2) spin symmetry. Comprehensive characterizations, including entanglement entropy, spin correlation, and chiral correlation, are carried out to distinguish the phase boundary between the above three phases. By tuning the on-site Coulomb interaction U to intermediate values, we observe for significantly large systems strong indications in favor of a chiral spin liquid. Specifically, for U10, we observe a plateau in the static chiral correlations vs. distance, and the estimated spontaneous chiral order parameter shows good agreement with ref. [1].


*This work is supported by the DFG WE4819/3-1, and DOE DE-SC0012704.

10:48AM R46.00013: Topological frustration: Quantum statistics of vortices from a dual theory of the XY ferromagnet*  SAYAK DASGUPTA (Presenter), Johns Hopkins University, SHU ZHANG, University of California, Los Angeles, IBRAHIMA BAH, OLEG TCHERNYSHYOV, Johns Hopkins University — The familiar concept of geometrical frustration can be extended to frustration induced by the topology of spin textures. For instance, in a magnetic vortex the spins on the periphery rotate in the easy plane, leaving the spins at the vortex core frustrated. To reduce the exchange energy, the core spins come out of the easy plane and point along the hard axis. There is a degeneracy resulting from the associated $\mathbb{Z}_2$ symmetry (polarization) which has well-known important consequences for the dynamics of a vortex. Here we show that topological frustration at the vortex core may induce a nontrivial quantum statistics of vortices. We extend the well-known mapping between the easy-plane ferromagnet and electrostatics in $d = 2$ spatial dimensions, introduced by Kosterlitz [1], to dynamical and quantum phenomena in a $d = 2+1$ spacetime. Ferromagnetic vortices behave like quantum particles with an electric charge equal to the vortex number and a magnetic flux equal to the transverse spin of the vortex core. Vortices with half-integer core spin exhibit fermionic statistics.


*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331.

Thursday, March 5, 2020 8:00 AM - 11:00 AM
8:00AM R47.00001: Chemical control of magnetism in $S = 1$ quantum materials: new twists on a seemingly old theme*  

[Invited] JAMIE MANSON (Presenter), JACQUELINE VILLA, DANIELLE Y. VILLA, ISABEL CALDERON-LIN, ZACHARY MANSON, NATHAN GRINALDS, ASHLEY SARGENT, Eastern Washington University, WILLIAM BLACKMORE, SAM CURLEY, PAUL GODDARD, Physics, University of Warwick, JOHN SINGLETON, NMFL, Los Alamos National Lab, MATTHEW STONE, Quantum Condensed Matter Div, Oak Ridge National Lab, ROGER JOHNSON, Physics, University of Oxford, VASILE O GARLEA, Quantum Condensed Matter Div, Oak Ridge National Lab, PASCAL MANUEL, ISIS, STFC RAL, CRAIG BROWN, NIST Center for Neutron Research, NIST — We aim to control the spatial exchange and single-ion anisotropies ($D$) in bespoke $S = 1$ Ni(II) quantum magnets. Early work led to $[\text{Ni(HF}_2\text{)(pyz)}_2\text{SbF}_6]$ which contains Ni-FHF-Ni chains ($J_{\text{FHF}}$) cross-linked by Ni-pyz-Ni segments ($J_{\text{pyz}}$) to form a tetragonal network [1]. The material undergoes $XY$-AFM order below $T_N = 12.2$ K with collinear Ni(II) moments confined to the $[\text{Ni(pyz)}_2]^{2+}$ plane. High-field $M(H)$ and inelastic neutron scattering (INS) revealed $D = J_{\text{FHF}} \gg J_{\text{pyz}}$. In the related square lattices [2,3], $\text{NiX}_2\text{(pyz)}_2$ ($X = F, Cl, Br, I$, NCS), the electronegativity of $X$ dictates the Ni(II) spin direction with $XY$-and Ising-like ground-states observed for $X = F, Cl$ and $X = Br, I$, NCS, respectively. We used INS to determine $J_{\text{pyz}}$ and $J_{\perp}$. Chemical substitution of pyz for pyrimidine (pym) affords unusual topologies and enhanced magnetic interactions along Ni-pym-Ni relative to Ni-pyz-Ni. Thus, we synthesized two new Q1D chains: staggered $[\text{Ni(pym)(H}_2\text{O)}_4\text{]SO}_4\bullet2\text{H}_2\text{O}$ and chiral $[\text{Ni(pym)}(\text{H}_2\text{O)}_4\text{]SiF}_6\bullet\text{H}_2\text{O}$, each showing multiple field-induced phase transitions below 5 K. Lastly, we will describe a unique 3D chiral Ni(II) framework that may display spin-liquid behavior at low temperatures. Time permitting, the structural and magnetic properties of these materials will be discussed.

*NSF DMR-1703003 (EWU), DMR-1157490 (MagLab), DoE, State of FL, ERC, EPSRC

References:
We report on a new molecule-based magnet NiI2(3,5-lutidine)4 characterized using x-ray diffraction, electron-spin resonance, magnetometry, inelastic neutron scattering and muon-spin relaxation. The system is a near-ideal realization of the $S = 1$ Haldane chain with intrachain exchange $J = 17.5$ K, energy gaps of 5.3 K and 7.7 K split by easy-axis anisotropy $D = -1.2$ K, and with no sign of magnetic order down to 20 mK. The value $D/J = -0.07$ implies one of the most isotropic Haldane systems yet discovered, while the ratio $\Delta/J = 0.40(1)$ (where $\Delta$ is the average gap size) is close to the ideal theoretical value, suggesting a very high degree of magnetic isolation of the chains. The Haldane gap is closed by orientation-dependent critical fields 5.3 T and 4.3 T, which are readily accessible experimentally. The fully polarized state occurs above 46.0 T. The results are explicable within the so-called fermion model, which is in contrast to other reported easy-axis Haldane systems. The flexible nature of this molecule-based material readily permits tuning via applied pressure and introduction of disorder along the exchange pathway.

*This project has received funding from the European Research Council (grant no. 681260). We also thank the NHMFL, EPSRC, STFC, NSF, DoE and the State of Florida.
8:48AM R47.00003: Magnetic ground-state of two new highly one-dimensional ferromagnetic chain compounds $M$(NCS)$_2$(thiourea)$_2$; $M = \text{Co, Ni}$.\* SAM CURLEY (Presenter), ROBERT C WILLIAMS, PAUL GODDARD, Department of Physics, University of Warwick, REBECCA SCATENA, STEPHEN BLUNDELL, Department of Physics, University of Oxford, PIERO MACCHI, Department of Chemistry and Biochemistry, University of Bern, THOMAS HICKEN, TOM LANCASTER, Centre for Materials Physics, Durham University, FAN XIAO, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, JAMES C ECKERT, Department of Physics, Harvey Mudd College, VIVIEN ZAPF, Los Alamos National Laboratory, National High Magnetic Field Laboratory, JACQUELINE VILLA, JAMIE MANSON, Department of Chemistry and Biochemistry, Eastern Washington University — Low-dimensional magnetic materials have garnered much attention from theorists and experimentalists alike for many years. Chains of low-spin, ferromagnetically (FM) or antiferromagnetically (AFM) coupled magnetic-ions can both harbour exotic magnetic ground-states: such as the gapped Haldane ground state in Heisenberg AFM chains, or the field-induced quantum paramagnetic state in Ising-like FM chains. In terms of physically realizing such systems, co-ordination chemistry has had great success in promoting crystal architectures that can lead to quasi-1D behaviours. Altering the bridging or non-bridging ligand species can modify both the Heisenberg exchange ($J$) and single-ion anisotropy ($D$). It is the interplay of these two parameters that ultimately determines the magnetic ground-state. To this end, we have recently synthesised two new, highly one-dimensional and isostructural molecule-based magnets; $M$(NCS)$_2$(thiourea)$_2$ [thiourea = $\text{CH}_4\text{N}_2\text{S}$, $M$ is Co ($S = 3/2$) or Ni ($S=1$)]. We employ a combination of magnetometry, heat capacity and muon spin-rotation in addition to theoretical charge density analysis, in an attempt to resolve the magnetic ground-state of both materials.

\*This project has received funding from the European Research Council (grant no. 681260).

9:00AM R47.00004: Cluster-Based Haldane States in Spin Cluster Chains TAKANORI SUGIMOTO (Presenter), KATSUHIRO MORITA, TAKAMI TOHYAMA, Tokyo Univ of Science, Katsushika — The $S=1$ Haldane state has attracted much attention due to its topological characters. This state emerges not only in the $S=1$ spin chain, but also in an $S=1/2$ two-leg spin ladder with a ferromagnetic rung interaction. Additionally, our recent study on low-temperature magnetism in a naturally occurring mineral Fedotovite, has shown the Haldane state consisting of cluster-based $S=1$ spins, in collaboration with experimental groups. In this compound, edge-shared tetrahedral spin clusters which include six spins in a cluster, are linked by a nearest-neighbor antiferromagnetic inter-cluster interaction in one dimension. The low-energy state in a cluster is a triplet and the inter-cluster interaction is perturbative as compared with the intra-cluster excitation energy, so that we can explain the low-temperature physics in an effective $S=1$ spin model obtained by projection into cluster's triplet states. Furthermore, we extend the cluster-based Haldane state to spin-cluster systems which have odd-number $S=1/2$ spins in a cluster, and find cluster-based Haldane state with breaking time-reversal symmetry. Thus, we will present several varieties of cluster-based Haldane states obtained in possible spin lattices.
A Novel Strongly Spin-Orbit Coupled Quantum Dimer Magnet: Yb$_2$Si$_2$O$_7$*

GAVIN HESTER, HARIKRISHNAN S NAIR, TIMOTHY REEDER, DANIELLE R YAHNE, TIMOTHY DELAZZER, Colorado State University, LÉO BERGES, DJAMEL ZIAT, Physics, Université de Sherbrooke, JAMES NEILSON, Colorado State University, ADAM ACZEL, GABRIELE SALA, Oak Ridge National Laboratory, JEFFREY A QUILLIAM, Physics, Université de Sherbrooke, KATE ROSS (Presenter), Colorado State University — The quantum dimer magnet (QDM) is the canonical example of 'quantum magnetism'. This state consists of entangled nearest-neighbor spin dimers and often exhibits a field-induced 'triplon' Bose-Einstein condensate (BEC) phase. I will discuss a new QDM in the strongly spin-orbit coupled, distorted honeycomb-lattice material Yb$_2$Si$_2$O$_7$. Single crystal neutron scattering, specific heat, and ultrasound velocity measurements reveal a gapped singlet zero field ground state with sharp, dispersive excitations. We find a field-induced magnetically ordered phase reminiscent of a BEC phase, with exceptionally low critical fields of $H_{c1} \sim 0.4$ T and $H_{c2} \sim 1.4$ T. Using inelastic neutron scattering we observe a Goldstone mode that persists throughout the entire field-induced magnetically ordered phase, suggestive of the spontaneous breaking of U(1) symmetry expected for a triplon BEC. However, in contrast to other well-known cases of this phase, the high-field ($H > 1.2$T) part of the phase diagram in Yb$_2$Si$_2$O$_7$ is interrupted by an unusual regime signaled by a change in the field dependence of the ultrasound velocity and net magnetization, as well as the disappearance of a sharp anomaly in the specific heat. These measurements raise the question of how anisotropy in strongly spin-orbit coupled materials modifies the field induced phases of QDMs.

Dimensionality of the BEC state in structurally healed Sr-doped BaCuSi$_2$O$_6$

DAGMAR WEICKERT (Presenter), MARCELO JAIME, Los Alamos Natl Lab, PASCAL PUPHAL, Paul-Scherrer-Institute, SHUSAKU IMAOJO, YOSHIMITSU KOHAMA, Tokyo University, JOOSEP LINK, RAIVO STERN, NICBP, Tallinn — In the last 20 years, more than a dozen quantum paramagnets have been identified to show properties consistent with the formalism of Bose-Einstein condensation (BEC) when a magnetic field is used to induce XY-type AFM order at cryogenic temperatures. Among them, BaCuSi$_2$O$_6$ orders between critical fields $H_{c1} = 23.5$T and $H_{c2} = 49$T, below $T_{c,max} = 4$K. However, BaCuSi$_2$O$_6$ additionally undergoes a structural phase transition at 90K into a monoclinic lattice at lower temperature causing a spatial modulation of the spin gap along the c-axis. This spin gap modulation is suspected to be the reason for a dimensional crossover in the magnetic excitations spectrum observed in the critical exponent of the phase transition close to $H_{c1}$. We discuss experimental results on newly synthesized single crystals BaCuSi$_2$O$_6$ doped with 10% Sr, structurally healed, which do not exhibit a phase transition at 90K and allow the investigation of the BEC close to $H_{c1}$ in the absence of spin gap modulation. We establish the $H-T$ phase diagram based on magnetization, magnetic torque, specific heat and magnetocaloric effect (MCE) measurements in DC and pulsed magnetic fields that address the dimensionality of excitations in the BEC critical exponents.
10:00AM R47.00007: Unconventional critical behavior in the quasi-one-dimensional $S = 1$ chain NiTe$_2$O$_5$  JUN HAN LEE, Ulsan Natl Inst of Sci & Tech, MARIE KRATOCHVÍLOVÁ, Seoul National University, HUIBO CAO, Oak Ridge National Laboratory, ZAHRA-SADAT YAMANI, Canadian Neutron Beam Centre, JUNGSOO KIM, University of Florida, JE-GUEN PARK, Seoul National University, GREGORY RANDALL STEWART, University of Florida, YOON SEOK OH (Presenter), Ulsan Natl Inst of Sci & Tech — The physical quantities develop with critical behavior near the (quantum) critical regime of correlated systems, such as superfluid density of two dimensional superconductor, surface critical behavior in topological phase, Higgs mode in quantum antiferromagnet, quantum criticality in multiferroics, quantum phase transition in two-dimensional electron system, etc. Despite the variety of complex interactions and correlations, the critical behavior only depends on global properties such as the spatial dimension, the symmetry of the order parameter, and the range of interaction. Recently we found a new quasi-one-dimensional chain compound NiTe$_2$O$_5$, in which spin-1 of Ni$^{2+}$ ions form a one-dimensional chain structure through NiO$_6$ octahedra’s edge-sharing. Although it undergoes a long-range antiferromagnetic (AFM) order with an archetypical anisotropic AFM anomaly at $T_N = 30.5$ K, the AFM order parameter develops with intriguing unconventional critical exponents. In this talk, we present magnetic properties and structure of NiTe$_2$O$_5$ and discuss its unconventional critical behavior.

10:12AM R47.00008: Magnetic phase diagram and anisotropy in the one-dimensional quantum spin system Rb$_2$Cu$_2$Mo$_3$O$_{12}$  SHOHEI HAYASHIDA (Presenter), DOMINIC BLOSSER, KIRILL POVAROV, ZEWU YAN, SEVERIAN GVASALIYA, ETH Zurich, ALEXEY PONOMARYOV, SERGEI ZVYAGIN, Helmholtz-Zentrum Dresden-Rossendorf, ANDREY ZHELUDEV, ETH Zurich — We report low temperature thermodynamic, magnetic and electron spin resonance (ESR) measurements on single crystal samples of a quantum spin chain material Rb$_2$Cu$_2$Mo$_3$O$_{12}$. In heat capacity measurement, phase transitions to magnetically ordered state are clearly observed, and the entire phase diagram is mapped out in detail. It is found that the criticalities of the transitions at lower and upper fields are dominated by three-dimensional order and one-dimensionality, respectively. The measured phase boundaries and ESR data prove that anisotropy heavily influences the magnetic state of Rb$_2$Cu$_2$Mo$_3$O$_{12}$ [1].

10:24AM R47.00009: Comparison of spin dynamics in green and black dioptase: from classical chains to quantum fluctuations*  ANDREY PODLESNYAK (Presenter), Oak Ridge National Lab, STANISLAV NIKITIN, Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany., OLEKSANDR PROKHNENKO, Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany, ALEXANDER KOLESNIKOV, Oak Ridge National Lab, TIMOTHY PRISK, National Institute of Standards and Technology, LAWRENCE (LARRY) M. ANOVITZ, Oak Ridge National Lab — The magnetic excitations of a gem crystal green dioptase Cu$_6$[Si$_6$O$_{18}$]·6H$_2$O and fully dehydrated black dioptase Cu$_6$Si$_6$O$_{18}$ have been studied by inelastic neutron scattering. The intrachain $J_c$ and interchain $J_{ab}$ interactions as well as the anisotropy of the $J_c$ have been determined. The observed spectrum of green dioptase contains two sharp magnetic modes and a prominent spin gap that is consistent with the ordered ground state of Cu moments coupled antiferromagnetically in spiral chains along the c axis and ferromagnetically in ab planes on the hexagonal cell. We found that dehydration has a dual effect on the magnetic interactions: it significantly increases the intrachain exchange interaction $J_c$, and simultaneously decouples the chains by suppressing $J_{ab}$. The spin dynamics of green dioptase are dominated by conventional magnon excitations, whereas the continuum of excitations observed in black dioptase indicates the presence of fractionalized spinons. We suggest that black dioptase behaves like a nearly ideal $S=1/2$ antiferromagnetic Heisenberg spiral chain with enhanced quantum fluctuations and weak spinon confinement $J_{ab}/J_c$~0.02.  

*This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

10:36AM R47.00010: Using muons to probe magnetic phases in quantum disordered systems through muon-induced distortions*  BENJAMIN HUDDART (Presenter), TOM LANCASTER, Durham University, FRANCIS L. PRATT, STFC — In muon-spin spectroscopy ($\mu^+\text{SR}$) experiments, concerns are often raised about the influence of the implanted muon on its local environment. In this talk, we will present examples where the distortions induced by the muon provide sensitivity to the magnetic state of the system. Transverse-field $\mu^+\text{SR}$ spectra for the strong-rung molecular spin ladder system (Hpip)$_2$CuBr$_4$ exhibit characteristic behaviour in each of the regions of the phase diagram [1]. Analysis of the muon stopping sites in this compound, obtained from density functional theory calculations, suggests that the magnetic field shift at the muon site in the quantum disordered phase results from a local muon-induced antiferromagnetic state. We propose that a similar mechanism enables the detection of field-induced transitions in the quantum spin liquids (QSLs) $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ and $\kappa$-(BEDT-TTF)$_2$Ag$_2$(CN)$_3$. In these cases, the field distributions seen by the muon correspond to those expected from adjacent ordered phases in the 2D triangular lattice QSL phase diagram. 


*BMH thanks STFC for support via a studentship. We thank EPSRC for financial support under grants EP/N024028/1 and EP/N024486/1.
We study the phases and phase transitions of a spin-1 chain with next-nearest neighbor (NNN) interaction $J_2$ and uniaxial single-ion anisotropy $D$ by density-matrix renormalization group method. We reconfirm the topological first-order transition of the $J_1$-$J_2$ chain by the bond reversal method [Q. Luo, et al., Phys. Rev. B 100, 121111(R) (2019)], and we show accurately that the transition occurs at $J_{2,t} = 0.7607(2)$. When considering a negative $D$, there is a spontaneously dimerized phase so as to avoiding the direct transition between the Neel phase and the NNN-Neel phase. The Neel--Dimer transition is of Gaussian type with central charge $c = 1$, while the NNN-Neel--Dimer transition belongs to the 2D Ising universality class. For the positive $D$ case, there is a gapless chiral phase with a broken parity symmetry. It separates the NNN-Haldane phase and the large-$D$ phase before the direct transition between the two. We also determine the topological critical points between the Haldane phase and the large-$D$ phase by the level spectroscopy technique supplemented by the Richardson method. The critical point is obtained with spectacular accuracy, $D_c = 0.96847256(2)$, for the frustration-free case.
8:00AM R48.00001: Chirality polarization and spectral bulk-boundary correspondence

AKITO DAIDO (Presenter), YOUICHI YANASE, Kyoto Univ — Surface physics dominated by bulk properties is attracting much attention. For example, bulk-boundary correspondence predicts topological boundary states. Another important context is the electric polarization: Surface charge is the bulk property modulo a quantum [1]. This relation is analogous to BBC, in the sense that physics apparently sensitive to the surface details is the bulk property. It is an interesting question whether this "BBC" can be generalized to the other physical quantities.

Recently, Tamura et al. proposed by numerics that surface accumulation of odd-frequency Cooper pairs is the bulk property [2]. This relation is named spectral bulk-boundary correspondence (SBBC). However, formal proof for SBBC has been lacking.

In this work, we prove SBBC based on the analogy with electric polarization: SBBC can be regarded as polarization of chiralities.


*This work was supported by Grant-in Aid for Scientific Research on Innovative Areas "J-Physics" (No.~15H05884) and "Topological Materials Science" (No.~18H04225) from JSPS of Japan, and by JSPS KAKENHI Grants No. 15K05164, No. 15H05745, No. 17J10588, No.~18H01178, and No.~18H05227.

8:12AM R48.00002: Exciton-induced Charge Fluctuations in One-dimensional Quasi-periodic “Metallic” Chains: A Possible Embodiment of Room Temperature Superconductivity

PAUL GRANT (Presenter), W2AGZ Technologies — It is well known that a purely periodic chain of odd-electron atoms, nominally expected to exhibit metallic behavior, is unstable to charge/spin spatial displacement which lowers its ground state energy by gapping its multi-degenerate Fermi surface, in this case consisting of nesting parallel sheets. It is largely for these reasons that superconductivity is not observed in highly one-dimensional metals -- it is simply energetically more favorable for CDW/SDW gaps to form, rather than a BCS state, at least one mediated by electron-phonon coupling. In this talk, we explore the hypothetical electronic properties of a nominally "metallic" quasi-periodic chain using both an analytical approach and computationally with density functional theory, searching for configurations which yield "gap-lets" sufficiently small to permit the formation of BCS pairs as the new energetically favored ground state. The particular embodiment we examine is a string of aluminum atoms with interatomic spacing determined by a Fibonacci sequence. We propose a path to attempt synthesis of such a structure for experimental examination, and perhaps leading to an entirely new class of higher temperature superconductors.

A New Superfast Method for Combinatorial Search of High-Temperature Hydride Superconductors under Extreme Pressures  TIANRAN CHEN (Presenter), TANER YILDIRIM, National Institute of Standards and Technology — Due to the low atomic mass and high electron-phonon coupling strength of hydrogen, hydride compounds under extreme pressures are most promising in the search for high-Tc superconductors. First-principles based computational search has become extremely important not only predicting new materials but also guiding high-pressure experimental measurements. However, the calculation of electron-phonon coupling and the corresponding Tc for a given system is usually computationally very expensive, limiting the application of computational search to a few numbers of candidate systems. In this work, we have developed a super-efficient and fast method for searching high-Tc hydride superconductors. We introduce new "metrics" that are strongly correlated to strong electron-phonon coupling and Tc but it is much faster to calculate them. Using our new method, we have searched more than 50,000 binary hydride superconductors and predicted many new high-Tc systems, one of which may even break the current record. Our work will not only greatly accelerate the discovery of new hydride superconductors but also give a detailed understanding of important factors that yield superconductivity near room temperature at high pressures.

Emergent unconventional superconductivity in doped valence bond solid insulators  ZIXIANG LI (Presenter), DUNGHAI LEE, University of California, Berkeley — In this talk, I will discuss the unconventional superconductivity and non-Fermi liquid behavior in the doped valence bond solid insulators. Through sign-problem-free Quantum Monte Carlo simulation, we investigate the superconductor emergent from the doped valence bond solid insulators, which shares many properties with the superconductivity in doped resonance valence bond phases. Close to the valence bond solid quantum critical point, we observe the Non-Fermi liquid properties from the transport behavior. Our study sheds new light on Cooper pairing in the presence of strong Coulomb interaction. Moreover, this result might point to a new direction for searching high-Tc superconducting materials.
Possible counterintuitive enhancement of superconductivity in ladder-type cuprates by longitudinal compression

KAZUHIKO KUROKI (Presenter), HIKARU SAKAMOTO, Department of Physics, Osaka University — We explore how the electron hoppings of the ladder type cuprates are affected when uniaxial compression or tension is applied to the lattice in the leg or rung directions, and investigate its consequences to superconductivity. For simplicity, we consider the two-leg ladder cuprate without the chains, that is, SrCu$_2$O$_3$, although this material is known to be difficult to dope carriers. By constructing a model based on first principles calculation, we surprisingly find that the ratio $t_r/t_l$, where $t_r$ ($t_l$) is the nearest neighbor hopping in the rung (leg) direction, is enhanced when the lattice is compressed in the leg direction or stretched in the rung direction. This counterintuitive manner of the hopping variation can be attributed to the on-site hybridization between Cu $d_{x^2-y^2}$ and Cu 4$s$ orbitals, which arises due to the low symmetry of the lattice. We apply the fluctuation exchange approximation to the model and study how superconductivity is affected under uniaxial deformation. Due to the above mentioned variation of the hoppings, we find that the superconducting transition temperature is enhanced when the lattice is compressed in the leg direction, opposed to an intuitive expectation. The effect is expected to be strong especially in the electron-doped regime.

Ground state phase diagram of the doped Hubbard model on a two-leg ladder

CHENG PENG (Presenter), YI-FAN JIANG, SIMES, SLAC National Accelerator Laboratory and Stanford University, YUVAL GANNOT, Stanford University, CHAO-MING JIAN, University of California, Santa Barbara, STEVEN KIVELSON, Stanford University, HONG-CHEN JIANG, SIMES, SLAC National Accelerator Laboratory and Stanford University — We have revisited the problem of the two-leg Hubbard ladder using DMRG methods but keeping larger number of states than in previous studies so as to obtain definitive results on the long-distance behavior of relevant ground-state correlation functions. In light of recent evidence that relatively small changes in the ratio of next nearest height for nearest neighbor hopping matrix, $t'/t$, can cause transitions between distinct ground-state phases, we have studied the model for a range of $t'/t$, electron density per site, $n$, and for several "intermediate" values of $U/t$. We find for a broad range of $t'/t$ the ground-state exhibits quasi-long-range singlet superconducting order. For $t'/t$ negative and large enough, two additional phases are found: One is characterized by commensurate charge-density-wave long-range order and a single gapless spin mode. Unexpectedly, for a relatively narrow range of negative $t'/t$, there exists an exotic intermediate phase with gapless charge and spin excitations, but one less gapless mode than for the non-interacting system.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under contract DE-AC02-76SF00515.
Finding the breakdown of the linear Holstein model using determinant quantum Monte Carlo*  STEVEN JOHNSTON (Presenter), PHILIP DEE, University of Tennessee, Knoxville, JENNIFER COULTER, Harvard — A large-scale effort is underway to determine when vertex corrections are required to the Migdal approximation for electron-phonon (e-ph) coupled systems. Most often, the underlying model for these studies is the simple Holstein Hamiltonian, which captures e-ph interactions as an on-site coupling of electrons to the linear displacement of the phonon field operators. When these displacements are large, however, introducing nonlinear corrections to the e-ph interaction can significantly alter measured correlations. Using determinant quantum Monte Carlo, we compared pairing and charge density wave correlations obtained with and without second-order nonlinear corrections. We find signs of disagreement between the linear and nonlinear models for relatively small values of the dimensionless e-ph coupling λ, and importantly, these discrepancies often occur in the same parameter regions where Migdal's theorem breaks down. Our results suggest that questions of the validity of Migdal's theorem go hand in hand with questions of the validity of the linear Holstein model.

*This work was supported by the SciDAC program funded by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

The superconducting $T_c$ and the metal-insulator transition in the Hubbard-Holstein model  TAE-HO PARK (Presenter), HAN-YONG CHOI, Sungkyunkwan Univ — We present that the maximum superconducting $T_c$ is on the phase boundary between metallic and insulating states of the normal state in the Hubbard-Holstein model. It is a prototype model including the local Coulomb interaction $U$ and the electron-phonon coupling $g$. We performed the dynamical mean field theory (DMFT) calculations employing the numerical renormalization group (NRG) technique and identified the normal state phase diagram for the metal-insulator transition. Interestingly, local maximum $T_c$ occurs along the lower critical phase boundary $g_{c1}$ of the 1st order metal-insulator transition in the normal state where the quantum fluctuation becomes maximum. Implications of this finding will be discussed in comparison with the quantum critical superconductivity. In addition, we obtained the electron-phonon coupling spectra $\alpha^2 F(\omega)$ and examined whether the maximum $T_c$ calculated from the Eliashberg theory lies on the $g_{c1}$. 
9:36AM R48.00009: Pairing correlations in the cuprates: a numerical study of the three-band Hubbard model*  
PEIZHI MAI (Presenter), Oak Ridge National Lab, STEVEN JOHNSTON, Department of Physics and Astronomy, University of Tennessee knoxville, THOMAS MAIER, Oak Ridge National Lab — We study the three-band Hubbard model for the copper oxide plane of the high-temperature superconducting cuprates using exact diagonalization, determinant quantum Monte Carlo, and dynamical cluster approximation (DCA) with an emphasis on pairing correlations. Using these methods, we provide a comprehensive view of pairing in the model. Specifically, we compute the pair-field susceptibility for these methods and study its dependence on temperature, doping, interaction strength, and charge-transfer gap. Using DCA, we also solve the Bethe-Salpeter equation for two-particle Green's function to identify the dominant pairing correlations and its orbital composition, and to determine the transition temperature to the superconducting state.

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

9:48AM R48.00010: Explaining the Anomalous Isotope Shift in Cuprate High Temperature Superconductivity  
DENNIS NEWNS (Presenter), GLENN MARTYNA, Pimpernel SSIT, NY, SOUMYA KANTI GANGULY, Physics, Indian Institute of Science — The pairing mechanism of cuprate High Temperature Superconductors is still controversial. A vibrational component to the pairing mechanism is suggested by the anomalous Isotope Shift (IS), which is of order the BCS value at dopings well below the maximum Tc, but is very low at dopings close to the maximum Tc. Here, based on the Fluctuating Bond Model [1] (FBM), we re-examine the IS issue focusing on the oxygen soft mode associated in the FBM with the pseudogap - knowing that a soft mode plus a van Hove singularity in the electronic density of states is one mechanism capable of leading to the cuprate-type anomalous IS [2]. A quantum mechanical treatment of the FBM model in Born-Oppenheimer approximation shows soft excitations of a few meV. Solving the Eliashberg equation we evaluate the IS, and will present the results.

10:00AM R48.00011: Tendency of nematicity in the extremely underdoped t-J model*

YIHSUAN LIU (Presenter), Institute of Physics, Academia Sinica, Nankang, Taiwan, WEI-LIN TU, Institute for Solid State Physics, The University of Tokyo, Kashiwa, Japan, TING-KUO LEE, Department of Physics, National Sun Yat-sen University, Kaohsiung, Taiwan — Underdoped cuprates exhibiting electronic nematicity have been reported by various measurements such as scanning tunneling microscopy (STM) [1, 2] and resistivity [3]. These results indicate that nematicity already exists in very lightly doped thin film, which motivates us to study the extremely underdoped t-J model and Heisenberg model via variational Monte Carlo (VMC) method and renormalization mean-field theory (RMFT). In the previous VMC study of the Heisenberg model, various groups have confirmed that the uniform RVB+AFM trial wave function has the lowest energy [4], which is very close to the best numerical estimation of the exact ground state energy. However, we found that various C4 broken states are almost degenerate with the uniform solution. Also, we will study the lightly doped cases with one hole only.


*The authors are grateful for the support of Taiwan Ministry of Science and Technology Grant MOST 108-2112-M-110-015

10:12AM R48.00012: Nematic superconductivity in twisted bilayer graphene*

DMITRY CHICHINADZE (Presenter), LAURA CLASSEN, ANDREY CHUBUKOV, University of Minnesota — Twisted bilayer graphene (TBG) shows insulating and superconducting phases in connection with an exceptional flattening of its lowest-lying energy bands. In the hole-doped case with the highest critical temperature the superconducting state is nematic, i.e. the threefold lattice rotation symmetry is broken inside the superconducting phase. We analyze superconductivity near Van Hove (VH) filling in TBG within an itinerant approach. In particular, we present a mechanism for nematic superconductivity, which originates in the interplay of two superconducting orders with similar critical temperatures. We argue that TBG can be properly described by patch models with six VH points for electron and twelve for hole doping reflecting the electron-hole asymmetry. We obtain the pairing interactions being dependent on twist-induced non-local interactions. For hole-doping, two channels with almost equal coupling constants are attractive. We show that the ground state is a nematic phase of coexistence. We find two possible mixed states, one is time-reversal symmetric, the other breaks time-reversal in addition to the lattice rotation symmetry.

*The work was supported by U.S. DOE, Office of Science, Basic Energy Sciences, under Award No. DE-SC0014402.
Magnetic and superconducting correlation in monolayer and twisted bilayer graphene

TIANXING MA (Presenter), Beijing Normal Univ — Using exact quantum Monte Carlo method, we identify the phase diagram of the half filled, the lightly doped and heavily doped graphene. At half filling, the system is driven to a Mott insulator with antiferromagnetic long range order by increasing interaction, and a transition from a $d+i d$ pairing to a $p+i p$ pairing is revealed, depends on the next-nearest hoping and the electronic fillings. We also examine the recent novel electronic states seen in magic-angle graphene superlattices. We reveal that an antiferromagnetically ordered Mott insulator emerges beyond a critical $U_c$ at half filling, and with a small doping, the pairing with $d+i d$ symmetry dominates over other pairings at low temperature. The effective $d+i d$ pairing interaction strongly increase as the on-site Coulomb interaction increases, indicating that the superconductivity is driven by electron-electron correlation. Our non-biased numerical results demonstrate that the twisted bilayer graphene share the similar superconducting mechanism of high temperature superconductors, which is a new and idea platform for further investigating the strongly correlated phenomena.

This work was supported by NSFC (Nos. 11774033 and 11974049) and Beijing Natural Science Foundation (No.1192011).

Superconductivity in the doped quantum spin liquid on the triangular lattice

HONG-CHEN JIANG (Presenter), SLAC - Natl Accelerator Lab — Broad interest in quantum spin liquid (QSL) phases was triggered by the notion that they can be viewed as insulating phases with preexisting electron-pairs, such that upon light doping they might automatically yield high temperature superconductivity. Yet despite intense efforts, definitive evidence showing that doping QSLs leads to superconductivity has been lacking. We address the problem of a lightly doped QSL through a large-scale density-matrix renormalization group study of the $t$-$J$ model on the triangular lattice with a small but non-zero concentration of doped holes. We provide direct evidences that doping QSL can naturally give rise to superconductivity. The ground state is consistent with a Luther-Emery liquid with power-law superconducting and charge-density-wave correlations but short-range spin-spin correlations. Specifically, the superconducting correlations are the dominant correlations on both four-leg and six-leg cylinders, indicating that long-range superconductivity would emerge in doping QSL in two dimensions.

This work was supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.
10:48AM R48.00015: Supoerconductiviy in the doped chiral spin liquid on triangular lattice*

YI-FAN JIANG (Presenter), HONG-CHEN JIANG, SLAC and Stanford Univ — Theory proposes that doping chiral spin liquid (CSL) can give rise to topological superconductivity. Yet it has been extensively studied in the past, definitive evidences showing this has been lacking. We address this problem by studying the t-J model supplemented by spin chiral interaction (with coupling $J^\chi$) on the triangular lattice using density-matrix renormalization group. It has been established that the ground state of the system at half-filling is a CSL when $0.32 \leq J^\chi / J \leq 0.56$, or equivalently $\nu=1/2$ bosonic fractional quantum Hall state. Interestingly, we find that the ground state of the system upon light doping the CSL is consistent with a Luther-Emery liquid, which is characterized by quasi-long-range superconducting and charge-density-wave correlations but with a finite spin gap and one gapless charge mode. Furthermore, we show that the superconducting correlations are the dominant correlations and its pair symmetry is consistent with d+id-wave.

*This work was supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract DE-AC02-76SF00515.

Thursday, March 5, 2020 8:00 AM - 10:36 AM

Session R49 DCMP: Superconducting Proximity Effect and Josephson Junctions IV Mile High Ballroom 1B - Thomas Bullard, UES, Inc.

8:00AM R49.00001: Search for Majorana bound states in niobium-Bi2Se3-niobium arrays and junctions* XIANGYU SONG (Presenter), YANG BAI, GUANG YUE, JAMES N ECKSTEIN, DALE J VAN HARLINGEN, ALEXEY BEZRYADIN, University of Illinois at Urbana-Champaign — Under the right conditions, Majorana bound states (MBS) are believed to live in lateral Josephson junctions formed by depositing s-wave superconductors onto the surface of topological insulator thin films, e.g., Bi2Se3.

We have fabricated and measured lateral superconductor-topological insulator-superconductor (S-TI-S) single junctions, square arrays, transmon geometries, and other geometries to look for the signatures of MBS.

Our experiments include Fraunhofer patterns on such patterns, which show some signature kinks at fields less then flux quantum, lifted nodes, and missing critical current maxima. We will discuss extensive measurement performed on niobium-Bi2Se3 hybrid structures in microwave resonators, which include kinetic inductance vs. magnetic field and the quality factor vs. magnetic field measurements. The possibility of making a transmon qubit with a topological insulator film will be discussed.

*The work is supported by NSF-DMR 1836710 grant and by Army Research Office under agreement W911NF1910067.
8:12AM R49.00002: Growth and Characterization of (Bi\textsubscript{x}Sb\textsubscript{1-x})\textsubscript{2}Te\textsubscript{3}/MgB\textsubscript{2} heterojunctions
LONG CHENG (Presenter), LIN LI, University of Waterloo, HUI ZHANG, XIAODONG MA, Hefei National Laboratory for Physical Sciences at the Microscale (HFNL), University of Science and Technology of China, GEORGE NICHOLS, PETER SPRENGER, DELER LANGENBERG, DAVID CORY, GUOXING MIAO, University of Waterloo — Topological insulator-superconductor heterostructure, which was predicted to be an ideal system to search Majorana Fermions, has been extensively studied in recent years. Zero bias conductance peak (ZBCP) in such system was reported as a signature of Majorana bound states by several groups. Here we report the growth of epitaxial (Bi\textsubscript{x}Sb\textsubscript{1-x})\textsubscript{2}Te\textsubscript{3} (BST) thin film on MgB\textsubscript{2} and study the vertical Josephson junction based on BST/MgB\textsubscript{2}. The interface of BST/MgB\textsubscript{2} was found to be chemically reactive. Substrate temperature has to be lowered than typical growth temperature of BST to inactivate the reaction. In addition, a 2.5nm thin Nb layer inserted in between BST and MgB\textsubscript{2} can significantly improve the interface quality with little reduction to the pairing gap. Finally, 50nm Nb thin film was deposited on top to form the Nb/BST/MgB\textsubscript{2} and Nb/BST/Nb/MgB\textsubscript{2} junction. The former one shows tunneling behavior due to the formation of insulating layer at the interface of BST/MgB\textsubscript{2}, while the latter one behaves more like a Josephson junction. ZBCPs were observed in both the junctions, which survive even above 4.2K, much higher than previously reported. Our study provides a new design for searching Majorana Fermions which may exist at a higher temperature than before.

8:24AM R49.00003: Shapiro steps as a thermal probe in superconducting nanobridges*
CONNOR SHELLY (Presenter), PATRICK SEE, IVAN RUNGGER, JONATHAN WILLIAMS, National Physical Laboratory — We present measurements of microwave-induced Shapiro steps in a superconducting nanobridge weak link in the dissipative branch of a hysteretic current-voltage characteristic. Typically the hot-spot Joule heating in nanobridges is suggested to extend many micrometers beyond the nanobridge itself and into the superconducting electrodes heating the system above the critical temperature. We demonstrate that the Shapiro steps can be used to infer a reduced critical current and an associated local temperature. The observation of the Shapiro steps in the dissipative branch of the IVC show that a finite Josephson coupling exists in the dissipative state, and although the nanobridge is heated, our thermal model shows that the temperature remains always below the critical temperature. This work provides evidence that Josephson behaviour can remain in thermally-hysteretic nanobridges and allows extension of the temperature range that nanobridge devices (e.g., SFQ circuits, nanoSQUIDs) can be operated in.

*This work is funded as part of a feasibility study funded by Innovate UK: Project number 102677. Co-funding by the UK NMS Programme.
8:36AM R49.00004: Towards Perfect Andreev Reflection in Graphene-NbSe$_2$ planar Josephson Junctions  ADAM KRISTOPHER WILLIAMS (Presenter), MITALI BANERJEE, CORY DEAN, Physics, Columbia University — Several theoretical proposals suggest that combining 2D superconductors with 2D semiconductors could provide a rich platform to study novel quantum phases such as Majorana zero modes — fractional quasiparticles localized at boundaries of topological superconductors. However, interfacing these two phenomena with high interfacial transparency remains a longstanding challenge. The rapidly growing catalogue of 2D Van der Waals materials provides a platform for making atomically clean interfaces between materials with a variety of properties. In this talk I will present newly developed techniques to assemble NbSe$_2$-graphene Josephson junctions such that we simultaneously improve the junction transparency while also maintaining high mobility in the graphene channel. Transparent graphene-NbSe$_2$ contacts as a platform to explore planar topological Josephson junctions will be discussed.

8:48AM R49.00005: Tunneling spectroscopy of c-axis epitaxial cuprate junctions*  DOUGLAS NATELSON (Presenter), PANPAN ZHOU, Physics and Astronomy, Rice University, LIYANG CHEN, Applied Physics Graduate Program, Rice University, ILYA SOCHNIKOV, Department of Physics, University of Connecticut, TSZ CHUN WU, MATTHEW FOSTER, Physics and Astronomy, Rice University, ANTHONY TRAVIS BOLLINGER, XI HE, IVAN BOZOVIC, Brookhaven National Laboratory — Tunnel junctions are valuable tools for electronic spectroscopy, with epitaxial structures minimizing extrinsic effects of disorder. We report tunneling spectroscopy measurements, over a broad temperature and bias range, in c-axis La$_{2-x}$Sr$_x$CuO$_4$/La$_2$CuO$_4$/La$_{2-x}$Sr$_x$CuO$_4$ heterostructures grown via atomic layer-by-layer molecular beam epitaxy. Above $T_c$ of the LSCO layers, these structures show the pseudogap, while below $T_c$, the devices show superconductor/insulator/superconductor (SIS) response. Down to 20 mK there is no Josephson critical supercurrent $I_c$, indicating strongly incoherent transport. Tunneling spectra show greatly suppressed coherence peaks. The $T=0$ zero-bias conductance remains at approximately 20-30% that of the normal-state, implying a substantial population of unpaired carriers. As temperature is raised, the superconducting gap fills in rather than closing at $T_c$. The spectra show an inelastic tunneling feature at $\sim 0.08$ eV, suppressed as $T$ exceeds $T_c$. We discuss how these properties are inconsistent with standard $d$-wave tunneling expectations, despite the structural perfection of the epitaxial stack.

*US DOE, BES, Materials Sciences and Engineering Division and award DE-FG02-06ER46337; Moore Foundation’s EPIQS Initiative grant GBMF4410; Welch Foundation Grant No. C-1809.
9:00AM R49.00006: Scanning Tunneling Spectroscopy Study of the Superconducting Proximity Effect in (110)-oriented Manganite/Cuprate and Nickelate/Cuprate Thin Films* 
RAINNI CHEN (Presenter), CHAO C ZHANG, CHRIS GRANSTROM, JOHN Y.T. WEI, Univ of Toronto — An anomalously long-ranged (~ 30 nm) superconducting proximity effect was previously reported in thin-film heterostructures of ferromagnetic La_{2/3}Ca_{1/3}MnO_3 (LCMO) and superconducting YBa_2Cu_3O_{7-δ} (YBCO), and attributed to the induction of spin-triplet pairing [1,2]. However, there remains debate over the existence of this long-ranged proximity effect, since scanning tunneling spectroscopy (STS) on c-axis LCMO/YBCO bilayers has failed to observe any direct and microscopic evidence of this effect [3]. In this work, we extend prior STS studies to (110)-oriented films, the orientation most likely to produce d-wave Andreev resonances that show up as zero-bias conductance peaks (ZBCP). We observe these ZBCPs ubiquitously on our unilayer YBCO films, but do not observe them on our bilayer LCMO/YBCO films down to an LCMO overlayer thickness of ~ 5 nm. The ZBCPs also do not appear on (110)-oriented LaNiO_3/YBCO bilayers, measured as a non-magnetic control. Our results are inconsistent with proximity-induced spin-triplet superconductivity in LCMO/YBCO structures.


*This work was supported by NSERC, CFI, OIT, and CIFAR.

9:12AM R49.00007: Absence of proximity induced superconductivity in Bi/Bi2212 heterostructure*  
ASISH KUNDU (Presenter), ILYA DROZDOV, ZEBIN WU, GENDA GU, TONICA VALLA, Condensed Matter Physics and Material Science, Brookhaven National Laboratory, Upton, NY, United States — Mixing of topological states with superconductivity could result in topological superconductivity, where the elusive Majorana fermions could be applied in fault-tolerant quantum computing. Recent study\(^{(1)}\) suggests that topological superconductivity might be possible to realize in a Bi /Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+δ}\) (Bi2212) heterostructure by inducing a pairing in the Rashba-spin–orbit-coupled states of Bi by proximity effect. Here, we present an angle-resolved photoemission spectroscopy study of ultrathin Bi films grown in-situ on Bi2212 that show the absence of proximity effect. We find that the electron transfer from the film to the substrate and the resulting severe underdoping of Bi2212 interface is a likely origin for the absence of proximity effect. We also propose a possible way of preventing a total loss of proximity effect in this system.

\(^{(1)}\) Shimamura et al., ACS Nano 12, 10977–10983 (2018).

*This work was supported by the US DOE, Office of Basic energy Sciences, contract no. DE- SC0012704
The proximity effect in disordered and quasiperiodic systems

GAUTAM RAI (Presenter), STEPHAN WOLFGANG HAAS, Univ of Southern California, ANURADHA JAGANNATHAN, Laboratoire de physique des solides, Université Paris-Sud — We investigate the superconducting proximity effect in one-dimensional hybrid rings with a superconducting and a normal part. We consider two cases: when the normal part is a) a weakly disordered crystal and b) quasiperiodic. We carry out self-consistent calculations using a real space mean field Bogoliubov-de Gennes type approach within the tight binding framework. For the disordered case we find that the decay of the superconducting order parameter into the normal region reflects the the band center anomaly—a cusp like deformation in the density of states around E=0 known to exist for weak disorder. The order parameter decay when the normal chain has a Fibonacci hopping sequence will be discussed as well, along with the key features that differentiate the proximity effect in the two cases.

Proximitized Josephson junctions in highly-doped InAs nanowires robust to optical illumination*

LILY YANG (Presenter), STEPHAN STEINHAUER, KTH Royal Inst of Tech, ELIA STRAMBINI, NEST-Pisa, Istituto Nanoscienze, THOMAS LETTNER, LUCAS SCHWEICKERT, MARIJN VERSTEEGH, KTH Royal Inst of Tech, FRANCESCO GIAZOTTO, VALENTINA ZANNIER, LUCIA SORBA, NEST-Pisa, Istituto Nanoscienze, DMITRY SOLENOV, Physics, Saint Louis University — We have studied the effects of optical-frequency light on proximitized InAs/Al Josephson junctions based on highly n-doped InAs nanowires at varying incident photon flux and at three different photon wavelengths. The experimentally obtained IV curves were modeled using a shunted junction model which takes scattering at the contact interfaces into account. The Josephson junctions were found to be surprisingly robust, interacting with the incident radiation only through heating, whereas above the critical current our devices showed non-thermal effects resulting from photon exposure. Our work provides guidelines for the co-integration of Josephson junctions alongside quantum photonic circuits and lays the foundation for future work on nanowire-based hybrid photon detectors.

*The fabrication and measurement at KTH are co-funded by Vinnova and Marie Curie Actions FP7-PEOPLE-2011-COFUND (GROWTH 291795), and the growth activity at NEST is cofunded by H2020-FETOPEN-2018-2020 (AndQC).
9:48AM R49.00010: Quantum phenomena in Unconventional 1D Josephson Arrays*  WENSEN LU (Presenter), KONSTANTIN KALASHNIKOV, PLAMEN KAMENOV, THOMAS J DINAPOLI, MICHAEL GERSHENSON, Rutgers University, New Brunswick — The largely unexplored regime of low transparency Josephson junction chains with low charging energy $E_C$ has attracted theoretical interest since it offers a platform to realize many-body effects in superconducting circuits [1] and quantum phase slip devices [2]. In this work we study the current-voltage characteristics (IVc) of Josephson junction with Josephson energy $E_J \sim E_C \sim 0.01-1K$ and temperature range 0.03-1K. We observed the suppression of switching current $I_{SW}$ and finite zero-biased-resistance $R_0$ for different $E_J/E_C$ and $E_J/T$ ratios due to thermally activated phase slips and macroscopic quantum phase tunneling. We will discuss the behavior of $I_{SW}$ and $R_0$ at different temperature and environmental impedance, and propose potential experimental conditions to observe many-body physics such as localization effects [1] and Bloch oscillations [2] as analogues to condensed matter systems.

1. Nonergodic metallic and insulating phases of Josephson junction chains, M. Pino, L. Ioffe, B. Altshuler, DOI: 10.1073/pnas.1520033113
2. Bloch oscillations in small Josephson junctions, K. Likharev, A. Zorin, DOI: 10.1109/TMAG.1985.1063671

*We acknowledge the funding from NSF with award number 1708954

10:00AM R49.00011: Proximity effects of niobium nano-hydrides on state of the art superconducting radio frequency Nb cavity*  ZUHAWN SUNG (Presenter), ALEXANDER ROMANENKO, ANNA GRASSELLINO, Fermilab — Nb hydrides are responsible for performance degradation at high accelerating field regime in a superconducting radio frequency cavity for the linear particle accelerator, known as high field Q slope (HFQS). Normal conductive Nb hydride precipitates at the cavity operation temperature , ~2K, and leads to breakdown of surface superconductivity due to proximity effect under RF magnetic field, from which significant power dissipation occurs on the cavity surface. In this study, precipitation of nano-meter scale Nb hydrides on a SRF Nb cavity surface is first directly observed using cryogenic atomic force microscopy, and statistical morphological features of Nb hydrides are compared with HFQS behaviors of state of the art SRF Nb cavities that have shown high accelerating gradient close to the theoretical limit, 50MV/m. Additionally, RF magnetic field enhancement due to Nb hydride topological properties are discussed.

*This work was partially supported by the United States DOE, Offices of Nuclear and High Energy Physics. Fermilab is operated by Fermi Research Alliance, LLC under Contract No. DE-AC02-07CH11359 with the U.S. Department of Energy.
10:12AM R49.00012: Low Temperature Annealing and the Generation of Superconductivity in Nickel-Bismuth Bilayers* MATTHEW VAUGHAN, NATHAN SATCHELL, MANNAN ALI, Univ of Leeds, CHRISTY KINANE, GAVIN STENNING, SEAN LANGRIDGE, ISIS Neutron and Muon Source, Rutherford-Appleton Laboratory, GAVIN BURNELL (Presenter), Univ of Leeds — Unconventional superconductivity has been suggested to be present at Ni/Bi interfaces in thin-film bilayers. We report a study of the structural, magnetic and superconducting properties of sputtered Bi/Ni bilayers. As-grown, our films do not display a superconducting transition. However, when stored at room temperature, after about 14 days our bilayers do develop a superconducting transition up to 3.8 K.

We perform structural characterization with X-ray diffraction and spin polarized neutron reflectometry, and measure magnetisation and low temperature electron transport for samples annealed at 70°C. We show that the onset of superconductivity in our samples is coincident with the formation of ordered NiBi$_3$ intermetallic alloy, known to be an s-wave superconductor. We find that the annealing process has a rather low activation energy of (0.86±0.06) eV. Gentle heating as typical for cleanroom processing will result in NiBi$_3$ formation which poses a challenge for studying distinct Bi/Ni interface behaviour.

*We acknowledge support from the UK STFC ISIS neutron and muon source (RB 1920455). The work was also supported financially by the UK EPSRC DTP and EP/M000923/1 and from the EU H2020 Marie Sklodowska-Curie Grant Agreement No. 743791 (SUPERSPIN).

10:24AM R49.00013: Superconducting Phase Slip Oscillations on Demand* IRIS DORN (Presenter), ARMEN GULIAN, Chapman Univ — Remarkable properties of phase slip centers (PSCs) have direct analog with weakly coupled superconductors (Josephson contacts, SNS-junctions, ScS systems, etc.). In typical 1-D wire models of these types, PSC oscillations arise in the geometric wire centers or, if more than one PSC, symmetrically to this center location. We add weak spots in the model, which shift the position of the PSCs away from the symmetric location in a degree dependent on the imperfection's character, by taking into account enhanced phonon feedback onto the Cooper-pair/normal metal system of the wire which generates these phonons. The inclusion of this effect into the time-dependent Ginzburg-Landau (TDGL) system of equations requires an additional function and corresponding equation in the TDGL system. Interestingly, the system finds there is a competition between the induced weak points and symmetry-induced locations. Thus using our approach the PSCs can be generated on demand and provides the opportunity to initiate PSCs at the required time and required place in the wire without changing its biasing properties with high accuracy theoretical modeling.

*ONR Grants N00014-16-1-2269, N00014-17-1-2972, N00014-18-1-2636, & N00014-1901-2265.
8:00AM R50.00001: Spin Hall magnetoresistance studies of differently strained ultrathin SrMnO$_3$ films
ARIJIT DAS (Presenter), ADAM J WATSON, ESWARA PHANINDRA VALLABHANENI, TAMALIKA BANERJEE, Univ of Groningen — The ability to tune magnetic ordering in a nominally antiferromagnetic insulator, making use of the co-dependence of the charge, spin and orbital degrees of freedom in transition metal oxides, opens a vast playing field in the area of antiferromagnetic spintronics. We use Spin Hall magnetoresistance (SMR) as a probe of the magnetic ordering in thin films of SrMnO$_3$ (SMO) when grown on two different substrates – SrTiO$_3$ (STO) and LaAlO$_3$ (LAO) - that changes the induced strain from tensile to compressive respectively. An in-plane magnetic field dependent angular measurement of the transverse resistivity of Pt Hall bars patterned on SMO films were studied for both cases. The compressively strained SMO film on LAO shows a 180° phase shift relative to the tensile strained SMO film on STO, suggesting a change in the magnetic ordering from antiferromagnetic to ferromagnetic. This is brought about by the presence of oxygen vacancies promoted by the underlying tensile strain in SMO on STO. This work shows the unique possibility of tailoring the magnetic properties in complex oxides with strain and the ability of interface spin-transport probes as SMR to fingerprint them, establishing their suitability for magnon transport studies.

8:12AM R50.00002: Orbital wave in the Raman scattering cross section of LaMnO$_3$*
PUREVDORJ MUNKHBAATAR (Presenter), Institute of Photonics and Information Technology, Jeonbuk National University, MYUNG-WHUN KIM, Department of Physics, Jeonbuk National University — We calculated the polarization-dependent Raman scattering cross-section spectra of LaMnO$_3$ below the A-type magnetic ordering temperature. Two strong peaks appear around the MnO$_6$ octahedra stretching phonon frequency. One mode shows Ag symmetry, while the other mode shows Bg symmetry. We found that the Ag symmetry peak is a Jahn-Teller phonon coupled to the orbital wave and the Bg symmetry peak is an orbital wave mode coupled to a Q2 phonon mode via the Jahn-Teller electron-phonon coupling.

*This research was supported by the National Research Foundation of Korea (Grants No. 2016R1D1A1B03934648 and No. 2016K2A9A1A09914398); by the National Research Foundation of Mongolia (Grant No. SSA 017/2016).
The Jahn-Teller (JT) distortion occurs in a single valance system where a structural distortion is needed to lift the orbital degeneracy. In the mixed valance system La$_{1-x}$Sr$_x$MnO$_3$ (LSMO), the JT transition remains robust and sharp. It is not clear if the distribution of Mn$^{3+}$ in Mn$^{4+}$ matrix plays an important role. On cooling, LSMO undergoes the cooperative JT transition to order orbitals, spin ordering transition, and the charge ordering transition[1]. Pair distribution function analysis of neutron powder diffraction data has previously been done to discuss the role of polarons in the transition[2,3]. With single-crystal neutron diffuse scattering (NDS), we have observed patterns that show an interesting evolution as it is cooled through three transitions. Weak rod-shaped NDS features along L with even H+K above $T_{JT}$ get enhanced as the temperature is cooled below $T_{JT}$, suggesting coherent scattering is developed above $T_{JT}$. The NDS features disappear below the charge ordering transition temperature $T_{CO}$, associated with the formation of superlattices. Potential models to interpret the observations will be discussed.


*This work was supported by National Science Foundation DMR-1720595.
**Visualization of Site- and Bond-Centered Charge Order in a Half-Doped Manganite**

ISMAIL EL BAGGARI (Presenter), Physics, Cornell University, DAVID J. BAEK, Electrical and Computer Engineering, Cornell University, MICHAEL J. ZACHMAN, Applied and Engineering Physics, Cornell University, DI LU, Physics, Stanford University, YASUYUKI HIKITA, Applied Physics, Stanford University, ELIZABETH NOWADNICK, Materials Science and Engineering, University of California Merced, HAROLD HWANG, Applied Physics, Stanford University, LENA KOURKOUTIS, Applied and Engineering Physics, Cornell University — Charge order instabilities, the ordering of electrons and spins into periodic structures, occur in many classes of correlated quantum matter. Within a superlattice, charge-ordered states may have distinct electronic patterns and symmetries, however, distinguishing between them is challenging. In half-doped manganites, for instance, both site-centered (stripe) and bond-centered (bi-stripe) orders have been proposed. Using cryogenic scanning transmission electron microscopy, we map the charge-ordered structure in a Nd1/2Sr1/2MnO3 thin film by measuring picoscale periodic lattice distortions. We find two distinct ground states coexisting over tens of nanometers. The first is consistent with site-centered order. The second represents bi-stripes which remarkably are not purely bond-centered. The bi-stripes are intermediate between bond- and site-centered order and break inversion symmetry.

*This work was supported by AFOSR (FA 9550-16-1-0305) and the NSF (NSF-MRI-1429155, DMR-1719875)*
8:48AM R50.00005: Probing Orbital Order in Magnetite with Resonant Elastic X-Ray Scattering*
NELSON HUA (Presenter), University of California, San Diego, JIANHENG LI, University of California, Davis, STJEPAN B HRKAC, ANATOLY SHABALIN, University of California, San Diego, ANDI BARBOUR, WEN HU, CLAUDIO MAZZOLI, STUART B WILKINS, Brookhaven National Laboratory, ROOPALI KUKREJA, University of California, Davis, ERIC FULLERTON, OLEG SHPYRKO, University of California, San Diego — The underlying mechanism driving the metal-insulator transition in magnetite and the presence of charge order in the low-temperature insulating state remain unresolved since Verwey first discovered this transition back in 1939. Standard X-ray diffraction studies are difficult to perform due to twinned domains, and the various studies investigating the bond lengths between Fe+2 and Fe+3 at the octahedral sites have shown at most a charge disproportionality. However, the presence of a Bragg forbidden (001/2) superlattice peak, which is only observable in the insulating state at resonant energies, is a hidden door into magnetite's charge and orbital states. We have used coherent soft x-rays at the Fe L-edge resonant energy to probe the orbital order at the octahedral Fe sites. An unexpected diffuse scattering ring about the (001/2) superlattice peak that exists in both the insulating and metallic phases was discovered simultaneously. By following the shape and intensity of this diffuse scattering ring in reciprocal space, we can map out the degree of correlated disorder of the Fe ions in both the metallic and insulating phases.

*The work at UCSD was supported by U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contracts No. DE-SC0001805.

9:00AM R50.00006: Metal-insulator transition with ferromagnetic background in the two-orbital model for manganites*
CENGIZ SEN (Presenter), Physics Department, Lamar University, ELBIO DAGOTTO, Physics Department, University of Tennessee — The complex spin, electron and phonon dynamics of manganese oxides continues to attract attention. In this talk, we present results of unbiased Monte Carlo simulations with fermionic exact diagonalization of the two-orbital model with Jahn-Teller phonons at filling x=1/3 on lattice sizes up to 15x15. We identify a region in the finite-temperature phase diagram with a metal-insulator transition upon increasing electron-phonon coupling. In the metal the spin background is ferromagnetic (FM) with uniform charge order, whereas the insulator shows diagonal stripes while retaining the FM background. We report resistivity and magnetization measurements alongside with spin and charge structure factors.

*The authors acknowledge support from the Advanced Computing Facility (ACF) at the National Institute of Computational Sciences (NICS).
9:12AM R50.00007: Gyrotropic birefringence via electromagnon resonance in multiferroic manganite

MAKIKO OGINO (Presenter), Applied physics, Univ of Tokyo, YOSHIO KANEKO, YOSHINORI TOKURA, Center for Emergent Matter Science (CEMS), RIKEN, YOUTAROU TAKAHASHI, Applied physics, Univ of Tokyo — The magnetoelectric (ME) coupling has been exemplified in the certain classes of crystalline solids including multiferroics and topological insulators. Since the ME coupling modifies the Maxwell’s equations, such ME materials give rise to the exotic electromagnetic phenomena. In particular, the light-matter interaction can induce the unconventional gyrotropy, which is called gyrotropic birefringence (GB), whereas its observation remains highly limited. We focus on the electrically active spin excitation i.e. electromagnon, inherent to the multiferroics, which potentially exhibits the enhanced optical ME effect. Here we report the first observation of GB on multiferroic manganite with spin-induced ferroelectricity by use of the time-domain terahertz polarimetry. The enhanced optical rotation arising from the GB was found on the electromagnon resonance. It is demonstrated that the GB is scaled by the bilinear coupling of ferroic order parameters $P \cdot M$ ($P$: Electric polarization, $M$: magnetization) in the magnetic field dependence. In addition, the quantitative spectral analysis reveals that the electromagnon and antiferromagnetic resonance cooperatively produce the enhanced GB, indicating the important role of inter-mode coupling for the enhanced dynamical ME effect.

9:24AM R50.00008: Torsional mode as order parameter in H-ErMnO$_3$: mode screening, Fröhlich resonance, bipolarons

NÉSTOR MASSA (Presenter), CONICET- Univ. Nac. La Plata, Argentina, AURELIEN CANIZARÈS, LEIRE DEL CAMPO, CNRS-CEMHTI, Orléans, France, KARSTEN HOLLDACK, HZB, BESSY II, Berlin, Germany, VINH TA PHUOC, GREMAN, Univ. François-Rabelais,Tours, France, PAULA KAYSER, CSEC-UE, Edinburgh, UK, JOSE ANTONIO ALONSO, ICMM-CSIC, Madrid, Spain — While far infrared absorption, normal reflectivity, and emission spectra of hexagonal ErMnO$_3$ give a quantitative picture of phonon softening and merging on heating, the torsional mode at ~306 cm$^{-1}$ (300 K), associated to the negative thermal expansion and a $c$ axis hybridization of O-2p with Er$^{3+}$ levels, displays at lock-in Tc~830 K a distinctive infrared line shape anomaly and reststrahlen screening within the context of a ferroelectric instability inferred for a Mott-Hubbard insulator. Since the longitudinal optical (LO) mode macroscopic field screening implies phonon dynamic coupling to charge fluctuations in an electron correlated insulating polar environment we used the above the gap $\lambda_{exc}$= 355 nm Raman line to turn on the Fröhlich mechanism at macroscopic field frequencies at which the interaction between carriers and the Coulomb long range, responsible of the TO-LO split, takes place. We found a new Raman activated band that has its contour red shifted overlapping the infrared reflectivity minimum. It implies a univocal visualization of a huge electron-lattice interaction concomitant with finding small polaron correlations for which that phonon mediates in the formation of high temperature H-ErMnO$_3$ mid-infrared bipolarons below the metal-insulator transition at ~1600 K.
9:36AM R50.00009: Doping evolution of the electronic structure in RENiO$_3$* JIARUI LI (Presenter), Massachusetts Institute of Technology MIT, ROBERT GREEN, University of Saskatchewan, ZHIHAI ZHU, GRACE H ZHANG, DA ZHOU, MIN GU KANG, Massachusetts Institute of Technology MIT, JERZY T. SADOWSKI, Brookhaven National Laboratory, RONNY SUTARTO, FEIZHOU HE, Canadian Lightsource, ZHEN ZHANG, YIFEI SUN, SHRIRAM RAMANATHAN, Purdue University, RICCARDO COMIN, Massachusetts Institute of Technology MIT — Rare earth nickelates (RENiO$_3$) exhibit metal-insulator transitions accompanied by the appearance of charge and spin order, at times concurrently. The understanding of the evolving ground state in these materials is hindered by the existence of multiple competing orders which are further coupled to various kinds of local perturbations (strain, defects, disorder). Very recently, control of carrier doping by means of oxygen stoichiometry has been achieved in RENiO$_3$, presenting an opportunity to study the broader electronic phase diagram of these systems. In this talk, I will present our recent soft X-ray spectroscopy, resonant scattering, and photoemission microscopy experiments on both pristine and electron doped RENiO$_3$. Our results reveal the doping evolution of the electronic structure in RENiO$_3$.

*This material is based upon work supported by the National Science Foundation under Grant No. 1751739

9:48AM R50.00010: Local metallic properties of LaNiO$_3$ detected using β-detected NMR VICTORIA KARNER (Presenter), ARIS CHATZICHRISTOS, DAVID L CORTIE, MARTIN H DEHN, OLEKSANDR FOYEVTSOV, KATERYNA FOYEVTSOVA, DEREK FUJIMOTO, ROBERT F KIEFL, University of British Columbia, PHILIP C. P. LEVY, RUOHONG LI, TRIUMF, RYAN M. L. MCFADDEN, University of British Columbia, GEORGE MORRIS, DAVID PEARSON, MONIKA K STACHURA, TRIUMF, JOHN TICKNOR, University of British Columbia, GEORG CHRISTIANI, GENNADY LOGVENOV, FRIEDERIKE WROBEL, BERNHARD KEIMER, Max Planck Institute for Solid State Research, JUNJIE ZHANG, JOHN MITCHELL, Argonne National Laboratory, W ANDREW MACFARLANE, University of British Columbia — The rare earth nickelates (RNiO$_3$) are a prototypical example of a metal-insulator transition in strongly correlated materials; LaNiO$_3$ is the only RNiO$_3$ that remains metallic. Here, we will compare measurements on a single crystal and a thin film of LaNiO$_3$ using β-detected NMR. Analogous to μSR, β-NMR is a sensitive local probe of the electronic and magnetic properties of materials through the coupling between the $^8$Li nuclear spin and the electromagnetic properties of the host material and; therefore, provides a unique, local perspective. We find clear evidence of metallic behaviour and no static magnetism. However, the detailed account of the data appears inconsistent with the commonly considered distorted perovskite structure[1].

References:
1. V.L. Karner et al. Phys. Rev. B., 100; 165109, 2019
10:00AM R50.00011: Electron- and Hole-Doping Effects on the Metal-Insulator Transition in “113” Nickelates [RNiO$_3$, $R = \text{Pr, Nd, (La,Y)}$] Prepared at High Oxygen Pressure*  
GREGORIO PONTI, ZACHARY P. KUKLINSKI, QUINN D. B. TIMMERS, JOHN MARKERT (Presenter), Department of Physics, University of Texas at Austin — We report x-ray diffraction, electrical resistivity, and other data on bulk polycrystalline materials prepared under high oxygen pressure (150–200 bar) at high temperature ($T \approx 1000^\circ$C). These conditions stabilize the nearly simple-perovskite “113” structure, RNiO$_3$. For the orthorhombic parent compounds with the largest rare-earth ions that exhibit a metal-insulator transition, $R = \text{Pr and Nd}$, we dope with divalent Sr and Ba (hole doping) and tetravalent Ce and Th (electron doping). Results for Nd$_{1-x}$A$_x$NiO$_3$ ($A = \text{Sr, Ce, Th}$) have been reported previously$^1$: for example, for Ce$^{4+}$, the net effect on the metal-insulator transition, $\partial T_{\text{MI}}/\partial x \approx -220$ K, was corrected for size effects to obtain a bare electron-doping effect, $\partial T_{\text{MI}}/\partial x_{\text{elec}} \approx -1100$ K. Remarkably in our study, we find that, for Pr$_{1-x}$Ce$_x$NiO$_3$, the shift in the metal-insulator transition temperature with concentration $x$ is positive, with a net $\partial T_{\text{MI}}/\partial x \approx +225$ K. Also, we find hysteresis in the metallic resistivity of rhombohedral La$_{1-x}$Ce$_x$NiO$_3$, perhaps a signature of low-$T$ pseudogap monoclinic short-range order.$^2$


*Support from The University of Texas, College of Natural Sciences Freshman Research Initiative.

10:12AM R50.00012: Large magnetic excitation gap in antiferromagnetic YNiO$_3$ detected by NMR*  
LUKAS KOROSEC (Presenter), ETH Zurich and University of Geneva, DARIUSZ GAWRYLUK, MARISA MEDARDE, Paul Scherrer Institute, TONI SHIROKA, HANS RUDOLF OTT, JOEL MESOT, ETH Zurich and Paul Scherrer Institute — The rare-earth nickelate perovskites (RENiO$_3$) are an archetypal family of strongly correlated electron materials. Their antiferromagnetic state with four nickel atoms per period remains poorly studied, even though it has been predicted to be a type-II multiferroic with large polarization. Currently, there is no agreement on the magnetic structure and low-energy spin model for bulk RENiO$_3$. We present $^{17}$O nuclear-spin–lattice relaxation measurements demonstrating the presence of a large gap of 30 meV in the magnetic excitation spectrum of YNiO$_3$.

NMR relaxation data on quadrupolar nuclei (spin > 1/2) such as $^{17}$O in a polycrystalline or powdered antiferromagnet often seem to contain an unphysical jump in the temperature-dependence of the apparent relaxation rate within the antiferromagnetic state. This jump occurs when the effects of the magnetic order and the electric quadrupole moment on the NMR spectrum become similar in magnitude. We have found a new theoretical expression, which allows us to determine the correct value of the relaxation time $T_1$ for quadrupolar nuclei in antiferromagnetic powders, thus getting rid of this unphysical discontinuity.

*This work was financially supported in part by the Schweizerische Nationalfonds zur Förderung der Wissenschaftlichen Forschung (SNF).
10:24AM R50.00013: Impact of low-temperature stripe freezing in \( \text{La}_{1.67}\text{Sr}_{0.33}\text{NiO}_4 \) *JOHN TRANQUADA (Presenter), Brookhaven National Laboratory, ADRIAN MERRITT, DMITRY REZNIK, University of Colorado at Boulder, VASILE O GARLEA, Oak Ridge National Laboratory, GENDA GU, Brookhaven National Laboratory — \( \text{La}_{1.67}\text{Sr}_{0.33}\text{NiO}_4 \) develops charge stripe order below 240 K and spin stripe order below 190 K. We have reconsidered a wide variety of experimental studies that indicate changes in the stripe correlations below \( \sim 50 \) K [1]. From new neutron diffraction measurements of a significant set of stripe-order peaks, we make the case that the charge stripes, which can be centered on either Ni or O sites, become predominantly Ni-centered at low temperature. This is a prerequisite for the one-dimensional spin fluctuations on charge stripes that are observed at low temperature.


10:36AM R50.00014: Many-body physics of single and double spin-flip excitations in NiO

ABHISHEK NAG (Presenter), HANNAH ROBARTS, Diamond Light Source Ltd, F WENZEL, Institute for theoretical physics, JIEMIN LI, Diamond Light Source Ltd, H. ELNAGGAR, Debye Institute for Nanomaterials Science, RU-PAN WANG, Institute for theoretical physics, A C WALTERS, MIRIAN GARCIA-FERNANDEZ, Diamond Light Source Ltd, F. M. F. DE GROOT, Debye Institute for Nanomaterials Science, MAURITS HAVERKORT, Institute for theoretical physics, KEJIN ZHOU, Diamond Light Source Ltd — Understanding many-body physics of elementary excitations has advanced our control over material properties. Here, we study spin-flip excitations in NiO using Ni L3-edge RIXS and present a strikingly different resonant energy behaviour between single and double spin-flip excitations. Comparing our results with single-site full-multiplet ligand field theory calculations we find that the spectral weight of the double-magnon excitations originates primarily from the double spin-flip transition of the quadrupolar RIXS process within a single magnetic site. Quadrupolar spin-flip processes are among the least studied excitations, despite being important for multiferroic or spin-nematic materials due to their difficult detection. We identify intermediate state multiplets and intra-atomic core-valence exchange interactions as the key many-body factors determining the fate of such excitations.
How the electronic structure of correlated oxides evolves with electron and hole doping is a fundamental question of importance for applications. We have studied structural and electronic properties of high-quality MBE-grown doped NiO thin films using a variety of experimental and theoretical methods. We find that both K- and In-doped films at concentrations below 10% exhibit good X-ray diffraction spectra. However, extended X-ray absorption fine structure (XAFS) spectra indicate broadening of the K-O bond length distribution, and an increased bond length, much larger than obtained using theoretical methods. Ab-initio molecular dynamics suggests the XAFS feature is due to K-O\textsubscript{\textit{v}}-K defect structures in the thin film. Spectroscopic ellipsometry shows a smooth but asymmetric evolution of a decreasing optical gap for hole (K) and electron (In) doping, consistent with the behavior of a charge transfer insulator. Analysis shows that the decrease of the optical gap is due to the emergence of an absorption peak below (in energy) the optical gap of un-doped NiO. Calculations using Dynamical Mean Free Theory are in good agreement with the measurements and show the emergence of occupied states just above the valence band edge, and with an asymmetry between hole and electron doping.
8:00AM R51.00001: Spin-momentum Locking in an Array of Defect Lines in Gated Bilayer Graphene
RAUL GUERRERO, Donostia International Physics Center (DIPC), Paseo Manuel Lardizabal 4, 20018 Donostia-San Sebastián, Spain, MARTA PELC, Centro de Física de Materiales, CFM-MPC CSIC-UPV/EHU, Paseo Manuel Lardizabal 5, 20018 Donostia-San Sebastián, Spain, LEONOR CHICO, Instituto de Ciencia de Materiales de Madrid (ICMM), Consejo Superior de Investigaciones Científicas (CSIC), C/ Sor Juana Inés de la Cruz 3, 28049 Madrid, Spain, WLODZIMIERZ JASKOLSKY, Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Torun, Poland, ANDRES AYUELA (Presenter), Centro de Física de Materiales, CFM-MPC CSIC-UPV/EHU, Paseo Manuel Lardizabal 5, 20018 Donostia-San Sebastián, Spain — Graphene can have defect lines with pentagons and octagons (8-55) that induce localized states [1]. This domain wall in gated bilayer graphene produces a change between AB to BA stacking and presents topological states in the gap [2-4]. In this work using density functional theory calculations, we investigate an array of these defect lines in bilayer graphene. We found that the band structure shows a magnetic phase in which the spin is locked to the momentum, as in topological insulators. We also follow the topological states that appear even without a gate because of the array of defect lines. We lastly study the differences in spin bands and identified topological states when engineering by doping and/or electric field. All these results are summing to the new interesting data of the correlated behavior of electrons with the stacking in two-dimensional materials [5].


8:12AM R51.00002: Effect of correlation on nearly flat bands in twisted bilayer graphene*
MANCHEON HAN (Presenter), YOUNG WOO CHOI, HYOUNG JOON CHOI, Department of Physics, Yonsei University, Seoul 03722, Korea — Recently, correlated insulating phases were observed experimentally in twisted bilayer graphene (TBG) at different doping concentrations. To study possible mechanisms for insulating phases, we investigate electronic and magnetic properties in TBG by performing dynamical mean-field theory calculations based on a minimal tight-binding Hamiltonian. We study variation in the spectral function of the nearly flat bands for a range of local interaction parameters, electron filling, and temperature. We compare our results with experimental reports and discuss the possibility of Mott insulating phase in this system.

*This work was supported by NRF of Korea (Grant No. 2011-0018306), KISTI supercomputing center (Project No. KSC-2018-CRE-0097), and the Graduate School of Yonsei University Research Scholarship Grants in 2018.
8:24AM R51.00003: Visualization of the flat electronic band in twisted bilayer graphene near the magic angle twist  IQBAL UTAMA (Presenter), University of California, Berkeley, ROLAND KOCH, Advanced Light Source, Lawrence Berkeley National Laboratory, KYUNGHOO LEE, University of California, Berkeley, NICOLAS LECOMTE, Department of Physics, University of Seoul, HONGYUAN LI, SIHAN ZHAO, LILI JIANG, JIA Yi ZHU, University of California, Berkeley, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, PAUL ASHBY, ALEXANDER WEBER-BARGIONI, Molecular Foundry, Lawrence Berkeley National Laboratory, ALEX ZETTL, University of California, Berkeley, CHRIS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Laboratory, JEIL JUNG, Department of Physics, University of Seoul, ELI ROTENBERG, AARON BOSTWICK, Advanced Light Source, Lawrence Berkeley National Laboratory, FENG WANG, University of California, Berkeley — Bilayer graphene was theorized to host a moiré miniband with flat dispersion if the layers are stacked at specific twist angles known as the “magic angles”. Recently, such twisted bilayer graphene (tBLG) with the first magic angle twist was reported to exhibit correlated insulating state and superconductivity, where the presence of the flat miniband in the system is thought to be essential for the emergence of these ordered phases in the transport measurements. Tunneling spectroscopy and electronic compressibility measurements in tBLG have revealed a van Hove singularity that is consistent with the presence of the flat miniband. However, a direct observation of the flat dispersion in the momentum-space of such moiré miniband in tBLG is still elusive. Here, we report the visualization of the flat moiré miniband by using angle-resolved photoemission spectroscopy with nanoscale resolution (nanoARPES). The high spatial resolution in nanoARPES enabled the measurement of the local electronic structure of the tBLG. We clearly demonstrate the existence of the flat moiré band near the charge neutrality for tBLG close to the magic angle at room temperature.

8:36AM R51.00004: Low Temperature Insulating State in hBN-Encapsulated Multilayer Graphene  NICHOLAS MAZZUCCA (Presenter), MARC W BOCKRATH, CHUN NING LAU, Ohio State Univ - Columbus, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science — Bilayer graphene is susceptible to strong electron-electron interactions at charge neutrality, leading to the possibility for spontaneous symmetry breaking and the associated opening of a gap at low temperatures, even in the absence of any external fields [1]. Recent experiments confirm this possibility for Bernal stacked graphene layers of thickness up to 8 layers [2-4], but this physics is only observed via transport in suspended devices of the highest quality. Here, we present evidence for the opening of a gap at low temperatures in multilayer graphene systems which are encapsulated in hBN. The dielectric environment of hBN not only alleviates the requirement for suspension, but also poses constraints on the nature of the interactions. Our results provide new insights into the insulating state of multilayer graphene systems, and help to facilitate their fabrication for potential applications.

8:48AM R51.00005: Signature of Viscous Electron Flow in Graphene Using a Scanning Probe Microscope  MICHAEL ZIRPOLI (Presenter), SAGAR BHANDARI, Slippery Rock Univ — Graphene is a single layer of carbon atoms held together in a hexagonal crystalline structure. Graphene has shown great promise in electronics and photonics because of its two-dimensional properties. These properties reduce the scattering of electrons that are seen in metals, and thus graphene has the ability to be much more conductive than commonly used conductors such as copper. In graphene, at certain range of temperature and electron density, electrons begin interacting with each other in such a way that they start acting together as a viscous fluid. The purpose of this paper is to model the viscous flow of electrons in graphene and analyze the fluid behavior. The model of an incompressible fluid using the Navier-Stokes equations will be created to examine this behavior. The goal is to construct the best geometry and determine suitable boundary conditions for the walls and circular obstacle. The walls act as the edge of the graphene strip, and the circular obstacle acts as the tip perturbation of a scanning probe microscope. The objective is to obtain a suitable geometry showing signature of viscous electron flow.

9:00AM R51.00006: Engineering of the electronic properties of an epitaxial graphene on an SiC(0001) substrate by manganese adatoms  JINWOONG HWANG (Presenter), JIEUN LEE, MINHEE KANG, Physics, Pusan National University, BYEONG-GYU PARK, Pohang Accelerator Laboratory, JONATHAN DENLINGER, SUNG-KWAN MO, Lawrence Berkeley National Laboratory, CHOONGYU HWANG, Physics, Pusan National University — The application of graphene in electronic devices requires an energy band gap with its remarkable properties. By using angle-resolved photoemission spectroscopy, we show that it is possible to decouple the graphene from substrate by manganese (Mn) intercalation concomitant with energy band gap opening. Upon introducing Mn adatoms, we observe a charge neutrality of the graphene band with energy band gap at the Dirac energy up to ~ 0.4 eV. In addition, the Mn-intercalated graphene shows fully screened energy-momentum dispersion as Mn 3d states play a role of a metallic background on graphene. These observations provides a viable route towards the engineering of the electronic properties of graphene.

9:12AM R51.00007: Lévy flights and Hydrodynamic Superdiffusion on the Dirac Cone of Graphene*  EGOR KISELEV (Presenter), JOERG SCHMALIAN, Institute for Condensed Matter Theory, Karlsruhe Institute of Technology — It is shown that hydrodynamic collision processes in graphene at the neutrality point can be described in terms of a Fokker-Planck equation with a fractional derivative. This is a consequence of the fact that the phase space dynamics of electrons is governed by Lévy flights: rare large-angle scattering events interrupting the small-angle scattering. Lévy flights give rise to superdiffusive dynamics of collective excitations. Implications for transport and relaxation processes will be discussed.

*We thank the European Commission’s Horizon 2020 RISE program Hydrotronics (Grant Agreement 873028) for support.
9:24AM R51.00008: Scanning tunneling microscopy and electronic transport of gold-decorated graphene devices*  JAKE RIFFLE (Presenter), CAITLYN MEDITZ, SHAWNA HOLLEN, Univ of New Hampshire — Past studies on graphene show that scattering from disorder can give rise to weak Anderson localization, but a disorder-driven quantum metal-insulator transition has not been observed. Using a low temperature scanning tunneling microscope (STM) on graphene field effect transistors, we present simultaneous STM and electronic transport measurements of graphene devices decorated with gold adatoms. These data show quasiparticle scattering off of gold adatoms on graphene on SiO2/Si. We study the microscopic scattering mechanisms, including the effects of charge puddles versus point-like disorder, and correlate these mechanisms with macroscopic electronic transport. These experiments are the first steps toward understanding the phase space near disorder-tuned metal-insulator quantum phase transitions in 2D materials.

*This work supported by NSF DMR #1709029

9:36AM R51.00009: Atomic Engineering of Monolayer Graphene: Inducing Kekulé Bond Order by Adatom Deposition*  AMY QU (Presenter), PASCAL NIGGE, CHRISTOPHER GUTIERREZ, JISUN KIM, University of British Columbia, STEFAN LINK, Max Planck Institute for Solid State Research, GIORGIO LEVY, MATTEO MICHIARDI, MICHAEL SCHNEIDER, SERGEY ZHDANOVICH, University of British Columbia, ULRICH STARKE, Max Planck Institute for Solid State Research, DOUGLAS ANDREW BONN, SARAH A BURKE, ANDREA DAMASCELLI, University of British Columbia — The Kekulé distortion (KD) periodically modifies the carbon-carbon bonds in graphene, resulting in a √3×√3 R30° superstructure and symmetry breaking between three previously equivalent hexagonal plaquettes. Previous scanning tunnelling microscopy (STM) experiments have shown that such a distortion induced by vacancies in the graphene substrate can produce charge density modulations corresponding to the superstructure [1]. Here, we induce a KD phase in monolayer graphene by low-flux deposition of a small number of lithium adatoms. Using angle-resolved photoemission spectroscopy (ARPES), we observe backfolding of the Dirac cones to Γ, as well as a gap opening (2Δ = 0.22 ± 0.02 eV) at the Dirac point. Low-energy electron diffraction (LEED) measurements also show the appearance of peaks corresponding to the new periodicity. Finally, we discuss the real-space behaviour of the adatoms by comparing STM data with predictions by a Monte Carlo toy model.

References


*This research was undertaken thanks in part to funding from NSERC, CIFAR, CFREF, CFI, the BC Knowledge Development Fund, and the University of British Columbia.
9:48AM R51.00010: Scanning Tunneling Spectroscopy of Coupled Graphene Quantum Dots

DANIEL WALKUP (Presenter), FERESHTE GHAHARI KERMANI, National Institute of Standards and Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, NIKOLAI ZHITENEV, JOSEPH STROSCIO, National Institute of Standards and Technology — In backgated graphene devices with hexagonal boron nitride (hBN) substrates, impurities in the hBN can be locally charged by applying a voltage pulse to the tip of a scanning tunneling microscope. These charges create a writeable, tunable potential landscape for the graphene charge carriers, which we use to create isolated or coupled quantum dots in graphene. Under a strong perpendicular magnetic field, the free carriers condense into Landau levels (LLs). In a single dot, the LLs form a concentric pattern of alternating compressible and incompressible strips at the Fermi energy. The incompressible strips act as tunnel barriers creating a confined, concentric quantum dot system. When two or more such dots are placed next to each other, their charges interact. Addition of carriers to the dots manifests itself as peaks in the tunneling dI/dV, which can be tracked through the space of tip position, sample bias, and backgate voltage. Here, we explore the interaction between the dots revealed in the avoided crossings of their two sets of peaks to examine an intricate interplay of Coulomb interaction and tunnel coupling in this novel confined electron system.

10:00AM R51.00011: Frictional drag between graphene and LaAlO3/SrTiO3 heterostructures*

QING GUO (Presenter), JIANAN LI, JEN-FENG HSU, Univ of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin–Madison, PATRICK IRVIN, Univ of Pittsburgh, BRIAN R D'URSO, Physics, Montana State University, JEREMY LEVY, Univ of Pittsburgh — Vertical stacking of heterostructures that combine layered materials offer new ways of combining interesting properties of dissimilar electronic materials. Over the past few years we have been integrating graphene with complex-oxide heterostructures, specifically, the LaAlO3/SrTiO3 system. Furthermore, conducting nanostructures can be written under graphene, producing interesting interactions between the two systems. Here we report Coulomb drag measurements between single-layer graphene and a conductive LaAlO3/SrTiO3 interface. Fabry-Perot oscillations are observed in both graphene and drag signal in graphene, which indicate the local doping in graphene by conductive atomic force microscope(c-AFM) lithography. While the drag resistance is greatly enhanced in SrTiO3 in the superconducting region, the drag in graphene remain unchanged. We also observed key differences between longitudinal drag and hall drag in both graphene and SrTiO3.

*JL acknowledges a Vannevar Bush Faculty Fellowship (ONR N00014-15-1-2847), and the Office of Naval Research (N00014-16-1-3152). The work at the University of Wisconsin-Madison was supported by the National Science Foundation under DMREF Grant No. DMR-1629270, AFOSR FA9550-15-1-0334 and AOARD FA2386-15-1-4046.
10:12AM R51.00012: Visualizing broken symmetry states in the zeroth Landau level of the graphene quantum Hall system  SUNGMIN KIM (Presenter), DANIEL WALKUP, Physical Measurement Laboratory, National Institute of Standards and Technology, JOHANNES SCHWENK, Laboratory of Nanostructure at Surfaces, Ecole Polytechnique Federale de Lausanne, YIHANG ZENG, Department of Physics, Columbia University, FERESHTE GHAHARI KERMANI, Department of Physics and Astronomy, George Mason University, SON LE, Physical Measurement Laboratory, National Institute of Standards and Technology, JULIAN BERWANGER, Institute of Experimental and Applied Physics, University of Regensburg, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, FRANZ J GIESSIBL, Institute of Experimental and Applied Physics, University of Regensburg, NIKOLAI ZHITENEV, Physical Measurement Laboratory, National Institute of Standards and Technology, CORY DEAN, Department of Physics, Columbia University, JOSEPH STROSCIO, Physical Measurement Laboratory, National Institute of Standards and Technology — In graphene, the combination of electron spin and two equivalent sublattice atoms results in a four-fold degeneracy of Landau levels. A number of competing quantum Hall isospin states inside the four-fold degenerate zeroth landau level of graphene have been suggested based on macroscopic transport measurements. Here we observe the broken symmetry states of the zeroth Landau level in graphene with Kelvin Probe Force Microscopy (KPFM) by using a millikelvin scanning probe microscope coupled with qPlus sensor. The field dependence of the energy difference between isospin states is suggestive of transitions between isospin configurations at certain magnetic field values. In addition, we show how the quantum Hall edge channels of zeroth Landau level spatially develop and disperse at the edge of Hall bar.

10:24AM R51.00013: Imaging ballistic and hydrodynamic electron flow in the Corbino geometry  CHANDAN KUMAR (Presenter), Department of Condensed matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel, JOHN BIRKBECK, DAVID PERELLO, School of Physics & Astronomy, University of Manchester, Manchester M139PL, United Kingdom, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science,1-1 Namiki, Tsukuba, 305-0044, Japan, ANDRE GEIM, School of Physics & Astronomy, University of Manchester, Manchester M139PL, United Kingdom, SHAHAL ILANI, JOSEPH SULPIZIO, Department of Condensed matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — Hydrodynamic flow is predicted to exhibit unique voltage patterns which are distinct from both the Ohmic and ballistic regimes. A flow geometry to best highlight these patterns is the Corbino disc, in which the current is driven from a circular central contact into an outer ring. In this geometry there are no walls, and so the electrons can only transfer momentum to either impurities or to other electrons. In the hydrodynamic regime in which the flow is dominated by such electron-electron scattering, momentum is conserved, leading to an expulsion of the electric field across the bulk of the disc and hence a constant electrostatic potential. In this situation, the device resistance may even be lower than in the fully ballistic regime, where the potential drops inversely with the radius. We present our initial results on imaging electron flow in high-mobility graphene Corbino discs using a nanotube single electron transistor. We image the voltage drop of the flowing electrons from the inner to outer contact, with the aim of distinguishing these unique spatial signatures of ballistic and hydrodynamic flow.
10:36AM R51.00014: Correlation-Driven Kekule’ Dimerization and Semimetal-Insulator Transition in Strongly Isotropically Strained Graphene* ERIO TOSATTI (Presenter), SANDRO SORELLA, International School for Advanced Studies, KAZUHIRO SEKI, TOMONORI SHIRAKAWA, SHOHEI MIYAKOSHI, SEIIJI YUNOKI, RIKEN — Freestanding graphene will spontaneously distort and become insulating under a large isotropic tensile strain. We calculate the ground state enthalpy (not just energy) of strongly strained graphene by an off-lattice quantum Monte Carlo correlated approach of great accuracy and variational flexibility, removing the limitations of earlier density-functional or rigid lattice approaches. Beginning with undistorted semimetallic graphene at low strain, we find [1] that multideterminant Heitler-London correlations stabilize between 8.5% and 15% tensile strain an insulating Kekule’ dimerized state. Closer to a crystallized resonating-valence bond than to a Peierls state, Kekule’ dimerization of graphene prevails over the competing antiferromagnetic insulating state favored by density-functional calculations which we conduct in parallel. The insulator gap grows from zero at onset to over 1 eV before mechanical failure near 15% strain, and is topological in nature, implying under certain conditions 1D metallic interface states lying in the bulk energy gap. [1] S. Sorella, et al., PRL 121, 066402 (2018).

*Support is acknowledged by RIKEN research contracts, by the Simons Foundation, and by ERC Advanced Grants MODPHYSFRICT and ULTRADISS. We thank Oleg O. Brovko for early collaboration.

10:48AM R51.00015: Enhancement of Ultrafast Photoluminescence from Deformed Graphene KUNG-HSUAN LIN (Presenter), EN-XIANG CHEN, HAO-YU CHENG, Academia Sinica, WEILIANG CHEN, National Taiwan University, MONIKA KATARIA, National Central University, YU-MING CHANG, YANG-FANG CHEN, National Taiwan University, WEI-BIN SU, Academia Sinica — We studied the correlation between the ultrafast photoluminescence and the morphology of graphene, and observed enhancement of the ultrafast photoluminescence from the deformed graphene. In comparison to the planar graphene, the enhancement factor of ultrafast photoluminescence could be up to several times at the highly curved region. We found that the intensity of photoluminescence from the uniaxially rippled graphene depends on the polarization of excitation light. Furthermore, Raman spectroscopy was used to measure the strain distribution. Pump-probe measurements were conducted to reveal the carrier dynamics. From the experimental results, two mechanisms were confirmed to mainly account for the enhancement of ultrafast photoluminescence from the deformed graphene. One is the deformation-induced strain increases the absorption of graphene. The other is the prolonged carrier relaxation time in the curved graphene.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R52 DCMP: Thin Film nucleation, growth, and morphology Mile
High Ballroom 1E - Daniel Dougherty, North Carolina State University
8:00AM R52.00001: Introducing open boundary conditions in modeling nonperiodic materials and interfaces  JAMES CHARLES (Presenter), SABRE KAIS, TILLMANN KUBIS, Purdue Univ — Simulations are essential to accelerate the discovery of new materials. We introduce the first method of open boundary conditions in material and interface modeling. The new method, which we named ROBIN (recursive open boundary and interfaces) allows for discretizing millions of atoms in real space, thereby avoiding any symmetry or order of the atom distribution. The computational costs are limited to solving quantum properties in a focus area. It is verified in detail that the impact of the infinite environment on that area is included exactly. Calculations of graphene with the same amount of 1) periodic (currently available methods) and 2) randomly distributed silicon atoms shows that assuming periodicity elevates a small perturbation into a strong impact on the material property prediction. Graphene was confirmed to produce a band gap with periodic substitution of 3% carbon with silicon in agreement with published periodic boundary condition calculations. Instead, 3% randomly distributed silicon in graphene only shifts the energy spectrum. The predicted shift agrees quantitatively with published experimental data. Periodic boundary conditions can be applied on truly periodic systems only. Other systems should apply an open boundary method.

8:12AM R52.00002: Morphology and Mechanical Response of a Compressed Cylindrical Shells*  HUNG-CHIEH FAN CHIANG (Presenter), HSIN-HUEI LI, TZAY-MING HONG, Physical Society of Taiwan — Uniaxially compressed cylindrical shells are common in our daily life, such as rolled-up sleeves and retreated package of drinking straws. The deformations are complex and unpredictable, but often contain arrays of diamond. Is there any other modes of pattern? How does the cylinder respond mechanically when these modes transit? To clarify these problems, we perform both experiments and Molecularly Dynamics simulation. A rod is inserted inside and coaxial to the cylindrical shell in both approaches to avoid folding. It turns out that there are five more different patterns, besides the famous Yoshimura diamonds. These six modes of deformation are respectively spiral, ladder, diamond, wrinkle, ridge, and sagging. Phase diagram is drawn in a 3D plot with the spacing between shell and rod, compression strain and compression rate as axes. Material properties are incorporated to render these three parameters dimensionless. Two main features that worth noting are that different modes are allowed to mix and mode transitions are always accompanied by the absorption or release of latent heat. Simulation reveals that plasticity may disrupt and cause nonuniformity of the pattern.

*Financial support from MoST in Taiwan under105-2112-M007-008-MY3 and 108-2112-M007-011-MY3.
8:24AM R52.00003: Up against a wall: interfacial free energies at curved surfaces*  SETH MARTIN (Presenter), BRIAN LAIRD, Univ of Kansas — Interfacial free energies drive diverse physical phenomena, from wetting and capillarity to dendrite growth in crystal systems. While the interfacial free energy, $\gamma$, is largely controlled by the microscopic interactions between different phases, the geometry of the interface also plays a role in tuning the interfacial free energy. Although several analytic theories that try to include these geometric effects on $\gamma$ have been proposed, experimental and simulation studies of curvature dependence of $\gamma$ are few. Here we present simulation results for the 2-dimensional hard-disk fluid model at curved, hard, structureless walls and use the simulation results to test the limits of currently available analytical theories for interfacial free energy, including Morphometric Thermodynamics.

*Funding was provided by the NSF, grant #1465226.

8:36AM R52.00004: Two-step Unconventional Protocol for Epitaxial Growth in One Dimension with Hindered Reactions*  JULIÁN A. SÁNCHEZ (Presenter), DIEGO LUIS GONZÁLEZ, Physics, Universidad del Valle, A.A. 25360, Cali, Colombia, THEODORE EINSTEIN, Physics, University of Maryland, College Park — We study the effect of hindered aggregation and/or nucleation on the island formation process in a two-step (rather than the conventional one-step) growth protocol. In the proposed model, the attachment of monomers to islands and/or other monomers is hindered by additional energy barriers which decrease the hopping rate of monomers to occupied sites. For zero and weak barriers, the attachment is limited by diffusion while for strong barriers it is limited by reaction. We describe the time evolution of the system in terms of the monomer and island densities, $N_1$ and $N$. We also calculate the gap length, capture zone, and island-size distributions. For all sets of barriers considered, we compare the results from this analytical model with those from kinetic Monte Carlo simulations. The behavior of the system depends on the ratio of the nucleation barrier to the aggregation barrier. The two-step growth protocol gives more control and understanding of the island formation mechanism by intrinsically separating the nucleation and aggregation processes into different times regimes. We discuss experimental implications

*The work of DLG and JAS was supported by the Vicerrectoría de investigaciones de la Universidad del Valle C.I. 1164. TLE was supported in part by US-NSF grant CHE 13-05892.
8:48AM R52.00005: Foamability of oil mixtures  
HOAI-PHUONG TRAN (Presenter), LAURENCE TALINI, FRANÇOIS LEQUEUX, ESPCI Paris — In the absence of stabilization mechanism of films of pure liquids, foams do not form in pure liquids. Froth formation is observed in liquid mixtures, among which, oil mixtures, and that effect is well documented in the literature. The higher film lifetimes has however not been understood in non-volatile liquids and in the absence of surface-active molecules. We have experimentally studied the foaming of binary mixtures of liquids, and found the foam lifetime depends not only on the nature of the liquids but also on the proportions of the two liquids. We suggest a stabilizing mechanism of thin films of liquid mixtures based on non-linear variations of the mixture's surface tension with its composition, analogous to Gibbs’ elasticity defined for surfactant solutions. We show that the variations of foam lifetime with mixture composition is quantitatively described by the model. Finally, we define an effective disjoining pressure for thin films that can be fully computed from the variations of the surface tension of any liquid mixture which surface tension does not vary linearly with composition.

9:00AM R52.00006: Coupled Sublattice Melting and Charge-Order Transition in Two Dimensions*  
TYLER SMITH (Presenter), Department of Physics and Astronomy, University of Tennessee, Knoxville, FANGFEI MING, State Key Laboratory of Optoelectronic Materials and Technologies, School of Electronics and Information Technology, Sun Yat-sen University, D.G. TRABADA, CESAR GONZALEZ, DIEGO SOLER-POLO, FERNANDO FLORES, JOSÉ ORTEGA, Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, HANNO H WEITERING, Department of Physics and Astronomy, University of Tennessee, Knoxville — Two-dimensional melting is one of the most fascinating and poorly understood phase transitions in nature. Theoretical investigations often point to a two-step melting scenario involving unbinding of topological defects at two distinct temperatures. Here we report on a novel melting transition of a charge-ordered K-Sn alloy monolayer on a silicon substrate. Melting starts with short-range positional fluctuations in the K sublattice while maintaining long-range order, followed by longer-range K diffusion over small domains, and ultimately resulting in a molten sublattice. Concomitantly, the charge-order of the Sn host lattice collapses in a multi-step process with both displacive and order-disorder transition characteristics. Our combined experimental and theoretical analysis provides a rare insight into the atomistic processes of a multi-step melting transition of a two-dimensional materials system.

*NSF DMR 1410265
9:12 AM R52.00007: Quantification of multiple crystallite orientations in complex thin film materials

JONATHAN OGLE (Presenter), DANIEL POWELL, ERIC AMERLING, University of Utah, DETLEF-M. SMILGIES, Cornell High Energy Synchrotron Source, Cornell University, LUISA WHITTAKER-BROOKS, University of Utah — As thin films and interfaces have become more intricate, the morphological and structural information also grows in complexity. An increasing amount of studies have focused on understanding correlations between crystallite orientation and electronic structure. Crystallite orientation within thin films is studied using grazing incidence wide-angle X-ray scattering (GIWAXS) patterns, where the Miller indices of a crystal structure are related to the scattering reflections. GIWAXS can be used to elucidate crystallite orientations within a thin film by comparing the azimuthal distribution of specific Miller indices. However, as thin film technologies advance, there is a growing need to quantify the orientational distribution of similar thin films or also for multiple orientations within a single thin film in a comparative manner. Herein, we present a new method for quantifying the orientational distribution of crystallites, dubbed the Mosaicity Factor (MF). The efficacy of this method will first be studied using a model system consisting of Gaussian distributions. We will highlight the strengths and capabilities of MF when characterizing multiple Gaussian shapes and overcoming signal noise. Case studies will be used to show the range of applications available and the strengths of MF.

9:24 AM R52.00008: The role of He and H on the structural evolution of He- and H-irradiated 6H-SiC

NABIL DAGHBOUJ (Presenter), Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, BINGSHENG LI, state key laboratory, university of science and technology china, MAURO CALLISTI, materials science and metallurgy, University of cambridge, HUSEYIN SENER SEN, Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, MIROSLAV KARLIK, Department of materials, Faculty of Nuclear sciences and Physical engineering, JIE LIN, XIN OU, state key laboratory of Functionnal materials for informatics, Shanghai Institute of microsystem and information technology, TOMAS POLCAR, Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague — The behavior of irradiated H and He ions in the 6H-SiC lattice was rather different. H irradiated with low fluence at RT, blisters were formed after annealing at 1100°C, while at high irradiation fluence no blister cavities were observed due to the formation of an amorphous layer. At an irradiation temperature of 450 and 900°C, amorphization of 6H-SiC did not occur and hydrogen-containing microcracks grew laterally below the surface. Thus blisters appeared on the surface of the samples irradiated at 900°C even without annealing. For He irradiation, regardless of the fluence and irradiation temperature, blisters did not form. The presented results are well supported by density functional theory calculations. The coalescence between two small bubbles is an exothermic process when the H₂-bubbles contain an unpaired hydrogen and endothermic process when the H₂-bubbles contain paired H atoms, but it is energetically cheap. On the other hand, activation of the coalescence of He bubbles is endothermic and energetically very expensive.

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Epitaxial growth of cubic WC$_y$(001) thin films

PEIJIAO FANG (Presenter), BAIWEI WANG, Rensselaer Polytechnic Institute, CHRISTOPHER MULLIGAN, Benét Laboratories, THOMAS MURRAY, SUNY Polytechnic Institute, SANJAY V. KHARE, University of Toledo, DANIEL GALL, Rensselaer Polytechnic Institute — Tungsten carbide films were sputter-deposited onto MgO(001) substrates at 400 °C in 5 mTorr Ar-CH$_4$ gas mixtures as a function of the CH$_4$ fraction $f_{CH_4} = 0.4$ - 6%. High resolution transmission electron microscopy (TEM) and x-ray diffraction ω-2θ scans, ω-rocking curves, and reciprocal space maps on $d = 10$ nm thick layers indicate epitaxial growth of rock-salt WC$_y$ with a cube-on-cube epitaxial relationship: (001)$_{WC}$ || (001)$_{MgO}$ and [100]$_{WC}$ || [100]$_{MgO}$. The measured out-of-plane coherence length matches the film thickness for $d = 10$ nm but remains nearly unaffected by a 60-fold increase in layer thickness to $d = 600$ nm. This suggests a critical thickness for epitaxial breakdown of ~ 10 nm, associated with the nucleation of misoriented grains as also observed by TEM. The relaxed lattice constant increases monotonically from 0.419 to 0.425 nm with increasing $f_{CH_4}$. Comparing these measured lattice parameters with first-principle predictions indicates a C-to-W ratio $y = 0.47$ - 0.68. However, composition measurements using energy-dispersive x-ray spectroscopy and Rutherford backscattering spectrometry yield measured C-to-W ratios of 0.57-1.25, suggesting that a considerable fraction (18 – 46 %) of C does not incorporate in the cubic phase but likely forms amorphous carbon.

InAs(111) Homoepitaxy with Molecular Beam Epitaxy

KEVIN VALLEJO (Presenter), TRENT ALAN GARRETT, KEVIN SAYTHAVY, KATHRYN SAUTTER, Micron School of Materials Science and Engineering, Boise State University, BAOLAI LIANG, California NanoSystems Institute, UCLA, PAUL J SIMMONDS, Micron School of Materials Science and Engineering, Boise State University — In this study we have mapped the growth parameters for optimal homoepitaxy of InAs on InAs(111)A substrates using molecular beam epitaxy. Increasing the substrate temperature reveals a transition from 2D flat island growth to step-flow. The optimized parameters we established (substrate temperature = 500° C, growth rate = 0.12ML/s and V/III ratio = 48) produce an atomically flat surface, free of 3D imperfections. We study material quality using photoluminescence and have established a relationship between InAs(111)A surface smoothness and light emission intensity. This work paves the way for integrating the 6.1 Å family of materials with the desirable properties of semiconductors with a (111) orientation. In addition, we will present preliminary results demonstrating the self-assembly of InGaAs quantum dots on these smooth InAs(111) surfaces, strongly indicating new paths towards ultra-low bandgap tunable light emitters for infrared optoelectronics.

*We acknowledge the support of the College of Engineering at Boise State University.
**10:00AM R52.00011: Droplet spreading on a surface exhibiting solid-liquid interface premelting**  
YANG YANG, Physics, East China Normal University, BRIAN LAIRD (Presenter), Chemistry, University of Kansas — We study, using molecular-dynamics simulation, the spreading kinetics and equilibrium shape of liquid Pb droplets on an Al(111) substrate. The Al-Pb solid-liquid interface (SLI) was found previously to exhibit interfacial premelting at temperatures below the Al melting point [1]. We examine here how premelting affects the spreading and compare with both hydrodynamic (viscosity dominated) and kinetic (interfacial friction dominated) spreading mechanisms. For premelted surfaces, kinetic spreading is observed at intermediate times, in contrast to low temperatures near the Pb melting point where the surface is faceted and the hydrodynamic mechanism dominates. We conclude that the presence of the premelting layer has a significant effect on the thermodynamics of the Al(111)/Pb SLI and that the induced surface disorder gives rise to a kinetic spreading mechanism. We also observe that the structure of the droplet contact line with the premelted surface resembles that seen in reactive wetting.


*Funding is acknowledged from the US National Science Foundation (CHE-0957102) (BBL) and from the Chinese National Science Foundation (11504110), 111Project (B12024) and ENCU Large Instruments Open Foundation (YY)*

**10:12AM R52.00012: Visualization of Nanorod Assembly and Dynamics on Liquid Surfaces**  
SATYAM SRIVASTAVA (Presenter), ZACHARY FINK, PAUL Y KIM, ALEXANDER E RIBBE, DAVID HOAGLAND, THOMAS RUSSELL, Univ of Mass - Amherst — The two-dimensional phase behavior of rod-like particles was studied by dispersing silica-coated gold nanorods on a liquid surface. Nanorods with aspect ratio ranging from 3 to 6 were synthesized, coated with silica, functionalized with polyethylene glycol (PEG), and then dispersed in ionic liquid 1-ethyl 3-methylimidazolium ethyl sulfate ([EMIM][EtSO4]). The dispersed rods, driven to the surface by the low surface energy of PEG, were observed directly on the surface of an ionic liquid droplet by scanning electron microscopy. Rod diffusion coefficients were calculated in dilute systems by tracking position and orientation of single nanorods. In concentrated systems, the nanorod packing was studied using an in-situ liquid cell to control volume and surface area of the droplet. The 2D packing was characterized by pair correlation function, translational order parameter, orientational order parameter, and Voronoi tessellation. Order parameters were calculated as a function of areal density and nanorod aspect ratio. An increase in local orientational order was observed at higher areal densities but a liquid crystalline phase was not observed due to low aspect ratio.

*NSF DMR-1807255.*
10:24AM R52.00013: Effects of short-range repulsive barriers on island nucleation  
SAMEER HAMADNA (Presenter), INDIRAS KHATRI, JACQUES AMAR, Univ of Toledo — A variety of effects such as strain and surfactants can lead to attachment barriers in thin-film growth. While several studies of the effects of attachment barriers on submonolayer growth have been carried out, the emphasis has been on rate-equations which do not take into account island geometry or coalescence and are primarily applicable to point-islands. Here we present the results of kinetic Monte Carlo simulations for the case of extended 2D islands with critical island-size $i = 1$ which were carried out to determine the dependence of the exponent $\chi$ (describing the dependence of the peak island density on deposition rate) on barrier strength and ratio $R = D/F$ of the monomer hopping rate $D$ to deposition rate $F$. In particular, we have studied two different cases, one with a barrier to island nucleation and attachment as well as the case with an island attachment barrier but no nucleation barrier. Our results indicate that in both cases - and in contrast to the case of no barrier for which $\chi$ is equal to $1/3$ - the asymptotic (large $R$) value of $\chi$ increases continuously with barrier strength, reaching a value close to $1/2$ in the limit of a very strong barrier and very large $R$. The effects of attachment barriers on island morphology and coalescence will also be discussed.

10:36AM R52.00014: X-ray Photon Correlation Spectroscopy Studies of Ion Beam Nanopatterning Kinetics and Dynamics  
PECO MYINT (Presenter), Division of Materials Science and Engineering, Boston University, XIAOZHI ZHANG, Department of Physics and Materials Science Program, University of Vermont, DENISE ERB, Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf e.V., ANDREI FLUERASU, LUTZ WIEGART, YUGANG ZHANG, National Synchrotron Light Source II, STEFAN FACSKO, Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf e.V., RANDALL HEADRICK, Department of Physics and Materials Science Program, University of Vermont, KARL F LUDWIG, Department of Physics & Division of Materials Science and Engineering, Boston University — Solid surfaces can be ultra-smoothened or patterned on the nanoscale by irradiating with a broad beam of energetic ions. Different nanopatterns can be achieved by varying target-ion combination, the energy of ions, ions’ incident angle or the temperature of the solid target. There are several theories that seek to explain nanopatterning processes, but a definitive fundamental understanding has not been reached. In this study, the surface sensitive X-ray technique of Grazing-Incidence Small-Angle X-ray Scattering (GISAXS) is used to do real-time investigations of nano-pattern formation on Silicon and Germanium due to $\text{Ar}^+$ and $\text{Kr}^+$ bombardment. The coherent X-ray beam that is utilized in these GISAXS experiments enables us to study not only the kinetics, but also the fluctuations around the average kinetics, i.e. the dynamics of the nanopatterning process. The X-ray Photon Correlation Spectroscopy (XPCS) two-time correlation function shows a novel behavior in the early stage, with memory stretching back to the beginning of the bombardment. During the late stage, the stationary intensity auto-correlations are computed to determine the correlation times as a function of length-scale.

*This work was supported by NSF grant DMR-1709380 (BU) and DOE grant DE-SC0017802 (UVM).
**10:48AM R52.00015: Recent Applications of Voronoi Tessellation and Analysis of Their Size Distributions with the Generalized Wigner Surmise**  
**THEODORE EINSTEIN (Presenter)**, University of Maryland, College Park — While Voronoi tessellation has long been applied in spatial studies, analysis of their cell-size distribution using the single-adjustable-parameter generalized Wigner surmise, \( P_\beta(s) = a s^\beta \exp(-b s^2) \), has only been done in the last decade. Here we discuss some intriguing examples: Mitko et al. (2019) consider the evolution of morphology during growth of island films of low-e dielectric films via vapor deposition polymerization. Löbl et al. (2019) probe infilling Al-droplet-etched nanoholes in an AlGaAs surface. In both cases, estimates of the critical nucleus size were extracted from the value of the exponent \( \beta \) determined from a fit to \( P_\beta(s) \). We discuss the results and their implications. In other tantalizing examples, the Voronoi cell-size was not [yet] analyzed using \( P_\beta(s) \). Brookes (2017) uses Voronoi analysis of cells on the outer layer of eye-banked corneas to assess their viability before transplanting. Konishi et al. (2017) studied the growth-rate dependence of the spatial distribution of self-assembled 2D quantum dots on InAs-GaAs. They also consider the influence of modest array size.

**Thursday, March 5, 2020 8:00 AM - 10:48 AM**

**Session R53 DCMP: Optical Spectroscopy of Heterostructures of 2D Materials** Mile High Ballroom 1F - Nathan Wilson

**8:00AM R53.00001: Optical Second-Harmonic Interference in Two-Dimensional Heterostructures**  
**WONTAEK KIM, SUNMIN RYU (Presenter)**, Pohang Univ of Sci & Tech — Atom-thick two-dimensional (2D) transition metal dichalcogenides (TMDs) with strong excitonic transitions in the NIR and visible range are excellent media for optical second-harmonic generation (SHG). SHG is not only a powerful structural method owing to its sensitivity to crystallographic symmetry, but also a coherent probe because of its instantaneous but non-dissipative response. In this talk, I will present our recent findings on SHG interference occurring in 2D TMD heterostructures. All 2D crystal samples were prepared by mechanical exfoliation and studied with a polarized SHG micro-spectroscopy setup powered by a tunable femtosecond Ti-sapphire laser. Polarization-resolved SHG polar plots of MoS\(_2\) homo-bilayers exhibited a six-petal pattern with six angular nodes like those of MoS\(_2\) monolayers. Remarkably, the SHG behavior of MoS\(_2\)/WS\(_2\) was much different from that of MoS\(_2\) bilayers in that the former lacked angular nodes. This anomalous angular background became larger for more staggered hetero-bilayers but decreased for increased fundamental wavelength. All the results were nicely explained by an SHG interference model considering material-dependent phase delay in their nonlinear response, which was corroborated with phase-resolved interferometric SHG measurements.
8:12AM R53.00002: Interlayer Exciton in atomically reconstructed MoSe2/WSe2 van der Waals Heterostructure  HSUN JEN CHUANG (Presenter), United States Naval Research Laboratory, AUBREY T. HANBICKI, United States Naval Research Laboratory/ Laboratory for Physical Sciences, MATTHEW ROSENBERGER, United States Naval Research Laboratory, VLADIMIR P. OLESHKO, National Institute of Standards and Technology, KATHLEEN M MCCREARY, SAUJAN V SIVARAM, IGOR MAZIN, BEREND THOMAS JONKER, United States Naval Research Laboratory — Interlayer exciton (ILE) can be created by artificially stacking MoSe2 onto WSe2 to form a heterostructure with type II band alignment. With hBN encapsulation and a relative rotational angle close to 60 degrees, well pronounced ILE emission is observed at room temperature and further splits into two distinct peaks (ILE1 and ILE2) at low temp. Furthermore, we demonstrate that the ILE emission peaks have opposite circular polarizations when excited by circularly polarized light. Ab initio calculations provide an explanation of this unique and potentially useful property and indicate that it is a result of the indirect character of both transitions. We further investigate the atomic structure arrangement of MoSe2/WSe2 by TEM and reveal that the heterostructure indeed reconstructs under a small twist angle (≤ 1°) between the TMDs. With a small twist angle, periodic domains form with commensurate stacking within the domain. On the other hand, a rigid moiré structure is also observed by TEM when a larger twist angle (≥ 3°) is applied. These results may provide fundamental insights into the mechanical and optical behavior of this exciting class of semiconductor heterostructure.

8:24AM R53.00003: Nonradiative energy transfer enhances Raman intensity in layered heterostructure  MEDHA DANDU (Presenter), Electrical Communication Engineering, Indian Institute of Science, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, AJAY SOOD, Physics, Indian Institute of Science, KAUSIK MAJUMDAR, Electrical Communication Engineering, Indian Institute of Science — Since the discovery of Graphene enhanced Raman scattering, layered materials and their heterostructures are emerging as promising candidates for realizing Raman enhancement on flat surfaces. While most of the Raman enhancement studies on these materials are based on charge transfer interaction, here, we experimentally demonstrate for the first time, a strong enhancement of Raman intensity through nonradiative energy transfer (NRET) in a layered heterostructure. We achieve a ten-fold Raman enhancement of a monolayer transition metal dichalcogenide (1L-TMD, such as 1L-MoS2 and 1L-WS2) stacked on a multilayer SnSe2. Spectral resonance, extreme spatial proximity and in-plane orientation of dipoles result in strong dipole-dipole coupling that enables NRET driven Raman enhancement even when a barrier layer like hBN is introduced between 1L-TMD and SnSe2. We corroborate the evidence for NRET driven Raman enhancement by decoupling it from other effects and demonstrating its tunability through modulation of spectral overlap between 1L-TMD and SnSe2 by varying the sample temperature. Observation of such non-local, uniform Raman enhancement over a wide junction area opens new ways to engineer sensing mechanisms using NRET in tandem with other existing enhancement techniques.
8:36AM R53.00004: Circular emission under linear excitation from interlayer excitons in WSe$_2$/MoSe$_2$ heterobilayer* XIN LU (Presenter), WEIJIE LI, SUDIPTA DUBEY, AJIT SRIVASTAVA, Emory University — We report circularly polarized emission from interlayer excitons in WSe$_2$/MoSe$_2$ heterobilayer under linear excitation at zero magnetic field. The magnitude and sign of the degree of circular polarization (DCP) varies spatially over the sample. The DCP is independent of excitation energy when incident laser is linearly polarized, however, can be modulated by circular pumping or magnetic field. This is in stark contrast with WSe$_2$ and MoSe$_2$ intralayer excitons where circular emission only occurs with an applied magnetic field or under circular pumping. The observation of circularly polarized emission, in absence of magnetic field and circular pumping, implies an effective time-reversal symmetry (TRS) breaking in the WSe$_2$/MoSe$_2$ heterobilayer. As different cool downs result in very similar spatial patterns of DCP, we rule out spontaneous TRS breaking in the sample. Due to the momentum space-indirect nature of interlayer excitons, there is a finite center-of mass momentum in the recombining exciton state. This, together with the ubiquitous inhomogeneous strain in exfoliated samples can explain our observations.

*NSF EFRI NewLAW grant #EFMA-1741691

8:48AM R53.00005: Dipole-dipole interactions between localized interlayer excitons in WSe$_2$/MoSe$_2$ heterobilayer* WEIJIE LI (Presenter), XIN LU, SUDIPTA DUBEY, LUKA MATEJ DEVENICA, AJIT SRIVASTAVA, Emory University — We explored localized interlayer excitons in WSe$_2$/MoSe$_2$ heterobilayer by low temperature (~ 4K) photoluminescence spectroscopy. With type-II band alignment, the localized interlayer exciton compromises of an electron from MoSe$_2$ and a hole from WSe$_2$, forming an out-of-plane electric dipole moment. We thus tuned its energy by hundreds of its linewidth via an external electric field. In addition to the field-tuneability, the permanent dipoles have repulsive dipolar interaction scaled as $\sim 1/r_{ex}^3$ where $r_{ex}$ is the interexcitonic distance. Here we observed a peak blueshifted from the localized interlayer exciton peak by $\sim 2$ meV with increasing incident power. The blue peak is assigned to be the biexciton peak due to the same synchronized jittering as the exciton and its superlinear power dependence. The similar $g$ factor and gate dependence of biexciton and exciton imply that the second excitation has negligible impact on the exciton wavefunction. The polarization of the biexciton and exciton under finite magnetic field is consistent with the spin-valley singlet nature of the dipolar molecule states. With the singlet configuration and dipolar interaction $\sim 2$ meV, the confinement length of the localized interlayer exciton is calculated to be $\sim 5$ nm.

*NSF EFRI NewLAW grant # EFMA-1741691.
9:00AM R53.00006: Confinement of long-lived interlayer excitons in WSe$_2$/WS$_2$ heterobilayers*  ALEJANDRO MONTBLANCH, DHIREN KARA, IOANNIS PARADEISANOS, CAROLA PURSER (Presenter), GANG WANG, Univ of Cambridge, PAWEL LATAWIEC, MARKO LONCAR, Harvard University, SEFAATTIN TONGAY, Arizona State University, ANDREA FERRARI, METE ATATURE, Univ of Cambridge — Recently, there has been an increased focus on controllable quantum gases with long-range anisotropic interactions to simulate condensed matter problems that have so far remained intractable. Interlayer excitons (IX) in transition metal dichalcogenides (TMDs), which have a permanent electric dipole moment, have emerged as an alternative pathway to realising quantum simulations in the solid state. Here, we create ultra-long-lived IX and demonstrate they can be trapped - an important prerequisite for future investigations. We do this by depositing a heterostructure of monolayer WSe$_2$ and WS$_2$ on a pre-patterned substrate. We observe lifetimes of IX approaching 200 μs at cryogenic temperatures, an order of magnitude longer than any previous IX and three orders for any TMD IX. Power-dependent PL evidences IX-IX interactions and the ability to confine single IX at pre-defined locations. The potential to create arbitrary trapping profiles for long-lived dipolar particles evidences the capability of TMDs to provide a unique avenue for probing exotic states of matter in degenerate gases and artificial lattices.

*We acknowledge funding from EU Graphene and Quantum Flagships, Royal Society UK, ERC Grants Hetero2D and PHOENICS, EPSRC, Marie-Sklodowska-Curie Actions Spin-NANO, NQIT.

9:12AM R53.00007: Mechanically tunable nonlinear optics from a van der Waals interface in twisted hexagonal boron nitride heterostructures*  NATHAN FINNEY (Presenter), KAIYUAN YAO, Mechanical Engineering, Columbia University, SAMUEL MOORE, Physics, Columbia University, FANG LIU, Chemistry, Columbia University, JENNY ARDELEAN, XINYI XU, Mechanical Engineering, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, XIAOYANG ZHU, Chemistry, Columbia University, DMITRI BASOV, CORY DEAN, Physics, Columbia University, P. JAMES SCHUCK, JAMES C HONE, Mechanical Engineering, Columbia University — In the bulk limit, the second harmonic generation (SHG) response from hexagonal boron nitride (BN) includes electric quadrupole and dipole contributions. Both the total layer number and layer parity play a critical role in determining the overall nonlinear optical response. Here we investigate micromechanical devices consisting of a rotatable crystal of bulk BN placed on top of another crystal of BN, where the relative rotational alignment of the two crystal lattices can be dynamically tuned via an atomic force microscope (AFM) in contact mode. We find significant angle dependence of the unpolarized SHG response where the SHG signal is strongly suppressed or enhanced depending on the stacking order (AA’ or AA, respectively) at the homojunction between the top and bottom BN. At intermediate rotation angles of the top BN crystal between 0 and 60 degrees, we observe continuous modulation of both the SHG intensity and polarization. The non-symmetry-selective third harmonic generation (THG) signal remains unchanged over all rotation angles, suggesting that the observed modulation in nonlinear optical response is induced by mechanically tuning the symmetry at the van der Waals interface between the crystals.

*Support by ProQM, an EFRC funded by US DOE/Office of Sciences/BES: DE-SC0019443
9:24AM R53.00008: Interlayer Exciton Fine Structure in MoSe$_2$/WSe$_2$ Heterostructure

SHENGNAN MIAO (Presenter), TIANMENG WANG, ZHIPENG LI, Rensselaer Polytechnic Institute, ZHENGGUANG LU, Natl High Magnetic Field Lab, SUFEI SHI, Rensselaer Polytechnic Institute — The realization of the valleytronics based on transitional metal dichalcogenides (TMDCs) is hindered by the short lifetime of the exciton. Recently, it is predicted that the long-lived interlayer exciton in aligned TMDC hetero-bilayer possesses fine structures with distinctive valley polarization selection rules, which can be utilized to lift this limitation. However, the revealing of the details of the interlayer exciton is hindered by the sample quality. Further, the Moiré effect due to small twist angle also complicates the spectroscopy signature of the interlayer exciton. In this work, we present a comprehensive study of the interlayer excitons through gate-dependent, magnetic-field dependent spectroscopy study. The valley polarization is investigated through photoexcitation spectroscopy (PLE) study, and the high valley polarization of interlayer exciton is also explored. Our work paves the way for future exploration and understanding of the fascinating interlayer excitonic physics and Moiré physics in TMDC heterostructures.

9:36AM R53.00009: Evidence of Purely Electronic Lattice at Interface of TMD/Bi$_2$Se$_3$ 2D Heterostructures Induced by Strong Interlayer Coupling*

ZACHARIAH HENNIGHAUSEN (Presenter), CHRISTOPHER LANE, IOANA G BUDA, VINEET K MATHUR, ARUN BANSIL, SWASTIK KAR, Physics, Northeastern University — Vertically-stacked 2D heterostructures are more than a sum of the individual layers, but a product of the interlayer coupling and twist angle. New properties emerge from interlayer orbital interactions and charge redistribution, further modulated by the interlayer atomic registry and moiré superlattice. This talk shows experimental and theoretical indications of a real-space, non-atomic lattice formed by significant charge redistribution in vertically stacked Bi$_2$Se$_3$/Transition Metal Dichalcogenide (TMD) 2D heterostructures. High-energy (200keV) selected area electron diffraction (SAED) patterns correspond excellently with simulations from the moiré superlattices, suggesting substantial charge redistribution at sites of high interlayer atomic registry. Density functional theory (DFT) predicts concentrated charge pools reside in the interlayer region, located at sites of high nearest-neighbor atomic registry, suggesting the non-atomic lattices are standalone, reside in the interlayer region, and are purely electronic.

References:

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DE-FG02-07ER46352
DE-AC02-05CH11231
DE-SC0012575
Post-9/11 GI Bill
9:48AM R53.00010: Investigation of interfacial charge transfer in hybrid system of Graphene-MoS$_2$ * SAJEDEH POURIANEJAD (Presenter), Joint School of Nanoscience and Nanoengineering, University of North Carolina at Greensboro, FREDERICK ARYEETEY, Joint School of Nanoscience and Nanoengineering, North Carolina A&T State University, OLUBUNMI AYODELE, Joint School of Nanoscience and Nanoengineering, University of North Carolina at Greensboro, SHYAM ARAVAMUDHAN, Joint School of Nanoscience and Nanoengineering, North Carolina A&T State University, TETYANA IGNATOVA, Joint School of Nanoscience and Nanoengineering, University of North Carolina at Greensboro — Heterostructures of two dimensional layered materials have exciting optical properties that encourage scientists to further study of their photodetector applications. Interactions and, in particular, charge transfer between the constituting layers plays a critical role in the electronic and optical properties. Heterostructure of a few layers of graphene/MoS$_2$ has been demonstrated as a promising candidate for diverse unique optoelectronic devices owing to the high transparency of graphene, the tunability of its Fermi level and, the magnificent optical properties of MoS$_2$. Here, the magnitude and the direction (i.e. electron or hole) of the charge transfer was investigated in a graphene/MoS$_2$ heterostructure. Confocal Raman microscopy and photoluminescence were used to study doping and strain configuration. The surface morphologies of MoS$_2$ and graphene were investigated by scanning electron microscopy. To correlate work function difference to charge-related phenomena, KPFM and EFM were carried out. We speculate that the tunable Fermi level in graphene allows excellent work-function match with MoS$_2$, resulting in low contact resistance.

*Samples were provided by The Pennsylvania State University 2DCC-MIP supported by NSF DMR-1539916. To JSNN, a member SENI C NSF ECCS-1542174).

10:00AM R53.00011: Trion light emission in type-I WSe$_2$/MoTe$_2$ van der Waals heterostructures HYEMIN BAE, SUK HYUN KIM (Presenter), Seoul Natl Univ, SEUNGMIN LEE, Yonsei Univ, OURI KARNI, AIDAN O’BEIRNE, ELYSE BARRÉ, Stanford Univ, SANGWAN SIM, Hanyang University, TONY F HEINZ, Stanford Univ, HYUNYONG CHOI, Seoul Natl Univ — Two-dimensional (2D) transition metal dichalcogenides (TMDs) are attractive materials to investigate the light-induced many-body excitons. The reduced Coulomb screening leads to a large exciton binding energy, and stacking two or more dissimilar TMDs provides easy way to build van der Waals (vdW) heterostructures. With this features TMDs enables us to study a variety body of excitons such as neutral exciton, charged excitons, type-II interlayer excitons, moiré excitons, and localized excitons. Here we perform photoluminescence (PL), reflection contrast (RC) and photoluminescence excitation (PLE) to investigate vdW type-I heterostructures. We report the spectroscopic identification in type-I heterostructure of trions, a quasiparticle composed of two electrons and a hole. In the heterostructure spectra, we observe a significant enhancement of the MoTe$_2$ A trion PL emission under the excitation in resonance with the WSe$_2$ trion resonances. The enhancement is interpreted as a transfer effect arising from trions initially created in either layer. We suggest that the trions generated in WSe$_2$ have a great influence on the MoTe$_2$ trion emission. Our results show possibilities for fundamental studies of many-body interactions in 2D TMDs heterostructures.
The bright side of defects in MoS$_2$ and WS$_2$ and a generalizable chemical treatment protocol for defect passivation

HOPE BRETSCHER (Presenter), ZHAOJUN LI, JAMES XIAO, Department of Physics, University of Cambridge, DIANA QIU, Department of Mechanical Engineering and Materials Science, Yale University, SIVAN REFAELY-ABRAMSON, Department of Materials and Interfaces, Weizmann Institute of Science, JACK ALEXANDER-WEBBER, Department of Engineering, University of Cambridge, ARELO TANOH, Department of Physics, University of Cambridge, YE FAN, Department of Engineering, University of Cambridge, GERAUD DELPORT, Department of Physics, University of Cambridge, CYAN WILLIAMS, SILVIA VIGNOLINI, Department of Chemistry, University of Cambridge, SAM STRANKS, Department of Physics, University of Cambridge, STEPHAN HOFMANN, Department of Engineering, University of Cambridge, STEVEN LOUIE, JEFFREY NEATON, Department of Physics, University of California, Berkeley, AKSHAY RAO, Department of Physics, University of Cambridge

Defects in transition metal dichalcogenides, such as MoS$_2$ and WS$_2$, are frequently considered responsible for quenching photoluminescence (PL) and lowering mobility, limiting many of the proposed applications. However, while many chemical treatments have been proposed to passivate defects, primarily assumed to be sulfur vacancies, the mechanism of this passivation is poorly understood. In this work, we illustrate how TFSI superacid treatment reveals an optical subgap state associated with sulfur vacancies. At room temperature, this subgap state contributes to enhanced quantum yields and lengthened emission lifetimes, compared to untreated samples, rather than quenching PL. Building on this understanding, we propose a generalizable treatment protocol to passivate defects in monolayer MoS$_2$ and WS$_2$, increasing photoluminescence and maintaining mobilities. This protocol opens up a route for solution-based, post-processing of samples, which could not only passivate defects, but also simultaneously tune properties and functionalize materials.

Probing the nonlinear response of strongly coupled plasmon-WSe$_2$ system

CHENTAO LI (Presenter), XIN LU, AJIT SRIVASTAVA, HAYK HARUTYUNYAN, Emory University

Plasmonic nanostructures have been previously shown to facilitate strong light-matter interactions in a wide variety of systems. With the recent progress in our understanding of 2D transition metal dichalcogenides (TMDs), studies on plasmon-exciton coupling in these systems have increasingly attracted considerable attention, demonstrating evidence of strong light-matter coupling in scattering spectra. However, more convincing evidences of strong coupling are still needed, including probing in nonlinear optical interactions, to give a direct access for studying near-field properties of the coupled system.

In this work, gold nanorods and WSe$_2$ flakes (TMD material) are successfully assembled to investigate the strong light-matter interaction. Rabi splitting and anti-crossing phenomena in dark-field spectra is utilized as signatures of strong-coupled candidates. Interestingly, simulation based on the classical oscillator model predicts that second harmonic generation (SHG) will show a pronounced spectral splitting in this regime, which can be further verified by SHG experiments with a femtosecond pulsed laser. Thus, we suggest that probing in the nonlinear regime may give a clearer evidence of strong coupling that could not be observed in linear measurements.

*NSF EFMA – 1741691*
Homogeneous Broadening of Excitons in Bilayer MoSe$_2$* KEVIN SAMPSON (Presenter), Department of Physics, University of Texas at Austin, SOPHIA HELMRICH, Department of Optics and Atomic Physics, Technische Universität Berlin, CARTER YOUNG, Department of Physics, University of Texas at Austin, NINA OWSCHIMIKOW, Department of Optics and Atomic Physics, Technische Universität Berlin, JACOB EMBLEY, KAI HAO, Department of Physics, University of Texas at Austin, ULRIKE WOGGON, Department of Optics and Atomic Physics, Technische Universität Berlin, XIAOQIN (ELAINE) LI, Department of Physics, University of Texas at Austin — In transition metal dichalcogenides (TMDs), the electronic band structure shifts dramatically when the thickness of a sample is reduced from bilayer to monolayer, producing a concurrent change in their optical properties. Exciton resonances form at the K points on the Brillouin zone boundary in both the monolayers and bilayers, however, we find that their quantum dynamics differ drastically. We perform two-dimensional electronic coherent spectroscopy (2DECS) on a MoSe$_2$ monolayer and bilayer to investigate the quantum decoherence (homogeneous linewidth) of various exciton resonances. We first identify the A-exciton and trion resonances in the monolayer. The bilayer A-exciton is shifted to lower energy, consistent with previous studies. Despite the presence of an inhomogeneous broadening, we were able to extract the homogeneous linewidth using 2DECS. Most notably, the homogeneous linewidth of the bilayer exciton exceeds that of the monolayer exciton and trion significantly. Because the band structure of a MoSe$_2$ bilayer evolves to an indirect bandgap, we expect that scattering with additional interlayer phonon modes would lead to additional dephasing, consistent with the increased homogeneous linewidths observed.

*We gratefully acknowledge funding from NSF DMR-1808042.

Electron relaxation and motion at coplanar 1T'/2H MoTe$_2$ homojunction imaged by time-resolved photoemission electron microscopy AIQIN HU (Presenter), XIAOLONG XU, WEI LIU, State Key Laboratory for Mesoscopic Physics, Frontiers Science Center for Nano-optoelectronics, Collaborative Innovation Center of Quantum Matter, School of Physics, Peking U, QUAN SUN, Research Institute for Electronic Science, Hokkaido University, QIHUANG GONG, YU YE, GUOWEI LU, State Key Laboratory for Mesoscopic Physics, Frontiers Science Center for Nano-optoelectronics, Collaborative Innovation Center of Quantum Matter, School of Physics, Peking U — One critical aspect of optoelectronic devices, such as transistors, diodes, and solar cells, is the internal motion of electrons through the interface between semiconductor and electrode. High spatial and temporal resolution imaging the movement of these electrons would provide unprecedented insight into this critical phenomenon. Here, employing the femtosecond time-resolved photoemission electron microscopy with an energy analyzer, we demonstrate imaging of carrier dynamics in space and time after photoexcitation at 1T'/2H MoTe$_2$ coplanar homojunction, a seamlessly contacted metal/semiconductor interface. The energy-resolved photoelectron images revealed a highly non-equilibrium distribution of photocarriers in space and energy. Combining the time-resolved images, we visualize the motion of electrons from metallic 1T'-MoTe$_2$ to semiconducting 2H-MoTe$_2$ within about 1 picosecond. And the carriers lifetime and transfer rate can be obtained from the modified rate equations set for the homojunction. Our findings provide a new insight for the in-plane semiconductor-metal heterostructure, and it will aid the development of future high-performance devices based on 2D materials.
8:00AM R54.00001: Self-duality of the integer quantum Hall to insulator transition: a composite fermion description*  
PRASHANT KUMAR (Presenter), KEVIN S HUANG, Stanford Univ, YONG-BAEK KIM, Physics, University of Toronto, SRINIVAS RAGHU, Stanford Univ — The integer quantum Hall to insulator transition (IQHIT) is a paradigmatic quantum critical point. Key aspects of this transition, however, remain mysterious, due to the simultaneous effects of quenched disorder and strong interactions. We study this transition using a composite fermion (CF) representation, which incorporates some of the effects of interactions. As we describe, the transition also marks a IQHIT of CFs: this suggests that the transition may exhibit self-duality. We show the explicit equivalence of the electron and CF Lagrangians at the critical point via the corresponding non-linear sigma models, revealing the self-dual nature of the transition. We show analytically that the resistivity tensor at the critical point is $\rho_{xx} = \rho_{xy} = e^2/h$, which are consistent with the expectations of self-duality, and in rough agreement with experiments.

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8:12AM R54.00002: Superuniversality of topological quantum phase transitions*  
ALEXANDER TYNER (Presenter), PALLAB GOSWAMI, Northwestern University — Since two topologically distinct phases cannot be adiabatically deformed into each other, they must be separated by a sharp phase transition. Therefore, our understanding of global phase diagrams of topological quantum materials remains incomplete without addressing the nature of topological quantum critical points. We will show that irrespective of underlying symmetry classes, the universal behaviors of several topological phase transitions at different spatial dimensions are controlled by massless Dirac fermion fixed points. Based on this idea of superuniversality, we will address the scaling properties of topological quantum critical points for different Altland-Zirnbauer symmetry classes.

*NSF DMR-1720319
8:24AM R54.00003: Identification of Topological Phase Transitions in Kitaev Quantum Spin Liquids
ARA GO, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, KYUSUNG HWANG, Department of Physics, Korea Institute for Advanced Science, BEOM HYUN KIM, Department of Computational Sciences, Korea Institute for Advanced Science, JI HEON SEONG (Presenter), EUN-GOOK MOON, Department of Physics, Korea Advanced Institute of Science and Technology — We investigate physical quantities of a spin model and argue that magnetic field angle dependence and resonant inelastic X-ray scattering may probe topological phase transitions in Kitaev quantum spin liquids (KQSLs). By using exact-diagonalization, spin-wave theory, and parton mean field analysis, characteristic signatures of topological phase transitions in KQSLs are obtained in a spin model with the Kitaev, Heisenberg, and off-diagonal symmetric terms. Especially, we find qualitative differences between KQSLs and zig-zag ordered phases. We also apply our results to a candidate system α-RuCl3 and provide smoking-gun experiments.

8:36AM R54.00004: Probing Topological Phase Transition Using Rotational Second-Harmonic Generation in (Bi\textsubscript{1-x}Sb\textsubscript{x})\textsubscript{2}Se\textsubscript{3} KUN ZHAO (Presenter), SILU HUANG, JISUN KIM, MATTHEW T CURTIS, JOEL E TAYLOR, Department of Physics & Astronomy, Louisiana State University, LOUIS H HABER, Department of Chemistry, Louisiana State University, RONGYING JIN, E WARD PLUMMER, Department of Physics & Astronomy, Louisiana State University — Topological phase transitions have attracted significant attention recently. (Bi\textsubscript{1-x}Sb\textsubscript{x})\textsubscript{2}Se\textsubscript{3} demonstrates a metal-insulator transition as well as a topological phase transition from a topological insulator to a normal insulator driven by isoelectronic substitution. Although this topological phase transition has been studied both theoretically and experimentally for thin films and single crystals, very conflicting results have been reported and the critical transition point is still under debate. The symmetric study of surface electronic symmetry has never been conducted. Rotational second-harmonic generation (RSHG) is a powerful and non-invasive nonlinear optical technique for probing the electronic symmetry originating from broken symmetry at the surface. In this talk, we symmetrically characterize the surface electronic symmetry and the topological phase transition using high-quality (Bi\textsubscript{1-x}Sb\textsubscript{x})\textsubscript{2}Se\textsubscript{3} single crystals. From the RSHG patterns, we confirm the Bi\textsubscript{2}Se\textsubscript{3} surface shows a C\textsubscript{3v} symmetry and the Sb\textsubscript{2}Se\textsubscript{3} surface shows a C\textsubscript{2v} symmetry. By analyzing the evolution of RSHG patterns with substitution concentration, the critical transition point is further derived. The interplay between the topological phase transition and the metal-insulator transition is also discussed.
8:48AM R54.00005: Topological Phase Transitions in a Hybridized Three-Dimensional Topological Insulator*  SU KONG CHONG (Presenter), Department of Physics & Astronomy, University of Utah, LIZHE LIU, FENG LIU, TAYLOR D. SPARKS, Department of Materials Science and Engineering, University of Utah, VIKRAM V. DESHPANDE, Department of Physics & Astronomy, University of Utah — As the three-dimensional (3D) topological insulator (TI) approaches its 2D thickness limit, quantum tunneling between top and bottom surfaces turns their gapless Dirac band into a gapped state at the Dirac points. Analytical formulation suggests that the hybridization gap scales exponentially with a decrease in number of layers while the system oscillates between topologically trivial and non-trivial insulators. This work explores the transport properties of a 3D TI in the inter-surface hybridization regime. By experimentally probing the hybridization gap as a function of TI thickness using three different methods, namely thermal activation, differential conductance, and quantum capacitance, we map the crossover from 3D TI to 2D insulating state. We detect gap-closing features in the moderate hybridization regime with a perpendicular electric field, suggesting topological phase transitions in the regime. In certain parameter spaces of the non-trivial insulator, we observe quantization of the longitudinal conductance at $2e^2/h$ indicating the quantum spin Hall state.

*This work is supported by National Science Foundation (NSF) the Quantum Leap Big Idea Grant No. 1936383. The National High Magnetic Field Laboratory is supported by NSF through NSF/DMR-1644779* and the State of Florida.

9:00AM R54.00006: Quasi-periodic dynamical phase transitions in multi-band topological insulators  NICHOLAS SEDLMAYR (Presenter), Institute of Physics, Maria Curie-Sklodowska University — Dynamical phase transitions are non-equilibrium phenomena where non-analyticities occur in dynamically evolving correlation functions, in analogy with the non-analyticities in the derivatives of the free energy for a standard phase transition. Topological phase transitions separate phases of equivalent symmetry but different topology. The ways in which these two phenomena can be connected has recently become a topic of great interest. Here we will report on dynamical phase transitions in many-band one dimensional topological insulators which demonstrate curious quasi-periodic, rather than periodic, dynamical phase transitions. Furthermore we will consider the role of the topologically protected edge states in the dynamics and connections with fidelity susceptibility and dynamical entanglement entropy.

9:12AM R54.00007: Topological multicriticality of spin-orbit coupled electrons in one dimension*  MARIANA MALARD (Presenter), DAVID BRANDAO, PAULO E. DE BRITO, University of Brasilia, HENRIK JOHANNESSEN, University of Gothenburg — A central tenet in the theory of quantum phase transitions (QPTs) is that a nonanalyticity in the ground state energy in the thermodynamic limit implies a QPT. Here we report on a finding that challenges this assertion. As a case study we take the phase diagram of a one-dimensional band insulator with spin-orbit coupled electrons with trivial and topological gapped phases separated by intersecting critical surfaces. The intersections define multicritical lines across which the ground state energy becomes nonanalytical, but with no phase transition taking place. We propose a simple picture for how multicriticality gives rise to this unexpected phenomenon.

*This work was supported by the Swedish Research Council through Grant No. 621-2014-5972.
9:24AM R54.00008: Construction of second-order topological phases protected by chiral symmetry  RYO OKUGAWA (Presenter), WPI-AIMR, Tohoku University, SHIN HAYASHI, TAKESHI NAKANISHI, MathAM-OIL, National Institute of Advanced Industrial Science and Technology — We investigate topological phase transitions of a model to construct two-dimensional second-order topological insulators protected by chiral symmetry. By the theory of the topological phase transitions, we propose second-order topological semimetallic and insulating phases with flat hinge bands in chiral-symmetric three-dimensional systems. We also demonstrate the various second-order topological phases by constructing a two-dimensional lattice model from the Su-Schrieffer-Heeger models and by stacking the lattice models.

9:36AM R54.00009: Piezoelectricity and Topological Quantum Phase Transitions in Two-Dimensional Spin-Orbit Coupled Crystals with Time-Reversal Symmetry*  JIABIN YU (Presenter), CHAO-XING LIU, Pennsylvania State University — Topological quantum phase transitions can be reflected by the sudden jump of certain physical response functions, e.g., the transition between quantum spin Hall state and normal insulator state featured by the jump of the two-terminal conductance. In this work, we demonstrate that the piezoelectric response can also change discontinuously across a topological quantum phase transition in two-dimensional time-reversal invariant systems with spin-orbit coupling. We study all gap closing cases for all 7 plane groups that allow non-vanishing piezoelectric tensor and find that any gap closing with 1 fine-tuning parameter between two gapped states changes either the Z2 invariant (characterizing the quantum spin Hall phase) or the "locally" stable valley Chern number (characterizing the valley Hall phase). The jump of the piezoelectric response is found to exist for all these transitions, and we propose the HgTe/CdTe quantum well and BaMnSb2 as two potential experimental platforms.

*We acknowledge the support of the Office of Naval Research (Grant No. N00014-18-1-2793), the U.S. Department of Energy (Grant No. DESC0019064) and Kaufman New Initiative research grant KA2018-98553 of the Pittsburgh Foundation.
Vortex and Surface Phase Transitions in Superconducting Higher-order Topological Insulators

SAYED ALI AKBAR GHORASHI (Presenter), William & Mary, TAYLOR L HUGHES, University of Illinois at Urbana-Champaign, ENRICO ROSSI, William & Mary — Topological insulators (TIs) having intrinsic or proximity-coupled s-wave superconductivity host Majorana zero modes (MZMs) at the ends of vortex lines. The MZMs survive up to a critical doping of the TI at which there is a vortex phase transition that eliminates the MZMs. In this work, we show that the phenomenology in higher-order topological insulators (HOTIs) can be qualitatively distinct. In particular, we find two distinct features.(i) We find that vortices placed on the gapped (side) surfaces of the HOTI, exhibit a pair of phase transitions as a function of doping. The first transition is a surface phase transition after which MZMs appear. The second transition is the well-known vortex phase transition. We find that the surface transition appears because of the competition between the superconducting gap and the local T-breaking gap on the surface.(ii) We present numerical evidence that shows strong variation of the critical doping for the vortex phase transition as the center of the vortex is moved toward or away from the hinges of the sample. We believe our work provides new phenomenology that can help identify HOTIs, as well as illustrating a promising platform for the realization of MZMs.

Topological invariants and edge modes at quantum criticality

RUBEN VERRESEN (Presenter), Harvard University, RYAN THORNGREN, Harvard CMSA, NICK G. JONES, University of Bristol, FRANK POLLMANN, Technical University of Munich, ASHVIN VISHWANATH, Harvard University — It is sometimes presumed that a finite correlation length is essential to stabilizing topological phenomena. This applies even to well-studied topological semi-metals, where one appeals to gapped degrees of freedom (in momentum-space). In this talk, I will show that this common wisdom is not justified: topological invariants and edge modes can survive at phase transitions. This leads to the novel notion of symmetry-enriched quantum criticality, examples of which are hiding in plain sight.

Landau-forbidden quantum phase transitions between bosonic Z2 symmetry-protected topological phases in 2+1D

MAXIME DUPONT, University of California, Berkeley, SNIR GAZIT, Hebrew University of Jerusalem, THOMAS SCAFFIDI (Presenter), University of Toronto — We perform a Quantum Monte Carlo study of quantum phase transitions between different classes of Z2 bosonic symmetry-protected topological (SPT) phases in 2+1D. This is made possible by an advantageous choice of basis which takes care of the sign problem that one might naively expect. Depending on the classes of SPTs considered, we find a variety of unusual intermediate symmetry-broken phases, as well as evidence for a quantum critical direct transition.
**8:00AM R55.00001:** Characterization for higher-order symmetry-protected topological phases by quantized Berry phases

HIROMU ARAKI (Presenter), YASUHIRO HATSUGAI, TOMONARI MIZOGUCHI, Department of Physics, University of Tsukuba — We propose the $Z_Q$ Berry phase as a topological invariant for higher-order symmetry-protected topological (HOSPT) phases for two- and three-dimensional systems. It is topologically stable for electron-electron interactions assuming the gap remains open. The integer $Q$ is determined by the rotational symmetry the system has. As a concrete example, we show that the Berry phase is quantized in $Z_4$ and characterizes the HOSPT phase of the extended Benalcazar-Bernevig-Hughes (BBH) model, which contains the next-nearest neighbor hopping and the intersite Coulomb interactions. In addition, we introduce the $Z_4$ Berry phase for the spin-model-analog of the BBH model. Furthermore, we demonstrate the Berry phase is quantized in $Z_4$ for the three-dimensional version of the BBH model. We also confirm the bulk-corner correspondence between the $Z_Q$ Berry phase and the corner states in the HOSPT phases.

**8:12AM R55.00002:** Evolution of planar topological phases in topocircuits

JUNKAI DONG (Presenter), Cornell University, VLADIMIR JURICIC, NORDITA, BITAN ROY, Lehigh University — Liberation of topological phases from the realm of electronic materials has been recently initiated by their realizations in highly tunable metamaterials, such as phononic and photonic systems, as well as in electric circuits. These classical systems facilitate engineering of various seemingly complex phases of matter, and unveil their topological or geometric properties. We here present a systematic evolution of two-dimensional topological insulators, starting from the analog of quantum anomalous and spin Hall insulators, supporting one-dimensional edge states in electric circuits, also known as topocircuits. Subsequently, we construct rotational symmetry breaking higher-order topological insulators (HOTIs), supporting pointlike corner modes protected by an antiunitary symmetry. The systemic reduction in localization of the topological boundary modes from the edge to the corners is detected from site and orbital selective measurement of the impedance. We also present a simple circuit model for three-dimensional HOTI.

**8:24AM R55.00003:** Magnetotransport in a second-order topological insulator

BENJAMIN LEVITAN (Presenter), TAMI PEREG-BARNEA, McGill University — The most salient feature distinguishing topological insulators from ordinary band insulators is their bulk-boundary correspondence: the topologically-nontrival nature of a bulk sample is signalled by the presence of protected gap-crossing electronic states, localized to the boundary of the sample. Higher-order topological insulators exhibit a somewhat more subtle bulk-boundary correspondence. They still possess protected gap-crossing states, but these are localized to a particular submanifold of the boundary. In the case of a three-dimensional, second-order topological insulator (SOTI), the protected states are localized to the one-dimensional "hinges" of a rectangular nanowire.

We theoretically examine the effects of an applied magnetic field in a model of an SOTI, considering the case where the field couples to the orbital electronic motion. Based on numerical calculations, we predict a clear magnetotransport signature reflecting the interplay between Landau level physics and the hinge modes of the SOTI.
8:36AM R55.00004: Many-Body Invariants for Topological Insulators: Multipole, Chern, and Hinge States  BYUNGMIN KANG (Presenter), School of Physics, Korea Institute for Advanced Study, GIL YOUNG CHO, Department of Physics, Pohang University of Science and Technology (POSTECH) — We propose many-body invariants for the broad classes of topological insulators including Chern insulators, chiral hinge insulators, and multipole insulators. Unlike band indices which only work for non-interacting band insulators, our invariants can detect non-trivial topology of quantum many-body wave functions hence applicable to fully interacting quantum systems. To this end, we design several unitaries whose expectation values on many-body ground states serve as the invariants. We show that the unitaries detect the coefficients of the topological field theory, which are the defining characteristics of topological insulators. This allows us to develop a new way of evaluating Chern numbers, and also the many-body invariant for chiral hinge insulator. Furthermore, we will also show that boundary observables such as the edge-localized polarizations and the corner charge can be measured purely by the many-body unitaries when endowed with appropriate background geometry.

8:48AM R55.00005: Gapless hinge states from adiabatic pumping of axion coupling  THOMAS OLSEN, Department of Physics, Technical University of Denmark, TOMAS RAUCH, Friedrich-Schiller-University, Jena, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, IVO SOUZA (Presenter), Centro de Física de Materiales, Universidad del País Vasco — We demonstrate that gapless chiral hinge states naturally emerge in insulating crystals undergoing a slow cyclic evolution that changes the Chern-Simons axion coupling θ by 2π. This happens when the surface (not just the bulk) returns to its initial state at the end of the cycle, in which case it must pass through a metallic state to dispose of the excess quantum of surface anomalous Hall conductivity pumped from the bulk. If two adjacent surfaces become metallic at different points along the cycle, there is an interval where they are in topologically distinct insulating states, with gapless chiral modes propagating along the connecting hinge. We illustrate these ideas for a 3D tight-binding model consisting of coupled Haldane-model layers. The surface topology is determined in a slab geometry using two different markers, surface anomalous Hall conductivity and surface polarization, and we find that both correctly predict the appearance of gapless hinge states in a rod geometry.

9:00AM R55.00006: Transport signature of helical hinge states of quasi-one-dimensional topological insulators*  YANFENG ZHOU (Presenter), FAN ZHANG, Department of Physics, The University of Texas at Dallas — Higher-order topological insulators exhibit protected corner or hinge states generalizing the bulk-boundary correspondence. The quasi-one-dimensional materials Bi₄Br₄ and Bi₄I₄ have been predicted to be prototypical examples of such topological matter with helical hinge states along the atomic chain direction. We examine the electronic behavior of their helical hinge states and predict unique signatures in transport experiment. We further show how these signatures depend on the applied electric and magnetic fields.

*This theoretical work at UTD is supported by Army Research Office under Grant No. W911NF-18-1-0416 and Natural Science Foundation under Grant No. DMR-1921581 through the DMREF program.
9:12AM R55.00007: Flux Response of Higher-Order Topological Insulators  FRANK SCHINDLER (Presenter), STEPAN TSIRKIN, TITUS NEUPERT, Univ of Zurich, ANDREI BERNEVIG, BENJAMIN WIEDER, Princeton University — One of the highlights of the past few years of topological condensed matter physics has been the discovery of new forms of 3D topological crystalline insulators that are characterized by gapped bulks and surfaces and gapless hinges. Incipient experimental signatures of the gapless hinge states of these “higher-order” topological insulators (HOTIs) have been observed in bismuth, MoTe$_2$, and WTe$_2$. However, these signatures have also attracted other explanations. Therefore, it is of intense interest to establish additional indicators of higher-order topology beyond anomalous hinge states. In this work, we use threaded π-flux to probe HOTIs with and without time-reversal symmetry. We establish a general framework that captures the 0D and 1D bound states, charge, and spin that accumulate on the flux cores and tubes. Our framework captures all previous results, such as the fractional charges bound to flux cores in Chern insulators. However, we also discover new examples. Specifically, we demonstrate that π-flux tubes in inversion- and time-reversal-symmetric HOTIs bind Kramers pairs of end states, which represent observable signatures of the anomalous “half” quantum spin Hall effect present on the surfaces of weak topological insulators and HOTIs.

9:24AM R55.00008: Disordered intrinsic higher-order topological insulators  JAHAN CLAES (Presenter), TAYLOR L HUGHES, University of Illinois at Urbana-Champaign — Higher order topological insulators are a novel phase of matter in which topologically protected modes appear at corners or hinges rather than surfaces. Unlike conventional topological insulators, higher-order topological insulators can be protected by either a bulk gap or a Wannier gap. Here, we study disordered models of higher-order topological insulators whose topological modes are protected by internal symmetries and a Wannier gap. Like conventional topological insulators, we find that the topological modes are stable against weak disorder. However, we also find that increasing disorder leads to a transition to a trivial state without the mobility gap closing, in striking contrast to the case of conventional disordered topological insulators, in which topological transitions only occur at mobility gap closings. Instead, the topological transition occurs during a real-space Wannier gap closing.

9:36AM R55.00009: Higher Order Topological Insulators in Amorphous Solids  ADHIP AGARWALA (Presenter), ICTS, VLADIMIR JURICIC, NORDITA, BITAN ROY, Lehigh University — We identify the possibility of realizing higher order topological (HOT) phases in noncrystalline or amorphous materials. Specifically, starting from two and three dimensional crystalline HOT insulators, accommodating topological corner states, we gradually enhance structural randomness in the system. Within a parameter regime, as long as amorphousness is confined by outer crystalline boundary, the system continues to host corner states, realizing an amorphous HOT insulator. However, as structural disorder percolates to the edges, corner states start to dissolve into amorphous bulk, and ultimately the system becomes a trivial insulator (devoid of corner modes), when amorphousness plagues the entire system. These outcomes are further substantiated from the scaling of the quadrupolar (octupolar) moment in two (three) dimensions with the scrambling radius. Therefore, HOT phases can be realized in amorphous solids, when wrapped by a thin crystalline layer.
9:48AM R55.00010: Pfaffian formalism for higher-order topological insulators  HEQIU LI (Presenter), KAI SUN, Univ of Michigan - Ann Arbor — We generalize the Pfaffian formalism, which has been playing an important role in the study of time-reversal invariant topological insulators (TIs), to 3D chiral higher-order topological insulators (HOTIs) protected by the product of four-fold rotational symmetry $C_4$ and the time-reversal symmetry $T$. This Pfaffian description reveals a deep and fundamental link between TIs and HOTIs, and allows important conclusions about TIs to be generalized to HOTIs. As examples, we demonstrate in the Letter how to generalize Fu-Kane's parity criterion for TIs to HOTIs, and also present a general method to efficiently compute the $Z_2$ index of 3D chiral HOTIs without a global gauge.

10:00AM R55.00011: Identifying Higher Order Topology and Fractional Corner Charge Using Entanglement Spectra*  PENGHAO ZHU (Presenter), Department of Physics and Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign, KIERAN LOEHR, Department of physics, Cornell University, TAYLOR HUGHES, Department of Physics and Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign — We study the entanglement spectrum (ES) of two-dimensional Cn-symmetric second-order topological insulators (TIs). We show that some characteristic higher order topological, e.g., the filling anomaly and its associated fractional corner charge, can be determined from the ES of atomic and fragile TIs. By constructing the relationship between the configuration of Wannier orbitals and the number of protected in-gap states in the ES for different symmetric cuts in real space, we express the fractional corner charge in terms of the number of protected in-gap states of the ES. We show that our formula is robust in the presence of electron-electron interactions as long as the interactions preserve rotation symmetry and charge-conservation symmetry. Moreover, we discuss the possible signatures higher order topology in the many-body ES. Our methods allow the identification of some classes of higher order topology without requiring the of nested Wilson loops or nested entanglement spectra.

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Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R56 DCMP: Cerium-Based Heavy Fermion Metals  Mile High Ballroom 2C - James Allen, University of Michigan
**8:00AM R56.00001: Interplay of CEF effects and RKKY interaction in Ce- and Yb-based heavy-fermion compounds**

GERTRUD ZWICKNAGL (Presenter), Institut f. Mathemat. Physik, Techn. Univ. Braunschweig, VILEN ZEVIN, The Racah Institute of Physics, The Hebrew University of Jerusalem — We calculate the influence of Crystalline Electric Field (CEF) effects on the indirect Ruderman-Kittel-Kasuya-Yoshida (RKKY) exchange interaction between local 4f moments in Ce- and Yb-compounds. Starting from a periodic Anderson model and neglecting spin-orbit effects among the conduction states, we show that the anisotropy of the CEF ground state manifests itself in the anisotropy of the effective exchange coupling constant $J(R, R')$ between two moments at sites $R$ and $R'$ while the interaction between two Kramers doublets is isotropic in pseudo-spin space. We evaluate the exchange constant for various models of the conduction states in tetragonal Ce- and Yb-122 compounds. The influence of spin-orbit interaction among the conduction electrons is discussed.

*Partially supported by the joint French-German ANR-DFG grant Fermi-NESt.

**8:12AM R56.00002: Crystal-field excitations and magnetic fluctuations of heavy-fermion metal CeB$_6$**

MAI YE (Presenter), Department of Physics and Astronomy, Rutgers University-New Brunswick, HSXANG-HSI KUNG, Department of Physics and Astronomy, University of British Columbia, PRISCILA ROSA, ERIC BAUER, Los Alamos National Laboratory, ZACHARY FISK, Department of Physics and Astronomy, University of California-Irvine, GIRSH BLUMBERG, Department of Physics and Astronomy, Rutgers University-New Brunswick — CeB$_6$ enters an antiferro-quadrupolar (AFQ) phase below $T_{AFQ}=3.2K$, in which the $T_{2g}$-symmetry quadrupoles order at a finite wave vector [Rep. Prog. Phys. 79, 066502 (2016)]. With its cubic lattice structure and 4f$^1$ Ce$^{3+}$ electronic configuration, this compound is considered a prototypical example of heavy-fermion metal with quadrupolar ordering. We study the crystal-field (CF) excitations and magnetic fluctuations at Ce$^{3+}$ sites by Raman scattering [Phys. Rev. Materials 3, 065003 (2019)]. The spectral linewidth of the CF transitions increases on cooling below 80K, at which the electric resistivity shows its maximum. This coincidence points to the relationship between the broadening of linewidth and Kondo physics. For quasi-elastic fluctuations, the temperature dependence of the static Raman susceptibility in the magnetic channel is consistent with the previously-reported magnetic susceptibility data. Such behavior implies that above $T_{AFQ}$, the tendency towards AFQ ordering induces ferromagnetic correlations which manifest as long-wavelength magnetic fluctuations.

*M.Y., H.-H.K. and G.B. was supported by NSF DMR-1709161. Sample synthesis at Los Alamos was performed under the auspices of DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering.*
Large Fermi surface expansion through anisotropic mixing of conduction and f electrons in the semimetallic Kondo lattice CeBi

PENG LI, ZHONGZHENG WU, FAN WU, CHUNYU GUO, Zhejiang Univ; YI LIU, University of Science and Technology of China; HAIJIANG LIU, Swiss Light Source, ZHE SUN, University of Science and Technology of China, MING SHI, Swiss Light Source, FANNY RODOLAKIS, JESSICA L MCCHESENY, Advanced Photon Source, CHAO CAO, Hangzhou Normal University, HUIQIU YUAN, FRANK STEGLICH, YANG LIU (Presenter), Zhejiang Univ — Using angle-resolved photoemission spectroscopy (ARPES) and resonant ARPES, we report evidence of strong anisotropic conduction-f electron mixing (c-f mixing) in CeBi by observing a largely expanded Ce-5d pocket at low temperature, with no change in the Bi-6p bands. The anisotropic Fermi surface (FS) expansion is accompanied by a pronounced spectral weight transfer from the local 4f$^{0}$ peak of Ce (corresponding to Ce$^{3+}$) to the itinerant conduction bands near the Fermi level. Careful analysis suggests that the observed large FS change (with a volume expansion of the electron pocket up to 40%) can most naturally be explained by a small valence change (~ 1%) of Ce, which coexists with a very weak Kondo screening. Our work therefore provides evidence for a FS change driven by real charge fluctuations deep in the Kondo limit, which is highly dependent on the orbital character and momentum and is made possible by the low carrier density.

Vanishing Hall number at a quantum critical point

NIKOLA MAKSIMOVIC (Presenter), TAYLOR COOKMEYER, IAN HAYES, EHUD ALTMAN, JAMES ANALYTIS, University of California, Berkeley — Certain types of quantum critical points, phase transitions at zero-temperature, have long been thought to underlie unconventional superconductivity in a variety of systems. We study the effect of particle-hole dilution in the unconventional superconductor CeCoIn$_5$, and discover an unusual critical point that connects two distinct Fermi liquids with different Fermi surface volumes without any apparent symmetry breaking. The signature of this transition is pronounced in the Hall number, which nearly vanishes at the phase boundary between the two Fermi liquids and exhibits a strong dependence on the applied magnetic field. The experiment provides evidence for a type of quantum critical point that fractionalizes conventional metallic quasiparticles into gapless spin excitations and gapped charge carrying excitations. Calculations are presented which suggest that the experimentally measured Hall resistivity in this material reflects the motion of charged particles in the fractionalized Fermi fluid.

*This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Energy Frontier Research Center.
8:48AM R56.00005: Quantum Critical Strange Metal and Fermi Surface Reconstruction in a large-$N$ Kondo Lattice Model  AAVISHKAR PATEL, TAYLOR COOKMEYER, ERIK ALDAPE (Presenter), EHUD ALTMAN, University of California, Berkeley — Quantum critical points in heavy Fermion materials, involving a change of the Fermi surface volume, have presented a long standing puzzle. One way to describe such a transition within a Kondo lattice model is through condensation of a slave Boson. However, this approach leads to a weakly coupled critical point, which fails to describe non-Fermi liquid behavior, such as the ubiquitously observed $T$-linear resistivity at criticality. We present a modified large-$N$ Kondo lattice model, which also describes a transition from a small Fermi surface to a heavy Fermi liquid with a large Fermi surface, but gives rise to $T$-linear resistivity at the critical point. In the large-$N$ limit we also compute the behavior of the Hall transport properties across the transition and compare the results to recent experiments with CeCoIn$_5$. We show under what conditions a strong enhancement of the Hall coefficient, seen in the experiment, is expected.

9:00AM R56.00006: Spectroscopic evidence for pre-formed heavy electron pairs and novel pairing mechanism in CeCoIn$_5$ (Part 1/2)*  KESHAV SHRESTHA (Presenter), National High Magnetic Field Laboratory, SHENGZHI ZHANG, Florida State University, LAURA GREENE, National High Magnetic Field Laboratory, JOE D THOMPSON, Los Alamos National Laboratory, YOU LAI, Florida State University, RYAN BAUMBACH, National High Magnetic Field Laboratory, KALYAN SASMAL, M BRIAN MAPLE, University of California, San Diego, WAN KYU PARK, National High Magnetic Field Laboratory — The heavy-fermion compound CeCoIn$_5$ shows unconventional superconductivity ($T_c=2.3$ K) with $d_{x^2-y^2}$-wave pairing symmetry[1]. Despite evidence for pseudogap in the normal state[2], their spectroscopic nature remains to be unraveled. Here, we present results from planar tunneling spectroscopy measurements on CeCoIn$_5$ along [001], [100], and [110] directions. While the nodal junction exhibits only a zero-bias conductance peak, the non-nodal junctions show sharp double peaks corresponding to the superconducting gap. Interestingly, they evolve continuously crossing the $T_c$, merging into a single broad peak at $T_p=5$K. From quantitative analyses of the conductance spectra, we have found that the gap persistent in the normal state originates from the formation of heavy electron pairs that condense into a coherent state below $T_c$. We will discuss the implications of our findings in the context of other measurement results in the literature along with the underlying pairing mechanism.


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The glue that binds heavy electrons into pairs in CeCoIn$_5$ ($T_c=2.3$K) is not known unambiguously yet. The origin of the neutron resonance peak[1] is still controversial[2] despite the original interpretation as evidence for the spin fluctuation mechanism. Also, the hump-dip feature expected in tunneling conductance is missing in scanning tunneling spectroscopy measurements[3]. Here, we present results from planar tunneling spectroscopy on CeCoIn$_5$, revealing the pairing gap opens at $T_p \sim 5$K. Interestingly, under a magnetic field, the pairing gap turns into a field-induced gap-like feature (FIG). The FIG increases linearly with the field and is observed only below $T_p$. This concomitance of the FIG with the pairing along with its linear field dependence strongly suggests that it is intimately tied to the underlying pairing mechanism. We will discuss these findings in the context of the composite pairing mechanism based on the cooperative two-channel Kondo effect[4].


*Supported by NSF/DMR-1704712(FSU), DOE, Office of BES&Division of MSE(LANL), NSF/DMR-1810310(UC-San Diego) & NSF/DMR-1644779 & the State of Florida(NHMFL).
Resonances in thermal conductivity of superconducting CeCoIn$_5$ in rotating magnetic field

DUK YOUNG KIM, SKKU, South Korea, Institute of Basic Science, SHIZENG LIN, ERIC BAUER, FILIP RONNING, ROMAN MOVSHOVICH (Presenter), Los Alamos Natl Lab — We performed thermal conductivity measurements of d-wave superconducting CeCoIn$_5$ in magnetic field up to 12 Tesla rotating in the a-b plane of this tetragonal compound, in a dilution refrigerator. The heat current $J$ was applied along the [100] direction, antinodal of the superconducting order parameter. In similar previous measurements we observed sharp field-magnitude independent resonances in thermal conductivity for field direction $\Theta = \pm 33^\circ$ away from the direction of the heat current $J$ applied along [110], the direction of the nodes. For heat current $J || [100]$ we observe the resonances at $\Theta = \pm 12^\circ$, complimentary to previous $33^\circ$ resonances, also independent of the magnitude of the magnetic field. The field direction with respect to the crystallographic direction, not the direction of the heat current, is therefore of importance. Our model calculation of the density of state in the normal CeCoIn$_5$ in magnetic field show sharp resonances as function of the field orientation. This suggests that the sharp resonances in thermal conductivity in superconducting CeCoIn$_5$ should be attributed to normal parts of the Fermi surface, which were suggested to exist in magnetic field.

*Work at Los Alamos was supported by the Los Alamos Laboratory Directed Research and Development program.

Thermal expansion of heavy-fermion CeRhIn$_5$ under pressure

SOONBEOM SEO (Presenter), SEAN THOMAS, FILIP RONNING, ERIC BAUER, JOE D THOMPSON, PRISCILA ROSA, Los Alamos National Laboratory — Antiferromagnetic CeRhIn$_5$ is a prototypical heavy-fermion compound. With applied pressure, the antiferromagnetic ordering of CeRhIn$_5$ disappears and an unconventional superconducting state emerges. Crystalline electric field (CEF) effects are known to be important in the determination of the ground state of heavy-fermion materials. However, CEF effects in CeRhIn$_5$ have not been studied under pressure because of the limiting volume and background of pressure cells. Here we probe the CEF scheme of CeRhIn$_5$ via thermal expansion measurements under pressure using the strain gauge method at high temperature and optical fiber sensors at low temperature. We report the temperature dependence of the linear thermal-expansion coefficient of CeRhIn$_5$ under pressure. Our results allow us to determine CEF splitting energies from the ground state to the excited state and observe the evolution of the phase transitions under pressure. We will discuss the pressure dependence of CEF effects in CeRhIn$_5$ in comparison with other 115 compounds.

*Work at Los Alamos was performed under the auspices of the US DOE, Division of Materials Sciences and Engineering. S. S. acknowledges support of the LANL LDRD program through a Director's Postdoctoral Fellowship.
9:48AM R56.00010: Ferromagnetic quantum critical point in heavy fermion compound CeRh₆Ge₄
BIN SHEN, YONGJUN ZHANG, MICHAEL SMIDMAN, Zhejiang Univ, MICHAEL NICKLAS, ROBERT BORTH, MPI-CPfS, AN WANG, HANOH LEE, FRANK STEGLICH, HUIQIU YUAN (Presenter), Zhejiang Univ — Due to the low energy scales, the ground state of heavy fermion compounds can be readily tuned by parameters such as pressure, magnetic fields or doping. There have been numerous studies into antiferromagnetic quantum criticality and unconventional superconductivity, which have been revealed a possible role for spin fluctuations in the superconducting pairing [1, 2]. However, ferromagnetism in heavy fermion systems has been less investigated and there is still short of evidence for the presence of ferromagnetic quantum critical point in a pure system [3]. Here we report various measurements of the ferromagnetic compound CeRh₆Ge₄ under pressure, which provide clear evidence for the existence of a ferromagnetic critical point, at which strange metal behavior is also observed [4].

References:

10:00AM R56.00011: Theoretical investigation of mixed valence compound CeRh₃ by means of 3d-4f resonant inelastic X-ray scattering
NORIMASA SASABE (Presenter), Japan Synch Rad Inst (JSRI) — Ce intermetallics, which are typical strongly correlated system, show the various phenomena, Kondo effects, magnetic ordering and so on. This variety is caused to the 4f electron behavior of Ce atoms, and the electron state needs to be investigated for the understanding of the phenomena.

X-ray core-level spectroscopy is an efficient technique to investigate the electronic state of strongly correlated systems. Recent years, experimental techniques have been rapidly developing and, especially, the progress in experimental resolution has enabled us to observe fine spectral features, which were not formerly observed. These advantages will enable us to observe spectral fine features related with the electron state related to Kondo effects and/or magnetic ordering of the Ce intermetallics.

In this study, the spectral calculation for 3d-4f resonant inelastic X-ray scattering (RIXS) of CeRh₃ is shown, and the character of the final state for 3d-4f RIXS is clarified by paying attention to the incident X-ray energy and polarization. This calculation is performed with an impurity Anderson model considering full multiplet effects in addition to a realistic band effect based on a local density approximation calculation.
10:12AM R56.00012: Low temperature characterization of single crystalline Ce$_2$Ni$_2$In

JANNIS MAIWALD (Presenter), MEIGAN ARONSON, University of British Columbia — Materials with the $R_2T_2X$ ($R$ = Ce,Yb; $T$=transition metal; $X$=main group element) stoichiometry span an extensive (~40) class of compounds. The underlying interactions of these tetragonal systems leads typically to dimerization of the 4f magnetic moments associated with the $R$ ions. These materials feature a broad range of physics, ranging from valence fluctuations, non-Fermi liquid behavior and heavy fermion ground states. Most recently fractional excitations have been observed in inelastic neutron scattering experiments performed on Yb$_2$Pt$_2$Pb. In this talk we will introduce Ce$_2$Ni$_2$In, as a new single crystalline addition to the 221 family of materials. We will discuss its synthesis, general characterization, measurements of the specific heat as well as directional dependent measurements of the magnetic susceptibility and electrical transport from room temperature down to 50 mK.

10:24AM R56.00013: Frist Principles Study of the Fermi Surface Topology of CeCu$_2$Si$_2$*

ROXANNE TUTCHTON (Presenter), Los Alamos National Laboratory, QIMIAO SI, Department of Physics and Astronomy, Rice University, JIAN-XIN ZHU, Los Alamos National Laboratory — Since the discovery of heavy-fermion superconductivity in CeCu$_2$Si$_2$, the material has attracted interest in the nature of superconducting pairing. So, it is essential to better understand the electronic Fermi surface topology and its role in strong antiferromagnetic fluctuations. We have performed electronic ground state calculations on CeCu$_2$Si$_2$ using the Gutzwiller approximation. This method captures the quasiparticle band renormalization from the strong onsite Coulomb repulsion. We have performed an analysis of the electronic structure and the Fermi surface topology by varying the interaction strength and taking into account the crystal-field splitting. Using the de Haas van Alphen effect, the extremal Fermi surface cross-sectional areas were calculated to quantify the quasiparticle mass renormalization in the energy bands. Our results confirm two Fermi surface sheets corresponding to the heavy and light quasiparticles, which is in agreement with the renormalized band method. We also discuss the connection of the Fermi surface topology to hot-spots in the magnetic susceptibility form factor measured by neutron scattering.

The LANL LDRD Program.
The DOE BES Program.
Quantum Criticality from Sequential Destruction of SU(4) Spin-Orbital-coupled Kondo Effect

SILKE BUEHLER-PASCHEN (Presenter), Vienna University of Technology, CHIA-CHUAN LIU, ANG CAI, Rice Univ, EMILIAN NICA, Arizona State University, RONG YU, Renmin University of China, KEVIN INGERSENT, University of Florida, QIMIAO SI, Rice Univ — Quantum criticality and the beyond-Landau physics of Kondo destruction [1,2] have recently been studied in systems with multipolar degrees of freedom. The compound Ce$_3$Pd$_{20}$Si$_6$ shows evidence of two consecutive Fermi surface collapsing quantum critical points (QCPs) as it is tuned from a paramagnetic to an antiferroquadrupolar and then to an antiferromagnetic state [3]. A theory was advanced [3] for a sequential destruction of spin-orbital-coupled Kondo entanglement in an SU(4) Bose-Fermi Kondo model, an effective model for a multipolar Kondo lattice. Here we report an analytical renormalization group calculation of the model with Ising anisotropy, using a Coulomb-gas representation. We show that a generic trajectory in the parameter space contains two QCPs associated with the destruction of the orbital and spin Kondo effects, respectively. Our work establishes a firm theoretical ground for the sequential Kondo destruction.


*NSF Grant No. DMR-1920740 & Welch Foundation Grant No. C-1411.

X-ray and neutron-diffraction studies of the CeOs$_4$Sb$_{12}$ valence transition at low temperatures and high magnetic fields

JOHN SINGLETON (Presenter), National High Magnetic Field Laboratory, Los Alamos National Laboratory, KATHRIN GOETZE, MATTHEW PEARCE, Physics, Warwick University, ZAHIRUL ISLAM, Advanced Photon Source, Argonne National Laboratory, ULRICH WELP, Argonne National Laboratory, PAUL GODDARD, Physics, Warwick University, ROGER JOHNSON, University College London, PASCAL MANUEL, ISIS Neutron Source, M BRIAN MAPLE, UCSD, PEI-CHUN HO, Physics, Fresno State University — CeOs$_4$Sb$_{12}$ exhibits a very unusual field- and temperature-driven valence transition that is accompanied by a drastic change in Fermi-surface topology. It is also a candidate heavy-fermion topological semimetal and sports a field-induced quantum-critical point at about 20 T. Single crystal x-ray diffraction in pulsed magnetic fields of up to 30 T using a unique instrumental combination at the Advanced Photon Source permitted a study of the change in unit-cell volume as the field swept through the valence transition. In addition, neutron-diffraction measurements probed the analogous structural changes as a function of temperature in zero magnetic field. Both measurements shed light on the unique “wedge-shaped” phase boundary that marks the valence transition in CeOs$_4$Sb$_{12}$.
8:00AM R57.00001: Epitaxial growth of stanene and antimonene on noble metal and oxidized metal surfaces  AIDI ZHAO (Presenter), School of physical science and technology, Shanghaitech University — Group-IV and group-V monoelement two-dimensional (2D) materials like stanene, antimonene or bismuthene has been theoretically proposed to be quantum spin Hall (QSH) insulator with large energy gaps for room-temperature use. However, to experimentally fabricate such ultra-thin materials with topologically nontrivial properties remains challenging. It requires accurate control over substrate-interface structures at the atomic level. We successfully grown an ultraflat stanene layer with an in-plane s-p band inversion together with a large spin-orbit-coupling-induced topological gap (~ 0.3 eV), which represents a first group-IV ultraflat graphene-like material displaying topological features in experiment. Such an in-plane s-p band inversion results in a nontrivial σ-orbital-derived QSH phase described by the Bernevig-Hughes-Zhang model and this QSH phase is more environmentally stable comparing to those π-orbital-derived QSH phases. We also successfully synthesized an antimonene film on Ag(111) surface showing an extraordinarily large tensile strain and bilayer stanene on an oxidized Cu(110) surface with large anisotropic strain.

8:12AM R57.00002: Effects of short-range order and interfacial interactions on the electronic structure of two-dimensional antimony-arsenic alloys*  QI AN (Presenter), School of Materials Science and Engineering, University of Science and Technology Beijing, MATTHIEU FORTIN-DESCHÊNES, Department of Engineering Physics, École Polytechnique de Montréal, GUANGHUA YU, School of Materials Science and Engineering, University of Science and Technology Beijing, OUSSAMA MOUTANABBIR, Department of Engineering Physics, École Polytechnique de Montréal, HONG GUO, Department of Physics, McGill University — The growth of two-dimensional (2D) antimony-arsenic alloys has been recently demonstrated using solid-source molecular beam epitaxy and this provides an additional degree of freedom to tailor their basic properties. With this perspective, we propose and conduct a comprehensive first principles investigation on this 2D group-V antimony arsenide (2D As$_x$Sb$_y$), in both free-standing form as well as on common substrates of Ge(111), Si(111), bilayer graphene and bilayer hexagonal boron nitride (h-BN). Structural and electronic properties of the 2D As$_x$Sb$_y$ are evaluated for different compositions, different types of atomic arrangements for each composition, different lattice matched interfacial configurations of the composite heterostructures for the four substrates. These systematic studies provide property benchmarks for this new class of group-V 2D materials and reveal microscopic origins of the interfacial interactions, orbital hybridization, charge transfer and the resulting electronic structures of the 2D alloy.

*This work is supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Natural Science Foundation of China (Grant No. 51571017 and 51871018).
LaBr, a layered magnetic material that is weakly bound by van der Waals interactions, is an ambient pressure electride and, using first-principles electronic structure calculations, we show that monolayer LaBr is potentially exfoliable, stable, retains the magnetic ordering of bulk LaBr and could also be an electride at ambient pressure.

Furthermore, in monolayer LaBr, we show that the two interstitial sites occupied by electrons have a strong tendency to bind with, e.g., hydrogen and we propose several new structures with composition of La, H and Br. We have calculated the composition phase diagram of LaBr with hydrogen, finding LaBr to be a potential promising candidate material for high-density hydrogen storage, and monolayer La$_2$HBr$_2$ to be a potential promising candidate 2D multiferroic material.

8:48AM R57.00005: Quasiparticle band structure of bulk and few-layer transition-metal dichalcogenides*  
HAN-GYU KIM (Presenter), HYOUNG JOON CHOI, Department of Physics, Yonsei University, Seoul 03722, Korea — We studied the work function, ionization energy, and electron affinity of bulk and few-layer transition-metal dichalcogenides (TMDs) in 2H phase using the density functional theory (DFT) and the GW approximation. We obtained DFT band energies of few-layer TMDs with respect to the vacuum level. For the vacuum level of bulk TMDs, we considered a sufficiently thick slab system which has a similar band gap with bulk. We introduced the GW approximation to obtain the quasiparticle energy shift of valence band maximum and conduction band minimum and estimated the work function, band gap, ionization energy, and electron affinity as functions of the number of layers. We compare our quasiparticle band energies of TMDs with available experimental reports.

*This work is supported by the NRF of Korea (Grant No.2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2018-CRE-0097).

9:00AM R57.00006: Single-particle spectral function formulated and calculated by variational Monte Carlo method*  
MAXIME CHARLEBOIS (Presenter), CCQ, Flatiron Institute, MASATOSHI IMADA, Science and Engineering, Waseda University — A method to calculate the one-body Green’s function for ground states of correlated electron materials is formulated by extending the variational Monte Carlo method. We benchmark against the exact diagonalization (ED) for the one- and two-dimensional Hubbard models of 16 site lattices, which proves high accuracy of the method. The application of the method to larger-sized Hubbard model on the square lattice correctly reproduces the Mott insulating behavior at half filling and gap structures of \( d \)-wave superconducting state in the hole doped Hubbard model, evidencing a wide applicability to strongly correlated electron systems.

*This work was supported by Fonds de recherche du Québec - Nature et technologies (FRQNT) and by a Grant-in-Aid for Scientific Research (No. 16H06345) from Ministry of Education, Culture, Sports, Science and Technology, Japan.
I present two 2D material systems where their crystallinities are paradoxically improved by defects during growth. First, I demonstrate that a new class of defect complex, interlayer Frenkel pairs, enhances the orientational epitaxy of transition metal dichalcogenides on hexagonal boron nitride, leading to experiments that achieve 95% consistency in orientational order by strongly suppressing inversion domains [1,2]. I will show how the stability of the defect complex originates from its electronic structure at the density functional theory level and discuss our recent extension to accelerated GW-level computations for defects. Second, I discuss our recent joint theory and experimental work on a 2D metal-semiconductor heterostructure hosting air-stable, crystalline 2D metals. Enabled by graphene defects in an initial graphene/SiC system, p-block metal atoms such as Ga, In, and Sn intercalate under graphene and bond covalently to the SiC beneath, forming lattice-matched 2D metals, as demonstrated by their calculated phase stabilities [3,4]. Based on first-principles calculations assisted by Wannier functions, I explain the presence of superconductivity in spite of the metals' free-electron-like electronic structure.


*Funding for this work was provided by the 2D Crystal Consortium National Science Foundation (NSF) Materials Innovation Platform under cooperative agreement DMR-1539916.
Structural and optical properties of bulk and monolayer GeSe: A Quantum Monte Carlo Study*  
HYEONDEOK SHIN (Presenter), Argonne Natl Lab, JARON KROGEL, PAUL KENT, Oak Ridge Natl Lab, ANOUAR BENALI, OLLE HEINONEN, Argonne Natl Lab — We have performed quantum Monte Carlo simulations of the monochalcogenide GeSe to study its structural and optical properties. 2D GeSe has received a great deal of attention due to its wide range of applications in industrial devices, such as photodetector, gas sensor, and anode material. Density functional theory (DFT) studies show that the monolayer has smaller lattice parameters than the bulk system, with small band gap energy (1~2 eV). However, DFT cannot conclusive determine if the monolayer has a direct or indirect band gap because of very small differences (~0.02 eV) between direct and indirect gaps. Moreover, the geometry for GeSe is not clear within DFT scheme because the DFT lattice parameters and atomic coordinates vary strongly with the particular exchange-correlation functional used. Using fixed-node diffusion Monte Carlo (DMC), we reproduce accurate lattice parameters and band gaps compared to the experimental values for bulk GeSe. For the monolayer, we find that the DMC optimal lattice parameters for the monolayer are close to the bulk ones, and DFT significantly underestimates its lattice parameters. Finally, we compute accurate DMC band gap energies at the optimal geometry for the monolayer.

*This work was supported by CPSFM, a DOE-BES center.

Tailoring of interlayer hopping integral at K valley in transition metal dichalcogenides*  
WEI-TING HSU (Presenter), JIAMIN QUAN, Department of Physics, The University of Texas at Austin, PENG-JEN CHEN, Institute of Atomic and Molecular Sciences, Academia Sinica, XIAOQIN (ELAINE) LI, Department of Physics, The University of Texas at Austin, JUNG-FU LIN, Jackson School of Geosciences, The University of Texas at Austin, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin — Interlayer electronic coupling plays a critical role in developing novel electronic metamaterials such as unconventional superconductivity in graphene and moiré excitons in transition metal dichalcogenides (TMDs), in which the potential landscape is determined by the interlayer hopping integral. In addition to the well-known effects of stacking configuration, a largely unexplored factor is the van der Waals (vdW) gap, which impacts the hopping integral exponentially. Here, by measuring the direct optical transitions, we quantitatively determine the interlayer hopping integral of K valley as ~40 meV in Bernal-stacked MoS$_2$. The vdW-gap dependence was further investigated by tuning the temperature and hydrostatic pressure. We observed a 2.4-fold enhancement at a reduced vdW gap of ~7%. The experimental results were compared with the density functional theory. Our work has shed light on designing the TMD-based moiré heterostructures in the future.

*This research was supported by the Welch Foundation (F-1672), the US Airforce (FA2386-18-1-4097), and the US National Science Foundation (DMR-1808751 and the MRSEC program DMR-1720595).
10:12AM R57.00010: The relationship between activation energy and band gap in a disordered 2D insulator  YANJUN HE (Presenter), BRIAN SKINNER, Ohio State Univ - Columbus — We study how the activation energy for conductivity is related to the band gap in a 2D band insulator that experiences a disorder potential created by charged impurities. This problem can be mapped to a problem of classical percolation, since the conductivity is limited by the rate at which electrons are activated from the chemical potential to a percolating energy contour in real space (the classical mobility edge). When impurities are sparse, we find that the activation energy is the same as in the disorder-free case, even though there is significant band bending. On the other hand, when the Coulomb disorder is strong enough to induce large, closely-spaced electron puddles, the activation energy reflects the Coulomb charging energy of large puddles, and has a critical dependence on the band gap that is characteristic of 2D percolation.

10:24AM R57.00011: The temperature dependence of the band structures in mono-layer, few-layer and bulk black phosphorus  SHENYANG HUANG (Presenter), FANJIE WANG, Fudan Univ, GUOWEI ZHANG, Northwestern Polytechnical University, CHAOYU SONG, YUCHEN LEI, QIAOXIA XING, CHONG WANG, Fudan Univ — Black phosphorus (BP), an emerging two-dimensional material, has attracted abundant research interests. However, the study of temperature dependence of the bandgap in few-layer BP is still lacking. Here we systematically investigated the temperature dependence of the electronic structures in mono-layer, few-layer and bulk BP. We found that the temperature dependence of the electronic structure has strong layer and transition-index dependence, which is closely related to the temperature dependent interlayer interaction. Surprisingly, the band gaps of monolayer and bulk BP showed opposite temperature effect. Such diverse behavior sheds light on the importance of van der Waals coupling in defining the electronic structures of 2D materials.

10:36AM R57.00012: Effective Hamiltonian for Extrinsic Spin-Orbit Coupling in 2D Materials  SEYED MOHAMMAD FARZANEH (Presenter), Electrical and Computer Engineering, New York University, Brooklyn, NY 11201, SHALOO RAKHEJA, Holonyak Micro and Nanotechnology Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801 — Inversion symmetry of a two-dimensional (2D) electron system can be broken by a perpendicular external electric field which lifts the spin degeneracy while it preserves the time-reversal symmetry. The resulting spin splitting, known as the Bychkov-Rashba (BR) spin-orbit coupling, can be used for spin manipulation solely using electric fields without an external magnetic field. However, the main limitation of the phenomenological BR Hamiltonian is that it is inapplicable to two-dimensional (2D) monolayer materials in which the crystal structure is different than that of conventional zinc-blende and wurtzite semiconductors. In this work, we use the theory of invariants to derive the effective Hamiltonian for 2D materials, such as phosphorene and transition metal dichalcogenides, without resorting to any phenomenological prefactor as that in the BR model. Owing to their vertical and lateral scalability and high electron mobility, 2D materials provide an excellent platform to realize semiconducting spintronics devices. We determine the bands that contribute to the extrinsic spin-orbit coupling of conduction electrons and calculate the prefactors in terms of k.p parameters.

*MRSEC Program of the National Science Foundation, Award Number: DMR-1420073
Metal-dependent interfacial properties in pthalocyanine-MoS$_2$ heterostructures*  
TEODOR STANEV (Presenter), SAMUEL H AMSTERDAM, QUNFEI ZHOU, Northwestern University, PIERRE DARANCET, Argonne National Lab, MARK C HERSAM, TOBIN MARKS, NATHANIEL PATRICK STERN, Northwestern University — Mixed-dimensional heterostructures made by combining 2D materials with other systems of different dimensionality can exhibit unique interfacial effects and modify the properties of the individual constituent layers. Organic molecules are an attractive building block for these structures due to their synthetically tunable properties and ease of processing. Here we discuss interfacial charge transfer in metallophthalocyanine (MPc) – MoS$_2$ heterojunctions. These interfaces show heterojunction-specific optical absorption transitions, strong Raman enhancement, and defect emission quenching in the MoS$_2$, all of which depend the identity of the single metal (M) atom at the MPc core. Temperature dependent optical and electrical characterization were carried out to characterize and to understand the interfacial interactions. The metal core dependence provides a ‘knob’ for controlling opto-electronic properties of both the interface and the underlying layer, highlighting the complex and tunable nature of 0D/2D van Der Waals interfaces.

*This work was supported by the National Science Foundation's MRSEC program (DMR-1720319) at the Materials Research Center of Northwestern University.

Thursday, March 5, 2020 8:00 AM - 10:24 AM

Session R58 DCP DCOMP DPOLY DCMP: DFT and Beyond VIII  
Mile High Ballroom 3B - Neepa Maitra, Rutgers University, Newark - Tag(s): Focus
8:00AM R58.00001: Ultrafast Spin Dynamics with TDDFT* [Invited]  PETER ELLIOTT (Presenter), Max Born Institute Berlin, Berlin, Germany — Laser-induced ultrafast spin dynamics can manipulate the magnetic moment of materials on femtosecond timescales, several orders of magnitude faster than traditional methods.

In the past few years, we have applied real-time time dependent density functional theory to study the induced spin dynamics and provide an overdue ab-initio perspective to this problem. We observed two main mechanisms for ultrafast change in local magnetic moments: 1) spin-orbit driven spin-flips[1] leading to ultrafast demagnetization and 2) optical inter-sublattice spin transfer OISTR[2].

OISTR was first predicted in Heusler compounds[2], but appears for a wide range of materials, including anti-ferromagnetic systems where it can be used to switch the material to a transient ferromagnetic state[3].

The signature of OISTR has been seen experimentally for several materials including Heusler compounds, Co/Cu interfaces[4], Ni/Pt multilayers, CoPt, and FeNi.

In this talk I will review our findings so far and hope to convince you that ultrafast spin dynamics has been a real success story for TDDFT.


In collaboration with: Peter Elliott (Max Born Institute Berlin, Berlin, Germany), J.K. Dewhurst (Max Planck Inst of Microstructure Physics), Eberhard K Gross (ritz Haber Center for Molecular Dynamics, The Hebrew University of Jerusalem), Sangeeta Sharma (Max Born Institute Berlin, Berlin, Germany)

*DPG TRR227.
**8:36AM R58.00002: A real-time TDDFT study of CDW phase under femtosecond optical pulse in monolayer 2H-NbSe2**

TOWFIQ AHMED (Presenter), JIAN-XIN ZHU, Los Alamos Natl Lab —

Abstract: Intense, transient electromagnetic (EM) fields have recently emerged as an exciting alternative for driving quantum materials into new phases by selectively coupling to specific degrees of freedom, making it possible to create transient and metastable states that do not exist in equilibrium. First principles study of such driven quantum phases are now possible, thanks to the velocity-gauge implementation of real-time time-dependent density functional theory (RT-TDDFT). Ultra-fast/femtosecond laser pump and probe can reveal important information in 2D transition metal dichalcogenides many of which exhibit short time-scale complex interplay between quantum phases such as CDW, valley polarization and superconductivity. In this study, we performed RT-TDDFT calculations to study how the higher-harmonic generation (HHG) behaves in CDW and non-CDW phases of monolayer NbSe2 under different laser field intensities. We simulated frequency dependent current spectra to identify the HHG modes in NbSe2 under intense laser field.

*This work was carried out under the auspices of the U.S. Department of Energy (DOE) National Nuclear Security Administration under Contract No. 89233218CNA000001. It was supported by the LANL LDRD Program (20190026DR).*

**8:48AM R58.00003: Emergence of band gaps, mass enhancement and Jahn-Teller distortions in AFM and PM 3d Oxides from polymorphous DFT**

ALEX ZUNGER (Presenter), University of Colorado, Boulder, JULIEN VARIGNON, CRISMAT, Normandie — A central feature in understanding the properties of 3d Oxides is their magnetic structure. While local moments are present both in the AFM and PM phases, the latter has traditionally been simplistically modeled as non-magnetic (NM) structure in which each atom was thought to have zero moment, (while the real condition is only that the total PM cell will have zero moment). This NM approximation underlying the N-DFT approach (N= Naive) has led to the opinion that DFT misses the Mott gap in PM insulators, effective mass enhancement effect, bond disproportionation and Jahn-Teller distortions. These discrepancies suggested in the literature invoking explicitly dynamically correlated approaches. We explored the alternative option of staying within (single determinant) DFT but getting rid of N-DFT. Instead of using a minimal unit cells, we use a supercell where the total moment is constrained to be zero but local moments and displacements that lower the total energy are allowed. This generalization creates finite band gaps in AFM and PM phases of ABO3 perovskites (except PM metals SrVO3 and CaVO3 ), disproportionation (in SmNiO3 and YNiO3), mass enhancement (in SrVO3 and doped SrTiO3) and explains the observed trends in JT distortions throughout the series.

*DOE-BES-MSE to CU Boulder.*
9:00AM R58.00004: Characterizing Single-Molecule Magnets using Density Functional Theory
HENRY FITZHUGH (Presenter), JAMES FURNESS, JIANWEI SUN, Tulane Univ — Single-molecule magnets are valued as prospective components in devices for information processing and storage. Computational modeling can aid in understanding and optimizing their magnetic properties. Many single-molecule magnets are too large for analysis using high-level wavefunction theories, making density functional theory (DFT) an attractive choice.

The magnetic properties of single-molecule magnets depend on a strong exchange interaction between orbitals and the spatial localization of spin orbitals, properties that have been challenging for conventional exchange-correlation functionals. It is therefore crucial to understand the relative effectiveness of DFT methods. Here we apply functionals at the meta-GGA, and local hybrid levels in conjunction with broken symmetry methods to single-molecule magnet systems with exchange-coupled metallic cores. We determine effective coupling parameters and other magnetic properties, and investigate the practical utility of the functionals.

*DOE under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents

9:12AM R58.00005: Exchange-correlation magnetic fields in spin-density-functional theory
EDWARD A PLUHAR (Presenter), CARSTEN A. ULLRICH, Physics and Astronomy, Univ of Missouri - Columbia — In spin-density-functional theory for noncollinear magnetic materials, the Kohn-Sham system features exchange-correlation (xc) scalar potentials and magnetic fields. The significance of the xc magnetic fields is not very well explored; in particular, they can give rise to local torques on the magnetization, which are absent in standard local and semilocal approximations. We obtain exact benchmark solutions for two electrons on four-site extended Hubbard lattices over a wide range of interaction strengths, and compare exact xc potentials and magnetic fields with approximations obtained from orbital-dependent xc functionals. The xc magnetic fields turn out to play an increasingly important role as systems become more and more correlated and the electrons begin to localize; the effects of the xc torques, however, remain relatively minor. The approximate xc functionals perform overall quite well, but tend to favor symmetry-broken solutions for strong interactions.

*This work was supported by Research Corporation and by DOE Grant No. DE-SC0019109.
9:24AM R58.00006: A benchmark of predicting magnetic structures using a combination of the cluster multipole expansion and LSDA* MARIE-THERESE HUEBSCH (Presenter), Graduate School of Frontier Sciences, University of Tokyo, TAKUYA NOMOTO, Department of Applied Physics, University of Tokyo, MICHI-TO SUZUKI, Institute for Materials Research, Tohoku University, RYOTARO ARITA, Department of Applied Physics, University of Tokyo — The cluster multipole (CMP) expansion for magnetic structures [1] provides a scheme to systematically generate candidate magnetic structures specifically including noncollinear magnetic configurations adapted to the crystal symmetry of a given material. A comparison with the experimental data collected on MAGNDATA [2] shows that the most stable magnetic configurations in nature are a linear combination of only few CMPs. Furthermore, a high-throughput generalized local spin-density approximation (LSDA) calculation, in which each candidate magnetic structure was considered as an initial guess, was performed using VASP [3]. We benchmark the predictive power of CMP+LSDA by testing whether CMP administers an appropriate list of candidate magnetic structures and LSDA reproduces the experimental magnetic configurations.


*CREST(JPMJCR18T3), Grants-in-Aid for Scientific Research, MEXT, Japan (16H06345).

9:36AM R58.00007: TDDFT for spin waves in two-dimensional systems: orbital-based approximations* MATTHEW ANDERSON (Presenter), CARSTEN A. ULLRICH, Univ of Missouri - Columbia — The collective dynamics of electrons with Dirac-like dispersions, such as in doped graphene, is not well described by the usual semilocal approximations of (TD)DFT, which are based on the traditional electron gas. Instead, we use orbital-based approximations, most notably the Singwi-Tosi-Land-Sjolander (STLS) approach, generalized to systems with noncollinear spin. We calculate spin-wave dispersions in magnetized two-dimensional systems of itinerant electrons.

*This work was supported by Research Corporation and by DOE Grant No. DE-SC0019109.
The effect of removal of self-interaction error on the magnetic exchange couplings

PO-HAO CHANG (Presenter), PRAKASH MISHRA, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas, El Paso — Spin coupling within and between molecules has played an important role in the design and development of molecular magnets, spintronics, and memory devices. Accurate theoretical determination of magnetic properties in molecular complexes has therefore become crucial. The Green's function (GF)-based approach, often used in solid-state physics, for computing exchange coupling can potentially offer additional insights into local pathway in exchange spin coupling. We implement this approach into the UTEP-NRLMOL and FLOSIC codes and apply it, along with Noodleman's spin-projected (SP) broken-symmetry approach, to study the exchange coupling in a set of molecules. In particular, we use Fermi-Lowdin self-interaction method to investigate the role of self-interaction error in predicting exchange-coupling with three (LSDA, PBE, and SCAN) non-empirical density functional approximations that correspond to the first three rungs of Perdew-Schmidt ladder of functionals.

*DE-SC0018331
DE-SC0006818

Self-interaction-corrected electronic structure of Fe-based single-ion magnetic molecule

ANRI KARANOVICH (Presenter), Virginia Tech, YOH YAMAMOTO, University of Texas at El Paso, KAI TREPTE, KOBLAR JACKSON, Central Michigan University, RAJENDRA R ZOPE, TUNNA BARUAH, University of Texas at El Paso, KYUNGWHA PARK, Virginia Tech — Density-functional theory (DFT) has been successful in predicting properties of various systems ranging from molecules to solids. However, self-interactions of electrons that do not cancel out in local and semi-local approximate exchange-correlation functionals, impede accurate prediction of properties. Recently, an effective way to perform self-interaction correction (SIC) has been proposed using localized Fermi-Lowdin orbitals (FLO) by introducing a Fermi orbital descriptor for each occupied orbital. We apply this method to a Fe-based single-ion magnetic molecule with large magnetic anisotropy barrier, using FLOSIC code, in order to study electronic and magnetic properties. We discuss calculated projected density of states as well as an energy gap between the highest-occupied molecular orbital (HOMO) and the lowest-unoccupied molecular orbital (LUMO) for the ground-state spin configuration. We further compare our SIC-calculated result to DFT calculations without SIC and DFT+U calculations.

*Funded by the Department of Energy Basic Energy Sciences grant No DE-SC0019033.
Computational support by Virginia Tech ARC and XSEDE SDSC DMR060009N
10:12AM R58.00010: Fermi-Lowdin orbital self-interaction correction on magnetic properties of Cu(II)-acetate monohydrate*  PRAKASH MISHRA (Presenter), Computational Science Program, University of Texas at El Paso, YOH YAMAMOTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas, El Paso — We study the magnetic properties of copper acetate monohydrate [Cu(CH3COO)2(H2O)]2 using the Fermi-Lowdin orbital based self-interaction corrected (FLOSIC) density functional method. Most common density functional approximations that often accurately predict equilibrium properties have a self-interaction error that tends to unphysically lower the energies of fractionally occupied state which leads to deviation from piecewise linear behavior of total energy between two integer occupations. This leads to delocalization of the orbitals which is more apparent in d-electron systems resulting in incorrect electron densities. We find that removing self-interaction error using FLOSIC improves the magnetic coupling constant resulting in better agreement with experiment. The performance of self-interaction corrected density functional approximations on the magnetic properties is studied. The effect of self-interaction correction on the orbitals, density and the zero field splitting parameters will be presented and discussed.

*This work is supported by US Department of Energy grant No. DE-SC0018331.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R59 DMP: Weyl semimetals, nonlinear optics  Mile High Ballroom 3C -
Tag(s): Focus

8:00AM R59.00001: Fermi surface instability in the antiferromagnetic Dirac material Ca1- xNaₓMnBi₂ LEONARDO DEGIORGI (Presenter), MATTEO CORASANITI, RUN YANG, ETH Zurich — The quasi-two-dimensional bismuth layer-like AMnBi₂ (A= alkaline as well as rare earth atom) lately advanced as an arena for the investigation of low-energy quasiparticle excitations in topological materials. The A= Sr or Ca compositions have attracted special attention because of the coexistence of the anisotropic Dirac cones with antiferromagnetic order. In a broader context, the title compound also provides an opportunity to study low-dimensional magnetism and its putative relationship to the electronic properties. This work describes novel results of reflectivity measurements from the far-infrared up to the ultraviolet that probe the optical response as a function of temperature. This gives access to the optical conductivity which captures the relevant energy scales shaping the electronic structure. We discover [1] a reshuffling of spectral weight, defined as the integral of the real part of the optical conductivity, for energy scales up to 0.2 eV. This occurs at the onset of the spin reorientation transition which also manifests as an anomaly in the dc transport data of the title compound. This may reveal the inclination towards a Fermi surface instability in topological materials.

8:12AM R59.00002: Evidence for Strong Electron-Phonon Coupling in Weyl Semimetals

GAVIN OSTERHOUDT (Presenter), Boston College, CHRISTINA GARCIA, Harvard University, VINCENT PLISSON, Boston College, JENNIFER COULTER, Harvard University, JOHANNES GOOTH, Max Planck Institute for Chemical Physics of Solid, BING SHEN, NI NI, Univ of California Los Angeles, CLAUDIA FELSER, Max Planck Institute, PRINEHA NARANG, Harvard University, KENNETH BURCH, Boston College

— Since the experimental discovery of topological semimetals (TSM) there has been a flurry of activity focused on identifying signatures of topological transport. However, many of the transport properties display behavior that is dominated by non-topological interactions with the phonon system. A deeper understanding of these TSMs therefore requires investigation of the coupling between the topological electronic system and the non-topological vibrational system. In this presentation we discuss our recent temperature dependent Raman measurements on multiple TSMs which reveal unusual temperature dependence of the linewidths. These linewidths indicate strong electron-phonon coupling in these materials, and furthermore, they show a preponderance of optical phonon decay into electron-hole pairs which seems to be a relatively general feature in TSMs.

*U.S. Department of Energy Award No. DE-SC0018675
National Science Foundation, Grant No. DMR-1709987
National Energy Research Scientific Computing Center Contract No. DE-AC02-05CH11231
Research Computing Group at Harvard University
DOE `\`Photonics at Thermodynamic Limits" Energy Frontier Research Center, Grant No. DE-SC0019140
U.S. Department of Energy, Award Number DE-SC0011978

8:24AM R59.00003: Second Order Nonlinear Responses in Chiral Weyl Semimetal CoSi

ELIZABETH DRUEKE (Presenter), RACHEL OWEN, MATTHEW W DAY, Univ of Michigan - Ann Arbor, SHANGJIE TIAN, CHANGE LI, HECHANG LEI, Renmin University of China, STEVEN THOMAS CUNDIFF, LIUYAN ZHAO, Univ of Michigan - Ann Arbor — The origin of the nonlinear responses in Weyl semimetals has become an increasingly contentious issue in recent years, with some of these effects being attributed to topology and others to symmetry. Part of this contention comes from the fact that the Weyl nodes are required by mirror symmetries in non-chiral Weyl semimetals to appear at exactly the same energy in the band structure, making it impossible to probe a single cone. Recently, chiral Weyl semimetals – with no mirror symmetries – have been observed with paired Weyl cones at significantly different energies (>100meV), allowing for cone discrimination based on choice of laser wavelength. Here, we present our study of the second order nonlinear responses in one such chiral Weyl semimetal, CoSi. In particular, we look at variation of the second harmonic generation (SHG) at multiple crystalline facets of CoSi, and the spatial inhomogeneity and temporal dynamics of its induced SHG. Further, we compare the SHG response strength to a variety of second order nonlinear crystals. Finally, we examine the spontaneous photocurrent response in CoSi.

*E. Drueke acknowledges support by NSF Graduate Research Fellowship Program under Grant No. DGE-1256260.
Magnetic-Field Dependence of Chirality-Resolved Optical Phonon in Weyl semimetal

KUNYAN ZHANG (Presenter), Pennsylvania State University, AMBER MCCREARY, National Institute of Standards and Technology, FEI HAN, MINGDA LI, Massachusetts Institute of Technology, ANGELA HIGHT WALKER, National Institute of Standards and Technology, SHENGXI HUANG, Pennsylvania State University — Weyl semimetal (WSM), the solid-state realization of chiral Weyl fermions, exhibits chiral zeroth Landau levels in the magnetic field contributing to novel transport and optical properties. While electronic transport has been a focus of studies, the optical response of WSM is relatively under-explored, yet it can also reflect the topological nature of WSM. For example, the chirality of the Weyl fermions can be determined by measuring the photocurrent using circularly polarized mid-infrared light. In this work, we study the chirality-resolved optical phonons in type-I WSM TaP under magnetic field, using Raman spectroscopy with excitations of both linear and circularly polarized lasers. Under magnetic field, the $B_{1}^{1}$ mode prohibited at zero field for 633 nm excitation can be evidently observed for linear polarization. With circularly polarized excitation, the measured phonon modes break the classical Raman tensor theory, and the symmetry-prohibited modes can be observed. Moreover, the phonon mode intensity exhibits non-reciprocity with polarizations of incident and scattered light ($\sigma+/\sigma+$ and $\sigma+/\sigma-$). Our observation is closely related to the chiral Landau levels and shows the capability of Raman spectroscopy in studying the magnetic field response of WSMs.

Unique Optical Responses of Weyl Semimetals

KENNETH BURCH (Presenter), Boston College — The isolation of electrons of different chirality in Weyl semimetals led to predictions of novel transport phenomena. Amongst these are the nonlinear responses and chiral anomaly. Here I will discuss our recent results on a range of Weyl semimetals. First I will focus on their nonlinear responses. Next, I will cover how Raman reveals surprisingly large electron-phonon coupling, that is relevant to their high mobility and potential for chiral transport.

Weyl Semimetals in Nanophotonics and Quantum Optoelectronics

CHRISTINA GARCIA (Presenter), PRINEHA NARANG, John A. Paulson School of Engineering and Applied Sciences, Harvard University — Weyl semimetals obtain their topological classification from the breaking of inversion or time-reversal symmetry. Consequently, they hold the potential for large optical nonlinearities and nonreciprocal behavior, making Weyl semimetals a very interesting materials class for optoelectronic and photonic applications. In this talk, we discuss our first principles calculations of optoelectronic properties of Weyl semimetals for integration with nanophotonic and plasmonic architectures. We discuss the coupling of atom-like emitters to cavities made from Weyl semimetals, designed with the idea of minimizing the loss penalty of conventional metals, as well as the use of Weyl semimetals for nonreciprocal thermal radiation control, which could avoid the applied magnetic field required in previous nanophotonic device designs. Finally, as an outlook, we will present a general computational approach to develop low-loss, highly nonlinear Dirac and Weyl semimetal materials for photonic information science.

*This work was supported by the DOE Photonics at Thermodynamic Limits Energy Frontier Research Center under Grant No. DE-SC0019140. C. G. also acknowledges support from the NSF Graduate Research Fellowship Program under Grant No. DGE-1745303.
10:00AM R59.00007: Large longitudinal circular photogalvanic effect in a chiral Weyl semimetal  ZHUOLIANG NI (Presenter), Department of Physics & Astronomy, University of Pennsylvania, KEFENG WANG, Department of Physics, University of Maryland, College Park, BING XU, Department of Physics, University of Fribourg, XINGYUE HAN, Department of Physics & Astronomy, University of Pennsylvania, KAUSTUV MANNA, Max Planck Institute for Chemical Physics of Solids, JOHNPIERRE PAGLIONE, Department of Physics, University of Maryland, College Park, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, LIANG WU, Department of Physics & Astronomy, University of Pennsylvania — Breaking all of the mirror symmetries in a chiral Weyl semimetal lifts the energy degeneracy of two Weyl points with opposite Chern numbers. One of the consequences is the large or even quantized circular photogalvanic effect (CPGE), which originates from one of the Weyl points by keeping the other node Pauli-blocked. Here, we report a large photocurrent generated by circularly polarized light in a chiral Weyl semimetal. Symmetry analysis shows that the photocurrent is consistent with the longitude CPGE in bulk. The second-order conductivity spectrum of CPGE in near-infrared and mid-infrared regions is then obtained and the condition of quantization is examined.

10:12AM R59.00008: Polarized Transient Reflectance Spectroscopy of Type II Weyl Semimetal NbIrTe$_4^*$  SAMUEL LINSER (Presenter), GIRIRAJ JNAWALI, SEYYEDESADAF POURNIA, IRAJ ABBASIAN SHOJAEI, HOWARD E JACKSON, LEIGH M SMITH, Department of Physics, University of Cincinnati, CONGCONG LE, FU-CHUN ZHANG, Kavli Institute of Theoretical Sciences, University of the Chinese Academy of Sciences, BRENDEN ORTIZ, STEPHEN WILSON, Materials Engineering, University of California, Santa Barbara — Weyl semimetals have attracted intense interest for exhibiting chiral Fermion states. Strong nonlinear effects such as 2$^\text{nd}$ harmonic generation and DC photocurrents via circular photogalvanic effect are seen. Less understood is the dynamic response of said chiral carriers. We present polarized transient reflectance of single nanoflakes of NbIrTe$_4$, employing ultrafast (140 fs) NIR pump and MIR probe pulses. We use a photo-elastic modulator to produce a ~50 kHz oscillation of the circular probe polarization from left to right handedness. DFT calculations predict the presence of 8 pairs of Weyl nodes with opposite chirality in the BZ of NbIrTe$_4$. We observe a typical transient response composed of a rapid (~500 fs) decay followed by a slow (~1 ns) relaxation. A sign change in the transient response is observed at ~0.5 eV, suggestive of a band-to-band transition between a band below the Fermi energy and near the Weyl nodes to some higher-lying state.

*$We acknowledge the financial support of the NSF through grants DMR 1507844, DMR 1531373, and ECCS 1509706. S.D.W. acknowledges the support of NSF DMR 1505549, and FZ acknowledges the support of the NSF of China through grant 11674278.
10:24AM R59.00009: Angle and Polarization-Resolved Resonant Raman Spectroscopy of the Type-II Weyl Semimetal NbIrTe₄

* IRAJ ABBASIAN SHOJAEI (Presenter), GIRIRAJ JNAWALI, SEYYEDESADAF POURNIA, SAMUEL LINSER, HOWARD JACKSON, LEIGH SMITH, Univ of Cincinnati, CONGCONG LE, FU-CHUN ZHANG, Kavli Institute of Theoretical Sciences, University of the Chinese Academy of Sciences, BRENDEN ORTIZ, STEPHEN WILSON, Materials Engineering, University of California, Santa Barbara — We perform polarized Raman spectroscopy measurements of single nanoflakes exfoliated from a single crystal of the layered ternary compound NbIrTe₄. By varying the angle between the polarization direction of incident light and the crystalline “a” axis, spectra indicate strongly anisotropic Raman peaks which are consistent with the broken inversion symmetry of the crystal, which is an essential enabling condition for a type II Weyl semimetal. We have used both 633 nm and 514 nm laser excitation with incoming and backscattered rays parallel to the c-axis normal to the flake with the “a” and “b” axes in the plane of the nanoflake. The comparison of these spectra shows an enhancement of Raman peaks and also changes in rotational symmetry for 633 nm excitation. This suggest a possible unresolved resonance with a state at lower energies. Density Functional Theory (DFT) calculations of this crystal (space group Pmn2₁) show close correspondence with both the frequency and symmetries of the modes detected in our measurement.

*We acknowledge the financial support of the NSF through grants DMR 1507844, DMR 1531373, DMR 1505549 and ECCS 1509706, and NSF of China through grant 11674278.

10:36AM R59.00010: Investigating the Energy Dependent Photogalvanic Effect in the Type-II Weyl Semimetal NbIrTe₄

* SEYYEDESADAF POURNIA (Presenter), GIRIRAJ JNAWALI, IRAJ ABBASIAN SHOJAEI, SAMUEL LINSER, HOWARD JACKSON, LEIGH M SMITH, Univ of Cincinnati, CONGCONG LE, Kavli Institute of Theoretical Sciences, FU-CHUN ZHANG, University of Hong Kong, STEPHEN WILSON, BRENDEN ORTIZ, University of California, Santa Barbara — We explore the photogalvanic effect in NbIrTe₄, a type II Weyl semimetal. NbIrTe₄ exhibits 8 pairs of Weyl nodes which are monopoles of Berry curvature with opposite ±1 chiralities. We measured the photoresponse for a full rotation of a quarter wave plate for energies ranging from 0.3 to 1 eV. The Photothermoelectric (PT), and Circular (CPGE) and Linear (LPGE) Photogalvanic responses were extracted by fitting the angular dependence of the signal. The PT response shows an onset at an energy at 0.3 eV, consistent with DFT calculations. The LPGE response is relatively constant over this energy range, while the CPGE response shows a strong increase at low energies as the excitation approaches the Weyl nodes at the Fermi energy. Surprisingly, a strong peak in the CPGE response is also seen in the range 0.5 to 0.7 eV. This suggests that the CPGE response may be enhanced by a transition between bands near the Weyl point and a higher lying state.

*We acknowledge the support of NSF grants DMR 1507844, 1531373, 1505549 and ECCS 1509706, and the NSF of China through grant 11674278.
Investigation of optical properties of 3D Dirac materials

FRANCOIS JOINT (Presenter), GREGORY S JENKINS, University of Maryland, College Park, ROBERT J. CAVA, Chemistry, Princeton University, DMITRI BASOV, Physics, Columbia University, HOWARD DREW, University of Maryland, College Park — 3D Dirac semimetals are newly discovered topological materials that are characterized by Weyl nodes with double degeneracy in the bulk. The electronic bands are protected from gapping by crystal symmetries and touch at special points in the BZ zone. A Dirac semimetal band structure has been observed in with ARPES but the study of their electric-optical properties has yet to be further developed. Here, we present spectral measurements on the 3D Dirac semimetal. Using FITR technics in reflectivity configuration, we have observed the electromagnetic response of the 3D Dirac material from the FIR up to the NIR frequency range in different electrical field polarization configuration. Our measurements reveal the presence of unusual collective excitations near the screened plasma frequency. We attribute these excitations as arising from the extra-term in the action of the electromagnetic field that originates from the chiral shift between the Weyl nodes. We will also present the optical response in an applied magnetic field.

*Work supported by DOE grant # DE-SC0005436

Thursday, March 5, 2020 8:00 AM - 10:48 AM

Session R60 DMP: Topological Superconductivity with 1D Modes

Mile High Ballroom 4A - Enrico Rossi, William & Mary College - Tag(s): Focus
8:00AM R60.00001: Interference effects in quanum Hall - superconductor hybrid devices

[Invited] GLEB FINKELSTEIN (Presenter), ANDREW SEREDINSKI, LINGFEI ZHAO, ETHAN ARNAULT, ANNE M DRAELOS, ALEXEY BONDAREV, TREVYN LARSON, MING-TSO WEI, Duke University, HENGMING LI, Physics, Appalachian State University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, NIMS, Japan, FRANCOIS AMET, Physics, Appalachian State University, HAROLD U BARANGER, Duke University — I plan to discuss our group's two recent results: realization of the quantum Hall-based SQUID in side-gated samples; and observation of the chiral Andreev edge states – hybrid electron/hole single particle modes running along the superconductor - quantum Hall interfaces.

1) We have developed graphene Josephson junctions with self-aligned side gates, which enable full control over the electrostatic potential near the sample edges. The gates allow us to tune the local electron density in a wide range, in particular inducing counterpropagating quantum Hall edge states along either side gate. The close spacing between these states allows them to efficiently couple through Andreev reflections and carry supercurrent. When both side gates are applied, superconducting channels are created on both sides of the junction, thereby realizing a gate-tunable quantum Hall-based SQUID.

2) We observe direct signatures of chiral Andreev edge states (CAES) – single particle modes running along the superconductor - quantum Hall interfaces. Semi-classically, the CAES can be interpreted as a result of multiple Andreev reflections of a single electron/hole skipping along the interface. Experimentally, we observe fluctuations of the signal propagating along the superconducting contact and interpret them in terms of interference between the CAES.

*Transport measurements conducted by L.Z., E.G.A., and A.S. were supported by the DOE Award No. de-sc0002765. Lithographic fabrication and samples characterization was performed by L.Z., M.-T. W., and A.S. with the support of NSF awards ECCS-1610213 and DMR-1743907. The measurement setup was developed by A.W.D., T.L., and G.F. with the support of ARO Award W911NF-16-1-0122. Numerical simulations conducted by A.B. and H.U.B. were supported by the DOE Award No. de-sc0005237. H.L. and F.A. acknowledge the ARO Award W911NF-16-1-0132. K.W. and T.T. acknowledge support from JSPS KAKENHI Grant Number JP15K21722.
We study a tight-binding model of a graphene nanoribbon in the integer quantum Hall state with one edge coupled to an s-wave superconductor. Along the superconducting edge at high field, we find two gapless electron-hole hybrid modes related by particle-hole symmetry. These modes have nearly equal electron and hole content and propagate more slowly than the corresponding pure vacuum-quantum Hall edge modes. The momentum difference between these modes leads to accumulation of a relative phase between them. This phase is tunable via gate voltage, magnetic field, or applied bias. We show that such phase variation gives rise to oscillations of the longitudinal resistance between electron-like and hole-like transport similar to those measured recently by Zhao et al. [1]. Armchair and zigzag nanoribbons lead to similar results because the valley degeneracy is broken by the superconductor.


*Research supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, under award No. DE-SC0005237.
8:48AM R60.00003: Hybrid quantum circuits in vertical magnetic fields  KAVEH DELFANAZARI (Presenter), Engineering Department & Cavendish Laboratory, University of Cambridge, UK, LLORENS SERRA, IFISC (UIB-CSIC) and Physics Department, University of the Balearic Islands, Spain, PENGCHENG MA, Cavendish Laboratory, University of Cambridge, UK, IAN FARRER, Department of Electronic and Electrical Engineering, University of Sheffield, UK, DAVID A RITCHIE, Cavendish Laboratory, University of Cambridge, UK, HANNAH J JOYCE, Engineering Department, University of Cambridge, UK, MICHAEL JOSEPH KELLY, Engineering Department & Cavendish Laboratory, University of Cambridge, UK, CHARLES G SMITH, Cavendish Laboratory, University of Cambridge, UK — Topological superconductors, that host Majorana zero modes and parafermions, can also be realized at the interface of superconductivity and the quantum Hall states in hybrid superconductor-semiconductor devices. Here, we present (i) two types of artificially engineered hybrid Josephson circuits fabrication methods, and (ii) sub-Kelvin temperature-dependent transport measurements at low and high magnetic fields $B$. We experimentally demonstrate that the 2D Josephson junctions and field-effect transistors under vertical magnetic fields show (i) an unusual magnetoconductance oscillations together with asymmetric $dI/dV$ curves at $B < 100$ mT, (ii) Superconducting correlation on quantum Hall states at $B$ up to 6 T, respectively. Our experimental results are qualitatively explained by a model considering the trivial and topological phase transitions in hybrid 2D Josephson junctions in vertical fields.

Topological superconductors (TS) represent a phase of matter whose properties are insensitive to local perturbations. This robustness renders TS suitable for application in quantum computing. The past decade has witnessed substantial progress towards a quantum bit using Majorana modes, the well-known non-Abelian modes in TS. However, because Majoranas lack a universal logic gate set, Majorana quantum bits are computationally limited. This important drawback can be overcome by parafermions, a novel set of non-Abelian modes whose array supports universal topological quantum computation. A primary route to synthesize parafermions involves inducing superconductivity in fractional quantum Hall (FQH) edge. Here we use high-quality van der Waals devices coupled to a narrow NbN which remains superconducting in the magnetic fields required for robust FQH. We find crossed Andreev reflection (CAR) across the narrow NbN that separates two counterpropagating FQH edges. Control experiments show that CAR vanishes with increasing temperature, excitation and magnetic field as expected from the theory. These results lay the groundwork for experimental parafermion research in condensed matter.

*Ö.G. acknowledges support by a Rubicon grant of the Netherlands Organization for Scientific Research (NWO).
9:24AM R60.00006: Chiral Majorana Mode in Topological Superconducting Element Hcp Thallium
MOTOAKI HIRAYAMA (Presenter), RIKEN, TAKUYA NOMOTO, RYOTARO ARITA, University of Tokyo — The chiral Majorana fermion is an exotic particle that is its own antiparticle. It can arise in a one-dimensional edge of topological materials, and especially that in a topological superconductor can be exploited in non-Abelian quantum computation. While the chiral Majorana mode (CMM) remains elusive, a promising situation is realized when superconductivity coexists with a topologically non-trivial surface state. Here, we perform the fully non-empirical calculation for the CMM considering superconductivity and surface relaxation and show that hexagonal close-packed thallium (Tl) has an ideal electronic state that harbors the CMM [1]. The $k_z = 0$ plane corresponds to the TCI with mirror Chern number $|N_M| = 2$. One of the Dirac points on the (01-10) surface is located almost at the Fermi level. Tl is a textbook-like s-wave superconductor and the gap function has no significant wave-number dependence. Only one of the two Dirac points is relevant for the gap opening due to the superconducting transition, and the CMM appears at the hinge under the Zeeman field. Our calculation indicates that Tl will provide a new platform of the Majorana fermion and quantum computation.


9:36AM R60.00007: Spontaneous thermal Hall conductance in superconductors with broken time-reversal symmetry*
FIRAT YILMAZ (Presenter), SUNGKIT YIP, Academia Sinica — The thermal Hall conductivities (THCs), $\kappa_{ij}$s have extensively been studied in recent condensed matter experiments. THC can spontaneously become non-zero for a time-reversal symmetry (TRS) broken system, and have a contribution from topologically protected edge states. In this talk, we focus on an additional bulk effect, the impurity pair breaking mechanism (IPM) in superconductors (SCs). Previously, the THCs were calculated for the chiral p-wave [1-2] SCs for point impurities. Motivated by d-wave TRS broken SCs; URu$_2$Si$_2$, SrPtAs including Sr$_2$RuO$_4$ which is recently suggested to be also possibly, we calculate THCs at finite temperatures and for finite size impurities using the non-equilibrium quasiclassical Green's functions.

We find that the IPM is dominant in $\kappa_{yx}$ at finite temperatures when compared to the topological contribution except at very low temperatures. There are two experimental signatures of IPM: 1. a non-monotonic temperature dependence, 2. sign change as a function of temperature depending on the scattering process.


*This work supported by Taiwan MOST with Project No: 107-2112-M001-035-MY3.
Microwave spectroscopy of semiconductor-nanowire-based superconducting qubits with Majorana bound states  RAMON AGUADO (Presenter), JESUS AVILA, CSIC - Madrid, ELSA PRADA, IFIMAC, UAM, Madrid, PABLO SAN-JOSE, CSIC - Madrid — Recent experimental efforts have focused on replacing the weak link in the Josephson Junction (JJ) of a superconducting qubit by electrostatically-gateable technologies compatible with high magnetic fields. Such alternatives are crucial in order to reach a regime relevant for readout of topological qubits based on Majorana bound states (MBS). We here focus on a system where a semiconducting nanowire forming the JJ is driven to a topological superconductor phase with MBS which coherently interact with the superconducting qubit degrees of freedom. Our fully microscopic theoretical description of this nanowire-based superconducting qubit allows to unveil new physics. This includes the magnetic field dependence of the qubit frequency, which follows the gap closing and the emergence of MBS in the topological phase. In this phase, the periodicity of the qubit spectrum with respect to $n_g$ can be either that of Cooper pairs $2e$ or single electrons $e$, depending on microscopic parameters such as the degree of Majorana energy splitting or the ratio of Josephson to charging energy $E_J/E_C$. Overall, the corresponding microwave spectroscopy presents nontrivial features, including a full mapping of zero energy crossings and fermionic parity switches in the nanowire owing to Majorana oscillations.

Decays of Majorana or Andreev Oscillations Induced by Steplike Spin-Orbit Coupling*  ZHAN CAO (Presenter), Southern University of Science and Technology, HAO ZHANG, Tsinghua University, HAI-FENG L'U, University of Electronic Science and Technology of China, WAN-XIU HE, Lanzhou University, HAIZHOU LU, Southern University of Science and Technology, XINCHENG XIE, Peking University — The Majorana zero mode in the semiconductor-superconductor nanowire is one of the promising candidates for topological quantum computing. Recently, in islands of nanowires, subgap-state energies have been experimentally observed to oscillate as a function of the magnetic field, showing a signature of overlapped Majorana bound states. However, the oscillation amplitude either dies away after an overshoot or decays, sharply opposite to the theoretically predicted enhanced oscillations for Majorana bound states. We reveal that a steplike distribution of spin-orbit coupling in realistic devices can induce the decaying Majorana oscillations, resulting from the coupling-induced energy repulsion between the quasiparticle spectra on the two sides of the step. This steplike spin-orbit coupling can also lead to decaying oscillations in the spectrum of the Andreev bound states. For Coulomb-blockade peaks mediated by the Majorana bound states, the peak spacings have been predicted to correlate with peak heights by a $\pi/2$ phase shift, which was ambiguous in recent experiments and may be explained by the steplike spin-orbit coupling. Our work will inspire more works to reexamine effects of the nonuniform spin-orbit coupling in experimental devices.

Ref: Z. Cao et al., PRL 122, 147701 (2019).

*NSFC
**10:12AM R60.00010: Nonlocal conductance in three-terminal hybrid Al/InSb nanowire devices**  
SEBASTIAN HEEDT (Presenter), Microsoft Quantum Lab Delft, FRANCESCO BORSOI, QuTech, Delft University of Technology, MARINA QUINTERO PEREZ, ALEXANDRA FURSINA, Microsoft Quantum Lab Delft, NICK VAN LOO, QuTech, Delft University of Technology, GHADA BADAWY, SASA GAZIBEGOVIC, Eindhoven University of Technology, KEVIN VAN HOOGDALEM, Microsoft Quantum Lab Delft, ERIK BAKKERS, Eindhoven University of Technology, LEO P KOUWENHOVEN, Microsoft Quantum Lab Delft — Majorana zero-energy modes (MZMs) emerge at the edges of a one-dimensional topological segment. Signatures of these modes are correlated zero-bias peaks (ZBPs) in the local conductance that emerge simultaneously at both edges. The energy gap that separates them from the continuum - the bulk topological gap - can be identified in the nonlocal conductance, which is insensitive to local Andreev levels or transmission resonances. Thus, it is a vital tool to distinguish nontopological zero-energy modes and MZMs. Here, we have realized hybrid three-terminal devices based on InSb nanowires. The proximity-induced superconductivity is achieved via selective shadow-wall deposition of Al thin films. We demonstrate a hard induced gap using voltage-bias spectroscopy and study the appearance of zero-bias peaks in the local conductance. Harnessing the three-terminal geometry, we investigate the evolution of the nonlocal conductance in a magnetic field before the transition to the normal state.

*European Research Council, Dutch Organization for Scientific Research, and Microsoft Corporation Station Q

**10:24AM R60.00011: Engineering Majorana Bound States with Periodic Structures**  
BENJAMIN WOODS (Presenter), TUDOR DAN STANESCU, West Virginia Univ — Majorana bound states within semiconductor-superconductor heterostructures are a promising platform for future topological quantum computation. Here we theoretically explore the effects of periodic potentials and periodic structures on the emergence and properties of topological superconductivity and Majorana bound states within 1D and quasi-1D systems. Three key findings suggest that periodic structures may possess some advantages over homogeneous systems in supporting topological superconductivity. The three findings to be discussed are (1) an increased region of parameter space in which the topological phase and Majorana bound states are realized, (2) an increasing topological gap as one moves to higher energy mini-bands, and (3) an increased robustness against disorder compared to homogeneous systems. We also explore several physical systems in which the periodic potential/structure can be engineered and discuss their outlook.

**10:36AM R60.00012: Topological Josephson effect in gate-tunable qubit devices**  
ANDREY ANTIPOV (Presenter), CAMERON KING, KEWEI LI, JOHN GAMBLE, BELA BAUER, GEORG WINKLER, ROMAN LUTCHYN, Microsoft Corp — Gate-tunable superconducting qubits that host Majorana zero modes realize an intermediate step to topologically protected qubits by storing the quantum state in topological degrees of freedom. In this talk I will present numerical simulations of such devices that combine superconducting proximity effect, orbital effects, electrostatic environment and realistic geometry. I will show the phase diagram and the key properties of these topological Josephson junctions, in particular the Josephson energy and Majorana coupling energy. Based on these I identify regimes of the surrounding electrostatic environment most favorable for realizing qubits and relate this to observable experimental features.
8:00AM R61.00001: Heisenberg-Kitaev physics in magnetic fields [Invited] MATTHIAS VOJTA (Presenter), LUKAS JANSSEN, Physics, Technische Universitaet Dresden — Kitaev's bond-anisotropic spin model on the honeycomb lattice describes an exactly solvable quantum spin liquid with emergent gauge fields and fractionalized excitations. By now, a number of honeycomb-lattice magnets have been proposed to host sizeable Kitaev interactions, driven by strong spin-orbit coupling, among them Na$_2$IrO$_3$, α-Li$_2$IrO$_3$, and α-RuCl$_3$. Given the strong spin anisotropies, their response to applied magnetic fields is particularly rich. In this talk, I will describe the behavior of the relevant Heisenberg-Kitaev models and their extensions in applied field, with focus on field-induced exotic phases and their experimental signatures. I will also discuss phases of the hyperhoneycomb-lattice extended Kitaev models relevant for β-Li$_2$IrO$_3$ and a mapping connecting them to their two-dimensional counterparts.

8:36AM R61.00002: Emergence of a field-driven U(1) spin liquid in spin-1 Kitaev systems SIMON TREBST (Presenter), CIARAN HICKEY, Univ Cologne, PANAGIOTIS PETER STAVROPOULOS, University of Toronto, CHRISTOPH BERKE, Univ Cologne, HAE-YOUNG KEE, University of Toronto — Recent proposals for spin-1 Kitaev materials, such as Na$_3$Ni$_2$SbO$_6$, have shown that these compounds naturally realize antiferromagnetic (AFM) Kitaev couplings. Interest in such AFM Kitaev systems has recently sparked by the observation of a transition to a gapless U(1) spin liquid at intermediate field strengths in the AFM spin-1/2 Kitaev model. However, all known spin-1/2 Kitaev materials exhibit ferromagnetic bond-directional exchanges. Here we discuss the physics of the spin-1 Kitaev model in a magnetic field and show, by extensive numerical analysis, that for AFM couplings it exhibits an extended gapless U(1) quantum spin liquid at intermediate field strengths. The close analogy to its spin-1/2 counterpart suggests that this gapless spin liquid exhibits a spinon Fermi surface.

8:48AM R61.00003: Ground-state phase diagram of the Kitaev-Γ model on a honeycomb lattice TAKAFUMI SUZUKI (Presenter), SEI-ICHIRO SUGA, Univ of Hyogo — We investigate the ground-state phase diagram of the Kitaev-Γ model on a honeycomb lattice by utilizing several numerical methods, such as the numerical exact-diagonalization method and the density-matrix-renormalization-group method. In this study, we focus on the effect of the anisotropic interaction; we connect the isolated dimer limit and the spin-chain limit by changing the coupling constants. From the numerical results, we find that there are three kinds of phases, namely the Tomonaga-Luttinger (TL) liquid phase and two kinds of magnetic ordered states, in the spin-chain limit. When the Γ interaction is positive and the Kitaev interaction is negative, the TL liquid is stable against the interchain couplings, which implies that the TL liquid survives up to the vicinity of the isotropic point or shows a crossover behavior. The dimer phases also survive in the vicinity of the isotopic limit. We expect that many states are competing around the isotropic point.
Large off-diagonal exchange coupling driven magnetic anisotropy and spin liquid states in the C$_3$-symmetric iridate K$_2$IrO$_3$* 

RAJYAVARDHAN RAY (Presenter), RAVI YADAV, SATOSHI NISHIMOTO, MANUEL RICHTER, JEROEN VAN DEN BRINK, IFW - Dresden — Honeycomb lattice spin-orbit insulators are promising candidates for realization of quantum spin liquid states. The iridate oxide K$_2$IrO$_3$ is an end member of the recently synthesized iridate family K$_x$Ir$_y$O$_2$, and features a C$_3$ point-group symmetry at the Ir sites. Using ab-initio techniques, we investigate the magnetic couplings in the proposed structural model for K$_2$IrO$_3$. We find that the higher point-group symmetry leads to strong magnetic anisotropy driven by the unusually large off-diagonal exchange couplings (Γ’s) as opposed to other spin liquid candidates considered so far. High magnetic frustration and large quantum fluctuations imply lack of magnetic ordering consistent with the experiments. Exact diagonalization calculations for the fully anisotropic K−J−Γ Hamiltonian reveal a rich phase diagram with competing magnetic as well as spin liquid states. Our study points out the importance of the Γ’s in stabilizing a spin liquid state and highlights an alternative route to stabilize spin liquid states for ferromagnetic K.

References:

*We acknowledge support from DFG through SFB 1143 Project No. A05, and ERDF and the Free State of Saxony via the ESF Projects No. 100231947 and No. 100339533 (Young Investigators group - CoSiMa).

Chemical tuning between triangular and honeycomb structures in a 5d spin-orbit Mott insulator* 

ROGER JOHNSON (Presenter), Department of Physics and Astronomy, University College London, INEKE BROEDERS, University of Oxford, KAVITA MEHLAWAT, Department of Physical Sciences, ISER, YING LI, Institut fur Theoretische Physik, Goethe-Universitat Frankfurt, YOGESH SINGH, Department of Physical Sciences, ISER, ROSE VALENTI, Institut fur Theoretische Physik, Goethe-Universitat Frankfurt, RADU COLDEA, University of Oxford — We report structural studies of the spin-orbit Mott insulator family K$_x$I$_y$O$_2$, with triangular layers of edge-sharing IrO$_6$ octahedra bonded by potassium ions. The potassium content acts as a chemical tuning parameter to control the amount of charge in the Ir-O layers. Unlike the isostructural families with Ir replaced by Co or Rh (y = 1), which are metallic over a range of potassium compositions x, we instead find insulating behaviour with charge neutrality achieved via iridium vacancies, which order in a honeycomb supercell above a critical composition x$_c$. By performing density functional theory calculations we attribute the observed behaviour to a subtle interplay of crystal-field environment, local electronic correlations and strong spin-orbit interaction at the Ir 4+ sites, making this structural family a candidate to display Kitaev magnetism in the experimentally unexplored regime that interpolates between triangular and honeycomb structures.

*RDJ acknowledges support from a Royal Society University Research Fellowship.
9:24AM R61.00006: Raman Scattering Investigation of a New Candidate for a Quantum Spin Liquid, the Magnetic Insulator, $\text{Ba}_3\text{Ir}_4\text{O}_{10}$*  
AARON SOKOLIK (Presenter), NICK PELLATZ, GANG CAO, DMITRY REZNICK, University of Colorado, Boulder —  
The insulator $\text{Ba}_3\text{Ir}_4\text{O}_{10}$ is a new candidate for a frustrated quantum spin liquid, which was reported to have a stabilized quantum spin liquid state down to 0.2 K. The frustration parameter of around 3800 is extremely high. The spin liquid is also extraordinarily sensitive to changes in the lattice parameters as shown with the effects from strontium doping. The replacement of approximately 2% of barium with strontium readily lifts the frustration parameter and this doped material has long-range order from an antiferromagnetic transition at 130 K. Raman spectroscopy results show that both materials are also strongly anisotropic. We will present a comparison of the results of Raman scattering experiments on Sr-doped and undoped samples of $\text{Ba}_3\text{Ir}_4\text{O}_{10}$.

*The work of A.S. N.P., and D.R. was supported by the NSF under Grants No. DMR-1410111 and DMR-1903888

9:36AM R61.00007: Ab-Initio insight into non-local charge fluctuations in optical conductivity for $\alpha$-$\text{RuCl}_3$ through a Wannier basis: Highlighting the role of chemistry in correlated electron systems  
CASEY EICHSTAEDT (Presenter), University of Tennessee, Knoxville, TOM BERLIJN, Oak Ridge National Laboratory, KEN BURCH, Boston College, ADOLFO GERMAN EGUILUZ, University of Tennessee, Knoxville — $\alpha$-$\text{RuCl}_3$ is one of the top contenders for hosting a quantum spin liquid as its exact ground state by possibly being a real material realization of Kitaev's anisotropic spin model. While there is still no consensus for the magnetic ground state, there is plenty of rich physics in the electronic excitations (i.e optical conductivity). We simulate the optical excitations of $\alpha$-$\text{RuCl}_3$, by invoking a parameter-free treatment of the Random Phase Approximation (RPA) to exact Time Dependent Density Functional Theory (TD-DFT) implemented using a Wannier basis. The calculated optical peak for $\alpha$-$\text{RuCl}_3$ (peak at ~1eV) is in very good agreement in location and absolute units with experiment. There are two key findings using this implementation. The first is the origin of the insulating gap in the ground state appears to be due to the interplay between relativity (spin-orbit coupling) and correlation (Hubbard U). The second finding is the surprising result that to converge the optical peak in the calculation, there are sizable Ru-Ru electron-hole pairs of Wannier d-like orbitals spanning beyond neighboring sites. This is determined due to the strong covalency built into the underlying solid state electronic structure of the underlying $\alpha$-$\text{RuCl}_3$, in particular the hexagonal arrangement of Ru atoms.
**9:48AM R61.00008:** New magnetic order revealed in α-RuCl$_3$ at intermediate magnetic fields using neutron diffraction  
CHRISTIAN BALZ (Presenter), ISIS Neutron and Muon Source, LUKAS JANSSEN, TU Dresden, PAULA LAMPEN-KELLEY, University of Tennessee, ARNAB BANERJEE, YAOHUA LIU, JIAQIANG YAN, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee, MATTHIAS VOJTA, TU Dresden, STEPHEN E NAGLER, Oak Ridge National Laboratory — It is well-known that an external magnetic field can induce a transition in α-RuCl$_3$ from a magnetically ordered state to a disordered state that may be related to the Kitaev quantum spin liquid. The overall temperature - magnetic field phase diagram of α-RuCl$_3$ is currently under intense scrutiny, and presently there is no universal agreement on the number of field induced phase transitions between the zero-field state and the high field polarized paramagnet. Single crystals with minimal stacking faults show a transition near $T_N = 7$ K at $B = 0$ T to a low temperature ordered phase that has a zigzag AFM structure in a single honeycomb layer, with a 3-fold periodicity perpendicular to the planes. For fields applied in the honeycomb plane perpendicular to a Ru-Ru bond there is evidence from magnetization, AC susceptibility, thermal transport [1], and magnetocaloric effect [2] data for an intermediate-field phase with a different magnetic order that precedes the disordered phase. Here we discuss neutron diffraction data that clarifies the magnetic structure in this phase. The intermediate ordered phase puts additional constraints on the minimal model magnetic Hamiltonian for α-RuCl$_3$.


**10:00AM R61.00009:** Phononic Structure of Kitaev Quantum Spin Liquid Candidate Material alpha-RuCl$_3$  
TOM BERLIJN (Presenter), ARNAB BANERJEE, YONGQIANG CHENG, Oak Ridge National Lab, SAI MU, UC Santa Barbara — While many studies have focused on the magnetic excitations in alpha-RuCl$_3$, its vibrational excitation spectrum has remained relatively unexplored. However, understanding phonons in RuCl$_3$ is important for example to analyze the controversial observation of the half-integer thermal quantum Hall effect. We investigate the phononic structure of alpha-RuCl$_3$ via Density Functional Theory calculations and Inelastic Neutron Scattering experiments.
10:12AM R61.00010: X-ray scattering studies of elementary excitations of $\alpha$-RuCl$_3$  BLAIR LEBERT (Presenter), SUBIN KIM, Physics, University of Toronto, VALENTINA BISOGNI, IGNACE JARRIGE, ANDI BARBOUR, NSLS-II, Brookhaven National Laboratory, AHMET ALATAS, AYMAN SAID, APS, Argonne National Laboratory, YOUNG-JUNE KIM, Physics, University of Toronto — We investigated the Kitaev quantum spin liquid candidate $\alpha$-RuCl$_3$ using resonant inelastic x-ray scattering (RIXS) and inelastic x-ray scattering (IXS). Our room temperature M$_3$-edge RIXS results revealed a spin-orbit exciton from which we extracted values for the spin-orbit coupling constant and trigonal distortion field energy which support the $j_{\text{eff}} = 1/2$ nature of $\alpha$-RuCl$_3$ [1]. I will discuss the potential of M$_3$-edge RIXS to study 4d transition metal systems and perspectives on low temperature measurements on $\alpha$-RuCl$_3$. Finally, I will present our IXS measurements of the dispersion of acoustic phonons in $\alpha$-RuCl$_3$ measured at 5 K.


10:24AM R61.00011: Raman scattering response in the Kitaev magnet beta-Li$_2$IrO$_3$ and its evolution in the magnetic field*  MENGQUN LI (Presenter), University of Minnesota, IOANNIS ROUSOCHATZAKIS, Loughborough University, NATALIA PERKINS, University of Minnesota — Raman scattering has been proven to be a powerful dynamical probe to study magnetic excitations in various frustrated magnets. Here we analyze theoretically the one- and two-magnon Raman scattering intensity in the Kitaev magnet beta-Li$_2$IrO$_3$ and its evolution in the magnetic field. Our analysis shows that the response is very sensitive to the polarization of light and the direction of the external magnetic field, reflecting a peculiar spin dynamics of this compound which arises due to the competition between anisotropic exchange interactions and applied magnetic field.

*We acknowledge the support of the US Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0018056.
10:36AM R61.00012: Giant linearly-polarized photogalvanic effect and second harmonic generation in zero-plateau quantum anomalous Hall systems*  LI YANG (Presenter), RUIXIANG FEI, WENSHEN SONG, Physics, Washington University in St. Louis — Combining quantum perturbation theory and first-principles simulation, we predict giant nonlinear optical responses (NLOs) in even septuple layers of MnBi\textsubscript{2}Te\textsubscript{4} family materials (MBTs), which are the zero-plateau quantum anomalous Hall systems (QAHs). The interlayer antiferromagnetic order breaks the inversion symmetry, and the amplitudes of injection current and second harmonic generation can be about one order of magnitude larger than those of the ferroelectrics, such as LiNbO\textsubscript{3} and BiFeO\textsubscript{3}. Moreover, unlike the injection current in ferroelectrics, we find that the injection photocurrent only emerges under a linearly polarized light in MBTs. Our analysis indicates that these giant linearly-polarized second-order NLOs are resulted from the parity-time symmetry, three-fold rotation symmetry, and large spin-orbit coupling. These enhanced NLOs are valuable for characterizing subtle magnetic orders in QAHs and shed light on photo-detecting and photovoltaic applications based on emerging magnetic topological materials.

*This work is supported by the National Science Foundation CAREER DMR-1455346 and EFRI2DARE-1542815, and the Air Force Office of Scientific Research grant FA9550-17-1-0304. The computational resources are provided by the Stampede of TACC through XSEDE.

10:48AM R61.00013: Berry Curvature Engineering by Gating Two-Dimensional Antiferromagnets  SHIQIAO DU (Presenter), Tsinghua University — Recent advances in tuning electronic, magnetic, and topological properties of two-dimensional (2D) magnets have opened a new frontier in the study of quantum physics and promised exciting possibilities for future quantum technologies. In this study, we find that the dual gate technology can well tune the electronic and topological properties of antiferromagnetic (AFM) even septuple-layer (SL) MnBi\textsubscript{2}Te\textsubscript{4} thin films. Under an out-of-plane electric field that breaks PT symmetry, the Berry curvature of the thin film could be engineered efficiently, resulting in a huge change of anomalous Hall (AH) signal. Beyond the critical electric field, the double-SL MnBi\textsubscript{2}Te\textsubscript{4} thin film becomes a Chern insulator with a high Chern number of 3. We further demonstrate that such 2D material can be used as an AFM switch via electric-field control of the AH signal. These discoveries inspire the design of low-power memory prototype for future AFM spintronic applications.

Thursday, March 5, 2020 8:00 AM - 10:48 AM

Session R62 DMP: Thermal Transport in Nanostructures I  Mile High Ballroom 4C
- Charles Harris, Sandia National Laboratories - Tag(s): Focus
**8:00AM R62.00001: Advanced Josephson junctions circuits and nanoscale devices: The phase-coherence in heat transport** [Invited] FRANCESCO GIAZOTTO (Presenter), CNR Scuola Normale Superiore — The emerging field of *phase-coherent caloritronics* (from the Latin word *calor*, heat) [1] is based on the possibility of controlling heat currents by using the phase difference of the superconducting order parameter. The goal is to design and implement thermal devices that can control energy transfer with a degree of accuracy approaching that reached for charge transport by contemporary electronic components. This can be done by making use of the macroscopic quantum coherence intrinsic to superconducting condensates, which manifests itself through the Josephson effect and the proximity effect. Here, I will initially report the first experimental realization of a heat interferometer. We investigate heat exchange between two normal metal electrodes kept at different temperatures and tunnel-coupled to each other through a thermal device in the form of a DC-SQUID. Heat transport in the system is found to be phase dependent, in agreement with the original prediction. After this initial demonstration, we have extended the concept of heat interferometry to various other devices, implementing the first quantum `diffractor` for thermal fluxes, realizing the first balanced Josephson heat modulator, and the first tunable 0-π thermal Josephson junction. Finally, I will conclude by showing the realization of the first phase-tunable Josephson thermal router. Thanks to the Josephson effect, this latter structure allows to regulate the thermal gradient between the output electrodes until reaching its inversion, and represents an important step towards the realization of caloritronic logic components, and quantum thermal machines.


*The European Union Seventh Framework Programme (FP7/2007-2013)/ERC Grant No. 615187 - COMANCHE, and Horizon 2020 and Innovation Programme under grant agreement No. 800923-SUPERTED are acknowledged for partial financial support.

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**8:36AM R62.00002: Topological Quantum Thermocouple** CHARLES STAFFORD, MARCO ANTONIO JIMENEZ VALENCIA (Presenter), Univ of Arizona — The flows of charge and heat in an open quantum system coupled to three macroscopic electron reservoirs are studied. It is shown that even without particle-hole asymmetry in the electronic structure, thermoelectric effects can be induced topologically by the Aharonov-Bohm effect. The Peltier effect is calculated, and the conditions of maximum cooling power are determined. The Carnot bound on the refrigeration coefficient is verified, and in so doing, a generalized relationship between the Peltier and Seebeck effects in multi-terminal quantum devices is derived. An apparent thermodynamic paradox involving persistent Peltier cooling in equilibrium is resolved by a rigorous treatment of heat flow at the quantum level.

*This work was supported by the U.S. Department of Energy (DOE), Office of Science, under Award No. DE-SC0006699.*
8:48AM R62.00003: Noise emitted by a temperature biased tunnel junction* SAMUEL LAROCQUE, EDOUARD PINSOLLE (Presenter), CHRISTIAN LUPIEN, BERTRAND M REULET, Université de Sherbrooke — Caloritronic in small systems has been of high interest in recent years since new ways to manipulate electronic heat currents at the nanoscale have been developed. The ability to make mesoscopic systems with well controlled temperature enables the study of quantum heat transport and out of equilibrium quantum thermodynamic, which is of fundamental interest. A tunnel barrier between two metallic electrodes forms the basic unit in the study of non-equilibrium physics and fluctuations. This system has been put to great use in the understanding of electronic transport whether at equilibrium where fluctuations are used as thermometer or in the presence of voltage bias where information on charge carrier can be accessed. In this talk we present calculations and measurements of the electrical noise in a metallic tunnel junction in presence of a thermal and voltage gradient, pushing farther our understanding of its non-equilibrium properties.

*We acknowledge technical help of G. Laliberté. This work was supported by the Canada Excellence Research Chair program, the NSERC, the CFREF, the MDEIE, the FRQMT via the INTRIQ, the Université de Sherbrooke via the EPIQ and the Canada Foundation for Innovation.

9:00AM R62.00004: Thermal Conductivity of Small Angle Twisted Bilayer Graphene* CHENYANG LI, ROGER LAKE (Presenter), University of California, Riverside — The effect of misorientation on the in-plane thermal conductivity of twisted BLG (TBG) is still poorly understood. The one experimental study found that interlayer misorientation could reduce the in-plane thermal conductivity by 50%. A recent theoretical study of TBG with the three smallest commensurate unit cells, 21.8°, 32.2°, and 13.2°, found that the thermal conductivity decreased approximately linearly as the commensurate lattice constant increased. What happens at smaller misorientation angles of 10° or less is still an open question. For this range of rotation angles, we perform large-scale, non-equilibrium molecular dynamics calculations of the thermal conductivity of TBG for twist angles down to 1.89°. The picture that emerges from this study is that the misorientation reduces the shear elastic constant C44 which increases the wrinkling of the TBG. The increased out-of-plane wrinkling then reduces the thermal conductivity.

*This work was supported in part by the National Science Foundation under awards 1307671 and 1433395. This work used the Extreme Science and Engineering Discovery Environment (XSEDE) which is supported by National Science Foundation Grant No. ACI-1548562 and allocation ID TG-DMR130081.
Heterostructures of two-dimensional materials (2D) are a promising platform for the observation of phonon interface transport and coherent-phonon effects. Layer thickness and orientation can be tuned during heterostructure fabrication which provides a variety of ways to control the thermal-transport properties of the system. Using the 3ω method, we measure the interfacial thermal resistance between two common 2D materials, hexagonal boron nitride (hBN) and graphene (Gr), to be significantly lower than previously reported Raman thermometry values. The uncertainty of our measurement is limited by the uncertainty in the literature value for the bulk thermal conductivity of hBN. We aim to provide a precise measurement of the cross plane thermal resistance of hBN flakes from the bulk-like down to the ballistic phonon transport regime and demonstrate that a variety of geometries of 3ω wires including a semicircle with 750μm diameter, measure the same cross plane thermal resistance of a 70nm thick SiO₂ film with a standard deviation of 4.7 m² K GW⁻¹.

*Measurements supported by US DOE Basic Energy Sciences #DE-FG02-03ER46028. Growth of hBN by K.W. and T.T. is supported by the Elemental Strategy Initiative conducted by the MEXT Japan A3 Foresight by JSPS and the CREST (JPMJCR15F3) JST.
Engineering ultrahigh thermal anisotropy in 2D van der Waals films

SHI EN KIM (Presenter), Pritzker School of Molecular Engineering, University of Chicago, JOONKI SUH, School of Materials Science and Engineering, Ulsan National Institute of Science and Technology, AKASH RAI, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, FAUZIA MUJID, Department of Chemistry, University of Chicago, CHIBEOM PARK, James Franck Institute, University of Chicago, ARIANA RAY, DAVID ANTHONY MULLER, School of Applied and Engineering Physics, Cornell University, DAVID CAHILL, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, JIWOONG PARK, Pritzker School of Molecular Engineering, University of Chicago — Thermally anisotropic materials, whose thermal conductivity differs depending on the direction of heat conduction, are technologically important for heat management and fundamentally intriguing in terms of their mechanism of heat transport. Previous studies have achieved thermal anisotropy through anisotropic bonding, fabricating heterostructures, and introducing low dimensional defects, giving rise to anisotropic ratios of 1-2 orders of magnitude. Herein we report an ultrahigh thermal anisotropy (~1000 at room temperature) in large-area thin films with tunable thicknesses made by stacking transition metal dichalcogenide (MoS\textsubscript{2} or WS\textsubscript{2}) monolayers. We measure an ultralow cross-plane thermal conductivity comparable to that of air, which can be attributed to interlayer rotation and the lack of lattice order. In the in-plane direction, a high thermal conductivity close to that of the single crystal counterpart is maintained due to the long-range lattice order and grain connectivity in the polycrystalline monolayers. The overall thermal anisotropy ratio in our films is higher than that of any man-made or natural material, demonstrating interlayer structure as a new degree of freedom for engineering thermal anisotropy in matter.

*This work is supported by the AFOSR (FA9550-18-1-0480).

Phonon Localization in Ultrathin Silicon Membranes with Surface Nanostructures

QUENTIN MOORE (Presenter), SANGHAMITRA NEOGI, University of Colorado, Boulder — Surface nanostructures have been shown to introduce new vibrational modes that locally couple with phonon modes of the base and impact in-plane phonon propagation. Nanoscopic surface imperfections have been experimentally and theoretically demonstrated to decrease the thermal conductivity (TC) of silicon (Si) membranes. However, the tunability of the coupling or hybridization mechanisms due to unique surface geometries, and the extent of their impact on phonon properties are not fully understood. Using direct non-equilibrium molecular dynamics (MD), we investigate the effect of periodic “nanofins” on the thermal properties of ultrathin Si membranes. Our study exhibits that these structures engender a distinct in-plane anisotropy in the TC of the membrane, and create unique localized temperature and phonon-induced strain profiles, in accordance with the surface structure periodicity. Further investigation, using lattice dynamics with the quasi-harmonic approximation, reveals a significant reduction in mode diffusivity, indicating phonon localization, approaching behavior similar to highly disordered solids, e.g., amorphous Si. These results further establish surface nanoengineering as a viable approach to meter and direct heat flow in future microelectronic/quantum technologies.
Surface phonon mode remarkably limits heat conduction in a silicon ultra-thin film*  

MICHIMASA MORITA (Presenter), TAKUMA SHIGA, Mechanical Engineering, Univ of Tokyo — Decrease of silicon channel thickness is efficient to suppress short channel effects, which is beneficial for further miniaturizing of MOS transistor. However, this causes larger reduction thermal conductivity, resulting in temperature rise of the channel region. Therefore, accurate analysis of heat conduction in thin film is needed for heat dissipation control. The Sondheimer model, which has been widely used, is known to be valid for reproducing heat conduction in the range of 50-100 nm thickness. However, since the Sondheimer model uses the bulk phonon property, the applicability of the model to ultra-thin film with several nanometers is doubtful. Here, in order to validate the model, we performed the anharmonic lattice dynamics explicitly considering atomic structure of the film to rigorously calculate thermal conductivity and phonon transport properties of the ultra-thin silicon film. Consequently we found that the Sondheimer model cannot reproduce spectral phonon transport properties of ultra-thin film because it ignores the change of phonon dispersion and presence of surface phonon. We will discuss this discrepancy in terms of surface phonon scattering to suggest the way to resolve this.

*JST PRESTO (JPMJPR1715).

Numerical study on the transition from coherent to incoherent phonon transport in a superlattice*  

TATSUKI ICHIKAWA (Presenter), TAKUMA SHIGA, Mechanical Engineering, Univ. of Tokyo — Superlattice has been widely investigated due to its capability of modulating phonon dispersion and suppressing transport. However, increases of superlattice periodicity and temperature cause phonon decoherence and then suppress the reduction of lattice thermal conductivity [1], which is well known as the issue for developing heat conduction control by superlattice. Here a criterion for which phonon coherence is preserved needed to be identified. Ref. [2] derived the phonon coherence condition with respect to wavelength and temperature as $\lambda \geq (\hbar v/ kBT)$ with speed of sound ($v$), however, we addressed this issue from different viewpoint, namely, the uncertainty associated with energy and momentum conservations; it should be satisfied that not only the multiplication of phonon frequency $\omega$ and relaxation time $\tau$ is large enough ($\omega \tau \gg 1$) but also fluctuation of momentum $\delta(hk/2\pi)$ is sufficiently smaller than reciprocal lattice vector $G(=2\pi/a)$ ($\delta(hk/2\pi) \ll hG/2\pi$), where $a$ denotes periodicity. These discussions finally result in the relationship $T \leq (hvg/kBa)$, where $vg$ denotes group velocity. By using molecular dynamics simulations, we will report the verification of this formula.


*PRESTO (JPMJPR1715).
10:12AM R62.00010: Nonequilibrium phonon distribution in current-driven nanostructures
GUANXIONG CHEN (Presenter), RYAN M FREEMAN, ANDREI ZHOLUD, SERGEI URAZHDIN, Department of Physics, Emory University — Electric energy of current flowing in materials or devices is dissipated mostly as Joule heat. However, in nanoscale systems, the generated phonons can escape before they thermalize, which can result in the breakdown of the Joule heating approximation.
We demonstrate a strongly non-equilibrium phonon distribution in current-driven metallic microwires, which cannot be described in terms of heat [1]. Our main observation is a linear dependence of resistance on current at cryogenic temperatures, qualitatively inconsistent with the effects of Joule heating, as confirmed by the simulations of heat flow. As the temperature is increased, the zero-current singularity becomes smoothed out, but the linear dependence remains apparent at sufficiently large currents even near ambient temperatures. A kinetic model based on the quasi-ballistic escape approximation for the nonequilibrium phonons generated by electron scattering reproduces our main observations. The demonstrated effects are important for optimizing thermal management in electronic and thermoelectric nanodevices, and for the analysis of current-induced thermal effects at nanoscale.


*Supported by the grant # DE-SC2218976 funded by the U.S. DOE Office of Science

10:24AM R62.00011: New regimes of nanoscale thermal transport from nanostructured heat sources on diamond probed using coherent EUV beams
BRENDAN MCBENNETT (Presenter), JOSHUA KNOBLOCH, BEGOÑA ABAD, TRAVIS D FRAZER, STROBE and JILA, University of Colorado and NIST, ALBERT BEARDO, LLUC SENDRA, JUAN CAMACHO, JAVIER BAFALUY, Departament de Física, Universitat Autònoma de Barcelona, WEILUN CHAO, Center for X-Ray Optics, Lawrence Berkeley National Laboratory, ROGER WIRTH FALCONE, Department of Physics, University of California, Berkeley, JORGE HERNÁNDEZ-CHARPAK, HENRY KAPTEYN, STROBE and JILA, University of Colorado and NIST, XAVIER ALVAREZ, Departament de Física, Universitat Autònoma de Barcelona, MARGARET MURNANE, STROBE and JILA, University of Colorado and NIST — Nanostructured materials make it possible to engineer properties that are unattainable using conventional bulk materials, with applications in next-generation energy efficient devices. However, macroscopic, diffusive transport models break down at length scales comparable to a material's dominant phonon mean free path. Moreover, there are few, if any, characterization techniques that can probe functional nanosystems. Here we use short wavelength (~30nm), ultrafast pulse (~10fs) extreme ultraviolet (EUV) beams to nondestructively probe nanoscale thermal transport in diamond. We first impulsively heat nickel nano-gratings fabricated on the diamond sample with an infrared pump laser and then extract thermal conductivity by monitoring surface relaxation with a time-delayed EUV probe. Diamond is an ideal candidate for validating emergent transport behaviors because its long phonon mean free path causes non-diffusive effects to appear at larger length scales. We compare our results to an advanced hydrodynamic transport model to isolate the contribution of viscous resistivity directly underneath the nanoheaters to thermal transport. Finally, we gain insight into non-diffusive cooling processes by examining the individual diffracted orders in the scattered EUV probe beam.
10:36AM R62.00012: Nanoelectronic thermometry and refrigeration for sub-millikelvin temperatures

JONATHAN PRANCE (Presenter), SAMULI AUTTI, Physics, Lancaster University, KESTUTIS GRIGORAS, VTT Technical Research Centre of Finland, ANTHONY GUÉNAULT, Physics, Lancaster University, DAVID GUNNARSSON, VTT Technical Research Centre of Finland, RICHARD HALEY, ALEXANDER JONES, YURI PASHKIN, Physics, Lancaster University, MIKA PRUNNILA, LEIF ROSCHIER, VTT Technical Research Centre of Finland, DMITRY ZMEEV, Physics, Lancaster University — It has recently been shown that magnetic refrigeration can be deployed on-chip to cool nanoelectronic devices below the base temperature of a dilution refrigerator [1, 2, 3]. This technique has the potential to unlock microkelvin electron temperatures in nanoscale structures and devices. However, there are still significant challenges in thermometry and thermal isolation to be overcome. In this talk, we present our recent work to lower the operating temperature of Coulomb blockade thermometers to ≈300µK, and to improve the base electron temperature reachable by demagnetisation refrigeration of on-chip copper.


*U.K. EPSRC (EP/K01675X/1, EP/N019199/1, EP/P024203/1 and EP/L000016/1)
European FP7 Programme MICROKELVIN (project number 228464)
European Union’s Horizon 2020 research and innovation programme (European Microkelvin Platform, grant agreement No. 824109, and EFINED, grant agreement No. 766853)
Academy of Finland through its Centers of Excellence Program (312294).
S.A. acknowledges financial support from the Jenny and Antti Wihuri Foundation via the Council of Finnish Foundations.

Thursday, March 5, 2020 8:00 AM - 10:48 AM

Session R63 DMP DCMP FIAP: Defects: Structure and Strain 2 Mile High

Ballroom 4D - Rachel Goldman, Univ of Michigan - Ann Arbor
8:00AM R63.00001: Dynamic Dark-Field X-ray Microscopy to Probe Mesoscale Defects and their Dynamics* [Invited] LEORA DRESSELHAUS-COOPER (Presenter), Lawrence Livermore Natl Lab — Many problems in semiconductor physics require a detailed understanding of material defects at the mesoscale (e.g. dislocations, stacking faults, twins, etc.). While techniques exist to probe material defects, they are mainly limited to surface measurements or rastered scans that cannot measure the dynamics of irreversible processes. Dark-field X-ray microscopy (DFXM) can now directly image defects in single- and poly-crystals, spatially resolving the lattice strain and inclination with high sensitivity (ε~10^{-5}) and resolution across hundreds of micrometers. I extend DFXM to study structural dynamics, resolving how material defects show how crystals respond disturbances in their surroundings. I will show real-time movies that visualize how long-range dislocation patterns evolve in both temperature and time and will extend this to high-intensity X-ray radiation damage to demonstrate dynamic DFXM's capabilities. These results present important opportunities for semiconductor physics, as they can now address important problems at the mesoscale. Results from these findings can directly connect to dislocation models that have previously relied on multi-scale modeling and indirect measurements for refinement.

*This work was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

8:36AM R63.00002: High-throughput identification of point defects in SiC JOEL DAVIDSSON (Presenter), VIKTOR IVADY, RICKARD ARMIENTO, IGOR ABRIKOSOV, Linkoping University — Qubits and single photon emitters are examples of point defects applications. Before a point defect can be utilized in these applications, an important step is to identify and understand both the defect type and different configurations. A promising way to identify a defect is to combine experimental data with ab initio calculations which include zero-phonon lines and hyperfine coupling parameters. In earlier work, we made a convergence study for divacancies in 4H-SiC. Due to the size of the supercell and the number of calculations needed, we restrict us to the PBE exchange functional. Based on our understanding of the convergence of these calculations, we made an automatic workflow that can calculate zero-phonon lines for many different defects. Each defect is calculated for a range of different configurations, charges, spins, and possible excitations. Currently, we are running these calculations in a high-throughput manner and producing a database for an array of different defects. We present the results from the workflow for various vacancy configurations in 4H-SiC. Our preliminary results suggest that with this choice of methodology, useful data are obtained at a feasible computational cost for a large number of defect types and configurations available in SiC.
8:48AM R63.00003: Theoretical Investigations of the Hyperfine Coupling in Group IV-Vacancy Centers in Diamond Using Hybrid Density Functional Theory*  
RODRICK KUATE DEFO (Presenter), EFTHIMIOS KAXIRAS, Harvard University, STEVEN RICHARDSON, Howard University, Harvard University — Recently, single-photon emitters comprised of Group IV (Si, Ge, Sn, and Pb)-vacancy centers in diamond have attracted considerable interest in the literature because of their potential applications in quantum information processing and quantum metrology. Because some of these Group IV-vacancy color centers are paramagnetic, their electronic properties can be experimentally characterized using electron paramagnetic resonance (EPR) which is a direct measure of the hyperfine interaction at a microscopic level. It has been demonstrated that an understanding of the core spin polarization is essential to providing accurate hyperfine tensors in a number of point defects in diamond, including the NV(-) center.\(^1,^2\) In this work we use density-functional theory (DFT) with the HSE06 exchange functional to compute the hyperfine tensors of several paramagnetic Group IV-vacancy centers in diamond and we compare our results with other experimental and theoretical results where available.  
*We acknowledge financial support from the NSF STC Center for Integrated Quantum Materials, NSF Grant Number No. DMR1231319.

9:00AM R63.00004: Theory on spectral diffusion and electrically driven interferometry of qubits*  
PÉTER UDVARHELYI, GERGO THIERING, VIKTOR IVADY, ADAM GALI (Presenter), Wigner Research Center for Physics — Scalable spin-to-photon interfaces require quantum emitters with strong optical-transition dipole moment and low coupling to phonons and stray electric fields. Here, we show that inversion symmetry is not a prerequisite criterion for a spectrally stable quantum emitter. We find that identical electron density in ground and excited states can eliminate the coupling to the stray electric fields. We demonstrate this effect on silicon-vacancy qubit in silicon carbide by first principles methods (SiC)\(^1,^2\). Our study opens an additional rationale in seeking promising materials towards the realization of robust spin-to-photon interfaces. Furthermore, we show by density functional theory that low-symmetry of defects can provide coherent optical and spin subsystems that can be harnessed to achieve electrically driven interferometry of SiC divacancy qubits\(^3\).  
\[3\] K. C. Miao et al., arXiv:1905.12780, accepted to Science Advances  
*NKFIH of Hungary Grant Nos. 2017-1.2.1-NKP2017-00001 and NVKP 16-1-2016-0043 as well as Grant Nos. NN127902 (EU QuantERA Nanospin project) and KKP129866, and from the EU Commission (ASTERIQS project with Grant No. 820394).
9:12AM R63.00005: Progress for high photon collection of color centers in quantum materials  
TONY ZHOU, PRESTON ZHOU (Presenter), GABRIEL SILVERMAN, KELECHI UKAH, LING XIE, AMIR YACOBY, Harvard University — Color centers in materials have attracted enormous amount of attention due to their interesting quantum properties for quantum computation, quantum optics\cite{1}, and quantum sensing applications\cite{2}. The most notable research has been focused on NV centers, SiV centers in diamond, divacancy in silicon carbide, and etc. There is also an increasing focus on defects, exciton physics in 2D materials. These collections of point-like entities share common optical technique in studies. Thus, efficient collection of each associated photons serves as the ultimate bottle neck in all applications. In this work, we present an effective approach to tackle this fundamental limit and use NV center as an example for its application\cite{3,4}.

\cite{1} B. Hensen, R. Hanson et al, Nature 2015, 526, 682.

9:24AM R63.00006: Modeling the Electronic Structure of Phosphorus Donor Clusters in Quantum Devices*  
QUINN CAMPBELL (Presenter), PETER A SCHULTZ, MITCHELL I BRICKSON, NOAH T JACOBSON, Sandia National Laboratories, LEON N MAURER, Google, EZRA BUSSMANN, SHASHANK MISRA, ANDREW BACZEWSKI, Sandia National Laboratories — Modeling the electronic structure of phosphorus donor clusters is essential for understanding and predicting the behavior of quantum devices fabricated using atomic precision advanced manufacturing (APAM) techniques. Scanning Tunneling Microscope (STM) lithography is one such technique for creating nanoelectronic devices by placing activated shallow dopants in silicon with atomic precision. To model these devices, we first use kinetic Monte Carlo parameterized from first principles calculations to predict the geometry of phosphorus donor clusters. From these geometries, we predict device performance by applying multivalley effective mass theory, developing a formalism for using a basis of anisotropic atomic orbitals for the envelope functions. We then compare the predicted electronic structure of these donor clusters to experimentally realized devices, reporting on observables such as charging energy and tunnel coupling.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.
9:36AM R63.00007: Electron paramagnetic resonance study of sodium guests in silicon clathrates, a cage-like crystalline silicon allotrope*  WILLIAM SCHENKEN (Presenter), Department of Physics, Colorado School of Mines, YINAN LIU, Department of Chemical and Biological Engineering, Colorado School of Mines, LAKSHMI KRISHNA, Department of Physics, Colorado School of Mines, AHMAD AFIF ABDUL MAJID, CAROLYN KOH, Department of Chemical and Biological Engineering, Colorado School of Mines, P CRAIG TAYLOR, REUBEN T COLLINS, Department of Physics, Colorado School of Mines — Si clathrates are cage-like crystalline Si allotropes with potentially exciting properties. They are synthesized in the presence of alkali guest atoms, e.g. Na, which occupy interstitial sites in the cages. However, Na guests degenerately dope the crystal. Realizing the potential of these materials requires fundamental understanding of guest properties in the host crystal structure. We present an EPR study of Na guests in Type II Si clathrate powders with ≤1 at. % Na. At low temperature, the spectrum shows four lines from the hyperfine interaction of the Na valence electron with the $^{23}$Na nucleus ($I=3/2$). We attribute a line to Si dangling bonds in a highly disordered phase surrounding each grain, and identify doublets around the four hyperfine lines as arising from interactions with a $^{29}$Si nucleus ($I=1/2$) in the surrounding cage. We estimate about half of the electronic wavefunction on the Si sub-lattice extends past the confining cage. Additional structure is observed halfway between the strong hyperfine lines, which we attribute to interactions of two $^{23}$Na nuclei ($I=3$) in adjacent cages. A relatively broad line is attributed to clustered sodium. The relative intensities show the Na distribution is inhomogeneous.

*This work was supported by NSF Award #1810463

9:48AM R63.00008: Quadrupolar interactions between acceptor pairs in p-doped semiconductors  ADAM DURST (Presenter), GENESIS YANG-MEJIA, Hofstra University, RAVINDRA NAUTAM BHATT, Princeton University — We consider the interaction between acceptor pairs in doped semiconductors in the limit of large inter-acceptor separation relevant for low doping densities. Modeling individual acceptors via the spherical model of Baldereschi and Lipari, we calculate matrix elements of the quadrupole tensor between the four degenerate ground states and show that the acceptor has a nonzero quadrupole moment. As a result, the dominant contribution to the large-separation acceptor-acceptor interaction comes from direct (charge-density) terms rather than exchange terms. The quadrupole is the leading nonzero moment, so the electric quadrupole-quadrupole interaction dominates for large separation. We calculate the matrix elements of the quadrupole-quadrupole interaction Hamiltonian in a product-state basis and diagonalize, obtaining a closed-form expression for the energy spectrum. All dependence on material parameters enters via an overall prefactor, resulting in surprisingly simple and universal results. This simplicity can be traced to the nontrivial vanishing of a particular Wigner 6-j symbol. Results are relevant to the control of two-qubit interactions in quantum computing implementations based on acceptor spins, as well as the thermodynamic properties of insulating p-type semiconductors.
10:00AM R63.00009: Nanoscale NV-detected Electron Spin Resonance at 115 GHz and 4.2 Tesla*  
BENJAMIN FORTMAN (Presenter), Dept. of Chemistry, Univ. of Southern California, JUNIOR PENA, SUSUMU TAKAHASHI, Dept. of Physics & Astronomy, Univ. of Southern California — The nitrogen-vacancy (NV) center is a promising candidate for single-spin electron spin resonance (ESR). NV-detected ESR enables ESR analysis for paramagnetic spins with sensitivity of a single spin. We have recently shown that the spectral resolution of NV-detected ESR is improved by carefully adjusting microwave (MW) pulse duration and intensity [1]. Pulsed ESR spectroscopy at high magnetic fields offers higher spectral resolution and greater spin polarization than measurements at lower magnetic fields. However, the shift to high fields requires a high frequency MW source whose output power is often much lower than that of a low frequency MW source. This results in incomplete population inversion due to limited excitation bandwidths and spin relaxation. Within this talk we present our development and application of adiabatic pulses at 115 GHz to overcome this challenge. We utilize these pulses to control the spin states of single NV centers and to perform ESR using a single NV center at a field of 4.2 Tesla [2].


*This work was supported by the National Science Foundation (DMR-1508661 and CHE-1611134).

10:12AM R63.00010: Defects in 4H-SiC Studied by Electrically Detected Magnetic Resonance and Electrically Detected Electron Nuclear Resonance*  
RYAN WASKIEWICZ (Presenter), BRIAN MANNING, DUANE MCCRARY, PATRICK LENAHAN, Pennsylvania State University — We utilize electrically detected magnetic resonance (EDMR) and electrically detected electron nuclear double resonance (EDENDOR) to observe defects responsible for recombination in fully processed 4H-SiC bipolar junction transistors (BJTs). The EDMR response in these devices is detected via spin dependent recombination (SDR) within the space charge region of the forward biased emitter-base junction with the collector grounded. (We link the observed response to silicon vacancies in the 4H-SiC.) We demonstrate the application of EDENDOR on these devices. To the best of our knowledge, this is the first demonstration of EDENDOR on a fully processed device. The EDENDOR measurements combines the power of EDMR with a nuclear magnetic resonance (NMR) excitation, allowing for the identification of magnetic nuclei near the observed defects. Our EDENDOR measurements indicate the presence of $^{14}$N nuclei near the silicon vacancies that are measured with EDMR. This work brings the unparalleled analytical power of ENDOR to applications with functional nanoscale devices.

*This work was supported by the Air Force Office of Scientific Research under award number NO. FA9550-17-1-0242.
10:24AM R63.00011: Hybrid spintronics as a novel platform for quantum sensing. ARTUR LOZOVOI (Presenter), HARISHANKAR JAYAKUMAR, DAMON DAW, CARLOS MERILES, The City College of New York — Defects in semiconductors are emerging as a robust solid-state platform for quantum sensing and quantum information processing. These applications demand efficient readout of the defect spin state with high fidelity. We propose a novel spin readout technique based on a non-local hybrid spin-to-charge conversion that takes advantage of drift and diffusion of the charge carriers in semiconductors in the presence of electric field. In this approach, spin-dependent generation of charge carriers from the target defects with superior spin properties is coupled to emitters with high quantum efficiency, optical cycling frequency and favorable photoionization properties. We implement this technique in type IIa diamonds and demonstrate that it provides higher sensitivity compared to the conventional spin readout techniques. We note that the proposed approach is universal in its nature and can be applied to spin-active impurities in other semiconductor materials. In addition to that, we use this technique to characterize charge dynamics and capture cross-sections of optically active and dark defects in diamond.

1. H. Jayakumar et al. Time-integrated qubit measurements using digital memories. (*submitted, under review*)

10:36AM R63.00012: High-density defect ensembles in SiC for superradiance and magnetometry* PETER BRERETON (Presenter), SETH RITTENHOUSE, JOSEPH WIEDEMANN, JEFFREY R VANHOY, US Naval Academy, JOHNN ABRAHAM, Johns Hopkins APL — The silicon vacancy in SiC has recently become of great interest as a platform for quantum sensing and quantum information processing. In particular, recent theoretical work has shown that the spin 3/2 multiplet of a single silicon vacancy in 4H-SiC can achieve magnetic field sensitivities sufficient to detect single nuclear spins [1]. However, there has been less work done in the high-density, radiatively coupled regime in SiC. Superradiant coupling between atoms [2] and nitrogen vacancies in diamond [3] has been demonstrated experimentally and has been proposed as a route toward ultra-sensitive quantum sensing in the solid state. We explore the details of the superradiant transition in the 4H-SiC silicon vacancy and show possible routes toward engineering suitable defect ensembles.


*This work was partially supported by the Office of Naval Research Grant N0001419WX00566

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R64 DMP DCOMP: Chiral and Polar Structures in Thin Film Oxides Mile High Ballroom 4E - Kaveh Ahadi, NC State University - Tag(s): Focus
**8:00AM R64.00001: Electric-field control of emergent chirality in PbTiO$_3$/SrTiO$_3$ superlattices** [Invited] MARGARET MCCARTER (Presenter), SUJIT DAS, University of California, Berkeley, CHRISTOPH KLEWE, Advanced Light Source, ELIZABETH P DONOWAY, University of California, Berkeley, PADRAIC SHAFER, Advanced Light Source, GERRIT VAN DER LAAN, Diamond Light Source, LANE WYATT MARTIN, RAMAMOORTHY RAMESH, University of California, Berkeley — Novel chiral phases in ferroelectric materials—the polar analogs of magnetic vortices and skyrmions—can be stabilized in superlattices of PbTiO$_3$ and SrTiO$_3$. These chiral structures emerge in low-dimensional ferroelectrics, where the competition among gradient, electrostatic, and elastic energies favors non-uniform polarization configurations. Such phases can lead to new functional properties such as negative capacitance as well as unique interactions with polarized light. The characterization of these new phases and their three-dimensional chiral structure remains a challenge due to limitations of conventional electron microscopy and X-ray diffraction techniques.

In this talk, I will discuss how resonant soft X-ray diffraction (RSXD) can be used to study chirality in the emergent polarization textures (polar vortices and skyrmions) that form in PbTiO$_3$/SrTiO$_3$ superlattices. RSXD provides an element-specific probe with which to study the chiral configuration of orbitals in these materials. I will show that circular dichroism in RSXD originates from chiral arrays of electric quadrupoles, which are intrinsically related to the electric polarization. The presence of circular dichroism points to the formation of helical spirals of electric polarization, akin to Bloch domain walls in magnetic materials. Furthermore, circular dichroism can be observed in second harmonic generation. By performing electric-field dependent second harmonic generation circular dichroism experiments, we can demonstrate a coupling between the electric field and the handedness of chiral polar vortices.

*This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under contract number DE-AC02-05-CH11231 and the National Science Foundation Graduate Research Fellowship under grant number DGE-1106400

**8:36AM R64.00002: Atomic Structure Underlying Vortex Polarization Domains in Hexagonal RMnO$_3$** SIZHAN LIU, New Jersey Inst of Tech, MATTHEW NEWVILLE (Presenter), ANTONIO LANZIROTTI, University of Chicago, SANG-WOOK CHEONG, Rutgers University, TREVOR TYSON, New Jersey Inst of Tech — Hexagonal phase RMnO$_3$ systems exhibit polarization domains with complex vortex patterns with density depending on the cooling rate from the high-temperature paraelectric phase. Detailed polarization mapping is being compared with spatially dependent structural and spectroscopic studies to related variations in the domain patterns with local atomic and electronic structure. Structural measurements reveal variations on the lengthscale of the changes in polarization.

*This work is supported by NSF Grant No. DMR-1809931.
**Negative capacitance in polar skyrmions**

SUJIT DAS (Presenter), University of California, Berkeley, ZIJIAN HONG, VLADIMIR A STOICA, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, MAURO A. P. GONÇALVES, Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), 5 avenue des Hauts-Fourneaux, L-4362 Esch/Alzette, Luxemburg, ERIC PARSONNET, SAHAR SAREMI, MARGARET MCCARTER, ARMANDO REYNOSO, DEREK MEYERS, VISHAL RAVI, University of California, Berkeley, HUA ZHOU, ZHAN ZHANG, HAIDAN WEN, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA, FERNANDO GÓMEZ-ORTIZ, PABLO GARCIA-FERNANDEZ, Universidad de Cantabria, JEFFREY BOKOR, University of California, Berkeley, JORGE INIGUEZ, Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), 5 avenue des Hauts-Fourneaux, L-4362 Esch/Alzette, Luxemburg, JOHN WILLIAM FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA, JAVIER JUNQUERA, Universidad de Cantabria, LONG Q. CHEN, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, SAYEEF SALAUDDIN, LANE WYATT MARTIN, RAMAMOORTHY RAMESH, University of California, Berkeley — Topological solitons such as magnetic skyrmions have drawn enormous attention as stable quasi-particle-like objects. The recent discovery of polar vortices and skyrmions in ferroelectric oxide superlattices, exhibiting exotic physical phenomena, has opened up new vistas to explore topology, emergent phenomena, and approaches for manipulating such features with electric fields [1,2]. Here, using macroscopic dielectric measurements, phase-field simulations, and second-principles calculations, we demonstrate that polar skyrmions in (PbTiO$_3$)$_n$/(SrTiO$_3$)$_n$ superlattices are distinguished by a sheath of negative permittivity at the periphery of each skyrmion which enables a strong enhancement of the effective dielectric permittivity as compared to the individual SrTiO$_3$ and PbTiO$_3$ layers. Electric-field-dependent X-ray scattering measurements, phase-field simulations, and second-principles calculations are used to determine the relative fraction of skyrmions and quantify the local dielectric susceptibilities. A large, electric-field tunable negative permittivity provides a fundamental framework to enable novel low-power electronics.

1. Das, S et al, Nature **568**, 368-372 (2019);

*Grant GBMF5307*
9:00AM R64.00004: Polar Domains in Strained SrTiO$_3$ Films  
SALVA SALMANI-REZAIE  
(Presenter), KAVEH AHADI, SUSANNE STEMMER, University of California, Santa Barbara — We report on the microscopic mechanisms of how the incipient ferroelectric SrTiO$_3$ transforms into a ferroelectric by epitaxial strain. These films have recently been shown to have enhanced superconducting transition temperatures when doped, pointing to a relationship between superconductivity and ferroelectricity order parameters. Here, using high-angle annual dark-field scanning transmission electron microscopy, we detect local polar regions at room-temperature in compressively strained and unstrained SrTiO$_3$ films, respectively. Our image analysis uses the average deviation of the Ti column from the cubic position as the polar order parameter. We find that unstrained SrTiO$_3$ stays paraelectric while compressively strained films show short-range cooperative displacements within nano polar regions at room temperature. The observation of polar regions may explain optical second harmonic generation (SHG) studies, showing a residual SHG signal at room temperature in strained SrTiO$_3$. Oxygen annealing suppresses the formation of polar regions, highlighting the importance of free carriers for the stability of the polar regions.

9:12AM R64.00005: Strain-Induced Ferroelectricity in Freestanding SrTiO$_3$ Membranes  
RUIJUAN XU (Presenter), Department of Applied Physics, Stanford University, JIAWEI HUANG, School of Science, Westlake University, ED BARNARD, The Molecular Foundry, Lawrence Berkeley National Laboratory, SEUNG SAE HONG, Department of Applied Physics, Stanford University, ED WONG, The Molecular Foundry, Lawrence Berkeley National Laboratory, VARUN HARBOLA, Department of Physics, Stanford University, PRASTUTI SINGH, Department of Applied Physics, Stanford University, BAI YANG WANG, Department of Physics, Stanford University, SHI LIU, School of Science, Westlake University, HAROLD HWANG, Department of Applied Physics, Stanford University — SrTiO$_3$ is known to exhibit quantum paraelectricity in which quantum fluctuations suppress ferroelectric ordering at low temperature. Despite the intrinsic paraelectric nature of SrTiO$_3$, epitaxial strain applied via the lattice mismatch in thin-film heterostructures can significantly enhance the ferroelectric transition temperature $T_c$. Here we utilize freestanding crystalline membranes to extend the lattice control of ferroelectric ordering in SrTiO$_3$. By dissolving a water-soluble buffer layer, we release SrTiO$_3$ films from substrates, and transfer the resulting freestanding membranes onto flexible substrates that can be dynamically stretched into various strain states. Using second harmonic generation microscopy, we probe the ferroelectric phase transition as a function of strain wherein we observe $T_c$ is significantly enhanced by strain. Upon applying 1.5% uniaxial strain, we observe robust room-temperature ferroelectricity with the notable feature of 180° ferroelectric domains using piezoresponse force microscopy. First-principle calculations and molecular dynamics simulations further reveal the structural nature at each given strain state and the order-disorder character of phase transition in strained SrTiO$_3$ membranes.
Manipulation of superdomains in Pb(Zr_{0.2}Ti_{0.8})O_3 epitaxial films grown on SrTiO_3 (110) substrates

YI-CHUN CHEN (Presenter), Department of Physics, National Cheng Kung Univ., HENG-JUI LIU, Department of Materials Science and Engineering, National Chung Hsing Univ., YUCHEN LIU, MENG-XUN XIE, YU-HUAI LI, SHENG-ZHU HO, Department of Physics, National Cheng Kung Univ., YI-CHIA CHOU, Department of Electrophysics, National Chiao Tung Univ., YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung Univ., JAN-CHI YANG, Department of Physics, National Cheng Kung Univ. — Various interesting physical properties arising from manipulating strain energy terms in epitaxial films have attracted great attention. For tetragonal Pb(Zr_{0.2}Ti_{0.8})O_3 (PZT) films, the large piezoelectric response mainly originates from the switching of 90-degree c/a domains due to the strain-relief-induced reorientation. In this study, we found a superdomain structure existing the epitaxial PZT films when grown on the (110)-oriented SrTiO_3 (STO). The in-plane strain from STO breaks the uniaxial symmetry of the tetragonal PZT film, and with suitable adjusting the strain energy, superdomains can be formed in long-range areas. We used X-ray diffraction, transmission electron microscopy, and piezoresponse force microscopy (PFM) to investigate the distortion of crystal and domain structures. The PFM images show periodic nanodomains with size about 50-80 nm in the superdomain region and indicate the coexistence of at least two distortions of the crystal. The superdomains can be effectively induced or erased by external fields. Based on systematical investigations, the mechanism to create superdomains by electric fields is concluded relating to the surface energy. This study provides basic understanding and control of this unique superdomain structure.

Low-temperature synthesis of BaTiO_3 thin film by molecular beam epitaxy

YEONGJAE SHIN (Presenter), JUAN JIANG, YICHEN JIA, FREDERICK J WALKER, CHARLES H AHN, Yale University — The perovskite oxide BaTiO_3 is a lead-free material with high performance ferroelectric/piezoelectric properties. Integrating BaTiO_3 with existing semiconductor technology requires the synthesis of high-quality BaTiO_3 in the thin-film form at low temperatures to decrease the thermal budget during device fabrication. We describe our synthesis of BaTiO_3 thin films by molecular beam epitaxy at various temperatures and find that coherently strained BaTiO_3 can be grown at a temperature as low as 280 °C. The growth mechanism and strain state of these films are characterized as a function of temperature using x-ray diffraction and in-situ reflection high-energy electron diffraction. Our results pave the way toward large-scale integration of BaTiO_3 with semiconductor technology.
Monoclinic Phase and Interphase Boundaries in Perovskite Ferroelectrics  
TYLER LIEBSCH (Presenter), VLADIMIR SOBOLEV, South Dakota School of Mines and Technology — The temperature intervals of phase coexistence, including the recent experimentally observed monoclinic phase, in ferroelectric BaTiO$_3$ have been investigated using the Landau-Ginzburg-Devonshire phenomenological approach. Comparison of the thermodynamic potential for all phases in BaTiO$_3$ showed that the monoclinic phase is metastable near the tetragonal-orthorhombic phase transition, in the absence of an electric field. The structure and width of the interphase boundaries separating domains of coexisting phases near the phase transitions have been analyzed. The temperature dependence of polarization distributions, width, and energy density of the interphase boundary separating the tetragonal and monoclinic phases as well as the orthorhombic and monoclinic phases were found. The obtained results for interphase boundaries were compared to previous experimental and theoretical results for the domain walls existing within the above-mentioned phases.

Surface Proximity Effect, Imprint Memory of Ferroelectric Twins, and Tweed in the Paraelectric Phase of BaTiO$_3$*  
NICHOLAS BARRETT (Presenter), CLAIRE MATHIEU, CHRISTOPHE LUBIN, SPEC, CEA, CNRS, Université Paris-Saclay, PASCALE GEMEINER, BRAHIM DKHIL, SPMS, Centrale Supélec, Université Paris Saclay, EKHAARD SALJE, Department of Earth Sciences, University of Cambridge — For post-CMOS electronics applications using ferroic materials, the surface can play a crucial role. Non-invasive techniques are required to study the chemistry and electronic structure underlying their unique electrical properties. The sensitivity of photoemission (PEEM) electron microscopy to local surface potential, chemistry and electronic structure makes it a useful tool for probing the ferroic surfaces. We present a PEEM study of the evolution of the domain structure in BaTiO$_3$(001) through the phase transition. At room temperature, in- and out-of-plane polarized domains are present with ferroelectric and ferroelastic domain walls. Adsorbate screening results in inversion of the electrostatic surface potential contrast. Domain-related structure above the Curie temperature ($T_C$) is observable. Ferroelectric memory persist up to 550 K. The domain-like structures above $T_C$ may be related to a combination of atomic relaxation, adsorbates and oxygen vacancies. Finally, we present some first results of PEEM imaging of domain wall creep at the surface of BaTiO$_3$ around $T_C$.

*Conseil Régional Île de France SESAME project MesoXcopy  
ERSRC (EP/PO24904/1) and the Levershulme trust (RP6-2012-564)  
ANR Investissements d’Avenir program (Labex NanoSaclay ANR-10-LABX-0035 and ANR11-EQPX0005-ATTOLAB)
10:12AM R64.00010: Coherent Acoustic Phonons and Ultrafast Carrier Dynamics in BaTiO3-BiFeO3 Films and Nanorods* RATHSARA R HERATH MUDIYANSELAGE (Presenter), BRENDEN A MAGILL, GITI KHODAPARAST, Virginia Tech, CHRISTOPHER J STANTON, Univ. of Florida, JADE HOLLEMAN, STEPHEN A MCGILL, NHMFL, Florida, MIN-GYU KANG, Penn State, HAN-BYUL KANG, Virginia Tech, SHASHANK PRIYA, Penn State — BiFeO3 has become a popular multiferroic material as an alternative to PZT since it is lead free. The addition of about 25% BaTiO3 in solid solution has been shown to substantially improve the coupling between electric, magnetic, optical, and structural orders parameters and offers the possibility of developing high speed multifunctional devices. We performed two-color (400 nm pump, 800 nm probe) time resolved transient reflectivity measurements of (1-x) BaTiO3-(x) BiFeO3, with x = 0.725 and BaTiO3-BiFeO3 nanorods. Our results show ultrafast carrier dynamics in BaTiO3-BiFeO3, which we interpret as diffusion of the photoexcited carriers away from the surface with an ambipolar diffusion constant that is below 1-2 cm²/s. The differential reflectivity also showed evidence of coherent acoustic phonons (CP) in both the films and nanorod samples at lower temperatures (100 K). The ability to generate strain via ultrafast optics can offer the intriguing possibility of dynamically manipulating and controlling electric and magnetic fields.

*This material is based upon work supported by the Air Force Office of Scientific Research under award numbers FA9550-17-1-0341, FA9550-16-1-0358 under DURIP2016 Program.

10:24AM R64.00011: Understanding the ferroelectric switching in freestanding BiFeO3 films QIWU SHI (Presenter), Department of Materials Science and Engineering, University of California, Berkeley; Sichuan University, YEN-LIN HUANG, HONGRUI ZHANG, XIAOXI HUANG, SUJIT DAS, RAMESH RAMAMOORTHY, Department of Materials Science and Engineering, University of California, Berkeley — The goal to achieve the low-voltage switching in BiFeO3 could be significant for reducing the energy consumption for the electric field control of magnetism, and promoting the prospect of ultra-low power ferroelectric memories. Although several strategies have been proposed, such as size scaling, strain engineering or achieving high-quality of crystals, the value of switching voltage has been still limited. In this work, we design the freestanding BiFeO3 films for elucidating the ferroelectricity without the “clamping effect” from substrate. Due to the release of the imposed strain from substrate, the lattice distortion and a reduced c/a value are observed. And the ferroelectric domain pattern of BiFeO3 shows a highly-order to disorder transition after freestanding. This inhomogeneous domain structure might be induced by the release of the clamping effect from the substrate and could be one of the reasons for the reduced switching voltage in the freestanding BiFeO3. It indicates that the freestanding methodology may pave a new pathway toward the next-generation low-power ferroelectric memory.
**10:36AM R64.00012: Manipulation of spin and the effective spin-orbit coupling in complex oxides**

WEICHUAN HUANG (Presenter), SUJIT DAS, University of California, Berkeley, USA, RUCHIRA CHATTERJEE, KATHERINE INZANI, EVAN SHERIDAN, SINÉAD GRIFFIN, Lawrence Berkeley National Laboratory, USA, VALENTIN V. LAGUTA, Czech Academy of Sciences, Prague, Czech Republic, YEN-LIN HUANG, Lawrence Berkeley National Laboratory, USA, HONGRUI ZHANG, RAMAMOORTHY RAMESH, University of California, Berkeley, USA — Electric field manipulation of spins and control of spin-orbital coupling have stimulated an intense interest due to their promise for new functionalities and power efficient device concepts. We are particularly interested in the manipulation of spin state (high spin to low spin) as well as their directionality, for example in a \(d^5\) state Fe\(^{3+}\) ion. Using Fe-doped PbTiO\(_3\) (Fe-PTO) as a model system, we present a systematic study of the thickness, temperature and electric field-dependent spin manipulations and spin-orbit coupling (SOC) effect in dilute magnetic ferroelectrics. Using laser MBE, we synthesized a series of Fe-PTO thin films with thickness range from 15 nm to 200 nm on various substrates in order to access systematically strained states in the Fe-PTO layer. Electron spin resonance from the Fe-site demonstrates a strong \(g\)-factor anisotropy from the normal to in-plane direction of the films. Moreover, we observed that the \(g\)-factor anisotropy systematically changes under tensile strain. These results demonstrate the manipulation of spins as well as effective SOC by subtle aspects of lattice strain/electric field.

*This work was supported by the CAPSL, one of the nCORE Centers as task 2759.002, and a SRC program sponsored by the NSF through CCF 1739635.

**10:48AM R64.00013: Octahedral rotations in Ruddlesden-Popper layered perovskites under pressure from first principles**

SRIRAM POYYAPAKKAM RAMKUMAR (Presenter), ELIZABETH NOWADNICK, Materials Science and Engineering, University of California, Merced — Octahedral rotations are ubiquitous in perovskite oxides and couple closely to their electronic and magnetic properties. Applying pressure to bulk perovskites tunes the octahedral rotation amplitudes, and in some cases changes the octahedral rotation pattern. While the pressure response of octahedral rotations in ABO\(_3\) perovskites has been well studied, the impact of pressure on layered perovskites such as the n=2 Ruddlesden-Popper (RP) phase A\(_3\)B\(_2\)O\(_7\) is much less explored. Here, we use density functional theory calculations to investigate the pressure response of several A\(_3\)B\(_2\)O\(_7\) layered perovskites. We find that these RPs have a distinct pressure response compared to ABO\(_3\) materials. In particular, while the pressure response of ABO\(_3\) perovskites often can be classified according to the charge state of the A- and B-site cations, we find that each of the A\(_3^{2+}\)B\(_2^{4+}\)O\(_7\) RPs that we study exhibits a different response to pressure. Using a Landau expansion, we show how the interplay between different energetic contributions in RPs leads to this diverse set of responses to pressure. Our results offer insight into how to tune the structure and hence properties such as ferroelectricity in layered perovskites.

**Thursday, March 5, 2020 8:00 AM - 10:00 AM**
8:00AM R65.00001: Large Tunability of Band Edges and Band Gaps in Colloidal Nanoplatelets

QUNFEI ZHOU (Presenter), Materials Research Science and Engineering Center, Northwestern University, YEONGSU CHO, Department of Chemistry, University of Chicago, SHENYUAN YANG, Institute of Semiconductors, Chinese Academy of Sciences, EMILY WEISS, Materials Research Science and Engineering Center, Northwestern University, TIMOTHY BERKELBACH, Department of Chemistry, Columbia University, PIERRE DARANCET, Center for Nanoscale Materials, Argonne National Laboratory — Colloidal semiconductor nanoplatelets (NPLs) are quasi-two-dimensional nanostructures, that exhibit outstanding physical and chemical properties for optoelectronic applications. Using first-principles density functional theory calculations, we demonstrate large tunability of NPLs band edge energies over a range of 5 eV through surface passivation by common organic molecules, and how this could be leveraged in controlling the functionality in mixed-dimensional heterojunctions and photocatalysis[1]. Meanwhile, ligands induce up to 300 meV band gap shifts, in addition to the shifts by quantum confinement dictated by the number of atomic layers in thickness. We developed simple quantitative theory describing the independent tunability of band edge and band gap shifts in terms of ligand-induced surface dipole, and strain, respectively, which can be used for controlled modification of photochemistry and optoelectronic properties for NPLs.


*Funded by NSF through Northwestern MRSEC grant DMR-1720139. Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
8:12AM R65.00002: Suppression of Impurity Phase in Cesium Halide Perovskites by using Pressure  
LANANH NGUYEN (Presenter), DUONG MINH NGUYEN, YOUNGJONG KANG, Hanyang Univ, LIN WANG, HPSTAR, JAEYONG KIM, Hanyang Univ — Cesium halide perovskites, Cs$_4$PbBr$_6$ are new promising candidates for the applications of wide band gap semiconductors. However, the unavoidable appearance of CsPbBr$_3$, during the growth of the host crystal significantly hinders the optical and electrical properties of the materials. We report the suppression of the CsPbBr$_3$ phase by applying pressure in an order of giga-pascal scale. The results of XRD revealed that the CsPbBr$_3$ phase disappeared at 2.6 GPa. No PL and band edge peak of CsPbBr$_3$ was observed at 3.0 GPa, which demonstrates the disappearance of the fluorescence from the UV irradiated sample. With further pressure, the XRD data showed a reversible phase transition from rhombohedral to monoclinic of Cs$_4$PbBr$_6$ at 2.6 GPa. The main peaks were stable under pressure up to 20.0 GPa. After releasing the pressure, a very small intensity of PL peak, the band edge, and XRD peaks for CsPbBr$_3$ phase were observed. The Cs$_4$PbBr$_6$ phase was recovered at ambient conditions. It is speculated that CsPbBr$_3$ crystals are sensitive to pressure with the distortion of [PbBr$_6$]$^{4-}$ network at moderately low pressure (<3.0 GPa), while Cs$_4$PbBr$_6$ crystals are much stable at high pressure (up to 20.0 GPa) due to the isolated octahedral PbBr$_6$$^{4-}$ ions interspersed Cs$^+$ cations.

8:24AM R65.00003: A Machine Learning Approach to the Analysis of X-ray Diffraction Patterns From Multilayered Thin Film Diffusion Couples*  
ALEXEI KANANENKA (Presenter), MATTHEW FORBES DECAMP, KARL UNRUH, Physics and Astronomy, Univ of Delaware — A machine learning approach based on Neural Network and Gaussian Process Regression algorithms has been developed to extract structural information from the x-ray diffraction (XRD) patterns of multilayered Au/Pt diffusion couples. These algorithms have been trained on a subset of about 100,000 simulated XRD patterns computed at various stages of diffusional mixing in multilayers containing a fixed number of bilayers but a fluctuating number of atomic planes in each (unreacted) Au and Pt layer. When used to analyze the simulated diffraction patterns, this approach has been successful in reconstructing the known composition profile and the number of unreacted Au and Pt planes in each layer.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR140076.
First principles study of hBN-AlN short-period superlattice heterostructures*  CATALIN SPATARU (Presenter), MARY H. CRAWFORD, ANDREW A. ALLERMAN, Sandia National Laboratories — We present a theoretical study [1] of the structural, electronic, and optical properties of hBN-AlN superlattice (SL) heterostructures using a first-principles approach based on standard and hybrid density functional theory. We consider a short-period (L < 10 nm) SL and find that its properties depend strongly on the AlN layer thickness L_{AlN}. For L_{AlN} less than ~1nm, AlN stabilizes into the hexagonal phase and the SL displays insulating behavior with type II interface band alignment and optical gaps as small as 5.2 eV. The wurtzite phase is formed for thicker AlN layers. In these cases, built-in electric fields lead to the formation of polarization compensating charges as well as two-dimensional conductive behavior for electronic transport along interfaces. We also find defect-like states localized at interfaces which are optically active in the visible range. [1] C.D. Spataru, M.H. Crawford and A.A. Allerman, Appl. Phys. Lett. 114, 011903, (2019).


Hydrogen passivation effect on the sealing problem of edge growth in h-BN*  WENJING ZHAO (Presenter), JUNYI ZHU, Physics, The Chinese University of HongKong — Edge kinetics in two dimensional structure has been the key to understand the growth. In this talk, we'll illustrate the intrinsic difficulty to fill out the last few atoms to the edge of hexagonal BN and define such a difficulty as a sealing problem. The physical origin is due to the accumulation of local strain energy of the reconstruction near edges. Specifically, the local distortion becomes severe when more atoms are imperfectly placed to fill the gap on the edge. To solve the sealing problem and reduce the energy barrier to form a perfect edge, it's possible to passivate the dangling bonds of the edge atoms to reduce the edge reconstruction by hydrogen. This new finding and growth strategy may largely enhance the crystal quality and growth rate.

*This work is supported by Hong Kong RGC/GRF under the project number of 14307219 and 14319416.
**9:00AM R65.00006: Epitaxial growth of atomically-sharp GeSn/Ge/GeSn tensile strained (≥1.5 %) quantum well on Si**  SIMONE ASSALI (Presenter), ANIS ATTIAOUI, PATRICK DEL VECCHIO, SAMIK MUKHERJEE, AASHISH KUMAR, OUSSAMA MOUTANABBIR, Ecole Polytechnique de Montreal — In a full-group IV integrated semiconductor platform for tensile-strained Ge the direct-band gap can be obtained when the Ge is grown on a lattice-mismatched Ge$_{0.87}$Sn$_{0.13}$ substrate. The main challenge is to increase the incorporation of Sn in Ge above the ~1at.% equilibrium composition. Major developments were recently achieved in the epitaxial growth of random GeSn alloys with composition above 16at.%. A biaxial tensile strain in a Ge layer up to ~1.5% was demonstrated when growing on a Ge$_{0.88}$Sn$_{0.12}$ substrate. However, despite the large amount of tensile strain in Ge, no information are available on the abruptness of the Ge-GeSn interface and on the possibility of the subsequent GeSn growth on top.

Here, we discuss the epitaxial growth of a tensile-strained GeSn/Ge/GeSn heterostructure(s-Ge) with sharp interfaces and in-plane biaxial strain above 1.5% grown on lattice-mismatched Ge$_{0.86}$Sn$_{0.14}$. The sharpness of the Ge/GeSn heterostructure interfaces will be addressed using TEM-EELS and atom probe tomography(APT) measurements. A defect-free s-Ge layer thickness in the 13-1.2nm range is achieved and its pseudomorphic nature will be discussed using STEM and XRD. The s-Ge QW platform is a new versatile platform to investigate LH spin-based qubits and high hole mobility electronics.

**9:12AM R65.00007: Field emission characteristics of solid-state, GaN-based vacuum nanoelectronic devices**  KESHAB R SAPKOTA (Presenter), ALBERT A TALIN, FRANCOIS LEONARD, Sandia National Laboratories, BARBARA A KAZANOWSKA, KEVIN S JONES, Engineering, University of Florida, BRENDON P GUNNING, GEORGE T WANG, Sandia National Laboratories — Vacuum nanoelectronics have notable advantages over conventional solid state devices. Vacuum channel devices are inherently robust in harsh environments and allow high frequency and power operation due to ballistic electron conduction. By shrinking the vacuum channel to nanoscale size well below the electron mean free path in air, these devices should be operable in air while maintaining the advantages of vacuum transport. Here we propose GaN as a superior materials platform compared to silicon or metals for solid-state, nanogap field emission devices based on its lower electron affinity, higher chemical stability, and high breakdown voltage. These novel GaN nanogap field emission device exhibit low turn-on voltage, high field emission current, and excellent on-off ratio. We will present experimental and modeling results on the field emission characteristics of these devices at various gap sizes and operating pressures.

*Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525*
9:24AM R65.00008: Classification of Critical Points in Energy Bands Based on Topology, Scaling and Symmetry  
NOAH YUAN (Presenter), LIANG FU, Massachusetts Institute of Technology  
MIT — A critical point of the energy dispersion is the momentum where electron velocity vanishes. At the corresponding energy, the density of states (DOS) exhibits non-analyticity such as divergence. Critical points can be first classified as ordinary and high-order ones, and the ordinary critical points have been studied thoroughly by Leon van Hove, whose DOS is particle-hole symmetric and logarithmically divergent. In this work, we describe and classify high-order critical points based on topology, scaling and symmetry. We show that high-order critical points can have power-law divergent DOS with particle-hole asymmetry, and can be realized at generic or symmetric momenta by tuning a few parameters such as twist angle, strain, pressure and/or external fields.

9:36AM R65.00009: Super-geometric electron focusing on the hexagonal Fermi surface of PdCoO$_2$  
MAJA BACHMANN (Presenter), AARON SHARPE, ARTHUR W BARNARD, Physics, Stanford University, CARSTEN PUTZKE, École Polytechnique Fédéral de Lausanne, MARKUS KOENIG, SEUNGHYUN KHIM, Max Planck Institut for Chemical Physics of Solids, DAVID GOLDHABER-GORDON, Physics, Stanford University, ANDREW MACKENZIE, Max Planck Institut for Chemical Physics of Solids, PHILIP MOLL, École Polytechnique Fédéral de Lausanne — The ultrapure delafossite metal PdCoO$_2$ exhibits a strikingly long mean free path of $\sim 20$ µm at temperatures below 20K. Owing to its peculiar Fermi surface, resembling a nearly perfect hexagon, the electron’s ballistic trajectories are mainly restricted into three directions, rendering PdCoO$_2$ an ideal material to investigate unusual anisotropic ballistic effects. We fabricate ballistic structures for transverse electron focusing from as-grown single crystals using focused ion beam machining, and demonstrate magnetic focusing up to 35 µm. Compared to typically studied materials with circular Fermi surfaces, the transverse focusing amplitude is strongly enhanced due to the large parallel sections of the hexagonal Fermi surface. We demonstrate this focusing enhancement experimentally, and corroborate it by transport simulations.
XUEDONG BAI (Presenter), Chinese Academy of Sciences, Institute of Physics — In-situ transmission electron microscopy (TEM) method is powerful in a way that it can directly correlate the atomic-scale structure with physical and chemical properties. Here, we will report on the construction and applications of the in-situ TEM setup including mechanical, electrical and optical holders, which were built by STM technique. So the manipulation and physical measurement have been realized inside TEM, where the real-time imaging of electrically and/or mechanically driven structural evolution at atomic scale has been carried out by the homemade in-situ TEM setup.

Exploring the lattice degree of freedom of metal oxides in transition between different structural phases may provide a route to the new properties in oxide materials. Here we report on the electrically driven oxygen vacancy ordering in CeO$_2$ films, and the experimental finding of strain-inhibited structural transition from perovskite to brownmillerite during the oxygen vacancy electromigration in epitaxial LaCoO$_3$ thin films, as well as the mechanically induced ferroelectric vortices transformation in PbTiO$_3$/SrTiO$_3$ superlattice will be included. This is a fundamental research for the future nanoelectronics such as memories and also the valuable insight into lattice-charge interactions at nanoscale.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R66 DCMP: Exploring the Relation Between Electron Nematicity and Superconductivity in Strongly Correlated Electronic Systems

Four Seasons 1 - Daniel Arovas, University of California, San Diego - Tag(s): Invited
Strain sensitivity and other experimental consequences of nematic-mediated superconductivity* [Invited] SAMUEL LEDERER (Presenter), Cornell University, EREZ BERG, Weizmann Institute of Science, EUN-AH KIM, Cornell University — In many unconventional superconductors, nematic quantum fluctuations are strongest where the critical temperature is highest, inviting the conjecture that nematicity plays an important role in the pairing mechanism. Recently, strontium-doped barium nickel oxide has been identified as a tunable nematic system that provides an ideal testing ground for this proposition. We therefore propose several sharp empirical tests, supported by quantitative calculations in a simple model of this material. The most stringent predictions concern experiments under uniaxial strain, which has recently emerged as a powerful tuning parameter in the study of correlated materials. Since uniaxial strain so precisely targets nematic fluctuations, such experiments may provide compelling evidence for nematic-mediated pairing in this and other materials, analogous to the isotope effect in conventional superconductors.

*SL was supported in part by a Bethe/KIC fellowship at Cornell. EB was supported by the European Research Council (ERC) under grant HQMAT (grant no. 817799) and by the Israel-USA Binational Science Foundation (BSF). Theoretical studies by SL and E-AK were supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award de-sc0018946.

Sixfold enhancement of superconductivity in a tunable electronic nematic system* [Invited] JOHNPIERRE PAGLIONE (Presenter), University of Maryland, College Park — The electronic nematic phase - in which electronic degrees of freedom lower the crystal rotational symmetry - is commonly observed in high-temperature superconductors. However, understanding the role of nematicity and nematic fluctuations in Cooper pairing is often made more complicated by the coexistence of other orders, particularly long-range magnetic order. Here we report the enhancement of superconductivity in a model electronic nematic system that is not magnetic, and show that the enhancement is directly born out of strong nematic fluctuations associated with a quantum phase transition. We present measurements of the resistance as a function of strain in Ba$_{1-x}$Sr$_x$Ni$_2$As$_2$ to show that strontium substitution promotes an electronically-driven nematic order in this system. In addition, the complete suppression of that order to absolute zero temperature leads to an enhancement of the pairing strength, as evidenced by a sixfold increase in the superconducting transition temperature. The direct relation between enhanced pairing and nematic fluctuations in this model system, as well as the interplay with a unidirectional charge density wave order comparable to that found in the cuprates, offers a means to investigate the role of nematicity in boosting superconductivity.

*This research was supported by the AFOSR Grant No. FA9550-14-10332, the Gordon and Betty Moore Foundation Grant No. GBMF4419 and GBMF4542, and the U.S. DOE Department of Energy, Office of Science, Basic Energy Sciences under award number DE-SC0012336 (theory) and DE-FG02-06ER46285 (x-ray experiments).
Historically, the antiferromagnetic insulator state of CuO$_2$ is transformed by hole-doping onto the oxygen sites, into an exotic quantum fluid that is usually referred to as the pseudogap (PG) phase. Its defining characteristic is a strong suppression of the electronic density-of-states for energies $E<D$, where $D$ is the pseudogap energy scale. Within the pseudogap phase, complex broken-symmetry phases have been detected by a very wide variety of techniques. First, there is the finite-Q charge-density-wave (CDW) state that is locally commensurate and unidirectional, with $4a_0$ periodicity and a $d$-symmetry form factor. Second, is the finite-Q pair-density-wave (PDW) state which is detected with superconducting-tip STM as having a $4a_0$ periodicity in the magnitude of Josephson currents and an $8a_0$ periodicity in its energy-gap modulations. Third, there is the nematic (NE) state which breaks rotational symmetry at $Q=0$.

Simultaneous measurements of the PDW and CDW phenomenology now reveal strong evidence that they are facets a single, fundamental, density wave (DW) state that breaks translational symmetry. More surprisingly, several characteristics of the NE state appear closely related to those of this DW state. For example, by simultaneously imaging the doping and energy dependence of the DW and NE states, we find that the maximum spectral intensity of these quite distinct forms of symmetry breaking always occurs at the same energy, and that this is always the pseudogap energy for hole-density $p<0.19$. We discuss how this perplexingly linked phenomenology of two highly distinct broken-symmetry states may be understood as the natural consequence of a vestigial nematic state within the pseudogap phase of Bi$_2$Sr$_2$CaCu$_2$O$_8$.

J.C.S.D. acknowledges support from the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4544, from Science Foundation Ireland under Award SFI 17/RP/5445, and from the European Research Council (ERC) under Award DLV-788932.
Strain-tuning nematic order and signatures of nematic quantum criticality* [Invited] IAN FISHER (Presenter), Department of Applied Physics and Geballe Laboratory for Advanced Materials, Stanford University — Quantum criticality associated with electronic nematic order has been suggested as a possible avenue for a range of exotic electronic effects, from non-Fermi liquid behavior to superconductivity. In order to study the behavior of metals proximate to such a quantum critical point, it is useful to establish effective tuning parameters that can drive the critical temperature of an electronic nematic phase to zero. I will describe how both symmetric and orthogonal antisymmetric strains can play this role, and demonstrate these effects in an archetypal Fe-based superconductor. For compositions progressively closer to the putative nematic quantum critical point, these tuning parameters become increasingly more effective, the precise variation of which provides evidence for a wide range of composition and temperature over which quantum critical fluctuations play a key role in shaping the properties of this family of materials. Additional evidence can be found in the temperature and doping dependence of the nematic susceptibility, which, by applying large magnetic fields, can be measured in the absence of superconductivity down to low temperatures. Further insights can be obtained by consideration of other model material systems, in particular materials that undergo ferroquadrupolar order of local 4f atomic orbitals.

*This work reflects several individual projects, and was supported in part by the Department of Energy, Office of Basic Energy Sciences under contract DE-AC02-76SF00515, and in part by the Gordon and Betty Moore Foundation EPiQS Initiative through Grant No. GBMF4414.
Divergent nematic susceptibility near the pseudogap critical point in Bi-cuprate superconductors* [Invited] TAKASADA SHIBAUCHI (Presenter), Univ of Tokyo-Kashiwanoha — In strongly correlated materials, superconductivity is often found near a magnetic quantum critical point (QCP) where a magnetic phase vanishes in the zero-temperature limit. Moreover, the maximum of superconducting transition temperature $T_c$ frequently locates near the magnetic QCP, suggesting that the proliferation of critical spin fluctuations emanating from the QCP plays an important role in Cooper pairing. In cuprate superconductors, however, the superconducting dome is usually separated from the antiferromagnetic phase and $T_c$ attains its maximum value near the verge of enigmatic pseudogap state that appears below doping-dependent temperature $T^*$. Thus a clue to the pairing mechanism resides in the pseudogap and associated anomalous transport properties. Recent experiments suggested a phase transition at $T^*$ but the key question is what kind of fluctuations are associated with the pseudogap. Here we report elastoresistance measurements of nematic susceptibility in $(\text{Bi,Pb})_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, which is sensitive to an electronic order with twofold in-plane anisotropy. The nematic susceptibility shows an anomaly at $T^*$ evidencing a phase transition with broken rotational symmetry. Near the pseudogap end point, nematic susceptibility becomes singular and divergent. This signifies the presence of a nematic QCP, which has emerging links to the high-$T_c$ superconductivity and strange metallic behaviours in cuprates.

This work has been done in collaboration with K. Ishida, S. Hosoi, Y. Teramoto, T. Usui, Y. Mizukami, K. Itaka, Y. Matsuda, and T. Watanabe.

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Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R67 DCMP DCOMP: Predictive Discoveries of Novel Two-Dimensional (2D) Materials Through Complementary High-Throughput Approaches Four Seasons 2-3 - Ismaila Dabo, Pennsylvania State University - Tag(s): Invited
We performed extensive density-functional theory calculations of the geometries, band structures, and Z2 topological invariants of 2D honeycomb materials. Using a recently developed artificial-intelligence approach (SISSO, Ref. 1) we identify the actuators ('material's genes') that govern the topological transition. We also draw a 'map of materials properties' which identifies the regions of metals, trivial insulators, and topological insulators. The latter region contains several million newly predicted topologically nontrivial alloyed materials.


*This work was partially funded by the NOMAD (Novel Materials Discovery) Center of excellence: https://nomad-coe.eu .
We have performed an extensive high-throughput screening of known inorganic materials, to identify those that could be exfoliated into novel two-dimensional monolayers [1]. The screening protocol first identifies bulk materials that appear layered according to a simple and robust chemical definition of bonding, determining then for all of these the binding energies of the respective monolayers, their electronic state (metallic vs insulating), magnetic configuration (ferro-, ferri- or antiferromagnetic), and phonon dispersions (to evaluate mechanically stability). Such protocol identifies a portfolio of close to 2,000 inorganic materials that appear either easily or potentially exfoliable. With further data ingestion, this initial portfolio has recently almost doubled, providing an extensive pool to investigate promising properties. First focus has been on the determination of the effective masses and mobilities (from the full solution of the Boltzmann transport equation) for electronic applications; of topological invariants; of superconductivity and charge-density waves; and of photocatalytic parameters for water splitting. Thanks to the use of the AiiDA (http://aiida.net) materials' informatics platform, all the high-throughput calculations can be performed and streamlined in fully searchable and reproducible ways, they are stored in a database with the full provenance tree of all parent and children calculations, and can be shared with the community at large in the form of raw or curated data via the Materials Cloud (http://www.materialscloud.org) dissemination portal.


*Support from the Swiss National Science Foundation through the Ambizione career program and the MARVEL National Centre for Competence in Research is greatly acknowledged.
SHENGBAI ZHANG (Presenter), Rensselaer Polytechnic Institute — Recent years have witnessed an amazing expansion in the family of 2D materials, which has led to many exotic physical properties distinctly different from their bulk counterparts. An example is the traditional II-VI compound semiconductors in their monolayer limit [1], for which the experiments have been catching up rapidly. Besides the monolayer honeycomb (MLHC) $h$BN-like structure, a double layer honeycomb (DLHC) structure was also predicted to be stable over a large portion of ordinary semiconductors [2]. It is becoming clear that when the thickness of a solid is below certain critical value, irrespective of its commonly-observed bulk form, a universal van der Waals stacking may happen, leading to unexpected physical properties. Taking GaAs, a well-known covalent semiconductor, as an example, non-trivial topological properties emerge as a result of the stacking of DLHCs [2], as well as the formation of an excitonic insulator (EI) where the excitonic binding energy magically becomes larger than its band gap [3]. In strongly-correlated 2D systems such as MX$_2$ where M = Ni, Co and X = Cl, Br, on the other hand, half excitonic insulator can also form where one spin channel is an ordinary semiconductor while the other spin channel is an EI, leading to Bose-Einstein condensation [4].


*Work in the US was supported by the US DOE Grant No. DE-SC0002623. The supercomputer time sponsored by NERSC under DOE contract No. DE-AC02-05CH11231 and the CCI at RPI are also acknowledged.
CLAUDIA DRAXL (Presenter), Physics Department, Humboldt University Berlin — 2D materials exhibit peculiar optoelectronic properties [1] that can be further tuned by stacking, functionalization, or creating interfaces [2-4]. Analysis based on many-body approaches provide us insight into their intriguing features. Making use of this information and the large data pool of the NOMAD Repository [5], we apply data-analytics tools to create a pool of fingerprints and find descriptors for particular properties. A novel approach, based on these fingerprints, will be demonstrated to unravel hidden similarities between materials.

[5] https://nomad-repository.eu

(*) Work performed in collaboration with Martin Kuban and Santiago Rigamonti

*Work supported by the NOMAD Laboratory (https://nomad-coe.eu) and the Deutsche Forschungsgemeinschaft (DFG), project numbers 182087777 - SFB 951 and 403180436 (ED 293/2-1).
10:24AM R67.00005: Epitaxial tellurene, phosphorene and MoTe$_2$ derivatives: from theoretical prediction to experimental observations* [Invited] MAOHAI XIE (Presenter), Physics Department, The University of Hong Kong — The family of 2D materials has been expanding continuously showing the diverse structural, symmetrical and electronic properties. Presently, there are two major categories of 2D materials experimentally obtainable: one is by exfoliation from bulk crystals (e.g., graphene) and the other is by epitaxial growth (e.g., silicene), and the latter is more versatile capable of synthesizing materials that would otherwise be not present naturally. In this presentation, some of our synergistic research efforts between theory, modeling, and experiments in the discoveries and further characterizations of a few members of the 2D materials family will be given. These include layered tellurium [1,2], metal-phosphorene network consisted of blue-phosphorene units linked by Au atoms [3,4], and a variational hexagonal phase of molybdenum telluride [5]. Each of these are achieved by molecular-beam epitaxy and their structural and electronic properties are characterized by scanning transmission electron microscopy, scanning tunneling microscopy and scanning tunneling spectroscopy. These materials show potentials of various applications.


*The works are financially supported by a Collaborative Research Fund (No. C7036-17W), a General Research Fund (No. 17304318), and a NSFC/RGC joint research grant (No. N_HKU732/17) from the Research Grant Council, Hong Kong Special Administrative Region, China.

Thursday, March 5, 2020 8:00 AM - 11:00 AM

Session R68 DQI: Control and Calibration Tools for Scalable Quantum Computing Four Seasons 4 - Robin Blume-Kohout, Sandia National Laboratories - Tag(s): Focus
Estimation of statistical significance in the quantum supremacy experiment with the Sycamore processor  

PING YEH (Presenter), ADAM ZALCMAN, SERGIO BOIXO, Google, Inc. — Google’s quantum supremacy experiment is based on sampling of output bitstrings of random quantum circuits [1]. To demonstrate quantum supremacy, it is critical to establish that the hardware fidelity at sampling time is not degraded to zero due to errors and the sampled bitstrings correspond to the expected noisy distribution. In addition, since the run time of classical approximate simulations is proportional to fidelity, it is important to verify that the fidelity is above a threshold at which classical simulation is estimated to be hard. In this talk, I will describe the methodologies for the statistical analyses and show that the bitstring distributions are extremely unlikely to be explained by noise alone and the fidelity is significantly above the threshold.


How OpenSuperQ is planning to fully calibrate and characterize a 100 qubit superconducting QPU over the weekend*

SHAI MACHNES (Presenter), NICOLAS WITTWER, FEDERICO ROY, Univ des Saarlandes, ANURAG SAHA ROY, Citizen scientist, KEVIN PACK, FRANK WILHELM, Univ des Saarlandes — The current methodology of designing control pulses for superconducting circuits often results in an absurd situation: simplified analytic models which do not predict gate fidelities to high accuracy, and calibrated pulse shapes which achieve good fidelities, but do not correspond to the model. For large number of qubits the QPU calibration is long and difficult, and determining a detailed error budget is nearly impossible.

To rectify the situation, we have implemented a novel procedure of Combined Calibration and Characterization (C3): An interative combination of open-loop pulse optimization, model-free tune-up and iterative model fitting and refinement, utilizing a high-performance TensorFlow simulator. It allows for a rapid, and largely automated bring-up process of QPUs. The result is a high-fidelity model, comensurate high-fidelity gates and a detailed error budget.

The above components are then utilized to implement machine-learning capabilities such as adversarial system characterization and automated experiment design, to further accelerate the process of gaining insight into the behaviour of our systems.

C3 software will be made available as an open-source project.

*Project OpenSuperQ (820363) EU Flagship Quantum Technologies, IARPA LogiQ grant W911NF-16-1-0114
As the era of NISQ is dawning, calibration and characterization of QPUs is becoming an increasingly complex task due to the growing amount of qubits and high fidelity requirements. To tackle this problem, we developed a machine learning driven approach for Combined Calibration and Characterization procedure, C^3. This talk focuses on the gate calibration task, where optimization algorithms are used to find the best pulse parameter values in a multidimensional space.

We present a strategy which is capable of optimizing dozens of parameters, optimizing both an entangling gate and the single qubit gates of the two qubits involved, and to do so significantly faster than previously possible.

To succeed in this endeavor we engaged in an in-depth study of the multitudes of gradient-free algorithms available. The result is a unique portfolio of algorithms, for fast initial convergence and high fidelities.

Finally, we present experimental results by several labs that applied the above methodology. We show how our method takes entire gate sets all the way from 0.85 fidelities to state-of-the-art fidelities, using our open-source software.

*Project OpenSuperQ (820363) of the EU Flagship Quantum Technologies. IARPA through the LogiQ grant No. W911NF-16-1-0114.
8:36AM R68.00004: Automatic Calibration and Characterization of Quantum Devices - Experimental Results on NISQ QPUs and Quantum Memory devices* SHAI MACHNES, NICOLAS WITTLLER (Presenter), FEDERICO ROY, Univ des Saarlandes, ANURAG SAHA ROY, Citizen scientist, KEVIN PACK, FRANK WILHELM, Univ des Saarlandes — The practical application of optimal control techniques, especially in superconducting settings, requires extensive calibration to reach high fidelities. By controlling both experiment and a high performance numerical simulation, the C3 procedure provides a framework to systematically design and apply even intricate open loop optimal control pulses.

We demonstrate the characterization and tune-up of a quantum computing device with a few qubit, as well as a quantum memory device composed of a transmon with a 3D microwave cavity. The memory experiment presents different challenges, as the control protocol involves high-power sideband transitions, leading to system dynamics that are incompatible with simple models for qubit-cavity interactions.

In both cases, we numerically simulate the measurement of gate sequences and, by comparing the results to experimental data, improve the model of the experiment, including both simple parameters such as qubit frequencies, as well as non-trivial aspects such as line responses and bandwidth limitations of the electronic equipment that distort and imposes constraints on control signals.

*Project OpenSuperQ (820363) of the EU Flagship Quantum Technologies. IARPA through the LogiQ grant No. W911NF-16-1-0114

8:48AM R68.00005: Active Learning of Hamiltonians ARKOPAL DUTT (Presenter), Massachusetts Institute of Technology, EDWIN PEDNAULT, CHAI WU, SARAH SHELDON, LEV S BISHOP, JOHN SMOLIN, IBM Thomas J. Watson Research Center, ISAAC CHUANG, Massachusetts Institute of Technology — Querying a quantum system produces measurement outcomes which originate from the Hamiltonian dynamics of the system and its environment. Learning a Hamiltonian from a class that best fits these observations is the Hamiltonian tomography problem. Prior work has focused on estimation and offline optimal experiment design. Here, we consider an active learner that is given an initial set of training examples and the ability to interactively query the quantum system to generate new training data. The goal is to then minimize the training data required for Hamiltonian learning. To this end, we present an efficient active learning algorithm based on Fisher information and assess its performance on recalibrating superconducting qubit systems based on the cross-resonance (CR) gate. The CR Hamiltonian has up to nine parameters and admits queries involving input state, measurement operator and interaction time. Practical challenges include exponential growth of number of parameters with number of qubits, and modeling different noise sources such as readout, and imperfect pulse shapes. We show that we can achieve a constant 30% reduction in queries compared to a uniformly random approach. We also describe a regime where we achieve Heisenberg limited convergence rate during learning.
9:00AM R68.00006: Optimizing Quantum Gate Frequencies for Google's Quantum Processors  PAUL KLIMOV (Presenter), JULIAN KELLY, KEVIN SATZINGER, ZIJUN CHEN, HARTMUT NEVEN, JOHN M MARTINIS, Google AI Quantum — A crucial component of operating a quantum processor is mitigating computational errors from energy-relaxation, dephasing, leakage, and control imperfections. In superconducting qubits, these sources of error can arise from control-electronics noise, control-pulse distortions, and the parasitic coupling of qubits to other qubits, two-level system defects, spurious microwave modes, and the control and readout circuitry. In frequency-tunable qubit architectures, it is possible to mitigate these sources of error by choreographing qubit gate frequencies over the course of quantum algorithms. This choreography maps to constructing and optimizing a high-dimensional, high-constraint, non-convex, and time-dependent objective over a search space that significantly exceeds the Hilbert-space dimension of the processor. In this talk, I will introduce the frequency optimization problem and the Snake optimizer that we developed to solve it for Google’s flagship quantum processors [1].


9:12AM R68.00007: Quantum Orchestration Platform Integrated hardware and software for design and execution of complex quantum control protocols  YONATAN COHEN (Presenter), ITAMAR SIVAN, NISSIM OFEK, LIOR ELLA, NIV DRUCKER, TAL SHANI, ORI WEBER, HANAN GRINBERG, MICHAEL GREENBAUM, Quantum Machines — The incredible progress in designing quantum systems, engineering their environment, and controlling them effectively, has led to significant improvements in coherence times, gate fidelities and the ability to integrate more qubits into a single quantum processor. While development of quantum processors remains the number one challenge, many bottlenecks exist in the classical control hardware layer as well as the software layer, where optimizations can play a critical role for near term quantum computing. Some examples include (1) feedback for error correction and repeat until success protocols, (2) complex calibrations, and (3) hybrid quantum classical algorithms. Here we present a new platform for designing quantum control protocols, executing them on a wide range of quantum hardware, and optimizing performance. The platform, called Quantum Orchestration Platform incorporates a unique FPGA architecture and integrates classical hardware and software in a novel way that allows for combining the most cutting-edge real-time control capabilities with an intuitive programming environment and programing language. We show examples and present results of several protocols, including multiqubit feedback and complex control flow.
9:24AM R68.00008: Quantum Orchestration Platform Integrated hardware and software for design and execution of complex quantum control protocols  ITAMAR SIVAN (Presenter), YONATAN COHEN, NISSIM OFEK, TAL SHANI, ORI WEBER, LIOR ELLA, MICHAEL GREENBAUM, HANAN GRINBERG, NIV DRUCKER, Quantum Machines — Quantum computing holds a great promise for immense computational power. In last years, it was suggested that noisy intermediate-scale quantum (NISQ) processors may already demonstrate an advantage over classical hardware for particular computational tasks which may be of commercial use. Nonetheless, significant additional technological progress, at every layer of the quantum computer, is required in order to advance from NISQ processors to ones capable of running fault-tolerant-quantum-computation (FTCC). In particular, for FTCC, multi-qubit real-time feedback capabilities have to be developed far beyond those we know today. Here we present the recently developed Quantum Orchestration Platform (QOP) allowing for general multi-qubit protocols to be run. The QOP is a scalable system designed to support hybrid quantum-classical algorithms with the outlook to FTCC, and is optimized for driving multiple qubits simultaneously as well as performing complex readout schemes and branching based on readout results with ultra-low latency feedback. In this talk, we will show examples for quantum-error-correction protocols and demonstrate how they are programmed and run with the QOP.

9:36AM R68.00009: High-Fidelity, Scalable Quantum-Classical Control Interface using Photonics*  JACKY CHAN (Presenter), APURVA S. GOWDA, PETER T. S. DEVORE, BRANDON W. BUCKLEY, JONATHAN L DUBOIS, JASON CHOU, Lawrence Livermore Natl Lab — Quantum computing (QC) has been hailed as the next big leap for the digital age; however, state-of-the-art QC devices have yet to surpass classical computers. One bottleneck is in the number of quantum operations that can be done within a qubit lifetime, also known as the "circuit depth". The circuit depth on current hardware is limited to 10-100 operations due to uncontrolled coupling to the classical environment, infidelities in the qubit operations and the gate operation time. Effective control signal generation is essential to extending the circuit depth by improving classical control over the quantum system. To address this need, we propose an RF-photonic implementation of a QC control interface, via high-fidelity, scalable quantum drive signal generation and fiber optic transport of this signal to the qubit. By increasing the signal dynamic range and bandwidth, the time per quantum gate operation can be reduced, thus widening the circuit depth bottleneck. Additionally, replacing RF cabling with optical fiber reduces waste heat and thermalization issues, improving scalability to larger qubit systems. We show experimental results from a single-channel system and discuss its extension to a multi-channel system via simulations.

*Prepared by LLNL under Contract DE-AC52-07NA27344.
9:48AM R68.00010: Automatic single qubit characterization with QubiC*  
YILUN XU  
(Presenter), GANG HUANG, Lawrence Berkeley National Laboratory, RAVI KAUSHIK NAIK, BRADLEY MITCHELL, Physics, University of California, Berkeley, DAVID SANTIAGO, Lawrence Berkeley National Laboratory, IRFAN SIDDIQI, Physics, University of California, Berkeley — Initial setup a physical qubit is a complex procedure which involve multiple instruments and multiple experiments and optimization. After the initial setup, they still need to be carefully calibrated routinely because the qubit is sensitive to the environment and the qubit itself can have slow drift so as to impact the gate fidelity.

The Qubit Control system (QubiC) combines the high-speed pulse generation, data acquisition, parallel processing, and deterministic high-throughput data exchange together through the FPGA. Based on this feature, we propose a single qubit characterization and gate optimization protocol which automatically find and tune the qubit. The automatic calibration executes a full suite of serialized and recursive tasks from initial device bring-up to qubit setup to gate optimization in few hours.

*This work was supported by the U.S. Department of Energy, Office of Science, Office of High Energy Physics, under Contract DEAC02-05CH11231.

10:00AM R68.00011: Optimal Control of Superconducting Qubits*  
MAX WERNINGHAUS  
(Presenter), DANIEL EGGER, IBM Research - Zurich, FEDERICO ROY, SHAI MACHINES, FRANK WILHELM, Saarland University, STEFAN FILIPP, IBM Research - Zurich — Fast and accurate two-qubit gates are a key requirement to perform complex algorithms on current quantum computers. Ideally, the duration of the gate should be much shorter than the coherence time of the system. However, shorter gates can result in unwanted loss of states from the computational subspace.

Optimal control theory aims to design fast control pulses suppressing such side effects of the driving field. Even with an accurately calibrated system model, control pulses require a tune-up to accommodate for parameter-drifts and model-inaccuracies. Here we present our work on optimal control algorithms, using a closed loop approach with direct experimental feedback to design complex pulses. This approach avoids errors from an inaccurate initial system model and uses information gained during the pulse optimization to update the model. We improve the interplay of control instruments and multidimensional optimization algorithms to speed up the tune-up of feedback-loops, reducing evaluation times from several minutes to a few seconds. With these measures, we achieve a reduction of gate errors by more than a factor of five for short pulses.

*we acknowledge the support of the European Commission Marie Curie ETN “QuSCo” (GA N°765267)
The promise of quantum computers is that certain computational tasks might be executed exponentially faster on a quantum processor than on a classical processor. A fundamental challenge is to build a high-fidelity processor capable of running quantum algorithms in an exponentially large computational space. Here we report the use of a processor with programmable superconducting qubits to create quantum states on 53 qubits.

We create ergodic dynamics by applying a sequence that alternates between a randomly chosen single-qubit gates and an entangling two-qubit gate. Measuring the output of these quantum circuits amounts to sampling from the underlying probability distribution and produces a set of bitstrings. We verify that the quantum processor is working properly using a method called cross-entropy benchmarking, which compares how often each bitstring is observed experimentally with its corresponding ideal probability computed via simulation on a classical computer. We discuss the computational complexity of the sampling problem and show how the results of computation in a $10^{16}$ dimensional Hilbert space can be verified. Furthermore, we demonstrate how our processor is programmable by showing how various algorithms can be implemented.

10:48AM R68.00013: Calibration of flux crosstalk in flux qubit based quantum annealers with persistent current readout devices*

XI DAI (Presenter), ANTONIO JAVIER MARTINEZ, DANIEL M TENNANT, DENIS MELANSON, ALI YURTALAN, SALIL BEDKIHAL, YONGCHAO TANG, University of Waterloo, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, RABINDRA DAS, DAVID K KIM, JONILYN YODER, STEVEN WEBER, ANDREW JAMES KERMAN, MIT Lincoln Laboratory, SERGEY NOVIKOV, STEVEN M DISSELER, JAMES I BASHAM, JEFFREY GROVER, Northrop Grumman, EVGENY MOZGUNOV, DANIEL A LIDAR, University of Southern California, ADRIAN LUPASCU, University of Waterloo — Quantum annealing with superconducting flux qubits requires reliable control of externally applied magnetic fluxes. We present results on the calibration of flux crosstalk in a device consisting of two flux qubits coupled by a chain of seven couplers. The device has 27 superconducting loops and 27 bias lines. The method relies on the use of flux detectors formed of RF-SQUID terminated waveguide resonators, attached to each qubit and coupler. An iterative version of the method is demonstrated, which is more tolerant to errors arising from persistent currents in the complete circuits. The ability to perform reliable crosstalk calibration and compensation allows maintaining high coherence qubit designs and eliminates overhead in designs that are robust against crosstalk. We discuss future extensions of this work, relevant for large scale annealing control.

*This material is based upon work supported by the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO) under Contract No. W911NF-17-C-0050. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Intelligence Advanced Research Projects Activity (IARPA) and the Army Research Office (ARO).
8:00AM R70.00001: Predicting γ'-Phase Stability in Co-Based Superalloys*  
HAYDEN SCOTT OLIVER (Presenter), CHANDRAMOULI NYSHADHAM, BRAYDEN BEKKER, GUS HART, Brigham Young Univ - Provo — The discovery of a cobalt-based γ/γ'-forming superalloy in 2006 inspired our computational investigation of the Co-Al-W system. We use the Moment Tensor Potentials (MTP) active-learning framework to predict the total energy, forces, and stresses for nearly 300,000 derivative superstructures in the Co-Al-W system. We report several new structures on the convex hull with the ordered L1_2-Co_3(Al, W) crystal structure, which may correspond to the experimentally discovered γ' phase. Small additions of tantalum, titanium, and vanadium lower the formation enthalpy of the L1_2 structure, which could act as γ' stabilizers at high temperature. While the total cost of the MTP analysis is about 1/1000th the cost of a similar result using DFT, the difference between calculated and predicted results is less than 3 meV/atom. MTP can be used for high-throughput phase stability analysis for many kinds of materials, such as high-temperature superalloys, multi-principle element alloys, high-Tc magnetic materials, superhard materials, and electrochemical materials.

*The authors are grateful for financial support from the Office of Naval Research (MURI N00014-13-1-0635). HSO is grateful for financial support at the Ames National Laboratory through the 2019 DOE SULI program.

8:12AM R70.00002: Elastic properties of the Ni-containing metallic glasses.*  
OLEKSIY SVITELSKI (Presenter), DANIELLE DUGGINS, DAVID S LEE, Gordon College, Wenham MA, ALEXEY SUSLOV, National High Magnetic Field Laboratory, Tallahassee FL — Several different acoustic techniques can be used to determine the elastic constants of a material. We use resonant ultrasound spectroscopy (RUS) and acoustic pulse-echo (APE) to investigate the elastic properties of Ni_{71.5}Cr_{5.6}Nb_{3.4}P_{16.5}B_{3}, a bulk metallic glass alloy (Ni-BMG). The sample was made by a counter-gravity suction casting technique. Modeling of the measured spectrum of acoustic resonances for the sample in its cylindrical geometry was done with finite element analysis (FEA). FEA gives a longitudinal modulus (C11) of 300 GPa, and a Youngs modulus (C44) of 50 GPa (+/-5%). We compare these values with literature values for other Ni-bearing bulk metallic glass alloys.

*This work was partially supported by NSF DMR award number 1709282. National High Magnetic Field Laboratory is supported by NSF/DMR-1644779 and State of Florida.
Undercooling of gold nanodroplets levitated in a quadrupole ion trap in high vacuum

Joyce Coppock (Presenter), Quinn Waxter, José Hannan, Samuel Klueter, University of Maryland, College Park, Hope Reynolds, Montgomery Blair High School, Maryland, Gregory Schare, Columbia University, New York, Bruce E Kane, Laboratory for Physical Sciences, 8050 Greenmead Dr., College Park, MD 20740 — A nanoparticle levitated in vacuum has minimal thermal contact with its surroundings and can be heated efficiently with a laser beam. Precise control of the temperature of a levitated particle could facilitate thermodynamic measurements of materials with very high melting points. To establish such a measurement technique using a well-characterized material, we levitate a charged 200 nm gold nanoparticle in an AC quadrupole electric field trap in a vacuum chamber and use a 532 nm laser to illuminate and heat it. Accurate measurements of the mass of the particle are used to deduce the internal temperature of the particle from the rate of mass erosion. We have observed undercooling of gold particles, a phenomenon in which a melted droplet remains liquid when cooled below the usual freezing temperature. In our preliminary measurements, particles have remained liquid to temperatures around 190 K below the freezing point and have persisted in this state in excess of two minutes without refreezing. We will discuss progress toward the precise control of the temperature of a gold nanoparticle and prospects for the measurement of other materials.

This work was supported by the Laboratory for Physical Sciences.

Thermodynamic theory of crystal plasticity – formulation and application to fcc copper

Charles Lieou (Presenter), Los Alamos National Laboratory, Curt A Bronkhorst, University of Wisconsin-Madison — We present a thermodynamic description of crystal plasticity. Our formulation is based on the thermodynamic dislocation theory (TDT) of Langer et al., which asserts the fundamental importance of an effective temperature that describes the state of configurational disorder and therefore the dislocation density of the crystalline material. We extend the TDT description from isotropic plasticity to crystal plasticity with many slip systems. Finite-element simulations show favourable comparison with experiments on polycrystal fcc copper under uniaxial compression. The thermodynamic theory of crystal plasticity thus provides a thermodynamically consistent and physically rigorous description of dislocation motion in crystals. We also discuss new insights about the interaction of dislocations belonging to different slip systems.
8:48AM R70.00005: Ab initio studies of TiPd-M (M= Os, Ru, Co) high temperature shape memory alloys*
RAMOGHLO DIALE (Presenter), Materials Modelling Centre, Private Bad x1106, Polokwane, South Africa, University of Limpopo, ROSINAH MODIBA, Future Production: Manufacturing, PO Box 395, Pretoria, 0001, South Africa, CSIR, PHUTI NGOEPE, HASANI CHAUKE, Materials Modelling Centre, Private Bad x1106, Polokwane, South Africa, University of Limpopo — The TiPd alloy has a potential for high temperature shape memory applications due to its martensitic transformation capability from B2 to B19 at 823 K. Previous studies indicated that B2 TiPd is unstable displaying a negative C at room temperature. In order to improve its properties, the effects of partial substitution of Pd with either Os, Ru or Co were investigated using density functional theory. The calculations are carried out within PBE-GGA for the exchange correlation functional. It was found that the heats of formation decrease with an increase in Os and Ru concentration and increases with Co addition. The ductility of TiPd-M (M= Os, Ru and Co) is predicted using Pugh’s ratio, Poisson’s ratio and Cauchy pressure. It was found that the structures showed positive C above 18.75 at. % Os, 20 at. % Ru and 31 at. % Co, displaying condition of stability. The calculated moduli confirm that alloying with Os effectively increases hardness and ductility better compared to Ru and Co. Partial substitution of Pd with Os and Ru was found more effective as a strengthening elements and may enhance the martensitic transformation temperature of B2 TiPd alloy.

*CSIR, NRF and DSI SARChI for financial support

9:00AM R70.00006: First-Principles Study on the Role of Doped In in Fe–Pd–In Systems
YASUTOMI TATETSU (Presenter), University Center for Liberal Arts Education, Meio University, KENSHI MATSUMOTO, RYOTA SATO, TOSHIHARU TERANISHI, Institute for Chemical Research, Kyoto University — Electronic states, for example, atomic positions, orbital hybridization, etc. determine crystal structures and these physical properties. The most stable crystal structure of binary Fe–Pd systems is known as a \( L_1^2 \)-type crystal structure[1, 2]. However, according to our latest experimental studies, a new Mille-feuille-like Fe–Pd structure is synthesized by adding a small amount of In, implying that In is the key to stabilizing the new system.
We performed first-principles calculations for the In-doped FePd\(_3\) systems in order to understand the role of In in terms of its stability. There are two symmetrically different sites for Pd in the new system, which are labeled e and g, and In prefers the e site. This result is consistent with our recent experiments. From our analysis, we find that the distance between Fe, Pd, and In is the key factor in stabilizing the new system.
9:12AM R70.00007: Molecular Dynamics (MD) Potential Development for Carbides

TYLER MCGILVRY-JAMES (Presenter), MUZTOBA RABBANI, Department of Physics, Astronomy, and Materials Science, Missouri State University, NIRMAL BAISHNAB, Department of Physics and Astronomy, University of Missouri, PUJA ADHIKARI, SARO SAN, Department of Physics and Astronomy, University of Missouri-Kansas City, ANDREW IAN DUFF, Daresbury Laboratory, Science and Technology Facilities Council, WAI-YIM CHING, Department of Physics and Astronomy, University of Missouri-Kansas City, RIDWAN SAKIDJA, Department of Physics, Astronomy, and Materials Science, Missouri State University — We utilized the reference-free (RF) MEAMfit code to generate many-body potentials of Embedded Atom Method (EAM) and Modified Embedded Atom Method (MEAM) for a variety of MC (M = Transition Metals, C = Carbon) systems with an emphasis on the M23C6 and MC carbide phases. These phases are the key ingredients to strengthen the Ni-based Superalloys at the grain boundary. By sampling of the results of energy, stress and force data from the DFT calculations, a set of transferable potentials can be produced and be utilized to model the mechanical properties of these carbides.

*Funding from DOE (NETL) Grant No. FE0031554 (Crosscutting Research Program) is gratefully acknowledged.

9:24AM R70.00008: Developing the Modified Embedded Interatomic Potential for Atomistic Simulations in Ni-Ti-Hf System

MEGHNATH JAISHI (Presenter), GARRITT TUCKER, AARON P. STEBNER, Mechanical Engineering, Colorado School of Mines — The NiTiHf alloy, owing to its superior mechanical behavior over the parent alloy NiTi (nitinol) has received a considerable attention in recent years as a promising alternative for shape memory and super-elastic applications. The substantial mechanical strength, and wide variability in martensitic transformation temperature of NiTiHf shape memory alloy have enabled its applications in numerous sectors ranging from bio-medical to aviation industries. However, the lack of atomic level understanding during its micro-structural engineering is inhibiting its further applicabilities. To unlock the atomic level information for an efficient shape memory application requires an interatomic potential to perform the atomistic simulations with a high predictive accuracy. Herein, we discuss the development of an optimized interatomic potential for NiTiHf system within the framework of modified embedded atom method (MEAM).
9:36AM R70.00009: Accelerating the computational design of multi-principle element alloys*  DUANE D JOHNSON (Presenter), RAHUL SINGH, PRASHANT SINGH, AAYUSH SHARMA, Ames Lab, GANESH BALASUBRAMANIAN, Lehigh University, PA — We present a metaheuristic hybrid Cuckoo-Search (CS) algorithm that overcomes NP-hard global optimization and produces ultrafast solutions for large-dimensional combinatorial problems, using Levy flights (global) and Monte Carlo (local) searches, which avoids local-minima traps that stagnate solutions. The hybrid-CS removes a roadblock to computational materials design of arbitrary MPEAs by enabling \`on-the-fly\' construction of optimized Super-Cell Random Approximates (SCRAPS) with extraordinary reduction in solution times, scaling linear with cell size and exhibiting strong scaling for parallel solution. For example, a 4-element, 128-atom cell [10^{73}+ space] in 45s or 5-element, 500-atom cell [10^{415}+ space] in 270s. For a 4-component 128-atom model, we find a factor of 12,600+ reduction in parallel [400+ in serial] execution over current limited strategies. SCRAPS has specified point and pair probabilities with proper Gaussian distributions. We present several example applications using electronic-structure-based energetics and phonons.

*Supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Science & Engineering Division. Work was performed at Ames Laboratory, which is operated by Iowa State University for the U.S. DOE under contract #DE-AC02-07CH11358.

9:48AM R70.00010: Ab initio typical medium theory of substitutional disorder*  ANDREAS OESTLIN (Presenter), Augsburg University, YI ZHANG, avli Institute for Theoretical Sciences, Beijing 100190, China, HANNA TERLETSKA, Middle Tennessee State University, VOICU POPESCU, Sophie-Scholl-Gymnasium Oberhausen, 46145 Oberhausen, Germany, KRZYSZTOF BYCZUK, Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Poland, LEVENTE VITOS, Uppsala University, SE-75121 Uppsala, Sweden, MARK JARRELL, Louisiana State University, Baton Rouge, Louisiana 70803, DIETER VOLLHARDT, Augsburg University, FLORIAN BEIUUSEANU, Faculty of Science, University of Oradea, RO-410087 Oradea, Romania, LIVIU CHIONCEL, Augsburg University — By merging single-site typical medium theory with density functional theory we introduce a self-consistent framework for electronic structure calculations of materials with substitutional disorder which takes into account Anderson localization. The scheme and details of the implementation are presented and applied to the hypothetical alloy Li_{1-c}Be_{c}, and the results are compared with those obtained with the coherent potential approximation. Furthermore we demonstrate that Anderson localization suppresses long-range magnetic order for a very low concentration of (i) carbon impurities substituting oxygen in MgO_{1-c}C, and (ii) manganese impurities substituting magnesium in Mg_{1-c}Mn_{c}O for the low-spin magnetic configuration.

*U.S. Department of Energy, Award Number DE-SC0017861 DFG, (German Research Foundation) - Projectnumber 107745057 - TRR 80/F6
10:00AM R70.00011: Prediction of Stability, Short-range Order, and Phase Selection in Multi-Principal-Element-Alloys*  PRASHANT SINGH (Presenter), ANDREY V. SMIRNOV, Ames Lab, PRATIK K RAY, Indian Institute of Technology Ropar, India, MATTHEW J KRAMER, Ames Lab, SEZER PICAK, Texas A&M University, College Station, TX, YURIY I. CHUMLYAKOV, Tomask State University, RAYMUNDO ARROYAVE, Texas A&M University, College Station, TX, K.G. PRADEEP, Indian Institute of Technology, Madras, India, IBRAHIM KARAMAN, Texas A&M University, College Station, TX, DUANE D JOHNSON, Ames Lab — We present the capabilities of KKR-CPA-based stability and short-range order (SRO) prediction in multi-component solid-solution alloys for general lattices. The refractory-based Al$_x$TiZrHf and Cantor-type FeMnCoCr are chosen to showcase the powerful predictive capabilities and insights found from our electronic-structure-based thermodynamic linear-response method. For Al$_x$TiZrHf (x=1) we discovered a vacancy-mediated mechanism for phase selection driven by vacancy-atom SRO. Our X-ray diffraction data finds a variant of gamma-brass with 4 vacancies per cell (not 2, as in typical brasses), which was indicated by the calculated SRO. For fcc FeMnCoCr, we monitor energy, stacking fault energy, and SRO and find quantitative agreement with single-crystal data.

*Supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Science & Engineering Division. Work was performed at Ames Laboratory, which is operated by Iowa State University for the U.S. DOE under contract #DE-AC02-07CH11358. We also acknowledge the NSF grant no. 1729350 (DMREF).

10:12AM R70.00012: Synthesis of nanocrystalline Mg-based alloy powders by mechanical alloying and their microstructural characterization  CELAL KURSUN (Presenter), DAN J. THOMA, JOHN H. PEREPEZKO, Materials Science and Engineering, University of Wisconsin - Madison — Nanocrystalline Mg$_{65}$Ni$_{25}$Y$_{5}$M$_{5}$ (M= Si, B, Ag) alloys have been produced by mechanical alloying from mixtures of pure crystalline Mg, Ni, Y and M powders using a Spex Industries Mill Model 8000 in order to characterize the influence of Si, B and Ag on the microstructure of Mg-Ni-Y alloy system. Microstructural evolution, thermal behavior and morphological changes of the mechanically alloyed powders at different stages of milling have been investigated using a variety of analytical techniques including x-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectrometry (EDX), differential scanning calorimetry (DSC) and transmission electron microscopy (TEM). The present results revealed that the crystallite size of Mg$_{65}$Ni$_{25}$Y$_{5}$M$_{5}$ (M= Si, B, Ag) powders decreased with increasing milling time and it was determined in the range of 18–30 nm by TEM observation. After 65 h of milling, different intermetallic phases such as Mg$_{24}$Y$_{5}$, MgB$_{2}$, Mg$_{2}$Ni and Mg$_{2}$Ni$_{3}$Si were obtained. According to SEM images, particle size of the powders decreased during mechanical alloying and their shape and distribution became uniform. The compositional homogeneity of the Mg$_{65}$Ni$_{25}$Y$_{5}$M$_{5}$ (M= Si, B, Ag) alloys after mechanical alloying were confirmed by EDX analyses.
**10:24AM R70.00013: Ab initio investigation of Pb-based solder replacements**  
MICHAEL WOODCOX (Presenter), Physics, Binghamton University, JOSHUA YOUNG, Chemical and Materials Engineering, New Jersey Institute of Technology, MANUEL SMEU, Physics, Binghamton University — Alloys have been the focus of a large amount of research across different disciplines due to the ability to manipulate inherent properties of different materials. Due to the tunable nature of these materials, industrial needs can be more readily met with materials that are designed towards a specific purpose, as opposed to bulk materials that may not fit a unique need. One specific area that can be satisfied through the alloy process is the removal of industrial components that are harmful to humans, or their environment, with alloys that are equally effective. In this work, we have used density functional theory (DFT) and *Ab Initio* Molecular Dynamics (AIMD) to model materials at temperatures below and above their melting points. From these simulations, we are able to calculate the temperature dependence of the mechanical properties of materials which increases the quantitative understanding of the physical nature of ductility and how these properties can be captured on short time scales using first principles techniques.

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**10:36AM R70.00014: The Temperature Evolution of Dislocation Dynamics in Aluminum**

LEORA DRESSELHAUS-COOPER (Presenter), Lawrence Livermore Natl Lab, PHIL COOK, BOKU, CAN YILDIRIM, CEA Grenoble, HUGH SIMONS, DTU, CARSTEN DETLEFS, ESRF, HENNING FRIIS FRIIS POULSEN, DTU, JON HENRY EGGERT, Lawrence Livermore Natl Lab — A material’s response to its surroundings depends on both its native properties and the imperfections (defects) in its structure. While techniques exist to probe material defects, they are mainly limited to surface measurements or rastered scans that cannot measure the dynamics of irreversible processes. Dark-field X-ray microscopy can now directly image defects in single- and poly-crystals, resolving the lattice tilt and inclination with high sensitivity over long length-scales. I extend this novel technique to time-resolved studies that measure real-time movies to visualize how dislocations evolve at thermal equilibrium. These movies resolve the creep dynamics of dislocations in high-purity single-crystal aluminum, directly measuring their mobility and interactions by measuring the strain with $10^{-5}$ resolution over hundreds of micrometers. Our results directly measure the dislocation velocity as a function of temperature, covering the final 6% of temperatures for $T < T_{\text{melt}}$. These findings have important implications for dislocation models that have relied on multi-scale modeling and indirect measurements.

*This work was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.*

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**Thursday, March 5, 2020 11:15 AM - 1:51 PM**

**Session S01 DAMOP DQI: Hybrid/Macroscopic Quantum Systems, Optomechanics, and Interfacing AMO with Solid State/Nano Systems**

**II 103 - Manuel Endres, Caltech** - Tag(s): Focus
11:15AM S01.00001: Exploring synthetic quantum matter in superconducting circuits [Invited]
RUICHAO MA (Presenter), Purdue University — Superconducting circuits have emerged as a competitive platform for quantum computation, satisfying the challenges of controllability, long coherence and strong interactions. Here we apply this toolbox to the exploration of strongly correlated quantum materials made of microwave photons. I will present our recent results on a new approach for preparing photonic many-body phases, where engineered dissipation is used as a resource to protect the fragile quantum states against intrinsic losses [1]. We build a strongly interacting Bose-Hubbard lattice and realize a dissipatively stabilized Mott insulator of photons. The dynamics of thermalization towards the Mott phase is probed using lattice-site- and time-resolved microscopy. In a separate experiment, we create Chern insulator lattices for microwave photons and observe topologically protected edge states [2]. I will discuss future directions to stabilize strongly correlated photonic states, study many-body dynamics in driven-dissipative settings, and engineer topological lattices to explore strongly interacting topological phases and realize robust encoding and transport of quantum information.


11:51AM S01.00002: Listening to Bulk Crystalline Vibrations with Superconducting Qubits*
VIJAY JAIN (Presenter), TAEKWAN YOON, CHAN U LEI, YIWEN CHU, LUIGI FRUNZIO, PETER T RAKICH, ROBERT SCHOELKOPF, Yale University — Superconducting circuits are a versatile platform for quantum computing owing to their scalability and reconfigurability, integration with high quality microwave resonators, and demonstrated ease in interfacing with hybrid quantum platforms. Recent work has demonstrated strong coupling to long-lived phonons of bulk acoustic waves (BAWs) of pristine crystalline substrates [1]. Despite achieving single-phonon control, a superconducting qubit piezoelectrically coupled to BAWs had a significantly reduced lifetime (T₁ = 7 us) compared to a naked transmon qubit (T₁ = 40 us), suggesting that uncontrolled coupling to BAW modes may be complicit in the qubit’s decoherence.

Here, we use the lifetime of a superconducting qubit to measure the local density of acoustic states in sapphire as a proxy for electro-mechanical decoherence. Varying the crystalline geometry can be used to systematically modify the qubit’s lifetime in order to ascertain how the coupling geometry leads to a mechanical Purcell effect. Our work offers insights into the design of compact quantum memories based on BAW resonators.


*We acknowledge support from US Dept of Energy Grant Nr. DE-SC0019406 and the Max Planck Research Award from the Alexander von Humboldt Foundation.
12:03PM S01.00003: Strong coupling of two individually controlled atoms via a nanophotonic cavity*  
PALOMA L OCOLA (Presenter), POLNUP SAMUTPRAPHOOT, TAMARA DORDEVIC, Harvard University, HANNES BERNIEN, University of Chicago, CRYSTAL SENKO, University of Waterloo, VLADAN VULETIC, Massachusetts Institute of Technology, MIKHAIL LUKIN, Harvard University — We demonstrate photon-mediated interactions between two individually trapped atoms coupled to a nanophotonic cavity. Specifically, we observe collective enhancement when the atoms are resonant with the cavity, and level repulsion when the cavity is coupled to the atoms in the dispersive regime. Our approach makes use of individual control over the internal states of the atoms, their position with respect to the cavity mode, as well as the light shifts to tune atomic transitions individually, allowing us to directly observe the anti-crossing of the bright and dark two-atom states. These observations open the door for realizing quantum networks and studying quantum many-body physics based on atom arrays coupled to nanophotonic devices.

*This work was supported by the Center for Ultracold Atoms, the National Science Foundation, AFOSR MURI, Vannevar Bush Faculty Fellowship, and ARL CDQI.

12:15PM S01.00004: Generating multipartite entangled states with Cavity Rydberg Polaritons*  
HADISEH ALAEIAN (Presenter), TILMAN PFAU, University of Stuttgart — Polaritons are superpositions of matter and photon states, whose effective masses are from the photonic part and their interactions originate from their matter part. While the small mass of the photons allows for observing quantum effects at higher temperatures, even up to the room temperature, the interaction allows creating collective many-body effects. In this work, I introduce a new type of quasi-particles called cavity-Rydberg polariton, with large interaction inherited from their strongly-interacting Rydberg constituents. In particular, I will show how this dipole-dipole interaction can be utilized to induce large non-linearity between discrete modes of an optical cavity. A property that can be further utilized to generate bipartite and tripartite entangled photons.

*IQST Young Investigator Award and Baden-Württemberg Foundation
12:27PM S01.00005: Parity switching in a semiconductor-based transmon qubit*  DEIVIDAS SABONIS (Presenter), OSCAR ERLANDSSON, ANDERS KRINGHØJ, Univ of Copenhagen, BERNARD VAN HECK, THORVALD LARSEN, TORSTEN KARZIG, DMITRY I. PIKULIN, PETER KROGSTRUP, KARL PETERSSON, Microsoft, CHARLES MARCUS, Univ of Copenhagen — Unpaired quasiparticles can adversely affect the performance of superconducting devices, including qubits based on Majorana zero modes. We study charge parity switching in a superconductor-semiconductor nanowire-based transmon device that shows Little-Parks oscillations of its frequency as a function of magnetic field. In the recovery regime, where a single flux quantum threads the cross-section of the wire transport measurements recently revealed signatures compatible with Majorana zero modes [1].

We read out the charge parity by dispersive monitoring of a readout resonator to which the transmon qubit is coupled. At zero magnetic field, we measure parity switching times in the range of 10-100 ms. As the magnetic field is increased toward the first closing of the superconducting gap, the switching time is decreased and is consistent with the superconducting gap reduction. In the recovery regime where the gap is re-opened, the switching time is reduced below the sensitivity of our measurement, putting a bound on the minimum observable Majorana hybridization energy in a full-shell nanowire system.


*Research supported by Microsoft Station Q and Danish National Research Foundation.
Suppression of charge dispersion by resonant tunneling in a single-channel transmon qubit

ANDERS KRINGHØJ (Presenter), Microsoft Quantum Lab Copenhagen and Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark, BERNARD VAN HECK, Microsoft Quantum Lab Delft, Delft University of Technology, 2600 GA Delft, The Netherlands, THORVALD LARSEN, OSCAR ERLANDSSON, DEIVIDAS SABONIS, Microsoft Quantum Lab Copenhagen and Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark, PETER KROGSTRUP, Microsoft Quantum Materials Lab and Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Kanalvej 7, 2800 Kongens Lyngby, Denmark, LUCAS CASPARIS, KARL PETERSSON, CHARLES MARCUS, Microsoft Quantum Lab Copenhagen and Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark — Motivated by the importance of understanding the underlying charge physics in superconducting qubits, we investigate the charge dispersion of a gate-controlled nanowire-based transmon. When approaching the pinch-off regime of the nanowire junction, we observe resonant behavior of the plasma frequency, which we attribute to the formation of a quantum dot in the junction. By measuring the charge dispersion while crossing a resonance, we observe that it is suppressed far below the range expected for a conventional transmon at comparable values of the Josephson and charging energies. The enhanced suppression can be explained and quantitatively modeled by the presence, at resonance, of a single transport channel with near-unity transmission. Our results establish an experimental validation of the theory of Coulomb oscillations in Josephson junctions in a previously unexplored regime. In addition, these results show that charge dispersion can be suppressed without the necessity of large $E_J/E_C$ ratios, potentially allowing a very large qubit anharmonicity.

This work was supported by Microsoft and the Danish National Research Foundation.

Efficient microwave measurement of superconducting optomechanical circuits

GABRIEL PETERSON (Presenter), University of Colorado, Boulder, SHLOMI KOTLER, FLORENT LECOCQ, KATARINA CICAK, X. Y. JIN, RAYMOND W SIMMONDS, JOSE AUMENTADO, JOHN TEUFEL, National Institute of Standards and Technology — Optomechanical interactions between electromagnetic modes and mechanical resonators have proven to be a valuable testbed for measurement and control of linear quantum systems. In this context, the light is considered as a meter that probes and influences the quantum state of the mechanical object. Reaching quantum limits of measurement and control therefore requires both that the optomechanical coupling overwhelms any decoherence and that the light is measured with sufficiently high efficiency. In microwave optomechanical systems, the first requirement has been demonstrated, but the second remains an experimental challenge, with state-of-art continuous linear measurements of microwave fields struggling to exceed 50% efficiency. Here I report recent progress to increase microwave measurement efficiencies to enable new regimes of ponderomotive squeezing and displacement sensing beyond the standard quantum limit.
1:03PM S01.00008: A Scalable Nanophotonic Platform for Rare Earth Ions* SUBHOJIT DUTTA (Presenter), University of Maryland, College Park, ELIZABETH GOLDSCHMIDT, Physics, University of Illinois, SABYASACHI BARIK, UDAY SAHA, EDO WAKS, University of Maryland, College Park — Rare earth ion ensembles doped in single crystals are a promising platform with widespread applications in optical signal processing, lasing and quantum information processing. The ability to engineer nanoscale patterns surrounding these ions would enable strong light matters interaction and open possibilities for a new generation of photonic devices. We present a new nanophotonic platform with Thulium ions doped in single crystal Lithium niobate thin films on insulator, that supports scalable top down fabrication. The ions in the thin film retain bulk like optical properties. We show spectral hole burning in a nanophotonic waveguide with powers upto 2 orders of magnitude lower than previously reported bulk waveguides. Such a platform paves way for on chip lasers and efficient ensemble quantum memories. The high electro-optic coefficient of lithium niobate coupled with densely patterned electrodes promises large stark tuning which may be useful for ensemble quantum memory protocols like CRIB. Lastly strong light matter interaction can lead to Purcell enhancement and the ability to isolate single ions as a long lived qubit.

*National Science Foundation (Award No. EFMA1741651)

1:15PM S01.00009: Spin-photon interfaces based on tin-vacancy centers in diamond MATTHEW TRUSHEIM (Presenter), Harvard University, LORENZO DE SANTIS, KEVIN CHEN, Massachusetts Institute of Technology, CHRISTOPHER CICCARINO, Harvard University, DIRK R. ENGLUND, Massachusetts Institute of Technology, PRINEHA NARANG, Harvard University — Color centers in diamond are quantum systems that can combine long-lived spin degrees of freedom with coherent optical transitions for applications in quantum networks and information processing. The tin-vacancy (SnV) center in diamond in particular combines the characteristic inversion symmetry of the Group IV-vacancy complexes with a large spin-orbit splitting of its ground-state orbitals, enabling the demonstration of long spin coherence times at accessible temperatures. Several challenges remain in the application and understanding of these centers, including a complete theoretical description of the electronic structure, universal spin control, and the engineering of efficient light-matter interaction. Here we discuss theoretical and experimental work towards coherent spin-photon interfaces based on SnV centers at liquid-helium temperatures.
1:27PM S01.00010: Investigating Microwave Raman Transitions Beyond the Rotating Wave Approximation in the Electronic Ground State of the Nitrogen-Vacancy Center  FLORIAN BÖHM (Presenter), NIKO NIKOLAY, SASCHA NEINERT, BERND SONTHEIMER, OLIVER BENSON, Humboldt University of Berlin — Up to now, spin manipulation experiments with the NV center were mostly limited to applying subsequent monochromatic microwave pulses, manipulating only single electronic transitions at a time. In our work we explore the possibility of applying multitone microwave pulses, allowing a full simultaneous control of all three electronic ground states of the NV center. This here presented spin manipulation scheme opens up new measurement possibilities, which could be used to increase the NV center's magnetic field sensitivity.

We will present the implementation of a spin-forbidden coherent population swapping between the $m_s = -1$ and $m_s = +1$ states, without undergoing the spin allowed transition into the $m_s = 0$ state via microwave Raman transitions and compare our experimental results with theoretical calculations. These Raman transitions are operated in a regime exceeding the rotating wave approximation (RWA). This has hardly been investigated as the RWA is traditionally applied in the single atom community. Due to the short coherence times, a low detuning has to be chosen, which in turn causes fast Raman transitions and a breakdown of the RWA. An indication for this is an experimentally observed beating signal which we want to utilize for faster and more robust population swapping.

1:39PM S01.00011: Solid-state defect based quantum modules  MICHAEL HANKS (Presenter), National Institute of Informatics (NII), MICHAEL TRUPKE, Vienna Center for Quantum Science and Technology, Universität Wien, WILLIAM MUNRO, NTT Basic Research Laboratories & NTT Research Center for Theoretical Quantum Physics, NTT Corporation, KAE NEMOTO, National Institute of Informatics (NII) — The development of technology required for quantum modules is likely to form the basis of any large-scale quantum information processing device. The question of the appropriate physical implementation of such technology remains, however, unsettled. In this presentation, we compare and contrast a number of different solid-state defects – including the nitrogen-, silicon-, and germanium-vacancy centers in diamond, as well as a variety of defects in silicon carbide – according to their suitability for quantum modules based on strong coupling to optical cavities. The primary aspects forming the basis of this comparison are Hilbert space size and connectivity, optical transition contrast and branching ratios, decay lifetimes, and the capability for robust information storage across multiple failed probabilistic optical operations. Our results show several promising candidates.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S02 GSCCM: Dynamic Compression II: Experiments 105 - Camille Chauvin
11:15AM S02.00001: Complex loading experiments to study multiphase strength in Cerium
BRIAN JENSEN (Presenter), M9 Shock and Detonation Physics, Los Alamos National Laboratory —
Understanding the mechanical properties of materials at extreme conditions is relevant to a wide range of dynamic phenomena related to geophysics and planetary science, general solid and fluid flow behavior, and applications for ballistics and armor development, for example. Efforts in recent years have used multiple-shock and release loading to examine material strength in metals including single crystal and polycrystalline aluminum. Despite these efforts, data that describes strength effects following a shock-induced, solid-solid phase transition is lacking. In this work, complex loading experiments were analyzed to examine the strength of cerium shocked to stress states that span the low-pressure phase transition up toward the melt boundary. The experimental results and data analysis will be presented along with a discussion on their implications and future work.

EMMA MCBRIDE (Presenter), SLAC - Natl Accelerator Lab —
Although vital, the direct measurement of temperature at extreme conditions, in particular in the warm dense matter regime is challenging. We combine a cryogenic jet with a chirped short pulse laser to generated a laser-driven shock-wave with a setup for performing high-resolution inelastic X-ray scattering measurement at the Linac Coherent Light Source (LCLS) to directly measure the evolution of temperature of laser-compressed argon. We use the principle of detailed balance to determine temperature directly, from the bulk sample probed by the X-ray beam. In addition, we measure the sample density using X-ray diffraction, and estimate the sound speed at extreme conditions from a direct measurement of the dispersion curve. The techniques described are applicable across a wide range of fields of plasma and warm dense matter science.

11:39AM S02.00003: Toward predictive pulsed power loss estimates to ensure dynamic materials properties experiment success*
ANDREW PORWITZKY (Presenter), BRIAN HUTSEL, Sandia National Laboratories — Successful execution of dynamic materials properties experiments on large scale pulsed power machines can involve over-taxing the pulsed power driver. Under some circumstances, electrical loses can alter the isentropic compression path of the sample material at high pressure, resulting in shock formation or a failure to reach the desired peak pressure. Loss models based on space charge limited ion emission, enhanced by electron flow current, are beginning to demonstrate potential for predictive modeling of materials experiments. We present the state of this effort and some of the challenges inherent in the use of the ion loss model.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
**11:51AM S02.00004: Electrical Conductivity of Tin Under Shock Conditions**  
RYAN CRUM (Presenter), MINTA C AKIN, DAVID BRANTLEY, RICKY CHAU, Lawrence Livermore Natl Lab — Electrical conductivity of materials under extreme conditions may provide the necessary information to obtain bulk temperatures, the location of phase boundaries, and pertinent knowledge for ongoing electromagnetic responses for planetary interiors. We introduce a means to study the electrical conductivity of metals, in this study tin, with an easily accessed melt boundary between 45 and 70 GPa on the principal Hugoniot. A plate impact methodology is implemented to drive the tin sample to high pressure and temperature states while the electrical resistivity and conductivity of the sample are recorded. We observe a stark jump in the electrical resistivity and conductivity associated with the melt boundary, further constraining the tin melt boundary. Through the Wiedemann-Franz law, we will address implications of whether the law holds and what the predicted temperature and thermal conductivity are under shock conditions.

*Work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.

**12:03PM S02.00005: Shock Driven Dynamics on the Benchtop: Generation and Characterization with Imaging and Spectroscopy**  
DMITRO MARTYNOWYCH (Presenter), JET LEM, KEITH ADAM NELSON, Massachusetts Institute of Technology MIT — We have developed a benchtop platform to generate shockwaves in materials and monitor the ensuing material response and chemistry. A thin layer (20-100 µm) of material is pressed between two glass plates, confining it to a planar geometry. A nanosecond laser pulse is focused into a circular “ring” pattern of 180 µm radius, launching a shock wave that propagates within the plane of the sample and focuses toward the circle’s center. Using a high-speed multi-frame camera, we have been able to record up to sixteen images of a single shock event with time intervals as short as 5 ns. Employing a host of spectroscopic techniques, we can further interrogate the structural and chemical nature of the shocked sample. This single-shot method of imaging and characterizing shocked samples has allowed us to investigate a variety of chemical and physical phenomena including cavitation, structural phase transitions, and chemical reactivity/decomposition.
Determining an orientation relationship for the diffusionless hcp-bcc phase transition in Mg under dynamic loading

MATTHEW BEASON (Presenter), BRIAN JENSEN, Los Alamos National Laboratory — For years, crystallographers have sought to decompose phase transitions into a series of dilations, shears, or contractions based on fundamental symmetries between the parent and product phases. Burger’s mechanism describes the bcc-hcp phase transition through two steps: a strain in the [001]_{bcc} direction followed by an internal shear of the (110)_{bcc} planes along the [1-10]_{bcc} direction displacing every alternate plane and resulting in the hcp structure. While such mechanisms may describe certain transitions under static conditions and provide a framework for theoretical studies, it is not clear that such an orderly process is relevant for a shock driven transformation. This presentation reports on experiments performed at the Dynamic Compression Sector (DCS) on the hcp-bcc phase transition of Mg. By performing in situ X-ray diffraction (XRD) on shock loaded Mg we have captured the orientation of the bcc phase at the shock state, allowing an orientation relationship to be established with the initial hcp lattice. This represents an important first step in ongoing efforts to develop a transition mechanism for the hcp-bcc phase transition under dynamic loading.

*Funding was provided by the Los Alamos National Laboratories Science Campaign.

Cellular Structures Imaged in the Detonation Front of Pure Liquid Nitromethane

ERIN NISSEN (Presenter), MITHUN BHOWMICK, DANA D DLOTT, University of Illinois at Urbana-Champaign — We developed a tabletop compression microscope, which uses laser driven flyer plates to generate 4-ns duration planar shocks in tiny cuvettes filled with the high explosive nitromethane. When the flyer velocity is 4.0 km/s, a detonation forms at a pressure of 19 GPa and a velocity of 6.25 µm/ns. We implemented a high-speed high-resolution camera in combination with photon Doppler velocimetry to watch how the reaction zone develops on the nanoscale. We captured, for the first time in pure liquid nitromethane, micron-scale structures, known as cellular structures in the detonation front. These cells are caused by a superdetonation, a shock traveling in a precompressed medium, that forms behind the shock front after a short delay. The superdetonation will collide with the original shock front and reflect transverse waves into the reacting material behind it. These waves bounce between the backwards traveling shock from the superdetonation and the shock front creating a complex reactive flow with a convoluted shock front. Applying the size of the cells measured in the front to known theory allows us to measure the reaction zone length.

*We acknowledge support from the DOE NNSA SSGF under cooperative Agreement No. DE-NA002135 and Army Research Office under W911NF-19-2-0037.
12:39PM S02.00008: Molecular Influence in Microparticle Impact Response of Elastomers
DAVID VEYSSET (Presenter), YUCHEN SUN, YOU-CHI MASON WU, STEVEN E KOOI, TIMOTHY M. SWAGER, KEITH ADAM NELSON, Massachusetts Institute of Technology MIT, ALEX J. HSIEH, Army Research Laboratory — Segmented elastomers have gained attention for their performance against high-velocity impacts through tailored segmental dynamics. The influence of molecular moieties has also been reported to be important on the dynamic behavior of polymers. In this work, we present impact measurements of laser-launched supersonic micro-particle impacts on polyurea and polyurethane elastomers. In a laser-induced projectile impact test (LIPIT), we accelerate solid microparticles to supersonic velocities up to 1 km/s through a laser-ablation process. The impact events are observed in situ using an ultra-high-speed multi-frame camera that can record up to 16 images with time resolution of each frame as short as 5 ns. We study the high-strain rate deformation response of elastomers to unravel the relation between microstructure and high-rate properties. In particular, we are interested in the influence of the nature and the extent of hydrogen bonding and the role of intermolecular interaction in the dynamic response of these polymers. We demonstrate that LIPIT is capable of quantifying the variation in dynamic stiffening observed among these elastomers upon impact at strain rate $\sim 10^8 \text{ s}^{-1}$.

12:51PM S02.00009: Hot Spot and Reaction Temperature of Insensitive High Explosives using Time-Resolved Optical Pyrometry
MEYSAM AKHTAR (Presenter), DANA D DLOTT, University of Illinois at Urbana-Champaign — The capability of time-resolved optical pyrometry of our dynamic shock microscope system enables us to explore the evolution of the hot spot and combustion temperatures of shocked insensitive high explosives with nanosecond time resolution. Primarily, we analyze plastic-bonded explosive (PBX) formulations of triaminotrinitrobenzene (TATB), 1,1-diamino-2,2-dinitroethene (FOX-7), and 2,6-Diamino-3,5-Dinitropyrazine-1-Oxide (LLM-105). These explosives are particularly interesting because they are powerful but insensitive to accidental initiation. These three insensitive explosives have a yellow color, which causes a significant absorption in the blue region of the visible spectrum. This deviation from thermal radiation complicates the pyrometry experiment and should be accounted for in the determination of the temperature.

The experiments used short-duration (4 ns) shocks using laser-launched flyer plates with velocities of 1-4.5 km/s. The dynamic shock microscope system has, in addition to the optical pyrometer, a high-speed Photon Doppler Velocimeter (PDV), high-speed imaging cameras. We have developed methods to mass-produce tiny well-characterized PBX charges in arrays with hundreds of charges. The tiny charges were 80% explosive and 20% binder.
1:03PM S02.00010: High-speed X-ray Phase Contrast Imaging Analysis of Microscale Shock Response of a Mock Additively Manufactured Energetic Material*  KARLA WAGNER (Presenter), ANDREW BODDORFF, AMIRREZA KEYHANI, GREGORY B. KENNEDY, Georgia Inst of Tech, DIDIER MONTAIGNE, Eglin Air Force Research Lab, MIN ZHOU, NARESH N THADHANI, Georgia Inst of Tech — X-ray phase contrast imaging (XPCI) is used to probe the interior of a mock additively manufactured energetic material (AMEM) under dynamic loading and determine the equation of state (EOS). AMEMs have a range of structural characteristics with a hierarchy of length scales and process-inherent heterogeneities. Many of these features are difficult to precisely control or avoid and it is important to understand how they affect the dynamic response of the AMEM. To this effect, XPCI is a technique that grants insight into micro- and meso-scale processes during a shock event. We use XPCI results to analyze the shock response of a mock AMEM loaded in different directions at several impact conditions. By tracking displacement of the shock front and features behind it, we can determine shock velocity and particle velocity. PDV was also used to measure the free surface velocity of the specimens and from that the particle velocities, which correlate well with those obtained from XPCI. The shock and particle velocity EOS is found to approximately follow \( U_s = 1.63U_p + 2619 \) with \( R^2 = 0.8 \). The experiments presented were performed at the DCS in the APS at Argonne National Lab, in collaboration with Brian Jensen at Los Alamos National Lab.

*This project is funded by DTRA grant HDTRA-18-1-004.

1:15PM S02.00011: Quantitative Assessment of the Interior Deformation of an Additively Manufactured Energetic Material Simulant under Shock Loading*  AMIRREZA KEYHANI, KARLA WAGNER, ANDREW BODDORFF, NARESH N THADHANI (Presenter), MIN ZHOU, Georgia Inst of Tech — The performance of energetic materials subjected to dynamic loading depends on the morphology of their microstructures. The geometric flexibility and versatility offered by additive manufacturing open new pathways to control the performance of these materials and functionally tailor them for given applications. Additively manufactured energetic materials (AMEM) have a wide range of microstructures with a hierarchy of length scales and heterogeneities which are difficult to control or avoid. To understand how they affect the response of such materials under shock loading, X-ray phase contrast imaging (XPCI) is used to probe the interior and quantify the deformation fields in the impacted samples. Two to four XPCI images were captured revealing the shock front and deformation. DIC analysis was then used to provide the first-ever assessment of the average strain fields inside the material under shock loading. The results show that the average axial strain in the samples depends on the intensity of shock loading and reaches as high as \( \sim 0.23 \) for impact velocities up to 1.5 m/k. The experiments presented were performed at the DCS in the APS at Argonne National Lab, in collaboration with Brian Jensen at Los Alamos National Laboratory.

*This project is funded by DTRA grant HDTRA-18-1-004.
1:27PM S02.00012: Inferring 3D Behavior of Dynamically Compressed Granular Materials from X-ray Tomography and Dynamic Radiography Measurements* ADYOTA GUPTA, KALIAT T RAMESH, RYAN HURLEY (Presenter), Johns Hopkins University — Dynamically compressed granular materials have primarily been studied using macroscopic measurements (e.g., VISAR, PDV). However, simulations and x-ray imaging measurements have revealed the rich, heterogeneous behavior occurring at the microscale during dynamic compression of granular materials: force chains, non-planar shock fronts, porosity-dependent shock velocities.

I will present the results of recent shock compression experiments performed on granular materials composed of spherical and angular particles at the Dynamic Compression Sector (DCS) of the Advanced Photon Source (APS). We integrate: (1) sample characterization with x-ray computed tomography (XRCT), (2) dynamic x-ray phase contrast imaging (XPCI) performed in situ, (3) an x-ray phase contrast or absorption image generation algorithm, and (4) an optimization algorithm to combining XRCT and XPCI to infer the time-evolution 3D particle positions. We are using this approach to understand the energy budget local heterogeneity, shock-front planarity, and porosity and inter-particle contact-network dependence of shock events.

*We acknowledge support from the Johns Hopkins University's Whiting School of Engineering and the Army Research Laboratory Cooperative Agreement Number 911NF-12-2-0022.

1:39PM S02.00013: Deviation from classical laws in shock-driven gas mixtures at moderate Mach numbers.* PETER VOROBIEFF (Presenter), HUMBERTO SILVA, CALEB WHITE, PATRICK J WAYNE, University of New Mexico — We conducted a series of experiments where planar shocks propagated through mixtures of helium and sulfur hexafluoride. Even at modest Mach numbers, the bulk temperatures and pressures measured in the shocked mixture deviated significantly from the predictions of both Dalton's and Amagat’s laws. As early as in the 1960s, it was already known that the behavior of gas mixtures in the immediate vicinity of a shock front was highly non-classical, however, our measurements show that the observed non-classical behaviors may persist far beyond the temporal and spatial scales associated with the shock passage. Simple molecular physics considerations can help explain some of the observed discrepancy. Numerical simulation of the experiments helps elucidate the observed disagreement between observations and models.

*This work was funded by NNSA grant DE-NA-0002913. We also acknowledge support from Sandia National Laboratories.
Laser-driven shock compression is a common method to study the equations of states (EOS) of materials under extreme conditions. The shock etalon method is an effective method to extract the shocked dynamic parameters of transparent materials. However, the sample surface reflection should be eliminated when using this method, which results in more time and efforts on the sample preparation. Here, we proposed a modified shock etalon method to measure the shocked dynamic parameters of transparent materials. The proposed method utilizes the \( p \)-polarized chirped probe pulse under the Brewster incident angle to eliminate the sample surface reflection, thus no extra efforts on the sample preparation are needed and can adapt the simplest solid transparent thin film samples. Simulation results show that the proposed method is feasible, accurate and robust on the shocked dynamics metrology for solid transparent materials. At last, the shock compression experiment with the proposed method is carried out on a polycarbonate thin film and the shocked dynamic parameters are obtained successfully, such as the shock velocity, the particle velocity and the shocked refractive index.


Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S07 DQI: Quantum Computing with Defects 102 - Viatcheslav Dobrovitski, Delft University of Technology
Towards fault-tolerant quantum error correction with spins in diamond

MOHAMED ABOBEIH (Presenter), JOE RANDALL, QuTech and Kavli Institute of Nanoscience Delft, Delft University of Technology, YANG WANG, QuTech, Delft University of Technology, SJOERD LOENEN, CONOR BRADLEY, QuTech and Kavli Institute of Nanoscience Delft, Delft University of Technology, BARBARA MARIA TERHAL, QuTech, Delft University of Technology, TIM HUGO TAMINIAU, QuTech and Kavli Institute of Nanoscience Delft, Delft University of Technology — Quantum error correction (QEC) is essential for reliable large-scale quantum information processing. Pioneering experiments have demonstrated QEC codes that could only correct specific types of errors using various physical platforms [1,2]. However, an experimental demonstration of a fault-tolerant QEC code that can correct any type of single-qubit error remains an open challenge. Here, I will present our progress towards the implementation of a fault-tolerant QEC code using a solid-state spin register in diamond. Recently, we have demonstrated that such a register can hold up to 10 qubits with high-fidelity universal control, coherence times up to one minute, and genuine multipartite entanglement [3]. Building upon these promising results, I will show how we can use non-destructive repeated parity measurements to encode a logical state in multiple C13 nuclear-spin qubits in diamond. These parity measurements might be further used to detect and correct arbitrary single-qubit errors on the logically encoded state, and are therefore an important step towards fault-tolerant quantum information processing.


Hardware-Efficient Quantum Error Correction with NV Center

MO CHEN (Presenter), DAVID LAYDEN, PAOLA CAPPELLARO, Massachusetts Institute of Technology MIT — The near-term intermediate-scale quantum (NISQ) era dawns with the demonstration of `quantum supremacy'. In the NISQ era, it is under debate if quantum error correction (QEC) is required. Although QEC is essential towards scalable universal quantum computation, it imposes a prohibitively high overhead for NISQ devices. To reduce the overhead, a hardware-efficient QEC approach has recently been employed and enjoyed experimental success [1]. Applying the same philosophy to our system—a quantum register consisting of one NV electronic spin and neighboring nuclear spins, we have carefully characterized the system and recently identified its dominant decoherence source [2]. Moving forward, we developed a hardware-efficient QEC code for such noise, which requires exponentially less overhead [3], and we are progressing in experiments towards one logical qubit consisting of two physical qubits.

Detection and control of large systems of nuclear-spin qubits in diamond

JOE RANDALL (Presenter), MOHAMED ABOBEIH, CONOR BRADLEY, FLORIS VAN DER GRONDEN, MAARTEN J DEGEN, HANS BARTLING, TIM HUGO TAMINIAU, Delft University of Technology — Nuclear spins in diamond are promising for their use as qubits in quantum computers and quantum networks, and for simulating many-body physics phenomena. Recently, we demonstrated the 3D imaging of a system of 27-nuclear-spin qubits using a nitrogen vacancy (NV) center in diamond [1], and a universally connected 10-qubit register formed of 9 nuclear spins combined with the NV center electron spin [2].

Building on these recent results, I will present new methods that allow us to extend control over more nuclear spin qubits. By combining precise knowledge of the nuclear spin environment with dynamic nuclear polarization techniques and selective readout protocols, we can prepare and measure individual nuclear spin qubits within a large interacting cluster. As well as extending the number of qubits available for quantum information applications, these techniques open the door to the quantum simulation of complex many-body physics phenomena using nuclear spins in diamond.


Hidden Silicon-Vacancy Centers in Diamond

CHRISTOPHER SMALLWOOD (Presenter), Physics and Astronomy, San Jose State University, RONALD ULBRICHT, Max Planck Institute for Polymer Research, MATTHEW W DAY, Physics, University of Michigan, TIM SCHRODER, Engineering and Computer Science, Massachusetts Institute of Technology, KELSEY M BATES, Physics, University of Michigan, TRAVIS AUTRY, JILA, University of Colorado and NIST, GEOFFREY DIEDERICH, Physics and Astronomy, University of Denver, EDWARD S BIELEJEC, Sandia National Laboratories, MARK SIEMENS, Physics and Astronomy, University of Denver, STEVEN THOMAS CUNDIFF, Physics, University of Michigan — Color centers in diamond—in particular, negatively charged silicon-vacancy (SiV\textsuperscript{−}) centers—have generated excitement recently as potential hardware elements in quantum networks and devices. The attention is due in part to the protective influence of diamond’s wide bandgap and weak magnetic susceptibility, and in part to the technology available for manipulating and detecting light at these photon energies. In spite of this, open questions remain concerning the optical properties of SiV\textsuperscript{−} centers and related defects, and there exist significant opportunities for elucidating these properties using nonlinear optical spectroscopy. Here we report measurements on a high-density sample of negatively charged SiV\textsuperscript{−} centers in diamond through the use of collinear optical multidimensional coherent spectroscopy (MDCS). Using the technique, we have uncovered a hidden population of centers that not typically observed in photoluminescence, and which exhibit a high degree of spectral inhomogeneity and longer-than-expected single-particle electronic $T_2$ dephasing times. The phenomenon is likely caused by strain, indicating opportunities for controllably mediating electronic coherence in color-center-based quantum devices.
Second-order Nonlinear Frequency Conversion and Integrated Color Centers in Silicon Carbide Nanophotonics

MELISSA GUIDRY (Presenter), DANIIL LUKIN, CONSTANTIN DORY, KIYOUL YANG, Stanford Univ, PRAFUL VASIREDDY, MAMDOUH NASR, EMILIO NANNI, SLAC National Accelerator Laboratory, Stanford University, JELENA VUCKOVIC, Stanford Univ — 4H-Silicon carbide photonics offer the unique prospect of monolithic generation and frequency conversion of quantum light on-chip, as the material hosts color centers with favorable spin coherence properties and has a strong second-order optical nonlinearity. We integrate single color centers into thin-film nanophotonic devices and demonstrate efficient second-harmonic generation using a doubly resonant microring resonator scheme, which may be modified for quantum frequency conversion to the telecommunications band. We introduce color centers into thin films via electron irradiation and study the optical stability of single defects.

National Science Foundation under grant number NSF/EFRI-1741660

Controlling the Silicon Vacancy in Silicon Carbide via Electric and Magnetic Fields

DANIIL LUKIN (Presenter), MELISSA GUIDRY, SHUO SUN, CONSTANTIN DORY, JELENA VUCKOVIC, Stanford Univ — The Silicon Vacancy in Silicon Carbide is an optically-active, spin-3/2 defect with a long spin coherence and potential for integration into large-scale nanophotonic circuits due to its narrow, stable optical transitions and small inhomogenous broadening. We demonstrate the optical transitions of the Silicon Vacancy are widely tunable via electric fields, which may enable multi-emitter scalability. We perform magnetic-field spectroscopy on single defects, and discuss the cavity-assisted spin-initialization protocols enabled by its fine structure.

U.S. Department of Energy, Office of Science, under Award DE-SC0019174

Computational identification of defect qubits in transition metal dichalcogenide WSe₂

JENG-YUAN TSAI (Presenter), JINBO PAN, QIMIN YAN, Physics, Temple University — Nitrogen-vacancy (NV) center in diamond serves as a leading solid-state qubit system due to its fidelity of manipulation at room temperature, while the search for novel solid-state systems with NV-like defects is highly desirable for the future development of solid-state quantum technologies. Two-dimensional solid-state systems are superior platforms to implement controlled manipulation of qubits. Our computational studies focus on point defects in WSe₂ as one of the well-known compounds in the family of transition metal dichalcogenides (TMDs). First-principle calculations based on density functional theory are adopted to study the formation energetics and electronic properties of point defects including intrinsic defects such as V₆ and Se antisite (W₆Se), and extrinsic defects such as V₆-N₆Se, V₆-P₆Se, and V₆-As₆Se. Our calculations show that both intrinsic and extrinsic defects can exhibit high magnetic moments and triplet ground states, which offer a set of defect candidates as qubits in this 2D TMD system. In addition, optical transition paths between ground and excited states will be discussed, which provide potential optical signatures for experimental verification.
12:39PM S07.00008: Probing the Coherent Spin Dynamics of Divacancies in Silicon Carbide with Spin Correlated Low-Field Magnetoresistance*  

STEPHEN MCMILLAN (Presenter), MICHAEL FLATTÉ, Univ of Iowa — Silicon carbide has attracted attention in the quantum information community due to remarkably long room temperature spin coherence times [1] and the potential for integration with the photonics and communications sectors due to divacancy energies in the near-infrared regime [2]. Isolated neutral divacancies are realizable and addressable via optically detected magnetic resonance [3]. The long coherence times of these individual deep centers suggest that they are ideal candidates for single spin sensing and quantum memory applications. We describe an approach we predict will allow exploration of the coherent spin dynamics of these divacancies through low-field magnetoresistance by addressing an individual divacancy with a spin-polarized scanning tunneling microscope (SP-STM) [4]. Measurement of the spin coherence time should be feasible and signatures of the local hyperfine interactions and single-spin exchange interactions should be resolvable.


*We acknowledge support from DOE BES through Grant No. DE-SC0016379.

12:51PM S07.00009: Site-controlled generation of tin-vacancy centers in diamond via shallow ion implantation and subsequent diamond growth*  

ALISON E RUGAR (Presenter), HAIYU LU, CONSTANTIN DORY, SHUO SUN, PATRICK J MCQUADE, ZHIXUN SHEN, NICHOLAS A MELOSH, JELENA VUCKOVIC, Stanford University — Color centers in diamond have garnered much interest in recent years as potential solid-state spin qubits. Paramount to implementing these color centers in scalable photonic systems is the development of techniques to generate high-quality, site-controlled emitters. This challenge is amplified for color centers with larger group-IV impurity atoms, which have emerged as otherwise promising emitters due to predictions of long spin coherence times without a dilution refrigerator. In the case of the tin-vacancy (SnV-) center, conventional site-controlled color center generation methods either damage the diamond surface or yield bulk spectra with unexplained features. In this talk we present a novel method to generate site-controlled SnV- centers with clean, consistent bulk spectra. We shallowly implant Sn ions and subsequently grow a layer of diamond via chemical vapor deposition. This method is compatible with nanophotonic device fabrication and can be extended to other color centers.

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SLAC LDRD
1:03PM S07.00010: Integrated Photonic Circuit for Generation and Isolation of Single Photons from Quantum Dot Ensembles  COREY MCDONALD (Presenter), TRAVIS AUTRY, RICHARD MIRIN, KEVIN SILVERMAN, National Institute of Standards and Technology Boulder — Practical quantum photonic technology must be scalable, highly isolated from noise, low loss, and have high stability of optical elements. These needs have motivated the development of photonic integrated circuits (PICs) for quantum optical devices. While significant progress has been made in silicon PICs, generating single photons depends on heralded, probabilistic processes such as spontaneous down-conversion. III-V quantum dots (QDs) have demonstrated deterministic, high-purity, single-photon and entangled-pair emission, including electrically-pumped QDs, providing a path towards source integration. We have previously demonstrated tungsten silicide waveguide-integrated superconducting single-photon detectors with low dark counts (~1 count per 1000 s) on a III-V PIC with waveguide-coupled LEDs. These detectors may allow in-situ measurement of on-chip single-photon sources. We will demonstrate on-chip generation of single photons from a QD ensemble, using ring resonators to isolate the emission of single dots. These circuits may be tuned thermally, and cascaded ring resonators may have sufficiently high Q-factors to isolate single transitions. On-chip detectors may be used to quantify single-photon purity using an integrated Hanbury-Brown and Twiss interferometer.

1:15PM S07.00011: Ab-initio and crystal-field calculations of defect properties of Er$^{3+}$ in yttria*  CUNEYT SAHIN (Presenter), University of Iowa, TIAN ZHONG, University of Chicago, MICHAEL FLATTÉ, University of Iowa — Wide band-gap oxides with rare-earth impurities exhibit narrow transitions with long coherence times and high quantum efficiency due to partially filled f orbitals. This allows the fabrication and usage of these materials in highly efficient optical amplifiers, high power lasers, data, and quantum information processing. We study electronic, structural, and spin properties of trivalent erbium impurities in yttria. First, we perform ab-initio calculations of the structural properties using the generalized gradient approximation and the pseudopotential method. We also calculate the electronic band structure and the density of states of the bulk and doped yttria. Then we proceed to compute the formation energies of erbium impurities. We also compute level splittings and g-tensors using a crystal field Hamiltonian. We show that the g-tensor is highly anisotropic, with a large component in one direction. The presence of an abundant isotope with a non-zero nuclear spin and anisotropic g-tensor suggest that an experimental control of the spin dynamics of this system is possible through the Zeeman and hyperfine interaction.

*Center for Emergent Materials, an NSF MRSEC under Award No. DMR-1420451, an NSF DMREF project under Award No. DMR-1921877, and an NSF EAGER Award No. 1843044
Quantum networks will require scalable quantum information processing architectures for fast data rates and reliable communication. Recently, the first memory-enhanced quantum repeater that beats direct photon transmission between two communication nodes was realized[1]. However, achieving the range and speed demanded by proposed quantum applications on the quantum internet requires quantum repeater nodes with many multiplexed memory qubits[2]. In particular, it is necessary to optically excite and measure multiple quantum memories fast and efficiently. In this talk, we will discuss recent experimental progress on multiplexed repeaters based on color centers in diamond, with a particular focus on the efficient fluorescence collection towards high-speed entanglement distribution.


*M. S. acknowledges support from MIT EECS Alan L. McWhorter fellowship. This work was supported by the National Science Foundation grant EFMA-1641064 and MIT Lincoln Laboratory.

1:39PM S07.00013: Atomic-scale control of tunneling in few-donor quantum dots  XIQIAO WANG (Presenter), University of Maryland, College Park, RANJIT KASHID, JONATHAN WYRICK, PRADEEP NAMBOODIRI, ALBERT RIGOSI, National Institute of Standards and Technology, FAN FEI, University of Maryland, College Park, RICHARD SILVER, National Institute of Standards and Technology — Donor-based quantum devices in silicon are a promising candidate for spin-based solid-state quantum computing and analog quantum simulation. Carefully designing the tunneling strength in tunnel-coupled quantum dots is critical to high fidelity performance of spin initialization, readout, spin-exchange operations. This presentation covers our results in atomic-scale control and characterization of tunneling in STM-patterned devices in the few-donor quantum dots regime. We present resonant tunneling spectroscopy analysis of the tunnel junctions in few-donor single-electron transistors and double-dot devices where the tunnel gaps are defined at the atomic-scale. We characterize the tunneling rates between few-donor quantum dots and atomically aligned single electron charge sensors and report their impact on spin-selective tunneling for spin initialization and readout in few-donor quantum dots.
1:51PM S07.00014: Seeking superconductivity with new, two-dimensional dopants super-saturated in silicon  KE TANG (Presenter), HYUN SOO KIM, ARUNA N RAMANAYAKA, National Institute of Standards and Technology, MICHAEL E HOENK, SHOULEH NIKZAD, APRIL JEWELL, Jet Propulsion Laboratory, JOSHUA POMEROY, National Institute of Standards and Technology — Realizing superconducting Josephson junctions within group-IV semiconductors would herald a new era of solid-state quantum computing. For some acceptors, super-saturated doping has been demonstrated to superconduct, e.g. boron-doped silicon having a \(T_c\) of 0.6 K [1]. Here we explore the possibility of superconductivity in similar material systems using both n-type (antimony) and p-type (aluminum) delta-doped layers. Low-temperature molecular beam epitaxy (MBE) has been used to embed atomically thin (2D) layers of antimony and aluminum atoms with dopant densities on the order of \((10^{13} - 10^{14})\text{ cm}^{-2}\). Mesa-etched Hall bar devices are fabricated on these delta layers and magnetotransport measurements at 4 K will be presented to study the material properties, such as carrier concentration and mobility. Temperature dependent measurements below 500 mK will be carried out in a dry dilution refrigerator to test for superconductivity. Comparisons between different dopant systems will also be presented.


2:03PM S07.00015: EPR spectroscopy of Er:CaWO\(_4\) at millikelvin temperatures*  MILOS RANCIC (Presenter), MARIANNE LE DANTEC, PATRICE BERTET, DENIS VION, CEA-Saclay, THIERRY CHANELIÈRE, Néel Institute, Grenoble Alpes University, PHILIPPE GOLDNER, Chimie ParisTech, SYLVAIN BERTAINA, PHANO, Institut Matériaux Microélectronique Nanosciences de Provence — Rare-earth-ions are interesting physical systems because they have long lived states and record coherence times, due the screening of the 4f valence shell by the 5s and 5p filled shells. Rare-earths with an odd number of electrons are also paramagnetic, with an electron-spin transition at GHz frequencies in magnetic fields less than 1 Tesla. For such transitions, coherence times around 50-100 us have been measured at temperatures as low as 1.4K [1]. Here we present results from our recent Electron-Paramagnetic-Resonance (EPR) studies of 0.005% Er:CaWO\(_4\). These measurements were recorded in a novel regime for this material: sub-Kelvin temperature down to 10mK, using a superconducting micro-resonator fabricated directly on the material surface and using a superconducting parametric amplifier for the microwave signals [2], [3]. We observe the longest recorded Hahn-echo decay for an electronic spin transition in an Erbium doped material, up to 1 ms.


*The authors acknowledge EU Grant No. 792727 (Project SMERC) and the French ANR through the Chaire Industrielle NASNIQ

Thursday, March 5, 2020 11:15 AM - 2:15 PM
11:15AM S08.00001: Asymmetric Sensing Dot for Scaleable Baseband Readout of Spin Qubits  
EUGEN KAMMERLOHER (Presenter), MATTHIAS KÜNNE, INGA SEIDLER, JARA-Institute for Quantum Information, RWTH Aachen University, D-52074 Aachen, Germany, ARNE LUDWIG, ANDREAS WIECK, Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44801 Bochum, Germany, LARS SCHREIBER, HENDRIK BLUHM, JARA-Institute for Quantum Information, RWTH Aachen University, D-52074 Aachen, Germany — High fidelity scalable readout is one of the key requirements for quantum computers with more than just a few qubits. Charge sensing dots are in this regard the most sensitive sensors for spin qubit readout. The most widespread readout technique is based on RF reflectometry, satisfying the requirement of high fidelity, but requires bulky, power-hungry components and is not well scalable. A more scalable alternative is to use transistors in close proximity to the qubit [1,2].

For best performance a high output swing of the sensor is desirable. We present experimental results in GaAs of an asymmetric sensing dot (ASD), improving the sensor response by a factor of 15 compared to conventional charge sensing dots. We perform charge sensing using a current biased ASD and observe a 2.36 mV swing in response to a (1,1)→(2,0) transition in a nearby double dot.

The improved voltage swing is due to a device design with a strongly decoupled drain reservoir from the sensor dot, mitigating negative feedback effects.

[1] M. J. Curry et al., APL 2015

11:27AM S08.00002: A Reservoir Computing Approach to Quantum State Measurement*  
GERASIMOS ANGELATOS (Presenter), HAKAN TURECI, SAEED KHAN, Princeton University — Quantum state measurement is an essential step in the probe or operation of any quantum system, and its optimization has accordingly been the focus of considerable ongoing research. Increases in the speed and fidelity of continuous measurements directly contribute to quantum information processing applications and the fundamental study of quantum systems. In this work, we propose a hardware-based reservoir computing system for quantum state measurement and discuss its performance when compared to conventional approaches. We theoretically analyze the readout of a superconducting circuit via direct coupling to a minimal reservoir computer and demonstrate how such a system provides a low latency approach to state measurement.

*We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC) and the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Award No. DE-SC0016011.
11:39 AM S08.00003: Neural Network assisted Superconducting Qubit Readout*  

BENJAMIN LIENHARD (Presenter), ANTTI VEPSALAINEN, Massachusetts Institute of Technology MIT, LUKE GOVIA, Raytheon BBN Technologies, YANJIE QIU, Massachusetts Institute of Technology MIT, DIEGO RISTÈ, MATTHEW WARE, Raytheon BBN Technologies, DAVID K KIM, MIT Lincoln Laboratory, RONI WINIK, Massachusetts Institute of Technology MIT, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, JONILYN YODER, MIT Lincoln Laboratory, GUILHEM RIBEILL, THOMAS A OHKI, HARI K KROVI, Raytheon BBN Technologies, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, Massachusetts Institute of Technology MIT, WILLIAM OLIVER, MIT Lincoln Laboratory, Massachusetts Institute of Technology — A significant error source in contemporary quantum processors is qubit-state readout. For a single qubit connected to a unique readout line, a linear matched filter is sufficient for high-fidelity readout. However, it is more resource efficient to frequency-multiplex multiple qubits on the same readout line. In this case, the single-qubit matched filters are no longer optimal. Rather, readout discrimination becomes a computationally intensive, multi-state classification problem. Here, we present a new approach to the readout problem based on neural networks. We discuss different types of neural network architectures and their readout discrimination performance compared to current readout methods when applied to experimental single and multi-qubit readout data.

*This research was funded in part by the ARO grant No. W911NF-18-1-0411; and by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

11:51 AM S08.00004: Single-Qubit Optimal Quantum Readout via Neural Networks  

WEI TANG (Presenter), Computer Science, Princeton University, ZHAOQI LENG, Physics, Princeton University, ANDREW HOUCK, Electrical Engineering, Princeton University, MARGARET MARTONOSI, Computer Science, Princeton University — High fidelity readout is an essential part of quantum computing. Conventional approaches for superconducting circuit readout rely on linear models. We explore the benefits of employing alternative classification schemes based on neural networks. We discuss different types of neural network architectures and their readout discrimination performance compared to current readout methods when applied to experimental single and multi-qubit readout data.

12:03 PM S08.00005: Dispersive readout for Majorana qubits  

THOMAS SMITH (Presenter), STEPHEN D BARTLETT, ARNE GRIMSMO, Univ of Sydney — We analyze the use of dispersive readout for qubits encoded in topological superconducting nanowires. Two models are considered: the Majorana transmon qubit and the Majorana box qubit. We model the interaction with each qubit and a readout resonator, and calculate the size of the qubit state-dependent dispersive shift of the resonator. We show that dispersive readout of Majorana qubits is protected against measurement-induced bit flips. Furthermore, we find that Majorana transmon qubits are well-suited to dispersive readout, producing dispersive shifts comparable to that of conventional superconducting transmons. Majorana box qubits produce more modest, but still potentially viable, dispersive shifts.
12:15PM S08.00006: Tracking non-Markovian quantum dynamics of a superconducting qubit with a recurrent neural network filter*  NOAH STEVENSON (Presenter), GERWIN KOOLSTRA, BRADLEY MITCHELL, AKEL HASHIM, Univ of California - Berkeley, SHIVA BARZILI, JUSTIN DRESSEL, Chapman Univ, IRFAN SIDDIQI, Univ of California - Berkeley — Precise quantum control of superconducting qubits necessitates determining the time-dependent Hamiltonian of control pulses with high fidelity. While continuous state tracking has proved effective for determining qubit time-evolution in regimes with Markovian dynamics, fast control pulses used for native quantum gates and entanglement generation can result in non-Markovian transient dynamics. We use quantum state tracking with continuous weak measurement to experimentally investigate non-Markovianity in a transmon superconducting qubit coupled to a readout resonator. By weakly measuring the qubit state during a Rabi oscillation sequence on a timescale comparable to the cavity decay rate, we isolate dynamics that are difficult to describe with single-qubit trajectory theory. We train a recurrent neural network to reconstruct the quantum trajectories, motivated by such a network's demonstrated ability to learn long-time correlations in sequential data, and estimate parameters of the stochastic master equation.

*This research was supported by the LPS HiPS program under ARO grant W911NF1810178.

12:27PM S08.00007: High-fidelity quantum state estimation via autoencoder tomography*  SHIVA LOTFALLAHZADEH BARZILI (Presenter), Chapman Univ, NOAH STEVENSON, BRADLEY MITCHELL, Univ of California – Berkeley, RAZIEH MOHSENINIA, Univ of Southern California, IRFAN SIDDIQI, Univ of California – Berkeley, JUSTIN DRESSEL, Chapman Univ —

We investigate the use of supervised machine learning, in the form of a denoising autoencoder, to simultaneously remove experimental noise while encoding one- and two-qubit quantum state estimates into a minimum number of nodes within the latent layer of a neural network. We decode these latent representations into positive density matrices and compare them to similar estimates obtained via linear inversion and maximum likelihood estimation. Using a superconducting multiqubit chip we experimentally verify that the neural network estimates the quantum state with greater fidelity than either traditional method. Furthermore, we show that the network can be trained using only product states and still achieve high fidelity for entangled states. This simplification of the training overhead permits the network to aid experimental calibration, such as the diagnosis of multi-qubit crosstalk.

*This research was supported by the LPS HiPS program under ARO grant W911NF1810178.
12:39PM S08.00008: Characterization and tomography of a hidden qubit*  MAREK PECHAL, MARC GANZHORN, MAX WERNINGHAUS, DANIEL EGGER, GIAN SALIS, STEFAN FILIPP (Presenter), IBM Research - Zurich — In circuit-based quantum computing it is typically assumed that the available gate set consists of single qubit gates acting on each individual qubit as well as an entangling gate between pairs of qubits. In some physical architectures, not all qubits may be addressable, but some may be hidden and only connected to another control qubit. In this case, no single qubit operations can be applied to the hidden qubit and its state cannot be measured directly, but entangling gates with the control qubit can be carried out. Tomography of the combined two-qubit system is still possible on the combined two-qubit system whenever an iSWAP-type interaction in combination with a controlled-phase gate and single qubit operations on the control qubit is available. In our experiment we use transmon-type superconducting qubits along with parametric tunable-coupler gates to realize both types of two-qubit interactions. We further discuss the tune-up process required to completely characterize the gate set used for tomography and we evaluate the resulting fidelities.

*This project has received funding from the EU H2020 under the Grant Agreement No. 828826.

12:51PM S08.00009: Quantum Rifling: Protecting a Qubit from Measurement Back-action DANIEL B SZOMBATI, ALEJANDRO GOMEZ FRIEIRO (Presenter), Univ of Queensland, CLEMENS MUELLER, IBM Research Zürich, TYLER JONES, MARKUS JERGER, ARKADY FEDOROV, Univ of Queensland — Quantum mechanics postulates that measuring the qubit's wave function results in its collapse, with the recorded discrete outcome designating the particular eigenstate the qubit collapsed into. We show this picture breaks down when the qubit is strongly driven during measurement. More specifically, for a fast evolving qubit the measurement returns the time-averaged expectation value of the measurement operator, erasing information about the initial state of the qubit, while completely suppressing the measurement back-action. We call this regime `quantum rifling', as the fast spinning of the Bloch vector protects it from deflection into either of its two eigenstates. We study this phenomenon with two superconducting qubits coupled to the same probe field and demonstrate that quantum rifling allows us to measure either one of the two qubits on demand while protecting the state of the other from measurement back-action. Our results allow for the implementation of selective read out multiplexing of several qubits, contributing to efficient scaling up of quantum processors for future quantum technologies.
Over the past decade tremendous progress has been made on spin qubits based on electron spins in silicon quantum dots. As with any qubit implementation, a critical requirement is the ability to read out the qubit rapidly, with high fidelity, and in a scalable manner. Much attention has been focused on improving single-electron transistors embedded in radio-frequency reflectometry circuits as charge detectors to detect, in combination with a spin-to-charge conversion scheme, electron spin states. While these are the most sensitive detectors to date, they come with additional resources that take up valuable space near the quantum dots (gate electrodes, electron reservoirs), which makes scaling up to two-dimensional spin qubit arrays difficult. More efficiently, read-out can be performed utilizing gates that are already in place for defining quantum dots by connecting those gates to a resonant circuit. This promising method of gate-based sensing has been developed for quantum dots with off-chip resonators, and only very recently achieved the sensitivity necessary for single-shot read-out of spins in silicon [1]. In this talk, I will describe the use of an on-chip superconducting microwave resonator to improve the sensitivity, aided by its high quality factor and impedance. Using Pauli Spin Blockade as the spin-to-charge conversion scheme, we demonstrate the gate-based read-out of a two-electron spin state in a single shot with an average fidelity of 98% in only 6 microseconds [2]. Furthermore, our latest work towards long-distance spin-spin coupling will be presented.


*This research was undertaken thanks in part to funding from the European Research Council (ERC Synergy Quantum Computer Lab) and the Netherlands Organisation for Scientific Research (NWO) as part of the NanoFront programme.
1:39PM S08.00011: Improving Multilevel Qudit Readout Fidelity During Relaxation Events via Hidden Markov Models

LUIS MARTINEZ (Presenter), YANIV J. ROSEN, JONATHAN L. DUBOIS, Lawrence Livermore National Laboratory — Quantum state determination with high fidelity is a requirement for quantum computation. However, qubit relaxation imposes a limiting constraint on readout fidelity. Longer readout measurement times increase the distinguishability between the qudit states, however state decay during a long readout pulse can obfuscate the measurement and result in misclassification of qudit state. To overcome this constraint, we demonstrate high-fidelity multi-state readout by detecting qubit relaxation with Hidden Markov Models on LLNL’s Quantum Design and Integration Testbed (QuDIT). The ability of Hidden Markov Models to account for relaxation and thermal excitation processes allows for longer readout times, extraction of transition probabilities, and higher readout fidelity.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was partially supported by the DOE ASCR quantum testbed pathfinder program and ASC Beyond Moore’s Law quantum effort. LLNL-ABS-795449

1:51PM S08.00012: Continuous Indirect detection of stabilizers for quantum error correction

YI-HSIANG CHEN (Presenter), TODD BRUN, Univ of Southern California — Measuring high-weight operators is an important problem in quantum computation. The conventional procedure to measure a high-weight operator involves multiple pairwise unitary operations, which may require a large number of quantum gates. We provide an alternative method to passively detect the value of an operator. This approach involves joint interactions between the system and continuously-monitored ancillary qubits. The continuous measurement outcomes of the monitor qubits reveal information about the values of the stabilizer generators. This information can be retrieved using an estimator, which is driven by the measurement outcomes. We also show that there is a more efficient way to read out the outcomes directly from the time average of the signals. The interaction Hamiltonian can use only two-local operators, based on techniques similar to perturbative gadgets. We apply this indirect detection scheme to the four-qubit Bacon-Shor code, where the two stabilizers are indirectly monitored using four ancillary qubits. Since it is an error-detecting code, we show that non-Markovian errors, e.g., the Hamiltonian 1/f noise, can be suppressed by the indirect detection. This detection scheme could be implemented in near-term experimental systems and operate in real time.

2:03PM S08.00013: Diagnosing Errors in Quantum Gates Using Continuous Measurements

JOHN STEINMETZ (Presenter), ANDREW N JORDAN, University of Rochester — We use continuous weak measurements to track a quantum gate operation as it develops in time, which allows us to identify the full time-dependent dynamics of any systematic errors. We account for measurement backaction such that it has no bearing on the error estimate. This diagnostic method is tested on imperfect single- and two-qubit gates, and is shown to accurately extract known time-dependent error pulses. This offers significant advantages over traditional quantum process tomography, as it provides the ability to identify the origin and nature of any deviations from the desired evolution, which can give insight into how to modify the gate pulse.

*We acknowledge funding from the US Army Research Office.
11:15AM S09.00001: Observing a Topological Transition in Weak-Measurement-Induced Geometric Phases*  
YUNZHAO WANG (Presenter), Department of Physics, Washington University in St. Louis, KYRYLO SNIZHKO, The Weizmann Institute of Science, ALESSANDRO ROMITO, Lancaster University, YUVAL GEFEN, The Weizmann Institute of Science, KATER MURCH, Department of Physics, Washington University in St. Louis — Quantum measurements induce backaction on quantum states resulting in measurement induced dynamics. A sequence of weak measurements can consequently realize a cyclic motion for the qubit state in Hilbert space and thus induce a geometric phase. As the measurement strength is varied between weak and strong regimes, we expect a topological transition corresponding to a change in the Chern number of the surface tracked by the qubit's cyclic motion. To experimentally measure this transition, we employ quantum non-demolition measurement of a superconducting transmon circuit in the strong dispersive regime. This transition is revealed as a quantized jump in the averaged geometric phase when tuning the strength for the measurement sequence, giving new insights into how weak measurements are a powerful tool for quantum control.

*NSF Grant PHY-1607156 and NSF Grant PHY-1752844 (CAREER)

11:27AM S09.00002: Microscopic magnetometry of neurons using a superconducting flux qubit*  
HIRAKU TOIDA (Presenter), KOJI SAKAI, IMRAN MAHBOOB, TETSUHIKO F. TESHIMA, KOUSUKE KAKUYANAGI, SHIRO SAITO, NTT Basic Research Labs — We have developed a microscopic magnetometer based on a superconducting flux qubit [1]. Using it, we have successfully obtained a magnetization signal from neurons. The neurons were cultured on parylene-C film in iron-rich medium to increase the number of spins in the cell. The film also worked as an insulator between the neurons and the flux qubit. The magnetization signal increased as a function of the inverse temperature and the Zeeman magnetic field. Considering that the control experiment without neurons showed no significant magnetization signal, this result strongly suggests that the signal originates from the spins in neurons. In the case of spins in neurons, because the spins distribute inhomogeneously in the cell, the contribution to the magnetization signal from the spins distant from the chip surface plays an important role, unlike the case of solid state spins [1]. To improve sensitivity to such widely distributed organic spins, a capacitively shunted flux qubit with a large loop size is developed and its design parameters are discussed [2]. [1] H. Toida et. al., Commun. Phys. 2, 33 (2019). [2] D. Marcos et. al., Phys. Rev. Lett. 105, 210501 (2010).

*This work was supported by CREST (JPMJCR1774), JST.
**11:39AM S09.00003: High contrast dual-mode optical and hyperpolarized $^{13}$C magnetic resonance imaging in diamond particles**  
XUDONG LV (Presenter), University of California, Berkeley, JEFFREY H WALTON, Nuclear Magnetic Resonance Facility, UC Davis, EMANUEL DRUGA, FEI WANG, ALESSANDRA AGUILAR, TOMMY MCKNELLY, RAFFI NAZARYAN, LAN WU, University of California, Berkeley, OLGA SHENDEROVA, Adamas Nanotechnologies, DANIEL VIGNERON, Department of Radiology and Biomedical Imaging, UCSF, CARLOS MERILES, Department of Physics, City College of New York, JEFFREY A REIMER, ALEXANDER PINES, ASHOK AJJOY, University of California, Berkeley — Multichannel imaging - the ability to acquire images of an object through more than one imaging mode simultaneously - has opened exciting new avenues in several areas from astronomy to biomedicine. Visible optics and magnetic resonance imaging (MRI) offer complementary advantages of resolution, speed and depth of penetration, and as such would be attractive in combination. In this work, we integrate optical and MR imaging in diamond particles endowed with a high density of quantum defects, Nitrogen Vacancy (NV) centers. Under optical excitation, NV centers fluoresce brightly in the visible, as well as electron spin polarize, allowing the hyperpolarization of lattice $^{13}$C nuclei. Leveraging the ability of optical and MR imaging to simultaneously probe Fourier-reciprocal domains (real and k-space), we elucidate a hybrid sub-sampling protocol in both conjugate spaces to vastly accelerate dual-image acquisition, while concurrently reducing the net optical power, by two orders of magnitude in sparse-imaging scenarios. In addition, we demonstrate background-free imaging in optical and MR domains respectively. This work portends new avenues for quantum-enhanced dual-mode imaging platforms and opens possibilities for new therapeutic avenues including in low-field MRI-guided endoscopy.

**11:51AM S09.00004: Expanding the possibility of quantum metrology with a mixture of superpositions of macroscopically distinct states**  
MAMIKO TATSUTA (Presenter), Univ of Tokyo, YUICHIRO MATSUZAKI, National Institute of Advanced Industrial Science and Technology, AKIRA SHIMIZU, Univ of Tokyo — A quantum sensor can beat the best sensitivity of a classical sensor, which is called the standard quantum limit (SQL), by the factor which scales with the square root of the system size. Sensitivity with such an enhancement is called the Heisenberg scaling. Although some specific examples that achieve the scaling have been studied, there is no general criteria about what kind of quantum states have the potential to achieve it. Here we prove that every state identified as a generalized cat state (GCS), i.e., superposition of macroscopically distinct states characterized by quantum coherence, can achieve it if used as a field sensor [1]. Importantly, even a mixture of exponentially large number of states can be identified as a GCS. We also show that GCSs beat the SQL in scaling despite the presence of dephasing which degrades the sensitivity. As a concrete example, we propose a protocol to generate a mixed GCS at finite temperature with donor spins in silicon. Its sensitivity is about 20 times better than that of a separable state even though it has an exponentially low purity.

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**12:03PM S09.00005: Weak Measurements of a Superconducting Qubit Reconcile Incompatible Observables**

JONATHAN MONROE (Presenter), TAEHO LEE, Washington University, St. Louis, NICOLE YUNGER HALPERN, Harvard University, KATER MURCH, Washington University, St. Louis — Traditional uncertainty relations dictate a minimal amount of noise in incompatible projective quantum measurements. The noise comes from the observables' not sharing an eigenbasis. However, not all measurements are projective. In particular, weak measurements are minimally invasive tools for obtaining partial state information without projection. Weak measurements obey an entropic uncertainty relation based on generalized measurement operators [Yunger Halpern et al. Commun. Phys. 2, 92 (2019)]. We experimentally test the entropic uncertainty relation with strong and weak measurements of a superconducting transmon qubit. We find that a weak measurement can reconcile the incompatibility of two strong measurements via the weak measurement's backaction.

*This work was supported by NSF grants PHY-1607156 and PHY-1752844.

**12:15PM S09.00006: Control-enhanced quantum parameter estimation through reinforcement learning**

HAN XU (Presenter), XIN WANG, City Univ of Hong Kong — Measurement and estimation of parameters are indispensable for science and engineering. One of the main goals in parameter estimation is to find systematic schemes achieving high precision. Schemes for quantum parameter estimation could focus on optimizing the probe, its interaction with the system and measurements. Recently, schemes that add controls during the evolution are realized for significantly improving the precision. However, the identification of the control-enhanced scheme is usually computationally demanding, because the controls depend on the parameter value and need to be re-optimized after each update of the estimation. Here we show an efficient way to identify the controls through reinforcement learning that can improve the precision for both single-parameter estimation and multi-parameter estimation. Reinforcement learning also shows great generalizability, namely the neural network trained under a particular value of the parameter can work for different values within a broad range. These results suggest that reinforcement learning can be an efficient alternative to conventional optimal quantum control methods.

*This work is supported by the Research Grants Council of the Hong Kong SAR (Grant Nos. CityU 21300116, CityU 11303617, CityU 11304018).

**12:27PM S09.00007: Optimal protocols for simultaneous measurement of multiple analytic functions with quantum sensor networks**

JACOB BRINGEWATT (Presenter), PRADEEP NIROULA, PRZEMYSLAW BIENIAS, University of Maryland, College Park, ALEXEY V GORSHKOV, National Institute of Standards and Technology — We expand on previous work for measuring analytic functions of input parameters of quantum sensor networks with qubit sensors. We consider the optimal bound with respect to different figures of merit for simultaneous measurement of multiple such analytic functions and propose protocols to achieve these bounds and thus Heisenberg scaling in the mean square error. We discuss conditions on the analytic functions where the possible speed-up over classical or sequential protocols is greatest and consider potential applications.
12:39PM S09.00008: Optimal control for quantum detectors  PARAJ TITUM (Presenter), KEVIN SCHULTZ, GREGORY QUIROZ, DAVID CLADER, Applied Phys Lab/JHU — Quantum systems are promising candidates for sensing of weak signals as they can provide unrivaled performance when estimating parameters of external fields. However, when trying to detect weak signals that are hidden by background noise, the signal to noise ratio is a more relevant metric than raw sensitivity. We identify, under modest assumptions about the statistical properties of the signal and noise, the optimal control to detect an external signal in the presence of background noise using a quantum sensor. We show this by considering the time-dependent control using the filter function formalism, and we use this formalism to derive the optimal protocol that maximizes the signal-to-noise ratio for the quantum detector. Interestingly, this optimal solution is the simple and well-known spin-locking control scheme. We further show, using numerical techniques, that this result is robust even when lifting some of our assumptions. These results show how that an optimal detection scheme can be easily implemented in near-term quantum sensors without the need for complicated pulse shaping.

12:51PM S09.00009: Optimal Control and Glassiness in Quantum Sensing  CHRISTOPHER TIMMS (Presenter), MICHAEL KOLODRUBETZ, University of Texas at Dallas — The extreme responsiveness of qubits to their external environment has proven to be very useful for the purpose of quantum sensing. While this is valuable for sensing small target fields, this also makes the qubits very susceptible to disruption by external noise. We simulate the use of quantum optimal control to control the qubits for sensing protocols. Our work extends the pioneering results of Poggiali et al [PRX 8, 021059 (2018)] by allowing the use of non-pi pulses. We show that this added complexity translates into both improved sensitivity and qualitative modifications of the control landscape. In particular, we explore the connection of the rough control landscape to that of a (classical) spin glass and comment on possible applications of this connection to improving quantum sensing more broadly.

1:03PM S09.00010: Statistical Certification of Majorana fermions  ABU ASHIK MD. IRFAN (Presenter), Indiana Univ - Bloomington, KARL MAYER, NIST, GERARDO ORTIZ, Indiana Univ - Bloomington, EMANUEL H KNILL, NIST — Physicists conjectured the existence of Majorana zero-energy modes in various condensed matter setups. Several experimental groups have even reported evidence of their existence by means that do not reflect or exploit its non-Abelian braiding statistics, a prerequisite for topological computation. What constitutes conclusive evidence for Majorana fermion detection? We present a quantum self-testing protocol that uses minimal assumptions and establishes strong conditions for Majorana fermion detection. We propose a contextuality witness $W$ which consists of putative Majorana fermion parity operators. The resulting Bell-like inequality $<W> \leq 3$ can be violated only if the system exhibits quantum contextuality. We further show that observing the ideal measurement statistics, leading to $<W>=5$, implies anticommutativity of the implemented Majorana fermion parity operators, a necessary prerequisite for the non-Abelian braiding statistics of Majoranas. Our protocol is robust to experimental errors. We obtain lower bounds on the fidelities of the state and measurement operators using both analytical calculations and a Semi Definite Programming approach. We also propose a protocol that certifies the gates which are implemented by the braiding of Majorana modes.
1:15PM S09.00011: Demonstration and Application of Long-lived state in a four-spin system hyperpolarized at room temperature*  KOICHIRO MIYANISHI (Presenter), NAOKI ICHIJO, MAKOTO MOTOYAMA, AKINORI KAGAWA, Graduate school of Engineering Science, Osaka Univ, MAKOTO NEGORO, Quantum Information and Quantum Biology Division, Institute for Open and Transdisciplinary Research Initiatives, Osaka Univ, MAKOTO MOTOYAMA, AKINORI KAGAWA, Graduate school of Engineering Science, Osaka Univ — A solution with hyperpolarized nuclear spins encoded into a long-lived state has been utilized for sensing chemical phenomena in vivo and in vitro. In a conventional way, nuclear spins are hyperpolarized at very low temperatures, and it needs a large-scale setup with a cryogenic instrument. In this work, we demonstrate the encoding of a four-nuclear-spin system hyperpolarized at room temperature into a long-lived state in a solution. Both room temperature hyperpolarization and quantum encoded sensor are a hot topic in quantum sensing. Experiments are performed for the aromatic protons in p-chlorobenzoic acid. The lifetime of spin polarization was increased 2.4 times by the quantum encoding. We apply the solution with the long-lived state as a sensor in ligand--receptor binding experiments.

*This work was supported by CREST (JST grant number JPMJCR16721) and PRESTO (JST grant number JPMJPR1666 and JPMJPR18G5). K.M. is supported by JSPS KAKENHI No. 19J10976 and Program for Leading Graduate Schools: Interactive Materials Science Cadet Program.

1:27PM S09.00012: Diamond quantum DC magnetometer with efficient digital signal processing*  YUTA MASUYAMA (Presenter), Natl Inst for Quantum & Radiological Science & Tech (QST), TAKAYUKI IWASAKI, MUTSUO HATANO, Tokyo Institute of Technology, TAKESHI OHSHIMA, Natl Inst for Quantum & Radiological Science & Tech (QST) — Nitrogen-vacancy (NV) centers in diamond are promising solid-state quantum sensors. The sensor can potentially monitor the real-time magnetic field at room-temperature toward the brain-machine interface. One of the biggest challenges is to implement a highly sensitive sensor in a compact system. The sensor based on a digital signal processing with the Fourier transform has an advantage of its simpler system than an analog type, but it is hard to monitor the real-time magnetic field because the method needs many computational resources.

Here, we demonstrate an alternative method of digital signal processing with less computational resources than the Fourier transform. The method uses a digital filter that effectively becomes a sinc filter utilizing the orthogonality of trigonometric functions by multiplication of the acquired data by a trigonometric function. The computational time of the method to compute the signal from n points of data is O(n), whereas the time with Fourier transform is O(n log n). We confirm our method with a large detection volume of the ensemble NV centers. Consequently, we obtained a DC magnetic field sensitivity of 2.4 nT/√Hz.

*This work was supported by MEXT Quantum Leap Flagship Program (MEXT Q-LEAP) Grant Number JPMXS0118067395.
Magnetic Measurement of SPIONs using NVs in Diamond

MAZIAR SALEH ZIABARI (Presenter), PAULI KEHAYIAS, JACOB D HENSHAW, TZU-MING LU, CHARLES HARRIS, EDWARD S BIELEJEC, DALE L HUBER, Sandia National Laboratories, VICTOR ACOSTA, University of New Mexico, MICHAEL P LILLY, ANDREW M MOUNCE, Sandia National Laboratories — Superparamagnetic iron oxide nanoparticles (SPIONs) have numerous biological, magnetic, and chemical applications. Their nontoxicity and functionalizability supports medical applications as temporally and spatially controlled nanovectors for drug delivery, markers for enhanced MRI sensitivity, and for externally controlled hyperthermia in tumors. While bulk magnetic properties of SPIONs have been the subject of numerous studies, the magnetic properties of single SPIONs aren't well understood. Nitrogen vacancy defects in diamond are particularly suitable for characterizing isolated nanoparticles due to their extreme sensitivity to local magnetic fields. We characterize the magnetic properties of SPIONs of varying size and density, deposited on the surface of NV implanted diamond.

This work was funded by the Sandia National Laboratory LDRD program and at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the DOE's National Nuclear Security Administration under contract DE-NA0003525.

Imaging nanoscale volumes of single spins with shallow nitrogen-vacancy quantum spin sensors in diamond

ZHIRAN ZHANG (Presenter), University of California, Santa Barbara, DOLEV BLUVSTEIN, Havard University, NICOLAS RYAN WILLIAMS, ANIA JAYICH, University of California, Santa Barbara — The single shallow nitrogen-vacancy (NV) center, as an atomic-sized quantum sensor, can be incorporated with scanning probe microscopy with the potential of imaging single molecule structure with atomic-scale resolution. Here we present NV-based imaging of electron spins patterned on the nanoscale structure, where we employ DNA origami, a powerful molecular self-assembly platform, to enable bottom-up patterning of single spin-containing molecules. Such molecular structures can serve as two-dimensional calibration ‘spin’ rulers for the development of NV nanometrology. Specifically, we demonstrate the synthesis of the Gd chelate labeled DNA origami structures and present images of these structures acquired with NV center T1 imaging. Lastly, we discuss the outlook for our imaging technique to image spin-labelled molecules at the single spin level.

We gratefully acknowledge support from DARPA DRINQS program (agreement D18AC00014).
2:03PM S09.00015: Time-resolved diamond magnetic microscopy of superparamagnetic nanoparticles*  NATE RISTOFF (Presenter), University of New Mexico, ABDELGHANI LARAOUI, University of Nebraska - Lincoln, ILJA FESCENKO, JOSHUA DAMRON, NAZANIN MOSAVIAN, JANIS SMITS, University of New Mexico, ANDREY JARMOLA, ODMR Technologies Inc., PAULI KEHAYIAS, Sandia National Laboratory, MAZIAR SALEHIZABARI, University of New Mexico, ANDREW M MOUNCE, DALE L HUBER, Sandia National Laboratory, VICTOR ACOSTA, University of New Mexico — Magnetic nanoparticles have many biomedical applications including hyperthermia for cancer therapy, magnetic resonance imaging, and magnetic relaxation imaging. These applications require that the magnetic nanoparticles have uniform magnetic properties, size and morphology. We report progress on a nitrogen vacancy (NV) center widefield magnetic microscope which measures the Neel relaxation and hysteresis curve of many single magnetic nanoparticles. In addition, we report on progress to correlate these relaxation measurements to particles size via scanning electron microscope (SEM).

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Thursday, March 5, 2020 11:15 AM - 1:15 PM

Session S15 DFD GSNP: Granular, Porous Media, & Multiphase Flows II
210/212 - Nathan Keim, California Polytechnic State University

11:15AM S15.00001: Nonlinear acoustic resonance and wave-induced softening in dense granular matter through flow heterogeneities  CHARLES LIEOU, Los Alamos National Laboratory, JEROME LAURENT, Institut Langevin, PAUL A JOHNSON (Presenter), Los Alamos National Laboratory, XIAOPING JIA, Institut Langevin — We report a series of experiments on the softening and compaction of a dense granular pack through traveling acoustic pressure and shear waves. Softening is manifested by a reduction the traveling-wave speed, as the amplitude of the disturbance increases beyond some threshold. We explain these seemingly contradictory observations using a theoretical model, based on shear transformation zones (STZs), that directly attributes these observations to dynamical heterogeneities and slipping contacts in the granular pack. Softening is accounted for by the increase of the fraction of STZs or slipping contacts as a function of increasing strain amplitude, while compaction is explained by an Ising-like correlation between STZs in the subyield regime. In so doing, we demonstrate the fundamental connection between nonaffine granular rearrangements, mesoscopic glassy dynamics, jamming and unjamming, and matter-wave interactions.
11:51AM S15.00002: Scaling and dynamics of impacts into cornstarch and water suspensions*  MARC BRASSARD (Presenter), NEIL CAUSLEY, The Naval Postgraduate School, JOSHUA DIJKSMAN, Wageningen University & Research, ABE CLARK, The Naval Postgraduate School — Impacts into dense suspensions, which consist of micron-scale particles suspended in a Newtonian fluid, undergo a dramatic solidification when subjected to sudden impact. Recent work has shown that the forces during the initial moments of impact are too large to be described by discontinuous shear thickening (DST), which is a steady-state description. Other descriptions, such as the added mass model proposed by Waitukaitis and Jaeger, capture some aspects of the dynamics well but fail to predict certain features. Here, we show results from experimental impacts into dense suspensions consisting of cornstarch particles and water. We vary the size, speed, mass, and shape of the projectile as well as the density of the suspension. We quantify the forces as a function of time using high-speed imaging and other sensors. We use scaling analysis to probe the underlying physical mechanisms and compare our results to existing descriptions.

*Funded by the Office of Naval Research, Grant No. N0001419WX01519 (program manager Roshdy Barsoum) and by the Office of Naval Research Global, Grant No. VSP 19-7-001.

12:03PM S15.00003: Peak Force Scaling During Impacts into Wet and Dry Granular Materials*  NEIL CAUSLEY (Presenter), NASSER F KRIZOU, MARC BRASSARD, The Naval Postgraduate School, JOSHUA DIJKSMAN, Wageningen University & Research, ABE CLARK, The Naval Postgraduate School — Impacts into granular materials, both wet and dry, are common in engineering and nature, but a fundamental description of the forces during impact is still lacking. Certain drag laws (e.g., Poncelet laws) and other rheological descriptions (e.g., inertial rheology for dry grains or discontinuous shear thickening for suspensions) are often successful in describing certain aspects of the forces, but these descriptions typically fail to capture the largest forces during the initial moments of impact. Here, we use experiments and simulations to study early time dynamics of impacts into wet and dry granular materials. We show that the magnitude and time scales of the peak forces obey power law scaling that is similar across the different types of materials we study, and we use dimensional analysis to isolate the relevant physical mechanisms. We find that existing models do not predict many of the scaling laws we observe, suggesting the need for new models to describe this process.

*Funded by the Office of Naval Research Grant No. N0001419WX01519 (program manager Roshdy Barsoum). Additionally, we acknowledge VSP 19-7-001 visitor grant from the Office of Naval Research Global.
12:15PM S15.00004: Proper Spatial Average Operators in a Heterogeneous Porous Medium
EHSAN TAGHIZADEH (Presenter), BRIAN DAVID WOOD, Oregon State Univ — In this work, we explore a wide range of kernel functions commonly used in Bayesian statistics to evaluate their functionality in attenuating geometrical fluctuations arising from sudden change in the porosity in a heterogeneous porous medium. Boxcar; single-, double-, and triple-convoluted boxcar; Epanechnikov; Tricube; Gaussian; Cosine; Logistic; Sigmoid; and Silverman are among weighting functions we examined for the cases where (1) a periodic homogeneous medium, (2) a quasi-periodic heterogeneous medium with a gradual porosity change, (3) a quasi-periodic heterogeneous material with a discontinuous jump in porosity, and (4) a disordered heterogeneous porous medium with a discontinuous jump in the porosity exist. We use an extended porous material's diffusion model developed based on volume averaging method recently reported by Battiato et al 2019 [1]. The model retains the zero- and first-order terms in the closure problem and neglects the second-order Taylor series. Results are promising in a sense that mollified version of some of those weighting functions can improve divergence of Taylor series approximation of the average flux of mass through the porous material.


12:27PM S15.00005: Fluid Flow with Suspended Soft Particles in Porous Media* SHUAIJUN LI (Presenter), JING FAN, The City College of New York — Transport of soft particles with flow in porous media is ubiquitous in many natural and engineering processes. For example, preformed-particle-gel (PPG) treatment is a common technique in enhanced oil recovery. While the measurable properties in this process are at the microscale, such as gel size, properties, and the macroscopic permeability directly correlates with the overall recovery efficiency. Therefore, it is desirable to find the quantitative relation between the macroscopic permeability and the relevant microscopic properties. However, this remains an unsolved problem. In this work, we study transport of mono-dispersed suspended soft particles in porous media. We start from analyzing a soft particle transport through a single pore throat and find the correlation between injection pressure and the properties of the soft particle. Based on this result, we then expand the analysis to macroscale. we find a quantitative relation between the macroscopic permeability and pore-scale properties in the presence of pore blockage. The work significantly improves our understanding on transport of soft particles in porous media and directly benefits the relevant industrial applications.

*Acknowledgment is made to the American Chemical Society Petroleum Research Fund for partial support
Granular packings with sliding, rolling and twisting friction*  ANDREW SANTOS (Presenter), ISHAN SRIVASTAVA, DAN STEFAN BOLINTINEANU, JEREMY LECHMAN, GARY GREST, Sandia National Laboratories, LEO SILBERT, Central New Mexico Community College — Intuition tells us that a rolling or spinning sphere will eventually stop due to the presence of friction. The resistance to rolling and spinning/twisting that stops one sphere also changes the microstructure of a granular packing of frictional spheres. Isostatic constraint counting allows packings of 3d spheres to span an average number of contacts per sphere between 6 to 2, depending on the types of frictional constraints. We perform discrete element modeling simulations to construct sphere packings implementing a range of frictional constraints under a stress-controlled protocol. The simulated granular packings are tested against the isostatic conjecture and are compared to experimental values. Stable packings are achievable at low volume fractions and average coordination numbers, circa 0.52 and 2.6 respectively, when the particles experience high resistance to sliding, rolling and twisting.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology &Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
SAND No. 2019-12577 A

Elastogranular Buckling of a Slender Ring*  DAVID SCHUNTER, JR. (Presenter), DOUGLAS HOLMES, Boston Univ — Thin flexible-walled structures provide utilitarian geometries in a variety of biological and engineering contexts. Whether describing the origins of certain vascular disorders, the mechanics of thin membranes, or in constructing domed architectures, understanding how these thin objects respond due to external forcing is crucial. Previous work has focused on thin structures deforming within media that, in general, have both compositional and mechanical homogeneity. In comparison, much less is known about the behavior of slender structures embedded in active or driven matter, such as a vibrating granular monolayer. By placing a thin elastic ring within a horizontally driven 2D granular bed, we investigate the phase space of buckling morphologies that arises under gradual compression of this coupled system. Varying the compression rate U, we see a crossover between two distinct regimes, with ring buckling geometries reflecting the degree of granular force homogeneity. These results will bring new insight into how flexible structures deform & pack within complex media, and will be relevant for geometric approaches to cell mechanics, the design of soft robots, the modeling of animal movements, and developing responsive, directable medical devices.

*NSF CMMI--CAREER 1454153
1:03PM S15.00008: Using time-dependent random resistor networks to capture the dynamics of flow in disordered porous media  AHMAD ZAREEI (Presenter), Harvard University, SHIMA PARSA, Rochester Institute of Technology, DAVID A WEITZ, ARIEL AMIR, Harvard University — The heterogeneous microstructure of a disordered porous medium determines the pore-level flow. Any changes to the micro-structure in a porous medium, such as solute retention during polymer flow (effectively "clogging" some pores in the network), affects the pore-level flow and alters the bulk behavior. In order to better understand the effect of microstructure on flow behavior, we study a model based on a disordered network of tubes, mathematically equivalent to a random resistor network. We show that this approximate model captures the observed velocity distribution in experiments on glass beadpack. We model the dynamics of structural changes during polymer retention, and show that the (dynamic) resistor network produces flow velocity distributions and bulk properties consistent with the experiments.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S16 DQI: Multi-mode and 3D-cavity Circuit QED Systems II  201 -

Yvonne Gao, Yale University

11:15AM S16.00001: Mediating interactions between superconducting microwave cavities with three-wave mixing, part 1*  STIJN DE GRAAF (Presenter), BENJAMIN CHAPMAN, YAXING ZHANG, SHANTANU O MUNDHADA, AKSHAY KOOTTANDAVIDA, NICHOLAS FRATTINI, LUKE BURKHART, ALEXANDER P READ, LUIGI FRUNZIO, STEVEN GIRVIN, MICHEL H. DEVORET, ROBERT SCHOELKOPF, Yale University — Engineering tunable bilinear couplings between microwave cavities provides a way to manipulate and entangle long-lived quantum states. Two-cavity gates, such as the beam splitter and exponential SWAP (eSWAP), have been successfully demonstrated using a driven transmon coupled to both cavities. However, the fidelity of these gates is limited by unwanted 4th order processes such as the AC Stark effect. By replacing the transmon's Josephson junction with a superconducting nonlinear asymmetric inductive element (SNAIL), we produce a bilinear interaction via its 3rd order nonlinearity while minimizing 4th order effects. This is expected to offer high fidelity two-cavity gates using all-RF control. I will discuss experimental design considerations and the theory behind the coupled-cavity device.

*We acknowledge support from the following sources:
National Science Foundation DMR-1609326
Army Research Office W911NF-18-1-0212
Army Research Office MURI Grant No. W911NF-16-10349
Max Planck Research Award-Alexander von Humboldt Foundation
11:27AM S16.00002: Mediating interactions between superconducting microwave cavities with three-wave mixing, part 2* BENJAMIN CHAPMAN (Presenter), STIJN DE GRAAF, YAXING ZHANG, SHANTANU O MUNDHADA, AKSHAY KOOTTANDAVIDA, NICHOLAS FRATTINI, LUKE BURKHART, ALEXANDER P READ, LUIGI FRUNZIO, STEVEN GIRVIN, MICHEL H. DEVORET, ROBERT SCHOELKOPF, Yale University — Quantum memories formed from three-dimensional superconducting microwave cavities provide the coherence and large Hilbert spaces needed for quantum error correction. To date, coupling between these memories has been primarily facilitated by transmons. There, four-wave mixing allows for the creation of beam-splitter, single-mode, and two-mode-squeezing interactions, from which gates can be built. Although this approach has proven to be flexible and robust, the engineered couplings are accompanied by unwanted Kerr and Stark effects, which can limit the fidelity of cavity-cavity gates. Here, we design the nonlinear coupling element to be an RF-driven three-wave mixer. The desired bilinear interactions may then be engineered while suppressing spurious fourth-order processes. In this talk, we present preliminary measurements of two microwave cavities coupled by such a three-wave mixing element.

*We acknowledge support from the following sources:
National Science Foundation DMR-1609326
Army Research Office W911NF-18-1-0212
Army Research Office MURI Grant No. W911NF-16-10349
Max Planck Research Award-Alexander von Humboldt Foundation

11:39AM S16.00003: Superconducting radio frequency cavities with seconds of photon lifetime in quantum regime ALEXANDER ROMANENKO (Presenter), ROMAN PILIPENKO, DANIIL FROLOV, SILVIA ZORZETTI, MOHAMED AWIDA, SAM POSEN, ERIC T HOLLAND, SERGEY A BELOMESTNYKH, ANNA GRASSELLINO, Fermilab — Superconducting radio frequency (SRF) cavities developed for accelerators are the highest quality factor (Q) man-made oscillators with record Q > 4e11, whereas Q~3e10 is a routine operation. Adopted for quantum regime, SRF cavities offer a route for multifold increase in photon lifetimes for applications in quantum computing and fundamental physics searches such as dark photons and axions. Initial demonstrations showed that the quantum regime lifetimes of tens of milliseconds can be achieved for SRF cavities "as-is", limited by the two-level-system (TLS) dissipation [1,2].

In this contribution we present the recent advancements [2] in the quantum regime performance of SRF cavities enabled by applying combined materials science investigations and vacuum heat treatments. We demonstrate the mitigation of the TLS dissipation and achievement of the 0.5 seconds of photon lifetime for 5 GHz and 2 seconds for 1.3 GHz cavities. Such cavities are currently being employed for several QIS type and fundamental physics applications such as dark photon searches, which we will summarize briefly as well.

11:51AM S16.00004: Exploiting tunable, ultrastrong nonlinearies of the cavity Cooper-pair transistor system for generating microwave quantum states*  WILLIAM BRAASCH, MILES BLENCOWE (Presenter), OSCAR D. FRIEDMAN, Dartmouth Coll, ANDREW D. ARMOUR, Physics and Astronomy, University of Nottingham, BENJAMIN BROCK, ALEXANDER J RIMBERG, Dartmouth Coll — The cavity Cooper-pair transistor (cCPT) device enables the engineering of a wide range of nonlinear, effective cavity oscillator interactions through the tunability of both its gate voltage and flux biases. Such nonlinearities can be strong even under low average photon number drives on the cavity. We utilize the recently developed Wigner current vector field (Wigner current) construct to give a geometrical analysis of the formation and possible stabilization of quantum microwave oscillator states in the presence of dissipation and noise for the cCPT.

*Supported by the National Science Foundation under grant Nos. DMR-1507383 and DMR-1807785

12:03PM S16.00005: Passive Error Correction with Grid States in a Non-Reciprocal Superconducting Circuit  MARTIN RYMARZ (Presenter), STEFANO BOSCO, JARA Institute for Quantum Information, RWTH Aachen University, Germany, ALESSANDRO CIANI, QuTech, Delft University of Technology, The Netherlands, DAVID PETER DIVINCENZO, JARA Institute for Quantum Information, RWTH Aachen University, Germany — Non-reciprocal circuit elements play an essential role for the practical realization of a solid-state quantum computer, independent of the chosen implementation. For that matter, non-reciprocal circuit elements often constitute the interface between the classical and quantum description of an electrical network. In electrical network theory, the gyrator proposed by Tellegen [1] in 1948 is considered to be the most fundamental non-reciprocal circuit element. The miniaturization of the actual device allows for the description of the gyrator within the lumped element model. Besides the incorporation of the gyrator into the theory of circuit quantum electrodynamics [2], we propose a non-reciprocal superconducting circuit comprising a gyrator, whose effective dynamics is described by the Hofstadter Hamiltonian [3]. Thus, the eigenstates of the system constitute grid states, which can be used for passive error correction in terms of the continuous variable code proposed in 2001 by Gottesman, Kitaev and Preskill [4].

12:15PM S16.00006: Cat-qubit operations preserving error structure*  JONATHAN GROSS (Presenter), Institut Quantique, Universite de Sherbrooke, SHRUTI PURI, Yale Quantum Institute, Yale University, ALEXANDRE BLAIS, Institut Quantique, Universite de Sherbrooke — A universal quantum computer will require error correction to perform in a fault-tolerant way, imposing substantial engineering challenges. Fortunately, many devices are subject to errors with structure that can be exploited to ease the burden of fault tolerance. Stabilized cat qubits in superconducting circuits push this principle to the extreme, with recent work identifying dramatic reduction of fault-tolerance requirements on this platform. Essential to this reduction is the ability to perform operations on the qubits that preserve the error structure, made possible by the infinite-dimensional Hilbert space in which the cats live. We present additional operations fulfilling this requirement and discuss their potential for near- and long-term applications.

*This work was undertaken thanks in part to funding from NSERC and the Canada First Research Excellence Fund. Shruti Puri also acknowledges support from ARO W911NF-18-1-0212 and NSF DMR-1609326.

12:27PM S16.00007: Multiplexed readout of four qubits in 3D cQED architecture using broadband JPA [Invited]  R VIJAY (Presenter), TIFR — Vijay has led the development of broadband quantum amplifiers, key to measurement in multiplexed systems.

1:03PM S16.00008: Waveguide Bandgap Engineering with an Array of Superconducting Qubits  JAN BREHMH (Presenter), ALEXANDER STEHLI, Karlsruhe Institute of Technology, ALEXANDER N. PODDUBNY, Ioffe Physical Technical Institute, TIM WOLZ, HANNES ROTZINGER, ALEXEY V. USTINOVO, Karlsruhe Institute of Technology — The interaction of qubits with free space instead of a cavity gives rise to several effects, which could play an important role for the implementation of a quantum computer. One of the most intriguing features is that in one-dimensional free space the interaction between qubits is of infinite range and can be tuned by varying the qubit separation [1]. In this work, we experimentally study an array of eight superconducting transmon qubits with local frequency control, which are all coupled to the mode continuum of a superconducting waveguide. The spacing between adjacent qubits is substantially smaller than the wavelength corresponding to their excitation frequency, eliminating almost completely the coherent exchange type interaction between qubits. By consecutively tuning the qubits to a common resonance frequency we observe the formation of super- and subradiant states as well as the emergence of a bandgap. Making use of the anharmonic level structure of the transmon qubit we study the nonlinear saturation of the collective modes with increasing photon number and electromagnetically induce a transparency window in the bandgap region of the ensemble.

1:15PM S16.00009: Quantum impurity simulation in a photonic crystal with superconducting circuits*  
ANDREI VRAJITOAREA (Presenter), Princeton University, RON BELYANSKY, REX LUNDGREN, University of Maryland, SETH P WHITSITT, ALEXEY V GORSHKOV, JQI-NIST, ANDREW HOUCK, Princeton University — Superconducting circuits have emerged as a rich platform for emulating synthetic materials composed of artificial atoms and photonic lattices. Here, we apply this toolbox for exploring the physics of a quantum impurity coupled to a photonic crystal. In previous experiments, strongly coupling a transmon qubit to the band structure of a stepped impedance waveguide filter has led to the first observation of atom-photon dressed bound states. In this work, we push the coupling strength even further to go beyond the single-photon limit. Our platform consists of a photonic crystal implemented as a linear array of 26 coupled microwave resonators, and a fluxonium qubit galvanically coupled to one resonator site. Tuning the coupling strength, we can reach a regime where counterrotating terms become relevant and multiphoton bound states participate in the single-photon scattering dynamics. Additionally, by probing the transmission response for each discrete bath mode subject to a qubit drive, we can extract the spin-bath susceptibilities that capture the many-body correlations between the impurity and the harmonic degrees of freedom in the crystal.

*This research is supported by the National Science Foundation under Grant no. PHY-1607160 and by the MURI under Grant no. W911NF-15-1-0397.

1:27PM S16.00010: High coherence bosonic modes in long Josephson junction chains  
NITISH JITENDRAKUMAR MEHTA (Presenter), ROMAN KUZMIN, NICHOLAS GRABON, VLADIMIR MANUCHARYAN, University of Maryland, College Park — Owing to high coherence and easy fabrication, 3-D Superconducting microwave cavities coupled to ancilla qubits are an attractive platform for the storage and manipulation of continuous variable quantum information. Recent experiments have demonstrated high fidelity QND readout, arbitrary control and remote entanglement of photonic states in these cavities[1]. Despite the progress, large size of the 3-D cavities poses a significant hurdle in scaling up the architecture. Here we present a way to get around the problem by using standing wave modes in 6mm long transmission line made out of two parallel chains of Josephson junctions[2]. Remarkably, we measure energy relaxation times exceeding 1ms in a setup with more than 20,000 junctions in one device.

Experimental Realization of the bosonic Kitaev-Majorana model  

JIMMY SHIH-CHUN HUNG, J. BUSNAINA, M.V. MOGHADDAM, CHUNG WAI SANDBO CHANG, ANANTHAPADMANABHA VADIRAJ, C.M. WILSON (Presenter), Institute for Quantum Computing, University of Waterloo — Superconducting quantum circuits (SQC) are a natural platform for quantum simulations of a wide variety of important lattice models, spanning condensed matter to high-energy physics. The varied toolbox of SQC allow the simulation of a variety of phenomena, including topological effects. Recently, McDonald et al proposed one such topological model that they dubbed the bosonic Kitaev-Majorana model. The model is a bosonic analog of the well-known fermionic Kitaev-Majorana model that has garnered great interest recently. Both models consist of a 1D chain connected by a hopping term but also subject to a pairing potential for the resident excitations. While the bosonic model does not reproduce all of the features of the original, it still exhibits a number of interesting topological features, such as chiral transport. Here we implement the bosonic Kitaev-Majorana model using a multimode superconducting parametric cavity. The nodes of the lattice are mapped to frequency modes of the cavity. The complex hopping terms are created by parametric pumping at mode-difference frequencies, while the pairing potential is induced by pumping at mode-sum frequencies. We present results for simulations on small lattices and discuss possibilities for scaling up the lattice size.

Driven quantum nonlinear resonators: new exact solution techniques and generalized photon blockade  

DAVID ROBERTS (Presenter), AASHISH CLERK, University of Chicago — Interacting driven-dissipative quantum resonators are at the forefront of research in quantum optics and quantum computing with superconducting circuits. We develop a new theoretical approach that allows one to non-perturbatively find the steady states of such systems. Our approach uncovers surprising phenomena in systems with an unusual three-photon coherent drive. This includes a new kind of generalized photon blockade effect, where interference causes a sharp cut-off in the system’s photon-number distribution despite without requiring extremely strong nonlinearity. This is distinct from standard photon blockade (which requires a strong nonlinearity), or the so-called “unconventional photon blockade” (which does not completely suppress high photon number states). We also describe a new kind of quantum bistability in these systems, which we can understand as a kind of interference between pairs of holomorphic functions in phase space. The effects we describe are well within the reach of current experiments in circuit QED, and could be harnessed for a variety of applications in quantum information processing.
 Encoding qubits in Bloch states of superconducting devices

THOMAS STACE (Presenter), Univ of Queensland, ARNE GRIMSMO, University of Sydney, CLEMENS MUELLER, ETH Zurich, JARED H. COLE, RMIT, DAT THANH LE, Univ of Queensland — We describe two related superconducting circuits, the transmon [1] and the dualmon [2] in terms of Bloch states that reflect periodic symmetries in their Hamiltonians. We use these two systems to illustrate a new scheme for encoding a qubit into superconducting qubits, using states in the lowest Bloch band. We discuss how these states are likely to be extremely robust against relaxation and noise, and suggest possible gates for controlling the state of such systems.


*This work was funded by the Australian Research Council Centre of Excellence in Engineered Quantum Systems CE170100009
11:51AM S17.00002: Logical Cooling for Noise Reduction in Analogue Quantum Simulation*
SUSAN M. CLARK (Presenter), CRAIG W. HOGLE, JAIMIE S. STEPHENS, KEVIN YOUNG, ROBIN
BLUME-KOHOUT, DANIEL L STICK, PETER MAUNZ, Sandia National Laboratories — Analogue
quantum simulation is arguably the most promising near-term application of quantum
computing. However, analogue simulators are susceptible to noise, and it is not known if realistic
noise destroys their computational power. Here, we report our progress using a technique to
remove errors in the computational basis of the system, without resorting to a full error
correcting scheme, to both measure and increase an analogue quantum simulator's robustness
to noise.

*SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2019-12836

12:03PM S17.00003: Characterizing the Propagation of Gate Errors in Experimental
Quantum Algorithms*  GABRIEL SAMACH (Presenter), MORTEN KJAERGAARD, AMY GREENE,
Massachusetts Institute of Technology, MOLLIE SCHWARTZ, MIT Lincoln Laboratory, ANDREAS
BENGTTSSON, Chalmers Institute of Technology, MICHAEL O'KEEFFE, MIT Lincoln Laboratory, CHRIS
MCNALLY, YOUNGKYU SUNG, Massachusetts Institute of Technology, PHILIP KRANTZ, Chalmers
Institute of Technology, JOCHEN BRAUMUELLER, RONI WINIK, Massachusetts Institute of Technology,
DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, JONILYN YODER, DANNA
ROSENBERG, KEVIN OBENLAND, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, SIMON
GUSTAVSSON, WILLIAM OLIVER, Massachusetts Institute of Technology — Universal quantum
computation requires a complete gate-set of single-qubit operations and a two-qubit entangling
gate. As research progresses towards useful applications of NISQ-era quantum processors,
infidelities in these operations limit the depth of algorithms accessible on near-term devices.
While Clifford Randomized Benchmarking provides a rough metric for the fidelity of operations in
a random quantum algorithm, this metric can fail to capture the buildup of coherent error in
algorithms with significant internal symmetry, such as Trotterization. In this talk, we present
recent measurements characterizing the propagation of gate errors in a Trotterized quantum
algorithm performed using >99.9% fidelity single-qubit and 99.7% fidelity controlled-phase (CZ)
gates between flux-tunable transmon qubits. We consider the role played by coherent and
incoherent gate errors in deep quantum circuits, and we look at how their propagation depends
on the choice of gate compilation.

*This research was funded in part by the ARO grant No. W911NF-18-1-0411 and the ASDRE via
MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. Opinions,
interpretations, conclusions, and recommendations are those of the authors and are not
necessarily endorsed by the US Government.
12:15PM S17.00004: Time-Dependent Simulation of Superconducting Quantum Circuits in the Presence of Non-Markovian Noise*  
SAM ALTERMAN (Presenter), ANDREW JAMES KERMAN, MIT Lincoln Laboratory — Understanding the practical impact of realistic noise on the performance of superconducting quantum circuits is vital to evaluating their prospects for potential applications and system architectures. This understanding is particularly limited at present for the more complex circuits involved in quantum annealing and reversible logic, which are subject to both damping and non-Markovian 1/f flux noise. In this presentation, we discuss a quantum trajectory-based dynamics simulation method for such circuits, and present progress towards its use in evaluating residual power dissipation in reversible logic circuits.

*This research is funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the U.S. Government.

12:27PM S17.00005: Low Rank Density Matrix Evolution for Noisy Quantum Circuits  
YI-TING CHEN (Presenter), COLLIN FARQUHAR, ROBERT PARRISH, QC Ware Corp — Quantum circuit simulators validate the accuracy of quantum computing hardware and facilitate the invention of quantum algorithms and the deployment of quantum solutions on real world problems. In this work, we present an algorithm for simulating noisy quantum circuits based on the fact that the effective dimensionality of a density matrix is low when the noise level is reasonable small. Under certain conditions on the noise level and circuit depth, we proof that the numerical rank of a density matrix grows only linearly with the number of qubits. This allow us to track the evolution of a compressed representation of a density matrix with exponentially less computational resource. We implement this algorithm in an in-house simulator, Quasar, showing that the low rank algorithm speeds up simulations more than two orders of magnitude against the standard full density matrix method, with a trade-off of small amount of error. We benchmark the performance of the algorithm with different noise channels, noise strength and circuit types. Finally, we implement instances of Grover's search algorithm, showing that the low rank evolution benefits not only random circuit simulations, but also structured quantum algorithms.

ROBIN HARPER, Univ of Sydney, WENJUN YU, Tsinghua University, STEVEN FLAMMIA (Presenter), Univ of Sydney — To achieve a scalable estimation of quantum noise we need to learn efficient and complete representations of that noise. We can do this by using descriptions that have clear and relevant physical assumptions baked in. Here I will present work on a scalable and complete protocol to learn a Pauli channel which only has $s$ non-negligible Pauli error rates. So long as the number of error rates scales polynomially with the number of qubits, then this is an efficient protocol and requires only $O(n \times s)$ experiments, linear in the number of qubits. The classical computational effort is also efficient in $n$. Learning these error rates is directly relevant to improving quantum error correction and we have already implemented this to efficiently learn all the errors on a 14-qubit quantum device.
**12:51PM S17.00007: Random Circuit Metrics for Performance Assessment and Model Testing** LUKE GOVIA (Presenter), GUILHEM RIBEILL, MATTHEW WARE, HARI K KROVI, Raytheon BBN Technologies — Random circuit metrics, such as cross-entropy benchmarking, have recently emerged as a powerful set of tools to assess the performance of quantum processors. A natural question is to what extent these techniques can be used to learn noise characteristics of the processor. Here, we present results on extensions of random circuit metrics to testing error models. We demonstrate for small processors built from superconducting qubits that analysis of random circuit distributions is a viable method to compare candidate error models for device operation. Such models feed directly into the debugging cycle, and can be used to guide future operation towards optimal performance, or in the design of future devices.

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**1:03PM S17.00008: Benchmarking tools for NISQ systems** DAVID MCKAY (Presenter), LEV S BISHOP, ANTONIO D CORCOLES, PETAR JURCEVIC, ABHINAV KANDALA, JIN-SUNG KIM, ISAAC LAUER, SETH MERKEL, ZLATKO MINEV, NEEREJA SUNDARESAN, SRIKANTH SRINIVASAN, MAIKA TAKITA, XUAN WEI, SARAH SHELDON, JAY M GAMBETTA, IBM TJ Watson Research Center — As the field marches towards quantum advantage with near-term quantum processors, it becomes imperative to characterize, verify, and validate performance. An outstanding scientific challenge in the community is a scalable set of metrics or experiments which can shed light on the usability of a device for near-term algorithms. Moreover, it becomes critical to explore techniques to extend the computational reach of noisy systems, be it through understanding underlying non-idealities, or more efficient circuit compilation. In this talk I will review the work we are doing at IBM to benchmark NISQ devices and I will discuss our recent results on quantum volume, large-scale entanglement and randomized benchmarking.

*This work was supported by the Army Research Office under contract W911NF-14-1-0124*
**1:15PM S17.00009: Model Refinement of Noisy Quantum Circuits Using Experimental Characterization**

MEGAN LILLY (Presenter), Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, Knoxville, TRAVIS HUMBLE, Quantum Computing Institute, Oak Ridge National Laboratory — Current quantum processing units represent noisy intermediate scale quantum systems that tend to be poorly characterized. Accurate modeling of these devices can provide insight into the underlying noise as well as methods for mitigating errors. We present a test-driven methodology for quantifying QPU performance and characterizing NISQ behavior that offers an alternative to costly experimental characterizations using standard tomographic methods. We demonstrate modeling of noisy gate operations by fitting experimental characterization circuits using a series of bootstrapped numerical methods. We generate parameterized gate models that are composed easily to model noisy quantum circuits. We demonstrate the effectiveness of this modeling method for applications of GHZ state preparation and the Bernstein-Vazirani algorithm using a family of superconducting transmon QPUs. We quantify the accuracy of the generated models using the total variation distance between experimental observations and numerically simulated results. Our results show that model refinement from test-driven experimental characterization offers an accessible methodology for approximating performance of NISQ devices.

*This work was supported by the Department of Energy Office of Science Early Career Research Program.

**1:27PM S17.00010: Modeling leakage in superconducting quantum computers**

FILIP WUDARSKI (Presenter), NASA Ames Research Center — Current quantum computing architectures are fragile and prone to various imperfections that limit computational capabilities. In order to better understand behavior of quantum hardware, we need to develop a theoretical framework that captures possibile sources of device errors.

Recent development in noise description allow us to characterize within statistical accuracy net effects of numerous unknown contributions. The most commonly used method for this is based on randomized Pauli channels (PC) approach, that can reflect circuit's fidelity.

In this talk, we discuss a potential extension to PC technique, that can in principle take into account leakage to non-computation basis. The method is based on Weyl matrices. We show the effect of projecting leakage subspace into a qubit space, and compare the method with PC. Finally, we briefly explain possibility of expanding this model to larger dimensions.

*We also appreciate support from the AFRL Information Directorate under grant F4HBKC4162G001 and the ODNI and the IARPA, via IAA 145483. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, AFRL, or the U.S. Government.
Benchmarking noise with Quantum alternating operator ansatz (QAOA) circuits with a symmetry

ZHUIHUI WANG (Presenter), MICHAEL STREIF, Quantum AI Lab, USRA; NASA Ames Research Center, ELEANOR RIEFFEL, Quantum AI Lab, NASA Ames Research Center — QAOA as a quantum heuristic algorithm has attracted a lot of interest with its simple iterative structure. We propose adapting a symmetry-preserving QAOA circuit for benchmarking noise. Consider the system consisting of a number of subsets of qubits, we design the QAOA such that it preserves certain quantity of the subsets (e.g., a constant Hamming weight). When errors are present, the evolution will quickly escape from the preserved subspace. We study how this escaping rate scales with the iteration of the circuit and system size. Our analysis shows for a wide range of local noise channels the escaping rate can be exactly obtained with only the knowledge of the error model, thanks to the non-increasing reverse causal cone with QAOA level with respect to noise. We show that the analysis is stable against inhomogeneity in the subsystem, hence our scheme is feasible for benchmarking local noises in realistic situations.

*We appreciate support from NASA Ames Research Center, NASA Advanced Exploration systems (AES) program, NASA Transformative Aeronautic Concepts Program (TACP), and the AFRL Information Directorate under grant F4HBKC4162G001. ZW is also supported by NASA Academic Mission Services (NAMS), contract number NNA16BD14C, and MS by USRA NAMS R&D Student Program.

Entanglement in superconducting qubits and quantum foundations

ARI MIZEL (Presenter), Lab for Physical Sciences — Leggett has proposed an experimental program to probe the limits of quantum mechanics using superconducting qubits. With this in mind, we consider the number of particles entangled in certain superconducting qubit states. Implications for quantum foundations are discussed.

Progress towards high-fidelity CZ gates in a tunable coupling architecture

CHRIS QUINTANA (Presenter), KEVIN SATZINGER, ANDRE PETUKHOV, ZIJUN CHEN, XIAO MI, YU CHEN, Google LLC — We describe progress towards implementing high-fidelity CZ gates in the Sycamore tunable coupling architecture.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S18 GSNP: Statistical Physics Meet Machine Learning

IBM TJ Watson Research Center - Tag(s): Invited
11:15AM S18.00001: Beyond Backprop: Different Approaches to Credit Assignment in Neural Nets [Invited]  IRINA RISH (Presenter), Computer Science and Operations Research (Département d'informatique et recherche opérationnelle), Université de Montréal / Mila - Quebec AI Institute —

Backpropagation algorithm (backprop) has been the workhorse of neural net learning for several decades, and its practical effectiveness is demonstrated by recent successes of deep learning in a wide range of applications. This approach uses chain rule differentiation to compute gradients in state-of-the-art learning algorithms such as stochastic gradient descent (SGD) and its variations. However, backprop has several drawbacks as well, including the vanishing and exploding gradients issue, inability to handle non-differentiable nonlinearities and to parallelize weight-updates across layers, and biological implausibility. These limitations continue to motivate exploration of alternative training algorithms, including several recently proposed auxiliary-variable methods which break the complex nested objective function into local subproblems. However, those techniques are mainly offline (batch), which limits their applicability to extremely large datasets, as well as to online, continual or reinforcement learning. The main contribution of our work is a novel online (stochastic/mini-batch) alternating minimization (AM) approach for training deep neural networks, together with the first theoretical convergence guarantees for AM in stochastic settings and promising empirical results on a variety of architectures and datasets.


12:27PM S18.00003: David Schwab Invited Talk [Invited] —

1:03PM S18.00004: Surya Ganguli Invited Talk [Invited] —


Despite tremendous success of Stochastic Gradient Descent (SGD) algorithm in deep learning, little is known about how SGD finds generalizable solutions in the high-dimensional weight space. By analyzing the SGD-based learning dynamics and the loss function landscape near solutions found by SGD, we discover a counter-intuitive relation between the weight fluctuation and the loss landscape – the flatter the landscape the smaller the weight variance. To explain this inverse variance-flatness relation, we develop a random landscape theory of SGD, which shows that noise strength (effective temperature) in SGD depends inversely on the landscape flatness and thus SGD serves effectively as a self-tuned (landscape-dependent) annealing mechanism to find the generalizable solutions at the flat minima of the loss landscape. Application of these new insights for preventing catastrophic forgetting will also be discussed.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S19 GMAG: New Opportunities in Spin Sensing, Manipulation and Resonance without Time-Varying Magnetic Fields 207 - Michael Flatté, Univ of Iowa - Tag(s): Invited
ALEXANDRE BOURASSA (Presenter), University of Chicago — The neutral divacancy (VV0) in silicon carbide (SiC) combines the advantages of a long lived spin system [1] and a near-infrared spin-photon interface [2] in a material compatible with state-of-the-art CMOS type fabrication techniques. Here, we use this scalable material to demonstrate a flexible quantum platform built by integrating and isolating single divacancies in a p-i-n diode structure.

This simple integration allows us to reduce electrical noise by engineering the defect's environment using charge depletion. This technique effectively eliminates spectral diffusion leading to optical linewidth narrowing approaching the transform limit. Broadly, this method could be generalized to produce ideal quantum emitters in various electrically “noisy” host materials. Additionally, field confinement in the junction enables wide tuning of the optical lines by almost a terahertz. Since this field is applied along the symmetry axis, the orbital splitting and associated mixing can be minimized. Finally, using electric fields and optical excitation, we show a method for deterministic charge state control of the divacancy.

Overall, we present a narrow, widely tunable and stable spin based single photon source ideal for communication networks and long-distance entanglement. These results demonstrate the power in combining highly coherent quantum spin system with scalable classical electronics.

Related publication:

Other References:

This work was performed in collaboration with C. P. Anderson, K. C. Miao, G. Wolfowicz, P. J. Mintun, A. Crook, H. Abe, J. U Hassan, N. T. Son, T. Oshima, and D. D. Awschalom

*Work supported by AFOSR, DARPA, NSF, ONR, VR and KAW
PATRICK LENAHAN (Presenter), Pennsylvania State University — We have investigated changes in current dominated by spin dependent recombination and spin dependent variable range hopping [1-3] in a variety of systems resulting from the application of relatively small magnetic fields. We compare the current changes resulting from the small magnetic fields to current changes induced by electrically detected magnetic resonance. Magnetic fields of order one mT can yield significant current changes in silicon and silicon carbide based metal oxide semiconductor (MOS) field effect transistors (MOSFETs), bipolar junction diodes and transistors, pin diodes, MOS gated diodes, amorphous silicon nitride, amorphous silicon dioxide and amorphous carbon thin films. These near zero magnetic field induced changes are easily observable at room temperature. The near zero magnetic field response is invariably a strong function of bias applied to the device structures; both the overall amplitude of the response and the “shape” of the response can be strongly influenced by the biasing conditions. In some cases one may also apply a time dependent biasing waveform to explore the kinetics of charge capture events. In this presentation I will discuss the potentially rich source of information about electronic transport which these electron spin based measurements can provide.

(Work done in collaboration with M. Flatte, U of Iowa, N. Harmon, U of Evansville, C.J. Cochrane, JPL/Cal Tech and others.)


*This project is sponsored by the Department of Defense, Defense Threat Reduction Agency under grant number HDTRA1-18-0012. The content of the information does not necessarily reflect the position or the policy of the federal government, and no official endorsement should be inferred.
Magnetoresistance Measurements as an Alternative to Magnetic Resonance Methods for Studying Paramagnetic Defects* [Invited] NICHOLAS HARMON (Presenter), Univ of Evansville — Magnetic resonance methods such as electronic paramagnetic resonance and other companion methods like electrically detected magnetic resonance have been popular for studying unpaired spins in a wide array of materials. In some situations resonance methods are not feasible — for instance when a system of interest is beneath conductive layers as in three-dimensional integrated circuits.

Recently an alternative approach to probing paramagnetic spins was devised which does not require any electromagnetic resonant field but instead magnetoresistance is measured near zero field [1]. The magnetoresistance arises from correlations between spin pairs that involve either a carrier recombining at a trap or hopping through a trap [2]. This magnetoresistance method can be used in electronic devices to great advantage by probing paramagnetic defect environments such as hyperfine and spin-orbit couplings. A theoretical description of the magnetoresistance effect utilizes a multi-spin stochastic Liouville equation [3] which provides agreement with recombination currents in MOSFETs. For high-nuclear spin defects, the theory predicts new resonances in the magnetoresistance that provide precise determination of hyperfine constants. These results offer a new means of analysis which does not rely on a resonator and are potentially applicable to systems inaccessible to conventional resonance methods.

This work was done in collaboration with the groups of M. E. Flatté (U of Iowa) and P. A. Lenahan (Penn. State U).


*The project or effort depicted was or is sponsored by the Department of the Defense, Defense Threat Reduction Agency, HDTRA 1-18-1-0012 and HDTRA 1-16-0008. The content of the information does not necessarily reflect the position or the policy of the federal government, and no official endorsement should be inferred.
HUIYAO CHEN (Presenter), Cornell University — Here we report on diamond mechanical resonator device engineering and its application to the acoustic control of NV center quantum states. We fabricate high quality diamond bulk acoustic resonators with gigahertz modes and integrated NV centers. Driving the resonator creates direct coupling of phonons to NV center electron spin and orbital states. At room temperature, we observe both single and double quantum spin transitions driven by phonons. Through improved device engineering, we demonstrate efficient acoustic control of NV center spin states using a semi-confocal high over-tone resonator. At cryogenic temperature, we probe the orbital states of a single NV center using photoluminescence excitation (PLE) spectroscopy. We show that the effects of phonon driving are spectroscopically revealed as Autler-Townes splitting and the occurrence of Raman sidebands. Lastly, we discuss how mechanical driving can be leveraged for decoherence protection based on phonon-dressed NV electronic states.


In collaboration with N. F. Opondo, B. Jiang, E. R. MacQuarrie, R. S. Daveau, S. A. Bhave and G. D. Fuchs.

*This work was supported by the Office of Naval Research (Grants No. N000141410812 and No. N000141712290) and by the DARPA DRINQS program (Cooperative Agreement #D18AC00024)
Nonlinear planar Hall effect* [Invited]  GIOVANNI VIGNALE (Presenter), Department of Physics and Astronomy, Univ of Missouri - Columbia, PAN HE, DAPENG ZHU, SHUYUAN SHI, HYUNSOO YANG, Department of Electrical and Computer Engineering and NUSNNI, National University of Singapore, STEVEN S -L ZHANG, Department of Physics, Case Western University, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory — An intriguing property of a three-dimensional (3D) topological insulator is the existence of surface states with spin-momentum locking, which offers a new frontier of exploration in spintronics. Here, we report the observation of a new type of Hall effect in a 3D topological insulator Bi$_2$Se$_3$ film. The Hall resistance scales linearly with both the applied electric and magnetic fields and exhibits a $\pi/2$ angle offset with respect to its longitudinal counterpart, in contrast to the usual angle offset of $\pi/4$ between the linear planar Hall effect and the anisotropic magnetoresistance. This novel nonlinear planar Hall effect originates from the conversion of a nonlinear transverse spin current to a charge current due to the concerted actions of spin-momentum locking and time-reversal symmetry breaking, which also exists in a wide class of non-centrosymmetric materials with a large span of magnitudes. This provides a new way to characterize and utilize the nonlinear spin-to-charge conversion in a variety of topological quantum materials.

* The work was partially funded by the Ministry of Education Academic Research Fund (MOE AcRF) Tier 1 (R-263-000- D61-114) and SpOT-LITE programme (A*STAR Grant No. A18A6b0057) through RIE2020 funds from Singapore. The work by S. S.-L. Z. and G. V. at the University of Missouri on initial development of the theoretical framework was supported by National Science Foundation (NSF) Grant No. DMR-1406568, and work by S. S.-L. Z. and O. G. H. at Argonne National Laboratory on further theoretical development, data analysis and manuscript writing was supported by Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Thursday, March 5, 2020 11:15 AM - 1:51 PM

Session S20 DBIO: Single-Molecule Techniques and Enzymes 301 - Helmut Strey, Stony Brook University
**11:15AM S20.00001: Multi-scanning of single DNA Molecules in a Dual Nanopore Device**

XU LIU, PHILIP ZIMNY, Ontera, YUNING ZHANG, McGill University, ANKIT RANA, ROLAND NAGEL, Ontera, WALTER W REISNER (Presenter), McGill University, WILLAM DUNBAR, Ontera — Single-molecule techniques can access to biomolecular information that is otherwise masked by ensemble averaging, and that can lead to new research discoveries or clinically applications. Solid-state nanopores offer a compact and electrical single-molecule sensing approach. However, single reads of molecules taken with solid-state nanopores generally do not possess sufficient quality for applications that otherwise require alignment of multiple reads of molecules from heterogeneous samples. Here we present a single-molecule manipulation and sensing approach based on a dual nanopore device that can linearize DNA and improve read quality by enabling repeated scanning at reduced speeds of the same molecule. A DNA molecule is first co-captured by the two pores with unbalanced voltage forces applied at the pores (tug-of-war state), and then repeatedly scanned back-and-forth by automated voltage control logic. The method enables detection of sequence-specific protein tags that are used for triggering the motion control during dual current sensing. We have achieved up to 100’s of scans, and analysis of multiple scans from a single molecule demonstrates a reproducible binding pattern, or molecular barcode, with tag spacings corresponding to expected sequence positions of the tags.

**11:27AM S20.00002: Computational design and interpretation of single-RNA translation experiments.**

* LUIS AGUILERA (Presenter), WILLIAM RAYMOND, KENNETH LYON, TATSUYA MORISAKI, TIMOTHY J. STASEVICH, BRIAN MUNSKY, Colorado State University — Recent advances in time-lapse fluorescence microscopy allow live-cell quantification of ribosome kinetics at single-molecule resolution. Here, we integrate single-molecule experimental data and stochastic models to investigate canonical and non-canonical translation processes. In a first study, we developed a new fluorescent tag system that allowed us to observe, for the first time, ribosomal frameshifting at single-molecule resolution. Our results corroborate that frameshifting is a bursty process, where the RNA stochastically switch between non-frameshifting and frameshifting state (Lyon, K., et al., 2019. Molecular Cell). In a second study, we developed novel stochastic models to estimate biophysical parameters, such as ribosomal elongation and initiation rates. Our methods were used to simulate single-molecule experiments under multiple imaging conditions and for thousands of human genes, and we evaluate which experiments provide accurate estimates of elongation kinetics. With this, we present an interpretation for the well-established experimental procedures, including Correlation Spectroscopy, ribosome Run-Off Assays, and FRAP (Aguilera, L., et al., 2019, Plos Comp Biology).

*This work was supported by the NIH (R35GM124747), NSF (DGE-1450032), and the WM Keck Foundation.*
11:39AM S20.00003: Single-Molecule Sensitivity in Mass Spectrometry Using Nanoscale Ion Sources*  NICHOLAS DRACHMAN (Presenter), MATHILDE LEPOITEVIN, BENJAMIN N WIENER, DEREK STEIN, Brown University — Electrospray ionization has revolutionized the analysis of biomolecules by softly transforming molecules in solution into gas-phase ions, which can be analyzed by mass-spectrometry. Due to the chaotic process by which the electrosprayed droplets break down into ever-smaller droplets, eventually yielding singly charged ions via ion evaporation, only a small fraction of the sample molecules makes it to the mass analyzer. We have shown that a nanoscale ion source allows ions to evaporate directly off of the meniscus, bypassing the wasteful droplet evaporation process. The small area of the liquid-vacuum interface also prevents significant evaporative heat loss, enabling the use of volatile solvents like water. This technique has been shown to work with simple salt solutions as well as aqueous solutions of biomolecules such as amino acids, nucleic acids, and small peptides. Adoption of these nanopore ion sources could drastically improve the sensitivity of mass spectrometry experiments and open the door to a wide range of potential applications, including single-molecule protein sequencing and single cell proteomic studies.

*Funding provided by Oxford Nanopore Technologies

11:51AM S20.00004: Brownian motion alone may not be sufficient to supply ribosomes with tRNA during translation elongation  AKSHAY J MAHESHWARI (Presenter), Bioengineering, Stanford University, EMMA DEL CARMEN GONZALEZ GONZALEZ, ALP M SUNOL, Chemical Engineering, Stanford University, DREW ENDY, Bioengineering, Stanford University, ROSEANNA ZIA, Chemical Engineering, Stanford University — The construction of artificial cells holds significant promise for biotechnology and medicine. However, substantial work remains to make such cells modelable. In particular, the set of functions necessary for life remains elusive, most acutely demonstrated by the existence of genes of unknown function that are essential for life1.

We hypothesize that some of the functions that remain unknown pertain to the physics of how molecules organize to produce cellular functions. To test our hypothesis we introduce translation elongation in E. coli as a model system. Due to its central role in protein production, elongation is likely to have undergone tremendous selective pressure to operate at the limits of physics. We construct a colloidal model of elongation and demonstrate that variable local volume densities around ribosomes at different growth rates may lead to competing trade-offs in tRNA transport and reaction. We then use lower-bounding simulations to show that tRNA transport via Brownian motion alone may be insufficient to recover experimentally determined elongation rates. Overall, we predict that currently unknown mechanisms for speeding up tRNA transport or biasing its spatial organization are implicated in translation elongation.

12:03PM S20.00005: Enhanced diffusion and enzyme dissociation at high substrate concentration  AH-YOUNG JEE (Presenter), Institute for Basic Science, KUO CHEN, Beijing National Research Center for Molecular Sciences, TSVI TLUSTY, Institute for Basic Science, JIANG ZHAO, Beijing National Research Center for Molecular Sciences, STEVE GRANICK, Institute for Basic Science — The concept that catalytic enzymes can act as molecular machines transducing chemical activity into motion has conceptual and experimental support, but much of the claimed support comes from experimental conditions where the substrate concentration exceeds $k_M$ (the Michaelis-Menten constant), meaning that it exceeds concentrations that are biologically relevant. Moreover, many of the enzymes studied experimentally to date are oligomeric. Urease, a hexamer of subunits, has been considered to be the gold standard demonstrating enhanced diffusion. Here we show that urease and certain other oligomeric enzymes of high catalytic activity above $k_M$ dissociate into their smaller subunit fragments that diffuse more rapidly, thus providing a simple physical mechanism of enhanced diffusion in this regime of concentrations. Data for urease are presented in the main text and the conclusion is validated for hexokinase and acetylcholinesterase with data presented in supplementary information. For substrate concentration regimes below $k_M$ at which these enzymes do not dissociate, we validate that enzymatic catalysis does lead to the enhanced diffusion phenomenon.

12:15PM S20.00006: Stochastic Simulation to Visualize Gene Expression and Error Correction in Living Cells* KEVIN Y CHEN, Chemistry, University of Cambridge UK, DANIEL M ZUCKERMAN, Biomedical Engineering, Oregon Health & Science Univ., PHIL NELSON (Presenter), Physics and Astronomy, Univ of Pennsylvania — Stochastic simulation can make the molecular processes of cellular control more vivid than the traditional differential-equation approach by generating typical system histories, instead of just statistical measures such as the mean and variance of a population. Simple simulations are now easy for students to construct from scratch, that is, without recourse to black-box packages. In some cases, their results can also be compared directly to single-molecule experimental data. After introducing the stochastic simulation algorithm, we give two case studies, involving gene expression and error correction, respectively. For error correction, several proofreading models are compared to find the minimal components necessary for sufficient accuracy in translation. Animations of the stochastic error correction models provide insight into the proofreading mechanisms. [Ref: KYC, DMZ, PCN, "The Biophysicist" in press.]

*This work was partially supported by NSF Grants PHY--1601894 and MCB--1715823. Some of the work was done at the Aspen Center for Physics, which is supported by NSF grant PHY--1607611.
12:27PM S20.00007: Single-pair measurements of nonradiative energy transfer efficiency between quantum dots and organic dyes reveals orientational variation  NOOSHIN SHATERY NEJAD (Presenter), CANDICE M. ETSON, Physics, Wesleyan University — Förster resonance energy transfer (FRET) is a technique that can be used to measure the nanoscale distances and to report on biomolecular dynamics at the single-molecule level. Organic dyes FRET pairs are commonly used in biophysical studies, but this approach suffers from the fact that the organic dyes have short bleaching lifetimes. Quantum dots have longer lifetimes, which makes them ideal for use as FRET donors in longer experiments. However, the energy transfer between quantum dots and organic dye molecule acceptors has not formerly been characterized at the single-molecule level. Therefore, we used TIRF microscopy to observe surface immobilized FRET pairs separated by known lengths of duplex DNA. We used two methods to construct these assemblies. In both cases, we observed broad distributions of FRET efficiencies and little correlation between duplex length and the average FRET efficiency. However, when we probe multiple donor-acceptor distances for a particular quantum dot, we observe the expected decrease in FRET efficiency with increasing duplex length. We attribute these contradictory observations to variations in the orientation factor for each single quantum dot, based on its inherent dipole moment and the location at which the DNA molecule is coupled to its surface.

12:39PM S20.00008: Bayesian nonparametrics allow for super resolution microscopy without photo-switching  IOANNIS SGOURALIS (Presenter), Arizona State University — Super resolution microscopy permits direct observation of biomolecules. However, due to noise, distinguish single molecules demands specialized analysis models that facilitate the interpretation of the acquired images. In such models, the positions of the molecules are represented by random variables and conventionally the total number of random variables in a model is kept fixed and finite. However, prevailing uncertainty in the number of individual molecules contributing photons to the images, makes existing approaches inappropriate as they rely on pre-specification of the number of unknown parameters. Switching of the fluorophores between bright and dark states, induced by experimental means (STORM, PALM, PAINT), ensures that each time at most one fluorophore is visible leading to a convenient solution. Nevertheless, photo-switching requires specialized fluorophores and long experiments necessary to collect photons from multiple switching events. In the talk, I will walk through recent modeling advances and highlight how Bayesian nonparametrics can be used to achieve super resolved localization of single molecules without photo-switching and so allowing for super resolution microscopy with less specialized fluorophores and significantly shorter experiments.
12:51PM S20.00009: Intensity Distribution of a Dilute Solution of Point Emitters under Gaussian Detection*  HELMUT STREY (Presenter), Stony Brook University — In single-molecule techniques, one often employs a Gaussian illumination profile to measure fluorescence intensities from a dilute solution of molecules. Typically such measurements are performed by single-photon detection and result in a sequence of single-photon arrival times. Here we develop a general framework for calculating the intensity distribution of a dilute solution of Point emitters under Gaussian Detection. We will show that the resulting Intensity distributions dramatically change character at low emitter concentrations when considering different dimensionalities of Gaussian Detection. In particular the one- and two-dimensional solutions are strongly structured, exhibiting discontinuities in their derivative at integer multiples of the brightness. This makes these distributions strong candidates for applications that distinguish and measure concentrations of mixtures of emitters of different brightnesses. Finally, we will discuss a maximum likelihood method to determine concentration and brightness from a sequence of single-photon arrival times.

*NSF (DMR Award 1106044), NIH (5R21DA03846702)

1:03PM S20.00010: Reliable Imaging of Dynamic Structures in Live-Cell Super-Resolution  OWEN ANDREWS (Presenter), IBRAHIM CISSE, Massachusetts Institute of Technology MIT — Super-resolution imaging by single-molecule localization is a powerful tool for visualizing structures inside of cells that are smaller than the diffraction limit. However, imaging in living matter poses a challenge because structures can be mobile and dynamic, yet single-molecule localization microscopy can require a long time to generate images. In this talk, I will present a metric for assessing image reliability, based on robust estimation of the density of detected molecules. This simple metric quantitatively defines the tradeoff between spatial and temporal resolutions, and their relationships to acceptable levels of noise in density estimation. I will discuss how this implies variations in resolution across a data set, and present a tool for visually assessing data quality.
1:15PM S20.00011: Controlled sliding of DNA knots in solid-state nanopores*  RAJESH SHARMA (Presenter), Center for Advanced 2D Materials, National University of Singapore, ISHITA AGRAWAL, Department of Biomedical Engineering, National University of Singapore, LIANG DAI, Department of Physics, City University of Hong Kong, PATRICK DOYLE, Department of Chemical Engineering, Massachusetts Institute of Technology, SLAVEN GARAJ, Center for Advanced 2D Materials, National University of Singapore — Knots in DNA are useful for investigating the static and dynamic physics of biopolymers in solutions. Recently, we showed nanopores that probe the equilibrium structures of DNA knots in solutions. With unprecedented statistics, our distributions of sizes of equilibrium DNA knots and their positions provide important insights relevant from biological, physical, and technological perspectives. Although nanopores enable statistically significant single molecule investigation, these distributions get biased due to sliding of knots through nanopores, adversely affecting the conclusions. Using our experiments and parametrized simulations, we demonstrate complete control over sliding of knots in nanopores over a molarity range of 1M-3M. We show that controlling the experimental parameters enabled the detection of equilibrium knots in both linear and circular DNA molecules. These results open up an exciting opportunity for statistically significant biophysical investigation of knots in single biomolecules, generating unprecedented insights useful from both scientific and technological perspectives.


1:27PM S20.00012: Optimal Control and Reinforcement Learning of Regulation and Enzyme Activities*  SAMUEL BRITTON (Presenter), MARK ALBER, University of California, Riverside, JENNIFER HURLEY, MEAGHAN JANKOWSKI, Department of Biological Sciences, Rensselaer Polytechnic Institute, JEREMY ZUCKER, Biological Sciences Division, Pacific Northwest National Laboratory, SCOTT BAKER, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, TINA KELLIHER, JAY DUNLAP, Geisel School of Medicine at Dartmouth, Department of Molecular and Systems Biology, WILLIAM CANNON, Research Computing Group, Pacific Northwest National Laboratory — Experimental measurement or computational inference/prediction of the enzyme regulation needed in a metabolic pathway is hard problem. Consequently, regulation is known only for well-studied reactions of central metabolism in various model organisms. In this study, we use statistical thermodynamics and metabolic control theory as a theoretical framework to calculate enzyme regulation policies for controlling metabolite concentrations to be consistent with experimental values. A reinforcement learning approach is utilized to learn optimal regulation policies that match physiological levels of metabolites while maximizing the entropy production rate and minimizing the heat loss. The learning takes a minimal amount of time, and efficient regulation schemes were learned that either agree with theoretical calculations or result in a higher cell fitness using heat loss as a metric. We demonstrate the process on four pathways in the central metabolism of Neurospora crassa (gluconeogenesis, glycolysis-TCA, Pentose Phosphate-TCA, and cell wall synthesis) that each require different regulation schemes.

*DOE SCGSR, NIH
1:39PM S20.00013: Binding Energies of Fn Cas12a  PETE RIGAS (Presenter), Cornell University — In recent years, CRISPR proteins have attracted much attention due to their use as a DNA binding platform, in which the protein undergoes steps of PAM attachment, crRNA-DNA inspection, and reconfiguration. Thermodynamically, we can model determinants of binding energies for different sites of the genome with a partition function that reflects energetic costs associated with base pair mismatches. From suitably chosen weights that assign higher energetic contributions to base pair mismatches among the first 6 positions of a DNA sequence, appropriate transition probabilities for a random walk $X$ will be defined so as to coincide with base pair mismatches. As $X$ approaches the position of binding, we stipulate that none of the transition probabilities of $X$ from all positions before $N$ vanish. Furthermore, with such a probabilistic approach, we will analyze the energy landscape of Fn Cas12a, leading to a more comprehensive understanding of how the binding energy of a sequence is dependent on individual base pairs. More broadly, this work will also study gRNA and DNA sequences that are conducive to binding in Fn Cas12a.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S21 GERA: Energy-related Thermal Phenomena 302

11:15AM S21.00001: Towards high power density, high efficiency thermophotovoltaic energy conversion system in the near field  ROHITH MITTAPALLY (Presenter), LINXIAO ZHU, ANTHONY FIORINO, Univ of Michigan - Ann Arbor, DAKOTAH THOMPSON, Univ of Wisconsin Madison, EDGAR MEYHOFER, PRAMOD REDDY, Univ of Michigan - Ann Arbor — Solid-state energy conversion holds promise for efficient extraction of electricity from different heat sources like solar and industrial waste heat. In particular, thermophotovoltaic (TPV) system involves a hot emitter radiating photons that excite electron hole pairs in a photovoltaic (PV) cell. Most TPV architectures in the far-field demonstrate very low power densities. Several theoretical proposals have shown that dramatic enhancement in power density can be achieved by reducing the gap to tens of nanometers where evanescent waves start contributing to power transfer. However, such demonstrations have been elusive due to the challenge of maintaining nano separations between a hot emitter (~1000 K) and a cold cell (~300 K). Here, we will first describe how high resolution calorimetry and custom-built nano-positioning platform have made possible, the first demonstration of ~40 fold increase in the power output, compared to far field, when the gap between the PV cell and thermal emitter at 650 K is reduced from ~10 µm to 60 nm. Further, we will describe ongoing efforts to achieve increases in both power output and efficiencies by engineering emitters that can reach high temperatures.
11:27AM S21.00002: Highly Efficient Solar Steam Generation by Glassy Carbon Foam Coated with Two-Dimensional Metal Chalcogenides*  
ZEESHAN TAHIR (Presenter), SUNGDO KIM, FARMAN ULLAH, Department of Physics, Univ of Ulsan, JOON I JANG, Department of Physics, Sogang University, YONG SOO KIM, Department of Physics, Univ of Ulsan — Steam generation by ecofriendly solar energy has immense potential in terms of low-cost power generation, desalination, sanitization and wastewater treatment. Herein, highly efficient steam generation in a bilayer solar steam generator (BSSG) is demonstrated which is comprised of a large-area SnSe-SnSe$_2$ layer deposited on glassy carbon foam (CF). Both CF and SnSe-SnSe$_2$ possess high photothermal conversion capabilities and low thermal conductivities. The combined bilayer system cumulatively converts input solar light into heat through phonon-assisted transitions in the indirect-bandgap SnSe-SnSe$_2$ layer, together with trapping of sunlight via multiple scattering due to the porous morphology of the CF. This synergistic effect leads to efficient broadband solar absorption. Moreover, the low out-of-plane thermal conductivities of SnSe-SnSe$_2$ and CF confine the generated heat at the evaporation surface, resulting in a significant reduction of heat losses. Additionally, the hydrophilic nature of the acid-treated CF offers effective water transport via capillary action, required for efficient solar steam generation in a floating form. A high evaporation rate (1.28 kgm$^{-2}$h$^{-1}$) and efficiency (84.1%) are acquired under one sun irradiation.

*National Research Foundation of Korea (NRF)

11:39AM S21.00003: Highly Efficient TiO$_2$ Nanorods@CF based Solar Steam Generator*  
SUNGDO KIM (Presenter), ZEESHAN TAHIR, ANH NGUYEN, JONGWOO PARK, YONG SOO KIM, Department of Physics, Univ of Ulsan — Harvesting solar energy via steam generation is an efficient way for brine and sewage water treatment. Directly bulk water heating with natural light yields low evaporation rates, owing to immense heat losses and its high heat capacity of water. Herein, we report styrofoam supported solar steam generator (SSG) comprised of glassy carbon foam (CF) covered with TiO$_2$ nanorods (TNRs). It shows a record high evaporation rate of 3.14 kgm$^{-2}$h$^{-1}$ under one sun irradiation. Such a high evaporation rate is mainly attributed to the synergetic effect of significant heat localization and reduction in enthalpy. Employing a low thermal conductivity, styrofoam naturally isolates the bulk water yielding an enhanced localization of heat. Concurrently, rapid water transport to SSG is ensured via a 2D air-laid paper as a wicking material. Moreover, the water molecules adsorbed in the form of clusters to the edges and tips of TNRs are more likely evaporate as clusters and thereby effectively reducing the enthalpy. Besides, the SSG offers broadband solar absorption displaying excellent photothermal conversion capability. Finally the facile method, low cost and longevity make our SSG a good candidate for application on a large scale.

*National Research Foundation of Korea (NRF)
11:51AM S21.00004: Continuum Model of Underground Thermal Energy Storage Applied to Efficiency Optimization  ANDERS CARLSSON (Presenter), Washington University, St. Louis — A major obstacle to extensive deployment of renewable energy sources is their seasonal intermittency. Borehole thermal energy storage (BTES) is an inexpensive technology that can mitigate this intermittency. Hot water is pumped from the center to the edge of an array of boreholes to heat it in the summer, and heat is discharged in winter by reversing the process. Mathematical modeling is key to efficiency improvement. I develop an approach to modeling BTES that is simpler than existing approaches that use either embedded symmetrized borehole temperature fields or explicit simulation of the full 3d geometry. This approach focuses on the average radial flow of water, and develops coupled 1d reaction-diffusion equations for the water and soil temperatures. These are supplemented by a time-dependent heat-transfer coefficient. With two adjustable parameters, the model fits four-year temperature data at 10-minute intervals from the Drake Landing Solar Community closely. I use the model to explore possible modifications to the charging and discharging strategies. A strategy in which heated water is discharged at variable distances can increase the efficiency by over 20% in some cases.

12:03PM S21.00005: Rattling-Induced Ultralow Lattice Thermal Conductivity in Simple Systems  RINKLE JUNEJA (Presenter), ABHISHEK SINGH, Indian Institute of Science — Rattling motion is one of the significant phenomena for achieving notable reduction in the thermal conductivity in complex crystal systems. To carry forward the advantages of rattling to simple crystal systems, we explored it in simpler cubic compounds AgIn$_5$S$_8$ and CuIn$_5$S$_8$. The weak and anisotropic bonding of Ag and Cu with the neighboring In and S causes the rattling motion, which result in very shallow anharmonic potential well for the rattlers Ag and Cu. The phonon spectra of these compounds have multiple avoided crossing of optical and acoustic modes, which are a signature of rattling motion. This leads to ultralow thermal conductivity. Even though Ag atoms contribute to the valence band states, the rattler modes of Ag do not scatter carriers significantly, leaving the electronic transport virtually unaffected. A combination of favorable thermal and electronic transport results in unprecedented figure of merit of 2.2 in p-doped AgIn$_5$S$_8$ at 1000 K. The proposed idea of having rattlers in simpler systems can be extended to a wider class of materials, which would accelerate the development of thermoelectric modules for waste energy harvesting.

Reference: ACS Appl. Mater. Interfaces, 11, 33894–33900, 2019
12:15PM S21.00006: On photon thermal Hall effect and persistent heat current in radiative heat transfer*  CHENG GUO (Presenter), YU GUO, SHANHUI FAN, Stanford Univ — We study the photon thermal Hall effect and the persistent heat current in radiative heat transfer. We show that the photon thermal Hall effect is not a uniquely nonreciprocal effect; it can arise in some reciprocal systems with broken mirror symmetry. This is in contrast with the persistent heat current, which is a uniquely non-reciprocal effect that can not exist in any reciprocal system. Nevertheless, for a specific class of systems with C4 rotational symmetry, we note that the photon thermal Hall effect is uniquely nonreciprocal, and moreover there is a direct connection between the persistent heat current and the photon thermal Hall effect. In the near-equilibrium regime, the magnitude of the photon thermal Hall effect is proportional to the temperature derivative of the persistent heat current in such systems. Therefore, the persistent heat current as predicted for the equilibrium situation can be probed by the photon thermal Hall effect away from equilibrium.

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12:27PM S21.00007: Self-sustaining Thermophotonic Circuits  BO ZHAO (Presenter), SIDDHARTH BUDDHIRAJU, PARTHIBAN SANTHANAM, KAIFENG CHEN, SHANHUI FAN, Stanford Univ — Photons represent one of the most important heat carriers. The ability to convert photon heat flow to electricity is therefore of substantial importance for renewable energy applications. However, photon-based systems that convert heat to electricity, including thermophotovoltaic systems where photons are generated from passive thermal emitters, have long been limited by low power density. This limitation persists even with near-field enhancement techniques. Thermophotonic systems, which utilize active photon emitters such as light-emitting diodes, have the potential to significantly further enhance the power density. However, this potential has not been realized in practice, due in part to the fundamental difficulty in thermodynamics of designing a self-sustaining circuit that enables steady-state power generation. Here, we overcome such difficulty by introducing a configuration where the light-emitting diodes are connected in series, and thus multiple photons can be generated from a single injected electron. As a result, we propose a self-sustaining thermophotonic circuit where the steady-state power density can exceed thermophotovoltaic systems by many orders of magnitude. This work points to possibilities for constructing heat engines with light as the working medium.
12:39PM S21.00008: Demonstration of thermal energy conversion though radiating optical rectennas for night harvesting applications  
AMINA BELKADI (Presenter), GARRET MODDEL, University of Colorado, Boulder — Night harvesting, where heat is harvested from the temperature difference between Earth and deep space, promises clean energy when sunlight is not available. The low efficiency of available thermal-to-electrical energy conversion technologies has been the largest barrier in the commercial pursuit of this technology. We present a new approach using radiating optical rectennas – femtosecond-fast metal-insulator-metal (MIM) diodes and micron-scale antennas – to overcome the limitations of low efficiency for low temperature differences (<100 °C). We experimentally demonstrate the basic principle of thermal-to-electrical energy conversion using a Ni-NiO-Al₂O₃-Cr-Au MIM diode-based optical rectenna, with a transmission line compensation structure to enhance the coupling efficiency between antenna and diode at terahertz frequencies. For a temperature gradient of 80° C, the device generates an open circuit voltage of 300 mV, corresponding to a power of at least 93 mW/m². Under practical operating conditions, this technology has the potential to exceed similar technologies exploiting radiative cooling.

12:51PM S21.00009: Relaxor-ferroelectrics: An efficient material for waste-heat harvesting*
AMRIT SHARMA (Presenter), MAKHES K BEHERA, SANGRAM K PRADHAN, CARL E BONNER, MESSAOUID BAHOURA, Norfolk State Univ — The need for efficient energy utilization is driving research to harvest waste-heat, which is ubiquitous, abundant, and free. Thermal energy harvesting for low power electronic devices using ferroelectric materials is one of the emerging areas of research because they possess spontaneous polarization and exhibit excellent pyroelectric coefficients. These materials are unique as they only sense time-dependent temperature change to generate electric power. We have grown lead-free BaZr₀.₂Ti₀.₈O₃ (BZT)/Ba₀.₇Ca₀.₃TiO₃ (BCT) multilayer heterostructures on SrRuO₃ (SRO) buffered SrTiO₃ (STO) single crystal substrates by optimized pulsed laser deposition (PLD) technique. We have developed a device with a capacitive structure of 200 nm thick BZT/BCT multilayer heterostructures sandwiched between platinum top and SRO bottom electrodes. The device demonstrates excellent pyroelectric current of ~600 nA in response to temperature fluctuation of 11 K using a laser diode of wavelength 850 nm with a repetition rate of 0.1 Hz and power 150 mW. Our findings suggest that the relaxor-ferroelectric thin film may be competitive with thermoelectric materials for low-grade thermal harvesting.

*NSF-CREST Grant number HRD 1036494 and NSF-CREST Grant number HRD 1547771.
Inorganic Multilayer Emitter for Passive Daytime Radiative Cooling

DONGWOO CHAE (Presenter), PIL-HOON JUNG, SOOMIN SON, YUTING LIU, HEON LEE, Department of Materials Science and Engineering, Korea university — Passive radiative cooling has been actively researched to compromise problems of active cooling. Passive radiative cooling refers to the cooling of a surface using optical properties without the supply of electricity from the external. In this study, Ag/Al₂O₃/Si₃N₄/SiO₂ multilayer structure was suggested and optimized by Particle Swarm Optimization (PSO). The multilayer was fabricated by E-beam evaporation and PECVD. Fabricated multilayer also has excellent radiative cooling properties with just three IR emissive layers of Al₂O₃, Si₃N₄, and SiO₂. In addition, since Al₂O₃, Si₃N₄, and SiO₂ is generally used as passivation layer, it has higher durability compared to polymer-based radiative cooler. The cooling temperature of the multilayer was measured using self-customized external cooling temperature measurement system. The cooling performance was calculated based on the optical properties of the multilayer using self-developed MATLAB tool. In Seoul which is mid-latitude and have relatively humid climate, the multilayer had cooling temperature of around 8°C during the daytime. And the calculated net cooling power and cooling temperature of the multilayer resonator was 66.0W/m² and 7.64°C respectively at T = 300K.

Low-temperature heat conduction in the Metal-Organic Framework Perovskite [C(NH₂)₃]Ni(HCOO)₃

DHARMENDRA SHUKLA (Presenter), Physics, Univ of Miami, THOMAS M. CARLINO, AMY M. SCOTT, Chemistry, Univ Miami, JOSHUA COHN, Physics, Univ of Miami — We report thermal conductivity (κ) measurements on single crystals of the metal-organic framework perovskite compound [C(NH₂)₃]Ni(HCOO)₃ in the temperature range 5K≤T≤300K. Measurements with heat flow along different crystallographic directions and under applied electric field will be presented and compared to κ measurements on the closely related compounds [C(NH₂)₃]X(HCOO)₃ (X=Zn, Cu).Thermal hysteresis, observed in the range 80K≤T≤300K, will also be discussed.


This material is based upon work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under grant No. DE-SC0008607, and by the Univ. Miami CAS Convergence grant.
Passive radiative cooling (PRC) of objects involves radiative heat loss into the cold outer space through the long wavelength infrared (LWIR) atmospheric transmission window. Due to its passive operation and net cooling effect, it is a promising alternative or complement to electrical cooling.\textsuperscript{1-2} For efficient PRC of objects, an unimpeded view of the sky is ideal. However, the view of the sky is often limited - for instance, the walls of buildings have $>50\%$ of their field of view subtended by the earth, while low-lying roofs are overshadowed by taller buildings. Moreover, objects on earth become heat sources under sunlight. Therefore, buildings with hot terrestrial objects in view experience reduced cooling or even heating.

We show that by using common materials with selective LWIR emittances, walls and roofs can radiatively cool to considerably lower temperatures than achievable by using traditional broadband emitters like paints. Cooling enhancements (theoretical and demonstrated) achieved by such materials opens opportunities for the appropriate selection and design of materials for building envelopes.


\*J.M. was supported by Schmidt Science Fellows, in partnership with the Rhodes Trust.
Neutron studies of the structure and dynamics of barocaloric Ammonium Sulfate*
HELEN WALKER (Presenter), Rutherford Appleton Lab, BERNET MEIJER, GUANQUN CAI, SHURONG YUAN, School of Physics and Astronomy, Queen Mary University of London, FRANZ DEMMEL, HELEN PLAYFORD, Rutherford Appleton Lab, ANTHONY PHILLIPS, School of Physics and Astronomy, Queen Mary University of London — Conventional vapour-compression refrigeration relies on refrigerants that contribute both to global warming and ozone depletion. Barocaloric materials, in which a large isothermal entropy change is associated with a pressure-induced phase transition, offer an eco-friendly alternative.

Recently a giant barocaloric effect has been demonstrated near the ferrielectric phase transition of ammonium sulfate [1], which is cheaply and widely available. The transition is associated with a symmetry change from Pnma to Pna2₁ at ~224 K at ambient pressure, while small changes in hydrostatic pressure drive giant inverse barocaloric effects near the ferrielectric phase transition.

The phase transition in (NH₄)₂SO₄ has been extensively studied, including crystallographic, Raman, reflectivity, NMR and infrared investigations, yet its exact nature is surprisingly still a matter of debate. We will present our neutron scattering experiments (total scattering, INS and QENS) probing the structure and dynamics of this material, which aim to identify the characteristics responsible for its exceptional barocaloric behaviour; and hence create a roadmap to develop new barocaloric materials and optimise their properties.


*Work supported by EPSRC grant EP/S03577X/1

A new source of thermal power
MILLICENT GIKUNDA (Presenter), PAUL MTHIBADO, Univ of Arkansas-Fayetteville — Due to an increasing need to produce self-charging, portable, implantable and wireless electronics with extended lifespans, development of energy harvesting systems is becoming increasingly important. Much emphasis has been placed on scavenging for vibrational energy as an alternative power source. A recent notable breakthrough is the discovery that when relaxed, sheets of freestanding graphene exhibit a rippled morphology, in which adjacent regions alternate between concave and convex curvature. These ripples form due to self-compression.

Here, I will discuss modelling ripple curvature inversion dynamic of freestanding graphene using Langevin's equation and fluctuation - induced current from freestanding graphene. I model one ripple as a Brownian particle in a double well potential with a minimum energy which corresponds to a ripple with concave and convex curvature. The particle is in contact with a thermal bath which is represented by an external white noise source. Interactions with the other ripples which occurs on longer time scales and keep the ripple out of equilibrium are mimicked by an Ornstein-Uhlenbeck colored noise.
11:15AM S22.00001: Adaptive robot morphology and behavioral control policy through responsive composite materials [Invited] REBECCA KRAMER-BOTTIGLIO (Presenter), Yale University — Robots generally excel at specific tasks in structured environments, but lack the versatility and adaptability required to interact with the real world. In this talk, I will introduce several soft robot platforms that can adapt both their shape and behavior to accommodate different tasks or environments. While actuation alone may temporarily change a robot’s shape, I will show that the ability to change resting shape is an advantage of soft robots, and that shape control can offset computationally-expensive tasks such as gait changes and obstacle avoidance. The focus will be on the responsive composites that enable these functional capabilities, including variable stiffness materials for move-and-hold shapeshifting applications, switchable stretchability materials for adaptive trajectories of volumetrically-expanding actuators, and stretchable circuitry for material-embedded computation.

11:51AM S22.00002: Robots and animals transition from less to more favorable modes to traverse obstacles RATAN SADANAND OTHAYOTH MULLANKANDY (Presenter), GEORGE THOMS, CHEN LI, Johns Hopkins University — Legged robots still struggle to robustly traverse obstacles in complex terrain using physical interaction, which animals do at ease. Recent studies revealed that cockroaches use body-beam interaction to traverse grass-like beam obstacles, probabilistically transitioning between locomotor modes. To understand what governs the direction of locomotor transitions between modes, we developed and studied a robophysical model traversing beams of variable stiffness. We discovered that, when viewed on a potential energy landscape resulting from body-beam interaction, different locomotor modes (system state trajectories) were attracted to different local minima basins. Regardless of beam stiffness, the system was always more likely to transition from less to more favorable modes (i.e., from lower to higher energy local minima) on the landscape, as long as kinetic energy fluctuation from oscillatory self-propulsion is sufficient to overcome the potential energy barrier in between. We made similar observations in cockroaches, despite their active behaviors. These physical principles are surprisingly similar to microscopic systems (e.g., protein-folding transitions on a free energy landscape). Our study is a step in establishing energy landscapes for locomotor transitions in complex terrain.
12:03PM S22.00003: Active adjustments help cockroaches traverse obstacles by lowering potential energy barrier  YAQING WANG (Presenter), RATAN SADANAND OTHAYOTH MULLANKANDY, CHEN LI, Johns Hopkins University — Robots predominantly navigate complex environments by using geometric models to avoid physical contact with obstacles. By contrast, animals easily traverse obstacles by using physical interaction controlled by active feedback. Our previous study revealed that cockroaches made active adjustments to traverse grass-like beam obstacles. As the animal pushed against the beams, its body pitched up. Then, the animal often quickly rolled into the gap between beams to traverse. In this process, the animal's head often flexed repeatedly, and one hind leg pushed against the ground while the other retracted. Here, we used physics modeling and robot experiments to understand the function of such active adjustments. We calculated system potential energy (resulting from gravity and beam elastic bending) as a function of head flexion. When the animal was in contact with the beams, head flexion lowered its potential energy barrier to transition from pitch to roll mode (by nearly half for the observed head flexion of 20°). We hypothesize that the animal uses proprioception (internal position and force sensing) to detect changes in beam resistive forces, which reflect the reducing transition barrier. We are developing a robotic physical model instrumented with force sensors to test this hypothesis.

12:15PM S22.00004: A template model reveals self-righting mechanism of a winged robot QIHAN XUAN (Presenter), CHEN LI, Johns Hopkins University — Animals and robots must self-right after flipping-over on the ground. Winged insects like many cockroaches push wings against the ground while flailing legs to generate lateral perturbation to self-right. Our previous study of a cockroach-inspired robot revealed the importance of good coordination (measured by phase) between wing pushing and leg flailing. Here, we elucidate the mechanism of phase dependence by developing a template model, validated against multi-body dynamics simulation. The model consists of a point mass body rotating in the sagittal plane, two massless wings, and a flailing leg with a point mass at its end. With modest wing opening and leg flailing, the model struggled to self-right, and successful righting relied on good coordination of the wings and leg. We used the model to calculate the potential energy barrier the body must overcome, mechanical energy input by the wings and leg, and energy dissipation due to collision and friction. With good phases, mechanical energy accumulation exceeded potential energy barrier; with bad phases, it did not do so. We used the template model to predict an optimal coordination strategy to increase self-righting probability. Our study highlighted the importance of appendage coordination in strenuous locomotor transitions.
12:27PM S22.00005: Testing the effect of scaling on microrobot locomotion performance
KAUSHIK JAYARAM (Presenter), University of Colorado, Boulder, ROBERT WOOD, Harvard University — The effects of scaling on locomotion performance has fascinated biologists, physicists and engineers alike. In particular, roboticists have exploited dynamic scaling to build systems at sizes varying from a tens of centimeters to several meters. Thanks to recent advances in manufacturing, insect-scale robotics is currently an exciting research direction and holds the promise of tremendous impact in areas of search-and-rescue and high-value asset inspection. However, most robots at this scale have simplified morphology and can only demonstrate basic mobility. Here, we present the newly designed HAMR-Jr, a 22.5mm, 320mg quadrupedal microrobot. With eight independently actuated degrees of freedom, HAMR-Jr is, to our knowledge, the most mechanically dexterous legged robot at its scale and is capable of high-speed locomotion (13.91 bodylengths/s) at a variety of stride frequency (1-200Hz) using multiple gaits. We achieved this using a design and fabrication process that is flexible, allowing us to exploit and implement the physics of scaling with minimum changes to our workflow. We further characterized HAMR-Jr’s open-loop locomotion and compared it with the larger scale HAMR-VI microrobot to demonstrate the effectiveness of scaling laws in predicting running performance.

12:39PM S22.00006: Tail control decreases jamming of a mechanics-dominated legged robot on rough terrain  DANIEL SOTO (Presenter), DANIEL I GOLDMAN, Georgia Inst of Tech — To develop robot locomotion principles which leverage mechanics to simplify control, we study a minimally aware quadrupedal RHex-type robot (~3kg, 20 cm long) walking on a rough terrain composed of blocks with Gaussian height distribution with mean and variance approximately leg length and one-quarter leg length respectively. This terrain resulted in failure modes due to limb jamming in protruding regions of the terrain. Performance was insensitive to gait symmetries (phasing and duty factor of limbs). To reduce jamming probability while maintaining the focus on minimal control and mechanics, we added a motor driven 10 cm long tail whose pitch and yaw actuation was uncoupled to limb dynamics. We experimented with a variety of open loop behaviors such as tapping, pulsing, and maintaining a constant angle with the body. We also developed a closed loop tapping scheme that triggered on IMU measured pitch and roll of the robot. Jamming probability could be reduced to near zero for open and closed loop schemes. The appropriate tail behaviors helped maintain either high or low “robot temperature” (variance of instantaneous velocity) relative to tail-less robot temperature.
12:51PM S22.00007: Modulation of robot orientation by exploiting leg-obstacle collisions through successive choices of gait* FEIFEI QIAN (Presenter), YONGXIN GUO, ANMOL KATHAIL, DANIEL KODITSCHEK, University of Pennsylvania — An environment can provide different affordances for locomotion based on a locomotor’s actions. Our study aims to explore how multi-legged robots can use various gaits to exploit the affordance of obstacle collisions to negotiate complex environments in different ways.

To allow assessment of obstacle affordances, we represent physical obstacles as a horizontal-plane disturbance field. For a given physical environment, the disturbance field is fixed. However, when a (structured) disturbance field couples with (periodic) locomotor gaits, there emerge stable fixed-point heading directions with substantial basins of attraction.

In this study, we show that the basins around these fixed-point headings depend sensitively on the locomotor gaits. We investigate the transit between these basins as a quadrupedal robot explores its 3-dimensional gait space (each dimension represents the relative phase difference between one pair of legs), and show that these gait-dependent basins allow the robot to take advantage of the repeated leg-obstacle collisions to robustly achieve desired sequences of headings without active steering.

*This research was supported by the National Science Foundation (NSF) under INSPIRE award, CISE NRI #1514882 and NRI INT award #1734355.

1:03PM S22.00008: A systematic approach to creating terrain-capable hybrid soft/hard myriapod robots YASEMIN OZKAN-AYDIN, ENES AYDIN, BAXI CHONG, DANIEL I GOLDMAN (Presenter), Georgia Inst of Tech — Multi-legged animals such as centipedes move effectively in diverse terrain. Their flexible body and limbs allow them to adapt their shape to the environment and traverse obstacles. To examine how the variation in body/limb forms of legged animals affects the mechanics of terrestrial locomotion, we built a multi-legged hybrid (soft/rigid) robot that has 8 segments (9 cm/segment), each with two out of phase legs. Back elements and limbs are driven by servo motors. We systematically tested the gait patterns with different leg contacts and body undulation provided by geometric mechanics on various environments including flat ground, obstacle course, stair climbing, and unstructured natural terrain. On flat ground, the robot with completely rigid parts moved in the same way as theoretically predicted gaits. As the complexity of the environment increases, adding flexibility into the robot body parts (legs, body joints, etc.) improved the locomotion performance by either reducing the effects of environmental disturbances or increasing stability.
1:15PM S22.00009: Basilisk Lizard Bipedal Locomotion on Sand, Mud, and Water: An Insight to Future Morphing Amphibious Robots  
HOSAIN BAGHERI (Presenter), MARCUS GAMBATESE, Arizona State Univ, DAVID LENTINK, Stanford University, HAMIDREZA MARVI, Arizona State Univ — With the astonishing development in robotics, one area that still remains an open challenge is their physical interaction with the outside world, beyond that of factory floors. In order for robotic devices to integrate and conquer obstacles introduced by the surrounding world, they will need to be able to traverse on and through diverse and alternating mediums and terrains. To address this desire of adaptive multi-modal locomotion, we look to the basilisk lizard as a form of inspiration and means of understanding how it can effectively run and transition from land to water, and vice versa. By shedding light on both active (i.e. gait, body dynamics) and passive (i.e. tail swing, toe fringes) mechanisms used by the animal, more competent robotic systems can be developed for the interaction and exploration of both terrestrial and aquatic environments. Notably, passive mechanisms do not require input power, sensing, or controls for operation. Through conducting animal experiments in both terrestrial and aquatic environments (and the transition between the two), the hierarchical physics of animal interaction with complex environments can be extracted and channeled towards the development of a bio-inspired amphibious robot for planetary exploration and search-and-rescue applications.

1:27PM S22.00010: Hierarchical control in sea star inspired locomotion*  
SINA HEYDARI (Presenter), Aerospace and Mechanical Engineering, University of Southern California, THEODORA PO, MATTHEW MCHENRY, Ecology and Evolutionary Biology, University of California, Irvine, EVA KANSO, Aerospace and Mechanical Engineering, University of Southern California — There is a growing effort to understand decentralized control mechanisms, particularly in application to robotic systems with distributed sensors and actuators. Sea stars, being equipped with hundreds of tube feet, are an ideal model system for studying decentralized sensing and actuation. The activity of the tube feet is orchestrated by a nerve net that is distributed throughout the body; there is no central brain. We developed mathematical models of the biomechanics of the tube feet and the sea star body. We then formulated hierarchical control laws that capture salient features of the sea star nervous system. Namely, at the component level, the individual tube feet follow a state-dependent feedback controller. At the system level, a directionality command is communicated to all tube feet. We studied the locomotion gaits afforded by this control model. We find that these minimally-coupled tube feet coordinate to generate robust forward locomotion on different terrains. Our model also predicts different gait transitions consistent with our experiments performed on Protoreaster nodosus. These findings offer a new paradigm for walking using soft actuators, with potential applications to autonomous robotic systems.

*Supported by Office of Naval Research (ONR) grant N00014-17-1-2062.
1:39PM S22.00011: Hopping with Elastic Restitution Is More Difficult Than It Seems  TAYLOR MCLAUGHLIN, MARION ANDERSON (Presenter), SHAI REVZEN, Univ of Michigan - Ann Arbor — Bouncing rubber balls and hopping on pogo sticks might suggest that building a robot that hops with a significant fraction of elastic energy restitution would be straightforward. Using spring steel legs with 99% restitution individually, we built a three-legged hopper. The hopper achieved a minute 11.2% restitution when using the springs in series with the actuators. We present five generations of three-legged hoppers: four have actuators in series with springs. Three different types of ground contact were tested. Our best design so far uses actuators in parallel with the springs, and achieves 49+/−5% restitution. This work will be of use to those interested in using elastic energy storage in legged locomotion.

1:51PM S22.00012: Recovery of Behaviors of Robots without Dynamics  GEORGE COUNCIL (Presenter), SHAI REVZEN, Univ of Michigan - Ann Arbor — For robots to function without humans on hand to fix them, they must be able to compensate for malfunctions that inhibit their ability to move all actuators.

The conventional choice would be to model the damaged robot, either by anticipating damage types and their effects on a known model, or by performing system identification on the damaged device. However, anticipating failure is fragile, and data-driven system ID of dynamics is expensive in time and robot wear-and-tear.

We instead suggest a method that leverages data from examples of successful motion to produce "behavior specifications" as constraints on outputs and states. By collecting time-series data from (nearly arbitrary) observation functions on a working robot, we defined a behavior as a list of differential constraints. The constraints, along with intrinsic constraints of physics, classify trajectories into those that yield a desired behavior, and those that do not.

For systems with many degrees-of-freedom, there are typically entire sub-manifolds of curves that meet the constraints. Assuming that the damaged robot retains enough control freedom to re-enforce our constraints, we can design an input that restores a desired behavior.

We demonstrate our method on a crawler in simulation, and on a dynamic hexapod in hardware.

2:03PM S22.00013: Modeling of the Primary Animal Gaits by Coupled Identical Raleigh-Van der Pol Oscillators  MASOUD ASADI-ZEYDABADI (Presenter), MOZHDEH SAFFARI-PARIZI, RANDALL TAGG, University of Colorado, Denver — Mathematical models based on coupled oscillators successfully describe animal gaits. The dynamics of individual oscillators (internal dynamics) in the network is nonlinear and must be at least two-dimensional to have a Hopf bifurcation. One example of this type of dynamics is a network of Rayleigh - Van der Pol oscillators which is used to produce primary gaits such as walk, trot, pace and bound. When these oscillators couple together, they produce patterns of relative phases that correspond to the different animal gaits. The patterns emerge through bifurcations as parameters describing the coupling are varied. At least eight cells are required to model the quadruped gaits.

Thursday, March 5, 2020 11:15 AM - 2:15 PM
11:15AM S23.00001: Protein condensates as aging Maxwell fluids [Invited] LOUISE JAWERTH (Presenter), for the Physics of Complex Systems, Max Planck Institute — Liquid-like protein condensates (LLPCs) are intracellular compartments that segregate material without the use of a membrane. The liquid-like behavior of the condensates is a defining characteristic and the viscosity, surface tension and other material properties determine how segregated species diffuse into and within condensates; they, thus, critically impact the biological function of the condensates. It has become increasingly clear that some LLPCs do not have time-independent material properties, but can, instead, transition to more solid, gel-like materials. Here, we present our efforts to quantify these new materials as they age in vitro. We measure the visco-elastic material properties of several proteins, (PGL-3, FUS and DDX4), by means of a combination of active and passive microrheology. At early times, we find that the droplets behave much like simple liquids but gradually become more elastic. Surprisingly, the changing mechanical properties can all be scaled onto a single master curve using one characteristic time scale which grows as the sample ages. This and other features we observe bear a striking resemblance to the behaviors observed in materials with glass-like aging. We consider protein condensates as soft glassy materials with age dependent material properties that we call Maxwell glasses. To gain insight into the molecular origins of this behavior, we present electron microscopy images of the condensates at different ages. Furthermore, we demonstrate how salt concentration tunes the characteristics of the aging process. Lastly, we speculate on possible molecular origins that might lead to the glass-like arrest we observe and how such arrest could be used for modulation of cellular biochemistry.

11:51AM S23.00002: Surface Fluctuations and Coalescence of Nucleolar Droplets in the Human Cell Nucleus* CHRISTINA M. CARAGINE (Presenter), SHANNON C HALEY, ALEXANDRA ZIDOVSKA, Physics, New York Univ NYU — The nucleolus is a membraneless organelle embedded in chromatin solution inside the cell nucleus. By analyzing the surface dynamics and fusion kinetics of nucleoli in live human cells, we find that the nucleolar surface exhibits subtle, but measurable, shape fluctuations and the radius of the neck connecting two fusing nucleoli grows as r(t)~t^{1/2} [1]. This is consistent with liquid droplets with low surface tension ~10^{-6} Nm^{-1} coalescing in a fluid of higher viscosity ~10^{3} Pa s, i.e. chromatin solution. We find the neck velocity, dr/dt, is comparable to the velocity of chromatin solution [2]. Surprisingly, nucleolar coalescence occurs in an active fluid, yet can be described by coalescence theory for passive liquid droplets, suggesting the measured quantities might be effective quantities. Our study presents a noninvasive approach, using natural probes to investigate material properties of the cell as well as to understand the physical interactions between nucleoli and chromatin solution [1,3].

*This work was supported by the National Institutes of Health Grant R00-GM104152 and by the National Science Foundation Grants CAREER PHY-1554880 and CMMI-1762506.
12:03PM S23.00003: Phase separation in the nucleus is limited by chromatin mechanics* 

YAOJUN ZHANG (Presenter), DANIEL LEE, Princeton University, YIGAL MEIR, Physics, Ben-Gurion University, CLIFF BRANGWYNNE, NED WINGREEN, Princeton University — Liquid-liquid phase separation is a fundamental mechanism underlying biological organization. While conventional theory predicts that a single phase-separated condensate would be energetically favored, both natural and synthetic condensates in cells typically appear as multiple dispersed droplets with suppressed growth dynamics. Here, we combine coarse-grained molecular dynamics simulations and theory of liquid-liquid phase separation to show that mechanical interactions with chromatin can constrain the size of droplets in the nucleus. The "gel-like" chromatin suppresses both droplet coalescence and ripening dynamics, resulting in a reduced scaling exponent for mean droplet radius versus time. Our work highlights the impact of the local mechanical environment on biomolecular condensate formation and growth, and further elucidates the role of mechanics in fundamental biological processes taking place in the cell nucleus.

*This work was supported in part by the NSF, through the Center for the Physics of Biological Function (PHY-1734030), the Graduate Research Fellowship Program (DCE-1656466, D.S.W.L.), NIH Grants R01 GM082938, U01 DA040601, and the HHMI.

12:15PM S23.00004: Subdiffusive Dynamics of Optogenetic Droplets Report on Local Chromatin Mechanics* 

DANIEL LEE (Presenter), Lewis-Sigler Institute for Integrative Genomics, Princeton University, SHUNSUKE SHIMOBAYASHI, YI-CHE CHANG, AMY R STROM, Department of Chemical and Biological Engineering, Princeton University, NED WINGREEN, Department of Molecular Biology; Lewis-Sigler Institute for Integrative Genomics, Princeton University, CLIFF BRANGWYNNE, Department of Chemical and Biological Engineering, Princeton University; Howard Hughes Medical Institute — DNA is organized into chromatin, a complex material which stores information and controls gene expression. Liquid-liquid phase separation is believed to be a principal mechanism governing its organization. Previous work with optogenetically activatable droplets demonstrated that liquid condensates displace chromatin. Here, we show that droplet growth dynamics are directly inhibited by chromatin. Generally, droplet radii follow a power law scaling with time, such that $R \sim t^\beta$. We observe an anomalously slow coarsening exponent during interphase but recover dynamics more consistent with classical theory when chromatin is condensed during mitosis. We show that this slowed growth is due to subdiffusion of individual condensates, a clear signature of elastic behavior in the nucleus. We further apply this framework to elucidate local mesoscopic mechanics of the nucleus in various biologically relevant contexts. Thus, our work demonstrates the use of engineered intracellular condensates as “probes” of local mesoscale nuclear organization.

*This work was supported by NIH Grant U01 DA040601, the Howard Hughes Medical Institute, and the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030) and the Graduate Research Fellowship Program (DCE-1656466).
Converting Stochastic Assembly into an Assembly Line: Non-Equilibrium Droplet Dynamics Assists Ribosome Formation  
TYLER HARMON (Presenter), FRANK JULICHER, Max Planck Institute for the Physics of Complex Systems — The nucleolus is a large liquid-like membraneless organelle responsible for the majority of the processing of ribosomal components and the assembly of ribosomes, which involves hundreds of proteins. It has been suggested that one of the primary functions of the nucleolus is to concentrate these proteins with the ribosomal RNA (rRNA), thereby significantly enhancing the binding rates and enzyme reaction speed for ribosome assembly and post-translational modifications.

Here we expand on this idea by considering the non-equilibrium effects that arise from having a constant rRNA flow outward from the center of a nucleolus and an inward flow of ribosomal protein (rProtein) from the nucleoplasm. We show numerically and analytically that the binding of specific rProteins to rRNA can be localized within a well-defined radial shell inside the nucleolus instead of being homogeneously distributed. By giving the different rProteins different physical properties, the different rProteins can be confined to bind to the rRNA at different radial distances from the transcription centers within the nucleolus. Thus, as rRNA molecules diffuse outward through the nucleolus, the rProteins can be added in sequential order like an assembly line.

Reentrant Liquid Condensation of Ribonucleoprotein–RNA Complexes  
MURALIKRISHNA RAJU (Presenter), RABIA LAGHMACH, DAVIT POTOYAN, Iowa State University — Intracellular Ribonucleoprotein (RNP) granules are membrane-less liquid condensates that dynamically form, dissolve, and mature into a gel-like state in response to a changing cellular environment. RNP condensation is largely governed by attractive inter-chain interactions mediated by low-complexity domains. Using an archetypal disordered RNP, fused in sarcoma (FUS), here we employ atomistic simulations to study how RNA, a primary component of RNP granules, can modulate the phase behavior of RNPs by controlling both droplet assembly and dissolution. Electrostatic interactions are found to be the primary driving force behind condensate formation. Monotonically increasing RNA concentration initially leads to droplet assembly via complex coacervation and subsequently triggers an RNP charge inversion, which promotes disassembly. We construct phase diagrams based on Droplet density and Shannon entropy calculations, wherein three distinct regimes can be identified based on RNA and peptide concentrations. Increasing salt concentration is found to inhibit the formation of liquid condensates and narrow the coexistence region. The internal organization and dynamics of the condensates are investigated as a function of RNA/peptide concentrations, RNA chain length and salt concentration.
12:51PM S23.00007: Size selection of phase-separated liquid droplets in strain-stiffening elastic networks*  SHENG MAO (Presenter), MIKKO HAATAJA, ANDREJ KOSMRLJ, Princeton University — Membraneless organelles are formed via phase separation inside cells, but it remains unclear how cytoskeleton affects this process. Recent experiments showed the size of separated droplets is controlled by the stiffness of the surrounding elastic network. This is in contrast to phase separation of liquid mixtures, which continue to coarsen indefinitely (Ostwald ripening). Motivated by these observations, we developed a model to investigate the coupling between the separating liquid mixture and the elastic network. We find that the elastic energy of distorted network effectively modifies the nucleation barrier and the critical nucleus size for the separating mixture. For a neo-Hookean elastic network we find that the coarsening proceeds indefinitely. On the other hand, for networks with sufficiently strong strain-stiffening considered in experiments we find that the elastic energy arrests the coarsening once droplets reach certain size. Furthermore, finite element simulations indicate that the interactions between droplets via the distorted elastic network are rather short-ranged, which explains why observed droplets in experiments achieve a uniform size.

*This work was supported by NSF through the Princeton University Materials Research Science and Engineering Center DMR-1420541.

1:03PM S23.00008: A hydrodynamic instability drives TPX2 protein droplet formation on microtubules and leads to branching microtubule nucleation*  SAGAR SETRU (Presenter), BERNARDO GOUVEIA, RAYMUNDO ALFARO-ACO, MATTHEW R KING, HOWARD A STONE, JOSHUA SHAEVITZ, SABINE PETRY, Princeton University — Microtubules are protein polymers with a variety of roles in biological cells. During cell division, many microtubules are generated by branching from the surface of preexisting microtubules. Recent work in vitro and ex vivo shows that the protein TPX2 drives the nucleation of branched microtubules by bringing augmin and the gamma-tubulin ring complex (gTuRC) to microtubules. It has also been shown that TPX2's ability to condense into a liquid phase is important for branching. Using atomic force microscopy, fluorescence imaging, electron microscopy, and hydrodynamic theory, we show that the dynamics of liquid TPX2 are crucial for nucleating branched microtubules. Initially, TPX2 coats the surface of microtubules in seconds, producing a cylindrical, liquid tube around the microtubule with an even thickness of 13-17 nm. Then, this layer loses stability due to surface tension, producing discrete droplets regularly spaced by 140-250 nm via a Rayleigh-Plateau mechanism. These droplets bind augmin and gTuRC to the microtubule surface, thus localizing where branches can form. Together, our work explains how the liquid phase of TPX2 leads to branching microtubule nucleation.

*We thank the NIH, NSF, Pew Scholars Program, Lucille & David Packard Foundation, HHMI, and PD Soros Fellowship.
Motif Sequences and Intracellular Phase Separation

BENJAMIN WEINER (Presenter), Princeton University, YIGAL MEIR, Ben-Gurion University, NED WINGREEN, Princeton University — Intrinsically Disordered Proteins (IDPs) lack a unique folded structure, and yet perform diverse and important functions inside cells. Recent work suggests that some IDPs promote the formation of membrane-less organelles via phase separation, helping cells spatially organize their biomolecules. Classical theories of phase separation focus on homopolymers, but IDPs have evolved particular sequences of interacting motifs. How does an IDP’s motif sequence determine its physical properties? We propose a statistical physics model of IDPs to elucidate the relationship between motif sequence, the phase boundary, and the partitioning of proteins between phases.

We find that motif sequences strongly influence the physical properties of model IDPs. Intuitively, each sequence has its own preference for inter- versus intra-protein bonds, which favor a condensed versus a dilute phase, respectively. As a result, the concentration of IDPs required for phase separation depends strongly on the motif sequence. Our work demonstrates the emergence of spatial order from conformational disorder, a process which may play a key role in intracellular organization.

*This work was supported in part by the National Science Foundation, through the Center for the Physics of Biological Function (PHY-1734030).

Coupling signaling cascades to membrane criticality

TAYLOR SCHAFFNER (Presenter), BENJAMIN B MACHTA, Yale University — Cellular biology has long understood spatial organization to be a crucial feature for determining function. Recent evidence suggests that thermodynamic phase separation may explain a range of structures in Eukaryotic cells. In particular, proximity to a liquid-liquid critical point may underlie membrane domains that are often termed lipid rafts. Such domains have been implicated in the functioning of many signaling cascades by localizing components to particular domains. Addition of ligand may lead to the formation of signaling platforms, and perturbations to membrane criticality often modify signaling outcomes. In order to create a theory that explains the interplay between signaling cascades and membrane criticality, here we present a model and Monte-Carlo simulation framework for proteins coupled to their surrounding lipid membrane using a 2D Ising model. We have additionally developed schematic diagrams that predict the effects of domain size on the outcome of various simple signaling cascade motifs. Our model naturally explains how changes in domain size arising from perturbations to membrane criticality can lead to changes in the rates of interaction amongst signaling components, eventually leading to altered signaling outcomes.

*Funded in part by NIH R01 GM129347
Wetting of Critical Membranes by Protein Droplets

MASON ROUCHES (Presenter), Molecular Biophysics and Biochemistry, Yale University, SARAH VEATCH, Biophysics, University of Michigan, BENJAMIN B MACHTA, Physics, Yale University — Phase-separated liquid-droplets of protein and RNA have recently been found as ubiquitous structures in cells – coordinating reactions, organizing cellular machinery, and protecting sensitive biomolecules. In two dimensions, the plasma membrane is organized by heterogeneities in lipid composition, with membrane domains posited to be a consequence of proximity to a miscibility critical point. These structures are linked by components that interact with both 2D and 3D phases such as lipidated proteins that partition into specific membrane phases. This leads protein droplets to localize to particular membrane domains, as seen in the post-synaptic structure, the immunologic synapse, and components of cell adhesion. Here, we consider the underlying thermodynamics of this interaction, constructing a minimal Landau theory describing the wetting of protein droplets to a near-critical membrane. The resulting phase diagram shows non-standard wetting behavior, where surface criticality greatly enhances a prewetting-like regime where bulk and surface phase separate together. We buttress these theoretical predictions with simulations of nearly critical Ising surfaces coupled to coacervating lattice polymers and link existing experimental observations to this phase diagram.

*NSF DMR-1905621

Probing the Dynamics of Optically Induced Protein Droplets with Single-Walled Carbon Nanotubes

HUGH HIGINBOTHAM (Presenter), SEBASTIAN COUPE, YOON JUNG, NIKTA FAKHRI, Massachusetts Institute of Technology MIT — Eukaryotic cells exhibit high levels of internal spatial organization, including a wide variety of membrane-less compartments. Protein-protein and protein-RNA interactions have been implicated as the primary factors responsible for these membrane-less structures, but how they are maintained and utilized by the cell is still poorly understood. Many proteins essential to the formation of these structures feature long intrinsically disordered regions (IDRs) that interact with each other and can induce demixing, as seen in many recent in vitro studies. However, quantitative characterization of these structures in vivo remains challenging due to the complexity of intracellular environments. Here, we use single-walled carbon nanotubes (SWNTs), which fluoresce in the near infrared and are photostable, to probe the local environment of optically induced protein droplets in vivo. The dynamics of SWNTs can reveal internal organization within these droplets and the influence of the intracellular environment on their mechanical properties.
Measuring protein concentrations in biomolecular condensates via quantitative phase microscopy

PATRICK MCCALL (Presenter), Max Planck Institute of Molecular Cell Biology and Genetics; Max Planck Institute for the Physics of Complex Systems; Center for Systems Biology Dresden, KYOOGHYUN KIM, Biotechnology Center, Technische Universität Dresden; Max Planck Institute for the Science of Light, JIE WANG, Max Planck Institute of Molecular Cell Biology and Genetics, ANATOL W. FRITSCH, Max Planck Institute of Molecular Cell Biology and Genetics; Max Planck Institute for the Physics of Complex Systems; Center for Systems Biology Dresden, ANDREY POZNYAKOVSKIY, Max Planck Institute of Molecular Cell Biology and Genetics, BENEDICT DIEDERICH, Leibniz Institute of Photonic Technology, MORITZ KREYSING, Max Planck Institute of Molecular Cell Biology and Genetics; Center for Systems Biology Dresden, RAINER HEINTZMANN, Leibniz Institute of Photonic Technology; Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, JOCHEN GUCK, Biotechnology Center, Technische Universität Dresden; Max Planck Institute for the Science of Light, SIMON ALBERTI, Max Planck Institute of Molecular Cell Biology and Genetics; Biotechnology Center, Technische Universität Dresden, JAN BRUGUÉS, Max Planck Institute of Molecular Cell Biology and Genetics; Max Planck Institute for the Physics of Complex Systems; Center for Systems Biology Dresden, ANTHONY HYMAN, Max Planck Institute of Molecular Cell Biology and Genetics — Many compartments in eukaryotic cells are protein-rich biomolecular condensates formed via phase separation from the cyto- or nucleoplasm. Although knowledge of condensate composition is essential for a full description of condensate properties and potential functions, measurements of composition pose a number of technical challenges. To address these, we use quantitative phase microscopy and optical diffraction tomography to measure the refractive index of model condensates, from which the protein concentration may be inferred. Here, model condensates are formed by phase separation of purified protein constructs derived from the primarily disordered RNA-binding domain (RBD) of TAF15. Surprisingly, we find that phase separation of TAF15(RBD) is attenuated only weakly by salt (0.05-3 M KCl) or temperature (10-50 °C), suggesting that Coulombic and entropic interactions, respectively, play only minor roles in controlling the phase equilibria. Interestingly, we also find that partition coefficients determined by fluorescence microscopy dramatically underestimate protein concentrations in condensates. A simple model including inner filter and excited-state saturation effects suggests that the discrepancy stems primarily from reduced fluorescence quantum yields in condensates.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S24 GSNP DSOFT DBIO: Glassy Dynamics: From Simple Models to Biological Tissues | 401 - Amy Graves, Swarthmore Coll
11:15AM S24.00001: Solving the equilibrium dynamics of particle systems in infinite dimensions* ALESSANDRO MANACORDA (Presenter), FRANCESCO ZAMPONI, Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université de Paris, F-75005 Paris, France, GRÉGORY SCHEHR, LPTMS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France — In the last years, a general framework to study the dynamics of particle systems in infinite dimensions has been developed. This theory can be applied to a wide class of physical cases both in and out of equilibrium, including the physics of glasses, colloids and active matter. On the other hand, even for the equilibrium - simplest - case, an analytical solution of the dynamical equations is out of reach. I will show how a numerical solution can be found, leading to the emergence of a dynamical transition in the case of short-ranged repulsive potentials. The numerical analysis for long times matches the predictions obtained by thermodynamical arguments at equilibrium, and provides new observations such as the behavior in time of the memory kernel and the critical scaling of the diffusivity when approaching the dynamically arrested phase. The consistency of the results at equilibrium is the first step to obtain new insights into non-equilibrium physical phenomena, which will represent the future direction of the research.

*This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement n° 723955 - GlassUniversality).

11:27AM S24.00002: Investigating Hydrogen Glass Dynamics in Amorphous Germanium and Amorphous Silicon-Germanium Alloys* BRENDA KNAUBER (Presenter), School of Physics and Astronomy, University of Minnesota, MOHAMMAD ALI ESLAMISARAY, Department of Mechanical Engineering, University of Minnesota, JAMES KAKALIOS, School of Physics and Astronomy, University of Minnesota — A hydrogen glass model has successfully accounted for stretched exponential relaxation (SER) of the conductivity and non-Gaussian $1/f$ noise in hydrogenated amorphous silicon (a-Si:H) thin films, in agreement with hydrogen diffusion studies. We have recently reported non-Gaussian $1/f$ noise in hydrogenated amorphous germanium (a-Ge:H) consistent with hierarchically constrained kinetics, reflected in log-normal noise power distributions, strong correlations between noise power octave bins and scaling of the second spectra. The similarities in the $1/f$ noise of a-Ge:H and a-Si:H motivated our study of current relaxation in a-Ge:H. However, unlike the a-Si:H SER decay of the conductivity, in a-Ge:H we find a time-dependent increase of the conductivity at constant temperature. For a-Ge:H, the stretched exponential power-law exponent and time constant are similar to that observed in a-Si:H, but only for temperatures above 390K. A set of hydrogenated amorphous silicon-germanium alloys are studied to investigate the transition in the noise statistics and conductivity relaxation as the alloy fraction changes.

*This work was partially supported by NSF grants DMR-1608937 and PHYS-1344251, the NINN Characterization Facility, the Minnesota Nano Center and the University of Minnesota.
11:39AM S24.00003: Towards a Unifying Scaling Theory of Rigidity Transitions*

FARSHID JAFARPOUR (Presenter), SEAN RIDOUT, ANDREA JO-WEI LIU, University of Pennsylvania — A large class of models describing various athermal disordered systems such as granular materials, living tissues, and polymer networks exhibit transitions from fluid or floppy states to rigid states. In some cases, the transition marks the boundary between the underconstrained region of parameter space to the overconstrained region, while in other cases, the transition takes place entirely in the underconstrained region as strain is varied. We study a spring-network model that exhibits both types of transitions and provide a unifying perspective based on a scaling ansatz for the rigidity transition in this model.

*This material is based upon work supported by the National Science Foundation under Grant No. NSF-DMR-1506625 and Simons Investigator Award 327939.

11:51AM S24.00004: Soft glassy dynamics and rheology: A damped soft-sphere model*

AMRUTHESH THIRUMALAIswamy (Presenter), ROBERT RIGGLEMAN, JOHN CROCKER, CBE, University of Pennsylvania — The mechanical response of a diverse family of seemingly disparate materials, like foams, cells, and emulsions, exhibiting a similar response to applied deformation, has largely defied explanation. One example being their rheology, where the complex modulus shows a weak power-law dependence on frequency, that we recently postulated could be a direct manifestation of the fractal energy landscape of these materials. In this work, we extend our previous study by performing bubble dynamics simulations with damped, non-inertial bubbles evolving similar to ripening observed in foams. We study the coarsening system in the dynamic scaling state, and the resulting physical and dynamic properties over a range of damping effects. As shown before, the under-damped system gives rise to spatially correlated dynamics with avalanches while traversing fractal paths in 3N-dimensional configuration space through super-diffusive motion. Further, we investigate the statistical nature of avalanches in time and their disappearance in the over-damped limit, and the corresponding changes in the rheology of the system. Lastly, we study the aging of the system after strong perturbations and look for signatures of self-organization in the dynamical steady state.

*NSF DMR-1609525
12:03PM S24.00005: Crystallization Instability in Glass-Forming Mixtures*  PADDY ROYALL (Presenter), Physics, University of Bristol, TROND INGEBRIGSTEN, JEPPE C DYRE, THOMAS SCHRODER, Department of Science and Environment, Roskilde University — Understanding the mechanisms by which crystal nuclei form is crucial for many phenomena such as gaining control over crystallization in glass-forming materials or accurately modeling rheological behavior of magma flows. The microscopic nature of such nuclei makes understanding hard in experiments, while computer simulations are hampered by short timescales and small system sizes. Here we use GPU simulations to reveal a general nucleation mechanism in mixtures. We find that the supercooled liquid of a prized model glass former is inherently unstable to crystallization, i.e., that nucleation is unavoidable on the structural relaxation timescale, for sufficient system sizes. This is due to compositional fluctuations leading to regions composed of one species which rapidly crystallize. This mechanism provides a minimum rate of nucleation in mixtures in general, and we show that it pertains to the metallic glass former copper zirconium.


* Royal Society, and Kyoto University SPIRITS fund, and European Research Council (ERC consolidator grant NANOPRS, Project No. 617266) JSPS Postdoctoral Fellowship, VILLUM Foundation’s Matter Grant (No. 16515).

12:15PM S24.00006: Cells on spheres: glassy dynamics of vertex models in curved space  DANIEL SUSSMAN (Presenter), Emory University — The analogy between cellular monolayers and aggregates on the one hand and jammed solids or colloidal glasses on the other has provided a powerful framework for probing questions of rigidity, motilitiy, and collective excitations in dense biological tissues. However, simple coarse-grained theoretical models of these systems — such as vertex or Voronoi models of confluent cells — have both an unusual zero-temperature rigidity transition and highly anomalous glassy dynamics. The underlying reasons for these atypical behaviors are poorly understood. Here we begin to discriminate between theoretical explanations by numerically studying cellular models embedded on the surface of a sphere. By introducing constant Gaussian curvature we lift the large degenerate space of zero-energy modes that contributes to the unusual jamming transition of vertex-like models, and explore how this changes the finite-temperature glassy dynamics.
12:27PM S24.00007: Anticipating Challenges of Propensity Measurements in Colloidal Systems*  CORDELL DONOFRIO (Presenter), ERIC WEEKS, Emory University — In order to study dynamics near the glass transition we simulate the Kob-Andersen binary glassformer in a series of isoconfigurational ensembles. This follows the work of Widmer-Cooper et al, (2004), where they used such an ensemble to define the propensity of each particle as the average motion of the particle, where the averaging is done across the ensemble. We seek to understand how sensitive the measurement of propensity is to the polydispersity of the particles. One could imagine attempting to measure propensity experimentally using a colloidal glass system, but these particles would have some distribution of size and there would always be the possibility for error when attempting to create an isoconfigurational copy of the system. We introduce polydispersity by splitting the population of each of the binary components into its own binary where half are increased in size and the other half are decreased in size by the same percentage. Experimental errors are then simulated by exchanging large and small variants each time a isoconfigurational copy is created. We find that the propensity signal is strengthened when polydispersity is increased, but decreased as more and more errors are introduced.

*NSF (DMR-1609763)

12:39PM S24.00008: Glassy behavior and memory effects in the elastic response of a disordered protein*  IAN L MORGAN, University of California, Santa Barbara, RAM AVINERY, ROY BECK, Tel Aviv University, OMAR SALEH (Presenter), University of California, Santa Barbara — We investigate the dynamic mechanical properties of an intrinsically-disordered protein derived from neurofilament tail domains. We use a single-molecule stretching technique, magnetic tweezers, to force a disordered polyprotein out of equilibrium, and observe the relaxation of its end-to-end extension. The relaxation is logarithmic and slow, enduring for minutes to hours. We explain our results in terms of a phenomenological model, originally developed for bulk glassy systems, that assumes relaxation is caused by the sum of many independent structural transitions with widely varying rates. Such a model makes sense for macroscopic systems but is surprising to observe in a single molecule. Yet, the model quantitatively accounts for both the force-dependence of the logarithmic relaxation, and our observation of a non-monotonic (Kovacs) relaxation when subjecting the protein to a multi-step force protocol. The Kovacs memory effect is an unambiguous signature that many independent and parallel structural transitions are contributing to the overall dynamic mechanical properties of the IDP. This is fundamentally different from previous examples of glassy behavior in folded proteins which rely on a heterogeneous population of conformations.

*NSF/MCB BSF Award #1715627
**12:51PM S24.00009: Crystallization properties of amorphous and supercooled liquid antimony**  
RICCARDO MAZZARELLO (Presenter), IDER RONNEBERGER, Institute for Theoretical Solid State Physics and JARA, RWTH - Aachen, YUHAN CHEN, WEI ZHANG, Center for Advancing Materials Performance from the Nanoscale, Xi'an Jiaotong University, Xi'an, China — Chalcogenide phase change materials are highly important for technological applications in data storage and neuro-inspired computing devices, which exploit the ability of these materials to undergo fast and reversible transitions between crystalline and amorphous states with pronounced electrical contrast. Antimony alloys form an important family of phase-change materials. Recent work has shown that even pure antimony can be employed in phase-change devices, in spite of its high proneness to crystallization. In this talk, we investigate the structural and crystallization properties of amorphous and supercooled liquid models of pure and alloyed antimony by ab initio molecular dynamics. We study the effects of quenching rate and finite size on the crystallization speed and elucidate how the dopants affect the short-range order and the crystallization kinetics.

**1:03PM S24.00010: Jammed solids held together with pins: The effect of pin geometry on structure and mechanical response**  
AMY GRAVES (Presenter), LIAM PACKER, BRIAN JENIKE, ARI LILOIA, Swarthmore College, SEAN RIDOUT, University of Pennsylvania — Currently, much is known about the theory and broad applicability of the jamming transition. Here, we address unanswered questions on the geometrical role that a scaffolding of fixed particles, or "pins", plays in structure and dynamical response of jammed, soft bi- or polydisperse particles. Our 2d system consists of particles and tiny pins which harmonically repel overlaps, fixed in various geometrical arrangements: square, triangular, or honeycomb lattices, or distributed randomly. While at low pin densities the jamming threshold, $\varphi_j$, decreases linearly with pin density, independently of pin geometry; at higher densities it reflects lattice-specific constraints on particle packing, and $\varphi_j$ may even increase with pin density. The distribution of bond angles may be anisotropic, and contact force distribution reflect the presence of pins. Changes in the linear elastic response can be seen in bulk and shear moduli, their scaling with pressure near jamming, and a Zener ratio indicating that pin geometry might break the mechanical isotropy of the jammed state.

*This work was supported by NSF DMR-1905474. We thank Swarthmore's Provost's Office, Division of Natural Sciences, Individual Donors, and Chapter of Sigma Xi. One of us (AG) is grateful for a Michener Sabbatical Fellowship.*
1:15PM S24.00011: Boundary and Interface Modes in Periodically Triangulated Origami
JAMES MCINERNEY (Presenter), School of Physics, Georgia Inst of Tech, BRYAN G CHEN, Physics, University of Massachusetts, LOUIS THERAN, School of Mathematics and Statistics, University of St. Andrews, CHRISTIAN SANTANGELO, Physics, Syracuse University, ZEB ROCKLIN, School of Physics, Georgia Inst of Tech — Origami is an important system for architectured materials because its mechanical response is controlled by the geometry of its crease pattern. While researchers are typically interested in the uniform deformations that arise from rigid folding, the role of boundaries and interfaces are important in design applications. Here, we investigate the linear modes of triangulated origami, for which the number of constraints matches the number of degrees of freedom, i.e. mechanical criticality. Such mechanically critical systems have zero modes on their boundaries which can be robustly moved from one side to the other, known as topological polarization. However, Chen et al. (2016) found triangulated origami does not admit such topological polarization. We first explain how this arises via a vertex duality in triangulated origami which prevents any net topological polarization. We then explore triangulated origami as an element of a recently identified symmetry class which can admit new types of modes at interfaces that depend on the geometry of the joined crease patterns.

1:27PM S24.00012: High Throughput Mechanical Quantification of Glassy Thin Films using Additively Manufactured Elastomeric Lattices  
RICHARD ARTHUR VAIA (Presenter), Materials and Manufacturing Directorate, Air Force Research Laboratory, ANESIA AUGUSTE, UES, Inc, ALLEN SCHANTZ, ANDREW GILLMAN, Materials and Manufacturing Directorate, Air Force Research Laboratory, ANDREW C TIBBITS, UES, Inc, PHILIP BUSKOHL, Materials and Manufacturing Directorate, Air Force Research Laboratory — Understanding the improved toughness, stiffness, and fracture resistance achieved with nanoscale thin films are crucial to numerous technologies, ranging from soft robotics to medicine, energy storage, and smart separation membranes. However, the development of structure-composition-processing-performance relationships are hinder by the lack of techniques that rapidly quantify the plasticity and failure mechanisms of these thin films, especially in relevant environments. In this work, we will discuss a high throughput concept to measure the elastic moduli, plasticity and failure strain of thin polymer films. Building from the copper grid technique developed by Lauterwasser and Kramer, we design an additively manufacture compliant elastomeric lattices to replace the traditionally rigid grid. The geometry of the lattice with differing Poisson's ratios transduces macroscopic, uniform, in-plane deformation into a wide range of local deformation fields at each lattice cell. By placing a thin polystyrene film on top of the lattice structure, each cell acts as a unique deformation stage, allowing simultaneous mapping of the yield and fracture envelope. Combining this with optical techniques and image processing, enables statistically robust analysis of various parameters in parallel.
1:39PM S24.00013: Classical E&M with a twist: A geometric Hall effect without magnetic field* NICHOLAS SCHADE (Presenter), DAVID I SCHUSTER, SIDNEY ROBERT NAGEL, University of Chicago — The classical Hall effect, the traditional means of determining charge-carrier sign and density in a conductor, requires a magnetic field to produce transverse voltages across a current-carrying wire. We demonstrate a fundamentally novel use of geometry to create transverse potentials along curved paths without any magnetic field. These potentials also reflect the charge-carrier sign and density, and they arise because a transverse electric field must accelerate the current radially in order to follow the curve. We demonstrate this effect experimentally in curved graphene wires where the transverse voltages are as large as millivolts. The potentials are consistent with the doping and change polarity as we switch the carrier sign. In straight wires, we measure transverse voltage fluctuations with random polarity demonstrating that the current follows a complex, tortuous path. This geometrically-induced potential offers a sensitive characterization of inhomogeneous current flow in thin films.

*NSF MRSEC

1:51PM S24.00014: Rigidity Transitions in Flexible Polymer Networks* JUSTIN LITTLE (Presenter), ROBJIN F BRUINSMA, University of California, Los Angeles — Granular media composed of hard paritcles undergo a rigidity transition with increasing volume fraction. We show that networks of flexible polymers in good solvent described by the Edward's Hamiltonian undergo first-order rigidity transitions as the excluded volume interaction is increased. At the transition point, the network acquires a finite shear modulus, and the density of the network becomes anisotropic. This transition is dominated by the eigenvalue spectrum of the Laplacian matrix of the network.

*We thank the NSF-DMR under Grant 1836404 for funding.

2:03PM S24.00015: Biological Regulatory Networks are Minimally Frustrated* SHUBHAM TRIPATHI (Presenter), PhD Program in Systems, Synthetic, and Physical Biology, Rice University, DAVID A KESSLER, Department of Physics, Bar-Ilan University, HERBERT LEVINE, Department of Physics, Northeastern University — How do biological regulatory networks differ from random networks? Multiple studies have attempted to answer this question by looking for topological features of biological networks that are absent in random networks, yielding few functional insights. Here, using a Boolean modeling framework to compare the dynamical behavior of five real biological networks to that of random networks with similar topological features, we show that biological networks possess sets of stable states that are minimally frustrated. These states exhibit gene expression patterns characteristic of canonical cell types and possess large basins of attraction due to which most cells end up in one the canonical types. The number of commonly observed cell types is thus restricted to the number of gene expression patterns in these minimally frustrated states. Random networks, with topological features similar to biological networks but with varying levels of hierarchy, do not possess such minimally frustrated stable states. Our analysis thus provides crucial insights into the design principles of biological regulatory networks.

*This work was supported by the National Science Foundation grants PHY-1427654 and PHY-1935762, and by the United States-Israel Binational Science Foundation grant no. 2015619.
Session S25 GSNP: Shell Buckling

11:15AM S25.00001: TBD [Invited]  OUSMANE KODIO (Presenter), Massachusetts Institute of Technology — tbd

11:51AM S25.00002: Postbuckling analysis of hyperelastic thick tube*  YU ZHOU (Presenter), YUZHEN CHEN, LIHUA JIN, University of California, Los Angeles — In recent years, mechanical instabilities of soft materials have been substantially investigated and utilized. Though tube structures are widely used and instabilities of thin-walled tubes are well studied, postbuckling behavior of hyperelastic thick tubes is elusive. It is well known that exact solutions of postbuckling are hard to obtain, especially for structures under three-dimensional finite deformation. In this presentation, we conduct buckling and postbuckling analysis for hyperelastic thick tubes undergoing finite deformation. We will briefly introduce the asymptotic expansion method for buckling and weakly postbuckling of elastic bodies and apply this theory to thick tubes. Our analytical results are validated by finite element simulations. As a result, a long tube prefers the Euler buckling mode, while a short tube prefers the barreling mode. Depending on the geometry, three kinds of postbuckling paths, including increasing force, snap-through and snap-back, are discovered. We summarize our results in two phase diagrams of buckling and postbuckling with respect to geometric parameters, which provide guidelines for utilization of tube structures.

*We acknowledge startup fund from Henry Samueli School of Engineering and Applied Science at UCLA and Hellman fellowship.

12:03PM S25.00003: Buckling in thin thermalized ribbons under longitudinal compression
PAUL HANAKATA (Presenter), ABIGAIL PLUMMER, SURAJ SHANKAR, DAVID ROBERT NELSON, Harvard University — Introducing kirigami cuts to thin sheets, ranging from macro to nanoscale, can allow for sensitive control of mechanical properties such as stretchability. The out-of-plane buckling due to in-plane compression can be a key feature in preventing failure upon stretching. While thin plate theory can predict critical buckling for thin frames and nanoribbons at very low temperatures, a unifying framework to describe the effects of thermal fluctuations on the buckling presents subtle problems. In analogy with understanding semi-flexible polymers with long persistence lengths, we address under what conditions a thin thermalized nanoribbon behaves like a classical plate and how its thermal modes compete with the buckling modes. We develop a mean field approach to understand how the critical buckling changes due to thermal fluctuations both above and below the buckling transition. We simulate thin graphene nanoribbons under axial compression using molecular dynamics simulations to test our predictions.
Poking and buckling of pressurized spherical shells  
AREFEH ABBASI, DONG YAN, MATTEO PEZZULLA, PEDRO REIS (Presenter), Ecole Polytechnique Federale de Lausanne — Imperfection sensitivity in shell buckling makes it difficult to predict the critical buckling conditions of shells with realistic distributions of defects. Recently, a non-destructive technique has been proposed and successfully applied to cylindrical shells [1,2], to access their landscape of stability using a probing force. It is still debatable whether this technique can also be used for spherical shells. Here, we combine precision experiments, finite element simulations and shell theory to explore the ability of a poking technique to determine the critical buckling pressure of a spherical shell containing a dimple-like defect. We find that the critical point can indeed be probed when the force is applied at the defect. However, when the poking is done further away from the defect, this becomes invisible to the probing and the shell buckles prior to the cue provided by the poking. Specifically, we quantify a threshold angle for the location of the probing force, beyond which poking no longer seems to be applicable as a non-destructive testing technique. The basis of our analysis is the localized nature of the deformation of shells under point-load indentation.


Multi-component assembly of microcompartments*  
SIYU LI (Presenter), YAOHUA LI, TAYLOR NICHOLS, NOLAN KENNEDY, DANIELLE TULLMAN-ERCEK, MONICA OLVERA DE LA CRUZ, Northwestern University — Many bacteria generate bacterial microcompartments (BMC) in their metabolic processes. These particles are protein-based shells that encapsulate enzymes spontaneously. Using all-atom and coarse-grained molecular dynamics, we study the mechanical properties of protein subunits and the assembly process. We find that the hexamers (PduA) are associated mainly due to the hydrogen bonding, the strength of which exactly corresponds to the region that BMC successfully formed. In addition, we observe cylinder and “samosa” shaped shells coexistent in solution when reducing the pentamer (PduN)-hexamer interaction. We calculate the free energy for each morphology thermodynamically and find that the cargo-hexamer attraction in cylinder/samosa compensates the energy loss of missing pentamers. We also discuss other thermodynamic parameters that can be used to control the shell morphology, which provides a prediction for future experiments.

*We thank DOE support of the grant DE-FG02-08ER46539 from the Department of Energy Basic Energy Science Office and the Sherman Fairchild Foundation.
12:39PM S25.00006: Shallowness effect on buckling of spherical shells  KANGHYUN KI (Presenter), JEONGRAK LEE, ANNA LEE, Pohang University of Science and Technology — We study the buckling of clamped spherical caps under uniform pressure. Since the 1960s, several theoretical and computational studies have addressed the non-monotonic relationship between the shallowness of the shells and its critical buckling pressure. However, there is a lack of precise experiments to corroborate these predictions. Using a recently developed technique, we fabricate polymeric spherical shells containing a precise geometric defect. We vary the shallowness of our shells by precisely changing the location of the clamped boundary conditions and measure the critical buckling pressure. Finite element simulations are conducted to analyze the buckling behavior of our shallow shells, in excellent agreement with the experiments. We find that the critical buckling pressure and the shallowness parameter have a decaying sinusoidal relationship, hence, the buckling strength of shallow shells can be larger or smaller than that of complete spherical shells. Moreover, this sinusoidal form is systematically characterized which is affected by a geometric defect.

12:51PM S25.00007: Circumferential Buckling of the Confined D-cone* LUCIA STEIN-MONTALVO (Presenter), KANANI ALMEIDA, DOUGLAS HOLMES, Boston Univ — Thin structures deform in dramatic ways to avoid stretching, and this strongly depends on how they are constrained. We observe that in-plane confinement forces the classical packed d-cone to deviate from its characteristic form. Instead of forming a cone with a single region of high stretching, thin, flexible plates wrinkle circumferentially in response to radial and packing-type confinement together. Geometry sets the limiting maximum wavenumber, but dynamic changes in morphology occur even as confinement increases quasi-statically. In a primarily experimental study, we investigate the role of confinement on shape selection, curvature distribution, stretching localization, and the resultant force as waves develop sequentially.

*We gratefully acknowledge financial support from NSF through CMMI-1824882.
1:03PM S25.00008: Investigating imperfection-sensitivity in shell buckling using a toy model

RAINER GROH (Presenter), ALBERTO PIRRERA, Univ of Bristol — Shell buckling is known for its extreme sensitivity to initial imperfections. It is generally understood that this sensitivity is caused by an unstable (subcritical) bifurcation, i.e. geometric imperfections rapidly erode the buckling load of the perfect shell. It is less commonly appreciated that subcriticality also creates a strong proclivity for spatially localised buckling modes. The ability of localisations to appear anywhere across the domain (spatial multiplicity) leads to a large set of possible trajectories to instability, with each trajectory affine to a particular imperfection signature. Using a toy model of a link system on a softening elastic foundation, we show that the spatial multiplicity of localisations leads to a large spread in buckling loads, even for indistinguishable random imperfections of the same amplitude. By imposing a dominant imperfection, the strong sensitivity to random imperfections is ameliorated, and the ability to control the trajectory to buckling via dominant imperfections or elastic tailoring, creates interesting possibilities for designing imperfection-insensitive shells.

*R.M.J.G. is funded by the Royal Academy of Engineering [RF\201718\17178]. A.P. is funded by the UK Engineering and Physical Sciences Research Council [EP/M013170/1].

1:15PM S25.00009: Newton’s method for experimental path-following of nonlinear structures

JIAJIA SHEN, RAINER GROH, ROBIN M NEVILLE, MARK SCHENK, ALBERTO PIRRERA (Presenter), Univ of Bristol — Traditional experimental testing of nonlinear structures has not evolved beyond the fundamental techniques of force control (dead loading) and displacement control (rigid loading). These two experimental paradigms face the same issues that computational solvers faced before numerical path-following; namely, limit points in the force-displacement response cannot be traversed by sole force or displacement control. To extend the capabilities of nonlinear testing methods, we have implemented an experimental analogue to numerical path-following. In addition to controlling the displacement at the primary load-introduction points, extra actuators and sensors are attached to control the overall shape of the structure. By perturbing the structure at these control points, and recording the resulting changes in reaction force, an “experimental tangent stiffness” matrix is computed, which is then used in a feedback control system based on Newton’s method. Using an experiment on a shallow arch, we demonstrate the capability of the test setup to path-follow stable and unstable equilibria and traverse limit points.

*R.M.J.G. is funded by the Royal Academy of Engineering [RF\201718\17178]. J.S. and A.P. are funded by the UK Engineering and Physical Sciences Research Council [EP/M013170/1].
EMMANUEL VIROT (Presenter), Harvard University, ANAIS ABRAMIAN, Institut Jean Le Rond d’Alembert, EMILIO LOZANO, TOBIAS SCHNEIDER, EPFL, SHMUEL RUBINSTEIN, Harvard University — What is the critical load required to crush a soda can or a space rocket shell? Surprisingly, there is no good way to estimate it, because of the high defect-sensitivity of the buckling instability.

Here we measure the response of (imperfect) soda cans to lateral poking and identify a generic stability landscape, which fully characterizes the stability of real imperfect shells in the case where one single defect dominates.

By using this new paradigm, we are able to accurately and non-destructively predict the buckling load of real imperfect shell structures, thereby promising drastic reductions of the costs of structural engineering experimental tests.

We will discuss the success rate of the method and the perspectives offered by such an approach.

NICHOLAS CUCCIA (Presenter), EMMANUEL VIROT, MICHAEL PHILLIP BRENNER, SHMUEL RUBINSTEIN, Harvard University — Materials under cyclic loading experience changes in their physical properties, commonly exhibiting structural fatigue, damage and eventually failure. There exists much interest in how a material ‘remembers’ the damage done to it, and few methods exist to, without irreversibly deforming the material, quantitatively describe this ‘memory’. Here, we explore the effects of cyclic loading on the stability of cylindrical shells with many small unknown defects (empty soda-cans). Using a custom-built multi-axial tester, we repeatedly load and unload our cans and generate stability landscapes by measuring the can’s response to non-destructive lateral poking at various axial loads. Here, we will show that cyclic loading changes the can’s reaction to poking, which can be visualized through the evolution of the can’s stability landscape.

We will also show how the initial defect structure of our shells can inform their overall fatigue and can be understood via topological features of our shell’s stability landscape.

*This research is supported by Harvard's Materials Research Science and Engineering Center (MRSEC) and the National Science Foundation (NSF) under Award Number DMR-1420570.
We study the bulging behavior of thin cylindrical balloons with various aspect ratios under internal pressure loading. Although the localized bulging of long circular tubes has been extensively studied experimentally and analytically, there is a lack of investigation on the deformation of short and moderate-length tubes. For non-cylindrical balloons, a recent simulation study on the inflation of spheroidal shells reported the boundary aspect ratio that determines the occurrence of localized bulging. We first experimentally investigate the bulging behavior of hyperelastic tubes under internal pressure by systematically varying the aspect ratio. We also explore the effect of prestretch both on the critical bulging pressure and the instability. Then, we compare our experimental results with analytical solutions. Furthermore, we combine multiple tube segments to achieve complex deformation. Our results can be used to understand inflatable biological structures and design soft pneumatic actuators.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S26 DBIO DPOLY GSNP: Physics of Genome Organization: From DNA to Chromatin: II 403 - Alexandre Morozov, Rutgers University, New Brunswick - Tag(s): Focus
11:15AM S26.00001: On the Border of Order: Chromosomal Organization in Space and Time*

[Invited] YAOJUN ZHANG, Princeton University, NIMISH KHANNA, Molecular Biology, University of California, San Diego, JOSEPH LUCAS, Physics, University of California, San Diego, CORNELIS MURRE, Molecular Biology, University of California, San Diego, OLGA DUDKO (Presenter), Physics, University of California, San Diego — Many biological processes, from antibody production to tissue differentiation, share a common fundamental step — establishing a physical contact between distant genomic segments. How do remote segments find each other on a remarkably short timescale despite being strung out over millions of base pairs along the DNA? What is the mechanism of the high degree of orchestration of remote genomic interactions? We address these questions in the context of adaptive immunity – the system that enables the individual to respond to a great variety of pathogens through a diverse repertoire of antibodies. Experimental data from live-cell imaging in B-lymphocytes reveal the signatures of anomalous diffusion that help us identify the dominant mechanism of genomic motion. Comparison of experimental and simulated data, along with insights from polymer physics, suggest that an interphase chromosome behaves as a network of cross-linked chains characteristic of a gel phase, yet it is poised near the sol phase, a solution of independent chains. Chromosome organization near the phase boundary provides the genome with a tradeoff between stability and responsiveness and orchestrates the timing of genomic interactions.

*The studies were supported by grants from the National Institutes of Health (U54DK107977) to O.K.D. and the National Institutes of Health (U54DK24230, AI082850, AI00880, and AI09599) to C.M. Y.Z. was supported by the Princeton Center for Theoretical Science, the National Science Foundation (Grant PHY1607612), and the NSF Center for the Physics of Biological Function (PHY1734030). Imaging was performed at the University of California, San Diego School of Medicine and supported by Core Grant P30 NS047101.


SWARNADEEP SETH (Presenter), ANIKET BHATTACHARYA, Univ of Central Florida — In an experimental “Tug-of-War” (X. Liu et al., Small 2019, 1901704), a DNA segment co-captured in both the pores in a Double-Nanopore system is subject to two equal and opposite biases at two pore locations for better control and repeated measurements of the same segment. We simulate a model system in three dimensions and use Brownian dynamics to reveal the details of the single file translocation. Specifically, we study the consequence of increased persistence length of the segment in between the pores due to the tug-of-war forces. We characterize the diffusive motion of the chain either for exact “Tug-of-War” with zero bias, or subject to a small net bias, and provide error estimates of the length translocated through the Double- nanopore from the velocity measurements. Furthermore, we compare the velocities of the individual monomers with the average velocity of the entire chain and explore measures to reduce the fluctuation in velocity along the chain.
12:03PM S26.00003: Studies of nucleosome-decorated DNA structures and deformations using a new analytical model*  
SEYED AHMAD SABOK-SAYR (Presenter), WILMA K OLSON, Rutgers University, New Brunswick — The two meters of DNA found in almost every human cell must be folded by many orders of magnitude to fit in the nucleus. The first step in this compaction involves the coiling of ~150 base pairs of DNA around a core of eight positively charged histone proteins. Understanding the biological processing of DNA requires knowledge of how the nucleosomes are arranged in space. We introduce a new analytical treatment of nucleosome-decorated DNA which is made up of three essential parts: nucleosomal DNA; protein-free stretches of DNA; and the intervening connectors. Every connector provides a physically smooth DNA pathway between a protein-bound and/or a protein-free segment. We have used this approach to study the energetically preferred configurations of torsionally relaxed, 360-base pair DNA rings with two evenly-spaced nucleosomes as well as rings of the same size with a single nucleosome subject to deformation in structure and/or variation in DNA wrapping. We have identified conditions where the closed DNA chain switches from one global configuration state to another. We are also using this model to study more complicated structures, such as the Simian virus 40 minichromosome, an assembly of ~20 nucleosomes on ~5200 base pairs of DNA supercoiling.

*Supported in part by USPHS GM 34809

12:15PM S26.00004: Long-lived memory and dynamics of liquefied chromatin  
EDWARD BANIGAN (Presenter), Massachusetts Institute of Technology MIT, HOUDA BELAGHZAL, TYLER BORRMAN, JOB DEKKER, University of Massachusetts Medical School, LEONID MIRNY, Massachusetts Institute of Technology MIT — Chromatin is organized into spatially segregated compartments, referred to as (active) euchromatin and (inactive) heterochromatin. Compartments are thought to be formed by phase separation, which may be facilitated by the underlying linear polymer structure of the genome. However, recent “liquid Hi-C” experiments in which chromosomes are fragmented into tiny segments reveal an hours-long spatial memory that does not rely on large-scale polymer connectivity. To understand the physical mechanisms and dynamics of this memory, we analyze Hi-C genome contact maps and perform polymer molecular dynamics simulations. In a heteropolymer simulation model, we find that strong interactions between inactive chromatin segments can lead to slow melting of inactive compartments, as in experiments. Surprisingly, in Hi-C maps, we find that contacts between segments separated by small genomic distances are maintained despite the fragmentation of the genome. Our model can only reproduce this counterintuitive behavior when such contacts are maintained by another cell nuclear structure, such as the lamina. Thus, while phase separation may globally compartmentalize chromatin, it is insufficient to dictate short-distance contacts, which instead may be maintained by specific, long-lived interactions.
12:27PM S26.00005: The Dynamic Archaeal Chromatin “Slinky” [Invited] SAMUEL BOWERMAN (Presenter), University of Colorado Boulder — Eukaryotic organisms package genomes that are significantly larger and more complex than genomes that are typically found in prokaryotes. The fundamental unit of compaction is the nucleosome, which is formed by histone heteromers – two H2A-H2B dimers flanking an H3-H4 tetramer – forming an octamer that binds approximately 147 bp of DNA. While histones were originally thought to only be present in eukaryotes, a plethora of histone sequences have been identified in a wide range of archaea, one of the prokaryotic domains of life. Our lab recently determined the structure of histone-based archaeal chromatin that showed striking similarities to eukaryotic nucleosomes, but crystal lattice packing and biochemical experiments suggested that archaea may form repeated stacking interactions, potentially forming long “Slinky-like” extended chromatin arrangements. Here, we utilize molecular dynamics simulations, cryoEM, and analytical ultracentrifugation to study the inherent dynamics of these putative chromatin slinkies. Formation of “Slinky stacking” interactions are observed to reduce system dynamics, and perturbing this interaction through stack-hindering mutations yields more flexible constructs and increases solution accessibility. The openness of the Slinky is also sensitive to the salt environment. We utilize these data to explore how inherent dynamics of archaeal Slinky chromatin may regulate transcription.

1:03PM S26.00006: 5-methyl-cytosine binding proteins loop DNA under nanoconfinement* MING LIU (Presenter), North Carolina State University, DAVID C. WILLIAMS, Department of Pathology and Laboratory Medicine, University of North Carolina at Chapel Hill, HONG WANG, ROBERT RIEHN, North Carolina State University — Methyl-binding domain proteins are a family of proteins that possess a domain to selectively bind 5-methyl cytosine in an CpG context. Members of the family interact with other proteins to modulate DNA packing. Stretching of DNA-protein complexes in nanofluidic channels with a cross-section of a few persistence lengths allows us to probe the degree of packing by such proteins. Here we demonstrate compaction by MeCP2 while MBD2 does not affect DNA configuration. By using atomic force microscopy (AFM), we determined that the likely mechanism for compaction by MeCP2 is the formation of bridges between distant DNA stretches and the formation of loops. We discuss the potential of both proteins for epigenetic mapping.

*We acknowledge funding from the NSF (DBI1353897) and the NIH (GM107559, GM123246)
1:15PM S26.00007: Nuclear chromatin patterns: modeling dynamics of intra-chromatin interactions and its impact on structure organization  RABIA LAGHMACH (Presenter), Iowa State University, MICHELE DI PIERRO, Center for Theoretical Biological Physics, Rice University, DAVIT POTOYAN, Iowa State University — The description of chromatin organization and its dynamics, at a large scale, are functionally important factors in the genome regulation function. Growing evidence suggests that chromatin within the nucleus has a liquid-like behavior mediated by phase separation into micro-droplets with distinct transcriptional states. The formation and spatial arrangement of chromatin droplets within the nucleus depending on their transcriptional states either active (euchromatin) or inactive (constitutive and facultative heterochromatin) genes are important features of the nuclear architecture. Understating mechanisms that control the dynamics and spatiotemporal regulation of droplets formation is a possible way to elucidate the relationship between nuclear architecture and gene regulation. Here, we introduce a mesoscale liquid model of nucleus (MELON) that incorporates dynamic of interactions between A-B-C chromatin compartments of the nucleus, as well as the affinity between constitutive heterochromatin and Lamina at the nuclear envelope and nucleus deformation. Using MELON framework, we show that phase separation together with surface tension effects and nuclear shape deformation is sufficient for recapitulating large-scale morphology and dynamics of chromatin along the life cycle of cells.

1:27PM S26.00008: Long-distance group dynamics of RNA polymerases via DNA supercoiling  SANGJIN KIM (Presenter), University of Illinois at Urbana-Champaign — Genes are often transcribed by multiple RNA polymerases (RNAPs) at densities that can vary widely across genes and environmental conditions. Here, we provide in vitro and in vivo evidence for a built-in mechanism by which co-transcribing RNAPs display either collaborative or antagonistic dynamics over long distances (>2 kb) through transcription-induced DNA supercoiling. In Escherichia coli, when the promoter is active, co-transcribing RNAPs translocate faster than a single RNAP, but their average speed is not altered by large variations in promoter strength and thus RNAP density. Environmentally induced promoter repression reduces the elongation efficiency of already-loaded RNAPs, causing premature termination and quick synthesis arrest of no-longer-needed proteins. This negative effect appears independent of RNAP convoy formation and is abrogated by topoisomerase I activity. Antagonistic dynamics can also occur between RNAPs from divergently transcribed gene pairs. Implications for genome organization and evolution will be discussed. Our findings may be broadly applicable given that transcription on topologically constrained DNA is the norm across organisms.
1:39PM S26.00009: Interplay of chromatin self-adhesion and lengthwise compaction on interchromosomal organization* SUMITABHA BRAHMACHARI (Presenter), VINICIUS CONTESSOTO, MICHELE DI PIERRO, JOSE N ONUCHIC, Rice Univ — Chromosome folding is driven by an interplay between two major forces: self-adhesion between specific chromatin segments and lengthwise compaction, which is in line with experimental observations of structure and dynamics of cellular chromosomes. We use a coarse-grained polymer model for chromosomes where centromeres and telomeres are treated as polymer blocks featuring respective self-adhesion, and simulate multiple chromosomes in a confined volume. We find that our scheme of lengthwise compaction drives the formation of chromosome territories, whereas, self-adhesive centromeres and telomeres tend to form localized clusters. We highlight the interplay between self-adhesion and lengthwise compaction, based on their relative strengths, that addresses a fundamental aspect of genome organization in the eukaryotic nuclei.

*This work was supported by the National Science Foundation and by the Welch Foundation (Grant C-1792).

1:51PM S26.00010: A minimal model for correlated chromatin dynamics* KUANG LIU (Presenter), ALISON PATTESON, Syracuse University, EDWARD BANIGAN, MIT, JENNIFER SCHWARZ, Syracuse University — The multiscale spatial structure of chromatin spans several decades from the nanometer scale to the micron scale. In addition to its nontrivial spatial structure, chromatin also exhibits nontrivial dynamics. For instance, correlated motion of chromatin on the length scale of microns over the time scale of tens of seconds has been observed. Correlations are diminished in the absence of ATP, suggesting that motor/enzymatic activity promotes chromatin collective dynamics. Therefore, we construct a minimal polymeric model to study the spatiotemporal properties of chromatin by simulating a Rouse chain with excluded volume interactions confined within a rigid, spherical shell that represents the lamina. We characterize the spatiotemporal properties of the chain in the presence of motor activity, crosslinking, and binding to the shell. These components model an active chromatin network with lamin-binding domains. We find correlated motion under several conditions, without the need for long-range forces. Notably, when chromatin is bound to the lamina, crosslinking and motor activity are required for strong correlations in chromatin motion. We also study the effects of a deformable lamina shell in order to study the coupling of correlated chromatin motion to nuclear shape.

*NSF-DMR-1832002
Due to the intrinsic twist of DNA, eukaryotic replication generates DNA supercoiling as the replisome unravels parental DNA. If not resolved, this supercoiling may intertwine chromatin fibers and result in significant topological challenges during chromosome replication. Since the replisome alone is incapable of driving its substrates out of torsional equilibrium, the generated supercoiling partitions ahead of or behind the replication fork to maintain a balance of torque. By making direct torque measurements, we demonstrated that a single chromatin fiber (as would be located ahead of a replisome) is torsionally soft, while a braided chromatin fiber (as would be located behind the replisome) is relatively stiff. These results imply that supercoiling on chromatin substrates is preferentially directed in front of the replication fork. We further showed that topoisomerase II relaxation displays a strong preference for a single chromatin fiber over a braided fiber, suggesting a synergistic coordination—the mechanical properties of chromatin inherently suppress intertwining during replication elongation by driving DNA supercoiling ahead of the fork, where it is more efficiently removed by topoisomerase II. This work highlights the fundamental role of physical principles in the cell.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S27 FIAP: Thermodynamic and Transport Properties 404 - Elena Cimpoiasu, US Naval Academy

11:15AM S27.00001: Charge Scattering Mechanisms in shallow InAs quantum wells*  ELENA CIMPOIASU, MATTHEW J. FOX (Presenter), US Naval Academy, SHAWN MACK, JOSEPH A. CHRISTODOULIDES, BRIAN R BENNETT, Naval Research Laboratory — We studied the charge scattering mechanisms present in In_{0.2}Al_{0.8}Sb/InAs/Al_{0.8}Ga_{0.2}Sb wells placed in close proximity to the surface of the heterostructures, at depths from 7 nm to 15 nm. The heterostructures were either unintentionally-doped, doped from below the channel or from above the channel. Measurements of sheet and Hall resistances were performed at T = 2K in variable magnetic field and under illumination with wavelengths of 400 nm up to 1300 nm. The charge density dependencies of the Hall mobility and quantum scattering time were used to infer the dominant mechanisms. We found that the transport quality of the sample is dominated by bottom interface roughness, and that reducing the asymmetry of the potential well results in improved charge transport as the scattering of interface roughness is reduced. This is, however, detrimental to the strength of spin-orbit coupling and to spin-based applications of these materials

*This work was supported by the Office of Naval Research.
Transport properties of exfoliated GaTe thin flakes

WENKAI ZHENG (Presenter), Natl High Magnetic Field Lab, JUSTIN FELDER, Chemistry, University of Texas at Dallas, ZACHARY BRYCE GORAUM, Physics, Florida State University, GREGORY MCCANDLESS, JULIA CHAN, Chemistry, University of Texas at Dallas, LUIS BALICAS — Metal mono-chalcogenide(MMCs), such as GaS, GaSe, InSe, and GaTe, have recently attracted much attention due in part to the evolution of their direct bandgap as a function of the number of layers. Although intrinsic MMC is nonmagnetic, a recent first principle calculation [1] predicts a Stoner-type magnetic instability that leads to the formation of a half-metallic and hence ferromagnetic ground state, which would make these materials interesting for spin transport or applications in spintronics. Here we discuss the temperature-dependent response of Field-Effect Transistors fabricated from GaTe single-crystals grown via a flux method, and measured through two and four-terminal configurations. We will also discuss the evolution of the Hall effect as a function of the temperature.

Bibliography

*We acknowledge support from NSF-DMR grant # 1807969.

Electronic Properties of Bismuth Iodide (Bi$_4$I$_4$) Thin Films

YULU LIU (Presenter), Ohio State Univ - Columbus, RUOYU CHEN, ASM, SHENG LI, XIAOYUAN LIU, University of Texas, Dallas, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science (NIMS), BING LV, FAN ZHANG, University of Texas, Dallas, CHUN NING LAU, Ohio State Univ - Columbus — Due to the gapless conductive surface states which are protected against perturbations, topological insulator materials have attracted much attention in this field. Bi$_4$I$_4$ is a quasi-one-dimensional van der Waals material, and its beta phase has been revealed by angle-resolved photoemission spectroscopy to be a topological insulator, thus offering a new platform for exploring topological phases. To date, all prior works on Bi$_4$I$_4$ are based on the bulk material. Here we report transport measurements of thin Bi$_4$I$_4$ films that are mechanically exfoliated Bi$_4$I$_4$ from bulk crystals. Devices in both alpha and beta phases are characterized. Their gate-tunable resistance demonstrates surface-dominated transport, which is further supported by the observation of weak antilocalization in magnetic fields. Moreover, the temperature behavior in b-Bi$_4$I$_4$ suggests that the inelastic scattering process at low temperature is dominated by the electron-electron interaction.
Amorphous silica (silicon dioxide) is one of the strongest glass formers known, and silicate glasses are by far the most widely produced for applications. Liquid-quenched silica shows tunneling two-level system density, as probed by low-temperature specific heat and internal friction, in the so-called universal glassy range observed for nearly all amorphous materials. We present low-temperature (down to 300 mK) specific heat and mechanical loss measurements on silica thin films grown at temperatures from 60 to 800 °C by e-beam evaporation. Results indicate that silica grown near room temperature shows TLS density, extracted from cryogenic specific heat, above the universal range. The mechanical loss, though high, is still within the universal range, and falls to the level of bulk silica as the growth temperature is increased to 800 °C. This is consistent with the observed increase in atomic density of approximately 10% as the growth temperature is raised 60 to 800 °C. These results are compared to previous work on amorphous silicon and tantala, with attention drawn to the somewhat unusual relative change of the sound velocity with temperature and how this changes systematically with growth temperature for the silica films.

*Supported by NSF Grants DGE 1752814 and DMR 1809498.

Amorphous silicon shows anomalous properties at low temperatures due to two-level systems, which affect both mechanical and electromagnetic oscillators. However, it is unclear whether the two-level systems responsible for these effects are the same. We performed mechanical and dielectric loss measurements of amorphous silicon films grown by electron beam deposition. Samples grown at 425 °C show a large reduction of mechanical loss and a mild reduction of dielectric loss compared to those grown at room temperature. Results indicate mechanical loss is related to mass density, while dielectric loss is to dangling bond density. Moreover, mechanical loss results show lower loss per unit volume for thicker films, while dielectric loss results show lower loss per unit volume for thinner films, suggesting an underlying structural and differential origin for both types of energy dissipation processes. Additionally, specific heat measurements show that the density of two-level systems extends far above the well-known glassy range, indicating that some interactions play a crucial role in creating the universal values of mechanical losses at low temperatures.

*We thank NSF DMR-1508828 and 1809498, Office of Naval Research, and Lawrence Livermore National Laboratory support.
**12:15PM S27.00006: Electrical Transport in Chemically Exfoliated Li$_x$CoO$_2$ in 2D Nanoflake**

**Form**  
KYLE CROWLEY (Presenter), KEVIN PACHUTA, SANTOSH KUMAR RADHA, Case Western Reserve University, HALYNA VOLKOVA, Centre des matériaux, MINES ParisTech, ALP SEHIRLIOGLU, WALTER LAMBRECHT, Case Western Reserve University, MARIE-HELENE BERGER, Centre des matériaux, MINES ParisTech, XUAN GAO, Case Western Reserve University — Layered oxides possess various novel electronic and magnetic phases, many of which remain either unexplained or continually debated. Li$_x$CoO$_2$ is one such material; one of the most commonly used cathode materials in rechargeable batteries, this oxide exhibits a rich landscape of properties, with many aspects still not fully understood. Li$_x$CoO$_2$ contains electrostatically stabilized layers, making it difficult to study in its few-layer, single-crystal form. Herein, a two-step process is utilized to chemically delithiate Li$_x$CoO$_2$ in the range 0.3<x<0.8. Li$_x$CoO$_2$ is then chemically exfoliated, producing nanoflakes 5-100nm thick. Electrical characterization of these individual nanoflakes reveals an insulating behavior upon contact formation, and suppression of metallic tendencies in the low-lithium range (x<0.75), likely due to termination effects of the surface lithium plane. Additionally, an anomaly in the temperature dependent resistance is observed in flakes of specific lithium content, indicating that this fabrication method is suitable for studying charge ordering phenomena in Li$_x$CoO$_2$. This technique offers potential for exploring Li$_x$CoO$_2$ in its two dimensional form, which has not been reported for single crystals to date.

*This work is supported by AFOSR grant# FA9550-18-1-0030.

**12:27PM S27.00007: Diamagnetic Susceptibility, Disorder, and Linear Magnetoresistance in Ag$_{2-\delta}$Te**

**Ian Leahy** (Presenter), PETER SIEGFRIED, University of Colorado, Boulder, HAROLD SCHNYDERS, Department of Physics, Grand Valley State University, MINHYEA LEE, University of Colorado, Boulder — The origin of linear magnetoresistance in Ag$_{2-\delta}$Te has historically sparked debate between several intrinsic and extrinsic mechanisms. We investigate the magnetotransport properties of the narrow-gap semiconductors Ag$_{2-\delta}$Te as a function of silver deficiency in order to quantify the role of disorder on their observed linear magnetoresistance. Built on our earlier work [1], we study the temperature and field dependence of the Hall angle and the diamagnetic susceptibility in order to develop a framework to quantify the disorder parameters, namely disorder potential $V_0$ and the characteristic lengths $\xi$, as a function of silver deficiency. These quantities will be compared as silver deficiency is varied. We will discuss the implication of our results in terms of generalized conditions for emergence of linear magnetoresistance.


**A portion of this work was performed at the National High Magnetic Field Laboratory which is supported by the National Science Foundation Cooperative Agreement Np. DMR-1644779 and the State of Florida.**
12:39PM S27.00008: Quantum Transport in Epitaxial Ultra Wide Bandgap Aluminum Gallium Oxide Tunnel Heterostructures*  
NICHOLAS TANEN (Presenter), CELESTA CHANG, VLADIMIR PROTASENKO, JONATHAN MCCANDLESS, DAVID ANTHONY MULLER, HUILI XING, DEBDEEP JENA, Cornell University — In this work, we studied the epitaxial growth of the wide-band gap, monoclinic beta-Ga$_2$O$_3$ (~4.4-4.9 eV) and (Al$_x$Ga$_{1-x}$)$_2$O$_3$ (~4.4-9.0 eV, Al% = 0-100) using molecular beam epitaxy on (010) beta-Ga$_2$O$_3$ substrates. We will discuss the optimum growth conditions for both materials and how the formation of Ga interstitial-divacancy complexes in unoptimized growths of (Al$_x$Ga$_{1-x}$)$_2$O$_3$ can lead to the formation of unwanted phases of Ga$_2$O$_3$ in our heterostructures. Additionally, tunnel barrier structures made with an (Al$_x$Ga$_{1-x}$)$_2$O$_3$ layer sandwiched between two n+ Ga$_2$O$_3$ layer are studied to explore tunneling behavior in this material system. The current-voltage characteristics are measured for a varying Al composition and the (Al$_x$Ga$_{1-x}$)$_2$O$_3$ barrier thickness. Using the Wentzel–Kramers–Brillouin approximation and Non-equilibrium Green's Function formalism, the current-voltage characteristics of these tunnel barrier devices are simulated and compared to experimental data. The above study helps identify the conduction band offset $\Delta E_c$ a critical unknown in this material family directly from transport. The $\Delta E_c$ thus found between beta-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ and beta-Ga$_2$O$_3$ is compared to those extracted from XPS, capacitance-voltage measurements, and also by DFT.  
*We acknowledge AFRL ACCESS, CCMR, CESI, CNF

12:51PM S27.00009: Lateral charge carrier transport properties of B-10 enriched hexagonal boron nitride epilayers*  
SAMUEL GRENADIER (Presenter), AVISEK MAITY, JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech Univ — Hexagonal boron nitride (h-BN) has emerged as a promising candidate for many technologically significant applications due to its unique physical properties. However, h-BN is one of the least studied members of the III-nitride materials system and many important fundamental properties including room temperature carrier mobility, lifetime and surface recombination velocity remain unexplored. We report Time-of-Flight (TOF) probed room temperature lateral carrier drift mobilities ($\mu$) and lifetimes ($\tau$) for both electrons and holes in highly resistive, wide bandgap h-BN epilayers. Photoconductive type detectors were fabricated from freestanding B-10 enriched h-BN material. We obtained values of $\mu_e$ ~ 34 cm$^2$/Vs for electrons and $\mu_h$ ~ 36 cm$^2$/Vs for holes and carrier lifetimes on the order of 10 $\mu$s. Surface recombination velocity (S) was then calculated by combining the $\mu$ from TOF with the ratio of S to $\mu$ (S/$\mu$) extracted directly from the bias voltage dependence of photocurrent. These results represent a valuable contribution to the understanding of the electrical transport properties of h-BN.  
*This research was supported by DOE ARPA-E (No. DEAR0000964). H. X. Jiang and J. Y. Lin are grateful to the AT&T Foundation for the support of Ed Whitacre and Linda Whitacre endowed chairs.
1:03PM S27.00010: Physical properties at the 157K-phase transition in Pr$_4$Ni$_3$O$_{10}$

SHANGXIONG HUANGFU (Presenter), Univ of Zurich, DARIUSZ GAWRYLUK, PSI, XIAOFU ZHANG, Univ of Zurich, EKATERINA POMJAKUSHINA, PSI, ANDREAS J SCHILLING, Univ of Zurich — As a member of the Ruddlesden–Popper Ln$_4$Ni$_3$O$_{10}$ series rare earth nickelates, the Pr$_4$Ni$_3$O$_{10}$ is constituted by three Ni-O layers piled up to a quasi-two-dimensional perovskite-like structure[i], and shows mixed Ni valent states of +2 and +3. A phase transition at ~ 157 K has already been observed in previous studies, which was interpreted as a charge-density wave (CDW) transition[ii][iii]. We have grown single crystals of Pr$_4$Ni$_3$O$_{10}$ in high oxygen pressure, and report on the physical properties around that phase transition, such as heat capacity, magnetization and electron transport. We observe a distinct anisotropy between in-plane and out-of-plane properties both in zero-field and in magneto-resistance. In addition, the magnetic susceptibility obeys a Curie-weiss law, with different Curie constants for the high temperature and the low temperature phases. We discuss a possible scenario in which a change of the d orbitals of the Ni ions at the Fermi level explains the changes in all these measured quantities at the phase transition.


1:15PM S27.00011: Charge transport mechanism near crystal edge of layered halide perovskites*

XIJJUN LIAN (Presenter), Florida State Univ, ENZHENG SHI, LETIAN DOU, Purdue University, HANWEI GAO, Florida State Univ — Halide perovskites show superior optical and electrical properties, which make this group of materials promising for highly efficient optoelectronic applications. Researchers have reported that there existed below-bandgap energy states at the edges of the layered perovskites and the presence of these lower energy states resulted in highly improved solar cell efficiency. In our work, the photophysics investigation near crystal edge unveiled the local charge transport mechanism and energy flow in layered halide perovskites, which will provide vital guidance for designing and engineering highly efficient optoelectronics based on this group of materials.

*The authors are thankful for the funding supports from the Office of Naval Research through the Young Investigator Program (N00014-18-1-2408)
1:27PM S27.00012: Dynamic disorder in BaTiS₃*  RAPHAEL HERMANN (Presenter), MICHAEL E MANLEY, BARRY WINN, Oak Ridge National Laboratory, KATHARINE L. PAGE, The University of Tennessee, AHMET ALATAS, Argonne National Laboratory, JAERYUN MOON, AUSTIN MINNICH, California Institute of Technology, JAYAKANTH RAVICHANDRAN, University of Southern California, Los Angeles — BaTiS₃ exhibits a hexagonal perovskite structure comprised of columns of sulphur coordinated Ti linked by barium making it a quasi-1D structure. Neutron pair distribution function measurements reveal that the Ti atomic displacement parameters increase with decreasing temperature. This observation suggest proximity to a ferroelectric type phase transition or, alternatively, dynamic disorder persisting in the ground state. A combination of phonon spectroscopy by inelastic x-ray scattering and inelastic neutron scattering supports the dynamic disorder scenario which extends into the quantum regime with Ti occupying a double-well potential. This unique dynamics have a profound consequence on the thermal conductivity and suggest a novel mechanism for thermal transport design.

*Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory and at the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357

1:39PM S27.00013: A High Throughput DFT Study of Half Heusler Solid Solution Mixtures ANDREW LEE (Presenter), SHASHWAT ANAND, Northwestern University, LOGAN WARD, Argonne National Laboratory, CHRISTOPHER MARK WOLVERTON, Northwestern University — Half heuslers exhibit properties well-suited for thermoelectrics. The best performing half heusler thermoelectrics such as TiNiSn, NbFeSb, and ZrCoBi-based systems are solid-solution alloys with disorder scattering which reduces thermal conductivity. However, only a handful of such alloy systems have been reported. Furthermore, these systems are studied with mixing on just one of the three sub-lattices at a time. Hence, a comprehensive study of solubility in mixed alloy systems can guide future choices of half heusler thermoelectrics. Here, we use DFT to calculate mixing energies and relative stabilities of around 1000 binary solid solutions using restrictions of isovalent substitution and single sublattice mixing. Half of these have mixing energies suitable for forming single phase alloys, when |E_mix| < 0.05 eV/atom (kBT @ 600K). We then extend our search to higher component mixtures and the unexplored concept of multi-sublattice mixing. Continuing with DFT is too slow given the combinatorically expanding composition space, so we develop a machine learning model to help classify mixing behavior. With trends identified from the model and DFT, we hope to better guide future experiments toward improved half heusler thermoelectrics.
**1:51PM S27.00014: Low temperature thermopower in CoSbS**  
QIANHENG DU (Presenter), State Univ of NY - Stony Brook, MILINDA ABEYKOON, YU LIU, Brookhaven National Laboratory, GABRIEL KOTLIAR, Rutgers University, CEDOMIR PETROVIC, Brookhaven National Laboratory — Thermopower of FeSb2 reaches colossal values of up to -45 mV/K, however, the physical mechanism is not well understood. In order to make progress and enable predictive materials design, it is important to discover new materials with high thermoelectric parameters and with tunable physical properties. Recently, it was shown that CoSbS could be a high-temperature thermoelectric material due to several positive factors that work simultaneously to enhance its thermoelectric performance. We report giant thermopower $S = 2.5$ mV/K in CoSbS single crystals [1], a material that shows strong high-temperature thermoelectric performance when doped with Ni or Se. Changes of low temperature thermopower induced by magnetic field point to mechanism of electronic diffusion of carriers in the heavy valence band. Intrinsic magnetic susceptibility is consistent with the Kondo-Insulator-like accumulation of electronic states around the gap edges. This suggests that giant thermopower stems from temperature-dependent renormalization of the noninteracting bands and buildup of the electronic correlations on cooling.


**S27.00015: Large magnetothermopower and anomalous Nernst effect in HfTe$_5$**  
JUNFENG HU (Presenter), BeiHang University, MARCO CAPUTO, Paul Scherrer Institute, EDUARDO BONINI GUEDES, EPFL, SA TU, BeiHang University, EDOARDO MARTINO, ARNAUD MAGREZ, HELMUTH BERGER, J. HUGO DIL, EPFL, HAIMING YU, BeiHang University, JEAN-PHILIPPE ANSERMET, EPFL — Topological quantum materials have stimulated a growing attention because they reveal novel aspects of condensed matter physics and point to new opportunities in materials science, in particular for thermoelectrics. Here, we experimentally study thermoelectric effects in HfTe$_5$, which was predicted to be at the boundary between strong and weak topological insulators. The magnetic field dependence of HfTe$_5$ thermoelectric properties attests to the anomalous character of this material, supported by our angle-resolved photoemission spectroscopy (ARPES) measurements. A possible topologically non-trivial band structure is proposed to account for our observations. Our results constitute a highly constraining set of data for any model of transport based on HfTe$_5$ band structure. Furthermore, the extraordinary thermoelectric properties suggest a new paradigm for the development of thermoelectric applications based on layered transition-metal chalcogenides.

*We acknowledge the support by NSF China under Grant Nos. 11674020, U1801661, by the Sino-Swiss Science and Technology Cooperation (No. EG 01-122016) for J. H., by the Program of Introducing Talents of Discipline to Universities in China "111 Program" No. B16001.
The theoretical limits of electron tomography have long been defined by the Crowther criterion, which relates 3D resolution to the number of projections acquired, and the dose fractionation theorem, which dictates total dose requirement across projections. However, these relations are invalid for aberration-corrected scanning transmission electron microscopy (STEM) where high convergence angles limit the ability to reconstruct objects larger than the depth-of-focus (c.a. 5 nm). We show overcoming the limitations of aberration-corrected STEM tomography requires collecting information beyond a traditional tilt series by acquiring a through-focal stack at every tilt. Here, information is no longer mapped to a plane in Fourier (k) space, but becomes a volumetric toroid.

Here we present a theoretical foundation for aberration-corrected electron tomography by establishing analytic descriptions for resolution, sampling, object size, and dose—with direct analogy to the Crowther criterion. The 3D structure of a contrast transfer function (CTF) for through focal tomography where every specimen tilt measures a toroid with petal-shaped cross-section. A remarkable feature of the 3D CTF is the overlapped regions that permit complete information collection—unachievable with conventional tomography. This breaks expected Crowther relationships and the maximum reconstructable object size is unlimited up to spatial frequency $k_c$. At resolutions beyond $2/k_c$, Crowther-like tradeoffs define the maximum object size (D) allowed for given 3D resolution (d).

When the tilt angle spacing becomes smaller than twice the convergence angle (2α) a continuum of information is measured and object size is unbounded at midband resolution. This occurs under typical instrument operation (> 25 mrad) and sampling (< 2° tilt). We show atomic resolution (1Å) 3D imaging is allowed across extended objects (> 20 nm) using currently available microscopes and modest specimen tilting (< 3°).
Phonons can be excited by fast electrons in two fundamentally different ways: by dipole scattering, which is similar to exciting the sample by infrared light, and by impact scattering, which bears a closer resemblance to neutron scattering. Dipole scattering occurs only in polar materials, and is characterized by small scattering angles (~0.1 mrad) and interaction distances of tens of nanometers. Impact scattering involves a direct interaction between the fast electron and an atomic nucleus, and leads to large scattering angles. Selecting the impact scattering (with an aperture in the diffraction plane) allows the vibrational signal to be imaged in materials such as h-BN with atomic resolution (0.2 nm).

The angular (momentum) distribution of vibrational scattering of fast electrons has also been explored. Attainable spatial resolution is then inversely related to the angular resolution. Optical and acoustic branches of vibrational scattering have been mapped in several materials while maintain a spatial resolution of a few nm. A change in the acoustic phonon signal has been observed at a single lattice defect in SiC, making it likely that the influence of lattice defects on thermal transport will be properly elucidated at last.

Dipole scattering provides another exciting experimental possibility: probing the sample from a small distance, by “aloof spectroscopy”. This approach limits the maximum energy that can be transferred to the sample with significant probability as 1/b, where b is the distance of the focused electron beam from the sample. In this way, vibrational properties of biological and other “fragile” materials can be probed without significant radiation damage, presently with about 5 meV energy resolution. This promises to revolutionize analysis in the electron microscope.
Heterogeneous nucleation at solid-liquid interfaces underlies a number of technologically important processes, from catalyst synthesis to fabrication of thin films, but remains poorly understood due to the dearth of techniques for quantifying nucleation energetics. In this talk, I will discuss development of a liquid cell transmission electron microscopy (LC-TEM) method for quantifying important parameters of heterogeneous nucleation, including supersaturation ratio and interfacial energy, and our efforts to utilize this approach to visualize nanoscale variations in nucleation kinetics at a solid-liquid interface. We quantify the supersaturation ratio of solute with numerical simulations of the electron beam induced chemistry during LC-TEM experiments, which enables fitting nucleation data using classical nucleation theory. Multiparticle tracking analysis applied to LC-TEM movies of nanoparticle nucleation reveals local variations in nucleation kinetics and preferential nucleation sites with nanometer scale spatial resolution. With this approach, we have demonstrated that heterogeneous nucleation of silver nanocrystals at a planar, uniform silicon nitride-water interface occurs preferentially in discrete nanoscale domains of the interface. Characterization of the solid-liquid interface with atomic force microscopy and covalent nanoparticle labeling revealed domains of surface functional groups on the interface acted as preferential nucleation sites. These results challenge previously held beliefs about nucleation on uniform interfaces, showing that nanoscale variations in surface chemistry can propagate nanoscale variations in nucleation kinetics.

*This work has been funded by ORAU (Award 17061851) and ACS PRF (61111-DNI10).
Nanocrystals often readily change structure and morphology during growth, self-assembly and applications when interacting with their environments. It imposes challenges as well as opens opportunities for the understanding and engineering of these nanostructures for practical applications. Due to the nanometer length scale and the dynamic nature of these transformations, in situ transmission electron microscopy (TEM) has become an indispensable technique for the investigation of these processes. Recently, the significant technical advances in in situ TEM have revealed many dynamic phenomena of nanocrystals with high spatial and temporal resolution that were previously unreachable. In this talk, I will show a few examples about the structural transformations of nanocrystals during growth and self-assembly in solution. Special attention has been made to the transient states, which may draw the system outside thermodynamic equilibrium. An understanding of the nanoscale dynamics and the intermediate states aid the future design of novel materials and devices.

*The project was funded by U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05-CH11231 within the in situ TEM program (KC22ZH). Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
The Intersection of Cryo, Laser Ablation, and Nanoscale Electron Imaging for Intact Battery Characterization

KATHERINE JUNGJOHANN (Presenter), Sandia National Laboratories — Characterization of intact batteries is challenging due to the great diversity of the component materials. For example, lithium anode batteries contain a stack consisting of a metal current collector, the lithium metal anode, a polymer separator saturated with lithium salts in an aprotic electrolyte, a transition metal oxide cathode, and another metal current collector. These components are generally stacked within a spring-loaded coin cell for electrochemical performance testing of the cell for repeated charge and discharge cycling. General characterization techniques require the disassembly of the stainless-steel coin cell, with analysis of each of the components individually. Here, we present a method for retaining the internal structure of the coin cell by cryogenic plunge freezing of the entire stack, followed by in-situ, athermal, ultrashort-pulse laser ablation to access the internal components in cross-section, followed by standard characterization using scanning electron microscopy and energy dispersive x-ray spectroscopy. This provides the complete structural and compositional analysis of the intact battery stack with nanometer resolution, where we have determined several failure modes of lithium metal anodes for use as rechargeable batteries.

*This work was funded by Sandia National Laboratories’ Laboratory Directed Research and Development program. It was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE’s National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S29 DSOFT DBIO GSNP DPOLY: Active Matter and Liquid Crystals in Biological Systems III

NOAH MITCHELL (Presenter), KITP, UC Santa Barbara, DILLON CISLO, University of California, Santa Barbara, SURAJ SHANKAR, Harvard, ZVONIMIR DOGIC, University of California, Santa Barbara, BORIS I SHRAIMAN, KITP, UC Santa Barbara, SEBASTIAN STREICHAN, University of California, Santa Barbara — A common theme in biology is the assembly of cells into tubes, which in turn develop into specific shapes for specific functions. In a large class of organs including the gut, a simple tube transforms into a coil of compartments. This process is particularly striking in the Drosophila melanogaster midgut -- a tube that folds and then coils into a helical configuration in only two hours. Using a combination of light-sheet microscopy, genetics, and computer vision techniques, we extract the full 3D dynamics of this organ with subcellular resolution. We present a quantitative account of the dynamics of folding and coiling of the midgut that links cellular motion and deformation to the macroscopic shape change of the organ.
11:27AM S29.00002: Dynamical self-consistent field-theory for active nematic liquid crystals: Nematic order and spatio-temporal structure in surface colonies of rod-like bacteria  DRAKE LEE (Presenter), ROBERT WICKHAM, Univ of Guelph — We present a dynamical self-consistent field theory for interacting, self-propelled rods that we use to study fascinating time-dependent, inhomogeneous structures observed in surface colonies of twitching *Pseudomonas aeruginosa* bacteria. We apply an extremal principle to an exact dynamical functional integral derived from the microscopic, many-body dynamics of self-propelled rods moving in two-dimensions. This reduces the problem to that of a single self-propelled rod moving in response to self-consistent, mean-force and torque fields. We address the thorny problem of calculating rod-rod interactions in this mean-field approximation. For uniform systems in two-dimensions, we observe that a continuous isotropic-nematic phase transition occurs at a critical rod concentration. The value of the critical concentration is independent of the magnitude of the self-propulsive force. We discuss our preliminary simulations of inhomogeneous, dynamical structures formed in motile bacteria surface colonies.

11:39AM S29.00003: Growth and dynamics of active nematic droplets of *Myxococcus xanthus* bacteria  CASSIDY YANG (Presenter), JOSHUA SHAEVITZ, Princeton University — *Myxococcus xanthus* is a rod-shaped soil bacterium that exhibits various forms of emergent collective phenomena using only short-range interactions. When starved, they collectively bead from surfaces to form 3D droplet-like aggregates known as fruiting bodies that are comprised of hundreds of thousands of cells and are crucial for sporulation and survival. The combination of active cellular motility and local nematic interactions generates increased pressures that drive the dewetting process. Unlike passive fluids that form axisymmetric spherical cap-shaped droplets, we find that these aggregates break symmetry and are often elongated in shape with non-uniform contact angles. We characterize the growth and dynamics of these active nematic droplets and make progress towards understanding the role of motility in the formation of stable fruiting bodies through tracking sparsely labelled cells.
11:51AM S29.00004: Solid-liquid transitions of deformable active particles*  
BENJAMIN LOEWE (Presenter), Department of Physics, University of California, Santa Barbara, MICHAEL CHIANG, DAVIDE MARENUZZO, School of Physics and Astronomy, University of Edinburgh, M CRISTINA MARCHETTI, Department of Physics, University of California, Santa Barbara — Experiments have established that confluent epithelial tissues exhibit solid-liquid transitions. Although epithelial tissues usually form a cell monolayer, there are situations in which that monolayer structure breaks, such as in cell extrusion and pseudo-stratified epithelia. To describe such situations, we have developed a multi-phase field model where cells are characterized by multiple scalar fields, and interact through steric repulsion. By reducing their deformability, these cells go from being highly-deformable with no overlap to almost-circular with high overlap, which can be thought of as a way to incorporate layering between cells. Using this model we have examined the interplay of cell deformability and cell motility in controlling the solid-liquid transition of ordered lattices. We find that by reducing cell deformability the melting transition changes from continuous to discontinuous: at finite overlap the system develops an intermittent region, alternating between crystalized and liquid states. Finally, by studying the formation of defect pairs in the intermittent region, we find that they correlate with spatial fluctuations of the cell-overlap, suggesting that cell extrusion is correlated with structural defects.

*This work was supported by NSF grant DMR-1609208.

12:03PM S29.00005: Uncovering the dynamic precursors to motor-driven contraction of active gels*  [Invited]  
JOSÉ ALVARADO (Presenter), University of Texas at Austin — Cells and tissues have the remarkable ability to actively generate the forces required to change their shape. This active mechanical behavior is largely mediated by the actin cytoskeleton, a crosslinked network of actin filaments that is contracted by myosin motors. Experiments and active gel theories have established that the length scale over which gel contraction occurs is governed by a balance between molecular motor activity and crosslink density. By contrast, the dynamics that govern the contractile activity of the cytoskeleton remain poorly understood. Here we investigate the microscopic dynamics of reconstituted actin–myosin networks using real-space video microscopy and Fourier-space dynamic light scattering. Light scattering reveals different regimes of microscopic dynamics. We uncover two dynamical precursors that precede macroscopic gel contraction. One is characterized by a progressive acceleration of stress-induced rearrangements, while the other consists of sudden, heterogeneous rearrangements. Our findings suggest a qualitative analogy between self-driven rupture and collapse of active gels and the delayed rupture of passive gels observed in earlier studies of colloidal gels under external loads.

*US Army Research Office under grant number W911NF-14-1-0396
12:39PM S29.00006: Microscopic simulations of a 3D active nematic composed of semiflexible polymers* MATTHEW PETERSON (Presenter), MICHAEL HAGAN, APARNA BASKARAN, Brandeis University — The field of active matter studies materials whose constituent particles can consume energy at the particle scale to produce motion. An active nematic has the additional constraint that these particles have nematic symmetry. Unlike a passive nematic, an active nematic can exhibit spontaneous creation and annihilation of topological defects. Recent work on 3D active nematics shows notable differences in the structure and dynamics of these defects compared to 2D systems—for example, defects tend to form as neutrally charged disclination loops. Here, we will use particle-based simulations to better understand the dynamical properties of dry active nematics in 3D, both in bulk and under confinement.

*We acknowledge support from the Brandeis NSF MRSEC, Bioinspired Soft Materials, DMR-1420382, and DMR-1855914.

12:51PM S29.00007: The structure and dynamics of microtubule bundles mediated by motor proteins BEZIA LEMMA (Presenter), Physics, Harvard, LINNEA LEMMA, Physics, Brandeis, SEBASTIAN FUERTHAUER, MICHAEL JOHN SHELLEY, Flatiron Institute, ZVONIMIR DOGIC, Physics, UC Santa Barbara, DANIEL NEEDLEMAN, Harvard — Mixtures of polar microtubule (MT) filaments and force-generating motor proteins self-organize by cross-linking and sliding MTs into dense networks of polar and apolar bundles. We can measure the geometric structure of these MT-based bundles using small-angle x-ray scattering and determine the polar structure of these materials by taking advantage of their chiral crystal lattice which produces constructive interference of second harmonic signal between polar-aligned MTs. A transition in the bundles' structure to a compressed square lattice corresponds to a change in the microtubules extensile sliding dynamics. These results are useful in understanding the dynamics of filamentous active materials. The quantified geometric packing of microtubule bundles can be incorporated into a framework of highly cross-linked active gel theories.

1:03PM S29.00008: Microscopic to mesoscopic: what can modular molecular motors teach us about the nature of active stress? STEVEN REDFORD (Presenter), University of Chicago, PAUL RUIJGROK, Stanford University, JONATHAN COLEN, University of Chicago, SASHA ZEMSKY, Stanford University, VINCENZO VITELLI, University of Chicago, ZEV BRYANT, Stanford University, AARON DINNER, MARGARET GARDEL, University of Chicago — Coarse-grained hydrodynamic theories have proven invaluable to our understanding of active nematic liquid crystals. In general, these treatments succeed despite coarse graining out the microscopic details of the material, because they account for certain mesoscopic consequences of microscopic change. For example, changing the elastic constants in the nematic governing equations can account for microscopic differences in mesogen length and rigidity. However, no such treatment accounts for the microscopic nature of the stress itself. Here, we step towards rectifying this discrepancy by experimentally tuning the properties of stress-generating myosin motors in an actin based active liquid crystal. Within this system, we can begin to understand how systematically varying the microscopic properties of these motors affects the resultant active flow.
1:15PM S29.00009: 2D Patterns of Active Stress ascribe 3D Deformations of Driven Actomyosin Networks  VIKRANT YADAV (Presenter), Department of Biomedical Engineering, Yale University, TAEYOON KIM, Weldon School of Biomedical Engineering, Purdue University, ENRIQUE DE LA CRUZ, Department of Molecular Biophysics and Biochemistry, Yale University, MICHAEL MURRELL, Department of Biomedical Engineering, Yale University — During morphogenesis 2D active stresses in actomyosin networks can lead to 3D deformation of epithelial sheets. Though there is consensus on role of stress, how in-plane activity morphs epithelial sheets out of plane is not clearly understood. To understand this relation, we design an invitro actomyosin network with tunable mechanical stiffness and activity. The active stresses can be locally programmed into the 2D actomyosin sheets by photoactivation of myosin motors. We demonstrate that an interplay between mechanics of sheet and activity leads to controlled 3D deformations. We show that the extent of 3D deformation of network is proportional to activity, but varies non-monotonically with stiffness. By controlling the shape and duration of activation protocol, we can create 3D deformations of various shapes with positive, negative, or zero gaussian curvature. Through experiments and agent-based simulations we show that local inhomogeneities in stiffness of actomyosin sheet are responsible for activity-driven out of plane deformations. These results open an arena for designing bio-inspired smart active materials with programmable deformations.

1:27PM S29.00010: Confinement effects on the phase behavior of collagen-like semiflexible polymers* RUSSELL SPENCER (Presenter), BAE-YEUN HA, University of Waterloo — Semiflexible polymers often self-assemble into aligned structures with emergent mechanical and optical properties. These properties depend on the particular molecular arrangement they form. Indeed, the main structural component of bone, skin and corneas is collagen, but their mechanical and optical properties are vastly different because of the way these molecules are arranged. In this talk, we discuss the phase behavior of collagen-like semi-flexible polymers in the presence or absence of confinement, focusing on isotropic, nematic and cholesteric phases. Using self-consistent field theory, we first investigate phase boundaries and locate regions where each arrangement is stable or metastable. We then consider confinement effects by introducing planar walls. Our results suggest that the presence of planar walls reduces allowed alignment directions to being parallel with the wall, allowing the ordering direction to be uniquely set by the geometry of the experimental setup. We discuss how they can be used to tailor materials.

*This work was funded by NIH 1R01EY028234-01 and NSERC.
1:39PM S29.00011: Shape study of Spindle-like microtubule tactoids using experiment and computation
SUMON SAHU (Presenter), Syracuse University, LENA HERBST, RYAN QUINN, UMass Amherst, JENNIFER L ROSS, Syracuse University — Mitotic spindles during metaphase are a fundamentally important puzzle of biophysics at the base of the question of how a cell divides its genetic material. Mitotic spindle self-assembly is inherently non-equilibrium with a vast parameter space. Factors that play a role as a system include microtubules, molecular motors, crosslinkers, and associated proteins, whose working principles are not yet clear. Recently, we reconstituted a minimal model system for creating microtubule-based spindle-like assemblies using microtubules and the plant-derived crosslinker, MAP65. Here we have extended our work to determine the important requirements for tactoid formation by exploring different crowders or viscosity agents to show that they do not play a significant role determining the formation or shape of the tactoids. Also, using a computational approach we have shown that similar steady state tactoids can evolve from growing filaments that follow a damped Langevin equation and Hookean type crosslinkers. We explored the phase space of this organization by varying initial conditions like filament number, orientation, and length as well as crosslinker number, binding dynamics. Using these two directions we are uncovering the principles behind spindle organization using tactoid as a model.

1:51PM S29.00012: Shear-induced gelation of self-yielding active networks*
DAVID GAGNON (Presenter), CLAUDIA DESSI, Georgetown University, ZVONIMIR DOGIC, University of California Santa Barbara, DANIEL BLAIR, Georgetown University — The activity of molecular motors reconfigures biopolymer networks and modifies their mechanical properties. Designing these active gels with tunable properties analogous to the cytoskeleton is a key prerequisite for creating biomimetic systems to study cellular behavior such as division and motility. Active gels form ephemeral networks with long-range but temporary active mechanical contacts. In this talk, I will describe how microscopic dynamics modify the macroscopic mechanical properties of extensile microtubule networks. Rheological measurements reveal a non-monotonic dependence on the applied shear rate. A simple phenomenological model, which describes the network as a collection of fluid-like and solid-like elements, quantitatively explains the shear-rate-dependent viscosity in terms of locally-measured activity-induced flows. Fast, active elements remodel the network and therefore do not transmit elastic stresses, while slow, temporarily crosslinked elements behave elastically until they break and reform under shear.

*Templeton Foundation Grant 57392 and U.S. Department of Energy, Office of Basic Energy Sciences award DE-199 SC0010432TDD

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S30 DSOFT GSNP: Origin of Rigidity and Yielding 502 - Sriram
Ramaswamy, Indian Institute of Science - Tag(s): Focus
11:15AM S30.00001: A statistical mechanical theory for the origin of rigidity in crystalline solids [Invited]  
SURAJIT SENGUPTA (Presenter), Hyderabad campus, Tata Institute of Fundamental Research (TIFR) — It is known that if local atomic rearrangements leading to exchange of neighbours are allowed, no crystalline solid can be rigid in the thermodynamic limit. The usual rigid, elastic, response to shape changes, a defining character of a crystalline solid, arises because the time needed for such rearrangements diverge as the magnitude of deformation approaches zero. Starting from these general considerations, we had shown that crystal rigidity arises as a consequence of a first order phase transition in an expanded parameter space [1]. The solid is subjected to not only elastic deformation but also to a fictitious external field, which penalises rearrangements, with the understanding that properties of real crystals are recovered by first taking the thermodynamic limit and then letting this field go to zero. Within this picture, we obtain a first order phase transition between a rigid crystal, N, and a crystal, M, where atoms rearrange to eliminate internal stress for any given deformation while maintaining crystalline order. The N-M phase boundary, in the thermodynamic limit, passes through the origin, where both field and deformation is zero. This picture gives us a fundamentally new viewpoint on the phenomenon of yielding, i.e. the loss of rigidity of a crystal when deformed beyond a limit, viz. the yield point. The phenomenon of yielding is now simply the nucleation of bubbles of the thermodynamically stable M phase within the metastable, rigid N crystal. An outcome of this theory is that the yield point is always a weak function of the rate of deformation and vanishes in the true quasistatic limit. The analytic form derived by us for the yield point as a function of the rate of deformation is able to explain experimental data over 15 orders of magnitudes in time [2]. We also discuss several details of yielding in Lennard Jones solids in 2 and 3 dimensions. 

11:51AM S30.00002: Critical Scaling of Avalanches with Strain Rate in Athermal, Disordered Solids*  
MARK ROBBINS (Presenter), Johns Hopkins University, JOEL CLEMMER, Sandia National Laboratory, KENNETH SALERNO, Army Research Laboratory — Molecular dynamics simulations are used to study critical behavior in slowly sheared disordered solids that are modeled as a bidisperse Lennard-Jones glass. The mean flow stress rises as strain rate to the power 1/β. Finite-size scaling is used to determine β and the exponent ν describing the divergence of the correlation length. The system length L varies from 55 to 1753 particle diameters in d=2 and 20 to 163 in d=3. Fluctuations in the stress and kinetic energy per particle scale as L^{-d/2}, implying that the largest avalanche scales as L^α with α < d/2. Temporal correlations are used to measure the dynamical exponent z relating the duration of an avalanche to its linear dimension. In contrast to lattice models, we find z>1, as required by causality. New scaling laws are derived for exponents describing the power law decay of the noise power spectrum with frequency and tested using finite-size scaling.

*This material is based upon work supported by the National Science Foundation under Grant No. DMR-1411144.
12:03PM S30.00003: Bauschinger effect in model glasses* SYLVAIN PATINET, ARMAND BARBOT, ISMAIL EL KORDE, MATTHIAS LERBINGER, DAMIEN VANDEMBROUCQ (Presenter), PMMH, ESPCI Paris, ANAÎL LEMAÎTRE, Laboratoire Navier, IFSTTAR — Once a material has experienced a significant plastic deformation, it it generally exhibits a softer stress response under reverse loading than under reloading in the original direction. The origin of this so-called Bauschinger effect, observable in various classes of materials remains poorly understood. We present here recent results obtained on two-dimensional model glasses at atomistic and mesoscopic scales. Using a numerical method developed in [1] we perform measurements of the local plastic thresholds in the steady state flow of a 2D model glasses under athermal quasi-static (AQS) deformation. Our results show evidence for the development of a forward-reverse asymmetry of the distribution of the residual strengths that can be directly connected with the Bauschinger effect [2].


*M.L. and S.P. acknowledge the support of French National Research Agency through the JCJC project PAMPAS under grant ANR-17-CE30-0019-01.

12:15PM S30.00004: Shear banding transition in granular materials under uniform and boundary shear* YIQIU ZHAO (Presenter), Department of Physics & Center for Nonlinear and Complex Systems, Duke University, Durham, North Carolina 27708, USA, JONATHAN BARES, Laboratoire de Mécanique et Génie Civil, Université de Montpellier, CNRS, Montpellier, 34090, France, HU ZHENG, Department of Geotechnical Engineering, College of Civil Engineering, Tongji University, Shanghai, 200092, China, JOSHUA SOCOLAR, Department of Physics & Center for Nonlinear and Complex Systems, Duke University, Durham, North Carolina 27708, USA —

We experimentally study shear band formation in a 2D granular material subjected to quasistatic shear using Couette apparatus with a base consisting of 21 rotating concentric rings. The rings can independently be controlled to interpolate between uniform shear and boundary shear in a layer of photo-elastic disks resting on them. Previous uniform shear experiments using this setup [PhysRevLett.123.158001] showed that a steady localized shear band forms at sufficiently large strains for packing fractions \( \varphi > 0.78 \). In the present work, we study how this transition is affected by the specific choice of the relative velocities of the rings. For \( \varphi < 0.78 \), the flow roughly follows the basal velocity profile. For \( \varphi > 0.78 \), we find that the steady flow profile is insensitive to the basal velocity profile, though the times needed to reach the steady flow regime are different. For \( \varphi \sim 0.78 \), a localized shear band forms and dissolves irregularly in association with the formation and yielding of a strong force network.

* Work supported by NSF grant DMR-1809762.
12:27PM S30.00005: Strain localization and shear band formation during tensile tests of disordered floating granular monolayers*   HONGYI XIAO (Presenter), ROBERT IVANCIC, GE ZHANG, ROBERT RIGGLEMAN, ANDREA JO-WEI LIU, DOUGLAS DURIAN, University of Pennsylvania — Understanding and predicting strain localization and shear band formation during deformation of amorphous solids is an ongoing challenge. In this study, quasi-static tensile experiments were performed using a model disordered solid consisting of a monolayer of polydisperse granular spheres with capillary attractions floating on an air-oil interface. Under tensile deformation, the strain in the monolayer gradually localizes into an inclined shear band, upon which failure occurs. The ductility of the monolayer can be tuned by using different particle sizes compared to the capillary length, which sets the interaction range. Using machine learning methods, we developed a scalar field, softness, that relates the local structure around particles and particle-level dynamics. We found that softness tends to increase around particles that have rearranged. Furthermore, planes that develop into shear bands tend to have higher than average softness prior to deformation and become even softer as the shear band forms. These results reveal the relation between structure and dynamics that leads to strain localization, which could potentially apply to a broad range of amorphous solids.

*Funded by NSF grants MRSEC/DMR-1720530

12:39PM S30.00006: Yielding and mechanical failure in (amorphous) solids [Invited]   JUERGEN HORBACH (Presenter), Institute for Theoretical Physics: Soft Matter, University of Duesseldorf, Germany — Recently, a Monte Carlo simulation study [1] has shown that yielding in crystalline solids is associated with an underlying quasi-static first-order phase transition. As a consequence, in the limit of a deformation with sufficiently low strain rate, the rigid response of a crystal due to a shape change of its boundaries corresponds to a metastable state that transforms to a stable state where internal stresses are eliminated, maintaining the crystalline order. A nucleation theory based on these findings predicts the yield point as a function of strain rate and shows agreement with data from experiment and molecular dynamics (MD) simulations over 15 orders of magnitude [2]. In the case of amorphous solids (glasses), a MD simulation study, using an athermal quasi-static (aqs) deformation protocol [3], have found a sharp stress drop in the stress-strain relation that marks the transition from an elastic response of the glass to plastic flow. In Ref. [3], this stress drop has been interpreted as a non-equilibrium first-order transition, leading to the occurrence of shear localization, i.e. shear banding, after the drop. Using MD simulations of a glassforming binary Lennard-Jones (LJ) mixture under shear, we study the conditions for the occurrence of shear bands at finite temperatures [4] and discuss the response of the LJ glass to an external shear in the limit of zero strain rate. We argue that there is no quasi-static first-order transition as in the case of crystalline solids.

1:15PM S30.00007: Unjamming and reentrant jamming of dense systems in the extreme active limit* DESHPREET BEDI (Presenter), Brandeis University, PINAKI CHAUDHURI, The Institute of Mathematical Sciences, CHANDAN DASGUPTA, Indian Institute of Science, BULBUL CHAKRABORTY, Brandeis University — Simulations of dense, athermal assemblies of self-propelled soft particles with infinite persistence time display intriguing mechanical properties as a function of the strength of the active propulsion force and the packing fraction of the system. Applying active propulsion to an initial, passively-jammed state results in unjamming and subsequent flow of the system. We find that there is a threshold force above which the system remains fluid indefinitely but below which the system experiences reentrant jamming, and that this threshold force increases as the density of the system is increased. Interestingly, we find that the average coordination numbers of both fluid and re-jammed states under active propulsion are larger than those of the passively-jammed states for a given packing fraction.

We analyze various network properties over time series of such systems to illuminate the structural differences between packings formed with passive and active constituents, as well as understand the underlying mechanisms of reentrant jamming in this extreme active limit. We also investigate the effect of the magnitude of the active force on jamming behavior.

*This work has been supported by NSF-CBET 1916877 and BSF-2016118.

1:27PM S30.00008: States of self-stress in disordered solids SHANG ZHANG (Presenter), LEYOU ZHANG, Univ of Michigan - Ann Arbor, VISHWAS VASISHT, IIT Palakkad, India, EMANUELA DEL GADO, Georgetown University, XIAOMING MAO, Univ of Michigan - Ann Arbor — We investigate the interplay between the mechanical responses of disordered solids and their states of self-stress (SSSs), which are equilibrium stress distributions in a mechanical network with force balanced on any component. SSSs are determined by the geometry of the network (they span the null space of the network's equilibrium matrix) and govern load-bearing abilities of this network. On the other hand the mechanical load changes the geometry and feedback to the SSSs. By presenting our results on SSSs in disordered solids generated by molecular dynamics simulations as well as jamming protocols, we explore the relation between SSSs in a disordered solid and the memory of how the mechanical network is prepared, as well as how they yield under stress.
1:39PM S30.00009: Local order and structural rearrangement in two-dimensional jammed systems under oscillatory shear  ERIN TEICH (Presenter), LARRY GALLOWAY, PAULO ARRATIA, DANIELLE BASSETT, University of Pennsylvania — Amorphous, jammed systems are abundant in nature and utilized often in man-made materials. The way in which their disordered structure evolves under the application of shear stress is an area of active investigation with consequences in contexts ranging from earth science to cancer research. Identifying local structural characteristics that influence macroscopic dynamics in these materials remains an ongoing challenge, and previous work has indicated generally that particles with ordered local environments are less likely to dynamically rearrange under shear. Here, we expand on this preliminary conclusion, and quantify it concretely in a two-dimensional colloidal jammed system subject to oscillatory shear. We analyze local crystallinity and identify crystal grains in these systems. We track structural correlations over time, and find that crystalline particles that are more interior within grains are less likely to rearrange. Moreover, propensity to rearrange occurs in a hierarchy according to the degree to which particles are “protected” within the grains. In addition, structural correlations qualitatively change at strain amplitudes above yield, where elasticity and viscosity become comparable, implying a transition in structural memory in the system.

1:51PM S30.00010: Yielding and transient shear banding in soft jammed solids  VISHWAS VASISHT (Presenter), Physics, IIT Palakkad, EMANUELA DEL GADO, Georgetown University — We have designed 3D numerical simulations of a soft spheres model, with size polydispersity and in athermal conditions, to study the transient shear banding that occurs during yielding of jammed soft solids. We have analyzed the effects of different types of drag coefficients used in the simulations and compare the results obtained using Lees-Edwards periodic boundary conditions with the case in which the same model solid is confined between two walls. While load curves and velocity profiles obtained in different conditions displays some differences, the presence of a stress-overshoot and a related transient banding phenomenon are a robust feature for overdamped systems and large enough samples. We use this computational approach to investigate the microscopic origin of the flow inhomogeneities and the role played by the confinement.
2:03PM S30.00011: Strain dependent hysteresis in nanoparticle aggregate dispersions visualized to explain origin of the Payne Effect and Spectral Hole Burning in cross-linked filled rubber*  
ZACH GAULT (Presenter), ZSOLT TERDIK, PETER JAMES LU, JOERG WERNER, DAVID A WEITZ, Harvard University — Filled rubbers are composite materials containing two interpenetrating phases: crosslinked elastomers, and a ‘filler’ consisting of nanoparticle particle aggregates. The nanoparticle aggregates form a system-spanning subnetwork that reinforces the elastomer network and introduces a new energy loss mechanism at low strains of only 1-5%. This loss mechanism, known as the Payne Effect, is one of the mechanical hallmarks of filled rubbers and is a major contributor to rolling friction in tires. We create a transparent model system to study the strain dependent hysteresis of nanoparticle aggregates. With this system we can directly observe microstructural changes of filler particle aggregates during \textit{in situ} shear deformation. We complement these observations with bulk rheological tests, including spectral hole burning, to gain new insight into the microscopic structural changes that occur during cyclic deformation.

*NSF Colloids Grant: DMR-1611089
Harvard MRSEC: DMR 14-20570

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S31 DSOFT DBIO GSNP: Emergent Collective Dynamics in Biology: from Microbes to Organs I  
503 - Miguel Ruiz Garcia, University of Pennsylvania - Tag(s): Focus

11:15AM S31.00001: Dynamics and self-organization of active surfaces [Invited]  
FRANK JULICHER (Presenter), Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — Biological cells are active systems and exhibit complex dynamic behaviours such as cell division, cell polarity establishment and cell locomotion. Such dynamic processes emerge from the collective interplay of many molecular components far from thermodynamic equilibrium. Active molecular processes such as the force generation of molecular motors along filaments of the cytoskeleton transduce chemical free energy to generate movements and mechanical work. The cell cortex, a thin film of active material assembled below the cell membrane, plays a key role in cellular symmetry breaking processes such as cell polarity establishment and cell division. I will present a minimal model of the mechano-chemical self-organization of the cell cortex that is based on a hydrodynamic theory of curved active surfaces and that can capture the emergence of shapes. Active stresses on this surface are regulated by a diffusing molecular species. We show that coupling of the active surface to a passive bulk fluid enables spontaneous polarization and the formation of a contractile ring on the surface via mechano-chemical instabilities. We discuss the role of external fields in guiding such pattern formation. Our work reveals that key features of cellular symmetry breaking and cell division can emerge in a minimal model via general dynamic instabilities. Self-organised active surfaces provide minimal models for the generation of shape and the emergence of dynamic patterns in basic cellular processes.
**11:51AM S31.00002: Microtubule Motility on Fixed and Diffusive Motor Proteins**

FERESHTEH MEMARIAN (Presenter), University of California, Merced, JOSEPH LOPES, Physics, Brandeis University, LINDA S. HIRST, University of California, Merced — Motor proteins transporting cargo by walking on microtubules (MTs). MTs are part of the cytoskeleton and are important in cell division, giving shape to the cell membrane. Here we investigate motor-based transportation and behavior of MTs. In a MT gliding assay, motor proteins adhere to the glass while MTs glide on them. MT behavior in gliding assay experiments with high MT concentration is compared with behavior on diffusing motor proteins and at similar concentration. An interesting twist on the standard gliding assay is to attach the motors to a lipid bilayer and let them diffuse on the membrane. Using fluorescence recovery after photobleaching (FRAP), we measured motor diffusion constants. We demonstrate the MT “snuggling” effect, i.e. they spontaneously align locally while gliding on the membrane-bound motor proteins. When MTs encounter each other for gliding assays, they simply cross over in the absence of a crowding agent. Furthermore, we observe that MTs exhibit collective motion, much like bird flocking, with diffusing kinesins, which is not replicable with fixed kinesins.

*We acknowledge the National Science Foundation grant DMR-1808926, NSF-CREST: NSF-HRD-1547848. The data was collected, in part, with a confocal microscope acquired through the NSF MRI Award DMR-1625733*

**12:03PM S31.00003: Modeling of the collective motion of microtubules with mobile kinesin motors**

MADHUVANTHI ATHANI (Presenter), FERESHTEH MEMARIAN, LINDA S. HIRST, DANIEL BELLER, University of California, Merced — The microtubule gliding assay, an in-vitro technique commonly used to study motility of motor proteins, also provides an opportunity to study the collective motion of microtubules as an active fluid. Computational modeling of this system usually studies the microtubule positions assuming a spatially uniform distribution of the motor proteins, which models the experiments where the positions of motors are fixed. We explore a modified setup where kinesin motors are mobile. We use Brownian Dynamics simulations to model the collective motions of microtubules with explicit consideration of the concentration of the motors. We investigate spontaneous dynamical spatial variation in microtubule density that is introduced by allowing diffusion and transport of the motors. We also address how the mobile kinesin motors change the phase diagram as a function of kinesin and microtubule densities.

*We acknowledge support from National Science Foundation NSF grant DMR-1808926, NSF-CREST: Center for Cellular and Bio-molecular Machines at UC Merced (NSF-HRD-1547848). The data in this work was collected, in part, with a confocal microscope acquired through the National Science Foundation MRI Award Number DMR-1625733.*
12:15PM S31.00004: Multi-functional crystalline frameworks self-assembled from amphiphilic DNA nanostructures.  RYAN BRADY, University of Cambridge, NICHOLAS BROOKS, Imperial College London, PIETRO CICUTA, University of Cambridge, LORENZO DI MICHELE (Presenter), Imperial College London — Several emerging technologies require the production of porous frameworks with a precisely controlled nanoscale morphology and stimuli-responsiveness. Due to the binding selectivity of nucleic acids, their facile synthesis and functionalization, DNA nanotechnology has emerged as a prime route for the production of programmable nanoscale materials. Nonetheless, the reliable preparation of crystalline, highly porous and functional 3D DNA frameworks remains elusive.

I will discuss a novel class of amphiphilic DNA building blocks dubbed “C-stars” that combine Watson-Crick base pairing and hydrophobic forces to self-assemble into 3D single crystals [1-3]. The lattice parameter of C-star crystals can be tuned over several nanometers, resulting in programmable pore size [2]. The robustness and versatility of our approach enables the modification of the amphiphilic building blocks with responsive motifs, which can be triggered to induce, among other effects, the isothermal melting of the network [2] and the reversible entrapment and release of protein cargoes [2], making C-stars an ideal platform for the design of smart nanomedical devices.


12:27PM S31.00005: Controlled membrane remodeling by DNA origami nanorods:
Experiments targeting the design principles for membrane-based materials*  SARAH ZURAW (Presenter), ANTHONY DUPRAT DINSMORE, Univ of Mass - Amherst, MAHSA SIAVASHPOURI, Physics, Brandeis Univ, ZVONIMIR DOGIC, Physics, UC Santa Barbara, THOMAS GERLING, HENDRIK DIETZ, Physics, Technical University of Munich — Membrane remodeling facilitated by the self-assembly of proteins on the membrane is essential for cellular function. Inspired by this system, we use DNA origami nanorods to illuminate the role of particle shape and adhesion on membrane reconfiguration. We combine giant unilamellar vesicles with oppositely charged nanorods and observe them with optical and electron microscopy. The binding affinity of the nanorods to the membrane is tunable via lipid composition, which reveals three primary behaviors. For weak particle binding vesicles adhere to one another and form a stable gel. At intermediate binding strengths the gel forms but is subsequently destroyed by avid binding of the nanorods. At higher binding strengths the vesicles rupture without forming a gel. Cryo transmission electron microscopy reveals in-plane ordering of rods on the membrane. These responses are robust and repeatable providing a physical understanding of the dependence on shape, binding affinity and concentration in membrane remodeling. The design principles derived from these experiments will lead to bio-inspired membrane materials that are stimuli-responsive and reconfigurable.

*This work is funded by the NSF Materials Research Science and Engineering Center (DMR-1420382) and a Spaulding Smith Fellowship.
12:39PM S31.00006: A coarse-grained model for lipid bilayer formation, fusion, and its hydrodynamics* YUAN-NAN YOUNG (Presenter), New Jersey Inst of Tech, SZU-PEI FU, ROLF RYHAM, Mathematics, Fordham University — In this paper a theoretical model for long-range, hydrophobic attraction between amphiphilic particles is developed to quantify the macroscopic assembly and mechanics of a lipid bilayer membrane in solvents. The non-local interactions between amphiphilic particles are obtained from the first domain variation of a hydrophobicity functional, giving rise to forces and torques (between particles) that dictate the motion of both particles and the surrounding solvent. The functional minimizer (that accounts for hydrophobicity at molecular-aqueous interfaces) is a solution to a boundary value problem of the screened Laplace equation. We reformulate the boundary value problem as a second-kind integral equation. Solving a mobility problem in Stokes flow is incorporated to obtain corresponding rigid body motion. The simulated fluid-particle systems exhibit a variety of multiscale behaviors over both time and length: Over short time scales, the numerical results show self-assembly for model lipid particles. For large system simulations, the particles form realistic configurations like micelles and bilayers. Over long time scales, the bilayer shapes emerging from the simulation appear to minimize a form of bending energy.

*Y.-N. Young was supported by NSF (DMS-1412789 and DMS-1614863).

12:51PM S31.00007: Phase separation and domain registry in giant multilamellar vesicles prepared with biologically-relevant lipid compositions.* DYLAN STEER (Presenter), CECILIA LEAL, University of Illinois at Urbana-Champaign — Lipids are amphiphiles that commonly form bilayer sheets in the form of vesicles when exposed to excess water. Most commonly lipids have been studied in the context of the plasma membrane and other unilamellar vesicles containing a single bilayer. However, several key biological systems such as the myelin sheath, tubular myelin, or pulmonary lipid-based membranes are known to rely on correlated stacks of lipid bilayers into onion-like multi-lamellar vesicles. Lateral ordering of lipids is well-understood mostly in single-bilayer systems. Most often, the macroscopic distribution of phases is only well-characterized for giant unilamellar vesicles. Here we report on the macroscopic arrangement of phase-separated domains in multilamellar forms with biologically-relevant compositions. We will show how the registration of individual domains results in large changes in macroscopic vesicle structure and properties. Confocal fluorescence microscopy allows direct visualization of phase separation, supported by SAXS and spectrometry studies of lipid ordering.

*Office of Naval Research N00014-16-1-2886
1:03PM S31.00008: Clustering dynamics of collectively migrating malignant lymphocytes
FARNAZ GOLNARAGHI (Presenter), DAVID A. QUINT, Department of Physics, University of California, Merced, NIR SCHACHNA GOV, Department of Chemical and Biological Physics, Weizmann Institute of Science, AJAY GOPINATHAN, Department of Physics, University of California, Merced — Multi-cellular aggregates such as cell clusters and tissues exhibit collective migration with complex emergent behaviors that are very different from the behavior of the constituent single cells. We focus on the migration of clusters of malignant lymphocytes, responsible for the metastases of lymphomas. Previous work has shown that, in chemokine gradients, these clusters show a number of novel collective phases including rotations that enhance their chemotactic efficiency. Here we study the attachment and detachment dynamics that ultimately guides the formation of the clusters, which is similar to the gas-liquid transition of passive (thermal equilibrium) systems. We aim to quantify cell cluster shape dynamics and chemotactic efficiency as a function of cellular parameters such as, cell-cell adhesion and alignment, contact inhibition and chemotactic response. In particular, we show that cell-cell adhesion and alignment are important regulators of cell cluster size and shape, which in turn affects their chemotactic efficiency. Our systematic approach will allow us to identify regions of parameter space that may shed light on candidate strategies for suppressing metastatic potential.

1:15PM S31.00009: Imaging the emergence of bacterial turbulence using light-powered E. coli
YI PENG (Presenter), Chinese Academy of Sciences, Institute of Physics, ZHENGYANG LIU, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota — The collective motion of bacteria leads to intermittent jets and swarming vortices, a fluid pattern often referred as bacterial turbulence. We investigate the emergence of the collective motion of Escherichia coli suspensions and explore the kinetic pathway towards bacterial turbulence. We map the phase diagram of bacterial flows as functions of bacterial concentration, bacterial swimming speed and the number fraction of active bacteria. A simple model based on two-body hydrodynamic interaction quantitatively predicts the phase boundary of the 3D phase diagram. Furthermore, we trigger bacterial turbulence by using genetically engineered light-powered E. coli, whose swimming speeds vary with light intensity. The kinetics show one step near the phase boundary and two steps with an intermediate state far above the phase boundary. The transition rate increases as the system moves deep inside the turbulent phase. Our research reveals the microscopic origin of bacterial turbulence and provides new insights into nonequilibrium phase transitions in active matter.

*NSF CBET-1702352, and DARPA YFA-D16AP00120
1:27PM S31.00010: Activity-induced phase transitions in confined bacterial suspensions

DIPANJAN GHOSH (Presenter), ZHENGYANG LIU, XIANG CHENG, University of Minnesota — Active matter exhibits fascinating emergent ordered structures absent in passive equilibrium systems and, therefore, has been extensively studied as a model to explore nonequilibrium phase transitions. Here, we study the emergence of collective order in confined suspensions of genetically engineered *Escherichia coli*, whose propulsion speed can be controlled via intensity of light. The suspensions, when placed in a Hele-Shaw cell having a gap thickness of 10 microns, show various ordered phases unseen in their three-dimensional counterparts. Using a bright-field microscope, we image the positions and orientations of individual bacterium through different phase transitions. We identify a transition from a disordered phase to a nematic phase characterized by a long-range orientational order and the formation of lanes. The dependence of transition dynamics on the concentration and swimming speed of bacteria is explored. Moreover, we examine the rise of bacterial polar ordering within the nematic phase. Our study provides an experimental benchmark for understanding the role of complex interplays between hydrodynamic and steric interactions responsible for the emergence of ordered phases in confined active systems.

*NSF CBET-PMP 1702352

1:39PM S31.00011: Comparing sperm collective swimming with flocking transition

ALLAN ODUOR, North Carolina A&T State Univ, YISHAK BILILIGN, Duke University, DANIEL SUSSMAN, Syracuse University, SOON HON CHEONG, SUSAN S SUAREZ, Cornell University, M. LISA MANNING, Syracuse University, CHIH-KUAN TUNG (Presenter), North Carolina A&T State Univ — In viscoelastic fluid, bovine sperm are able to interact and align with their neighbors to swim in clusters. The formation of the polar liquid phase, or large flocks of sperm, however, did not solely depend on the number density and the alignment mediated by the fluid, but was strongly influenced by the initial conditions. If a pulse of flow was used to create an aligned initial condition, hundreds of sperm were able to form a flock swimming in the same direction. This suggests that the transition is first-order, with strong hysteresis. Analyzing these flocks, we found the decay of the orientation correlation function to be linear on a log-log plot. From our finite flock sizes, there was no indication that the correlation function decayed to a non-zero value, as suggested theoretically for the polar liquid phase. Further, the effective exponents of the correlation function were found to vary for the same flock at different time points, which made us wonder about some of the premises of continuum theoretical models. From tracking individually swimming sperm, we found that the rotational noise is an exponential decay, while the speed follows a Gamma distribution. Neither is commonly used in theoretical models.

*NSF HRD 1665004, NIH R15HD095411, APS Bridge Program MSI Travel Grant.
1:51PM S31.00012: Correlations in suspensions of microswimmers  ALEXANDER MOROZOV  
(Presenter), Univ of Edinburgh — Recent years witnessed a significant interest in physical properties of self-propelled particles that can extract energy from the environment and convert it into directed motion. One of the most striking consequences of this ability is the appearance of collective motion in self-propelled particles suspended in a fluid observed in recent experiments and simulations: at low densities particles move around in an uncorrelated fashion, while at higher densities they organise into jets and vortices comprising many individual swimmers.

Here, we present a novel kinetic theory that predicts the existence of strong correlations even below the transition to collective motion. We calculate the velocity-velocity correlation functions and the effective diffusivity of passive tracers, and reveal their non-trivial density and velocity dependence. The theory is in quantitative agreement with our recent Lattice-Boltzmann simulations (J. Stenhammar et al., Phys. Rev. Lett. 119, 028005 (2017), D. Bardfalvy et al., Soft Matter 15, 7747 (2019)), and captures the asymmetry between pusher and puller swimmers below the transition to collective motion. We discuss the consequences of these correlations for the nature of the transition to collective motion.

2:03PM S31.00013: Collective migration of bacteria in disordered media  TAPOMOY BHATTACHARJEE (Presenter), DANIEL AMCHIN, FELIX S KRATZ, JENNA A OTT, SUJIT DATTA, Princeton University — While bacterial motility is well-studied on flat surfaces or in unconfined liquid media, most bacteria are found in disordered porous media, such as biological gels and tissues, soils, sediments, and subsurface formations. Understanding how porous confinement alters bacterial motility is therefore critical to modeling the progression of infections, applying beneficial bacteria for drug delivery, and bioremediation. We recently discovered that isolated cells of *E. coli* move through disordered media via intermittent hopping and trapping, reminiscent of thermally-activated transport. Here, we use direct visualization and 3D bioprinting to investigate how this behavior manifests in multicellular communities in porous media. We find that cellular chemotaxis drives collective migration—and that this process depends sensitively on pore-scale confinement, colony density, and differential metabolism of nutrients. Our results thus expand the current understanding of collective migration, which focuses on populations in homogeneous environments, to the case of bacteria in disordered porous media.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S32 DPOLY DSOFT DCP: Dynamics of Glassy Polymers Under Nanoscale Confinement III  504 - Jane Lipson, Dartmouth College - Tag(s): Focus
11:15AM S32.00001: A Novel Technique for the Characterization of Freestanding Ultrathin Film Mechanics*  
LUKE GALUSKA (Presenter), SONG ZHANG, School of Polymer Science and Engineering, Univ of Southern Mississippi, ERIC MUCKLEY, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, DAKOTA EHLENBERG, School of Polymer Science and Engineering, Univ of Southern Mississippi, ILIA IVANOV, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, XIAODAN GU, School of Polymer Science and Engineering, Univ of Southern Mississippi — The contribution of nanoconfinement to ultrathin film mechanics has challenged the field for many years. Our previous work utilized a pseudo-free-standing tensile test which relies on water as a support and has successfully been employed throughout many systems. However, the effect of water on the mechanics of nanoconfined films is unclear. Here, we developed a novel truly free-standing (in air) tensile platform to study sub-100 nm thick films. Tensile characterization of stiff glassy polymer such as polystyrene and soft semicrystalline poly(3-hexylthiophene-2,5-diyl) films has been achieved at sub-80 nm thicknesses. We report negligible differences between the moduli obtained from on water and in air measurements, leading us to conclude that water plays an insignificant role despite other factors such as confinement, which is evident in the reduced modulus of PS with decreasing thickness. Our current work is to utilize this newly developed free-standing tensile platform to provide in-situ characterization of ultrathin film deformation mechanics across multiple size scales.

*NSF Award # DGE – 1449999

11:27AM S32.00002: Chains entanglements and flow within the mobile surface layers of glassy polymers*  
BAIO ZUO (Presenter), ZHIWEI HAO, XINPING WANG, Department of Chemistry, Zhejiang Sci-Tech University, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — The existence of a mobile surface layer of several nanometers thick has been established as critical to dynamical deviations in nanostructured polymers. Several questions arise, such as i) How are segments in this region entangled? and ii) How do polymers in this region flow especially when polymer size is larger than thickness of the surface layer? Herein, we design a creep experiment to investigate rheology in this layer. In this experiment, a micro-droplet was placed atop polymer surfaces to induce a nanometer deformation, called a wetting ridge, by the vertical component of surface tension of the droplet. The time evolution of the height of the wetting ridge, reflecting polymer relaxation at different length scales, was monitored. Results show that segments in the very thin surface layer are readily entangled. The terminal relaxation time was scaled by molecular weight ($M_w$) with a power law of 1.5. We proposed a 2D entanglement and limited flow to explain the phenomena. Within the surface layer, segments were entangled in direction parallel to the surface, but free of entanglements in film thickness direction. Flow of polymer in surface layer was constrained by the glassy underlying bulk, resulting in lower $M_w$ dependence.

*National Natural Science Foundation of China (21973083)
**11:39AM S32.00003: Entanglement Effect on Mechanical Properties of Ultrathin Glassy Polymer Films**

CYNTHIA BUKOWSKI (Presenter), ALFRED J CROSBY, Univ of Mass - Amherst —

Entanglement density is known to influence the large strain and failure responses of glassy polymer films. For ultrathin films, recent extension measurements show that failure strength decreases severely as film thickness decreases below the average size of an unconfined chain. The hypothesized cause for this effect is the loss of interchain entanglements as polymers statistically interact with themselves more than neighbors when confined. To provide more insight into how entanglements control the failure mechanisms of glassy polymers, especially in ultrathin films, we introduce polymer chains shorter than the entanglement molecular weight to control the entanglement density by effectively swelling the entanglement network. Specifically, we blend short (10.5 kDa or 61.8 kDa) and long (151.5 kDa) polystyrene chains and measure the changes in mechanical properties using The Uniaxial Tensile Tester for UltraThin films (TUTTUT). For 100 nm films, we observe a decrease in yield stress and work to failure with increasing diluent concentration that is diluent length dependent. These results establish the framework of how entanglement density affects mechanical properties of ultrathin polymer films.

*NSF DMR-1904525, NSF DMR-1608614

**11:51AM S32.00004: Effect of Confinement on Modulus and Fracture of Thin Conjugated Polymer Films For Organic Electronics**

XIAODAN GU (Presenter), Univ of Southern Mississippi, DONGSHAN ZHOU, Nanjing University, SIMON RONDEAU-GAGNÉ, University of Windsor —

In this talk, I will discuss our research on understanding the glass transition phenomena and thin-film mechanical property for those rigid conjugated polymers. This class polymers are electronically active and find great potential in future solution-processed electronics. Since those polymers are predominantly used in thin-film devices (e.g. <100nm), thus confinement effect plays a key role in those thin films. I will discuss our research journey using a thin-film tensile tester to study those novel class of polymers down to 20nm supported on the water surface. Specifically, we found the confinement effect plays a critical role in the modulus and fracture behavior of polymeric materials. I will also discuss the effect of the backbone rigidity on the thin film mechanical property studied by neutron scattering.

*Department of Energy, Basic Science Research, EPSCoR and Neutron Scattering Program DE-SC019361
12:27PM S32.00005: Mechanical Relaxations of Free-standing Polymer Films*  
HAILIN YUAN (Presenter), OPHELIA TSUI, Hong Kong University of Science and Technology — Young’s modulus of free-standing polystyrene films with thicknesses, \( h \), from 48 nm to 100 μm was studied as a function of temperature and relaxation time. For the \( h \leq 115 \) nm or \( h \geq \sim 3.5 \) mm films, data could be fit to a single Kohlrausch-Williams-Watts (KWW) function, with the former showing relaxation times shorter than the bulk (denoted \( t_s \)) and the latter similar to the bulk (\( t_{\text{bulk}} \)). For the films with thicknesses in between, data could be described by a double KWW function with relaxation times of \( t_s \) and \( t_{\text{bulk}} \), respectively. We found that \( t_s \) is similar to the fast relaxation time observed in previous optical anisotropy relaxation experiment. However, the apparent thickness found here of the film portion where fast relaxations take place is \( \sim 100 \) times larger. Our result shows that mechanical relaxations are much more susceptible to perturbations by the free surface than molecular relaxations are. Confinement effects may have far bigger impact on the properties of polymers than previously contemplated.

*We acknowledge supports of the Research Grant Council of Hong Kong through the Projects 16303418 and 16301919.

12:39PM S32.00006: Effects of Nanoparticles Motion on a Bound Layer in Strongly Attractive Polymer Nanocomposites  
HAMED EMAMY (Presenter), Columbia Univ, FRANCIS STARR, Physics Department, Wesleyan University, SANAT KUMAR, Columbia Univ — The attractive interactions between polymers and nanoparticles (NPs) in polymer composites can lead to the formation of a "bound" layer around the nanoparticle (NP) with very slow dynamics. Previous simulations show that this bound layer has a significantly larger relaxation time compared to polymer matrix. However, these studies have been done for a NP that is fixed at its initial position and does not move during simulation (infinitely massive NP). Here, we perform molecular dynamics simulations for polymer composites, where the NP can move in the polymer matrix. We explore the degree to which the NP diffusion affects nanocomposite dynamics. To explain the effects of NP diffusion, we study the dynamical properties of polymer composites, e.g., scattering function, relaxation time. We find that the motion of the NP reduces the bound layer relaxation time significantly. We show that the bound layer diffuses with NPs, and that results in shorter relaxation time. We also study the effects of NP motion on the glass transition temperature.
Annealing a polymer system at temperatures above its $T_g$ can induce the growth of an irreversibly adsorbed layer at the polymer-substrate interface which can impact the system's bulk properties. Several efforts have been made to explore the implications of irreversibly adsorbed layer growth in thin films, however consideration has not yet been given to polymer nanocomposites, whose high processing temperatures and significant interfacial area may especially favor irreversible adsorption. Herein, we describe the local effects of irreversible adsorption in polystyrene-silica nanocomposites. By combining direct, local techniques such as fluorescence spectroscopy and TEM imaging, we elucidate the relationship between irreversibly adsorbed layer thickness and the corresponding local $T_g$ perturbances, as well as how these parameters evolve with annealing time. The insights provided by this characterization of local interfacial dynamics may inform future endeavors towards the engineering of new and improved polymer nanocomposite materials.

*This material is based upon work supported by the NSF GRFP under Grant No. DCE-1656466. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the NSF.*

How the conformations and dynamics of surface bound chains influence neighboring chains are fundamental to adhesion and reinforcement mechanisms in polymer films and nanocomposites. Efforts to investigate adsorbed chains in melt films rely on solvent washing conditions to expose such near-surface chains. However, we find that the adsorbed layer thickness remaining from this protocol is entirely determined by the solvent washing conditions used, with only the time in solution needed to reach this final adsorbed amount affected by prior treatment of the melt film. These observations are consistent with surface diffusion and exchange measurements of adsorbed chains in solution demonstrating that surface bound chains are highly mobile, even for the case of strong adsorption. By directly comparing solution grown adsorbed layers with those formed by solvent washing melt films, we leverage the wealth of information on polymer adsorption in solution developed over several decades to inform us about polymer conformations in the melt. We investigate how these different populations of surface bound chains alter local glass transition properties of neighboring homopolymer chains, and compare them to end-tethered grafted chains.
**1:15PM S32.00009: Property enhancements and dynamic gradients in P2VP-silica nanocomposites**  
TONG WEI (Presenter), JOHN TORKELSON, Northwestern University — A fluorescence technique is used to probe the glass transition temperature ($T_g$) associated with α-relaxation dynamics at different locations in poly(2-vinylpyridine) (P2VP)-silica nanocomposites. The interfacial layer $T_g$ ($T_{g,\text{inter}}$) is determined using pyrene dye molecule covalently labeled to filler surface. The average matrix $T_g$ ($T_{g,\text{matrix}}$) is determined using evenly dispersed, free pyrene dye in the polymer matrix. For the first time, we decouple the interfacial dynamics from the rest of polymer matrix in nanocomposites. In 2.1 kg/mol P2VP nanocomposites containing 0.5 vol% nanoparticle, $T_{g,\text{inter}}$ is 21 °C higher than in neat P2VP $T_g$, indicating that the α-relaxation dynamics are significantly slowed down due to H-bonding between P2VP and silanol groups on the filler surface. The $T_{g,\text{matrix}}$ is only 3 °C higher than neat P2VP due to the low fraction of interfacial regimes at low filler loading. Both $T_{g,\text{inter}}$ and $T_{g,\text{matrix}}$ increase with increasing filler loading. At same filler dispersion and filler loading, 110 kg/mol P2VP nanocomposites exhibit a much reduced $T_g$ enhancement relative to 2.1 kg/mol P2VP nanocomposites. We hypothesize that 2.1 kg/mol P2VP chains can orderly pack and align at the filler surface, leading to higher H-bonding density and stronger $T_g$ enhancement.

**1:27PM S32.00010: Polymer conformations and dynamics in polymer nanoparticle composite with high nanoparticle loading**  
EMILY LIN (Presenter), ROBERT RIGGLEMAN, University of Pennsylvania — Polymer nanoparticle composites (PNC) with high loadings of nanoparticles (>50%) are an interesting class of material for a wide range of applications. Recent experiments have shown that these highly loaded PNC exhibit simultaneously improved strength and stiffness without compromising, sometimes even improving, the toughness compared to neat systems. These PNCs also show a large increase in the polymer glass transition temperature and viscosity, suggesting a slowdown in both segmental and chain-scale dynamics due to confinement. The goal of this work is to understand how confining polymers to the cavities of a random close packed nanoparticle solid affects polymer conformations and dynamics from the segmental to the chain scale. We performed molecular dynamics simulation of both entangled and unentangled coarse-grained polymer equilibrated in the voids of a nanoparticle packing. We varied the polymer fill fraction and compared the dynamics of the polymer in PNC to the pure polymer system, finding that the changes in the dynamics depend on the number of nanoparticles in contact with a polymer. Finally, we deformed the PNC uniaxially to track rearrangement behavior of nanoparticles and polymer segments to provide a molecular view of the toughening mechanism in these materials.
1:39PM S32.00011: Direct probing of the fracture behavior for pseudo-free-standing polymeric ultra-thin films*  SONG ZHANG (Presenter), Polymer Science and Engineering, Univ of Southern Mississippi, MASATO KOIZUMI, LIHUAN JIN, MECHANICAL AND AEROSPACE ENGINEERING, California State University, Los Angeles, XIAODAN GU, Polymer Science and Engineering, Univ of Southern Mississippi — The understanding of fracture mechanics of free-standing ultra-thin polymeric films is crucial for modern technology that heavily relies on thin films, including the semiconductor industry and coating. Past decades have witnessed improved understanding of several physical properties of the ultra-thin film, however, their fracture behavior is rarely explored due to limited testing methods on hard-to-handle samples. In this work, we reported a new testing methodology that not only can directly measure the fracture energy of ultra-thin films floated on the water, but also visualize the local stress field during the deformation through the wrinkling pattern of the film. Using polystyrene as a model system, we demonstrated for the first time the existence of a critical molecular weight/thickness, below which the fracture energy increases consistently, and above which levels up. Later, this method was applied to other polymeric thin films for further demonstration of its broad applicability to both stiff and soft materials.

*We thank the financial support from U.S. Department of Energy, Office of Science, Office of Basic Energy Science under award number of DE-SC0019361.

1:51PM S32.00012: Glassy, Conjugated Polymer Nanoparticles Formed by a Semiflexible Polymer: A Molecular Dynamic Study*  SUPUN SAMINDRA KAMKANAM MOHOTTALALAGE (Presenter), Department of Chemistry, Clemson University, Clemson, SC, United States, 29634, GARY GREST, Sandia National Laboratories, Albuquerque, NM, United States, 87123, DVORA PERAHIA, Department of Chemistry/Department of Physics, Clemson University, Clemson, SC, United States, 29634 — Conjugated polymers confined into nano dimensions form long-lived luminescent particles (polydots), with potential as bio markers, where the chain dynamics and conformation determine the photophysics in the confined state. Here we probe the structure and dynamics of semiflexible polymers MEH-PPV confined to their nano dimension, using fully atomistic molecular dynamics (MD) simulations as the temperature is varied. We find that the polymer swells below $T_g$ and $R_g$ increases linearly with temperature. A transition takes place at 605-610 K. This transition is attributed to transformation of glass-like particle to a more dynamic state. The auto correlation function of the backbones of the confined chains, were calculated and analyzed in terms of KWW stretched exponentials, yielding correlation times of $\sim$3.5 ms. This semiflexible polymer remains in its confined state over a broad temperature range. In comparison with polydots formed by rigid polymers, backbone flexibility results in a tighter packing and formation of internal correlations of the side chains.

*NSF CHE 1308298
2:03PM S32.00013: On the stability of initiators for surface-initiated controlled radical polymerization  CHRISTIAN PESTER (Presenter), Pennsylvania State University — The covalent attachment of polymers has emerged as a powerful strategy for the preparation of multifunctional surfaces. Patterned, surface-grafted polymer brushes provide spatial control over a variety of physical properties and allow for fabrication of ‘intelligent’ substrates which selectively adapt to their environment. However, the route towards such patterned polymer brush surfaces often remains challenging, creating a demand for more efficient and less complicated fabrication strategies. Here, we describe recent advances in our group in reduction photolithography to produce topographically and chemically pattern polymer brushes by using light-mediated controlled radical polymerization. We highlight recent work on expanding our technique towards photoinduced electron/energy transfer (PET) reversible addition–fragmentation chain transfer (RAFT) polymerization. We present findings regarding the long-term stability of the surface-grafted initiating sites and discuss reproducibility of SI-PET-RAFT and other polymerization techniques.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S33 DPOLY FIAP DSOFT GSNP: Physics of Foams: Fundamentals and Applications 505 - Kshitish Patankar, Dow - Tag(s): Focus

11:15AM S33.00001: Bubble Nucleation in Polymer-CO₂ Mixtures* [Invited] ZHEN-GANG WANG (Presenter), Division of Chemistry and Chemical Engineering, California Institute of Technology — Bubble nucleation is a critical first step in the foaming process, but its theoretical understanding is still rather incomplete. While the classical nucleation theory (CNT) offers a qualitative picture of the process, more advanced theories are needed to better describe molecular details. Here, we combine the string method with the state-of-the-art density functional theory (DFT) to investigate bubble nucleation in CO₂-supersaturated polymers. Nucleation in our study is initiated by saturating the polymer liquid with high pressure CO₂ gas and subsequently reducing the pressure to ambient condition. The string method is used to find the minimum free energy path on the free energy landscape that connects the metastable CO₂-supersaturated state with a well-developed bubble. The nucleation pathway, i.e., the evolution of the density profiles in the formation of the nuclei, as well as the nucleation barrier, are obtained as a function of the temperature and the initial pressure. We present an incipient-phase analysis which allows identification of phases that can form from the metastable CO₂-supersaturated parent phase. As result of an underlying metastable transition from an incipient CO₂-rich-vapor phase to an incipient CO₂-rich-liquid phase, there can be two kinds of nucleating bubbles, a liquid-like bubble and a vapor-like bubble, which can differ substantially in their nucleation barrier. We apply our theory to three common polymers: polystyrene, polymethylmethacrylate, and a commercial polyol. We also examine the effects of adding a third volatile component to the polymer-CO₂ mixture.

*The Dow Chemical Company is acknowledged for funding.
11:51AM S33.00002: Equilibrium coexistence between polyol, CO2, and a physical blowing agent at elevated pressures*  
HUlkUAN CHAO (Presenter), Dow Chemical Company Foundation, ANDREW YLITALO, JULIE KORNFIELD, California Institute of Technology, VALERIY GINZBURG, WEIJUN ZHOU, THOMAS FITZGIBBONS, Dow Chemical Company Foundation, ZHEN-GANG WANG, California Institute of Technology — Rigid polyurethane (PU) foams are widely used as thermal and acoustic insulation materials. The insulation properties depend critically on the size and distribution of cells from nucleation and growth of small-molecule bubbles during foaming. To achieve desired cell structures, the foaming recipe needs to be formulated. Besides reactants (polyols, isocyanates and water), the recipe typically contains physical blowing agents (PBAs) to increase the nucleation rate of bubbles. However, due to complex chemical and physical reactions, how PBAs affect the bubble formation are not understood. As a fist step to approach the issue, we develop a liquid-state theory of a ternary foaming system (PBA, CO2 and polyols) and study the phase behaviors of the system at manufacture-relevant conditions. Our results show a transition in the system from a liquid-vapor into a liquid-liquid coexistence via an intermediate triple-phase coexistence with increasing amount of PBA. When the polyol-rich phase in the coexistence is destabilized (e.g. upon rapid decompression), we find the incipient phase that metastably coexists with the polyol-rich phase changes its nature from a vapor-like to a liquid-like PBA/CO2-rich phase with increasing weight fraction PAB in the polyol-rich phase.

*Dow UPI. 227027AQ

12:03PM S33.00003: Microfluidic Approach to Study Bubble Nucleation in Polymeric Foams for the Development of DFT-based Models  
ANDREW YLITALO (Presenter), HUIKUAN CHAO, Caltech, THOMAS FITZGIBBONS, VALERIY GINZBURG, WEIJUN ZHOU, Dow Chemical, ZHEN-GANG WANG, JULIE KORNFIELD, Caltech — Bubble nucleation sets the structural foundation of a foam, yet remains poorly understood. Single-component classical nucleation theory predicts erroneous nucleation barriers, particularly when applied to foaming of multicomponent liquids used to produce lightweight, functional materials. Multicomponent theories are limited by lack of (1) thermodynamic and (2) nucleation rate data for validation. For the first, we used gravimetry-axisymmetric drop shape analysis (G-ADSA) in the Di Maio lab (U Naples) to measure equilibrium compositions and interfacial tension of polymer-CO2 mixtures up to 8MPa, which validated PC-SAFT and DFT models from the Wang group (Caltech) that enable string method calculations of the nucleation barrier. For the second, we developed a microfluidic hydrodynamic-focusing apparatus that linearly decreases pressure from 10MPa to as low as 0.1MPa within 100ms while observing bubble nucleation and growth. The instrument, designed for use with optical microscopy, X-ray scattering, thermography and FTIR, will be described. This approach to validating multicomponent theories of bubble nucleation can be extended to study complex effects of additives on foaming and enable design of foam composition and processing conditions to achieve desired material properties.
12:15PM S33.00004: An Off-Lattice Sanchez-Lacombe Related Equation of State Extensible to Polymeric Foams*  

HASSAN ALAM (Presenter), Physics and Astronomy, University of Waterloo, CHUL B. PARK, Mechanical & Industrial Engineering, University of Toronto, RUSSELL B THOMPSON, Physics and Astronomy, University of Waterloo — We have extended an off-lattice model of the Sanchez-Lacombe equation of state for pure polymeric systems by including internal degrees of freedom to polymer chains. The extension allows us to predict glass transition temperatures of pure polymeric systems at different pressures. To find unknown parameters of the model only two experimental values are required, namely, the glass transition temperature of the pure polymer at atmospheric pressure and the change in isobaric heat capacity of the pure polymer across the glass transition. The model is also successful in predicting the behavior of isobaric heat capacities of polymer melts as a function of temperature. The model shows that the Gibbs-DiMarzio criterion for the glass transition is invalid for the Sanchez-Lacombe equation of state. Thus, we proposed a new criterion for glass transition temperature calculations. Predictions of the model are compared with a lattice-based version of the Sanchez-Lacombe equation of state for several pure polymeric systems. The proposed model can be extended to multi-component polymeric systems and thus to retrograde vitrification in polymeric foams.

*Natural Sciences and Engineering Research Council of Canada

12:27PM S33.00005: Experimental Test of the Border-Crossing Model of Diffusive Coarsening in Wet Foams*  

DOUGLAS DURIAN (Presenter), ANTHONY CHIECO, University of Pennsylvania — For dry foams, the transport of gas from small high-pressure bubbles to large low-pressure bubbles is dominated by diffusion across the thin soap films separating neighboring bubbles. For wetter foams, the film areas become smaller as the Plateau borders and vertices inflate with liquid. So-called \"border-blocking\" models can explain some features of wet-foam coarsening based on the presumption that the inflated borders totally block the gas flux; however, this approximation dramatically fails in the wet/unjamming limit where the bubbles become close-packed spheres. Recently we accounted for the ever-present border-crossing flux by a new length scale defined by the average gradient of gas concentration inside the borders that is proportional to the geometric average of film and border thicknesses. We also showed how the well-known $dA/dt=K(n−6)$ von Neumann law is modified by the appearance of terms that depend on bubble size and bubble shape as well as the concentration gradient length scale. Here we extend this theory and describe on-going experiments to test it by measurement of area changes for six-sided bubbles, which would neither grow nor shrink if perfectly dry. Indeed we find six-sided bubbles that change area with time, and we find that they do so in good accord with our prediction based on their size and shape and degree of wetness.

*NASA Grant 80NSSC19K0599
1:03PM S33.00006: Experimentally Testing a Generalized Coarsening Model for Quasi-Two-Dimensional Wet Foams* ANTHONY CHIECO (Presenter), DOUGLAS DURIAN, University of Pennsylvania — In dry foams, a bubble's area grows or shrinks according only to its number of sides, \( \frac{dA}{dt} = K_0(n-6) \). While exact for a purely two dimensional foam with no liquid content this von Neumann law is increasingly violated for wetter quasi-2d foams. These latter foams have Plateau borders that are inflated with liquid and extend into the z-plane. Accounting for the size of the Plateau borders and gas that diffuses through both the Plateau Borders and thin films separating two bubbles, we modify von Neumann's law to a no-fit general coarsening equation where bubble size and shape now matter. To test this experimentally, we measure the growth rate of individual bubbles in quasi-2d foams of variable wetness confined between parallel plates. Interestingly, some 6-sided bubbles grow and others shrink - in direct violation of the usual von Neumann law but in agreement with our generalized version. We will show the coarsening of 6-sided bubbles and other violations of von Neumann's law for n-sided bubbles are driven predominantly by the bubble shape which is a key ingredient in our model.

*We would like to thank NASA Grant 80NSSC19K0599 for funding this research.

1:15PM S33.00007: Intelligent Design of Cellular Solids for Impact Mitigation MARCOS REYES-MARTINEZ (Presenter), National Institute of Standards and Technology, MENG SHEN, University of Chicago, EDWIN P CHAN, CHRISTOPHER SOLES, National Institute of Standards and Technology, NIDHI PASHINE, SIDNEY ROBERT NAGEL, HEINRICHA M. JAEGER, JUAN DE PABLO, University of Chicago — Disordered networks, comprised of random arrangements of bonds and nodes, offer degrees of mechanical tunability not accessible to periodic systems. These networks have emerged as the basis of a new class of metamaterials allowing for precise control over density (\( \rho \)), bulk (\( K \)), shear (\( \mu \)) modulus, and Poisson's ratio (\( \nu \)). Here, we demonstrate bond pruning and global node position optimization as effective routes for designing cellular materials with isotropic auxetic properties, and for independently controlling \( \mu \) and \( K \). We show how bond pruning controls \( \rho \), \( \mu \) and \( K \). Node position optimization allows for the tunability of \( \nu \) from \(-0.3\) to \(-0.5\), control over two orders of magnitude of \( K \) with almost no change to \( \mu \) and minimal change in foam density. We use multi-resin 3D-printing to extract the 2D and 3D disordered networks out of the simulation box and systematically study how the tunability of elastic constants affect their dynamic deformation behavior. We explore how node bending stiffness can affect global elastic properties and quantify how it affects the range of elastic tunability. This study demonstrates the power of top-down design of disordered network metamaterials and how such level of tunability can affect the next generation of materials for impact mitigation.

1:27PM S33.00008: Heat transfer of low-density styrenic foam ANSON WONG (Presenter), MARK RICKARD, Safety & Construction, DuPont — The heat transfer characteristics of extruded styrenic foams with various carbonaceous additives were reported. The effects of cellular morphology and type of additives on the thermal conductivity of the foams were analyzed with a predictive model. The total thermal conductivity as well as hemispherical reflectance and transmittance were measured. Comparison between the theoretical and experimental results was made to assess the performance of the predictive model.
Human Comfort and the Physics of Foams

KAORU AOU (Presenter), WENBO XU, LAURA DIETSCHE, DOUGLAS BRUNE, MANOJ THOTA, Dow Chemical Co — Human Comfort and the Physics of Foams is a current topic in the bedding and furniture industry. Polyurethane (PU) foams are thermally insulating, cushioning materials. Flexible open cell PU foams are used in padding materials for furnitures and bed mattresses, where insulation can be useful, but depending on the local climate, insulation can lead to localized heating that can lead to discomfort. In order to maintain comfort, two factors are needed: (1) preventing overheating, and (2) good cushioning (absence of pressure points). Thermal comfort simulation was conducted using the ASHRAE Human Comfort model, coupled with a multiphysics model taking into account natural convection of air, thermal conduction and mass (water vapor) diffusion phenomena. It is demonstrated that effective diffusivity of water vapor through foam is the critical parameter that determines whether the human body is able to regulate its skin temperature. Pressure relief measurements and simulations were also conducted, using an indenter held at a constant temperature of 23 and 34 °C. The relative insensitivity of the contact pressure to indenter temperature is reported.

*Authors thank support from The Dow Chemical Company for the research.

Foam formation in microfluidic EDGE devices: tuning the bubble size

BOXIN DENG, KARIN SCHROËN, JOLET DE RUITER (Presenter), Agrotechnology and Food Sciences, Wageningen University — The stability and flow properties of foams crucially depend on the bubble size and its distribution. Microfluidic devices are capable of producing extremely monodisperse yet small foam bubbles at low energetic cost. Upscaling towards an array of parallelized pores allows to increase the throughput of the device, but increases complexity of bubble formation due to possible pore-pore and bubble-bubble interactions. We use so-called partitioned-EDGE microfluidic chips with which we can produce bubbles in an array of rectangular pores. Pore height is minimized to (sub)micron size in order to produce bubbles down to 20 micron in diameter. The size of a single bubble formed at a pore is independent of pressure for the lower range of applied gas pressures (spontaneous formation mechanism), followed by bubble size increase (blow-up) at higher gas pressures. Here we discuss the final bubble size obtained for high gas flow rate through an array of parallel pores, which induces additional bubble-bubble interactions that can be modified by shear flow rate and stabilizer (protein) concentration. Surprisingly, monodisperse foams with a coefficient of variation around 10% can be produced, irrespective of these additional complexities.
2:03PM S33.00011: Phoamtonic designs yield sizeable 3D photonic band gaps*  MICHAEL ANDREAS KLATT (Presenter), PAUL J STEINHARDT, SALVATORE TORQUATO, Princeton University — We show that it is possible to construct foam-based heterostructures with complete photonic band gaps. Three-dimensional foams are promising candidates for the self-organization of large photonic networks with combinations of physical characteristics that may be useful for applications. The largest band gap found is based on 3D Weaire-Phelan foam, a structure that was originally introduced as a solution to the Kelvin problem of finding the 3D tessellation comprised of equal-volume cells that has the least surface area. The photonic band gap has a maximal size of 16.9% (at a volume fraction of 21.6% for a dielectric contrast of 13) and a high degree of isotropy, properties that are advantageous in designing photonic waveguides and circuits. We also present results for two other foam-based heterostructures based on Kelvin and C15 foams that have somewhat smaller but still significant band gaps.


*This work was supported by the Princeton University Innovation Fund for New Ideas in the Natural Sciences.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S34 DPOLY FIAP DMP: Organic Electronics I: Microstructure and Mechanical Property 506 - Stephanie Lee, Stevens Inst of Tech - Tag(s): Focus

11:15AM S34.00001: Advances in Non-Fullerene Organic Photovoltaics* [Invited]  SAMSON JENEKHE (Presenter), University of Washington — Recent progress in molecular engineering of organic small-molecule and polymer semiconductors and in engineering of the blend active layer morphology has pushed the state-of-the-art organic photovoltaic (OPV) device efficiency above 15%, narrowing the gap with theoretical values. In this talk I will discuss our work in both of the main classes of OPV devices: (i) all-polymer solar cells (all-PSCs) composed of both donor and acceptor polymers; and (ii) blends of a small-molecule non-fullerene acceptor (NFA) with a donor polymer. We have found that binary blends of new random copolymer acceptors with a known donor polymer can spontaneously self-organize into optimal bulk heterojunction morphologies without the use of any solution processing additives; thereby, enabling highly efficient all-PSCs with low energy loss and near unity internal quantum efficiency. Another example is our finding of the different roles of charge transport, blend morphology, and blend photophysics in dictating the photovoltaic properties of NFA/polymer blends, highlighting the importance of fused-ring NFAs in suppressing geminate and bimolecular recombination and enabling improved photocurrent and fill factor.

*Work supported by the National Science Foundation (NSF) and the Office of Naval Research (ONR).
11:51AM S34.00002: Revealing the Microstructure of the Active Layer of Ternary Organic Solar Cells using Energy-Filtered TEM  ISMAIL ALPEREN AYHAN (Presenter), ENRIQUE D GOMEZ, Chemical Engineering, The Pennsylvania State University — Fullerene-free ternary organic solar cells have emerged as a promising class of devices with higher efficiencies when compared with solar cells that encompass binary active layers. Compared with traditional fullerene acceptors, non-fullerene acceptors have stronger absorption in the visible and near-infrared, which helps to generate high photocurrent for solar cells. Nevertheless, controlling phase separation and domain size in the photoactive layer morphology is crucial to enable efficient charge separation, transport and collection. Here, we demonstrate high-efficiency devices by combining the organic semiconductors with complementary light absorption, using PTB7-Th as donor, and IDIC, COi8DFIC, Eh-IDTBR, and O-IDTBR as acceptors. The combination of Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS), Energy-Filtered Transmission Electron Microscopy (EFTEM), Resonant Soft X-ray Scattering (RSoXS) reveals the impact of crystallization on the mesoscale morphology. We show that ternary systems composed of compatible nonfullerene acceptors exhibit fibril-like nanostructures in the active layer, leading to devices with efficiencies in excess of 10%. The morphology suggests that compatibility between two of the three components is important for maximizing performance in devices.

12:03PM S34.00003: Solution Processed Organic and Inorganic Transistors – Application in Inverter Circuits*  JOHN BARRON (Presenter), ALEC PICKETT, JAMES GLASER, SUCHISMITA GUHA, Department of Physics and Astronomy, University of Missouri, Columbia, MO, USA — In the fabrication of organic field-effect transistors (FETs), the usage of high κ dielectrics lowers the operating voltage and enhances device performance. Polymer ferroelectrics open the path not just for high κ values but allow processing of the films via electrical poling. Poled ferroelectric dielectrics in p-type organic FETs is seen to improve carrier mobility and reduce parasitic current when compared to unpoled devices using the same dielectric. Furthermore, n-type inorganic FETs using solution processed ZnO have shown improved performance when the semiconductor layer is subjected to a UV-ozone treatment. FETs were fabricated using the ferroelectric polymer poly(vinylidene fluoride-trifluoroethylene) (PVDF-TrFE) as the dielectric insulator and the electron donor-acceptor polymer diketopyrrolopyrrole-dithienylthieno[3,2-b]thiophene (DPP-DTT) for the semiconductor layer, with devices showing mobilities as high as 0.4 cm²/Vs when electrical poling was utilized. ZnO thin film FETs were fabricated with SiO₂ as the dielectric layer, yielding carrier mobilities on the order of 10⁻² cm²/Vs. Both p- and n-type FETs were used in a voltage inverter circuit, showing promising characteristic gain.

*This work was supported by National Science Foundation under Grant No. ECCS-1707588
12:15PM S34.00004: Electric field-induced second harmonic generation imaging of organic thin-film devices* PAYAL BHATTACHARYA (Presenter), Physics and Astronomy, University of Missouri-Columbia, OKSANA OSTROVERKHOVA, Physics, Oregon State University, PING YU, SUCHISMITA GUHA, Physics and Astronomy, University of Missouri-Columbia — The application of an electric field is an effective mechanism for breaking the symmetry in otherwise symmetric molecular systems. Electric-field induced second harmonic generation (EFISHG) provides a tool for investigating chromophore orientation in nonlinear optical (NLO) materials and understanding transport at the semiconductor-dielectric interface in thin film transistors. A microscopic imaging platform in the reflection geometry has been developed for measuring second harmonic generation (SHG) and EFISHG signals from organic thin-film devices. The polymer poly(vinylidene fluoride) (PVDF), with its low glass transition temperature, provides a medium for orienting embedded NLO molecules under the application of external fields. Malonitrile based NLO chromophores were mixed with PVDF to form thin films. An in-plane electric field upwards of $6 \times 10^5$ V/m yields a strong EFISHG signal. The SHG signal is seen to increase with the magnitude of the applied in-plane field and decreases upon the application of a vertical electric field. We further apply this technique to small molecule based organic transistors, where the application of a source-drain potential breaks the symmetry and allows the investigation of carrier transport using an EFISHG signal.

*NSF under Grant No. ECCS-1707588

12:27PM S34.00005: Structure of vapor-deposited glasses within a few nanometers of organic-organic interfaces is bulk-like MARIE FIORI (Presenter), KUSHAL BAGCHI, University of Wisconsin - Madison, MICHAEL TONEY, SLAC National Accelerator Laboratory, MARK EDIGER, University of Wisconsin - Madison — Vapor-deposited (PVD) glasses are used in OLED devices as <50 nm layers, each deposited onto the layer below it. The bulk structure of a >100 nm PVD glass depends on the temperature at which it was deposited; it is unaffected by the substrate. The distance over which the substrate perturbs the structure of a PVD glass is unknown. In this work, we prepare PVD films made of 60 alternating 10 nm layers of organic semiconductors, DSA-Ph and Alq3, creating 60 interfaces. The large number of organic-organic interfaces allows us to access the X-ray scattering of the structure near the organic substrate. GIWAXS of films with 60 interfaces is virtually identical to the sum of the scattering of thick films of the pure components, indicating that the organic substrate perturbs the glass structure for <2 nm. When deposited at or below 0.8 °Tg, we find that the DSA-Ph molecules at organic interfaces lie parallel to the substrate. We expect that this is true for all PVD glassy films of rigid, flat molecules like DSA-Ph, ensuring good π-π orbital overlap at the organic-organic interface, allowing for efficient charge transport across the interface and into the semiconductor layer.
12:39PM S34.00006: Polymer light-emitting diodes with an emitting layer based on a nano-confined semiconducting polymer blend  ANIELEN RIBEIRO, KATHARINA LANDFESTER, PAUL BLOM, JASPER MICHELS (Presenter), Max Planck Inst — Blending a visible light-emitting organic semiconductor with an insulator alleviates the trap-limited nature of the electron current. Solution-processed organic light emitting diodes (OLEDs) comprising such a blend as emissive layer exhibit a two-fold increase in luminous efficiency with only 10% semiconductor. This low content of semiconductor can only be achieved with polymeric emitters. Hence, polymer-LEDs are considerably more cost-effective than devices based on small molecular emitters. However, due to the reduced translational entropy, polymers typically exhibit a low miscibility. In principle, macro-phase separation can be avoided if the molecular weight is kept low, which is however disadvantageous due to low charge carrier mobilities. An alternative strategy is to impose a nano-confinement. We prepare aqueous nanodispersions of poly(p-phenylenevinylene)-based emitters, blended with polystyrene. Macro-phase separation is fully suppressed, as confirmed by scanning force microscopy. Despite the fact that fabricating OLEDs from aqueous nanoparticle dispersions poses considerable risks of strong field inhomogeneity and high leakage currents, we succeed in fabricating such devices highly reproducibly and at efficiencies similar to the non-particle based reference devices.

12:51PM S34.00007: Sub-Turn-on Exciton Quenching Modulated by Spontaneous Orientation Polarization in Organic Light-Emitting Devices* JOHN BANGSUND (Presenter), JACK R VAN SAMBEEK, RUSSELL J HOLMES, University of Minnesota — Many common materials used in organic light-emitting devices (OLEDs) show preferred molecular orientation in thin films. In molecules with a permanent dipole moment, this can lead to spontaneous orientation polarization (SOP) of the film and can generate a large interface charge. This polarization charge is compensated in a device by the accumulation of charge carriers, typically holes, in the adjacent layer. While it has been speculated that these accumulated charges can quench excitons and accelerate degradation, no direct demonstration of these effects has been made. Here, we show that electron transport layers exhibiting SOP induce substantial exciton quenching prior to device turn-on, reducing the peak external quantum efficiency by ~20% relative to layers without SOP. In addition, we find that the accumulated charges accelerate degradation of emitter photoluminescence efficiency under optical pumping. We further show that SOP can be eliminated by substrate heating during deposition, thereby improving device efficiency and stability. These findings confirm that SOP is an important material parameter that must be considered when optimizing efficiency and lifetime of OLEDs.

*Work supported by DuPont Electronics and Imaging and the NSF GRFP, Grant No. 00039202.
Influence of Acceptor Type and Polymer Molecular Weight on the Mechanical and Photovoltaic Properties of Polymer Solar Cells [Invited]  BUMJOON KIM  
(Presenter), KAIST — The mechanical robustness of polymer solar cells (PSCs) is of great importance to ensure the long-term stability and enable their use as power-generators in flexible and stretchable electronics. Here, we present a comparative study of the mechanical properties of small-molecule acceptor (SMA)-based, polymer acceptors (PA)-based, and fullerene-based PSCs. We chose ITIC, P(NDI2OD-T2), and PCBM as three representative acceptor materials and blended them with the same polymer donor. To understand the difference between the mechanical properties of SMA-based and PA-based PSCs, we control the number-average molecular weight ($M_n$) of P(NDI2OD-T2) from 15 to 163 kg mol$^{-1}$ in all-PSCs. The high $M_n$ PA-based-PSCs exhibited a high strain at fracture of 31.1%, which is 9- and 28-fold higher than those of SMA-PSCs and PCBM-PSCs, respectively. The superior mechanical robustness of all-PSCs is attributed to using a PA above the critical molecular weight ($M_c$), which produces tie molecules and polymer entanglements that dissipate substantial mechanical strain energy with large plastic deformation. The connectivity between the crystalline domains generated by PA tie chains leads to high charge mobilities and photovoltaics performances of all-PSCs. Also, this feature explains very high donor:acceptor composition tolerance of all-PSCs in the photovoltaic and mechanical performances. Therefore, our work highlights the importance of incorporating high $M_n$ PAs above the $M_c$ for producing the PSCs with excellent mechanical robustness and device performance.

Mechanically-durable high performance OPVs using semi-interpenetrating networks*  ZHIQI HU, CHANGXU SUN, JOSHUA JACKSON, TANGUY TERLIER, RAFAEL VERDUZCO  
(Presenter), Rice Univ — Organic photovoltaic (OPVs) devices offer a number of unique advantages over conventional single crystal silicon solar cells, including simple and low-cost fabrication and reduced weight. However, OPV devices exhibit poor durability to mechanical deformations. Here, we study the use of an elastic semi-interpenetrating network to improve the mechanical durability of the active layer of OPV devices based on the high-performance PBDBT-2F:ITIC donor:acceptor blend. The elastic interpenetrating network is synthesized *in situ* after solution deposition of the donor:acceptor blend along with reactive thiol-ene small molecules. We systematically investigate the effects of strain on the network-stabilized active layer structure and show that network-stabilized devices outperform pristine devices above a critical bending strain and number of bending deformations. The elastic interpenetrating network suppresses crack formation and improves durability to high-curvature and repeated bending deformations. This work describes a general route to high performance flexible devices and detailed design parameters that influence performance.

*We acknowledge support from National Science Foundation under Grant No. CMMI-1352099 and Welch Foundation under Grant No. C-1888.
1:51PM S34.00010: Mechanically-Robust and High-Performance Thin Film Transistors with Regioregular-block-Regiorandom Poly(3-hexylthiophene) Copolymers  HYEONJUNG PARK (Presenter), BOO SOO MA, JIN-SEONG KIM, YOUNGKOWON KIM, KAIST, HYEONG JUN KIM, University of Massachusetts, Amherst, DONGUK KIM, HONGSEOK YUN, JUNGHUN HAN, KAIST, FELIX SUNJOO KIM, Chung-Ang University (CAU), TAEK-SOO KIM, BUMJOON KIM, KAIST — We develop mechanically-robust and high-performance organic thin film transistors (OTFTs) based on poly(3-hexylthiophene) (P3HT) regioblock copolymers (block-P3HTs). These block-P3HTs consist of regioregular (rre) and regiorandom (rra) P3HTs, where the crystalline rre block allows efficient charge transport while the amorphous rra block provides mechanical robustness and inter-domain connection. A series of block-P3HTs, having different molecular weight (M_n) of rra blocks with fixed M_n of rre blocks, are prepared and they all exhibit high hole mobility due to the formation of well-developed edge-on crystallites. In addition, mechanical robustness of block-P3HT thin films is remarkably enhanced with the longer rra block, finally leading to 30.2% of elongation at break, which is 100 times higher than rre P3HT homopolymer. In particular, the noticeable enhancement of both elongation at break and toughness is observed between the M_n of rra block, 8 and 20 kg mol\(^{-1}\), indicating that the critical molecular weight of rra P3HT plays an important role in mechanical response of the block-P3HT thin films. This study provides good strategies for high-performance soft electronics to improve the mechanical properties of electroactive materials without disruption of optoelectrical properties.

2:03PM S34.00011: Multiscale-ordered, highly stretchable polymer semiconductor through nanoconfinement  JIE XU (Presenter), Nanoscience and Technology Division, Argonne National Lab — Semiconducting polymers have been developed as a key component to enable skin-like wearable electronics, but their electrical performance must be improved while maintaining good mechanical stretchability. To substantially improve their charge carrier mobility under strain, we reported a novel and genetic approach that combines advanced solution processing with nanoconfinement effect to achieve multi-scale ordering and high stretchability in conjugated polymers. Here, the increased polymer chain dynamics under nanoconfinement significantly reduces the modulus of the conjugated polymer and largely delays the onset of crack formation under strain. As a result, our fabricated semiconducting film can be stretched up to 100% strain without affecting mobility. By using solution shearing with a patterned microtrench coating blade, macroscale alignment of conjugated-polymer nanostructures was achieved along the charge transport direction. In conjunction, the nanoscale spatial confinement aligns chain conformation and promotes short-range π–π ordering, substantially reducing the energetic barrier for charge carrier transport. As a result, the mobilities of stretchable conjugated-polymer films have been enhanced up to threefold and maintained under a strain up to 100%.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S35 DPOLY: Electrostatic Complexation of Proteins and Protein Mimics  507 - Samanvaya Srivastava, University of California, Los Angeles - Tag(s): Focus
The Effect of Protein Surface Charge Distribution on Protein-Polymer Complexation*

Sieun Kim, Hrsh Sureka (Presenter), Massachusetts Institute of Technology MIT, Basak Kayitmazer, Bogazici University, Bradley Olsen, Massachusetts Institute of Technology MIT — Charge patches on protein surfaces have been known to play a significant role in the coacervation and complexation of proteins with one another and with polymers; however, quantifying this patchiness has remained elusive. We present a methodology for quantifying the charge patchiness of protein surfaces and measure how the patchiness of a panel of proteins—engineered to have the same charge, but different charge distributions—affects complexation with a variety of polyelectrolytes. The panel complexed most strongly with the strong polycation used, poly(1-methyl-4-vinylpyridinium iodide), with the proteins with the largest patches complexing over a broader range of polymer-protein ratios than those with smaller patches. Only weaker complexation was seen with the other polyelectrolytes screened, which may have been driven by the weak net negative charge of the mutants. However, the mutant with the largest patches was found to form soluble complexes with both of the weak polyanions tested, hyaluronic acid and poly(acrylic acid). A cutoff between 0.25 and 0.3 in the patchiness parameter was predictive for whether the mutants would complex with any of the polymers tested (particularly qP4VP).

*Supported by DTRA (HDTRA1-16-1-0038).

Influence of charge heterogeneity and charge regulation in complexation between proteins and weak polyelectrolytes.

Rituparna Samanta (Presenter), Venkatraghavan Ganesan, University of Texas at Austin — We discuss the complexation of weakly dissociating proteins in the presence of oppositely charged polyelectrolytes using coarse-grained molecular simulations. We have used single chain in mean field simulation method with constant pH ensemble in a semi-grand canonical framework to include the charge dissociation effects. Through results (adsorption and bridging) pertaining to one and two proteins and several polyelectrolytes, we compare the influence of charge regulation and charge heterogeneities on proteins. Our results demonstrate that the charge regulation exerts bridging by polymers higher than that due to charge patches. We discuss the influence of different parameters such as polyelectrolyte concentration, number of charge patches, pH etc.
11:39AM S35.00003: Coacervate gel composites: Phase behavior and topologically frustrated dynamical hierarchy*  DI JIA (Presenter), MURUGAPPAN MUTHUKUMAR, Univ of Mass - Amherst — We report the discovery of a novel coacervate gel composite state and experimental results on the phase behavior and dynamics of this state. This state is qualitatively different from the traditional coacervate liquid states composed of oppositely charged macromolecules formed via liquid-liquid phase separation. The cross-linking of one of the components of our system induces a new dynamical state for the oppositely charged guest polymer. In this state, the guest molecule is topologically frustrated exhibiting a hierarchy of internal chain dynamics, and is non-diffusive, although the water content in the coacervate gel is very high. In addition, we find rich phase behaviors as a function of cross-linking of one component, charge stoichiometry, pH, and salt concentration. An interlude of an coacervate-emulsion phase prior to the gel formation and its response to cross-linking at different experimental control variables will be presented.

*Support from NSF DMR-1504265 is gratefully acknowledged.

11:51AM S35.00004: SAXS Investigations of Structure and Phase Behavior of Polyelectrolyte–Nanoparticle Assemblies  ADVAIT HOLKAR (Presenter), JESSE TOLEDO, SAMANVAYA SRIVASTAVA, University of California, Los Angeles — Aqueous mixtures of oppositely charged polyelectrolytes (PE) and nanoparticles (NP) self-assemble into dense complexes. This self-assembly forms the basis of diverse phenomena ranging from flocculant action in water treatment, where the PE-NP flocs phase separate and sediment, to DNA compaction around histone proteins into chromatin. Factors such as the PE length, architecture and concentrations; NP charge, morphology and concentrations; and solution conditions (pH and ionic strength) play key roles in directing these PE-NP assemblies. In this presentation, we will delineate fundamental investigations into the phase behavior and structure of polycation-silica NP assemblies using small angle X-ray scattering, turbidimetry and thermogravimetric analysis with systematic variation of PE sizes and flexibility, NP sizes, and a wide range of concentrations of both components. Trends in interparticle spacings and correlations as well as fractal dimensions of assemblies with varying PE and NP concentrations will be discussed, presenting a comprehensive narrative of the hierarchical structure of PE-NP self-assemblies. Near-contact compaction of NPs in the PE-NP assemblies above a critical ratio of PE and NP concentrations will be highlighted.
12:03PM S35.00005: Stabilizing Membraneless Polyelectrolyte Complex Coacervates Towards Inherent Coalescence  
AMAN AGRAWAL (Presenter), ALAMGIR KARIM, Chemical and Biomolecular Engineering, University of Houston — Although recent interests in polyelectrolyte coacervates have shown their advanced applications such as microscale bioreactors with enhanced transcription rates, these applications are, however, usually limited to spatially isolated coacervate droplets or those with lipid or polymer membrane because of membraneless droplets’ instability towards coalescence. In this experimental work, we systematically explored the role of the droplet size distribution (~1-10 μm), negative to positive monomer ratio, and salt concentrations in governing the zeta potential and the long-term stability of droplets. We worked with a well-studied coacervate system: PDDA - ATP. Near-uniform size droplets were formed using a PDMS based microfluidic flow-focusing system in the laminar flow (Re<2100). As has been shown earlier, droplets with narrow size distribution had higher stability and coalesced slowly, over a period of several days, as compared to polydisperse droplets which were stable only for minutes to hours before coalescing. This work has an important consequence as this analysis allows us to understand the stability of various phase-separated liquid systems formed in vivo which finds applications ranging from protein storage to neurodegenerative diseases.

12:15PM S35.00006: Protein Purification by Complex Coacervation  
RACHEL KAPELNER (Presenter), ALLIE OBERMEYER, Columbia University — Proteins are an important class of biomolecules with applications across many industries, including as therapeutics and biocatalysts. Their use in some industries, such as the food and pharmaceutical industries, require a high degree of protein purity for their products. Therefore, a highly selective, yet high throughput and low-cost purification method is of great interest to purify proteins from cell lysate. Complex coacervation, the liquid-liquid phase separation of oppositely charged polyelectrolytes, shows promise as a protein purification technique. Previous work in the field, however, has only addressed separating a protein of interest from a relatively simple mixture. In this work, we demonstrate the utility of complex coacervation as a platform to purify proteins from cell lysate. Using a spectroscopic method, we designed a high throughput approach to screen protein purity and recovery from cell lysate. We were then able to assess how protein and polymer design properties and solution conditions impact protein purity and recovery from cell lysate.
12:27PM S35.00007: Effects of therapeutic chemical modifications on polyelectrolyte properties of oligonucleotides  
JEFFREY VIEREGG (Presenter), ALEXANDER E. MARRAS, MATTHEW TIRRELL, University of Chicago — Polyelectrolyte complex micelles (PCMs), core-shell nanoparticles formed by complexation of polyelectrolytes and polyelectrolyte - hydrophilic neutral block copolymers, are an interesting laboratory for studying polyelectrolyte physics. They also provide an attractive solution to the longstanding problem of delivering therapeutic nucleic acids into cells, as nucleic acids are highly charged anions and are efficiently complexed by cationic polyelectrolytes. We recently published a set of structure-property data that provides rules for constructing DNA oligonucleotide PCMs with well-controlled morphology and low polydispersity and have found that they are applicable to several other polyelectrolytes, suggesting the possibility of developing general principles for PCM self-assembly. DNA oligonucleotides are accessible and chemically stable but are not bioactive, motivating investigation of how chemical modifications affect oligonucleotides' polyelectrolyte properties. Surprisingly, we find that even single atom changes (e.g. DNA to RNA, or phosphate to phosphorothioate) can have large effects on the properties of the resulting PCMs. I will discuss these, and their interpretation, which highlight the need to include chemical information in models of polyelectrolyte complexation.

12:39PM S35.00008: From Monomer Sequence to Self-Assembly in Polyelectrolyte Coacervation*  
GARY MIN CHIANG ONG, University of Illinois at Urbana-Champaign, TYLER LYITTLE, Chemistry, University of Wisconsin Madison, CHARLES SING (Presenter), University of Illinois at Urbana-Champaign — Oppositely-charged polyelectrolytes can undergo an associative phase separation known as complex coacervation, forming dense polymer phases that maximize favorable electrostatic interactions. This interaction motif can be harnessed to drive polymer assembly, via the incorporation of opposite charges on pairs of block copolymers. We present a recent theory developed to describe the equilibrium phase behavior of complex coacervation, capable of predicting both the correlated molecular structure of the bulk coacervate phase as well as matching experimental phase diagrams. We incorporate this model into a self-consistent field theory (SCFT) of polyelectrolyte self-assembly to predict phase diagrams, revealing a correspondence between salt concentration in charge-driven assembly and temperature in solvophobicity-driven assembly. We also show the limits of blockiness, mapping out the transition between micro-phase separated and macro-phase separated polymers as a function of the monomer sequence on a polyelectrolyte.

*We acknowledge funding from NSF CAREER Award DMR-1654158.
12:51PM S35.00009: Sequence-Controlled Complex Coacervation of Random Polyelectrolytes
ARTEM RUMYANTSEV, NICHOLAS JACKSON, BOYUAN YU, JEFFREY M TING, WEI CHEN, MATTHEW TIRRELL, JUAN DE PABLO (Presenter), University of Chicago — The primary sequence of monomers along a backbone of heteropolymers impacts their physical properties. Random heteropolymers with the sequences following a first-order Markov process arise from statistical copolymerization of different monomers. In this work, we study complex coacervation of oppositely charged, random polyelectrolytes, i.e., polyanions and polycations containing statistically distributed charged and uncharged units. It is shown that increasing blockiness of charged monomers in the primary structure of the random polyelectrolytes favors the formation of dense coacervates. Charge blockiness also improves coacervate salt resistance and increases the width of the two-phase solution region. This effect is due to the enhanced cooperativity of Coulomb interactions between oppositely charged monomers within the coacervate. Our findings demonstrate that the solution phase behavior can be controlled through the design of the Markov monomer sequences, which are governed by the kinetics of statistical copolymerization.

1:03PM S35.00010: Concentration and separation of proteins using polyion condensates*
SASKIA LINDHOUD (Presenter), Nanobiophysics, University of Twente — When oppositely charged macromolecules are mixed in aqueous systems at the right conditions, i.e., ionic strength, mixing ratio, pH, etc., solutions phase separate in a condensed phase which is rich in macromolecules and a dilute phase. The so formed polyion condensate can be liquid-like or solid-like. In both cases proteins can be captured in the condensate phase. This protein partitioning strongly depends on the ratio between the oppositely charged macroions. The cellular fluids contain liquid-like domains with similar properties to polyion condensates. This is not surprising since these cellular structures consist of intrinsically disordered proteins (IDPs) which are zwitterionic in nature, these readily phase separate in vitro, or contain RNA, which is negatively charged, and IDPs with high amount of basic residues. These cellular condensates are expected to selectively partition other biomacromolecules. Cellular condensates are very complex multi-component systems, which can be mimicked using simple polyion condensates, consisting of synthetic oppositely charged polyelectrolytes. In this talk I will discuss two features of these polyion condensates which can be linked to the cellular condensates. First of all their ability to concentrate proteins and second that the partitioning of proteins can be very selective. This selectivity can be used to separate two types of proteins. Both these features are also important for extraction processes in chemical engineering. This talk will therefore conclude by discussing the possibility to use these condensates as tunable extraction media for biorefinery applications.

*The authors acknowledge funding from the Netherlands Organization for Scientific Research (NWO) VENI (#722.013.013) and VIDI (# 723.015.003) grants
1:39PM S35.00011: Complex coacervation of polymerized ionic liquids in non-aqueous solvents
MINJUNG LEE (Presenter), RYAN HAYWARD, Univ of Mass - Amherst — The formation of polyelectrolyte complex coacervates within solutions of two oppositely charged polymers is a topic of great recent interest. Studies to date have focused almost exclusively on polyelectrolyte mixtures in water or aqueous solvent mixtures. In this study, polymerized ionic liquids (PILs) were used to investigate the effects of solvent on complex coacervation in non-aqueous solvents. We constructed phase diagrams of PIL mixtures in non-aqueous solvents via experiments using UV-Vis and quantitative $^{19}$F-NMR spectroscopy, and found a substantial difference between two solvent systems in terms of the salt resistance, i.e., the concentration of added salt where complex coacervates are destroyed. Through these studies we seek to provide insight into the role of dielectric constant and solvent/polymer interactions on complex coacervation.

*This research was supported by the National Science Foundation Division of Materials Research (NSF DMR-157384)

1:51PM S35.00012: Computational Investigation of Sequence-Controlled Complex Coacervation in Statistical Copolymers
BOUAN YU (Presenter), NICHOLAS JACKSON, ARTEM RUMYANSEV, JUAN DE PABLO, Pritzker School of Molecular Engineering, University of Chicago — Control of the monomer sequence of polymeric materials provides a pathway for the design of materials that mimic biomacromolecular complexity. In practice, this control can be achieved by tuning the reaction kinetics of random polymerization of different monomers, where the primary sequence distribution follows a first-order Markov chain. In this work, classical Gibbs ensemble and molecular dynamics simulations are used to explore the phase diagrams of polyelectrolyte coacervates with distinct monomer sequences controlled by a simple model for statistical copolymerization. Our results are summarized in phase diagrams that are in line with our previous theoretical findings and experimental observations including the fact that high charge “blockiness” within the sequence results in denser coacervates. Simulations also explore the important role of salt ion specificity as manifested by excluded volume interactions, and how these effects influence complex coacervate thermodynamics. The results presented in this work provide a deeper understanding of how chemical sequence can be used to control complex coacervation.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S36 DCOMP: Ultrafast Dynamics of Coupled Electrons and Atomic Motions: Experiments and Precise Simulations
Andre Schleife, University of Illinois at Urbana-Champaign - Tag(s): Invited
11:15AM S36.00001: Terahertz frequency switching in topological Weyl semimetals [Invited]
AARON LINDENBERG (Presenter), Stanford Univ — I will describe femtosecond-resolution crystallographic measurements probing dynamic switching responses driven by terahertz light pulses in topological Weyl semimetals, focusing on the 2D transition metal dichalcogenide WTe$_2$. We describe a new mechanism for driving large amplitude interlayer shear oscillations with ~1% strain amplitudes, leading to a topologically distinct metastable phase. We further show that such shear strain serves as an ultrafast, energy-efficient means to induce more robust, well-separated Weyl points or to annihilate all Weyl points of opposite chirality. I will also discuss new efforts investigating other means for manipulating the topological phase diagram and interlayer stacking of this material through the application of pure electric fields and through doping/intercalation as probed by both optical and transport measurements. This work defines new possibilities for ultrafast manipulation of the topological properties of solids and for the development of new types of topological optoelectronic devices.

11:51AM S36.00002: Observables of real-time lattice dynamics in time-dependent density functional theory [Invited] HANNES HUEBENER (Presenter), Max Planck Institute for the Structure and Dynamics of Matter — I will discuss real-time simulations of lattice vibrations in solids and their signatures in spectroscopy. In particular signatures of electron-phonon coupling in optical and electron spectroscopies have long been used to investigate materials. With the increasing interest in controlling and manipulating materials properties in a non-equilibrium state, such signatures become relevant also in time-resolved measurements. I will discuss how real-time time-dependent density functional calculations can be used to understand spectral features of electron-phonon coupling of driven electronic structure in solids. A useful interpretative tool that emerges from such a treatment is the picture of a dressed electronic structure, which allows to discuss effects in driven systems without referring to perturbation theory.

12:27PM S36.00003: Toward Precise Ab Initio Simulations of the Ultrafast Dynamics of Electrons and Phonons [Invited] MARCO BERNARDI (Presenter), Caltech — Recent progress in combining density functional theory and related ab initio methods with kinetic equations are enabling spectacular advances in computing carrier dynamics in materials from first principles. We will first review this framework and early ab initio calculations of electron scattering rates and carrier thermalization, and then discuss recent developments. The talk will focus on a numerical approach to evolve in time the coupled Boltzmann transport equations (BTEs) of electrons and phonons, using ab initio electron-phonon and phonon-phonon interactions together with a parallel algorithm to explicitly time step the BTEs. Our approach can simulate the electron and phonon dynamics up to hundreds of picoseconds (with a femtosecond time resolution), and the accuracy of the interactions used in the calculations can be validated by computing transport properties. We show example calculations on graphene and semiconductors, for which we compute carrier cooling rates, mode-resolved phonon dynamics, transient absorption, and time-resolved structural snapshots and diffuse X-ray scattering. We will show how this approach can be extended to include excitons, by discussing calculations of exciton-phonon interactions and real-time exciton dynamics. We will outline code development efforts, open problems and future directions.
1:03PM S36.00004: Recent advances in light induced superconductivity [Invited] ANDREA CAVALLERI (Presenter), Max Planck Inst Structure & Dynamics of Matter — I will discuss how coherent electromagnetic radiation at infrared and TeraHertz frequencies can be used to drive collective excitations in solids and especially experiments in which superconducting correlations can be induced at temperatures higher than the thermodynamic transition temperature. I will discuss results in cuprates, doped fullerenes and recent work in organic salts. By comparing these examples a clearer microscopic picture is emerging for driven unconventional superconductivity.

1:39PM S36.00005: Time-dependent potential energy surfaces from the exact factorization: A predictive first-principles approach to ultra-fast non-adiabatic dynamics [Invited] EBERHARD K GROSS (Presenter), Fritz Haber Center, Institute of Chemistry, The Hebrew University of Jerusalem — Some of the most fascinating phenomena in physics and chemistry, such as the process of vision, as well as exciton dynamics in photovoltaic systems involve the coupled motion of electrons and nuclei beyond the adiabatic approximation, i.e. processes not captured by the dynamics on a single Born-Oppenheimer surface. To go beyond the adiabatic approximation is notoriously difficult as one has to start from the full Hamiltonian of interacting electrons and nuclei. We deduce an exact factorization [1] of the full electron-nuclear wave function into a purely nuclear part and a many-electron wave function which parametrically depends on the nuclear configuration and which has the meaning of a conditional probability amplitude. The equations of motion of these two wave functions provide an ideal starting point to develop efficient algorithms for the study non-adiabatic phenomena. The successful prediction of ultrafast laser-induced isomerization processes [2], the description of decoherence [3], calculations of the molecular Berry phase without invoking the Born-Oppenheimer approximation [4] and accurate predictions of vibrational spectroscopy [5], especially dichroism, will demonstrate the power of this new approach. To tackle non-adiabatic phenomena in solids, such as laser-induced phase transitions, the equations of motion of the exact factorization are “density-functionalized” [6], leading to a coupled set of Kohn-Sham equations for electrons and phonons [7].

11:15AM S37.00001: Atomically thin van der Waals magnets: a career in flatland [Invited]
EFREN NAVARRO-MORATALLA (Presenter), Univ de Valencia — Layered magnetic materials are at the origin of modern magnetism and among the very first compounds to be explored at cryogenic temperatures. The phenomenon of magnetic ordering in layers has tantalized condensed matter physicists ever since the theory put forward by Mermin and Wagner demonstrating that long-range ordering in low dimensions is forbidden in an isotropic spin lattice. In order to confirm this hypothesis, many experiments have been performed in the aforementioned layered crystals as an approximation of a two-dimensional (2D) spin lattice. However, interlayer coupling in bulk systems is not negligible and an approach for the study of true 2D magnetism had been for a long time. With the avenue the 2D materials a genuine approach to correlated states in low-dimensions has been unlocked. In this talk I will narrate the launch of my independent research carrier, which has been intimately tied to our discovery of the first free-standing 2D ferromagnet made out of a single layer of a ferromagnetic insulator: chromium triiodide. I will try to stimulate for risk taking and multidisciplinarity in condensed matter physics careers and provide insight into timely research opportunities.

11:51AM S37.00002: Electrocatalysis from two-dimensional materials: an ERC project [Invited]
DAMIEN VOIRY (Presenter), University of Montpellier — Electrochemical reactions can afford hydrogen gas (H2) and small organic molecules from water and CO2, respectively and therefore offers promise for the production of fuels. Owing to their reduced dimensionality, two-dimensional (2D) materials have emerged as interesting platforms for studying electrocatalysis. In addition, their properties can largely be tuned by changing their elemental composition, their thickness and their atomic structure.
In 2018, our activity received support from the European Research Council (ERC) for exploring the influence of the defects, the crystal structure and the electronic properties on the catalytic performance towards the reduction of CO2. By developing engineering strategies, our group aims at investigating the electrocatalytic properties of 2D materials including transition metal dichalcogenides and quasi-2D transition metals. To do so, we have recently reported the fabrication of electrochemical microcells using microfabrication techniques. This device architecture allows testing individual nanosheets in order to precisely quantify the activity from the edges and the basal planes. In my talk, I will illustrate how the ERC grant was pivotal in developing my research activities in Europe.

References:
12:27PM S37.00003: Obtaining an ERC Starting Grant* [Invited]  TOMA SUSI (Presenter), Univ of Vienna — The European Research Council (ERC) is the continent's pre-eminent source of competitive funding to support investigator-driven frontier research across all fields. The ERC was designed by researchers and its funding decisions are made by disciplinary peers solely on the basis of scientific excellence. This 'bottom-up' approach allows the scientists themselves to identify new opportunities in any field of research, rather than being led by priorities set by politicians. Grants are awarded through open competition to projects headed by starting and established researchers who are working or moving to work in Europe.

In 2014, I discovered that the scattering of energetic electrons can cause silicon impurities to move through the graphene lattice, revealing a potential for atomically precise manipulation using the focused electron probe. To develop this into a practical technique, improvements in the description of beam-induced displacements, advances in heteroatom implantation, and a concerted effort towards the automation of manipulations were required in a multidisciplinary effort combining computational and experimental work in a custom-modified scanning transmission electron microscope electron microscope.

In this talk, I will describe my journey from designing a high-risk, high-reward frontier research project to writing a successful proposal and presenting it to my peers in a grant interview. After successfully receiving the grant and completing the grant negotiations, I started my project in October 2017. The generous support of 1.5 million euros over five years from an ERC Starting Grant allowed me to start my own research group devoted to this topic, and gave ample visibility within my university. This and the fact the grant is tied to my person and transferrable to another institution directly contributed to the tenure track position I received at the University of Vienna in 2019.

*Toma Susi is supported by the European Research Council (ERC) Grant 756277-ATMEN.

1:03PM S37.00004: PHYSICS FOR SOCIETY: GRAND CHALLENGES IN THE HORIZON 2050 [Invited] CARLOS HIDALGO (Presenter), European Physical Society — The talk will provide an overview of the EPS action designed to address the social dimension of science and the grand challenges in Physics that will bring radical change to developed societies and to provide basic understanding of nature on the Horizon 2050.

Although the quest for knowledge in itself is not necessarily susceptible to ethical evaluation, science abandons its ethical neutrality when it addresses the way in which knowledge is generated and when one considers the impact of its technological applications on individuals and society. Some consequences of being science (as a whole) a non-ethically neutral actor in Society will be addressed.

This action, developed within the framework of the EPS Forum Physics and Society, should reach a broad audience that is willing to explore a future shaped by science. A target audience is young people looking for perspectives in physics.
FRANCESCO DI STASIO (Presenter), Istituto Italiano di Tecnologia — Colloidal semiconductor nanocrystals (commonly referred to as Quantum Dots) are one of the earliest examples of Nanomaterials as their initial discovery dates back to 1986. Nevertheless, they still attract considerable attention thanks to their versatile chemical synthesis, desirable properties for optoelectronics and rich photophysics. Since 2013, my research effort has been dedicated to the development of optoelectronic devices based on colloidal semiconductor nanocrystals. Nanocrystals based II-VI semiconductors have served as a model system for understanding the strong correlation between chemical synthesis and physical properties, as well as the development of technological applications such as solar cells, lasers and light-emitting diodes (LEDs). Such knowledge is employed nowadays for the development of the newly discovered lead-based perovskites (general formula: APbX3, where A = Cs or an organic moiety and X = Cl, Br or I).

In this talk, I will present some recent results on NC light-emitting diodes (LEDs) based on PbS and perovskite nanocrystals, operating both in the visible and in the infrared spectral range. The efficiency of NC-LEDs has now reach important milestones thanks to interdisciplinary collaboration between physicists, chemists and material scientists. Yet, LEDs based on ensemble of nanocrystals (i.e. nanocrystal films) show good performance in terms of efficiency and luminance but their applicability is still limited to standard consumer electronics products such as displays and illumination.

The future challenge is to exploit colloidal semiconductor nanocrystals for single-photon generation under electrical excitation, thus leading to a novel class of non-classical light sources. In this playground, the ERC has provided me support through a starting grant. In the last part of my talk I will describe how “connecting the dots” between different research fields has led me to a successful grant application.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S38 DQI: Optimal Quantum Control 607 - Matthew Grace, Sandia National Laboratories - Tag(s): Focus
11:15AM S38.00001: Variational quantum control for single- and two-qubit transmon gates*  
ANDRES RUIZ CHAMORRO, ERIK TORRONTEGUI, JUAN JOSE GARCIA-RIPOLL (Presenter), Instituto de Fisica Fundamental — Transmon are among the most successful qubits in the superconducting world, enabling the largest gate-based quantum computations to-date. In this talk I will present a new set of techniques to design single-qubit and two-qubit gates for transmon qubits, which can be used to tune qubit frequencies, implement direct or cavity mediated CZ interactions [1], and √SWAP gates with tuneable couplers. The technique is based on variational estimates of the transmon qubit state dynamics, and provides semi-analytical controls that can be further tuned to develop more robust protocols. With minor efforts, methods provide various orders of magnitude improvement in fidelity over earlier techniques based on fast-quasi-adiabatic passages or conventional square or segmented pulses, as used in current experiments.


*This material is based upon work supported by the Air Force Office of Scientific Research under award number FA2386-18-1-4019. This work has been supported by funding from project PGC2018-094792-B-I00 (MCIU/AEI/FEDER, UE) and CAM/FEDER Project No. S2018/TCS-4342 (QUITEMAD-CM).

11:27AM S38.00002: Universal gates for protected superconducting qubits using optimal control*  
BRIAN BAKER (Presenter), Northwestern University, MOHAMED ABDELHAFEZ, University of Chicago, ANDRAS GYENIS, PRANAV MUNDADA, ANDREW HOUCK, Princeton University, DAVID I SCHUSTER, University of Chicago, JENS KOCH, Northwestern University — In this talk I will discuss the use of quantum optimal control theory to realize quantum gates for two protected superconducting circuits: the heavy-fluxonium qubit and the 0-π qubit. Utilizing automatic differentiation facilitates the simultaneous inclusion of multiple optimization targets, allowing one to obtain high-fidelity gates with realistic pulse shapes. For both qubits, disjoint support of low-lying wave functions prevents direct population transfer between the computational-basis states. Instead, optimal control favors dynamics involving higher-lying levels, effectively lifting the protection for a fraction of the gate duration. For the 0-π qubit, offset-charge dependence of matrix elements among higher levels poses an additional challenge for gate protocols. To mitigate this issue, we randomize the offset charge during the optimization process, steering the system towards pulse shapes insensitive to charge variations. Closed-system fidelities obtained are 99% or higher, and show slight reductions in open-system simulations.

*We gratefully acknowledge support from the Army Research Office through Grant Nos. W911NF-15-1-0421 and W911NF-19-1-0016.
11:39AM S38.00003: Uncomputability and complexity of quantum control  DENYS BONDAR
(Presenter), Tulane Univ, ALEXANDER N PECHEN, Steklov Mathematical Institute of Russian Academy of Sciences — In laboratory and numerical experiments, physical quantities are known with a finite precision and described by rational numbers. Based on this, we deduce that quantum control problems both for open and closed systems are in general not algorithmically solvable, i.e., there exists no algorithm that can decide whether dynamics of an arbitrary quantum system can be manipulated by accessible external interactions (coherent and dissipative) such that a chosen target reaches a desired value. This conclusion holds even for the relaxed requirement of the target only approximately attaining the desired value. These findings does not preclude an algorithmic solvability for a particular class of quantum control problems. To arrive at these results, we develop a technique based on establishing the equivalence between quantum control problems and Diophantine equations, which are polynomial equations with integer coefficients and integer unknowns. In addition to proving uncomputability, this technique allows to construct quantum control problems belonging to different complexity classes. In particular, an example of the control problem involving a two-mode coherent field is shown to be NP-hard, contradicting a widely held believe that two-body problems are easy.

11:51AM S38.00004: Robust control for tight SWAP cold atom sensors  MICHAEL HUSH
(Presenter), VIKTOR PUCINCIC, PER LIEBERMANN, ANDRE CARVALHO, HARRY SLATYER, RAJIB CHAKRAVORTY, HARRISON BALL, MICHAEL BIERCUK, Q-CTRL — Cold atom sensors currently provide state-of-the-art performance under lab conditions. Deploying these in tight-SWAP conditions, however, presents a variety of challenges arising from laser instabilities, such as power, frequency, and phase fluctuations. We demonstrate that robust control techniques - related to dynamic decoupling and dynamically-corrected composite pulses - can significantly improve the sensitivity of cold atom sensors in tight SWAP conditions, achieving performance commensurate with state-of-the-art lab conditions. We derive these robust control pulses using a custom numerical-optimization package, producing control solutions robust to specific coloured noise spectrums, and with relevant experimental constraints including bandwidth limitations. Our robust protocol is benchmarked against standard atom interferometry protocols, showing comparable sensitivity under ideal conditions, and over an order or magnitude improvement in a simulated field-deployed environment including realistic laser fluctuations.
Optimizing quantum circuits subject to cross coupling

PER LIEBERMANN (Presenter), HARRISON BALL, HARRY SLATYER, Q-CTRL, MACHIEL S BLOK, VINAY RAMASESH, University of California, Berkeley, ANDRÉ CARVALHO, VIKTOR PUCINCIC, RAJIB CHAKRAVORTY, MICHAEL HUSH, MICHAEL BIERCUK, Q-CTRL — We present a new optimization technique which creates time-optimized circuits capable of combating unwanted crosstalk in transmon circuits. The low anharmonicity of transmons allows for the performance of quantum computations with either qubits or qutrits realized using the three lowest energy levels of the device. Unfortunately when employed in circuits residual ZZ-type couplings can lead to error sources which degrade algorithmic performance. We demonstrate the optimization of complex Unitaries on up to five qutrits using SU(2) and SU(3) operations. Based on a custom GPU-compatible optimization toolkit, high-fidelity and robust circuits are generated by optimizing both applied SU(N) operations and their timing in the circuit. We further demonstrate the ability to find robust solutions optimized to account for additional time-varying noise processes. We compare numeric with analytic results and GPU-optimization speeds with CPU-limited methods. Overall this approach forms a new kind of optimized circuit compilation which trades-off algorithmic execution time for improved overall error performance in a deterministic fashion.

High fidelity unitary evolution using constrained control fields.

THALES FIGUEIREDO ROQUE (Presenter), Max Planck Inst for Sci Light, AASHISH CLERK, University of Chicago, HUGO RIBEIRO, Max Planck Inst for Sci Light — The problem of coherent errors, where the quantum unitary evolution is corrupted by populating spurious states (leakage error) or accumulates the wrong phase (phase error), is generic to a variety of situations. This type of errors often arise because it is a difficult task to find control fields that would generate with high accuracy a desired unitary evolution. The task becomes even more complex when taking into account experimental constraints: unavailable control fields, bandwidth limitations, amplitude limitations, etc. Here we attack a class of problems where suitable controls are known in an idealized scenario, but unwanted perturbative interactions disrupt the desired unitary evolution. We show how a recently-proposed Magnus expansion based algorithm for quantum control [1] can be modified to find control fields that both suppress coherent errors and are compatible with experimental constraints. In this talk, we focus on presenting the general method and revisit the problem of single qubit gates in a transmon qubit.

Quantum optimal control in a ZZ-free qubit architecture

ROSS SHILLITO (Presenter), Institut quantique and Département de Physique, Université de Sherbrooke, RONI WINIK, Research Laboratory of Electronics, Massachusetts Institute of Technology, CATHERINE LEROUX, AGUSTIN DI PAOLO, Institut quantique and Département de Physique, Université de Sherbrooke, JOCHEN BRAUMUELLER, MORTEN KJAERGAARD, ANTTI VEPSALAINEN, Research Laboratory of Electronics, Massachusetts Institute of Technology, DAVID K KIM, JONILYN YODER, MIT Lincoln Laboratory, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, WILLIAM OLIVER, MIT Lincoln Laboratory, ALEXANDRE BLAIS, Institut quantique and Département de Physique, Université de Sherbrooke — Quantum optimal control is a powerful technique for improving the performance of quantum gates. Numerical methods, such as GRAPE, have been demonstrated to reduce infidelity of single- and two-qubit gates by several orders of magnitude. In this talk, we demonstrate the application of quantum optimal control in a newly proposed architecture in which the ZZ-interaction is inherently suppressed. We explore the parameter regimes of this system to optimize the performance of a cross-resonance gate on this architecture.

This research was funded in part by the ARO grant No. W911NF-18-1-0411; and by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

This work was undertaken thanks in part to funding from NSERC and the Canada First Research Excellence Fund.

A comparative study for reinforcement learning and traditional algorithms on state transfer problem

XIAOMING ZHANG (Presenter), XIN WANG, City Univ of Hong Kong — While reinforcement learning (RL) has been widely used in quantum control problems, it remains unclear whether RL is the most suitable algorithm when the control has specific constraints. We perform a comparative study on the efficacy of three RL algorithms: tabular Q-learning, deep Q-learning and policy gradient, as well as stochastic gradient descent and Krotov algorithms, in the problem of quantum state preparation. Overall, the deep Q-learning and policy gradient algorithms outperform others when the problem is discretized, e.g. allowing discrete values of control and when the problem scales up. Moreover, the reinforcement learning algorithms can also adaptively reduce the complexity of the control sequences. Our work provides insights into the suitability of reinforcement learning in quantum control problems.

This work is supported by the Research Grants Council of the Hong Kong SAR (Grant Nos. CityU 21300116, CityU 11303617, CityU 11304018).
12:51PM S38.00009: A geometric approach to dynamically corrected gates* [Invited]  EDWIN BARNES (Presenter), Virginia Tech — Future technologies such as quantum computing, sensing and communication demand the ability to control microscopic quantum systems with unprecedented accuracy. This task is particularly daunting due to unwanted and unavoidable interactions with noisy environments that destroy quantum information through decoherence. I will present recent progress in understanding and modeling the effects of noise on the dynamics of a qubit and show how this can be used to develop new ways to slow down decoherence. I will then describe a new general theory for dynamically combatting decoherence by driving qubits in such a way that noise effects destructively interfere and cancel out. This theory exploits a rich geometrical structure hidden within the time-dependent Schrödinger equation.

*We acknowledge support from the U.S. Army Research Office (Grant No. W911NF-17-0287) and from the U.S. Office of Naval Research (Grant No. N00014-17-1-2971).

1:27PM S38.00010: Application of Pontryagin's Minimum Principle to Grover's Quantum Search Problem  CHUNGWEI LIN (Presenter), Mitsubishi Electric Research Lab — Grover's algorithm is one of the most famous algorithms which explicitly demonstrates how the quantum nature can be utilized to accelerate the searching process. In this work, Grover's quantum search problem is mapped to a time-optimal control problem. Resorting to Pontryagin's Minimum Principle we find that the time-optimal solution has the bang-singular-bang structure. This structure can be derived naturally, without integrating the differential equations, using the geometric control technique where Hamiltonians in the Schrödinger's equation are represented as vector fields. In view of optimal control, Grover's algorithm uses the bang-bang protocol to approximate the optimal protocol with a minimized number of bang-to-bang switchings to reduce the query complexity. Our work provides a concrete example how Pontryagin's Minimum Principle is connected to quantum computation, and offers insight into how a quantum algorithm can be designed.
1:39PM S38.00011: Variational quantum gate optimization on superconducting qubit system*  HEYA KENTARO (Presenter), Research Center for Advanced Science and Technology, The University of Tokyo, YASUNARI SUZUKI, NTT Secure Platform Laboratories, NTT Corporation, YUTAKA TAKEDA, AKHIL PRATAPS SINGH, Research Center for Advanced Science and Technology, The University of Tokyo, SHINGO KONO, KOH-ICHI NITTOH, KOICHI KUSUYAMA, Center for Emergent Matter Science, RIKEN, SHUHEI TAMATE, YUTAKA TABUCHI, Research Center for Advanced Science and Technology, The University of Tokyo, KEISUKE FUJII, Graduate School of Engineering Science, Osaka University, YASUNOBU NAKAMURA, Research Center for Advanced Science and Technology, The University of Tokyo — Hybrid quantum-classical (HQC) algorithms aim at realizing the quantum advantage in shallow depth quantum circuits with an aid of classical computation. Recently, HQC algorithms have been extensively studied with the expectation that they may solve practical problems in the near future. However, the quantum gate fidelities directly limit the sizes of executable problems in quantum computers without quantum error correction. While HQC algorithms require fewer quantum gates, the state-of-the-art gate fidelities are still insufficient to deal with practical problems. In this presentation, we propose a gate optimization method, where high-fidelity multi-qubit gates are generated by optimizing parametrized quantum circuits consisting of tunable high-fidelity single-qubit gates and fixed multi-qubit gates with limited controllability. We call the method variational quantum gate optimization (VQGO) and demonstrate it on a superconducting qubit system.

*This work is partly supported by JST ERATO (JPMJER1601) and MEXT Q-LEAP (JPMXS0118068682).

1:51PM S38.00012: Using Algebra to Dissect Quantum Optical Evolution for Quantum Control*  RILEY E MARTELL, Washington University in Saint Louis, JEAN-FRANCOIS VAN HUELE (Presenter), TY BEUS, MANUEL BERRONDO, Brigham Young Univ - Provo — Quantum control is the ability to affect quantum systems through judicious selection of dynamical parameters and their time dependence. Wei-Norman factorization [Wei and Norman, Proc. Amer. Math.Soc.15, 327 (1964)] is a powerful method to parametrize the quantum mechanical evolution operator before applying it to specific states. We first illustrate this method on the dynamics of optomechanical oscillators. We then extend the method to the pseudo-dynamics associated with the squeeze operator and characterize its action on a variety of optical states. This leads to improved insight into quantum control at a level accessible to undergraduates.

*Supported by NSF Award #1757998

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S39 DCOMP GDS DMP: Machine learning for quantum matter IV  703 - Linda Hung, Toyota Research Institute - Tag(s): Focus
11:15AM S39.00001: Self-learning projective quantum Monte Carlo simulations guided by restricted Boltzmann machines [invited] SEBASTIANO PILATI, University of Camerino, ESTELLE INACK (Presenter), Perimeter Inst for Theo Phys, PIERBIAGIO PIERI, University of Camerino — Projective quantum Monte Carlo (QMC) simulations have been successfully used to simulate various relevant quantum many-body systems. They are systematically implemented in a two-step approach, in which a variational ansatz inspired by theory is first optimized using traditional variational optimization techniques. Later, the optimized ansatz is used as a guiding wave function in projective QMC simulations. In this work, we present a novel method that uses unsupervised machine learning techniques to combine the two steps above. It adaptively trains the guiding wave function (represented by a restricted Boltzmann machine) within QMC simulations, thus avoiding the need for separate variational optimization. On the one hand, this approach greatly increases the efficiency and accuracy of projective QMC simulations. On the other hand, it provides a new way to develop ground-state ansatzes, complementary to the common variational optimization schemes. We present extensive benchmarks that demonstrate the efficiency of our self-learning method.

11:51AM S39.00002: Self-learning Hybrid Monte Carlo method for first-principles molecular simulations YUKI NAGAI (Presenter), MASAHIKO OKUMURA, Japan Atomic Energy Agency, KEITA KOBAYASHI, RIST, MOTOYUKI SHIGA, Japan Atomic Energy Agency — We propose a novel approach called Self-Learning Hybrid Monte Carlo (SLHMC) which is a general method to make use of machine learning potentials to accelerate the statistical sampling of first-principles density-functional-theory (DFT) simulations. The trajectories are generated on an approximate machine learning (ML) potential energy surface. The trajectories are then accepted or rejected by the Metropolis algorithm based on DFT energies. In this way the statistical ensemble is sampled exactly at the DFT level for a given thermodynamic condition. Meanwhile the ML potential is improved on the fly by training to enhance the sampling, whereby the training data set, which is sampled from the exact ensemble, is created automatically.


12:03PM S39.00003: On-the-fly machine learning algorithm for accelerating Monte Carlo sampling: Application to the stochastic analytical continuation* HONGKEE YOON (Presenter), MYUNG JOON HAN, Korea Adv Inst of Sci & Tech — We present a new Monte Carlo method whose sampling is assisted by modern machine learning (ML) technique. In order to improve the MC sampling efficiency in high dimensional problems, we suggest ML generative model as being a part of MC sampler. We apply this ML+MC method to a long-standing numerical problem in quantum many-body physics, namely, analytic continuation. In our scheme, ML sampler naturally satisfies physical constraints such as detailed balance because it is combined with the conventional Markov chain MC procedure. Furthermore, massive data sets generated by MC procedure provides the on-the-fly ‘learnings’ for ML sampler. Remarkable improvement has been achieved in terms of both convergence speed and the quality of continuation result. The same approach can be applicable to various other problems for which MC algorithm has been used.

*This work was supported by the National Research Foundation of Korea (NRF) (2018R1A2B2005204) and NRF (2018M3D1A1059001).
12:15PM S39.00004: Automatic Differentiable Monte Carlo: Theory  SHIXIN ZHANG
(Presenter), ZHOU-QUAN WAN, HONG YAO, Tsinghua University — Differentiable programming emerges as the new programming paradigm empowering the rapid development of deep learning as it has been shown equally powerful in computational physics. Here we propose a general theory framework with detach function techniques enabling infinite order automatic differentiation on Monte Carlo expectations with unnormalized probability distributions. By introducing automatic differentiable Monte Carlo (ADMC), we can leverage state-of-the-art machine learning framework and toolbox to traditional Monte Carlo approaches in statistics and physics by simply implementing relevant Monte Carlo algorithms on computation graphs.

12:27PM S39.00005: Automatic Differentiable Monte Carlo: Applications  ZHOUQUAN WAN
(Presenter), SHIXIN ZHANG, HONG YAO, Tsinghua University — Differentiable programming emerges as the new programming paradigm empowering the rapid development of deep learning as it has been shown equally powerful in computational physics. By introducing automatic differentiable Monte Carlo (ADMC), we can leverage state-of-the-art machine learning frameworks and techniques to traditional Monte Carlo approaches in statistics and physics by simply implementing relevant Monte Carlo algorithms on computation graphs. We show the power of ADMC by three specific applications from physics and statistics: 1. Locate the critical temperature for 2D Ising model; 2. Compute Fisher matrix with automatic differentiation setup; 3. End-to-end, easy-to-implement, automatic differentiable variational Monte Carlo on 2D Heisenberg model with general neural network wavefunction anstaz. We further discuss about other potential possibilities that ADMC bring us in the innovations and breakthroughs of Monte Carlo methods.

12:39PM S39.00006: Optimal Real-Space Renormalization-Group Transformations with Artificial Neural Networks*  JUI-HUI CHUNG, YING-JER KAO (Presenter), Natl Taiwan Univ — We introduce a general method for optimizing real-space renormalization-group transformations to study the critical properties of a classical system. The scheme is based on minimizing the Kullback-Leibler divergence between the distribution of the system and the normalizing factor of the transformation parametrized by a restricted Boltzmann machine. We compute the thermal critical exponent of the two-dimensional Ising model using the trained optimal projector and obtain a very accurate exponent $\gamma_t=1.0001(11)$ after the first step of the transformation.

12:51PM S39.00007: Machine-learning-accelerated predictions of optical properties of condensed systems based on many-body perturbation theory*  SIJIA DONG (Presenter), MARCO GOVONI, Materials Science Division, Argonne National Laboratory, GIULIA GALLI, University of Chicago — Accurate and efficient predictions of absorption spectra of molecules and solids are essential for the understanding and rational design of broad classes of materials, including photo-absorbers in solar and photo-electrochemical cells and defective insulators and semiconductors hosting optically addressable spin-defects. We present an approach to improve the efficiency of first principles calculations of absorption spectra of complex materials at finite temperature, based on the solution of the Bethe-Salpeter equation (BSE) [1]. We use machine learning techniques to predict the spectra of snapshots extracted from ab initio molecular dynamics simulations, and we use data generated by explicitly solving the BSE for a small subset of snapshots. We present results for nanoclusters, solids, liquids, including water, and semiconductor-water interfaces.


*The work was supported by Advanced Materials for Energy-Water Systems (AMEWS) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences (DOE-BES), and Midwest Integrated Center for Computational Materials (MICCoM) as part of the Computational Materials Science Program funded by DOE-BES.

1:03PM S39.00008: Machine Learned Spectral Functions for the Quantum Impurity Problem  ERICA STURM (Presenter), Brookhaven National Laboratory, MATTHEW R CARBONE, Department of Chemistry, Columbia University, DEYU LU, ANDREAS WEICHSELBAUM, ROBERT KONIK, Brookhaven National Laboratory — Machine learning techniques can greatly reduce simulation times by providing highly accurate approximations, thus circumventing the need for more expensive models. This work leverages a feed-forward neural network (NN) to predict the spectral functions of the single impurity Anderson model (SIAM) as a function of five physical parameters including the Coulomb interaction U, hybridization constant Γ, impurity energy ε_d, magnetic field B, and temperature T. The NN was trained on ~670,000 unique SIAM system spectral functions generated by Wilson’s Numerical Renormalization Group (NRG). The NN predicts the spectral function with a mean absolute difference of less than 3% compared to the ground truth. The ability to efficiently predict a spectral function for the quantum impurity problem can improve the computation time for dynamical mean field theory and related methods that investigate strong correlation in condensed matter systems.

References
1:15PM S39.00009: Finding New Mixing Strategies for Self Consistent Field Procedures Using Reinforcement Learning*  
DANIEL ABARBANEL (Presenter), HONG GUO, McGill Univ — Density mixing is a technique to improve the convergence for self-consistent field (SCF) procedures, and is used extensively to calculate electronic structure and transport properties in the context of density functional theory (DFT). Typically, a single mixing method will be chosen for the whole of a SCF calculation, but recent research suggests that alternating the mixing strategy between subsequent SCF iterations can improve the time of convergence. There are many untested SCF mixing methods beyond those already discovered that can be constructed using combinations of established methods. We present a new method to discover mixing strategies by applying a reinforcement learning algorithm (RLA). The state space of the RLA consists of SCF parameters such as the density, potential and convergence error. The action space of the RLA consists of previously developed mixing methods including simple mixing, Broyden mixing and Pulay mixing, with the crucial point being that the RLA is able to alter the mixing strategy in situ.

*Supported by the Natural Sciences and Engineering Research Council (NSERC) and McGill University

1:27PM S39.00010: Machine learning spin dynamics in the double-exchange systems  
PUHAN ZHANG (Presenter), PREETHA SAHA, GIA-WEI CHERN, Univ of Virginia — The double-exchange (DE) mechanism plays an important role in our understanding of the colossal magnetoresistance phenomenon. It describes itinerant electrons interacting with local magnetic moments through the Hund's rule coupling. Although extensive effort has been devoted to studying the equilibrium properties of the DE models, dynamical phenomena in these systems remain much less explored, partly due to the expensive computational cost of their microscopic simulations. For example, in Landau-Lifshitz dynamics (LLD) simulations of the DE systems, the electron tight-binding Hamiltonian has to be solved at every time-step in order to obtain the torque acting on the local spins. Here we propose a machine learning (ML) technique that can solve the dynamics of the DE model in linear time complexity. Our approach is similar to the ML-based force prediction in quantum molecular dynamics. In our method, a deep-learning neural network trained by dataset from small system simulations is used to directly predict the effective local exchange force. We will also present our ML-enabled large-scale LLD simulation of phase separation phenomena in DE systems.

1:39PM S39.00011: Machine learning of high-throughput DFT electron densities  
LINDA HUNG (Presenter), DANIEL SCHWEIGERT, ARJUN BHARGAVA, CHIRRANJEEVI GOPAL, Toyota Research Institute — Kohn-Sham density functional theory (DFT) provides a good balance between accuracy and efficiency, and its utility has given rise to high-throughput DFT databases including the Materials Project and the Open Quantum Materials Database. In this talk, we demonstrate how electron density datasets from these databases can be used to train machine learning models that complement and enhance the capabilities of DFT. We quantify the accuracy of neural networks that predict electron densities, and also report the trends observed in electronic structure-property relationships.
1:51PM S39.00012: Machine learning as a solution to the electronic structure problem
BEATRIZ GONZALEZ DEL RIO (Presenter), RAMAMURTHY RAMPRASAD, School of Materials Science and Engineering, Georgia Institute of Technology — An essential component of materials research is the use of simulations based on density functional theory (DFT), which imposes severe limitations on the size of the system under study. A promising development in recent years is the use of machine learning (ML) methodologies to train surrogate models with DFT data to predict quantum-accurate results for larger systems. Many successful ML models have been created to predict higher-level DFT results such as the total potential energy and atomic forces, and initial steps have been taken to create deep-learning based ML methodologies that can predict fundamental DFT outputs such as the charge density, wave functions and corresponding energy levels [1]. Here, we explore the applicability of this latter methodology using convolutional and recurrent neural networks to learn and predict the electronic charge density and the density of states of carbon, for a large variety of allotropes spanning from metallic to insulating behavior. Further improvements to the speed, accuracy and versatility of this DFT-emulation methodology will also be presented.


*This work was supported by National Science Foundation under award number 1900017.

2:03PM S39.00013: Machine learning spectral indicators of topology
NINA ANDREJEVIC (Presenter), Massachusetts Institute of Technology, JOVANA ANDREJEVIC, CHRISTOPHER RYCROFT, Harvard University, MINGDA LI, Massachusetts Institute of Technology — Topological materials discovery has emerged as an important frontier in condensed matter physics due to the exceptional properties arising from nontrivial band topology. Recent theoretical methods based on local and global symmetry indicators have been used to identify several thousand candidate topological materials, yet experimental determination of materials’ topological character often poses significant technical challenges. X-ray absorption spectroscopy (XAS) is a widely-used characterization technique of materials’ local geometric and electronic structure, as it is sensitive to the symmetry and local chemical environment of constituent atoms; thus, it is a potentially useful encoding of topological character. Here, we study the effectiveness of XAS as a predictor of topology using machine learning methods to disentangle key structural information from the complex spectral features. We discuss the utility of experimental spectra to inform materials’ topology and compare the predictive power of individual absorbing elements.

*N.A. acknowledges NSF GRFP support under Grant No. 1122374.
J.A. acknowledges NSF GRFP support under Grant No. DGE-1745303.
11:15AM S40.00001: Direct measurement of ion mobility by electrophoretic NMR and implications for correlated migration in liquid electrolytes [Invited]  
MONIKA SCHÖNHOFF (Presenter), FLORIAN SCHMIDT, MARC BRINKKÖTTER, MARK PHILLIP ROSENWINKEL, PINCHAS NÜRNBERG, University of Muenster — In studies of ion transport in electrolytes, multinuclear (1H, 7Li, 19F) electrophoretic NMR (eNMR) allows to directly measure electrophoretic mobilities, extracting them from the ion drift velocity in an electric field. For example, in Li salt-in-Ionic Liquid systems a negative mobility of Li⁺ may occur, implying a drift direction opposite to the expectation for a cation. This was attributed to a vehicular transport of Li in net negatively charged Li-anion clusters. Their stoichiometry can be deduced from the effective charge. Employing compositional variations, such as using asymmetric anions or high Li salt concentrations, a transition from a vehicular to a structural transport mechanism of Li⁺ can be achieved. In further liquid electrolytes, containing organic additives or in glyme-based solvate ionic liquids, a drift of uncharged molecules in the electric field can be identified by 1H eNMR. Thus, conclusions on their correlated transport, due to coordination to Li⁺ are possible, shedding light on the mechanisms governing Li transport. In summary, electrophoretic NMR elucidates transport mechanisms on a molecular level, and provides unique information; in particular, where correlated motion of different ion species is involved.

11:51AM S40.00002: Modulation of ion transference number by dynamic hydrogen bond network  
VERA BOCHAROVA (Presenter), Oak Ridge National Lab, ZANETA WOJNAROWSKA, University of Silesia in Katowice, Poland, ANDREW ERWIN, Georgia Tech, NISHANI JAYAKODY, STEVEN GREENBAUM, Hunter College of The City University of New York, IVAN POPOV, Oak Ridge National Lab, CATALIN GAINARU, Technische Universität Dortmund, Germany, SHIWANG CHENG, Michigan State University — Ionic liquids (IL) are important materials with potential to be used in various technologies because of their non-toxicity, non-flammability, and high ionic conductivity. Although high conductivity in ionic liquids can be achieved, their relatively low transference number remains a problem. Ionic materials with high transference number are required to design high power batteries. In the present talk, we demonstrate that addition of small nanoparticles capable of formation of hydrogen bonds can reduce electrostatic interaction between ions in IL which improves ion dissociation. Furthermore, with increase in concentration of nanoparticle a clear evidence of network formation has been obtained from rheology. By studying various aspects of diffusion, conductivity, and dynamics in the network at ambient and elevated pressure, we found that formation of the network promotes decoupling between ion conductivity and structural relaxation and controls ion diffusion trough hydrogen bond network. Our studies provide fundamental insights into decoupling phenomena which is a major mechanism of conductivity in solid ion conductors. Furthermore, introduction of additional interaction into IL seems to be a promising direction to control diffusion of the ions.
12:03PM S40.00003: Ionic Association, Solvation and Gelation in Super-Concentrated Electrolytes*  MICHAEL MCELDREW (Presenter), Massachusetts Institute of Technology MIT, SHENG BI, ZACHARY GOODWIN, ALEXEI A. KORNYSHEV, Chemistry, Imperial College London, MARTIN BAZANT, Massachusetts Institute of Technology MIT — In super-concentrated electrolytes, ion-ion association can become extensive and complex. When the extent of ion association reaches a certain threshold, infinite percolating ionic gel networks can be formed spontaneously. We developed a thermodynamic model of reversible ionic association and gelation in super-concentrated electrolytes accounting for the competition between ion solvation and ion association. Our model is able to predict the populations of ionic clusters of different sizes as a function of salt concentration, as well as capture the onset of ionic gelation. We benchmark our model against molecular dynamics simulations of aqueous LiTFSI electrolyte for a large range of salt concentrations. We find that the ionic association and gelation observed in the molecular simulations are captured nearly quantitatively by our theory. The extent of ionic association and gelation greatly affects both the fraction of “free” ions in solution that can carry ionic current, as well as the viscosity of the mixture. Thus, knowledge of what governs these phenomena is essential in understanding the transport properties of super concentrated electrolytes.

*We acknowledge the Amar G. Bose Research Grant and Imperial College-MIT seed fund grant.

12:15PM S40.00004: Unsupervised learning of ion dynamics in electrolytes using graph dynamical networks*  TIAN XIE (Presenter), ARTHUR FRANCE-LANORD, YANMING WANG, YANG SHAO-HORN, JEFFREY C GROSSMAN, Massachusetts Institute of Technology MIT — Understanding the dynamical processes that govern the performance of functional materials is essential for the design of next generation materials to tackle global energy and environmental challenges. Many of these processes involve the dynamics of individual atoms, ions, or small molecules in condensed phases, which are difficult to understand due to the complexity of local environments. Here we present graph dynamical networks [1], an unsupervised learning approach for atomic scale dynamics in arbitrary phases and environments from molecular dynamics simulations. We apply the methodology to ion dynamics in polymer electrolytes, and show how important features related to ion-ion correlations can be automatically captured. With the large amounts of molecular dynamics data generated every day in nearly every aspect of materials design, this approach provides a broadly applicable, automated tool to understand atomic scale dynamics in material systems.


*This project is supported by the Toyota Research Instutue (TRI), and used computational ressources of Google Cloud, NERSC, and XSEDE.
**12:27PM S40.00005: Ion clustering in electrolytes: impact on correlated transport and voltage stability**  
ERIC FADEL (Presenter), Materials Science And Engineering, Massachusetts Institute of Technology MIT, NICOLA MOLINARI, School of Engineering and Applied Sciences, Harvard University, ARTHUR FRANCE-LANORD, Materials Science And Engineering, Massachusetts Institute of Technology MIT, BORIS KOZINSKY, School of Engineering and Applied Sciences, Harvard University, JEFFREY C GROSSMAN, Materials Science And Engineering, Massachusetts Institute of Technology MIT — The study of ionic transport is an important tool for the optimization of the performance of Lithium ion batteries. The diffusion of Lithium ions across the electrolyte system often exhibits complex correlated motion, which remain relatively poorly understood. Building on previous studies showing the existence of cluster motion in different electrolytes (solid polymers, ionic salts ...) we study the fundamentals of the clustering behavior, to provide insights into cluster formation. In particular, we develop algorithms to describe conditions for clustering to appear, the nature and composition of these clusters, the distribution in size, composition and diffusion coefficient of clusters during transport. We also investigate the lifetime of cluster and relate it to the transport properties of the electrolyte, particularly with regard to the recently reported negative transference number in a variety of systems. This study is also linked back to our work on the voltage stability of organic electrolytes, that shows how the stability of anions in these systems is weakened by the presence of the solvent, and increased by the presence of cations. Therefore, clustering behavior would impact not only the diffusion properties but also the voltage window of the electrolyte.

**12:39PM S40.00006: Molecular Dynamics Simulations of FcMIM-based Ionic Liquids**  
QING GUO (Presenter), Michigan Technological Univ, KAHCHUN LAU, California State University, Northridge, RAVINDRA PANDEY, Michigan Technological Univ — Room temperature ionic liquids (RTILs) are salts in liquid state below 100 °C, and have attracted great attention as electrolytes candidates in battery systems due to properties such as low vapor pressure, high ionic-conductivity, and large operation temperature window, etc. In this talk, we will present the results of Molecular Dynamics simulations identifying the structural characteristics of the ferrocene-imidazolium-based ionic liquids and their aqueous solutions. We will also provide atomistic view of the system to facilitate fundamental understanding at molecular level which is critical for improvement in the electrolyte properties for battery systems.

*Financial support from Alfred P Sloan Foundation is acknowledged.*
Adaptive dimensionality reduction for accelerated calculations of ionic conductivity in correlated electrolytes

NICOLA MOLINARI, YU XIE, IAN LEIFER (Presenter), BORIS KOZINSKY, Harvard University — Molecular dynamics (MD) computation of the ionic conductivity of correlated electrolytes does not allow for the use of the familiar mean square displacement, instead requiring to collect statistics on the total ionic flux fluctuations, which leads to the need of much longer trajectories to obtain converged results. We propose a way to systematically reduce the noise in the conductivity and diffusivity calculations from MD in regimes of moderate correlation (Haven ration 0.5-2). For systems with a time-independent correlation structure, we use spectral decomposition of the short-time position covariance matrix to learn the optimal set of diffusion eigenmodes and perform the analysis of the full MD trajectory in that basis. The proposed method allows to significantly decrease the uncertainty of conductivity estimates.

Asymmetric composition of ionic cluster and correlated transference number in water-in-salt electrolytes

ZHOU YU (Presenter), LEI CHENG, Argonne Natl Lab — The recent research breakthrough on “water-in-salt” electrolytes opens up exciting new avenues for expanding the electrochemical window of aqueous electrolytes. Subsequent work from the electrolyte community found the solvation environment of ions in the “water-in-salt” systems dictates ion mobility. In this work, the crosslinked heterogeneous ion and water domains were captured by molecular dynamics (MD) simulations and small-angle X-ray scattering techniques. The asymmetric composition of ionic clusters composed of more TFSI\(^-\) ion than Li\(^+\) ion was first observed in the water-in-salt electrolyte. The decay of the Li-TFSI association correlation function is faster than that of the residence correlation function for the large percolated ionic clusters with asymmetric composition, which implies that the Li\(^+\) ion can hop through the TFSI\(^-\) ions in the ionic cluster. Furthermore, a reasonably high correlated transference number (i.e., ~0.32) can be maintained even in 20 m electrolytes due to a weak negative correlation between the motion of cations and anions featuring heterogeneous ionic regions.

*This research was supported by the Joint Center for Energy Storage Research (JCESR), a U. S. Department of Energy, Energy Innovation Hub.
1:15PM S40.00009: Ion-ion correlations from aggregation and the Nernst-Einstein equation*

ARTHUR FRANCE-LANORD (Presenter), JEFFREY C GROSSMAN, Massachusetts Institute of Technology

MIT — We present a new approximation [1] to ionic conductivity well suited to dynamical atomic-scale simulations, based on the Nernst-Einstein equation. Ionic aggregates constitute the elementary charge carriers, and are considered as non-interacting species. This approach conveniently captures a dominant effect of ion-ion correlations on conductivity, namely short range interactions in the form of clustering. In addition to providing better estimates to the conductivity at a lower computational cost than exact approaches, this new method allows to understand the physical mechanisms driving ion conduction in concentrated electrolytes. As an example, we consider Li⁺ conduction in poly(ethylene oxide), a standard solid-state polymer electrolyte. Using our newly developed approach, we are able to reproduce recent experimental results reporting negative cation transference numbers at high salt concentrations, and to confirm that this effect can be caused by a large population of negatively charged clusters involving cations.


*This project is supported by the Toyota Research Institute (TRI), and used computational ressources of NERSC.

1:27PM S40.00010: Transport anomalies in electrolytes emerging from strong ionic correlation

NICOLA MOLINARI (Presenter), Harvard University, JONATHAN PRADANA MAILOA, Robert Bosch LLC, BORIS KOZINSKY, Harvard University — Electrolytes control battery recharge time and efficiency, anode/cathode stability, and ultimately safety, consequently electrolyte optimization is crucial for the design of modern energy storage device. Electrolytes containing ionic liquids (ILs) possess superior chemical stability, however, poor transport properties are hindering their applicability. These systems possess high degrees of ion-ion correlation, therefore posing a non-trivial yet crucial and interesting challenge to understanding their transport properties.

Here we present molecular dynamics analysis of transport properties in IL-based electrolytes. First, we show that intra- and inter-species correlation can lead to anomalously low and even negative Li transference numbers. Second, we computationally quantify the recently measured negative Li transference number in IL-based electrolytes, and extend this surprising result to a vast range of different chemistries, suggesting a universal behavior of this class of electrolytes. Additionally, we show that lithium-containing clusters carry a negative charge. Third, we leverage our microscopic understanding to suggest and test modifications to increase the cation transference number.
1:39PM S40.00011: Exploring the ion solvation environments in solid-state polymer electrolytes at different concentrations through free-energy sampling.  
SIDDHARTH SUNDARARARAMAN (Presenter), DAVID PRENDERGAST, Lawrence Berkeley National Laboratory — A major obstacle to improving the performance of Li ion solid state polymer electrolyte batteries is that the exact mechanism of ion conduction in such systems is not well understood. A deeper understanding of solvation from atomistic simulations would prove to be a great stride towards overcoming this challenge. Unfortunately, systematic differences were observed in local forces predicted by various classical force fields in literature and ab-initio results for the system of interest (PEO/LiTFSI). Hence, parameters in the GAFF potential were modified to predict various structural features like bond length, angles and dihedrals in closer agreement with ab-initio estimates, resulting in significant improvements in the local interactions between atoms. These accurate classical force fields were then applied to the study of ion solvation cages and transport in these electrolytes at different ion concentrations. Accelerated molecular dynamics and free-energy sampling techniques were employed to explore the distribution of solvation cages within these electrolytes, their variation with concentration and hopping between them as a possible mechanism of transport. These insights will go a long way towards understanding the mechanism of ion solvation and conduction.

1:51PM S40.00012: Ion Correlation and Collective Dynamics in Organic Electrolytes and Ionic Liquid Mixtures: From Dilute Solutions to the Ionic Liquid Limit  
CHANG YUN SON (Presenter), Chemistry, Pohang University of Science and Technology, JESSE G. MCDANIEL, Chemistry, Georgia Tech — Quantifying ion association and collective dynamical processes in electrolytes is essential for fundamental property interpretation and optimization for electrochemical applications. The extent of ion correlation depends on both the ion concentration and dielectric strength of the solvent; ions may be largely uncorrelated in sufficiently high-dielectric solvents at low concentration, but properties of concentrated electrolytes are dictated by correlated and collective ion processes. In this work, we utilize molecular dynamics simulations to characterize ion association and collective ion dynamics in electrolytes composed of binary mixtures of BMIM$^+$BF$_4^-$ and various organic solvents, water, and LiTFSI salt. We illustrate different physical regimes of characteristically distinct ion correlations for the systematic range of electrolyte concentrations and solvent dielectric strengths. Electronic polarization and solvent dielectric controls the extent of ion pairng and clustering, changing the dominant ion correlation mechanism characterized by quantifying the fractional self and distinct contributions to the net ionic conductivity. The analysis also shed light on understanding the negative transference number observed in ionic liquid mixtures and concentrated polymer electrolytes.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S41 GMAG DMP DCOMP: Emergent magnetism in correlated electron systems II  
707 - Bruce Gaulin, McMaster University
11:15AM S41.00001: Scanned-probe study of spin pumping from Y$_3$Fe$_5$O$_{12}$ into two-dimensional materials using ferromagnetic resonance force microscopy  GUANZHONG WU (Presenter), DONGYING WANG, Department of Physics, The Ohio State University, RYAN MUZZIO, Department of Physics, Carnegie Mellon University, YANG CHENG, GUIXIN CAO, Department of Physics, The Ohio State University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, CHUN NING LAU, FENGYUAN YANG, Department of Physics, The Ohio State University, SIMRANJEET SINGH, JYOTI KATOCH, Department of Physics, Carnegie Mellon University, MARC BOCKRATH, P CHRIS HAMMEL, Department of Physics, The Ohio State University — Driving a ferromagnet to resonance will generate spin current normal to the interface with an adjacent normal metal due to spin pumping. Spin angular momentum dissipation in normal metal will lead to increasing damping in the ferromagnet. This phenomenon is less understood in the case of the ferromagnet/two-dimensional materials interface. Graphene, the best-known two-dimensional material, has a spin diffusion length of order of 1um, making it a poor spin sink. However, there are reports of detectable spin pumping from Y$_3$Fe$_5$O$_{12}$ (YIG) into CVD grown graphene that is attributed to large Rashba-Edelstein effect at the YIG/Graphene interface. Here we report a study of spin pumping in YIG/graphene heterostructures using local, force detected ferromagnetic resonance (FMR). This technique can detect FMR in an area of a few microns and, therefore, enables study of exfoliated two-dimensional materials, which have better crystal quality than CVD grown materials. We discuss spin pumping in pristine graphene as well as graphene/transition metal dichalcogenide bilayers studied using scanned ferromagnetic resonance force microscopy. We will also discuss the surprising discovery of a magnetic uniaxial anisotropy induced in a thin YIG film by the transition metal dichalcogenide overlayer.

11:27AM S41.00002: Localized gap states in oxides and their anti-doping*  OLEKSANDR MALYI (Presenter), ALEX ZUNGER, University of Colorado, Boulder — In standard unreactive doping, adding charge carrier to a compound results in a shift of the Fermi level towards the conduction band for electron doping and towards the valence band for hole doping. We point out a curious case of anti-doping where p-type (n-type) doping results in band gap opening, moving the previously occupied (unoccupied) bands to the principal conduction (valence) band and reducing conductivity. We find that this is a generic behavior for a class of materials and find inverse-design principles for detecting such materials. For instance, early transition metal oxides where the sum of composition-weighed formal oxidation states is positive (e.g., TiO$_{2-x}$, CeO$_{2-x}$, Ba$_2$Ti$_6$O$_{13}$ and Ba$_4$Ti$_{12}$O$_{27}$) tend to form in the band gap an intermediate trapped electron band localized on reduced cation orbitals. Upon p-type doping of such materials, hole annihilates a trapped electron on just one cation; consequently, electronically equivalent cation sublattices in the undoped compound become electronically distinct after doping, i.e., symmetry breaking. We give specific theoretical predictions for target compounds where hole and electron anti-doping might be observed experimentally for the first time.

*This work is supported by NSF-DMR-EPM.
11:39AM S41.00003: Charge disorder induced magnetic order  JINNING HOU (Presenter), Tsung-Dao Lee Institute, YUTING TAN, Natl High Magnetic Field Lab, WEI KU, Tsung-Dao Lee Institute — We propose a scenario of inducing magnetic order via charge disorder in systems with coexisting local moment and itinerant degrees of freedom. By disrupting quantum magnetic fluctuation originated by the itinerant carriers, the long-range magnetic order of the local moment can emerge. We demonstrate this mechanism using realistic spin-model for the undoped FeSe as an example and demonstrate the appearance of anti-ferromagnetic order with enough disruption. This mechanism provides a possible resolution to the observation in many strongly correlated materials, for example the ruthenates [1] in which clean non-magnetic samples turns magnetic with introduction of small number of impurities during synthesis.


11:51AM S41.00004: Magnetic avalanches induced by magnetic sweep rate in a cluster glass  SHALINEE CHIKARA (Presenter), CMS, National High Magnetic Field Laboratory, GIA-WEI CHERN, Department of Physics, University of Virginia, NEIL HARRISON, JOHN SINGLETON, NHMFL, Los Alamos National Laboratory, LEONARDO CIVALE, Quantum Material Group, Los Alamos National Laboratory, JOHN MITCHELL, Materials Science Division, Argonne National Laboratory, VIVIEN ZAPF, NHMFL, Los Alamos National Laboratory — We study magnetic avalanches in La$_{1-x}$Sr$_x$CoO$_3$ and show that we can induce these avalanches for certain magnetic field sweep rates. La$_{1-x}$Sr$_x$CoO$_3$ with 0.1 ≤ x ≤ 0.15 are magnetic cluster glasses consisting of magnetic Co clusters seeded by Sr dopant atoms, surrounded by non-magnetic Co ions. For certain ranges of magnetic field sweep rates, large and random steps are observed in the magnetization, consistent with near-system-size magnetic avalanches. Beyond this range, magnetic field sweep rates produce smooth curves of magnetization vs magnetic field. We develop a model effectively showing that the magnetic interactions between the clusters are controlled by the magnetic field sweep rate.
**12:03PM S41.00005: The Role of Charge Doping in High Entropy Perovskite Oxides**

ALESSANDRO MAZZA (Presenter), YOGESH SHARMA, ELIZABETH SKOROPATA, WENRUI ZHANG, Materials Science and Technology Division, Oak Ridge National Lab, THOMAS HEITMANN, University of Missouri Research Reactor, TIMOTHY R CHARLTON, Neutron Sciences Division, Oak Ridge National Lab, JOHN WILLIAM FREELAND, Argonne National Lab, THOMAS ZAC WARD, Materials Science and Technology Division, Oak Ridge National Lab — Disorder is an important aspect of correlated quantum systems. As examples, it can be used to manipulate superconductivity, magnetic ordering, and enable scaling of non-fermi liquid responses. While synthesis of new quantum materials is generally focused on creating perfect crystals comprised of only a few elemental building blocks, we will present our recent efforts to create high quality single crystals with a high degree of configurational elemental disorder on sublattice sites. Complex crystal structures comprising two or more sublattices, such as those in the perovskite family, are particularly promising. This is due to the nearest neighbor cations on one configurationally disordered sublattice being tied together by an intermediate common and uniform anion sublattice. We will present our recent stabilization of single crystal epitaxial films of the ABO$_3$ perovskite, La(Cr$_{0.2}$Mn$_{0.2}$Fe$_{0.2}$Co$_{0.2}$Ni$_{0.2}$)O$_3$. Hole doping the A site with Sr is shown to give access to unexpected functional responses, as demonstrated by transport, magnetometry, x-ray spectroscopy, and neutron studies.

*This work was supported by the DOE Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

**12:15PM S41.00006: Classification of materials with phonon angular momentum and microscopic origin of angular momentum**

SINISA COH (Presenter), University of California, Riverside — We group materials into five symmetry classes and determine in which of these classes will phonons generically carry angular momentum. In some classes of materials, phonons acquire angular momentum via the forces induced by relative displacements of atoms out of their equilibrium positions. However, for other materials, such as ferromagnetic iron, phonon angular momentum arises from the forces induced by relative velocities of atoms. These latter effects are driven by the spin-orbit interaction.

*This work was supported by grant NSF DMR-1848074.
12:27PM S41.00007: The Role of Oxygen Vacancies in the Magnetic and Electronic Structure of La$_{0.7}$Sr$_{0.3}$MnO$_3$ * ZACHARY ROMESTAN (Presenter), Department of Physics and Astronomy, West Virginia University, A. C. GARCIA-CASTRO, School of Physics, Universidad Industrial de Santander, XU HE, Physique Théorique des Matériaux, Université de Liège, MIKEL HOLCOMB, ALDO H ROMERO, Department of Physics and Astronomy, West Virginia University — Perovskite manganites host a variety of phenomena such as (anti)ferromagnetism, charge and orbital order, metal-insulator transitions, and colossal magnetoresistance that are highly sensitive to charge carrier density and crystal structure. As with cation substitution, oxygen vacancies can provide control over these parameters through electronic doping and steric effects. In our investigation, we consider the role of oxygen vacancies on the magnetic, electronic, and structural properties of La$_{0.7}$Sr$_{0.3}$MnO$_3$-$\delta$ within the DFT+U formalism. In order to isolate the effects of the vacancies, we utilize the Virtual Crystal Approximation to treat the La/Sr content. We report the cases when $\delta = 0.125$, 0.25, and 0.5. For each system, we consider all symmetry inequivalent vacancy sites. We optimize each structure to determine the energetically favorable vacancy sites and magnetic ordering. For the low energy structures, we determine the vacancy formation energy, electronic structure, magnetic structure, magnetic exchange coupling parameters, and conductivity. From the results, we correlate the calculated properties with the effects of the vacancies on the orbital character.

* Bridges and Stampede XSEDE-NSF supercomputers and DMREF-NSF 1434897, NSF OAC-1740111 and DOE DE-SC0016176 projects.

12:39PM S41.00008: Insulating antiferromagnetism in VTe DAVID PARKER (Presenter), LIURUKARA D SANJEEWA, XIAOPING WANG, VALENTINO COOPER, YAOHUA LIU, ATHENA S. SEFAT, Oak Ridge National Lab — We report a comprehensive theoretical and experimental study on the vanadium monotelluride VTe, which crystallizes in the NiAs hexagonal structure. First principles calculations reveal a complex hierarchy of magnetic interactions and energy scales, with the ground state theoretically determined as an \((1/2,0,1)\) antiferromagnetic ordering with insulating character and a band gap of 0.5 eV. These interactions vary significantly from a nearest-neighbor or extended Heisenberg-like model, suggesting a similarity to the parent state of the iron-based superconductors and the possibility of superconductivity if appropriately doped. Experimental synthesis and characterization efforts find a substantially off-stoichiometric orthorhombic structure (a defect NiAs structure) with composition V$_{0.85}$Te, and an apparent Neel point of some 45 K. Our first principles calculations find the stoichiometric phase VTe to have a negative Vanadium defect formation energy, thus explaining the formation of the off-stoichiometric phase.
12:51PM S41.00009: On-chip terahertz characterization of the antiferromagnet CaFe$_2$O$_4$*

DANIEL HELIGMAN (Presenter), RACHEL RESNICK, Ohio State Univ - Columbus, LUNYONG ZHANG, Laboratory for Pohang Emergent Materials and Max Plank POSTECH Center for Complex Phase Materials, Pohang University of Science and Technology, Pohang 790-784, Korea, JAE WOOK KIM, Physics and Astronomy, Rutgers University, SANG-WOOK CHEONG, Rutgers University, Physics and Astronomy, and Laboratory for Pohang Emergent Materials and Max Plank POSTECH Center for Complex Phase Materials, Pohang University of Science, ROLANDO VALDES AGUILAR, Ohio State Univ - Columbus — We report on the magnetic excitations of the antiferromagnet CaFe$_2$O$_4$ as measured with time-domain terahertz spectroscopy via an on-chip device. This material has been previously measured with a free-space terahertz apparatus, showing a magnon excitation at ~725 GHz below the material's Neel temperature of 200 K. We have observed a possible first-order phase transition between 60 K and 120 K, indicating the coexistence of two different magnetic phases. For this experiment the material was measured with a device that generates a terahertz pulse confined to a transmission line. We report on the results of this experiment.

*Funding for this research was provided by the Center for Emergent Materials: an NSF MRSEC under award number DMR-1420451

1:03PM S41.00010: Ferrimagnetism in High Entropy Transition Metal Spinel Oxides*

GRAHAM JOHNSTONE (Presenter), ALANNAH HALLAS, University of British Columbia — High entropy oxides (HEOs) have a crystal structure comprised of chemically ordered oxygen anions and an equimolar proportion of five metal cations randomly distributed over their sublattice. The imposition of large disorder allows configurational entropy to overcome the enthalpy of formation and stabilize a new high entropy phase. HEOs have potential applications ranging from ferroic multifunctionality to reversible energy storage. Studies of the magnetic properties of HEOs to date have been limited to (MgCoNiCuZn)$_{0.2}$O, which has a rock-salt structure. This material undergoes a long-range antiferromagnetic ordering transition at $T_N$=113K despite intense disorder and a 40% magnetic dilution. Here, we present the discovery of three 3$d$-transition metal based ferrimagnetic spinel type HEOs. The high entropy phase is confirmed by Rietveld refinement of powder x-ray diffraction data and elemental microprobe analysis. Magnetic susceptibility measurements of these HEOs suggest that all three transition into ferrimagnetic ordered states between $T$=300K and 400K, followed by a spin reorientation around 100K. In this talk we will present a robust characterization of their magnetic and electronic ground states via heat capacity and resistivity measurements.

*SBQMI
**1:15PM S41.00011: Giant Electric Field Modulation of Magnetism in Ferrimagnetic Heusler Heterostructures**  QILONG SUN (Presenter), SOHEE KWON, NICHOLAS KIOUSSIS, California State University, Northridge — The demand for high efficient magnetoelectric random access memory (MeRAM) requires the search of novel materials and magnetic tunnel junction stacks with voltage-controlled magnetic anisotropy (VCMA) efficiency greater than the 1000 fJ/(Vm) challenge. In this talk, we will present predictions of *ab initio* electronic structure calculations of the VCMA of Ir/Mn$_3$Ga/MgO heterostructures, in which the ultrathin ferrimagnetic Mn$_3$Ga has the tetragonal DO$_{22}$ structure. We find that the Mn$_{\text{II}}$-Mn$_{\text{II}}$ (Mn$_{\text{I}}$-Ga-) terminated interfaces exhibit large out-of-plane (in-plane) magnetic anisotropy (MA). More importantly, the calculations reveal colossal PMA and VCMA efficiency of about one order of magnitude higher than the values reported today. We demonstrate that both the MA and VCMA depend critically on the heavy metal thickness. We also predict a sign reversal of the VCMA efficiency from the Mn$_{\text{II}}$-Mn$_{\text{II}}$ to the Mn$_{\text{I}}$-Ga-terminated interface. Our results show that the dominant contribution to both the PMA and VCMA arises from the strong spin-orbit-coupling of Ir and the E-field induced shift of the Ir $d$-derived orbitals. These findings provide useful guiding rules in the design of more energy-efficient ferrimagnetic-based MeRAM devices.

**1:27PM S41.00012: Hybrid Purification and Sampling Approach for Thermal Quantum Systems**  JING CHEN (Presenter), MILES STOUDENMIRE, Simons Foundation — We propose an algorithm combining two methods for studying finite-temperature quantum systems with tensor networks. One approach is the ancilla method, which gives high-precision results but scales poorly at low temperatures. The other is the minimally entangled typical thermal state (METTS) sampling algorithm which scales better than the ancilla method at low temperatures and can be parallelized, but requires many samples to converge. Our proposed hybrid of these two purifies physical sites in a small central spatial region with partner ancilla sites, sampling the remaining sites by the METTS. Observables measured within the purified cluster have much lower sample variance than in the METTS approach, while sampling the sites outside the cluster reduces their entanglement and the computational cost of the algorithm. The sampling steps of the algorithm remain straightforwardly parallelizable. The hybrid approach also solves an important technical issue with METTS that makes it difficult to benefit from quantum number conservation. By studying $S=1$ Heisenberg ladder systems, we find the hybrid method converges more quickly than both the ancilla and METTS algorithms at intermediate temperatures and for systems with higher entanglement.

*The project is supported by Simons Foundation.*
Fermi surface investigation of intermetallic La$_2$Pt$_3$Ge$_5$*  

ELIZABETH GREEN (Presenter), National High Magnetic Field Laboratory, JOHANNES KLOTZ, KATHRIN GOETZE, HLD (HZDR) / TU Dresden, TOBIAS FOERSTER, MARC UHLARZ, HLD (HZDR), ALIX MCCOLLAM, HFML-Nijmegen, JENNIFER NEU, THEO SIEGRIST, National High Magnetic Field Laboratory, TINO GOTTSCHALL, HLD (HZDR), JOACHIM WOSNITZA, HLD (HZDR) / TU Dresden, KEFENG WANG, CEDOMIR PETROVIC, Brookhaven National Laboratory — Rare-earth intermetallic compounds, specifically those in the R$_2$T$_3$X$_5$ family (where R is rare-earth, T is transition metal, and X is p-block element), have garnered interest due to their novel electronic and magnetic properties. Though they have been a topic of research for decades, detailed Fermi surface studies have been lacking. To fill this void, we performed de Haas-van Alphen effect measurements on La$_2$Pt$_3$Ge$_5$, which was reported to have the highest critical temperature in the R$_2$T$_3$X$_5$ family, $T_c \sim 8.1$ K [1], though the presence of superconductivity is a topic of debate [2]. Our results from a high-quality sample evidence several small pockets in the Fermi surface. Electronic band structure calculations and the implications of our results will be discussed.


*A portion of this work was performed at the NHMFL, which is supported by NSF Coop. Agreement No. DMR-1644779 and the State of FL. We acknowledge the support of HLD at HZDR and HFML, members of EMFL. Work at BNL is supported by the U.S. DOE under Contract No. DE-SC0012704. JN and TS acknowledge support from the NSF under grant NSF/DMR-1606952.*

High-field resonant torsion magnetometry as a probe of magnetic phases in honeycomb lattice Na$_2$IrO$_3$*  

CHRISTOPHER POCS (Presenter), IAN LEAHY, PETER SIEGFRIED, GANG CAO, Physics, University of Colorado, Boulder, ARKADY SHEKHTER, DC Facility, National High Magnetic Field Laboratory, ROSS MCDONALD, NHMFL-PFF, Los Alamos National Laboratory, MINHYEA LEE, Physics, University of Colorado, Boulder — We probe magnetoanisotropy of the quasi-2d honeycomb antiferromagnet Na$_2$IrO$_3$ via resonant torsion magnetometry in pulsed fields up to 65T. In recent years, this material has received much experimental and theoretical attention as a candidate for realizing Kitaev spin-liquid physics. At low temperatures, Na$_2$IrO$_3$ has a robust zigzag AFM ground state and unambiguous signatures of any field-induced transition out of this state have remained elusive so far. Our analysis of the magnetoanisotropy reveals unusual field and angular dependence at high field and a possible signature of a field-driven transition to a quantum disordered state, providing strong evidence for a potential quantum spin liquid phase at high field. We will discuss how resonant torsion magnetometry can extract detailed thermodynamic information and show how it is used to map the entire magnetic free energy in real space from data at only a handful of low symmetry angles. These results are compared to the case of related Heisenberg Kitaev material RuCl$_3$.

*A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by the National Science Foundation Cooperative Agreement No. DMR-1644779*, the State of Florida and the United States Department of Energy.
2:03PM S41.00015: Quasi-2D magnon identification in antiferromagnetic FePS$_3$ via magneto-Raman spectroscopy  
JEFFREY SIMPSON (Presenter), Towson Univ, AMBER MCCREARY, THUC MAI, ROBERT MCMICHAEL, JASON E DOUGLAS, NICHOLAS BUTCH, CINDI DENNIS, ANGELA HIGHT WALKER, NIST, ROLANDO VALDES AGUILAR, Ohio State Univ — The recent discovery that van der Waals-bonded magnetic materials retain long range magnetic ordering down to a single layer stimulates a thorough magneto-Raman study of one such material, FePS$_3$, a large spin ($S = 2$) Mott insulator where the Fe atoms form a honeycomb lattice. Bulk FePS$_3$ was shown to be a quasi-2D Ising antiferromagnet, with additional features in the Raman spectra emerging below the Neel temperature ($T_N \approx 120$ K). Using temperature and magnetic field dependent Raman spectroscopy as an optical probe of magnetic structure, we demonstrate that one of these Raman-active modes below $T_N$ is a magnon with a frequency of $\approx 3.7$ THz (122 cm$^{-1}$). Contrary to previous work, which interpreted this feature as a phonon, our Raman data shows the expected frequency shifting and splitting of the magnon as a function of temperature and magnetic field, respectively, were we find the $g$-factor $= 2$. In addition, the symmetry behavior of the magnon is studied by polarization-dependent Raman spectroscopy and explained using the magnetic point group of FePS$_3$. Temperature dependence of the Raman-active phonons will also be discussed.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S42 GMAG: Spin-Orbit Torques  
Thursday, March 5, 2020 11:15 AM - 2:03 PM

11:15AM S42.00001: Partitioning the spin-orbit torque in heavy metal/ferromagnet heterostructures*  
FEI XUE (Presenter), University of Maryland & National Institute of Standards and Technology, PAUL HANEY, National Institute of Standards and Technology — In heterostructures composed of heavy metals and ferromagnets, the spin-orbit torque is the result of reduced symmetry and the presence of spin-orbit coupling. In order to optimize the spin-orbit torque efficiency, we provide a general scheme to identify the contributions to the intrinsic spin-orbit torque due to the wave-function change induced by an external electric field in the steady state. Using a toy model of a bilayer system with atomic p-orbitals, we find both spin current from spin Hall effect and Berry curvature-like pseudo-magnetic field contribute to the torque. We next apply our analysis to first-principles calculation of spin-orbit torque in multilayer Pt/Co and 1T'-WTe2/Co systems. The additional in-plane symmetry breaking in 1T'-WTe2 allows for an unconventional out-of-plane torque. We find that the atomic orbital current can be transferred to spin current at the interface heavy metal layer, which is the dominant spin current contribution to the torque. The contributions identified by our partitioning scheme in the ferromagnet/heavy metal heterostructure could shed light on how to improve the spin-orbit torque switch efficiency.

*F.X. acknowledges support under the Cooperative Research Agreement between the UMD and the NIST PML, Award 70NANB14H209, through the UMD.
11:27AM S42.00002: Bulk versus Interface Contributions to the Spin-Orbit Torque in Ferromagnetic Heterostructures*  FARZAD MAHFOUZI (Presenter), NICHOLAS KIOUSSIS, California State University, Northridge — We present an ab initio-based theoretical framework which elucidates the origin of the bulk versus interface contributions to the spin-orbit torque (SOT) in Heavy-Metal(HM)/Ferromagnet(FM) heterostructures. We find that (i) the Field-Like (FL) SOT is dominated by the interface component and (ii) both components contribute to the Damping-Like (DL) SOT on equal footing. We demonstrate that the FL-SOT can be expressed in terms of the non-equilibrium spin-resolved orbital moment accumulation. The calculations reveal that the experimentally reported oxygen-induced sign-reversal of the FL-SOT in Pt/Co bilayers is due to the significant reduction of the majority-spin orbital moment accumulation on the interfacial HM atoms.

*The work is supported by NSF ERC-Translational Applications of Nanoscale Multiferroic Systems (TANMS)- Grant No. 1160504.

11:39AM S42.00003: Spin-orbit torque generated by amorphous Fe\textsubscript{x}Si\textsubscript{1-x}  CHENG-HSIANG HSU (Presenter), Electrical Engineering and Computer Science, University of California, Berkeley, JULIE E KAREL, Materials Science and Engineering, Monash University, NIKLAS ROSCHEWSKY, DINAH SIMONE BOUMA, Physics, University of California, Berkeley, SCOTT BENNETT, ALEXANDER NGUYEN, Materials Science and Engineering, Monash University, SURAJ S CHEEMA, Materials Science and Engineering, University of California, Berkeley, SHEHRIN SAYED, Electrical Engineering and Computer Science, University of California, Berkeley, FRANCES HELLMAN, Physics, University of California, Berkeley, SAYEEF SALAHUDDIN, Electrical Engineering and Computer Science, University of California, Berkeley — Despite the tremendous amount of work that has gone into spin-orbit torque and spin current generation in heavy metals, questions on the origin of the underlying physics still remain, often stemming from the challenge in differentiating between spin currents that are generated from the bandstructure of the heavy metal, and other sources, such as inversion symmetry breaking at the interface and or scattering. Here we report observation of spin-orbit torque under room temperature in fully amorphous non-magnetic Fe(x)Si(1-x)/cobalt bilayer via spin-torque ferromagnetic resonance and harmonic Hall measurements. Both techniques provide a consistent spin Hall angle of about 3%. According to the conventional theory of the spin Hall effect, a spin current in an amorphous material is not expected to have any contribution from the bandstructure. Despite this fact, our observation of a reasonably strong spin-orbit torque paves a new avenue for understanding the underlying physics of spin-orbit interaction.
11:51AM S42.00004: Transverse and parallel spin-torque ferromagnetic resonance for improved measurements of spin-orbit torques  SABA KARIMEDDINY (Presenter), JOSEPH MITTELSTAEDT, ROBERT BUHRMAN, DANIEL RALPH, Cornell University — We present a method to quantify the contribution of the spin-pumping/inverse-spin-Hall-effect (SP-ISHE) voltage to spin-torque ferromagnetic resonance (ST-FMR) measurements of spin-orbit torques. In this approach the resonant homodyne voltages transverse to and parallel to the applied microwave current are measured simultaneously. We leverage the fact that spin-pumping only contributes as a symmetric Lorentzian to derive consistency conditions which allow the SP-ISHE to be separated from the rectification signals associated with the spin-orbit torque. The method does not require knowledge of parameters such as the effective spin mixing conductance and spin diffusion lengths of heavy metals. Our findings show that for some material combinations SP-ISHE can alter the ST-FMR signal significantly, and the relative sign of rectification and SP-ISHE is unambiguously determined.

12:03PM S42.00005: Interfacial contributions to spin-orbit torque and magnetoresistance in ferromagnet/heavy-metal bilayers*  KIRILL BELASHCHENKO (Presenter), ALEXEY KOVALEV, Department of Physics and Astronomy, University of Nebraska - Lincoln, MARK VAN SCHILFGAARDE, Department of Physics, King's College London — The thickness dependence of spin-orbit torque and magnetoresistance in ferromagnet/heavy-metal bilayers is studied [1] using the first-principles non-equilibrium Green’s function formalism combined with the Anderson disorder model. A systematic expansion in orthogonal vector spherical harmonics is used for the angular dependence of the torque. The damping-like torque in Co/Pt and Co/Au bilayers can be described as a sum of the spin-Hall contribution, which increases with thickness in agreement with the spin-diffusion model, and a comparable interfacial contribution. The magnetoconductance in the plane perpendicular to the current in Co/Pt bilayers is of the order of a conductance quantum per interfacial atom, exceeding the prediction of the spin-Hall model by more than an order of magnitude. This suggests that the "spin-Hall magnetoresistance," similarly to the damping-like torque, has a large interfacial contribution unrelated to the spin-Hall effect.

*This work was supported by NSF through DMR-1609776 (K.B.) and Nebraska MRSEC DMR-1420645 (K.B. and A.K.), DOE grant DE-SC0014189 (A.K.), and EPSRC CCP9 Flagship Project EP/M011631/1 (M.v.S.).
**Field-free spin-orbit torque switching of Cr-induced perpendicular magnetization**  

TSAO-CHI CHUANG (Presenter), Department of Physics, National Taiwan University, CHI-FENG PAI, Department of Materials Science and Engineering, National Taiwan University, SSU YEN HUANG, Department of Physics, National Taiwan University — Current-induced spin-orbit torque (SOT) switching in a heterostructure with perpendicular magnetic anisotropy (PMA) has attracted great attention, as a new writing method for spintronic devices. However, this highly attractive switching scheme is often accompanied by an unfavorable external magnetic field. In this work, we show that the 3d Cr, without any heavy metals and the MgO layer, can induce strong interfacial PMA and deliver deterministic SOT switching. Most importantly, we demonstrate field-free SOT switching in 3d Cr without any complex schemes, including asymmetrical layers, pattern structure, and additional ferromagnetic or antiferromagnetic layers. We show that the underlying cause for the deterministic field-free switching lies in the slanted columnar microstructure for the otherwise uniform thin films. The direction of oblique columnar structure dictates the up and down orientations of the PMA layer, resulting in polarity-controlled field-free SOT switching [1]. Our results uncover the significant role of 3d materials and shed light on field-free SOT magnetization switching.
Current-induced spin-orbit torques have attracted a considerable amount of attention in recent years. The typical structure for studying the spin-orbit torque is a ferromagnetic metal/ nonmagnetic material bilayer. Most research has focused on the spin-orbit torque generated externally by the nonmagnetic material, overlooking the possibility that the ferromagnetic metal can generate spin-orbit torque on itself. We recently discovered that a ferromagnetic metal can in fact generate equal and opposite spin-orbit torques at its surfaces, which is termed as the anomalous spin-orbit torque, due to its analogy to the anomalous spin Hall effect. The strong anomalous spin-orbit torque may challenge our current understanding of spin-orbit torque in bilayer/multilayer systems. It also provides new opportunities that ferromagnet itself can be a source of spin-orbit torques.

Spin-orbit driven spin depolarization in the ferromagnetic Weyl semimetal Co$_3$Sn$_2$S$_2$* SANDEEP HOWLADER (Presenter), Department of Physical Sciences, IISER Mohali, SURABHI SAHA, Department of Physics, Indian Institute of Science, RITESH KUMAR, Department of Physical Sciences, IISER Mohali, VIPIN NAGPAL, SATYABRATA PATNAIK, School of Physical Sciences, Jawaharlal Nehru University, TANMOY DAS, Department of Physics, Indian Institute of Science, GOUTAM SHEET, Department of Physical Sciences, IISER Mohali — Co$_3$Sn$_2$S$_2$ has recently emerged as a ferromagnetic Weyl semimetal. Previous experiments and theoretical investigations of the band structure have provided an indication of the possibility of half-metallicity in this compound. However, our spectroscopic investigations have shown that a spin-polarized super-current flows through a Nb/Co$_3$Sn$_2$S$_2$ point contact with a large Andreev reflection indicating a huge deviation from half-metallic character. In fact, we have observed a 50% spin polarization at the Fermi level. Theoretical calculation of the electronic density of states with inclusion of spin-orbit coupling showed that this deviation stems from a spin depolarizing effect near the Fermi energy. Additionally, the calculations revealed a particle-hole asymmetry that explains our experimental observation of asymmetric Andreev reflection spectra.

*SERB EMR/2016/003998

Spin Orbit Torque in Graphene/Co Heterosystem KENAN SONG (Presenter), AURELIEN MANCHON, UDO SCHWINGENSCHLOGL, King Abdullah Univ of Sci & Tech (KAUST) — The spin-orbit torque (SOT) technique has opened new horizons for the development of innovative magnetic devices beyond memories and data storage. When graphene is attached to the surface of Co (001), the inversion symmetry is broken, which results in the onset of a built-in perpendicular electric field. As a result, in the presence of the large spin-orbit coupling of Co, Rashba effect emerges at the interface. Therefore, a spin density driven by a net current can be achieved at the interface, bringing SOT into such a heterostructure. With density functional theory, we show that Co atoms at the interface exhibit spin-momentum locking, which is in line with the experiments. Around the Fermi level, the graphene Dirac cones couple with the Co 3d states around the K and K' points, resulting in a spin texture odd in momentum k. This special spin texture promotes current-driven SOT. We then project the band structure obtained by first principles onto Wannier orbitals to get the tight-binding Hamiltonian. Non-equilibrium properties then are calculated using the Kubo formula. Our results show that the SOT can be used to electrically control the magnetization of the Co layer and to realize fast electronic device.
1:27PM S42.00010: Time-evolution of spin-orbit torque and magnetization in Rashba ferromagnet from multiscale time-dependent-quantum-transport/classical-micromagnetics formalism UTKARSH BAJPAI (Presenter), BRANISLAV NIKOLIC, Univ of Delaware — Spin-orbit torque originates in a ferromagnetic material when the nonequilibrium electronic spin density emerging due to spin-orbit coupling is noncollinear to the local magnetization. In this work, we investigate the time-evolution of spin-orbit torque in a Rashba ferromagnet using a recently developed quantum-classical hybrid framework where quantum electrons described by time-dependent nonequilibrium Green functions (TDNEGF) are self consistently coupled to local magnetization dynamics described by classical-micromagnetics using the Landau-Lifshitz-Gilbert (LLG) equation. It has been previously shown that such a self-consistent TDNEGF+LLG framework microscopically generates a spatially inhomogeneous and time-dependent dynamical Gilbert damping [1] through a memory kernel, contrary to conventional micromagnetics where a static Gilbert damping parameter is introduced phenomenologically. Here, we explore the influence of Rashba spin-orbit coupling on the resulting time-dependent spin-orbit torque, magnetization dynamics and dynamical Gilbert damping parameter in our TDNEGF+LLG framework which is further compared to the Gilbert damping parameter and magnetization dynamics evaluated using the scattering matrix theory.


1:39PM S42.00011: Theoretical study of spin torque and domain wall motion on ferromagnetic Kagome lattice SEHOON KIM (Presenter), KENTARO NOMURA, Institute for Materials Research, Tohoku University — We theoretically study spin torque and domain wall motion induced electrically in a ferromagnetic Kagome lattice, which has spin-orbit coupling. For details, we suppose the exchange interaction with an inhomogeneous magnetic texture of uniaxial magnetic anisotropy and the spin-dependent second-nearest neighbor hopping acting as the spin-orbit coupling. Because of the chiral edge conduction, electric charges are accumulated around the domain wall. We calculate the spin polarization of localized charges as a response of the electric field by the Kubo formula. As a result, the spins of localized charges are polarized and exert spin torque on the domain wall. Firstly, we discuss the spin torque and domain wall motion in two-dimensional limits of the ferromagnetic Kagome lattice. [1] Second, we extend the 2D model to thin films of Kagome-lattice shandite, [2] which are more realistic. All of the two models cause non-adiabatic spin-transfer torque on the domain wall reducing the intrinsic threshold current. These results and discussions suggest a good comparison between ideal models and realistic models in terms of spin torques in topological materials.

Current-induced unidirectional magnetoresistance in FeRh/Pt bilayers

JULIE SHIM (Presenter), Physics, University of Illinois at Urbana-Champaign, HILAL SAGLAM, Materials Science Division, Argonne National Laboratory, KISUNG KANG, Materials Science and Engineering, University of Illinois at Urbana-Champaign, JUNSEOK OH, Physics, University of Illinois at Urbana-Champaign, YI LI, Materials Science Division, Argonne National Laboratory, WEI ZHANG, Physics, Oakland University, MATTHEW GILBERT, Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, ANDRE SCHLEIFE, AXEL HOFFMANN, Materials Science and Engineering, University of Illinois at Urbana-Champaign, JOSEPH SKLENAR, Physics and Astronomy, Wayne State University, NADYA MASON, Physics, University of Illinois at Urbana-Champaign — Antiferromagnetic (AFM) spin-orbit torque oscillators are important due to potential applications ranging from magnetic random-access memory to THz emitters. However, AFM spin-torque oscillators operate in the THz-range, and direct observation of THz magnetization dynamics is difficult. Previously, in ferromagnetic spin-torque oscillators, current-induced unidirectional magnetoresistance (UMR) signals accompanied the emission of microwave radiation at the ferromagnetic resonance frequency [1,2], which implies that observations of UMR may provide indirect evidence of AFM-resonance. Here we present transport results on magnetron sputtered AFM FeRh/Pt films, fabricated into nanowire geometries. A current-induced UMR is observed, in addition to anisotropic magnetoresistance effects. These findings suggest a route toward designing AFM spin-orbit torque oscillators.


*This work was undertaken as part of the Illinois Materials Research Science and Engineering Center, supported by the National Science Foundation MRSEC program under NSF award number DMR-1720633. Sample growth was supported by the Department of Energy, Office of Science, Materials Science and Engineering Division.

Thursday, March 5, 2020 11:15 AM - 1:51 PM

Session S43 DCOMP DMP: Computational Design and Discovery of Novel Materials IV: 2D and Layered Materials - Kai-Ming Ho, Iowa State University - Tag(s): Focus
11:15AM S43.00001: Computational Discovery at the Interface of Chemistry and Materials: 1D Carbon Nanothreads and 2D Polar Metals* [Invited] VINCENT CRESPI (Presenter), YUANXI WANG, BO CHEN, TAO WANG, NADIRE NAYIR, BOYANG ZHENG, ADRI C.T. VAN DUIN, Pennsylvania State University, ROALD HOFFMANN, Cornell — The total number of equilibrium crystal structures composed from subsets of the periodic table is likely bounded fairly strictly by phase separation of multi-component mixtures. In contrast, the design space afforded by metastable structures is essentially unbounded: the key challenge here is to craft kinetic constraints that access structures with compelling properties. One strategy to this end deploys the immense design power of synthetic organic chemistry within a solid-state context to produce carbon nanothreads of diverse compositions and properties as ordered lattices comprising uniquely one-dimensional sp³ or mixed sp²/sp³ macromolecules at the ultimate juncture between crystalline rigidity and molecular control. These systems exhibit unique behaviors as the thinnest possible objects whose rigidity is maintained by covalent bonds. In two dimensions, kinetic control in service of unique structure can also be obtained by crafting similarly unique synthesis "containers", for example the gallery between silicon carbide and epitaxial graphene, which can host a broad family of epitaxial, air-stable, crystalline two-dimensional polar metals with record-breaking optical nonlinearities, excellent surface-enhanced Raman performance, and intriguing prospects for the integration of metals into quantum heterostructures. In both cases, predictive computational theory can provide strong guiding principles.

*This work was supported by the National Science Foundation, under the Centers for Chemical Innovation (CHE-1832471), Materials Research Science and Engineering Center (DMR-1420620), and Materials Innovation Platform (DMR-1539916) programs.

11:51AM S43.00002: Robust Half-Metallicity and Perfect Spin Filtering in 2D oxide layer* ARQUM HASHMI (Presenter), Center for Computational Sciences, University of Tsukuba, Japan, KENTA NAKANISHI, Graduate School of Pure and Applied Sciences, University of Tsukuba, Japan, MUHAMMAD UMAR FAROOQ, Department of Physics, Southern University of Science and Technology, Shenzhen, China, TOMOYA ONO, Department of Electrical and Electronic Engineering, Kobe University, Japan — We use first-principles calculations to demonstrate the transition metal oxide monolayer (ML) of Cr₂O₃ as an ideal candidate for next-generation spintronics applications. Cr₂O₃ ML has a honeycomb-kagome lattice that possesses the kagome band characteristics, where the Dirac and strongly correlated fermions coexist around the Fermi level. Furthermore, the classical Heisenberg Hamiltonian shows strong FM interactions between Cr spins, and the Cr³⁺ ions are in a low-spin state leading to a spin S = 3/2. Cr₂O₃ ML possesses a robust half-metallic behavior with a large spin gap of ~ 3.9 eV and a high T_c = 190 K. We also find that Cr₂O₃ ML displays an intrinsic Ising ferromagnetism with a giant PMAE of ~ 0.9 meV. More importantly, NEGF calculations reveal that the Cr₂O₃ ML exhibits an excellent spin filtering effect.

*This research was partially supported by MEXT as a social and scientific priority issue (Creation of new functional devices and high-performance materials to support next generation industries) to be tackled by using post-K computer, JSPS KAKENHI Grant No. 19K15381, and JSPS Core-to-Core program (Controlled Interfacing of 2D materials for Integrated Device Technology).
**12:03PM S43.00003: Giant polarization charge density at ScN/GaN interfaces**

NICHOLAS ADAMSKI (Presenter), Department of Electrical and Computer Engineering, University of California, Santa Barbara, CYRUS DREYER, Department of Physics and Astronomy, Stony Brook University, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara —

GaN is a wurtzite semiconductor that exhibits a large spontaneous polarization, while ScN is a semiconducting nitride that takes the nonpolar rocksalt crystal structure. Due to small lattice mismatch between ScN and GaN, it is possible to create a polar-nonpolar interface between the two materials.

Using density functional theory and the Berry-phase method, we examine the formal polarization of rocksalt ScN along the [111] direction, finding a polarization discontinuity of -1.358 Cm$^{-2}$. We confirm this finding with explicit ScN/GaN supercell calculations. The polarization discontinuity causes a high-density electron gas to form on the N-polar GaN/ScN interface, and a hole gas to form on the Ga-polar interface, with carrier concentrations up to $8.5 \times 10^{14}$ cm$^{-2}$. The large polarization difference and low lattice mismatch make ScN a promising material for integration with III-nitride electronic and optoelectronic devices.

*This work is supported by AFOSR.

**12:15PM S43.00004: Quasi-Binary Transition Metal Dichalcogenide Alloys: Thermodynamic Stability Prediction, Scalable Synthesis and Application**

ZAHRA HEMMAT, The University of Illinois at Chicago, JOHN CAVIN (Presenter), Washington University, St. Louis, ALIREZA AHMADIPARIDARI, ALEXANDER RUCKEL, The University of Illinois at Chicago, SUNG BEOM CHO, Korea Institute of Ceramic Engineering and Technology, ROBERT KLIE, The University of Illinois at Chicago, ROHAN MISHRA, Washington University, St. Louis, AMIN SALEHI-KHOJIN, The University of Illinois at Chicago —

Quasibinary alloying in transition metal dichalcogenides (TMDCs) has been successfully used to improve applications including optoelectronics and catalysis. However, the vast compositional space of possible TMDC alloys remains largely unexplored. To guide the synthesis of such alloys, we present ab-initio calculations of equilibrium phase diagrams for 25 TMDC alloys: $M_{1-x}M'_{x}X_{2}$ and $MX_{2(1-x)}X'_{2x}$ ($M,M' = V, Nb, Ta, Mo, W; X,X' = S, Se$). We verify the predictions made by these phase diagrams by synthesizing a subset of 12 alloys using scalable chemical vapor transport. We demonstrate the ability to exfoliate these alloys into few-layers. One of these alloys, Nb$_{1-x}$Ta$_{x}$S$_{2}$, is shown to have outstanding thermal stability, exceptional CO$_{2}$ reduction activity with near zero overpotential, and excellent energy efficiency in a Li-air battery. Our work highlights the large number of TMDC alloys accessible to a scalable synthesis-process. By expanding beyond group VI TMDC alloys, this study lays the groundwork for studying how alloying in group V TMDCs affects novel properties such as superconductivity, magnetism, and topological properties.

*Acknowledgments: This work was funded by NSF DMREF-1729787.
12:27PM S43.00005: First-principles prediction of optomechanically controlling phase transition of IV-VI semiconductors  
JIAN ZHOU (Presenter), Xi’an Jiaotong Univ — Diffusional phase-change materials, such as Ge-Sb-Te alloys, are used in rewritable nonvolatile memory devices (PC-RAM). This order-disorder transition contains a large latent heat and requires breaking of chemical bonds. It is thus highly desired to develop new phase change materials with diffusionless and order-to-order transitions to accelerate the read/write kinetics, reduce energy dissipation, and eliminate fatigue. Two-dimensional materials are considered as potential phase change materials. For example, one famous 2D material example is transition metal dichalcogenide monolayer which exists in 2H and 1T' structures. However, it always requires mechanical, electrical, or electrochemical contacts and patterning to trigger phase transition. Non-contacting optical readout/write with focused laser would be preferable in many circumstances, especially for low-dimensional materials which are easily optically accessible. Here, we computationally illustrate an optomechanical strategy, which uses a linearly polarized laser pulse with selected frequency. We will give a few examples of such ultrafast diffusionless martensitic phase transition in various materials. With no or only a few chemical bonds breaking, the phase transition would occur very fast and requires low energy input.

12:39PM S43.00006: Predicting synthesizable multi-functional edge reconstructions in two-dimensional transition metal dichalcogenides*  
GUOXIANG HU (Presenter), ANH PHAM, VICTOR FUNG, XIAHAN SANG, RAYMOND UNOCIC, PANCHAPAKESAN GANESH, Center for Nanophase Materials and Sciences, Oak Ridge National Laboratory — Two dimensional transition metal dichalcogenides have attracted great interest due to their exceptional properties, especially at the edges. Recently, more complex edge reconstructions were discovered experimentally. This poses intriguing questions: what is the whole family of synthesizable reconstructed edges and what are they good for? Here, we develop a high-throughput *ab initio* based computational approach to shed light on this. Using MoS$_2$ as a model, we screened hundreds of edge configurations, leading to predictions of new reconstructions with record thermodynamic stability in addition to the discovered ones. We find that the reconstructed edges can be optimized as catalysts for a wide range of reactions and suited for applications in information storage, spintronics, and topologically protected dissipationless transport from their exhibited wide distribution of work function, half-metallicity, magnetic variations, and intriguing topologically protected edge-states.$^{1,2}$ *Our work reveals the existence of a wide family of synthesizable, reconstructed edges, thereby opening a new field of intrinsic edge engineering of 2D materials as multifunctional materials.*  
1. JMCA, 2019, 7, 18357.  

*This work was supported by the ORNL-LDRD program and CNMS at ORNL.*
Hybrid assemblies of two-dimensional octagonal monolayers of C and BN*  

PRASHANT VIJAY GAIKWAD (Presenter), ANJALI KSHIRSAGAR, Univ of Pune — In the dominating regime of hexagonal family, 2D octagonal monolayers (o-MLs) have emerged recently. High coordination cluster assembly route [J. Phys.: Condens. Matter 29, 335501 (2017)] is employed to form o-MLs of C and BN and their hybrid assemblies. The o-MLs are dynamically and thermally stable. Most of the MLs reveal charge transfer among atoms and asymmetric sp$^2$ hybridization. Hybrid assemblies can be tuned from metallic to insulating (4.13 eV). Stacking of zigzag buckled o-MLs forms stable body centered tetragonal bulk phase of C and BN. Dynamically stable nanotubes (NT), obtained by cutting chunk, with diameter 3.6 Å and 3.57 Å for o-C and o-BN respectively, can also be realized as vertically stacked o-rings and can be contrasted with the rolling of hexagonal ML. We thus report a CNT with a size smaller than the reported theoretical limit and synthesized experimentally till now.

Present work has established octagonal ring as a basic unit to form 1D, 2D and 3D materials of groups IV, III-V and II-VI. Studies of their properties, possible constraints, mechanism for stabilization, bonding and hybridization are fascinating and can unlock unusual facts for many applications.

*DST Nanomission Council, Government of India (DST/NM/NS- 15/2011(G))

Theoretical studies on excitonic and half-metallic properties in 2D chalcogenides  

XIAOLONG ZOU (Presenter), NANNAN LUO, SHUQING ZHANG, Tsinghua University — In this talk, I will present theoretical investigation on two classes of chalcogenides with interesting properties, i.e., the saddle-point excitons and half-metallicity. First, monolayer b- and γ-phase group-IV monochalcogenides (MX, M = Ge or Sn; X = S or Se) are shown to possess saddle-point and camel's back like band structure, respectively. While saddle-point exciton in b-MX leads to its strong adsorption, render them promising for solar cell applications with power conversion efficiencies as large as 1.11%,[1] a high-temperature exciton gas to electron-hole liquid transition can be achieved in γ-MX. Second, a class of CoGa$_2$X$_4$ (X= S, Se or Te) monolayer with triangular lattice exhibits intrinsic in-plane half-metallic ferromagnetism. The half-metal gaps are large enough (about 0.5 eV) to make them stable against the spin flip under weak external disturbances. We have systematically investigated the underlying origin of the ferromagnetism and predicted their high transition temperature $T_C$.[2]

Reference:
1:15PM S43.00009: New 2D massless Dirac fermion systems and quantum spin Hall insulators based on sp–sp\(^2\) carbon sheets  MINWOO PARK (Presenter), Physics, Konkuk University, YOUNGKUK KIM, Physics, Sungkyunkwan University, HOONKYUNG LEE, Physics, Konkuk University — Graphene was identified as a quantum spin Hall (QSH) insulator when considering spin-orbit coupling (SOC), which opens a band gap at the Dirac points. This discovery has initiated new research efforts to study the QSH effect on its application for quantum computing and spintronics. Nevertheless, the SOC strength of graphene is too small (~40 µeV) to induce the topological insulator phase in an experimentally achievable temperature regime. Here, we design two-dimensional sp–sp\(^2\) hybrid carbon sheets to discover new Dirac systems, hosting the QSH phase. We find that 21 out of 31 new carbon sheets are identified as Dirac fermion systems without SOC, distinct from graphene in the number, shape, occurring Dirac cones. Furthermore, we find 19 out of the 21 new Dirac fermion systems become QSH insulators with a sizable SOC gap. It is enhanced up to an order of meV, allowing for the QSH effect at experimentally accessible temperatures. Besides, based on the 26 Dirac fermion systems, we find a correlation between the number of Dirac points without SOC and the resultant QSH phase. We hope our findings contribute to new prospects for the design of topological materials with desired properties.

1:27PM S43.00010: A first principle study on the role of Li intercalation in the structural transition from a few-layer black to blue phosphorene*  MD RAJIB KHAN MUSA (Presenter), MING YU, Physics and Astronomy, University of Louisville — A systematic study on the role of Li intercalation played in the structure transition from a few-layer black to blue phosphorene has been carried out from first principle calculations based on the density functional theory. It is found that, depending on Li concentration and configuration intercalated on black phosphorene surface, the structure of the black phosphorous is either maintained its A17 symmetry, transferred to blue phosphorene with A7 symmetry, or distorted to form zigzag chains. Specifically, it was found that within a certain Li configurations intercalated on black phosphorene, Li atoms could play as ‘catalysts’ to drive the specific P atoms moving along specific directions, resulting bond breaking and forming, and subsequently, transforming a few-layer black to a few-layer blue phosphorene. This study opened a new pathway that, at a certain high rate Li intercalation, a feasible transition pathway from black to blue phosphorene. The role of the Li intercalation induced phase transition will be further studied and discussed, which will guide us to identify the specific conditions for such structural transformation.

*Acknowledgement: We acknowledge support from the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award # DE-SC0019348
1:39PM S43.00011: The role of Configurational entropy in real time mass sensing.* Sudeep Adhikari (Presenter), Kevin Stuart David Beach, Univ of Mississippi — We present a theoretical framework for determining the mass deposited on a mechanical resonator subject to a flux of incoming particles of a single species. We consider the specific example of a vibrating nanostring and infer the history of mass deposition events from the frequency shifts in real time using a numerical optimization algorithm that correctly compensates for the configurational entropy. Our approach is tested against simulated data and is shown to perform well. We extend this model for a two particle system and try to comment on its applicability over a multi-particle deposition.

*University of Mississippi Graduate School and Advisor.

S43.00012: A Computational Study of Layered Sulfides for CO2 Reduction Photocatalysts*

Hao Yu (Presenter), Department of Physics, Southern University of Science and Technology, Elizabeth A Peterson, Jeffrey B Neaton, Department of Physics, University of California, Berkeley — The CO2 reduction reaction (CO2RR) is central to artificial photosynthesis, a means of using excess CO2 in atmosphere to generate solar fuels. While advances have been made in improving efficiency and selectivity of known catalysts for CO2RR, new materials are needed to realize scalable platforms for solar fuels generation. The high valence bands seen in low-band gap layered sulfides show promise for meeting the high redox potentials required for CO2RR, and motivate a focused high-throughput search with first-principles density functional theory (DFT). Our calculations, using van der Waals (vdW) dispersion corrections, lead to nearly a dozen photocatalyst candidates, many which are not identified by prior studies. Refining Materials Project crystal structures with vdW corrections, we find excellent agreement with experimental lattice parameters for our candidate photocatalysts. For the identified materials, we perform HSE06 band edge calculations. The alignment of the band edges with CO2RR potentials and implications for experiments on the newly identified layered sulfide compounds are discussed.

*This work is supported by the Department of Energy via the Joint Center for Artificial Photosynthesis and NERSC.
Stabilized Penta-silicene: An Elemental Ferroelectric Material with High Curie Temperature

YAGUANG GUO (Presenter), QIAN WANG, Peking Univ — The compatibility of Si semiconductor technology with current electronic devices has led to continuing search for new Si-based materials with novel properties. The recent synthesis of penta-Si nanoribbons is a new addition to this family. However, penta-silicene, a two dimensional (2D) sheet composed of only Si pentagons, was found to be unstable in penta-graphene-like configuration. Using first-principles calculations and a thorough analysis of its imaginary frequencies, we show that penta-silicene can be made dynamically stable by tilting the Si dimers to reduce the Coulomb repulsion between them. The consequence of this tilting leads to an interesting discovery: the stabilized penta-silicene breaks the centrosymmetry, resulting in intrinsic ferroelectricity with a high Curie temperature of 1190 K. This realizes the spontaneous electrical polarization in a pure 2D Si system, which has the potential to work as a future non-volatile phase change material.

*This work is supported by grants from the National Science Foundation China (No. 21773004 and 11974028), and the National Key Research and Development Program of China (No. 2017YFA0205003). Y. G. acknowledges the Project funded by China Postdoctoral Science Foundation (No. 2019M650289).

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S44 DCOMP DMP: Electrons, Phonons, Electron Phonon Scattering, and Phononics V

704 - Xiulin Ruan, Purdue University - Tag(s): Focus
11:15AM S44.00001: Characterization of Thermal Effects in Wide Bandgap Semiconductor Materials and Devices* [Invited] SAMUEL GRAHAM (Presenter), Georgia Inst of Tech — Wide bandgap electronics made from nitrides (e.g., Gallium Nitride (GaN)) and oxides (e.g., Gallium Oxide (Ga$_2$O$_3$)) are currently under development due to their potential to create some of the most advanced RF and power electronic devices in the world. However, the thermal response of these devices under applied electric fields can create large power densities (RF and power electronics) that must be understood. For many of these devices, the electrothermal response plays a strong role in both the acceptable operation or long-term failure and reliability of the devices. Thus, tools that can help elucidate these responses and provide a method to help design better devices is of critical need for this field.

In this talk we will discuss advancements in thermal characterization techniques that have allowed new insights into electrothermal behavior in GaN and Ga$_2$O$_3$ materials and devices. Specifically, a focus on the role of device architecture and material processing will be addressed. For GaN and Ga$_2$O$_3$ RF and power electronics, the role of thermal interfaces in the heat dissipation of both lateral and vertical device architectures will be discussed. We will cover aspects of semiconductor-semiconductor as well as metal-semiconductor interfaces and their roles in device thermal management. A highlight will be the use of plasma activated bonding to provide ultralow thermal resistance interfaces that allow for heterogenous integration of nitrides and oxides with high thermal conductivity substrates. Finally, we will discuss the implications of these effects on device behavior through experiments and modeling.

*ONR MURI Grant No. N00014-18-1-2429 and AFOSR GAME MURI Program (Grant No. FA9550-18-1-0479)

11:51AM S44.00002: Direct solution to the space-time dependent Peierls-Boltzmann transport equation using an eigendecomposition method CHENGYUN HUA (Presenter), Oak Ridge National Lab — Nonlocal thermal transport is generally described by the Peierls-Boltzmann transport equation (PBE). However, solving the PBE for a general space-time dependent problem remains a challenging task due to the high dimensionality of the integro-differential equation. In this work, we present a direct solution to the space-time dependent PBE with a linearized collision matrix using an eigendecomposition method. Furthermore, we show that there exists a generalized Fourier type relation that links heat flux to the local temperature, and this constitutive relation is valid from ballistic to diffusive regimes. Combining this approach with ab initio calculations of phonon properties, we demonstrate that the derived solution gives a more accurate description of thermal transport in crystals that exhibit weak anharmonicity than the commonly-used single-mode relaxation time approximation and thus will lead to an improved understanding of phonon transport in solids.
12:03PM S44.00003: Calculation of mode Gruneisen parameters made simple  ANGELO BONGIORNO (Presenter), CUNY College of Staten Island — Gruneisen parameters measure the degree of anharmonicity of a material. These parameters can be used to calculate the coefficient of thermal expansion, as well as the thermal conductivity of a material. The existing method to calculate mode Gruneisen parameters relies on the (quasi-)harmonic approximation, and the numerical differentiation of phonon frequencies computed at different volumes (through the use of energy schemes based on either classical force fields or a first principles approach). Here we present a new method to calculate mode Gruneisen parameters. This method involves two steps. First, the calculation of the harmonic frequencies at only the equilibrium volume of a material. Second, for each normal mode, a few self-consistent field calculations are needed to calculate the corresponding mode Gruneisen parameter. In this talk, we discuss the conceptual basis of the new method, its technical implementation and validation, its advantages and disadvantages, and selected applications. In particular, our method in combination with a density functional theory approach is used to calculate mode Gruneisen parameters and the coefficient of thermal expansion of silicon and aluminum.

12:15PM S44.00004: Density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials: the magnetic case  ANDREA URRU (Presenter), ANDREA DAL CORSO, International School for Advanced Studies — We discuss the extension of density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials to magnetic materials [1]. We avoid the computation of the response at -q by using explicitly the time-reversal operator, which is applied to the Sternheimer linear system and to its self-consistent solutions, an approach that has been introduced for the calculation of magnons [2]. We validate our implementation by comparison with the frozen phonon method in fcc Ni and in a monatomic ferromagnetic Pt wire, and present an application to MnBi. We are working to extend the technique to the computation of the phonon dispersions of magnetic polar insulators.

References:

Photothermal imaging as a new tool for the investigation of the temperature-dependent properties of the medium in nanoscale  MARYAM ZAHEDIAN (Presenter), BOGDAN DRAGNEA, Chemistry, Indiana University Bloomington — Photothermal imaging is a powerful technique to detect small light-absorbing nanoparticles down to 1.4 nm with a high spatial resolution (1). The signal magnitude is proportional to the absorption cross-section of the nanoparticle as well as properties of the medium. Finite thermal diffusivity of the medium causes a phase delay in the response of the heat dissipation. The phase delay at each point integrated over the resolution disk is identified as the photothermal signal phase that depends on the material property (2). In this study, first, we demonstrate that the photothermal phase is capable of monitoring the local medium modifications, with high sensitivity. Second, we determine that, with the aid of simulation, information about the temperature-dependent properties of the medium, such as heat conductivity is attainable in nanoscale.


Thermal Transport in Phosphorene  GUANGZHAO QIN (Presenter), Department of Mechanical Engineering, University of South Carolina, ZHENZHEN QIN, Zhengzhou Univ — Phosphorene, a novel elemental 2D semiconductor, possesses fascinating chemical and physical properties which are distinctively different from other 2D materials. The rapidly growing applications of phosphorene in nano/optoelectronics and thermoelectrics call for comprehensive studies of the thermal transport properties. In this talk, based on the theoretical and experimental progresses, the thermal transport properties of single-layer phosphorene, multilayer phosphorene (nanofilms), and bulk black phosphorus are summarized to give a general view of the overall thermal conductivity trend from single-layer to bulk form. The mechanism underlying the discrepancy in the reported thermal conductivity of phosphorene is discussed by reviewing the effect of different functionals and cutoff distances on the thermal transport evaluations. This review then provides fundamental insight into the thermal transport in phosphorene by reviewing the role of resonant bonding in driving giant phonon anharmonicity and long-range interactions. In addition, the extrinsic thermal conductivity of phosphorene is reviewed by discussing the effects of strain and substrate, together with phosphorene based heterostructures and nanoribbons.
**12:51PM S44.00007: Thermoelectric properties of half-Heusler TaFeSb from first-principles electron-phonon scattering calculations**

NATALYA FEDOROVA (Presenter), ANDREA CEPELLOTTI, BORIS KOZINSKY, Harvard University — We investigate thermoelectrics transport properties of half-Heusler TaFeSb within the Boltzmann transport formalism, using first principles calculations of the electronic relaxation times. Our goal is to explore the microscopic origin of exceptionally high ZT values (up to 1.52 at 973 K) recently reported from the experimental measurements of transport properties of TaFeSb-based compounds. In particular, we focus on the effects arising from the electron-phonon interaction. For that we calculate corresponding scattering rates using Wannier-Fourier interpolation of electron-phonon matrix elements as well as the recently developed electron-phonon averaged (EPA) approximation. We discuss the likely mechanisms of high ZT in TaFeSb-based systems and possible ways to further improve thermoelectric properties of half-Heusler compounds.

*This work is supported by Swiss National Science Foundation (grant number P2EZP2_178532)*

**1:03PM S44.00008: Thermal phonons with micron-scale mean free paths in ultra-drawn polyethylene**

TAEYONG KIM (Presenter), Division of Engineering and Applied Science, California Institute of Technology, STAVROS X. DRAKOPOULOS, IGNACIO MARTIN-FABIANI, Department of Materials, Loughborough University, ANDREW ROBBINS, Division of Engineering and Applied Science, California Institute of Technology, SARAH RONCA, Department of Materials, Loughborough University, AUSTIN MINNICH, Division of Engineering and Applied Science, California Institute of Technology — Heat conduction in highly oriented polymers is of fundamental and practical interest. It is well-known that the thermal conductivity of certain polymers such as polyethylene (PE) increases by orders of magnitude with drawing, but the microscopic properties of phonons responsible for heat conduction have remained difficult to access experimentally. Here, we report the observation of thermal phonons with micron-scale mean free paths (MFPs) in ultradrawn polyethylene using transient grating spectroscopy. The MFPs are comparable to those in covalent single crystals such as Si despite the imperfect nature of the sample’s microstructure. Further, the sample exhibits a decrease in thermal conductivity with increasing temperature above 200 K, indicating that anharmonic scattering is dominant over reflections from domains between crystallites. Our work provides new insights into the microscopic origin of high uniaxial thermal conductivity of ultradrawn polymers.

**1:15PM S44.00009: Accelerated Screening of Electron-Phonon Transport in 2D Materials**

JENNIFER COULTER (Presenter), BORIS KOZINSKY, Harvard University — Numerous experimental and theoretical studies have identified promising 2D materials for thermoelectric applications. These materials can exhibit an advantageous combination of electrical and thermal properties, sometimes resulting in large thermoelectric figure-of-merit values. Using an in-house method to perform accelerated screening of transport properties through first-principles electron-phonon calculations, we consider thermoelectric effects in a broader set of 2D materials. From these calculations, we consider how specific electronic and vibrational properties relate to thermoelectric potential, and identify the best candidate materials for use in application. Additionally, we consider the practical importance of substrate effects on the electron-phonon interaction and transport properties of these materials.
1:27PM S44.00010: Simulations of thermoelectric coefficients using DFT bandstructures and energy dependent scattering rates* PATRIZIO GRAZIOSI (Presenter), CHATHURANGI KUMARASINGHE, NEOPHYTOS NEOPHYTOU, School of Engineering, University of Warwick — Performance prediction for thermoelectric (TE) materials requires extracting DFT bandstructures and computation of TE coefficients using Boltzmann transport equation (BTE). The constant relaxation time approximation is commonly employed due to complexities in accurately computing scattering rates.
In this work, we describe the construction of an advanced simulator, which couples generic bandstructures (e.g. from DFT) with BTE, utilizing the full numerical energy/momentum/valley dependences of all states in the extraction of the relaxation times. The method provides more predictive capabilities and accuracy, but also considers all scattering mechanisms (acoustic, non polar optic and polar phonons, ionized impurities) independently, as well as intra- and inter-band transitions.
We show that according to the scattering physics under consideration, the performance ranking between different materials and their doping and temperature dependence varies significantly compared to constant relaxation time consideration.

*This work is funded by the Marie Sklodowska-Curie Actions (Grant agreement No. 788465) and from the European Research Council (ERC) under the European Union's Horizon 2020 Research and Innovation Programme (Grant Agreement No. 678763).

1:39PM S44.00011: Zero-Point renormalization of the band structure within Quasiparticle Self-consistent GW SAVIO LARICCHIA (Presenter), NICOLA BONINI, MARK VAN SCHILFGAARDE, Department of Physics, King's College London — The reliability of Density Functional Theory (DFT) for the electron-phonon coupling in many materials, including even simple sp-bonded compounds, has been questioned in recent years. Hybrid functionals and quasiparticle GW corrections suggest that nonlocal exchange-correlation enhances the electron-phonon interaction as a consequence of an improved description of the electronic screening. This has highlighted the need to move beyond local exchange-correlation functionals within DFT, but complete field-theoretic investigations are still missing in literature. In this talk I will introduce the development of a field-theoretic methodology which is able to predict on an equal footing electronic quasiparticles and phonons as well as their interaction. Such an approach has been implemented within the Quasiparticle Self-consistent GW (QSGW) formalism which describes well the electronic properties for a wide range of materials, including many where standard DFT fails. The reliability of a such field-theoretic methodology will be discussed with applications ranging from the renormalization of the optical gap of nonpolar semiconductors to the renormalization of the Fermi surface of correlated materials such as FeSe.
Quantum coherent coupling between a zone-center phonon and two acoustic phonons was observed in two GaAs/AlAs superlattices (8 nm/8 nm and 5.4 nm/5.4 nm) at ambient temperature. Using degenerate coherent phonon spectroscopy, a multi-cycle oscillation feature appears in the time-resolved phonon amplitudes of both samples, as a result of the coherent energy exchange between a driving phonon mode near first Brillouin zone center and two target acoustic phonon modes. This feature resembles the photon resonant parametric down/up-conversion processes, as well as the reversible coherent energy exchange between the optical field and a mechanical oscillator, suggesting quantum coherent coupling between the driving and target phonon modes. In the 8nm/8nm superlattice, the coupling strength increases nonlinearly at high pump fluences, which may eventually reach an extreme state where all three phonon modes share the same coherent state, as predicted by Orbach in the 1960’s.

*National Science Foundation (NASCENT, Grant No. EEC-1160494; CAREER, Grant No. CBET-1351881, CBET-1707080, Center for Dynamics and Control of Materials DMR-1720595), and the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under award No. DE-SC0013599.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S45 DCOMP GSNP: Computational Methods for Statistical Mechanics: Advances and Applications II
Coupled Molecular Dynamics and Spin Dynamics display very attractive features that allow to get new insights of the intriguing interplay between structure and magnetism in Fe-based alloys. Each atom is treated as a moving particle, eventually charged, supporting a classical spin. Coordinate dependent on both magnetic exchange and magnetic anisotropic functions ensure minimal coupling between the spin and the lattice degrees of freedom to translate the well known magneto-elastic behavior of magnetic materials. These functions need well crafted magnetic and mechanical Hamiltonian parametrized on \textit{ab-initio} calculations to recover the size dependence of the energy barriers and characteristic time scales of the magnetization relaxation of condensed phases. The equations of motion (eoms) come naturally from the Nambu dynamics that formulates covariant Poisson brackets for classical fields that encode the constrained structure of the topological space of spins. To solve these coupled eoms in practical simulations, numerical integration algorithms based on decomposition methods have to be considered, that preserve the structure of the flow of canonical variables in such an extended phase space. Consequences of such schemes will be discussed in details from the point of view of the known invariant quantities. To mimic experimental conditions, various statistical ensembles have to be generated to monitor the physical properties by varying external temperature for instance, as a stochastic connection. One consequence is that the positions, momenta and spins of all the atoms become, in return, varying quantities evolving through stochastic instead of deterministic differential equations of motion. The challenge to compute these quantities in parallel and examples provided by the SPIN package in the open source LAMMPS code are discussed.

*J. Tranchida and coworkers, Sandia National Laboratories, Multiscale Science Department, P.O. Box 5800, MS 1322, Albuquerque, NM 87185
Quantum-accurate multiscale modeling of ramp compressions and magneto-elastic phase transitions in iron* JULIEN TRANCHIDA (Presenter), ATTILA CANGI, MITCHELL WOOD, AIDAN THOMPSON, MICHAEL PAUL DESJARLAIS, Sandia National Laboratories — Magnetic spin fluctuations have a significant impact on the thermodynamic properties of magnetic metals. Accurately predicting magneto-structural phase transitions in compressed iron hence requires accounting for those effects.

We achieved this by constructing a magneto-elastic Hamiltonian. Following the Spectral Neighbor Analysis Potential approach, a machine-learning interatomic potential for iron was trained on ab initio calculations performed on the pressure and temperature range of interest. This potential was combined to a magnetic Hamiltonian accounting for transverse and longitudinal spin fluctuations.

Leveraging the numerical capability combining lattice and magnetic degrees of freedom that was recently implemented in LAMMPS, large scale spin-lattice simulations of ramp compressions and phase transitions in iron are performed based on the developed Hamiltonian.

*Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Absolute entropy calculation from liquid state correlation functions* MICHAEL WIDOM (Presenter), Carnegie Mellon Univ, MICHAEL GAO, National Energy Technology Lab —

Because entropy is a function of thermodynamic state it can be determined without need for thermodynamic integration. Concepts from information theory relate the entropy of a liquid metal to its correlation functions, which can be accurately determined from ab-initio molecular dynamics. This relationship is equivalent to the "S2" method that has previously been applied to model liquids. We demonstrate the accuracy of the approach by calculating the absolute entropy of liquid aluminum entirely from first principles, and demonstrate excellent agreement with experimental data.

*This work was supported by the Department of Energy under grant DE-SC0014506.
12:15PM S45.00004: Absolute free energies from ab-initio calculation: application to phase stability of liquid metal alloys*  YANG HUANG (Presenter), Carnegie Mellon Univ, MICHAEL GAO, National Energy Technology Lab, MICHAEL WIDOM, Carnegie Mellon Univ — Absolute liquid state entropies calculated using the "S2" method can be combined with ab-initio enthalpies to predict absolute Gibbs free energies. We apply this method to model the phase behavior of the liquid alkali metal alloy Li-Na, which is known to phase separate, compared with Na-K, which exhibits a eutectic. Our ab-initio simulations employ hybrid Monte Carlo/molecular dynamics to accelerate sampling of the ensemble and provide accurate pair correlation functions for the entropy calculation. Both alloys exhibit effective unlike-atom repulsion, but the weaker repulsion of Na-K allows an entropically stabilized eutectic, while the stronger repulsion of Li-Na overwhelms the entropy below a high temperature critical point which we approximately locate.

*This work was supported by the Department of Energy under grant DE-SC0014506.

12:27PM S45.00005: Investigation of Fe by means of atomistic spin dynamics coupled with ab initio molecular dynamics simulations  DAVIDE GAMBINIO (Presenter), BJORN ALLING, Linkoping University — Ab initio molecular dynamics (AIMD) is a mature approach for the investigation of nonmagnetic materials. Magnetism in condensed matter, however, introduces a further challenge for the theoretical community. A recently developed method that allows to take advantage of the accuracy of AIMD and couples the magnetic and vibrational degrees of freedom is the atomistic spin dynamics - ab initio molecular dynamics (ASD-AIMD) method [1]. In this approach, the atomic and magnetic dynamics are run in parallel while communicating with each other. The applicability of the method has been shown in the study of CrN, a semiconducting system with well localized magnetic moments. Here, we employ ASD-AIMD simulations to investigate Fe near its Curie temperature. Being Fe a ferromagnetic metal, temperature induces fluctuations not only on the transversal magnetic degrees of freedom, but also on the longitudinal ones, which are often considered irrelevant for a system like bcc Fe. In our simulations we include this type of excitations through a mean-field entropic term, and we compare results in absence of this effect. This work is a pre-step in the calculation of free energy differences in magnetic systems with ab initio accuracy.

Spin dynamics simulations on Surface for a nanoscale Heisenberg antiferromagnet  
ZHUOFEI HOU (Presenter), University of Georgia — Monte Carlo and spin dynamics techniques with fourth-order Suzuki-Trotter decompositions of the exponential operator have been used to perform large-scale simulations of the dynamic behavior of a nanoscale, classical, Heisenberg antiferromagnet on a simple-cubic lattice at a temperature below the Néel temperature 1. A classical isotropic Heisenberg model with an antiferromagnetic nearest-neighbor exchange interaction was studied. A simple-cubic lattice with free boundary conditions was used. The assumption of q-space spin-wave reflections with broken momentum conservation due to free-surface confinements was developed and used to explain multiple excitation peaks for wave vectors within the first Brillouin zone appear in the spin-wave spectra of the transverse component of dynamic structure factor in the nanoscale classical Heisenberg antiferromagnet. In this study, we applied the same simulation techniques to the nanoscale classical Heisenberg antiferromagnet we studied before for studying spin dynamic behavior on the surfaces of a nanoscale antiferromagnet.


Effective diffusion in rough potential energy landscapes*  
THOMAS GRAY (Presenter), Univ of Cambridge — Diffusion in spatially rough, confining, one-dimensional energy landscapes is treated using Zwanzig's proposed formalism, which is based upon the Smoluchowski Equation. Disagreement between its predictions and the results of numerical simulations is observed. We use the configurational partition function to amend Zwanzig's formalism, and resolve the disagreement. The analogous over-damped Langevin Equation is proposed, and a numerical simulation scheme offering potentially significant reductions in computational time is derived. The case of random roughness is treated. We then extend the above into higher dimensions and calculate effective diffusion coefficients for motion in non-confining, rough, multi-dimensional potential energy landscapes. This leads us to propose an expression for the mean first-passage time from one potential minimum to any one of the immediately adjacent potential minima. As before, simulation schemes offering significant improvements upon those derived from the unmodified Langevin Equation are obtained. Good agreement between our theory's predictions and both numerical simulation schemes - unmodified and modified - is observed.

*EPSRC Funding
1:03PM S45.00008: Stefan–Maxwell diffusivities extracted from molecular dynamics simulations via Onsager’s regression hypothesis*  
CHARLES MONROE, MAXIM ZYSKIN (Presenter), University of Oxford — We report on our development of a method to measure macroscopic diffusion coefficients in silico by analysing molecular-dynamics (MD) data. Application of Onsager’s regression hypothesis to the macroscopic constitutive laws for multicomponent Stefan–Maxwell mass transport allows application of Casimir’s fluctuation theory, which shows how the decay rates of certain autocorrelation functions relate to macroscopic mutual diffusivities. The autocorrelation functions are then determined numerically, using periodic MD simulations in the Gibbs ensemble. As an illustrative example, we compute the diffusivities for a ternary Lennard–Jones gas mixture, a case where the diffusivities measured by MD can be compared to diffusivities determined analytically by the Chapman–Enskog kinetic theory. The ultimate application of this method will be to quantify component activities and transport properties in liquids, with the ultimate aim of studying electrochemical transport properties in electrolytic solutions.

*Faraday Institution battery challenge grants FIRG003 and FIRG007

1:15PM S45.00009: Machine Learning the Effective Hamiltonian in High Entropy Alloys with Large DFT Datasets*  
XIANGLIN LIU (Presenter), JIAXIN ZHANG, Oak Ridge National Lab, YANG WANG, CARNEGIE MELLON UNIVERSITY, MARKUS EISENBACH, Oak Ridge National Lab — The development of machine learning sheds new light on the Monte Carlo simulation of complex alloys. One major challenge, however, is that machine learning models are generally data-hungry, while the data from density functional theory (DFT) are computationally expensive. To solve this problem, we use the atomic local energy as the target variable, and harness the power of the linear-scaling DFT method to obtain large DFT data sets. This method is used to calculate the energy data of a range of MoNbTaW refractory high entropy alloys, with machine learning techniques including kernel ridge regression, Gaussian process, and artificial neural network applied to construct the effective Hamiltonian. The results demonstrate that machine learning model built on the configurational space, which naturally incorporates non-linear and multi-site interactions, can efficiently and accurately predict the DFT energy.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division and Laboratory Directed Research and Development funding. This research used resources of the Oak Ridge Leadership Computing Facility, which is supported by the Office of Science of DOE under Contract No. DE-AC05-00OR22725.
1:27PM S45.00010: Quantifying the disassembly of viral capsids from a multiscale molecular simulation approach*
HORACIO ANDRES VARGAS GUZMAN (Presenter), Soft Matter Theory Department, Institute Josef Stefan, CHRISTOPHER COOPER, Department of Mechanical Engineering, Technical University Federico Santa Maria, ADOLFO POMA, Institute of Fundamental Technological Research, Polish Academy of Sciences — Molecular simulation of large biological systems, such as viral capsids, remains a challenging task in soft matter research. On one hand, coarse-grained (CG) models attempt to make feasible the description of the entire viral capsids. On the other hand, novel development of molecular dynamics (MD) simulation approaches, like enhance sampling which attempt to overcome the time scales required in biophysics. Those methods have a potential for delivering molecular structures and properties of biological systems. Nonetheless, exploring the process on how a capsid disassembles by all-atom MD simulations has been rarely attempted. Here, we propose a methodology to analyze the disassembly process of viral capsids quantitatively. In particular, we look at the effect of pH and charge of the genetic material inside the capsid, and compute the free energy of a disassembly trajectory by combining CG simulations to a Poisson-Boltzmann solver. We employ such multiscale approach on the triatoma virus as a test case, and find that even though an alkaline environment enhances the stability of the capsid, the resulting deprotonation of the internal solvent generates an electrostatic repulsion that triggers disassembly.

*This research has been supported by the Slovenian Research Agency P1-0055

1:39PM S45.00011: Exploring the Potential of Parallel-Biasing in Flat Histogram Methods*
SHANGHUI HUANG (Presenter), JONATHAN K. WHITMER, University of Notre Dame — Metadynamics, a member of the "flat histogram" class of advanced sampling algorithms, has been widely used in molecular simulations to drive exploration of states that are separated by high free energy barriers and promote the sampling of full free energy landscapes. A recently proposed variant, parallel bias metadynamics (PBMetaD) promises to aid in exploration of free energy landscape along multiple important collective variables by exchanging the n-dimensional free energy landscape required by standard methods for n one-dimensional marginal free energy landscapes. In this study, we systematically examine how parallel biasing affects convergence of free energy landscapes along each variable relative to standard methods, and the effectiveness of the parallel biasing strategy for addressing common bottlenecks in the use of advanced sampling to calculate free energies.

*NSF DMR-1751988
1:51PM S45.00012: Superfluidity and dimensional cross-over in Quasi-1D systems* PER BOLLMARK (Presenter), ADRIAN KANTIAN, Uppsala Univ — 1D systems cannot attain long-range order (LRO) but have a wide range of other benefits. One method to cure the missing LRO is to construct an infinite array of weakly coupled 1D systems.

We consider a 3D array of one-dimensional repulsive bosons. If the bosons are hard-core they can model the electron-pairs in e.g. a quasi-1D USC such as the Bechgaard and Fabre salts. Static Mean-Field (SMF) combined with Density Matrix Renormalization Group (DMRG) reduces the full 3D model to a self-consistently treated 1D one, enabling calculation of ground and thermal equilibrium states. This approach is motivated by the low cost of such an implementation and further allows the simulation of real-time/frequency dynamics.

This model exhibits a phase transition from a 3D superfluid (SF) to a 1D Mott insulator (MI) that forms the basis of the more complex behavior in the USCs. Interestingly, the order parameters indicating the different phases suggest a mix between first- and second-order transitions.


*This work is supported by the ERC Starting Grant from the European Union's 2020 research and innovation programme under grant agreement No. 758935.
11:15AM S46.00001: Kondo effect in a spinon metal [Invited] ANDREJ ZORKO (Presenter), MATJAZ GOMILSEK, ROK ZITKO, MARTIN KLanjSEK, MATEJ PREGELJ, Jozef Stefan Institute, QINGMING ZHANG, School of Physical Science and Technology, Lanzhou University — The Kondo screening of localized impurities possessing magnetic moments is traditionally associated with exchange scattering of conduction electrons. This nontrivial display of many-body physics is common to ordinary metals and was recently found also in various more complex conducting systems, such as quantum dots, graphene, and topological insulators. Moreover, the Kondo effect was theoretically predicted for certain electric insulators in which emergent fractional magnetic excitations can effectively take over the role of itinerant electrons in screening the impurities’ magnetic moments [1-4].

Indeed, our experimental study of the kagome lattice antiferromagnet Zn-brochantite, ZnCu$_3$(OH)$_6$SO$_4$, with a spin-liquid ground state has finally confirmed these theoretical predictions [5]. Although in this material the charge degrees of freedom are frozen, an effect conceptually identical to the traditional Kondo effect takes place. This is possible because the magnetic spinon excitations of Zn-brochantite behave like quasi-free fermions with a Fermi surface and thus, regarding their interactions with localized impurities, closely resemble itinerant electrons in a metal. The observed Kondo response is, however, to a certain degree modified from the ordinary case, which is attributed to spinon-spinon interactions. The discovered spinon-based Kondo effect thus provides a prominent platform for characterizing enigmatic spin-liquid states through impurities acting as in situ local probes of the host magnetic state.


11:51AM S46.00002: Dynamics of jammed spin liquid on the kagome bilayer SHENG ZHANG (Presenter), PREETHA SAHA, DEPEI ZHANG, SEUNGHUN LEE, GIA-WEI CHERN, Univ of Virginia — The Heisenberg antiferromagnet on the kagome bilayer is one of the canonical frustrated spin systems. It also provides a basic model for the compound SCGO that triggered the interest in highly frustrated magnets. The source of the seemingly glassy behavior observed in SCGO at temperatures below $T_g \approx 3.5 \rightarrow 7$ K remains unclear even after decades of intensive study. In particular, previous works [1], including our own [2], seem to indicate that dilution alone does not engender a spin glass in its classical spin-liquid ground state. Instead, it is suggested that the glassy behavior likely originates from the interplay between disorder and the coplanarity tendency due to quantum fluctuations-[1,3]. In this work, we study the dynamical properties of an effective Hamiltonian that incorporates the collinear/coplanar tendency through a biquadratic spin interaction. We report unusual relaxation dynamics and the dynamical structure factor of the effective model and discuss their experimental implications.
12:03PM S46.00003: Electron-nuclear hyperfine coupling in quantum kagome antiferromagnets from first-principles calculation and a reflection of the defect effect*

SHUNHONG ZHANG (Presenter), ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, YI ZHOU, Institute of Physics, Chinese Academy of Science, FENG LIU, Department of Materials Science and Engineering, University of Utah, ZHENG LIU, Institute for Advanced Study, Tsinghua University — The discovery of ideal spin-1/2 kagome antiferromagnets Herbertsmithite and Zn-doped Barlowite represents a breakthrough in the quest for quantum spin liquids (QSLs), and nuclear magnetic resonance (NMR) spectroscopy plays a prominent role in revealing the quantum paramagnetism in these compounds. However, interpretation of NMR data that is often masked by defects can be controversial. Here, we show that the most significant interaction strength for NMR, i.e. the hyperfine coupling (HFC) strength, can be reasonably reproduced by first-principles calculations for these proposed QSLs. Applying this method to a supercell containing Cu-Zn defects enables us to map out the variation and distribution of HFC at different nuclear sites. This predictive power is expected to bridge the missing link in the analysis of the low-temperature NMR data.

*NSFC (11774196, 11774306) and Tsinghua University Initiative Scientific Research Program. National Postdoctoral Program for Innovative Talents of China (BX201600091) and the Funding from China Postdoctoral Science Foundation (2017M610858) US-DOE (DEFG02-04ER46148). National Key Research and Development Program of China (No. 2016YFA0300202), and the Strategic Priority Research Program of Chinese Academy of Sciences (XDB28000000).

12:15PM S46.00004: Thermal conductivity of the quantum spin liquid candidate herbertsmithite

PATRICK BOURGEOIS-HOPE (Presenter), PIERRE LEFLOÎC, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, Universite de Sherbrooke, PHILIPPE MENDELS, Universite Paris-Sud, MATIAS VELAZQUEZ, Universite de Bordeaux — Hosting a $S = 1/2$ system on a kagome lattice, herbertsmithite (ZnCu$_3$(OH)$_6$Cl$_2$) is a leading candidate in the search for quantum spin liquids. Despite the absence of magnetic ordering down to very low temperature and several probes detecting a significant density of low-energy states, a debate persists on whether this material has gapless spinon excitations. Our thermal conductivity measurements down to 60 mK show no signs of the $T$-linear contribution to heat conduction that is expected from mobile spinons. Instead, our results suggest that the low-energy spin excitations in herbertsmithite are either localized or gapped.
12:27PM S46.00005: Diverse $S=1/2$ distorted kagome Hamiltonians in titanium fluorides
HARALD JESCHKE (Presenter), Okayama University, HIROKI NAKANO, TORU SAKAI, University of Hyogo
— We determine the connection between highly frustrated kagome based Hamiltonians and a recently synthesized family of materials containing Ti$^{3+}$ $S = 1/2$ ions [1]. With the help of a combination of all electron density functional theory and numerical diagonalization techniques, we establish the Heisenberg Hamiltonians for the distorted kagome antiferromagnets Rb$_2$NaTi$_3$F$_{12}$, Cs$_2$NaTi$_3$F$_{12}$, and Cs$_2$KTi$_3$F$_{12}$. We determine magnetization curves in excellent agreement with experimental observations. Our calculations successfully clarify the relationship between the experimental observations and the magnetization-plateau behavior at 1/3 height of the saturation and predict characteristic behaviors under fields that are higher than the experimentally measured region. We demonstrate that the studied Ti(III) family of materials interpolates between the kagome strip and kagome lattice. Further members of this family of materials are also considered.


12:39PM S46.00006: The origin of trimerized phase in $S=1$ kagome magnet Na$_2$Ti$_3$Cl$_8$*
ARPITA PAUL (Presenter), University of Minnesota, CHIA-MIN CHUNG, Ludwig-Maximilians-Universitat Munchen, HITESH CHANGLANI, Florida State University, TURAN BIROL, University of Minnesota — The kagome magnet Na$_2$Ti$_3$Cl$_8$ with $S=1$ spins undergoes a structural transition involving trimerization or breathing distortion of the underlying kagome lattice as the temperature lowers. We investigate the magnetic ground state of this compound by constructing a model spin Hamiltonian based on first-principles density functional theory and analyzing it using exact diagonalization and density matrix renormalization group methods. Along with the nearest neighbor Heisenberg and biquadratic exchanges, we propose a new exchange term fourth order in spins - ring exchange that does not originate from spin-orbit coupling and involves simultaneous hopping of electrons from one site to its two neighboring sites. The parameters that our first principles calculations give for the high temperature crystal structure place this compound to the ferroquadrapolar region of the phase diagram predicted by exact diagonalization and density matrix renormalization group calculations. We thus suggest that a spin - lattice coupling favors the trimerized phase over the quadrapolar phase, even though density functional theory alone does not predict a lattice instability.

*NSF DMREF Grant No. DMR-1629260 and Minnesota Supercomputing Institute
12:51PM S46.00007: Dynamical properties of site-diluted Heisenberg antiferromagnetic on the kagome bilayer  PREETHA SAHA (Presenter), DEPEI ZHANG, SEUNG-HUN LEE, GIA-WEI CHERN, Univ of Virginia — We present spin dynamical simulations of the site-diluted Heisenberg antiferromagnet with nearest neighbor interactions on a quasi-2D kagome bilayer. This geometrically frustrated lattice consists of two kagome layers connected by a triangular-lattice layer. We combine Monte Carlo method with precessional spin dynamics simulations to compute the dynamical structure factor of the classical spin liquid and study the thermal and dilution effects. The low frequency and long wavelength dynamics of the classical spin liquid in kagome bilayer is dominated by spin diffusion [1]. In the presence of spin vacancies, the dynamical properties of the diluted system can be understood within the two population picture [2,3]. The spin diffusion of the “correlated” spin clusters gives rise to an exponentially decaying autocorrelation function. On the other hand, the diffusive dynamics of the quasi-free “orphan” spins leads to a distinctive long time power-law tail in the autocorrelation function. We discuss the implications of our work for the glassy behaviors observed in the frustrated magnet SrCr$_{9p}$Ga$_{12-9p}$O$_{19}$ (SCGO).


1:03PM S46.00008: Search for simplex solid and spin liquid phases in highly frustrated S=1 antiferromagnets* [Invited] HITESH CHANGLANI (Presenter), Physics, Florida State University — Quantum spin liquids are enigmatic phases of matter characterized by the absence of symmetry breaking and conventional quasiparticles. The search for their realisation in actual magnetic materials has targeted, but is not limited to, materials involving the geometrically frustrated triangular, kagome and pyrochlore geometries with low spins. Indeed, while there have been significant efforts to synthesize quantum spin liquid materials in spin-1/2 systems in two dimensions, fewer efforts have been devoted to three dimensions and higher spins. In this talk, we show that both these criteria may be too restrictive. We thus expand our search to spin-1 frustrated antiferromagnets which are abundant in nature but where few theories or results exist to understand their general properties and behavior. Motivated by recent realizations of S=1 kagome and pyrochlore geometries, we address the question of their quantum many-body ground state. For kagome, a spin liquid state known as the Hexagonal Singlet State, motivated by the Affleck Kennedy Lieb Tasaki state in one dimension, is found to be competitive in energy. However, for the pure Heisenberg model it loses out to a symmetry broken trimerized (simplex solid) ground state, a conclusion we derive from density matrix renormalization group calculations. We show that this finding is relevant to the recently synthesized S=1 kagome material Na$_2$Ti$_3$Cl$_8$ which shows a large trimerized distortion in its low temperature phase. For the S=1 pyrochlore case, our search bears fruit - we find a nearly idealized Heisenberg model in NaCaNi$_2$F$_7$. Our results show strong evidence for a quantum spin liquid phase based on both its static and dynamical properties.

*Supported by Florida State University and the National High Magnetic Field Laboratory. The National High Magnetic Field Laboratory is supported by the National Science Foundation through NSF/DMR-1644779 and the state of Florida.
1:39PM S46.00009: Magnetoresistance Study of Kagome Artificial Spin Ice with Fibonacci Distortions*  JUSTIN WOODS (Presenter), BARRY W FARMER, Univ of Kentucky, YONG-LEI WANG, Nanjing University, WAI-KWONG KWOK, Material Sciences, Argonne National Laboratory, LANCE ERIC DE LONG, Univ of Kentucky — Nanofabrication techniques allow magnetic thin films to be lithographically patterned into arrays of interacting macro-spins designed to exhibit emergent physical properties. We study the effects of continuous symmetry breaking on the magnetoresistive behavior of frustrated Kagome (alt. honeycomb) ASI whose periodic lattice is aperiodically distorted by repeated application of a substitution algorithm: A Fibonacci sequence of binary digits is mapped into short (d1) and long (d2) primitive lattice translations, which alters the magnetic moments and angular coordination of the three-fold Kagome vertices. Kagome arrays with variable distortions are patterned in series to permit simultaneous longitudinal and transverse magnetoresistances measurements in external magnetic fields. The direction and magnitude of applied field was varied to produce distinct, interesting differences in the magnetoresistance response of the distorted Kagome arrays, compared to the undistorted arrays.

*Research supported by the University of Kentucky's DOE Grant DE-SC0016519. Research at Argonne National Laboratory was conducted in the Division of Materials Research and the Argonne Center for Nanoscale Materials with the support of U.S. DOE Office of Basic Energy Sciences Contract No. DE-AC02-06CH11357.

S46.00010: Tuning the Two-step Melting of Magnetic Order in Dipolar Kagome Ice by Quantum Fluctuations  YAO WANG (Presenter), STEPHAN HUMENIUK, YUAN WAN, Institute of Physics, Chinese Academy of Sciences — Complex magnetic orders in frustrated magnets may exhibit rich melting processes when the magnet is heated toward the paramagnetic phase. In this talk, we show that one may tune such melting processes by quantum fluctuations. We consider a kagome lattice dipolar Ising model subject to transverse field and focus on the thermal transitions out of its magnetic ground state, which features a root 3 by root 3 magnetic unit cell. Our quantum Monte Carlo (QMC) simulation suggests that, at weak transverse field, the root 3 by root 3 order melts by way of an intermediate, magnetically charge ordered phase where the lattice translation symmetry is restored whilst the time reversal symmetry remains broken[1]. By contrast, at moderate transverse field, QMC simulation suggests the root 3 by root 3 order melts through a floating Kosterlitz-Thouless (KT) phase. The two distinct melting processes are likely separated by a multicritical point identified in Ref.[2].

References:

Non-coplanar magnetic order and topological magnons in tripod kagome antiferromagnet $\text{Yb}_3\text{Mg}_2\text{Sb}_3\text{O}_{14}$*  
ZHILING DUN (Presenter), Georgia Inst of Tech, OWEN BENTON, Riken center for Emergent Matter Science, XIAOJIAN BAI, Georgia Inst of Tech, NICHOLAS BUTCH, NIST center for neutron research, HAIDONG ZHOU, University of Tennessee, MARTIN MOURIGAL, Georgia Inst of Tech — Kagome antiferromagnet is one of the most studied models for geometrical frustration which is expected to be a topological magnon insulator in the presence of Dzyaloshinskii–Moriya interactions. The recent discovered tripod kagome materials provide us a platform to explore such ideas with strongly spin-orbit coupled rare earth ions. Using elastic neutron scattering measurements, we show that one of the tripod kagome compounds, $\text{Yb}_3\text{Mg}_2\text{Sb}_3\text{O}_{14}$, orders into a strongly non-coplanar magnetic ground state below 0.88 K which calls for large antisymmetric exchanges. Inelastic neutron scattering experiment on polycrystalline samples reveals both dispersive and flat magnon bands which can be fitted by an anisotropic exchange Hamiltonian derived from a symmetry analysis. Along with numerical calculations, our results unveil $\text{Yb}_3\text{Mg}_2\text{Sb}_3\text{O}_{14}$ as a candidate to host topological non-trivial magnon bands.

*The work at Georgia Tech was sponsored by the Department of Energy under DE-SC-0018660.

**Thursday, March 5, 2020 11:15 AM - 1:39 PM**

**Session S47 GMAG DMP FIAP DCOMP: Spin Phenomena in Topological Insulators 710/712 - Cuneyt Sahin, Univ of Iowa - Tag(s): Focus**
Topological Insulator/Magnetic Insulating Oxide: A Platform for Efficient Spin Current Transport* [Invited]

PENG LI (Presenter), Auburn University, STEVEN S-L ZHANG, Case Western Reserve University, LAUREN RIDDIFORD, Stanford University, TIMOTHY PILLSBURY, Penn State University, JINJUN DING, Colorado State University, JAMES KALLY, Penn State University, ALEXANDER GRUTTER, National Institute of Standards and Technology, GAURAB RIMAL, University of Wyoming, CHONG BI, Stanford University, GYORGY CSABA, Pazmany Peter Catholic University, J SAMUEL JIANG, JUNJIA DING, Argonne National Laboratory, WEI ZHANG, Oakland University, JINKE TANG, University of Wyoming, WEIGANG WANG, University of Arizona, OLLE HEINONEN, VALENTYN NOVOSAD, Argonne National Laboratory, AXEL HOFFMANN, University of Illinois at Urbana-Champaign, NITIN SAMARTH, Penn State University, YURI SUZUKI, Stanford University, MINGZHONG WU, Colorado State University — Topological insulators (TIs) hold great promise for spintronic devices due to their large charge-to-spin conversion efficiency. It has been demonstrated that a TI can induce a spin-orbit torque to switch the magnetization of a magnetic metal. However, it is unclear if this is due to the topological surface state (TSS) because the electrons from the magnetic metal can suppress TSS. Here we discuss experiments that identified bona fide surface state-induced spin-orbit torques in topological insulator/magnetic oxide bilayers. In Bi$_2$Se$_3$/BaFe$_{12}$O$_{19}$, a large spin-orbit torque from Bi$_2$Se$_3$ switched the magnetization of BaFe$_{12}$O$_{19}$. When the magnetization was switched by a magnetic field, a current in Bi$_2$Se$_3$ can reduce the switching field by about 4000 Oe. The switching efficiency at 3 K is 300 times higher than at room temperature. When BaFe$_{12}$O$_{19}$ is replaced with Mg(Al,Fe)$_2$O$_4$, efficient spin pumping in the bulk-dominated regime was found at room temperature. These results highlight the promise of topological insulator/ferromagnetic insulating oxide bilayers as a platform for studying topological surface states in the context of spin-to-charge interconversion.

*Funding: The fabrication and characterization of the samples and the electrical measurements were supported mainly by the U.S. National Science Foundation under grant no. EFMA1641989. The data analyses were supported mainly by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under award DE-SC0018994. Work at PSU was supported by the Pennsylvania State Two-Dimensional Crystal Consortium-Materials Innovation Platform (2DCC-MIP) under the U.S. National Science Foundation grant no. DMR-1539916. Work at Argonne was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. Work at UW was supported by the U.S. National Science Foundation under grant no. DMR-1710512. Work at Arizona was supported by the NSF under grant no. ECCS-1554011.
**11:51AM S47.00002: Nonlinear Hall effect in topological insulator-ferromagnet heterostructures**

YANG WANG (Presenter), YONG WANG, TAO WANG, YU-SHENG OU, YI JI, MATTHEW F DOTY, BRANISLAV NIKOLIC, STEPHANIE ANN LAW, JOHN Q XIAO, University of Delaware — Topological insulators (TIs) are a new class of materials which have insulating bulk bands and gapless helical surface states. The unique spin-momentum locking property leads to large charge-to-spin conversion efficiency which can be used to manipulate the magnetization in an adjacent ferromagnetic layer via spin-orbit torques (SOTs). However, more rich phenomena can happen in topological insulator/ferromagnet bilayers. Here, we report current-nonlinear Hall effect in Bi$_2$Se$_3$/CoFeB heterostructures measured by second harmonic Hall voltage method, which is commonly used to extract SOTs in TI/FM bilayers. By field dependence analysis and magneto-optical Kerr effect spin-orbit torque measurement, the origin of the second harmonic Hall voltage is mainly attributed to asymmetric magnon scattering mechanism. We further show that the second harmonic Hall resistance might be linked to quantum interference effect in TIs.

*This work is supported by the U.S. DOE, Office of Basic Energy Sciences, under contract number DE-SC0016380.

**12:03PM S47.00003: Nonlinear planar Hall effect**

PAN HE, Department of Electrical and Computer Engineering, National University of Singapore, SHULEI ZHANG (Presenter), Materials Science Division, Argonne National Lab, DAPENG ZHU, SHUYUAN SHI, Department of Electrical and Computer Engineering, National University of Singapore, OLLE HEINONEN, Materials Science Division, Argonne National Lab, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, HYUNSOO YANG, Department of Electrical and Computer Engineering, National University of Singapore — An intriguing property of a three-dimensional topological insulator (TI) is the existence of surface states with spin-momentum locking. We report the discovery of a new type of Hall effect in a TI Bi$_2$Se$_3$ film [1]. The Hall resistance scales linearly with both the applied electric and magnetic fields and exhibits a $\pi/2$ angle offset with respect to its longitudinal counterpart, in contrast to the usual angle offset of $\pi/4$ between the linear planar Hall and anisotropic magnetoresistance. This novel nonlinear planar Hall effect originates from the conversion of a nonlinear transverse spin current to a charge current due to the concerted actions of spin-momentum locking and time-reversal symmetry-breaking, which also exists in other non-centrosymmetric materials [e.g., WTe$_2$ and the 2DEG on the SrTiO$_3$(001) surface] with a large span of magnitude.


*P. H, D. Z, S. S, and H. Y. was partially supported by the A*STAR's Pharos Programme; work by S.Z. and G.V. at the Univ. of Missouri on initial development the theoretical framework was supported by NSF; work by S. Z. and O. H. at Argonne Nat'l Lab on further theoretical development and data analysis was supported by DOE, Office of Science, BES, Material Sciences and Engineering Division.
12:15PM S47.00004: Nonlinear Hall signatures of ferroelectric switching in atomically thin WTe$_2$

BENJAMIN T. ZHOU (Presenter), CHENG-PING ZHANG, XUEJIAN GAO, Hong Kong University of Science and Technology, KAIFEI KANG, KIN FAI MAK, School of Applied and Engineering Physics, Cornell University, KAM TUEN LAW, Hong Kong University of Science and Technology — Recent experiments have observed nonlinear Hall effects (NLHEs) in atomically thin WTe$_2$, an ultrathin ferroelectric material which may enable miniaturizing ferroelectric memories. However, signatures of ferroelectricity in NLHEs have remained elusive. In this work, we demonstrate that the direction and magnitude of nonlinear Hall currents can be highly sensitive to the ferroelectric polarization in WTe$_2$. In particular, there exists a wide experimental regime in which different polarization states are associated with opposite Hall current directions. We point out that such strong NLHE signatures of ferroelectricity originate from polarity-dependent Berry curvature dipoles, which arises from the broken mirror symmetry under strong out-of-plane displacement fields near polarity-switching points. Our work establishes the polarity-dependent NLHE as a novel scheme for fast and nondestructive reading in WTe$_2$-based ferroelectric memory devices.

12:27PM S47.00005: Magnetization control of ferromagnetic materials based on topological insulator Sb$_2$Te$_3$ sputtered thin films

SOFIA FERREIRA TEIXEIRA (Presenter), Department of Physics and Astronomy - University of Porto, IFIMUP, ALEXANDER VANSTONE, Blackett Laboratory, Physics Department, Imperial College London, ANA L. PIRES, Department of Physics and Astronomy - University of Porto, IFIMUP, WILL R BRanford, Blackett Laboratory, Physics Department, Imperial College London, JOÃO P. ARAÚJO, Department of Physics and Astronomy - University of Porto, IFIMUP, LESLEY COHEN, Blackett Laboratory, Physics Department, Imperial College London, ANDRÉ M. PEREIRA, Department of Physics and Astronomy - University of Porto, IFIMUP — Topological Insulators (TI) are a recent category of materials. 3D TIs host a protected metallic state on their surface while having an insulating bulk. The state appears in the form of a spin-textured Dirac cone. Due to these properties, several applications are foreseen. However, a better fundamental understanding of the relationship between the TI surface and bulk states is required.

In this paper, the structural and electrical properties of a uniform nanocrystalline Sb$_2$Te$_3$ thin film fabricated by ion beam sputtering will be reported. We show that the thin film bulk conduction is dominated by Variable Range Hopping. However, the presence of the weak antilocalization cusps on the magnetoresistance at low temperatures and low magnetic fields is also analyzed and found to be consistent with the existence of a TI surface state, having a phase coherence length of ~60 nm and a single 2D channel open at 2 K. Following these properties, the preliminary results of ferromagnetic resonance spin current generation and magnetization control of Sb$_2$Te$_3$ - Py thin films bilayers will be discussed, including our estimate of the spin Hall angle. As these bilayers were made using a scalable inexpensive method, the results offer promising opportunities for future applications in spintronics.
Persistence of spin memory in the insulating state of the crystalline phase-change material SnSb$_2$Te$_4$ revealed by magnetotransport measurements

NICHOLAS BREZNAY (Presenter), Harvey Mudd College, JOHANNES REINDL, HANNO VOLKER, MATTHIAS WUTTIG, RWTH Aachen University — Understanding the driving mechanisms for quantum materials, whether strongly correlated, strongly disordered, or characterized by nontrivial band topology, often derives from precise studies of electronic lifetimes. Sufficiently long electronic spin and phase-coherence lifetimes result in weak localization or (in the presence of strong spin-orbit coupling) antilocalization, effects that can be used to spectroscopically probe complex materials. Here we identify a distinct, complementary phenomenon that can also be used to probe electronic lifetimes in strongly disordered materials [1]. We find an unexpected spin sensitive hopping conductivity in the phase change material SnSb$_2$Te$_4$ that can be tuned with disorder. An isotropic magnetoconductance arises from disruption of spin correlations that inhibit hopping transport, the recently described ‘spin memory’ effect [2], whose occurrence signals that the spin plays a previously overlooked role in the disorder-driven transition between weak and strong localization in spin-orbital materials. [1] J. Reindl, H. Volker, N. Breznay, M. Wuttig, npj Quantum Materials (2019). [2] O. Agam, I. Aleinder, B. Spivak PRB 89, 100201(R) (2014).

Observation of magnetoresistance effects in a heterostructure of Bi$_2$Se$_3$ and a ferromagnet with perpendicular magnetic anisotropy*

JUNSEOK OH (Presenter), University of Illinois at Urbana-Champaign, VINCENT HUMBERT, Unité Mixte de Physique CNRS/Thales, JOSEPH SKLENAR, Wayne State University, BORA BASA, MATTHEW GILBERT, NADYA MASON, University of Illinois at Urbana-Champaign — Topological insulators (TIs) have insulating bulk states and topologically protected gapless boundary states that exhibit spin momentum locking and prohibited backscattering. Such unusual properties of topological surface states (SSs) in three dimensional TIs make the material much favorable for spintronic applications. However, the properties of these SSs can be largely modified in the presence of ferromagnetism in out-of-plane direction which breaks the time reversal symmetry. We report magnetoresistance (MR) signals in a heterostructure of 3D TI Bi$_2$Se$_3$ and Co/Pt multilayer with perpendicular magnetic anisotropy. In particular, the abrupt switching between the high and low MR states was observed for temperature lower than 1K and for field along in-plane and out-of-plane directions. This MR is incompatible with the magnetization behavior of the ferromagnetic layer and thus attributed to the magnetic ordering in the TI. Our observations indicate the possible existence of proximity magnetized SSs in Bi$_2$Se$_3$ with out-of-plane spin component.

*This work is supported by DARPA under ONR 14-17-1-3012.
1:03PM S47.00008: Bi-linear magnetoresistance in surface states of topological insulator: the role of Rashba-Edelstein effect and relaxation processes  ANNA DYRDAL (Presenter), JOZEF BARNAS, Faculty of Physics, Adam Mickiewicz University in Poznan, ALBERT FERT, Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud — Magnetoresistance effects scaling linearly with both external electric and magnetic fields are currently of great interest. These phenomena may be observed even in a uniform layer of material with strong spin-orbit coupling (SOC). A recent theoretical description of this bi-linear magnetoresistance (BMR) assumes a hexagonal warping of the band structure, which enables electron backscattering [1]. However, the experimental data on the topological insulator α-Sn(001) (a material without hexagonal symmetry) indicate that BMR can also exist in materials without hexagonal warping. Thus, one may expect another mechanisms contributing to the BMR in systems with isotropic energy spectra.

We will present our recent study on BMR of surface electronic states in TIs and in 2D Rashba gas [2]. The mechanism is based on the interplay of current-induced spin polarization and scattering processes due to peculiar spin-orbit defects. Additionally, we will discuss the role of the particle-hole asymmetry term and compare our approach with other theoretical descriptions and available experimental data.

[1] P. He, et al., Nat. Phys. 14, 495 (2018);

1:15PM S47.00009: Nonreciprocal second harmonic generation in CuB$_2$O$_4$  SHINGO TOYODA (Presenter), RIKEN CEMS, MANFRED FIEBIG, ETH Zurich and RIKEN CEMS, TAKA-HISA ARIMA, YOSHINORI TOKURA, RIKEN CEMS and University of Tokyo, NAOKI OGAWA, RIKEN CEMS and JST-PRESTO — In a matter with broken time-reversal and space-inversion symmetries, optical responses can differ for the photons propagating in the opposite directions. The so-called nonreciprocal optical effect has been observed ranging from GHz to X-ray. Especially, CuB$_2$O$_4$ is known to show huge nonreciprocal effects for the linear optical response, such as absorption, luminescence and refraction. In this study, we have investigated nonreciprocity of second harmonic generation. It is demonstrated that such gigantic nonreciprocal effects can show up for not only linear optical responses but also for nonlinear optical responses.

CuB$_2$O$_4$ shows nonreciprocal absorption at 1.405 eV, which corresponds to the intratomic transition of Cu$^{2+}$ hole [1]. In addition, it has been reported that the large second harmonic signal appears at this transition [2]. Therefore, we expect nonreciprocal second harmonic generation at this photon energy. By carefully tuning the amplitude and phase of electric-dipole and magnetic-dipole transitions, we realize very large nonreciprocal signal reaching 97 %. The temperature dependence and magnetic-field dependence will also be discussed in the presentation.

**S47.00010: Magnetic torque of holmium antimonide topological semimetal**

NARAYAN POUDEL (Presenter), Idaho National Laboratory, M. MOFAZZEL HOSEN, University of Central Florida, DARIUSZ KACZOROWSKI, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, MADHAB NEUPANE, University of Central Florida, KRZYSZTOF GOFRYK, Idaho National Laboratory — The family of compounds AX, where A = Lanthanides or Actinides and X = pnictides, have drawn a great scientific interest recently due to their unusual magneto-transport properties and potential non-trivial nature of the topological ground state. HoSb in one of the candidates of this family that shows antiferromagnetic transition at 5.7 K. Our recent magneto-transport and ARPES studies indicate the presence of the Rashba-type surface-states and non-trivial semimetallic characteristics in this material. In non-trivial magnetic semimetals it is important to understand the interplay between topology and magnetism. In HoSb, however, this behavior is still not well-understood. In order to account for this issue, we have initiated detailed studies of magnetic torque of HoSb along the three crystallographic directions, and in the antiferromagnetic and paramagnetic phases. We show that in this cubic system the torque exhibits large magnetic anisotropy in antiferromagnetic phase and an angle dependence indicates the presence of complex magnetic structure below the Neel temperature. We will discuss implications of these studies in the context of the presence of non-trivial topological state in this material.

*This work is supported by INL LDRD and DOE's Early Career Research Programs

**S47.00011: Large Spin-to-Charge Conversion Induced by Hybrid Rashba- and Surface-State in Topological Insulator Heterostructures**

RUI SUN (Presenter), Chinese Academy of Sciences, Institute of Physics, SHIJIA YANG, North Carolina State University, Department of Physics, YANG XU, Chinese Academy of Sciences, Institute of Physics, ERIC VETTER, DALI SUN, North Carolina State University, Department of Physics, LI NA, LEI SU, YAN LI, YANG LI, ZIZHAO GONG, ZONGKAI XIE, QEEMAT GUL, WEI HE, XIANGQUN ZHANG, ZHAO HUA CHENG, Chinese Academy of Sciences, Institute of Physics — Efficient spin-to-charge conversion at room temperature is of great value in spintronics applications. Recently, Topological insulators (TIs) have emerged as some of the most efficient spin-to-charge converters because of their correlated spin-momentum locking at helical Dirac surface states. While endeavors have been made to pursue large “charge-to-spin” conversions in novel TI materials using spin-torque-transfer geometries, the reciprocal process “spinto-charge” conversion, characterized by the inverse Edelstein effect length ($\lambda_{IEE}$) in the prototypical TI material (Bi$_2$Se$_3$), remains moderate. Here, we demonstrate that, by incorporating a “second” spin-splitting band, namely, a Rashba interface formed by inserting a bismuth interlayer between the ferromagnet and the Bi$_2$Se$_3$ (i.e., ferromagnet/Bi/Bi$_2$Se$_3$ heterostructure), $\lambda_{IEE}$ shows a pronounced increase (up to 280 pm) compared with that in pure TIs. We found that $\lambda_{IEE}$ alters as a function of bismuth interlayer thickness, suggesting a new degree of freedom to manipulate $\lambda_{IEE}$ by engineering the interplay of Rashba and Dirac surface states. Our finding launches a new route for designing TI- and Rashba-type quantum materials for next-generation spintronic applications.
Charge-density modulations are inevitably accompanied by a distortion of the crystalline lattice. Electronic or phononic origins of charge order are therefore difficult to distinguish. Here we propose a mechanism which traces the charge-density wave formation in underdoped cuprates to the incipient softening of a bond-buckling phonon. The momentum dependence of its coupling to the electrons in the copper oxygen planes favourably selects the incommensurate and axial ordering wavevector. But, it requires strong electronic correlations via their cuprate specific renormalization of the weight and the dispersion of quasiparticles to enable a unique enhancement of the charge susceptibility near the $B_{1g}$-phonon selected wavevector. The frequency of the $B_{1g}$ phonon softens by a few percent, and a lattice instability with concomitant finite range charge-density wave correlations will form locally, if nucleated by materials’ defects or dopant disorder.

*Natural Sciences and Engineering Research Council (NSERC) of Canada.
Deutsche Forschungsgemeinschaft through TRR 80.

Superconducting order in the doped Holstein model* 

The Holstein model (HM) is a tight-binding Hamiltonian which describes the interaction between electrons and local phonon modes on a lattice. Although charge density wave (CDW) order dominates at half-filling, the electron-phonon interaction is known to give rise to superconducting (SC) order away from half-filling. We use Quantum Monte Carlo simulations to explore the onset of SC order in doped systems through measurements of the s-wave pair susceptibility. We provide estimates for the critical temperature of the SC transition, obtained through a scaling analysis, for various values of the electron-phonon coupling $\lambda$ and phonon frequency $\omega$. We complement our calculation of the pair susceptibility with measurements of the electron kinetic energy and nearest-neighbor charge correlator.

*This work was supported by the Department of Energy, grant DE-SC0014671.
The interplay between electron-electron correlations and disorder has been a central theme of condensed matter physics over the last several decades, with the possibility that interactions might cause delocalization of an Anderson insulator into a metallic state, and the disrupting effects of randomness on magnetic order and the Mott phase both being central themes of investigation. Here we extend this physics to explore electron-phonon interactions and show, via exact quantum Monte Carlo simulations, that the suppression of the charge density wave correlations in the half-filled Holstein model by disorder can stabilize a superconducting phase. We discuss the relationship of our work to studies of the disorder quenching of the charge ordered phase in ZrTe$_3$ through Se doping, and the interplay with the observed superconductivity in that material, reproducing the qualitative features of the phase diagram in the temperature-disorder strength plane.

*The work of B.X. and R.T.S. was supported by the Department of Energy (DOE) under grant No.DE-SC0014671. N.C.C. was supported by the Brazilian funding agencies CAPES and CNPq. E.K. acknowledges support from the National Science Foundation (NSF) under Grant No.MR-1609560. GGB was supported by the University of the Côte d'Azur IDEX Jedi and Beijing CSRC.
11:51AM 548.00004: Charge ordering due to topological reconstruction of the Fermi surface*  DANKO RADIĆ (Presenter), Department of Physics, University of Zagreb, Faculty of Science, ANATOLY M. KADIGROBOV, Theoretische Physik III, Ruhr-Universitaet Bochum, ALEKSA BJELIŠ, Department of Physics, University of Zagreb, Faculty of Science — Numerous experiments in recent years indicate presence of charge ordering such as charge density wave (CDW) in layered 2D materials among which we single out HiTC cuprates in pseudogap regime and intercalated graphite. External magnetic field leads to the stabilization of long-ranged CDW. We show that topological reconstruction of the Fermi surface (FS), appearing as a consequence of spontaneously created CDW of such wave vector to bring closed electron pockets to touching, lowers the total energy of electron condensate. Opening the gap Δ at the touching points transforms the chain of closed electron pockets into a continuous open FS. Such CDW appears as rather peculiar quantum phase transition, with nonstandard dependence of condensate energy on Δ for coupling constant of responsible interaction exceeding the critical value [PRB 97 235439]. It appears in the regime opposite to the standard CDW mechanism related to the FS nesting. Introducing external magnetic field, and taking into account magnetic breakdown, even more strengthens the spontaneous FS reconstruction because open FS does not undergo the energy-increasing Landau quantization [PRB 100 115108]. Reconstruction in two directions changes sign of the Hall constant.

*HRZZ IP-2016-06-2289, QuantiXLie KK.01.1.1.01.0004

12:03PM 548.00005: Enhanced electron-phonon coupling for charge-density-wave formation in La$_{1.8-x}$Eu$_{0.2}$Sr$_x$CuO$_4$  YINGYING PENG, Peking Univ, ALI HUSAIN, MATTEO MITRANO, XIAOLAN SUN, THORMAS JOHNSON, ALEXANDER ZAKRZEWSKI, GREG MACDOUGALL, University of Illinois at Urbana-Champaign, ANDI BARBOUR, IGNACE JARRIGE, VALENTINA BISOGNI, Brookhaven National Laboratory, PETER ABBAMONTE (Presenter), University of Illinois at Urbana-Champaign — Charge density waves (CDW) are prevalent in all copper-oxide superconductors and their connection to high-temperature superconductivity is hotly debated. A key issue is that, although widely studied, that the microscopic origin of CDW is still unclear. For conventional CDWs in metals, electron-phonon coupling (EPC) plays an important role for the CDW formation. Resonant inelastic X-ray scattering (RIXS) has recently become an effective tool to directly determine the momentum dependence of the electron-phonon coupling strength. Here we present the first RIXS study of the CDW and Cu-O bond-stretching phonons in La$_{1.8-x}$Eu$_{0.2}$Sr$_x$CuO$_4$ compounds. By varying the sample doping and temperature, we show that the EPC is surprisingly enhanced around the CDW wave vector. Our results support a picture in which lattice excitations play a central role in the formation of the CDW, and furthermore exhibit a feedback effect in which the CDW enhances the EPC.
Observation of two types of charge-density-wave orders in superconducting La$_{2-x}$Sr$_x$CuO$_4$*  

JIAJIA WEN (Presenter), HAI HUANG, SANG JUN LEE, SLAC - Natl Accelerator Lab, HOYOUNG JANG, PAL-XFEL, Pohang Accelerator Laboratory, JASON KNIGHT, SLAC - Natl Accelerator Lab, YOUNG SANG LEE, Stanford University, MASAKI FUJITA, K. M. SUZUKI, SHUN ASANO, Tohoku University, STEVEN KIVELSON, Stanford University, CHI-CHANG KAO, JUN-SIK LEE, SLAC - Natl Accelerator Lab — Density wave orders, including charge- and spin-density-wave (CDW/SDW), have been widely observed in cuprate superconductors. However, to fully elucidate the relationship between the density wave orders and high temperature superconductivity (SC) has been challenging. Here we use resonant soft X-ray scattering to study the CDW order in superconducting La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) over a broad doping range. We discover two types of CDW orders in LSCO, namely CDW stripe order and CDW short-range order (SRO). They exhibit distinct interactions with SC that are not simply competitive. While the CDW-SRO is suppressed by SC, it is partially transformed into the CDW stripe order which keeps growing with developing SDW stripe order below the superconducting $T_c$. Our findings suggest that the stripe orders and SC are inhomogeneously distributed in the superconducting CuO$_2$ planes, and point to the emergence of a heterogeneous low temperature state as a result of the intricate interplay between CDW, SDW, and SC in LSCO.

*This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-76SF00515. M.F. is supported by Grant-in-Aid for Scientific Research (A) (Grant No. 16H02125) and Scientific Research (C) (Grant No. 16K05460).

Observation of an extended charge density wave boundary beyond the LTT phase in optimally doped LBCO  

SANG JUN LEE (Presenter), SLAC - Natl Accelerator Lab, SANGJUN LEE, University of Illinois Urbana Champaign, HAI HUANG, SLAC - Natl Accelerator Lab, YOUNG-IL JOE, WILLIAM B DORIESE, NIST, JASON KNIGHT, DONGHUI LU, SLAC - Natl Accelerator Lab, JOEL N ULLOM, PAUL SZYPRYT, DANIEL SWETZ, NIST, PETER MICHAEL ABBAMONTE, University of Illinois Urbana Champaign, JUN-SIK LEE, SLAC - Natl Accelerator Lab — Charge density wave (CDW) correlation in cuprates has been deemed a key ingredient to understand high-Tc superconductivity (SC). Since CDW is intertwined with other phases in a complicated way, determining the phase diagram of CDW is of critical importance. Here we focus on an archetypal La-based cuprate La$_{2-x}$Ba$_x$CuO$_4$ (LBCO) that has shown an interesting CDW behavior. The onset of CDW appears correlated with the low-temperature tetragonal (LTT) phase transition in the underdoped region whereas there is a big discrepancy above x=1/8. Particularly at the optimal doping of x=0.155, CDW was reported to occur at more than 20 K below the LTT transition. This contrasting behavior has not been well understood. Here, we present a resonant soft X-ray scattering (RSXS) study of CDW in optimally-doped LBCO, where we utilized a novel TES spectrometer with unprecedented sensitivity. Surprisingly, we detected short-ranged CDW up to T ~ 115 K, which is much higher than not just the previously reported CDW onset temperature but also the LTT transition temperature. We also observed behavior that suggests a positive correlation between CDW and SC, which are thought to be in general competing with each other. In this presentation, we will further discuss the implications of these new findings.
12:39PM S48.00008: Doping dependence study of CDW and its excitations via high
resolution RIXS*

HAIYU LU (Presenter), MATTHIAS HEPTING, MAKOTO HASHIMOTO, SU-DI CHEN, SLAC National Accelerator Laboratory, SHIGEYUKI ISHIDA, YOSHIYUKI YOSHIDA, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology, ABHISHEK NAG, MIRIAN GARCIA-FERNANDEZ, Diamond Light Source, RICCARDO ARPAIA, Chalmers University of Technology, GIACOMO GHIRINGHELLI, LUCIO BRAICOVICH, Politecnico di Milano, BRIAN MORITZ, EDWIN HUANG, SLAC National Accelerator Laboratory, KURT KUMMER, NICHOLAS B BROOKES, European Synchrotron Radiation Facility, KEJIN ZHOU, Diamond Light Source, ZHIXUN SHEN, THOMAS DEVEREAUX, WEISHENG LEE, SLAC National Accelerator Laboratory — Although it is now well established a charge
order (CO) is ubiquitous high-temperature superconducting cuprates, its doping dependence, interplay with superconductivity, and more importantly, its relevance to the putative quantum critical fluctuation inside the superconducting dome remain an active area of research. To gain further insights, it is necessary to conduct a comprehensive doping and temperature
dependence study. High energy resolution momentum-resolved resonant inelastic soft x-ray scattering (RIXS) experiments at the Cu L3-edge has been performed on the high-temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ with 8 different doping concentration throughout the phase
diagram, including antiferromagnetic, underdoped, optimally doped, and overdoped regime, at the superconducting critical temperature Tc and well below the Tc. Doping and temperature
dependence of the CDW, the associated phonon softening, and excitations will be discussed.

*This work is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy
Sciences, Materials Sciences and Engineering Division, under contract DE-AC02-76SF00515

12:51PM S48.00009: Resonant x-ray scattering studies of nematicity and charge order in the
La-based superconducting cuprates

TIMOTHY BOYLE (Presenter), MORGAN WALKER, ZITONG ZHAO, WILLIAM MOORE, EDUARDO H DA SILVA NETO, University of California, Davis, ALEJANDRO RUIZ, ALEX FRANO, University of California, San Diego, SANTIAGO BLANCO-CANOSA, Donostia International Physics Center, ZHAO W LI, HANJIE GUO, ALEXANDER KOMAREK, Max Planck Institute, CHRISTIAN SCHÜSSLER-LANGEHEINE, ENRICO SCHIERLE, Helmholtz-Zentrum Berlin, RONNY SUTARTO, FEIZHOU HE, Canadian Light Source, FABIO BOSCHINI, University of British Columbia — Charge-density waves (CDWs) are ubiquitous in the cuprates, however it is often difficult to distinguish between their different patterns and rotational symmetries. Additional phases, such as superconductivity and nematicity, further enrich the interplay between the low temperature phases in the cuprates and rotational symmetry. In particular, the La-based materials show an orthorhombic (LTO) to tetragonal (LTT) phase transition, with the LTT stabilizing stripes within the CuO$_2$ planes. Recent resonant inelastic x-ray scattering (RIXS) experiments also indicate the presence of high-temperature CDW correlations in these materials. In this study we use resonant x-ray scattering (RXS) to probe the energy and temperature dependent CDW correlations. We interpret our results in terms of the effects of uniaxial strain to the CDW correlations to uncover the nature of their interplay with nematic order.
**1:03PM S48.00010: X-ray scattering study of the role of charge-order in enhancing the superconducting transition**

MAXIME LEROUX (Presenter), LNCMI-Toulouse, CNRS, ZAHIRUL ISLAM, APS synchrotron, Argonne National Laboratory, VIVEK MISHRA, Oak Ridge National laboratory, JACOB RUFF, CHESS synchrotron, Cornell University, JOHN TRANQUADA, Brookhaven National Laboratory, MATTHEW SMYLIE, Hofstra University, PRASHANTA NIRAULA, ASGHAR KAYANI, Western Michigan University, GENDA GU, Brookhaven National Laboratory, WAI-KWONG KWOK, ULRICH WELP, Argonne National Laboratory — We combined proton irradiation (PI) and x-ray scattering to controllably tune and probe the competition between superconductivity (SC) and spatially modulated orders (e.g. charge order, CO). In particular, in La$_{2-x}$Ba$_x$CuO$_4$ (LBCO) complementary magnetization, tunnel diode oscillator, and resistivity measurements discovered that, despite being a d-wave superconductor, disorder induced by PI increases the superconducting critical temperature ($T_c$) by up to 50 % (4 K to 6 K) near $x = 1/8$ doping. X-ray scattering revealed that this $T_c$ increase coincides with a substantial suppression in CO strength and correlation length, providing clear evidence of strong competition between CO and bulk SC in LBCO. Insight from scattering and TDO suggest this competition originates from the cancellation of the interlayer Josephson coupling between CuO$_2$ planes.

*Experiments:

ANL, US DoE, Office of Science, Materials Sciences and Engineering Division.
BNL, US DoE, Office of Science, Materials Sciences and Engineering Division, under Contract DE-SC0012704.
APS synchrotron, DoE Office of Science, ANL, under Contract DE-AC02-06CH11357.
CHESS synchrotron, NSF and NIH/NIGMS under NSF Award DMR-1332208.

**1:15PM S48.00011: Time-resolved resonant soft x-ray scattering study on charge density wave in YBCO**

HOYOUNG JANG (Presenter), MINSEOK KIM, INTAE EOM, PAL-XFEL, Pohang Accelerator Laboratory, MASAKI FUJITA, IMR, Tohoku University, JUN-SIK LEE, SSRL, SLAC National Accelerator Laboratory — Charge order / charge density wave (CO/CDW) have been observed in the most of cuprate superconductor families by x-ray scattering and they are considered as ubiquitous features in cuprate superconductors. To understand their properties and relation to superconductivity, the CDW have been investigated as a function of temperature, external magnetic field, doping, and other conditions.

In this study, we have investigated the temporal dynamics of the CDW in YBa$_2$Cu$_3$O$_{6+x}$ single crystal using time-resolved resonant soft x-ray scattering (tr-RSXS) at the newly developed RSXS endstation of the PAL-XFEL. Using infrared optical pump, CDW correlation changes within a few picosecond time window. Detailed results, i.e. temperature and fluence dependence, will be discussed in the presentation.

*Supported by National Research Foundation (Korea), Grant-in-Aid for Scientific Research (Japan), and Department of Energy (USA)
1:27PM S48.00012: Search for charge density wave order in (Y_{1-x}Pr_x) Ba_2Cu_3O_7* KALYAN SASMAL (Presenter), ALEJANDRO RUIZ, BRANDON GUNN, Department of Physics, University of California, San Diego, JUN-SIK LEE, SSRL, SLAC National Accelerator Laboratory, JESSICA L MCCCHESNEY, FANNY RODOLAKIS, Advanced Photon Source, Argonne National Laboratory, ALEX FRANO, M BRIAN MAPLE, Department of Physics, University of California, San Diego — High-\( T_c \) superconductivity in cuprates occurs in proximity to competing low-temperature density-wave-order states. Superconductivity appears when spin order of the parent compound is destroyed and for underdoped compounds it competes with charge density wave (CDW) order. Resonant elastic soft x-ray scattering (RSXS) combines x-ray scattering with x-ray spectroscopy, making it possible to probe a variety of exotic spin, charge, orbital and structural ordering phenomena. We report on the growth and characterization of single crystals of Y_{1-x}Pr_xBa_2Cu_3O_7 cuprate superconductors with \( 0 < x < 1.0 \) by means of XRD, magnetic susceptibility, and electrical resistivity measurements, as well as RSXS measurements performed to probe the relationship between CDW order, the pseudogap, and high \( T_c \) superconductivity in this unexplored system.

*Research supported by US DOE: DE-FG02-04ER46105, NSF: DMR 1810310

1:39PM S48.00013: Visualizing charge ordering in a charge-transfer insulating cuprate* ILIJA ZELJKOVIC (Presenter), HE ZHAO, ZHENG REN, BRYAN RACHMILOWITZ, Boston College, JOHN SCHNEELOCH, University of Virginia, RUIDAN ZHONG, Princeton University, GENDA GU, Brookhaven National Lab, ZIQIANG WANG, Boston College — Although numerous symmetry-broken electronic states have been detected in metallic and superconducting cuprates at relative high carrier doping, there still exists little information about the “parent” state of cuprates after the first few charge carriers are introduced. The bottleneck in large part lies in the difficulty of synthesizing and characterizing bulk cuprates in the very lightly doped insulating regime at low temperatures. We demonstrate that by annealing the surface of optimally-doped superconducting Bi_2Sr_2CaCu_2O_{8+x} (\( T_c \sim 91 \) K) in ultra-high vacuum, we can reduce the oxygen dopant density near the surface and extend the hole doping range to achieve the previously inaccessible charge-transfer insulating state at low temperature (Zhao et al., Nat. Mater. 18, 103 (2019)). At this low doping, we discover a unidirectional charge-stripe order with a commensurate 4\( a_0 \) period, the same as the charge ordering wave vector previously seen across the pseudogap phase and the superconducting dome. Our work provides strong evidence that charge ordering in cuprates is unlikely to be related to the pseudogap phase.

*We gratefully acknowledge the support from the NSF Grant No. 1654041, the Army Research Office Grant No. W911NF-17-1-0399 and the DARPA Grant No. N66001-17-1-4051.
The effect of magnetic field on the charge density wave in La$_{2-x}$Sr$_x$CuO$_4$ near the critical end point

MENGZE ZHU (Presenter), ALEXANDER PETSCH, Univ of Bristol, OLEH IVASHKO, Deutsches Elektronen Synchrotron DESY, ELIZABETH BLACKBURN, Lund University, LAUREN CANE, Univ of Bristol, MARTIN VON ZIMMERMANN, Deutsches Elektronen Synchrotron DESY, STEPHEN HAYDEN, Univ of Bristol — The interplay between superconductivity and other competing tendencies has been intensely investigated in high temperature cuprate superconductors. In underdoped La- based cuprates, the charge and spin orders appear to be intertwined to form stripes with the incommensurability $\delta_{\text{charge}} = 2\delta_{\text{spin}}$ [1]. In contrast, in YBa$_2$Cu$_3$O$_{6+x}$ (YBCO), charge density waves (CDW) and spin density waves (SDW) emerge at different doping indicating that they might compete with each other. These competing tendencies can be tuned by a magnetic field. In YBCO, a magnetic field can give rise to a ferro-type long-range CDW in-phase along the $c$ direction, distinct from the short-range anti-phase CDW at zero field [2,3]. Here, we study the effects of a magnetic field on the CDW of La$_{2-x}$Sr$_x$CuO$_4$ ($x = 0.132$), a composition close to the end point of the SDW where no SDW is observed at zero field. We find that the magnetic field induces a CDW such that its intensity grows linearly with field. A similar increase in the SDW intensity is observed for the SDW suggesting that the SDW and CDW modulations are strongly coupled as required for example in stripe theories.


Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S49 DCMP: Electronic Structure of Superconductors
(photoemission, etc.) Mile High Ballroom 1B - Anton Vorontsov, Montana State University, Bozeman

11:15AM S49.00001: ARPES Study on the Electronic Structure of Ferromagnet Rb$_{0.93}$Co$_{1.87}$Se$_2$ JIANWEI HUANG (Presenter), HAN WU, Department of Physics and Astronomy, Rice University, ZHICAI WANG, HONGSHENG PANG, School of the Gifted Young, University of Science and Technology of China, SUNG-KWAN MO, Advanced Light Source, Lawrence Berkeley National Lab, ALEXANDER F KEMPER, Department of Physics, North Carolina State University, ROBERT J BIRGENEAU, MENG WANG, Department of Physics, University of California, Berkeley, MING YI, Department of Physics and Astronomy, Rice University — As an isostructural analogue of AFe$_2$Se$_2$ (A=K,Rb,Cs) iron-based superconductors, ACo$_2$Se$_2$ (A=K,Rb,Cs) exhibits distinct magnetic ground states without manifestation of superconductivity. Specifically, in Rb$_{0.93}$Co$_{1.87}$Se$_2$, a ferromagnetic transition occurs at 83K. Here we use angle-resolved photoemission spectroscopy to study the electronic structure of Rb$_{0.93}$Co$_{1.87}$Se$_2$ across the ferromagnetic transition. Clear spin-splitting of bands of different orbitals are observed across the transition. Detailed comparison with first-principle calculations both in the normal state and the magnetic state will be presented. The contribution of different orbitals to the ordered moment as well as the nature of the ferromagnetism in Rb$_{0.93}$Co$_{1.87}$Se$_2$ will be discussed.
11:27AM S49.00002: ARPES studies of model cuprate high-temperature superconductor*

SUDHEER ANAND SREEDHAR (Presenter), Physics, University of California, Davis, ZACHARY ANDERSON, YANG TANG, MARTIN GREVEN, Physics and Astronomy, University of Minnesota, ROBERT J BIRGENEAU, Physics, University of California, Berkeley, MING YI, Physics and Astronomy, Rice University, INNA VISHIK, Physics, University of California, Davis — HgBa$_2$CuO$_{4+d}$ (Hg1201) is a model single-layer cuprate which has uniquely elucidated the cuprate phase diagram via transport, scattering, and optics studies, but it has received relatively little ARPES study owing to the difficulty in cleaving and achieving good photoemission cross-section. We will discuss recent progress in identifying three energy scales of interactions near the node and evaluating their evolution with doping, temperature, and momentum. We will also discuss recent progress in identifying experimental conditions which optimize antinodal spectra.

*SAS and IV supported by Air Force Office of Scientific Research grant #FA9550-18-1-0156.

11:39AM S49.00003: Further evidence of concurrent mass enhancement and superconductivity in a topological state*

NADER ZAKI (Presenter), GENDA GU, PETER JOHNSON, Brookhaven National Laboratory — Previously$^{1,2}$, we reported on the concurrent onset of mass enhancement at the Dirac point below the superconducting transition in FeSe$_x$Te$_{1-x}$. In this talk, we will review these results and provide more evidence of this phenomenon using low energy laser-based ARPES measurements. Given the increased interest in this system, due in part to the co-existence of superconductivity and non-trivial topology, our results show that this system is even more complicated than perhaps previously presumed and may require re-interpretation of recent experimental reports.

$^1$2019 APS March Meeting (talk: K05.00009)
$^2$arXiv:1907.11602 [cond-mat.supr-con]

*The work carried out at Brookhaven was supported in part by the U.S. DOE under Contract No. DE- SC0012704 and in part by the Center of Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy.
11:51AM S49.00004: Evolution of Electronic Spectral Weight in the Hubbard ladder
MASANORI KOHNO (Presenter), Natl Inst for Materials Sci — Although the number of electronic bands is usually considered invariant in a conventional band picture, the electronic states can generally emerge, grow, and disappear as the electron density changes in strongly correlated systems. Here, the evolution of the electronic states as a function of the electron density is illustrated in the Hubbard ladder in the strong Coulomb repulsion and strong intra-rung hopping regime using the non-Abelian dynamical density-matrix renormalization group method and perturbation theory. An emergent mode in the low-electron density regime grows with the electron density and plays a significant role in the dimer Mott physics at quarter filling, whereas an originally non-interacting band at zero electron density loses the spectral weight and disappears in the Mott transition at half filling, which leads to the spin excitation of the Mott insulator. The emergence and disappearance of electronic states, which have almost been overlooked in conventional band theory and Fermi liquid theory, are particularly important in understanding of the physics around the Mott transition.

12:03PM S49.00005: Non-local correlation effect in iron-based superconductors* KARIM ZANTOUT (Presenter), Goethe University Frankfurt, STEFFEN BACKES, Centre de Physique Theorique, Institut Polytechnique de Paris, ROSER VALENTI, Goethe University Frankfurt — While experimental studies of many iron-based superconductors observe momentum-dependent effects like the so-called blue/red shift that describes opposite energetic shifts of electron- and hole-parabolas with respect to bandstructure calculations, DMFT by construction is not able to capture such features. We therefore present a momentum-dependent and dynamical many-body method, the Two-Particle Self-Consistent (TPSC) approach, and apply it to an ab-initio-derived multi-orbital Hubbard model.
Multi-orbital TPSC assumes the irreducible interaction vertex to be an orbital-dependent constant, which is self-consistently determined from local spin and charge sum rules. Those are immediate representatives of the Pauli principle. We disentangle the contribution of non-local correlations in LiFeAs and show that in the local approximation, i.e. after momentum-averaging the self-energy, one recovers dynamical-mean field theory (DMFT) results. The comparison of our results to experimental data shows that non-local correlations in LiFeAs are decisive to describe the spectral function, Fermi surface and scattering rates.

*We thank the German ResearchFoundation (Deutsche Forschungsgemeinschaft) for financial support.
**12:15 PM S49.00006: Electronic structure and superconductivity in unconventional cuprates**

*KUN JIANG (Presenter), Boston College, CONGCONG LE, FU-CHUN ZHANG, Kavli Institute of Theoretical Sciences, University of Chinese Academy of Sciences, ZIQIANG WANG, Boston College, JIANGPING HU, Institute of Physics, Chinese Academy of Sciences — We study the recently discovered 73K high-$T_c$ superconductor $\text{Ba}_2\text{CuO}_{3+\delta}$ at $\delta \approx 0.2$ grown under high pressure. Neutron experiments find that the polycrystal exhibits a structure similar to $\text{La}_2\text{CuO}_4$, but with dramatically different lattice parameters due to the CuO$_6$ octahedron compression. The octahedron compression leads to an \{\em inverted\} Cu $3d\ e_g$ complex with the $d_{x^2-y^2}$ orbital sitting below the $d_{3z^2-r^2}$ orbital and an electronic structure highly unusual compared to the conventional cuprates. We conjecture that the material realizes a new path of in-plane positional oxygen doping, where the doped oxygens create matrices of compressed $\text{Ba}_2\text{CuO}_4$ embedded in $\text{Ba}_2\text{CuO}_3$. Constructing a strongly correlated two-orbital model at hole doping $x = 2\delta$ of the Cu $d^9$ state, we show that the multi-orbital exchange interactions lead to an antiphase $d$-wave superconducting state, i.e. a nodal $d_{\pm}$ pairing state. These findings suggest that the class of unconventional cuprates with liberated orbitals as doped two-band Mott insulators can be a direction for realizing high-$T_c$ superconductivity.

*The work is supported by the U.S. Department of Energy, Basic Energy Sciences Grant No. DE-FG02-99ER45747.

**12:27 PM S49.00007: Photoemission studies of BSCCO-2212 across the phase diagram with in-situ control of doping**

*ILYA DROZDOV (Presenter), GENDA GU, TONICA VALLA, Brookhaven National Laboratory — I will present angle-resolved photoemission studies of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ enabled by oxide MBE [1]. Single crystals were cleaved and annealed in ultra-high vacuum or in ozone (O$_3$) to reduce or increase the doping level. Photoemission studies have been carried out on a wide range of dopings spanning the superconducting dome and covering the previously inaccessible, metallic, non-superconducting phase on the overdoped side (OD0K). This allowed us to study the evolution of the Fermi surface with doping [2], the reconstruction of the Fermi surface due to the superstructure modulation [3], and the renormalization of the electronic spectrum concomitant with the onset of superconductivity [4]. In this talk, I will focus on the sample preparation aspects and cover the first two results.


*US DOE, BES, contract no. DE-SC0012704.
Disappearance of Superconductivity Due to Vanishing Coupling in the Overdoped Cuprate Superconductors

TONICA VALLA (Presenter), ILYA DROZDOV, GENDA GU
Condensed Matter Physics and Materials Science, Brookhaven National Laboratory — In high-temperature cuprate superconductors, superconductivity is accompanied by a "plethora of orders" and phenomena that may compete, or cooperate with superconductivity, but which certainly complicate our understanding of origins of superconductivity. While prominent in the underdoped regime, these orders weaken or completely vanish with overdoping. Here, we approach the superconducting phase from the more conventional highly overdoped side. We present angle-resolved photoemission studies of Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ single crystals cleaved and annealed in ozone to increase the doping all the way to the non-superconducting phase. We show that the mass renormalization in the antinodal region of the Fermi surface, associated with the structure in the quasiparticle self-energy, that possibly reflects the pairing interaction, monotonically weakens with increasing doping and completely disappears precisely where superconductivity disapears. This is the evidence that in the overdoped regime, superconductivity is determined by the coupling strength. A strong doping dependence and an abrupt disapearance above $T_c$ eliminate the conventional phononic mechanism of the observed mass renormalization.

*This work was supported by the US DOE, Office of Basic Energy Sciences, contract no. DE-SC0012704.

ARPES on Unusual Superconducting Properties of Single-Layer FeSe/SrTiO$_3$ Films

YU XU (Presenter), QINGYAN WANG, HONGTAO RONG, DINGSONG WU, Chinese Academy of Sciences, Institute of Physics, YONG HU, University of Science and Technology of China, XINXUAN GUO, LIN ZHAO, GUODONG LIU, Chinese Academy of Sciences, Institute of Physics, ZUYAN XU, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences , Beijing 100190 , China, XINGJIANG ZHOU, Chinese Academy of Sciences, Institute of Physics — Single-layer FeSe films grown on SrTiO$_3$ substrates have attracted much attention because of their record high superconducting critical temperature and distinct electronic structure. Here we report MBE growth of very high-quality single-layer FeSe/STO films, and systematic investigations of their electronic structure and superconducting properties by high-resolution angle-resolved photoemission spectroscopy measurements. Two ellipse-like electron pockets are clearly resolved at one Brillouin zone corner and obvious band splitting is observed. The anisotropic superconducting gap along the Fermi surface is measured with high precision. In particular, we observe very strong superconductivity-induced band back-bending that extends to rather high binding energy. The implications of these observation on superconductivity mechanism of the single-layer FeSe/SrTiO$_3$ films will be discussed.
1:03PM S49.00010: Angle-resolved photoemission spectroscopy of in-situ grown cuprate heterostructures by molecular beam epitaxy  ZHUOYU CHEN (Presenter), YUNTIAN LI, YONG ZHONG, SLAVKO REBEC, TAO JIA, Stanford University, MAKOTO HASHIMOTO, DONGHUI LU, ROBERT G MOORE, SLAC National Accelerator Laboratory, ZHIXUN SHEN, Stanford University — The molecular beam epitaxy (MBE) system in-situ connected to the beam-line angle-resolved photoemission spectroscopy (ARPES) in Stanford Synchrotron Radiation Lightsource (SSRL) enables rational design of complex material systems and direct electronic structure measurements. The in-situ connected scanning tunneling microscopy (STM) further enables electronic property mapping in the spatial dimensions. Particularly, cuprate films and heterostructures grown atomic-layer-by-layer are of great interest to be explored. In this talk, we will present the newest results about ARPES on cuprate heterostructures.

1:15PM S49.00011: Improved Understanding of Gap Dynamics from Time- and Angle-Resolved Photoemission Spectroscopy of a Nonequilibrium Superconductor*  TIANRUI XU, DANIEL EILBOTT (Presenter), Physics, University of California, Berkeley, CLAUDIA FATUZZO, Materials Science Division, Lawrence Berkeley National Laboratory, TAKAHIRO MORIMOTO, Applied Physics, University of Tokyo, JOEL MOORE, ALESSANDRA LANZARA, Physics, University of California, Berkeley — Time- and angle-resolved photoemission spectroscopy (tr-ARPES) has shown to be a useful tool in studying non-equilibrium states of matter. However, the absence of time-translation invariance presents a challenge to understanding the underlying dynamics of the system from the measurements in a straightforward manner. In equilibrium, ARPES intensity is understood to be \( I(k, \omega) \propto f(\omega) A(k, \omega) \) with broadening, where \( f(\omega) \) is the Fermi-Dirac distribution, and \( A(k, \omega) \) is the electronic spectral function. Here we study how one should interpret \( I(k, \omega, t) \), now as a function of time \( t \). We focus our study on tr-ARPES measurements of a non-equilibrium superconducting system where the superconducting gap changes with time. With a focus on situations where the standard quasi-static analysis method fails, we present a possible better way to obtain superconducting gap dynamics.

*Funding from the Department of Energy as a part of the Ultrafast Materials Program; the NSF Graduate Research Fellowship Program; the Gordon and Betty Moore Foundation.
1:27PM S49.00012: Gap opening in monolayer FeSe/TiO$_2$(100) at low doping  CHENHUI YAN (Presenter), Pritzker School of Molecular Engineering, University of Chicago, BRENDAN D. FAETH, Department of Physics, Laboratory of Atomic and Solid State Physics, Cornell University, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University, SHUOLONG YANG, Pritzker School of Molecular Engineering, University of Chicago, KYLE M. SHEN, Department of Physics, Laboratory of Atomic and Solid State Physics, Cornell University — Monolayer FeSe grown on SrTiO$_3$(001) has been established to host a high-temperature superconducting state, with the gap-opening temperature between 60 and 70 K. On the other hand, it was shown that monolayer FeSe exhibits an insulating gap when the electron doping level is below 0.09 electron per iron atom. This insulating gap is temperature independent, in contrast to the gap-opening phenomenology in superconducting monolayer FeSe. Here we grow monolayer FeSe on rutile TiO$_2$(100), and show that the gap opens below 40 K with an electron doping of 0.08 electron per iron atom. This doping level is lower than the previously reported doping threshold for superconductivity. We will discuss the origin of this gap.

1:39PM S49.00013: Strong particle-hole asymmetry in a 200 Kelvin superconductor*  SOHAM GHOSH (Presenter), YUNDI QUAN, WARREN E PICKETT, University of California, Davis — The superconducting state of metals have long provided a classic example of particle-hole symmetry at low energy. We present fermionic self-energy results based on first-principles theory for the electron-phonon coupling in H$_3$S which illustrates strong particle-hole asymmetry in the dynamics arising from the underlying sharp structure in the fermionic density of states. We evaluate the momentum-resolved and zone-averaged spectral densities and interacting thermal distribution function, all of which clearly illustrate strong particle-hole asymmetry. The results allow us to study the infrared conductivity and to note that the strength and position of extrema are affected by electron-phonon coupling.

*The project was supported by NSF Grant No. DMR 1607139.
1:51PM S49.00014: Band structure motif and bosonic excitations in the fluctuating superconductivity of overdoped cuprates* YU HE (Presenter), Physics, University of California at Berkeley, SU-DI CHEN, Applied Physics, Stanford University, MAKOTO HASHIMOTO, SSRL, SLAC National Laboratory, SHAN WU, XIANG CHEN, YU SONG, Physics, University of California at Berkeley, HIROSHI EISAKI, AIST, Japan, ZHIXUN SHEN, Applied Physics, Stanford University, ROBERT J BIRGENEAU, Physics, University of California at Berkeley — Superconducting fluctuation is one of the central discussions in the physics of high-Tc superconductivity, especially when the system is optimally doped. Recent years have seen a renewed interest in this topic regarding overdoped cuprates, where the expectation is to seek a resolution closer to various BCS premises. However, a series of transport and optical experiments reveal substantial departure from the conventional wisdom.

We combine angle-resolved photoemission spectroscopy (ARPES) with inelastic neutron scattering (INS), and aim to provide a holistic view on this issue on overdoped single crystal Bi-2212. In particular, we discuss the role of the van Hove point on the electronic structure and the partial flat band around it [1]. The relation between electronic structure and the underlying magnetic excitation will also be discussed in the context of d-wave pairing and pair-breaking [2].


*Miller Institute for Basic Research in Science
Department of Energy, Office of Science, Basic Energy Sciences

2:03PM S49.00015: Interface-enhanced superconductivity of single layer FeSe grown on non-TiO2 based oxides* YUAN-HE SONG (Presenter), XIA LOU, XIAOYANG CHEN, RAN TAO, TIANLUN YU, RUI PENG, HAICHAO XU, State Key Laboratory of Surface Physics, Department of Physics, and Advanced Materials Laboratory, Fudan Univ, HAO RU, YI-HUA WANG, Department of Physics and State Key Laboratory of Surface Physics, Fudan Univ, ZHENG CHEN, YAN-WU XIE, Department of Physics, Zhejiang Univ, QINGHUA ZHANG, LIN GU, XUETAO ZHU, JIANDONG GUO, Institute of Physics, Chinese Academy of Sciences, DONGLAI FENG, State Key Laboratory of Surface Physics, Department of Physics, and Advanced Materials Laboratory, Fudan Univ — The single layer FeSe film on SrTiO3 indicates that interfaces can play a significant role in high-temperature superconductivity. Here we report a new FeSe-based interface, single layer FeSe grown on non-TiO2 based oxides by molecular beam epitaxy (MBE) method, was successfully obtained. The structure of the interface was determined by high resolution transmission electron microscopy (HRTEM). The angle-resolved photoemission spectroscopy (ARPES) shows that it is superconducting with a large gap, while the ex-situ mutual inductance measurements indicate it has a high onset temperature for diamagnetism. This heterostructure can provide a new platform for understanding the interface-enhanced superconductivity.

*The National Natural Science Foundation of China

Thursday, March 5, 2020 11:15 AM - 2:03 PM
Unraveling the Mott-Peierls intrigue in Vanadium dioxide

ADRIANO AMARICCI (Presenter), MICHELE FABRIZIO, SISSA, FRANCESCO GRANDI, Department of Physics, Erlangen University — Vanadium dioxide is one of the most studied strongly correlated materials. The nature of the rutile metal to monoclinic insulator transition in this system triggered a longstanding debate about which comes first, the Mott localisation or the Peierls distortion. Here, we show that the electronic correlations and the lattice vibrations conspire to stabilise the monoclinic insulator, and so they must be treated on equal footing. We design a minimal model for VO2 that includes all the important physical ingredients: the electronic correlations, the multi-orbital character, and the two components antiferrodistortive mode that condenses in the monoclinic insulator. We solve this model by dynamical mean-field theory within the adiabatic Born-Oppenheimer (BO) approximation. Consistently with the first-order character of the metal-insulator transition, the BO potential has a rich landscape describing the distorted and undistorted phases, and which translates into an equally rich thermodynamics that we uncover by the Monte Carlo method. Remarkably, we find that a distorted metal phase intrudes between the low-temperature distorted insulator and high-temperature undistorted metal, which sheds new light on the debated experimental evidence of a monoclinic metallic phase.

Correlation induced emergent charge order in metallic vanadium dioxide thin films

CHRISTOPHER SINGH, LOUIS F. J. PIPER, Binghamton University, HANJONG PAIK, DARRELL SCHLOM, Cornell University, WEI-CHENG LEE (Presenter), Binghamton University — Understanding the metal-insulator transition in vanadium dioxide is complicated by symmetry breaking structural transitions accompanying correlated electronic transitions. Resolving this problem though is at the heart of many scientific and technological advancements. To that end, we develop a cross-phase, symmetry-consistent approach to treat structural distortions and electronic correlations in epitaxial VO2 films from first principles. By adopting a uniform Bravais symmetry across several epitaxial growth configurations, we demonstrate the exquisite sensitivity of correlation physics to apical bond lengths in the presence of lattice symmetry breaking, and discover emergent charge order preceding the dimerized insulating phase even in the metallic rutile phase. We discuss the deep physical implications for the phase diagram of VO2, and argue for the unparalleled significance of correlation physics and sample quality in light of this result.

*This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0024.
11:39AM S50.00003: Probing the Mott transition in \(V_2O_3\) with Pair Distribution Function Analysis

ETHAN FLETCHER (Presenter), BENJAMIN FRANDSEN, Department of Physics and Astronomy, Brigham Young University, KENTARO HIGASHI, HIROSHI KAGEYAMA, Department of Energy and Hydrocarbon Chemistry, Kyoto University — \(V_2O_3\) is a popular system for studying Mott insulators, which are materials that are driven into an insulating state by strong electron correlations. Despite decades of research, a complete understanding of the metal-insulator transition in \(V_2O_3\) has not been conclusively established. Here, we present comprehensive atomic and magnetic pair distribution function (PDF) analyses of \(V_2O_3\) using both x-ray and neutron total scattering measurements, shedding new light on the mechanism of the transition from the point of view of short-range structural and magnetic correlations on both sides of the transition. The results allow us to thoroughly examine the transition from the metallic state to the insulating state with complementary sensitivity provided by the x-rays (sensitive to the vanadium displacements) and neutrons (sensitive to the oxygen displacements and magnetic correlations). We discuss the implications of these results in the context of other recent experimental and theoretical studies of \(V_2O_3\).

11:51AM S50.00004: Nanosecond fluctuators in \(V_2O_3\) film within the metal-insulator-transition

LIYANG CHEN (Presenter), PANPAN ZHOU, Rice Univ, YOAV KALCHEIM, IVAN SCHULLER, University of California, San Diego, DOUGLAS NATELSON, Rice Univ — Vanadium sesquioxide (\(V_2O_3\)) is an archetypal Mott insulator, and exhibits a first-order transition at 160 K between a low temperature monoclinic, antiferromagnetic insulator and a high temperature, rhombohedral, paramagnetic, metallic phase. Resistive noise as measured through electronic transport can be used as a probe of the fluctuating dynamics of the two-phase domain structure. We measure noise spectra at both low frequencies (up to 300 kHz) and radio frequencies (between 200 MHz and 1 GHz). At low current densities the noise power is quadratic in bias current, as expected for resistive fluctuations probed nonperturbatively by the current. The low frequency noise generally resembles flicker-type \(1/f^\alpha\) noise, often taking on the form of Lorentzian noise dominated by a small number of fluctuators as the insulating phase is approached. The presence of radio frequency noise power that is quadratic in the bias current allow identification of domain fluctuations with lifetimes below 1 ns, comparable to timescales seen in non-equilibrium pump-probe studies of the transition.

*U.S. DOE office of Science/Basic Energy Science Award DE-FG02-06ER46337.
Vannevar Bush Faculty Fellowship Grant No. N00014-15-1-2848.
Energy Frontier Research Center US DOE Award No. DE-SC0019273.
Low-temperature metallic phase in V$_2$O$_3$ films due to structural confinement

YOAV KALCHEIM (Presenter), COLINE ADDA, NAREG GHAZIKHANIAN, HENRY NAVARRO, PAVEL SALEV, JAVIER DEL VALLE, IVAN SCHULLER, Department of Physics, University of California San Diego — We show that high purity V$_2$O$_3$ films grown on certain substrates exhibit a suppressed metal insulator transition (MIT) and in some cases even a reentrant metallic phase at low temperature. This occurs only in films which have the c-axis in the out-of-plane direction. For this lattice orientation the MIT entails a structural expansion which is entirely in the film plane. As the MIT progresses, some expansion into the low temperature monoclinic phase occurs but in-plane confinement prohibits a full expansion of the lattice. Instead, a coexisting metallic phase is stabilized down to the lowest temperatures measured. This low temperature metallic phase exhibits structural and electrical properties which are distinct from the high temperature metallic phase.

*Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019273.

Controlled growth of VO$_2$ Nanowires by direct conversion of V$_2$O$_5$ solution film

GAVIN BLAIR, ABIN JOSHY, ANDREW STEELY, JIANG WEI (Presenter), Tulane Univ — Vanadium dioxide is known to exhibit fascinating properties due to its phase transition from insulating to metallic phase at 340 K. Effectively growing single-crystal VO$_2$ nanowires has been difficult to realize in a controlled, repeatable way. Through the use of a chemical vapor deposition using solutions of V$_2$O$_5$, we realized a consistent growth of single crystals with their size ranging from nanowires to microbeams. A comprehensive understanding of the growth mechanism has also been obtained. With combined probing techniques, including an Enhanced Darkfield Optical Microscopy, Atomic Force Microscopy, and Raman Microspectroscopy, we captured the dynamics of growth, along with the stoichiometry and crystal structure for nanocrystals at different growth stages. We revealed that the growth starts with the vaporization of V$_2$O$_5$, followed by dense seed nucleation on the substrate, and then the growing of large crystals as a result of consuming neighboring seeds.

The new method of VO$_2$ nanowires growth based on V$_2$O$_5$ film provides a simpler and more economical solution for their application in industry.

*This research is supported by the US Department of Energy under grant DE-SC0014208
Observation of the voltage-triggered insulator to metal transition in a VO$_2$ thin film as a function of temperature.* 

ALYSON SPITZIG (Presenter), XUGUANG WANG, MICHAEL ARUMAINAYAGAM, DILEK YILDIZ, JASON HOFFMAN, JENNIFER E. HOFFMAN, Harvard University — VO$_2$ undergoes an insulator to metal transition with a resistivity change up to five orders of magnitude upon heating through 340 K. The transition has also been observed via current-voltage (IV) measurements as a sharp jump in the current when sweeping the applied voltage. We have previously used the tip of an atomic force microscope (AFM) to map the local current response of voltage-biased polycrystalline VO$_2$ thin films[1]. We have fit the IV curve immediately preceding the transition to the temperature-dependent Poole-Frenkel conduction mechanism and calculated the local temperature of the film. While these measurements were nominally performed at room temperature, we calculated an increased local temperature of 335 K immediately preceding the transition, confirming the role of Joule heating in our voltage-biased, tip-sample geometry. Here, we extend these measurements to a wider temperature range to further understand the effects of Joule heating on the voltage-triggered insulator to metal transition in VO$_2$ thin films. ([1] Spitzig et al. arXiv:1903.03062v1)

*This work is supported by STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319, the Gordon and Betty Moore Foundation’s EPIOS Initiative Grant No. GBMF4536, and Canadian NSERC CGS-M graduate fellowship.

Selective phonon-mode excitation revealed by tracing the pathway of photo-induced structural-phase-transition in single-crystal VO$_2$* 

JUNJIE LI (Presenter), WEI WANG, LIJUN WU, Brookhaven National Laboratory, OLIVIER DELAIRE, Duke University, JING TAO, YIMEI ZHU, Brookhaven National Laboratory — The Metal-Insulator (M-I) transition in VO$_2$ that is associated with a monoclinic-rutile (M-R) structure phase transition has been extensively studied due to the potential application of its fast electrical/optical switch properties. It remains a big challenge to reveal the transition pathway to fully understand the underlying mechanism. In this study, we use MeV ultrafast electron diffraction to monitor the structure evolution in single-crystal VO$_2$ under femtosecond laser excitation. The M-R phase transition was observed at a high sample temperature (T = 314 K) under a specific pump fluence of 16 mJ/cm$^2$. Crystallographic structural analysis reveals that the atomic motions have a two-step dynamics. During the first a few ps, both stretching and rotation A$_g$ phonon modes are involved in the collective vanadium motions. Then only rotation A$_g$ phonon mode is continuously excited in the following hundreds of ps. Moreover, such the M-R phase transition cannot be observed at a much lower sample base temperature (T = 77 K), indicating a certain role of thermal fluctuation in this photo-induced phenomenon.

*supported by the Materials Science and Engineering Divisions, Office of Basic Energy Sciences of the U.S. Department of Energy under Contract No. DESC0012704
12:51PM S50.00009: Probing the insulator-to-metal transition in VO$_2$ using non-contact atomic force microscopy*  
MICHAEL ARUMAINAYAGAM (Presenter), ALYSON SPITZIG, XUGUANG WANG, LARISSA LITTLE, DILEK YILDIZ, JASON HOFFMAN, JENNIFER E. HOFFMAN, Harvard University — Vanadium dioxide (VO$_2$) undergoes an insulator-to-metal transition (IMT) when heated above a critical temperature of 340 K. The role of Joule heating and applied electric field in inducing this transition is an active area of research. In this study, the IMT of VO$_2$ thin films grown using oxygen plasma molecular beam epitaxy are examined using non-contact atomic force microscopy (AFM) in ultrahigh vacuum. By measuring the dissipated power through a qPlus AFM tuning fork, the competing effects of Joule heating and applied electric field are assessed. With this non-invasive and highly sensitive technique, we can measure the IMT as a function of tip-sample distance and bias voltage.

*This work is supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319, the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant No. GBMF4536, and the Canadian NSERC CGS-M graduate fellowship.

1:03PM S50.00010: Resistive switching and filament formation in VO$_2$ vertical devices*  
MINHAN LEE (Presenter), Materials Science and Engineering, University of California-San Diego, SHAOBO CHENG, Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, JAVIER DEL VALLE, Center for Advanced Nanoscience, Department of Physics, University of California-San Diego, YIMEI ZHU, Department of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, IVAN SCHULLER, Center for Advanced Nanoscience, Department of Physics, University of California-San Diego — Vanadium oxides exhibit electrically-triggered, volatile, resistive switching and provide a promising opportunity to mimic spiking neurons for neuromorphic computing. The control of the physical properties of these oxides is an important requirement to develop oxide electronics for future technology. However, a detailed understanding of the non-volatile filamentary formation in these Mott materials is still lacking. In this work, we investigated the mechanisms behind volatile and non-volatile resistive switching in electrically-driven VO$_2$ vertical devices. By using electrical transport measurement and in-situ transmission electron microscopy, the metal-insulator transition properties of the conductive filament and its nanoscale lattice structure are studied. Our works address the important issues in resistive switching based neuromorphic technologies.

*Work supported by the Quantum Materials for Energy-Efficient Neuromorphic Computing (Q-MEEN-C) Energy Frontier Research Center (EFRC), funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0019273.
The acoustoelectric (AE) effect, which manifests itself as the generation of a DC current by a propagating acoustic wave, may convey crucial information on the interdependence between the structural and electronic properties of strongly correlated oxides. We observed that acoustic waves may be coupled not only to an electronic but also to a magnonic state of these materials. In this work, we studied the AE effect in non-magnetic (VO$_2$, V$_2$O$_3$) and ferromagnetic La$_{0.7}$Sr$_{0.3}$MnO$_3$ wires grown on top of piezoelectric LiNbO$_3$ substrates. It was observed that the resistance change across a metal-insulator transition results in a significant enhancement of the AE current in the vanadates wires. Additionally, we show that the sign of the AE current differs for excitations produced by bulk and surface acoustic waves. Importantly, it was observed that the AE current in the La$_{0.7}$Sr$_{0.3}$MnO$_3$ wire can be significantly tuned by applying an external magnetic field. Our work provides a new platform for surface acoustic wave devices based on Mott transitions.

This research was supported by the Office of Basic Energy Science, U.S. Department of Energy, BES-DMS funded by the Department of Energy's Office of Basic Energy Science, DMR under grant DE FG02 87ER-45332.

VO$_2$ displays a first-order metal-insulator phase transition near 340 K. Accompanying this electronic transition is a structural transition. The connection between these two transitions is unclear, with electronically-driven and structurally-driven models providing conflicting results. Electron doping with molybdenum enhances metallicity and reduces the structural transition temperature; between 17% and 19% Mo, we find that the long-range structural transition is suppressed entirely while the electronic transitions remain similar. Diffuse x-ray scattering measurements were performed on a single crystal of the V$_{0.81}$Mo$_{0.19}$O$_2$. In the low-temperature insulating phase, sharp rods are observed, indicating two-dimensional ordering of atomic displacements. The slight oscillation of these rods about the [110] direction in reciprocal space can be explained by weak, inherently frustrated coupling between the ordered planes. Such fragile embedded order is predicted by an Ising-like ferrodistortive model proposed by Lovorn and Sarker. 3D-ΔPDF analysis of the diffuse scattering and structural simulations provide a clear picture of the local order in this system.

This work was supported by the US DOE, Office of Science, Basic Energy Science, Materials Sciences and Engineering Division.
1:39PM S50.00013: Nonequilibrium-induced quantum fluctuations in resistive phase transition  JONG E HAN (Presenter), State Univ of NY - Buffalo — We investigate the quantum mechanical origin of resistive phase transitions in solids driven by a constant electric field in the vicinity of a metal-insulator transition. The mean-field theory [1] showed that the self-consistent Landau-Zener mechanism reproduced main experimental features, and we show that it is equivalent to the empirical resistor network theories based on electronic scenarios applicable to systems like VO$_2$. Despite the qualitative agreement, reliable quantitative predictions for the switching electric-field has remained elusive. Theoretical estimates based on the Landau-Zener mechanism are typically orders of magnitude larger than experimentally observed threshold electric-fields of kV/cm for the insulator-to-metal transition in transition metal oxides and chalcogenides. We investigate the similarities between the resistive switching and the charge-density-wave (CDW) system. Motivated by the CDW theories, we construct a Lagrangian for the gap parameter and investigate the role of the quantum fluctuations to the gap parameter as a quantum variable. We discuss how quantum corrections affect the nonequilibrium resistive transition.


1:51PM S50.00014: Emergent properties in films of transition metal oxides*  D. LAHNEMAN (Presenter), P. MCARDLE, H. JIANG, M. M. QAZILBASH, Department of Physics, College of William & Mary, T. SLUSAR, H.-T. KIM, Metal-Insulator-Transition Laboratory, Electronics and Telecommunications Research Institute (ETRI), A. BISWAS, Department of Physics, University of Florida, F. KEILMANN, Fakultät für Physik & Center for NanoScience (CeNS), Ludwig-Maximilians-Universität — Transition metal oxides exhibit diverse emergent phenomena such as strongly correlated Mott insulating states, magnetic and structural phase transitions, and metal-insulator transitions. Many of these emergent states occur at nanometer length scales which cannot be accessed with traditional infrared focusing methods due to the Abbe diffraction limit. However, scattering-type scanning near-field infrared microscopy (S-SNIM) can circumvent the Abbe diffraction limit and probe optical properties with spatial resolution of tens of nanometers. We have coupled table-top plasma light sources developed in-house to a commercial S-SNIM apparatus from Neaspec GmbH to demonstrate broadband infrared nano-spectroscopy. This is used to study the novel nanoscale properties of ultrathin vanadium dioxide (VO$_2$) film on rutile titanium dioxide (TiO$_2$) substrate. Due to strain from the substrate, the metal-insulator transition in the VO$_2$ film occurs at a temperature of 305 K which is much lower than in bulk VO$_2$. We also study the surface metallic layer induced by vacuum-annealing of insulating strontium titanate (SrTiO$_3$) crystals and extract the dynamical properties of the free charge carriers.

* M.M.Q. acknowledges support from ETRI and the National Science Foundation (NSF).

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S51 DCMP: Graphene: Electron interactions Mile High Ballroom 1D - George Kioseoglou, Univ of Crete
11:15AM S51.00001: Fabry–Pérot Quantum Hall Interferometry in Graphene  YUVAL RONEN
(Presenter), THOMAS WERKMEISTER, Harvard University, DANIAL HAEI NAJAFABADI, University of Massachusetts Lowell, ANDREW PIERCE, BOBAE JOHNSON, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, AMIR YACOBY, PHILIP KIM, Harvard University — The fractional quantum Hall effect (FQHE) manifests when a large magnetic field is applied to a 2-dimensional electron gas with strong electron-electron interactions. The excitations of this highly correlated phase are expected to possess anyonic exchange statistics. Inspired by experiments in GaAs heterostructures that have attempted to demonstrate anyonic exchange statistics via quantum Hall interferometry, we explore the possibility of determining quasiparticle charge and statistics by measuring quantum Hall interferometers in graphene heterostructures. We utilize hBN-encapsulated monolayer graphene with top and bottom graphite gates to electrostatically define interferometers in the FQHE regime. We demonstrate that two quantum point contacts (QPC), which individually act as beam splitters for quantum Hall edge states, cascaded in series forms a Fabry–Pérot interferometer. We will discuss development toward realizing Aharanov-Bohm dominated interference.

11:27AM S51.00002: Optical conductivity of graphene with second-nearest neighbors coupling*  ENRIQUE MUNOZ (Presenter), Physics, Pontifical Catholic University of Chile, HORACIO FALOMIR, Physics, Universidad Nacional de La Plata, MARCELO LOEWE, Physics, Pontifical Catholic University of Chile, RENATO ZAMORA, Centro de Investigacion y Desarrollo de Ciencias Aeroespaciales (CIDCA), Fuerza Aerea de Chile — Optical transparency experiments show that optical conductivity depends on the fine structure constant, as it can be fully explained within the effective theory of two-dimensional relativistic Dirac fermions. In this work, we investigate how this property is affected by second-nearest-neighbors coupling t'. Within a field theoretical representation in the continuum approximation arising from an underlying tight-binding atomistic model, we obtain the dependence of the optical conductivity on frequency, temperature and finite chemical potential. We investigated the model in the Keldysh contour representation at zero temperature[1], as well as in Matsubara space for finite temperature and chemical potential[2]. Our results reproduce the universal and experimentally verified value at zero frequency and, more importantly, they reveal that a small but still measurable shift in the conductance minimum at finite temperatures arises as a function of the second-nearest neighbors hopping t’, thus providing the possibility to directly measure this parameter in transport experiments.

References:


*We thank Fondecyt No 1190361 for financial support.
The equilibration dynamics of spin-polarized quantum Hall edges at graphene p-n junction

ARUP KUMAR PAUL (Presenter), MANAS SAHU, CHANDAN KUMAR, Indian Institute of Science - Dept of Physics, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Namiki 1-1, Ibaraki 305-0044, Japan., ANINDYA DAS, Indian Institute of Science - Dept of Physics — The understanding of equilibration dynamics of quantum Hall (QH) edges is essential to realize an electron interferometer, which has the potential to exhibit fractional statistics and quantum entanglement. Recently, graphene pn junction with spin-valley polarized QH edges showed an ideal platform for an electron interferometer. However, the interplay of different scattering mechanisms in equilibration of polarized QH edges at the graphene pn junction remain elusive. In this report, we have carried out the conductance together with shot noise measurements for symmetry broken QH edges co-propagating along a pn junction. The pn junction was realized in a dual graphite gated hexagonal boron nitride (hBN) encapsulated graphene device. Earlier studies with unpolarized QH edges showed incoherent processes as the dominant scattering mechanism for mode mixing. However, Our results reveal that the mode mixing dynamics of the polarized QH edges are much more intricate depending on the spin sequence of QH edges. A complete crossover from incoherent to fully coherent scattering regime was observed by tuning the number of participating polarized QH edges at the pn junction, which will pave the way to design the electron quantum optics experiments based on polarized QH edges of graphene.

Light-induced anomalous Hall effect in graphene*

JAMES MCIVER (Presenter), BENEDIKT SCHULTE, FALK-ULRICH STEIN, TORU MATSUYAMA, GREGOR JOTZU, GUIDO MEIER, ANDREA CAVALieri, Max Planck Inst Structure & Dynamics of Matter — In this talk I will discuss our recent observation of an anomalous Hall effect in monolayer graphene driven by a femtosecond pulse of circularly polarized light [1]. This was achieved using an ultrafast device architecture based on photoconductive switches. The dependence of the Hall effect on a gate potential used to tune the Fermi level reveals multiple features that reflect a Floquet-engineered topological band structure [2], similar to the band structure originally proposed by Haldane [3]. This includes an approximately 60 meV wide conductance plateau centered at the charge neutrality point, where a gap of equal magnitude is predicted to open. We find that when the Fermi level lies within this plateau, the non-equilibrium anomalous Hall conductance saturates around 1.8±0.4 e^2/h.

References

*The research leading to these results received funding from the European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013)/ERC Grant Agreement no. 319286 (QMAC). J.W.M. received funding from the Alexander von Humboldt Foundation.
12:03PM S51.00005: Landau Levels in Bilayer Graphene under Pressure*  BRET GREEN
(Presenter), JORGE OSVALDO SOFO, Pennsylvania State University — Bilayer graphene in a magnetic field hosts various ordered phases near neutrality, built from 8 low-energy Landau levels labeled by orbital n=0,1, valley ξ=+,− and spin σ=↑,↓. Phase energies depend strongly on interactions and the variables magnetic field, interlayer bias, and pressure. We find the ground state as function of these variables using a Hartree-Fock treatment including the effects of metallic gates, layer separation, layer thickness. Gates screen long-range interactions, separation weakens intervalley interactions, and thickness weakens the Coulomb blockade between layers; these effects distort the phase diagram but do not change its topology. We find that pressure strengthens the noninteracting scale relative to the Coulomb energy, which drives phase transitions to occur at lower fields. This stabilizes two orbitally polarized states not yet predicted or observed, adding to previously-identified valley-, spin-, and partially polarized states.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE1255832. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author and do not necessarily reflect the views of the National Science Foundation.

12:15PM S51.00006: Ballistic to hydrodynamic crossover in twisted bilayer graphene
ISABELLE PHINNEY (Presenter), DENIS BANDURIN, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — At elevated temperatures, electron-electron (e-e) collisions dominate transport in high-mobility graphene, causing the flow of charge carriers to resemble that of classical fluids or gases and allowing for a hydrodynamic description [1][2]. However, experimental conditions are typically such that the onset of fluidity and truly hydrodynamic phenomena occur in a regime where electron-phonon scattering becomes significant. Twisted bilayer graphene (TBG), which has already seen success as a host for the study of strongly interacting electron systems [3], can provide an exceptional alternative platform to study hydrodynamic electron flow due to reduced Fermi velocity and thus a higher e-e scattering rate. Here we show that, at liquid helium temperatures, such devices exhibit micrometer-scale ballistic transport, probed using transverse magnetic focusing. At higher temperatures, we observe the development of a negative potential in the vicinity of the current injecting contact, which can be attributed to the onset of hydrodynamic electron behavior.

12:27PM S51.00007: Hydrodynamic electron flow in a graphene-based device with engineered edge conditions*  
RUPINI KAMAT (Presenter), ARTHUR W BARNARD, JOE FINNEY, Stanford Univ, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, MARC KASTNER, DAVID GOLDHABER-GORDON, Stanford Univ — Hydrodynamic electron flow is expected to emerge in the regime where electron-electron interactions dominate over all other interactions. In this regime, electrons should flow like a viscous fluid. Evidence of such behavior in graphene has been found experimentally in the form of superballistic flow through constrictions [1] and negative local resistance measurements [2]. Hydrodynamic electron transport may strongly depend on boundary conditions, which can range from no-slip (all tangential momentum is dissipated at the boundary) to no-stress (the boundary exerts no force on the fluid). To isolate the impact of boundary conditions on hydrodynamic electron flow, we have fabricated a graphene device in a pipe geometry with the first half of the pipe having smooth edges and the second half having jagged edges. Through a combination of simulations and transport measurements with this device, we tune between the two extreme boundary conditions and identify the impact of edge geometry on the flow profile of a viscous electron fluid.


*This work is supported by the NSF Graduate Research Fellowship under Grant DGE-1656518 and the U.S. D.o.E. under Contract DE-AC02-76SF00515.

12:39PM S51.00008: Hydrodynamic and Ballistic AC transport in two-dimensional Fermi Liquids  
MANICHANDRA MORAMPUDI, GITANSH KATARIA, DESHDEEP SAHDEV (Presenter), Quazar Technologies Pvt. Ltd, RAVISHANKAR SUNDARARAMAN, Materials Science and Engineering, RENSSELAER POLYTECHNIC INSTITUTE — Electron transport in clean two-dimensional systems with weak electron-phonon (e-ph) coupling can transition from an Ohmic to a ballistic or a hydrodynamic regime. The ballistic regime occurs when electron-electron (e-e) scattering is weak whereas the hydrodynamic regime arises when this scattering is strong. Despite this difference, we find that vortices and a negative nonlocal resistance believed to be quintessentially hydrodynamic are equally characteristic of the ballistic regime. These non-Ohmic regimes cannot be distinguished in DC transport without changing experimental conditions. Further, as our kinetic calculations show, the hydrodynamic regime in DC transport is highly fragile and is wiped out by even sparse disorder and e-ph scattering. We show that microwave-frequency AC sources by contrast readily excite hydrodynamic modes with current vortices that are robust to disorder and e-ph scattering. Current reversals in the non-Ohmic regimes occur via repeated vortex generation and mergers through reconnections (movie : vimeo.com/261891439). Crucially, AC sources give rise to strong spatiotemporal correlations across the entire device that unambiguously distinguish all regimes.
12:51PM S51.00009: Dynamic response functions of graphene with short-range interactions*  MEGHA AGARWAL (Presenter), EUGENE MISHCHENKO, OLEG STARYKH, University of Utah — We consider a short-range interaction between electrons in graphene and determine their dynamic response functions, such as a longitudinal and a transverse electric conductivity and a polarization function. The calculations are performed to all orders in the interaction by taking into account the self-energy renormalization of the electron velocity and using a ladder approximation to account for the vertex corrections, ensuring that the Ward identity (charge conservation law) is satisfied. We discuss whether a collective mode can exist in this system corresponding to the propagation of electric polarization of correlated electron-hole pairs.

*M.A. and E.M are supported by the Department of Energy, Office of Basic Energy Sciences, Grant No. DE-FG02- 06ER46313.
OS is supported by NSF DMR Grant No. 1928919.

1:03PM S51.00010: Detecting Hall viscosity in the absence of inversion or time reversal symmetries  MUHAMMAD IMRAN (Presenter), University of Florida — The Hall viscosity is experimentally observed in graphene. The Hall viscosity is characterized by the induced voltage with its polarity opposite to the Hall voltage. A formula is derived for the induced voltage entering from the Hall viscosity for the prototype models of bilayer graphene in the absence of time reversal symmetry and the semiconductor heterostructures with strong spin orbit coupling. The fault tolerant Hall viscosity is predicted to be observed in the non-local resistance measurement.

1:15PM S51.00011: Reciprocal and non-reciprocal energy and momentum drag between 1D and 2D conductors  LAUREL ANDERSON (Presenter), AUSTIN K CHENG, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, PHILIP KIM, Harvard University — Double-layer drag experiments are an exceptionally sensitive tool for studying interactions in low-dimensional systems, since the drag response depends on long-range Coulomb interactions rather than particle exchange. Graphene in particular has exhibited unusual drag effects near charge neutrality that have been attributed to competing energy and momentum transfer between the layers. We have performed measurements of 1D-2D drag resistance between a single carbon nanotube (CNT) and monolayer graphene separated by a few-layer boron nitride flake. At high temperatures, the drag response is symmetric under interchange of the drive and drag layers, and resembles momentum transfer from drive to drag layer. This layer reciprocity is broken near the charge neutrality point of graphene at lower temperatures, which can be attributed to energy transfer or thermoelectric effects. Intriguingly, the high-temperature drag response decays with distance from the CNT slower than expected from the Ohmic diffusive current distribution. This suggests additional electron interactions coming into play near charge neutrality in the graphene layer.
1:27PM S51.00012: Cavity quantum electrodynamics with cyclotron resonance transitions in graphene  
YASHIKA KAPOOR (Presenter), JORDAN RUSSELL, ELLIE IRENE HUNT, REBECCA LIM, ERIK HENRIKSEN, Washington University, St. Louis — Cyclotron resonance transitions between highly-degenerate Landau levels are good candidates to achieve the ultrastrong coupling regime in cavity QED, as shown recently for GaAs quantum wells [1]. Graphene provides a similarly ideal platform, with the additional advantage of a strongly anharmonic Landau level spectrum so that a two-level system may be readily explored. We have recently demonstrated graphene cyclotron transitions with quality factor Q~500 at a field of 8 T. Incorporated into cavities with either thin metal or dielectric mirrors, we estimate that cooperativities C~100 and reduced coupling strengths \( \eta \sim g/\omega \sim 0.2 \) can be reached using graphene in an infrared cavity. We will present initial results of measurements on such graphene cavity QED devices and outline prospects for reaching higher coupling strengths.  

1:39PM S51.00013: Cyclotron Resonance in Dual-Gated Bilayer Graphene  
JORDAN RUSSELL (Presenter), JESSE BALGLEY, YASHIKA KAPOOR, Washington University, St. Louis, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ERIK HENRIKSEN, Washington University, St. Louis — We report observations of cyclotron resonance in boron nitride-encapsulated, dual-gated bilayer graphene by way of transmission infrared magnetospectroscopy. The inter-Landau level transitions \(-2 \rightarrow 1\) and \(1 \rightarrow 2\) are studied at a fixed magnetic field of 13 T as a function of the Landau level filling factor, \( \nu \), and the layer symmetry-breaking perpendicular electric displacement field, \( D \). Varying \( D \) at \( \nu = 4 \) yields a direct and high-resolution measurement of the optical bandgap in bilayer graphene at low energies. For increasing \( D \) at \( \nu = 0 \) we observe a varying number of transitions as the K and K' valleys diverge, while a sharp change in the CR energies signals the transition to a layer polarized state at finite \( D \). A detailed description of the data requires consideration of band parameters beyond the lowest order inter- and intra-layer hopping terms. Measurements at \( D = 0 \) reveal a pronounced electron-hole asymmetry and many-body interaction effects as \( \nu \) is varied.  

1:51PM S51.00014: Dynamic gauge field and quantum pumping in graphene nanoelectromechanical resonators*  
RUI PU (Presenter), DU XU, State Univ of NY - Stony Brook —  
Quantum pumping generates charge or valley current through periodic variation in its internal parameters. Graphene, with its large electron mobility and strong coupling between electronic properties and mechanical strain, is a promising candidate for the experimental realization of quantum pumping. Here we study the case of graphene nanoelectromechanical resonator suspended over a gate electrode as a quantum charge pump. The deformation of graphene sheet from electrostatic potential induces a cyclic modulation of carrier density as well as an effective dynamic gauge potential. By explicit breaking of spatial inversion symmetry, we observed a finite charge pumping current near the mechanical resonance frequency. We also explore the possibility of generating valley current in graphene nanoelectromechanical resonators.  

*This work is funded by NSF award DMR-1808491
11:15AM S52.00001: Symmetry breaking of in-plane anisotropic magnetoresistance with temperature in La-doped Sr$_2$IrO$_4$ film* MINGRUI LIU (Presenter), HONGXIA XUE, JIANCHAO MENG, Beijing Normal Univ, RUIPENG BAI, Chinese Academy of Sciences, WEIMIN JIANG, ZHE ZHANG, JINGZHOU LING, LIN HE, RUIFEN DOU, CHANGMIN XIONG, JIACAI NIE, Beijing Normal Univ — Electron-doped Sr$_2$IrO$_4$ has been the subject of recent attention because of its similarities with hole-doped La$_2$CuO$_4$. However, direct evidence of its superconductivity has not yet been observed, which has led to various unresolved issues related to this material. In this study, a 14-nm thick La-doped Sr$_2$IrO$_4$ film was grown on a (001) SrTiO$_3$ substrate. We found that the fourfold component of the in-plane anisotropic magnetoresistance disappears and is replaced by a twofold symmetry as the temperature increases. Variable-temperature x-ray diffraction and spatially resolved optical second-harmonic generation experiments eliminate the possibility of crystal structural distortion. The temperature dependence of direct current magnetization measurements indicates that a change in the spin structure may account for the symmetry breaking, similar to the nematic ordering of iron-based and other superconductors. These provide a perspective on these materials that helps elucidate the nature of magnetic interactions and explores the expected superconductivity of iridates.

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11:27AM S52.00002: Rock-salt type superconductor/ferromagnet heteroepitaxial junction: LaO/EuO* KENICHI KAMINAGA (Presenter), DAICHI OKA, HIROFUMI OKA, TOMOTERU FUKUMURA, Tohoku University — We report the first synthesis of rock-salt type superconductor/ferromagnet heteroepitaxial junctions using ferromagnetic semiconductor EuO [1]. As the superconducting layer, we deposited LaO with the maximum $T_c$ of 5.2 K onto EuO. The small lattice mismatch made it possible to synthesize a high-quality heteroepitaxial junction with an atomically sharp interface that realizes the ideal magnetic proximity effect. The magnetization of LaO/EuO heteroepitaxial junctions was governed by the ferromagnetic EuO layer. The saturation magnetization of 7 $\mu_B$/Eu atom at 5 K was equivalent to that of EuO thin film. Owing to the sharp interface and the strong magnetization, superconductivity in 21 nm thick LaO layer was fully suppressed by only 6 nm thick EuO layer. This system can be used for a new heteroepitaxial platform of superconducting spintronics devices. [1] K. Kaminaga et al., Chem. Lett. 48, 1244 (2019).

*This work is supported by JSPS-KAKENHI (Nos. 26105002, JP17J05331, 18H03872, 18H03876, 19K15440), and the Mitsubishi Foundation.
11:39AM S52.00003: Growth and electronic structure of LTO/STO heterostructure: Multimodal studies*   HAWOONG HONG (Presenter), FRIEDERIKE WROBEL, XI YAN, ANAND BHATTACHARYA, DILLON FONG, Argonne Natl Lab — LTO/STO interfaces have interesting features including 2-DEG, superconductivity and magnetism. These systems may realize complex-oxide based electronic devices. LTO is supposed to be insulators. However, PLD produced films, under compressional stress, behave like metal. It also undergoes transition to a Mott insulator below -145° C. Advanced photon source has beamlines suited for complex oxide studies. Sector-33 oxide-MBE allows operando studies of x-ray diffraction and RHEED measurements during the growth of oxide films. One can also transfer the sample in a UHV vacuum suitcase to soft-xray ARPES station at the beamline 29. Soft-xray ARPES provides significant enhancement in the penetration depth and one can study the interfaces in addition to the surfaces of samples. Deposition by alternating lanthanum and titanium did not produced pure phase of LaTiO3. Interestingly, the 6 unit cell sample from alternating deposition showed 2-DEG features in ARPES. LaTiO3 films could be successfully produced through codeposition of lanthanum and titanium. However, x-ray diffraction measurements showed the films from codeposition easily became rough after the growth.

*Work at the Advanced Photon Source was supported by the DOE, under Contract No. DE-AC02-06CH11357.

11:51AM S52.00004: Coherent lattice motion in freestanding perovskite films probed by ultrafast electron diffraction*   YIFAN SU (Presenter), ALFRED ZONG, ANSHUL KOGAR, Massachusetts Institute of Technology, DI LU, SEUNG SAE HONG, HAROLD HWANG, Stanford University, NUH GEDIK, Massachusetts Institute of Technology — Advances in femtosecond lasers make it possible to coherently generate specific phonon modes in crystals. These coherent lattice vibrations enable one to pinpoint specific atomic motion on the picometer scale, and this knowledge, in turn, helps one to realize ultrafast control of material property by laser pulses. In this experiment, we performed ultrafast electron diffraction on a 20-nm freestanding film of La_{0.67}Ca_{0.33}MnO_{3}. Following photoexcitation, we observed a 0.15 THz acoustic phonon extracted from Bragg peak intensity, position and width. By tracing the coherent oscillations in these three channels for more than 20 Bragg peaks, we are able to reconstruct in real space the unconventional atomic trajectory following the arrival of the laser pulse.

*Gordon and Betty Moore Foundation; U.S. Department of Energy
12:03PM S52.00005: Stoichiometry-Dependence of Electronic Properties in LaVO$_3$ Thin Films

BIWEN ZHANG (Presenter), JADE HOLLEMAN, Physics, Florida State University, YAN XIN, STEPHEN A MCGILL, National High Magnetic Field Laboratory, CHRISTIANNE BEEKMAN, Physics, Florida State University — LaVO$_3$ (LVO) has been proposed as a promising material for photovoltaics because its strongly correlated 3d electrons can facilitate creation of multiple electron-hole pairs per incoming photon, which would lead to increased device efficiency. Our group grows thin films of LVO on SrTiO$_3$ substrates using pulsed laser deposition. We control the La:V ratio of the films from ~60:40 to ~40:60 by adjusting laser fluences. We find that while V-rich films show behaviors that are similar to bulk LVO, films that are La-rich show remarkable differences in optical measurements, and more rich temperature dependent transport behaviors, which indicates the presence of electronic phase separation. This study allows us to better understand the complex physical properties of strongly correlated insulators paving the way for their use as absorbers in high performance photovoltaics.

*A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreements No. DMR-1157490 and No. DMR-1644779, and the State of Florida. S.M. acknowledges support under grant NSF DMR-1229217.

12:15PM S52.00006: Oxygen vacancy induced electronic phenomena of KTaO$_3$

SHASHANK KUMAR OJHA (Presenter), SANAT KUMAR GOGOI, MANISH JAIN, SRIMANTA MIDDEY, Indian Institute of Science — Emergent two-dimensional electron gas (2-DEG) at complex oxide interfaces has been a subject of huge interest over the last fifteen years. The discovery of 2-DEG at the interface between LaAlO$_3$ and SrTiO$_3$ has lead to a massive search for other 2-DEG systems. Various mechanisms viz. polar catastrophe, cationic intermixing and oxygen vacancy have been proposed to explain the origin of interfacial conduction. Since more than one mechanism can be operative simultaneously, well-defined understanding remains a challenge. In this work, we report on sole effect of oxygen vacancy on electronic structure modification of a prototypical perovskite KTaO$_3$ by deliberately creating oxygen vacancies in a pristine single-crystalline sample. Oxygen deficiency turns KTaO$_3$ into a metal which shows many interesting quantum transport phenomena such as Shubnikov-de Haas oscillations, anomalous Hall effect. Ab-initio calculations find the existence of vacancy induced local magnetic moments on Ta around vacancy and the skew scattering of conduction electrons by these local moments lead to the observation of anomalous Hall effect.
12:27PM S52.00007: Effect of Growth Conditions on the Formation of a 2-Dimensional Electron Gas at Antiferromagnetic LaCrO3 /SrTiO3 Interfaces*  ATHBY AL-TAWHID (Presenter), North Carolina State University — The realization of a high mobility two-dimensional conducting interface between a polar anti-ferromagnet, LaCrO3 (LCO) and non-polar SrTiO3 (STO) has important implications for the interfacial coupling of electronic and magnetic degrees of freedom. To realize such an interface, we examine the effect of growth conditions and post growth treatment on the structural and electronic properties of the polar/non-polar(LCO/STO) interfaces. Growth at high temperatures and low oxygen partial pressure followed by post growth annealing in Oxygen results in a 2-dimensional electron gas(2-deg) at the interface. The dimensionality of the conducting layer is confirmed by electric and magneto transport measurements. Growth at a lower temperature or higher partial oxygen pressure leads to an insulating interface. High-resolution synchrotron X-ray-based structural determination of the atomic-scale structures of both metallic and insulating LCO/STO interfaces shows structural differences between the two cases attributed to competing mechanisms present to alleviate the interfacial polar discontinuity.

*This material is based upon work supported by the National Science Foundation under Grant No. NSF DMR1751455.

12:39PM S52.00008: Interfacial mechanical coupling at the interface of Pb$_{0.2}$Zr$_{0.8}$TiO$_3$/LaNiO$_3$/SrTiO$_3$ heterostructures  CLAUDIA LAU (Presenter), CRISTINA VISANI, STEPHEN ALBRIGHT, Yale University, ZHAN ZHANG, Argonne National Lab, ANKIT DISA, Max Planck Institute for the Structure and Dynamics of Matter, DIVINE KUMAH, North Carolina State University, CHARLES H AHN, FREDERICK J WALKER, Yale University — The coupling of ferroelectric polarization to thin films of the conducting oxide LaNiO$_3$ results in large changes of conductivity at an epitaxial ferroelectric-LaNiO$_3$ interface. The observed changes in conductivity are larger than what is expected from band theory, implying the importance of electronic and structural correlations. To characterize the structural changes at the interface, specially designed capacitor structures are fabricated from thin films of PbZr$_{0.2}$Ti$_{0.8}$O$_3$ deposited on epitaxial LaNiO$_3$. The device geometry is optimized for in operando synchrotron x-ray diffraction measurements of crystal truncation rods in order to identify the atomic-scale structural changes responsible for the changes in conductivity. These structural changes include rotations of the LaNiO$_3$ oxygen octahedra, which are characterized via measurement of half-order Bragg peaks. The octahedral rotations exhibit a hysteresis loop as the applied voltage is swept through the coercive field of the ferroelectric and are correlated with the conductivity of the channel, with larger rotations leading to reduced conductivity.
Zero-Bias Anomalies Observed in the Tunneling Spectra of Sr$_3$(Ru$_{0.84}$Mn$_{0.16}$)$_2$O$_7$° YIFAN YANG (Presenter), Louisiana State University, Baton Rouge, MINGMING FU, QIANG ZOU, Center for Nanophase Materials Sciences Oak Ridge National Laboratory Oak Ridge, TN 37831, USA, RONGYING JIN, Louisiana State University, Baton Rouge, ZHENG GAI, Center for Nanophase Materials Sciences Oak Ridge National Laboratory Oak Ridge, TN 37831, USA, JIANDI ZHANG, E WARD PLUMMER, Louisiana State University, Baton Rouge — The partial substitution of Mn for Ru in the bilayer ruthenate Sr$_3$(Ru$_{1-x}$Mn$_x$)$_2$O$_7$ stabilizes long-range antiferromagnetic (AFM) ordering with the highest transition temperature $T_N = 82$ K for $x = 0.16$ [1]. Here, we report the observation of a well-defined symmetric zero-bias anomaly (ZBA) at 5.2 K in the scanning tunneling spectroscopy (STS) of $x = 0.16$. The temperature dependence of the ZBA shows thermal broadening and does not correlate with the bulk AFM transition. Consistent with this observation, there is no change in the ZBA with the application of a magnetic field (9T). This is in contrast to the case for $x = 0$, in which the ZBA is asymmetric about zero bias and magnetic field dependent which gradually vanished at 11T [2]. The more symmetric and narrower ZBA in $x = 0.16$ could originate from the distinct surface properties [3]. We will discuss the relationship between doping (disorder), the surface properties, and ZBA.


*NSF

Tuning the electronic properties of the 4d transition metal oxide LaRhO$_3$° JUAN JIANG (Presenter), TAEKYUN LEE, SANGJAE LEE, SOHRAB ISMAIL-BEIGI, FREDERICK J WALKER, CHARLES H AHN, Yale University — Perovskite transition metal oxides exhibit various novel properties due to strong correlations among their d electrons. These correlation effects are well known in the 3d transition metal oxides, such as LaCoO$_3$, where multiple spin states can be observed. Electronic correlations are expected to change as the transition metal is changed from a 3d element to a 4d element in the same column of the periodic table, for example changing from Co to Rh. To explore these changes, we grow epitaxial La$_{1-x}$Sr$_x$RhO$_3$ thin films with Sr concentrations as large as 50% using molecular beam epitaxy. Hall measurements show a sign change from hole-like conduction for low doping to electron-like conduction for a large doping level of $x=0.3$. Systematic changes in electronic structure as a function of doping are predicted by theory and may provide a basis for understanding electronic correlations in transition metal oxides.

*This work is supported by a grant from the Department of Energy, Basic Energy Sciences under grant number DE-SC0019211.
1:15PM S52.00011: Engineering Coercivity of SrRuO$_3$ thin film by SrTiO$_3$ capping layer  

EUN KYO KO (Presenter), Center for Correlated Electron Systems (CCES), Institute for Basic Science (IBS), JUNSIK MUN, Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, HAN-GYEOL LEE, JINKWON KIM, Center for Correlated Electron Systems (CCES), Institute for Basic Science (IBS), MIYOUNG KIM, Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, LINGFEI WANG, TAE WON NOH, Center for Correlated Electron Systems (CCES), Institute for Basic Science (IBS) — Oxide heterostructures have a high potential for spintronics applications due to their well-defined heterointerfaces and vast functionalities. Understanding and utilizing the advantages of oxide spintronics requires effective control of magnetism, such as engineering coercivity ($H_C$). SrRuO$_3$ (SRO) is an itinerant ferromagnet with high tunable electron-electron correlation and spin-orbit coupling. It could be a good candidate for exploring spintronics applications due to the recently discovered exotic topological properties. [1, 2]

Here, we reported our recent result on controlling $H_C$ of SRO ultrathin film by a SrTiO$_3$ (STO) capping layer. The film was deposited by pulsed laser deposition. By controlling the thickness and growth oxygen partial pressure of STO capping layer, we can tune the $H_C$ of SRO films by an amplitude over 100%. Such an effective modulation of $H_C$ is highly related to the oxygen vacancies transferred from STO capping layer to SRO film.


1:27PM S52.00012: Effects of Tungsten Doping on Magnetic and Material Properties of VO$_2$/Ni Bilayers  

LOGAN SUTTON (Presenter), JOSE DE LA VENTA, JOSHUA P LAUZIER, Colorado State University — Magnetic hybrid materials show increasing promise as candidates for magnetic storage and magnetic sensors under a wide range of operating environments. Strain coupled materials are a type of magnetic hybrid materials that show a strong potential for precise control over magnetic properties. Vanadium oxides are a class of compounds which have structural phase transitions (SPTs) at various temperatures, making them ideal candidates in the fabrication of hybrid materials of this nature. Previous work has shown sputtered vanadium oxide/ferromagnetic bilayers have large changes in magnetization and coercivity at the vanadium oxide transition temperature. In this study, a sol-gel synthesis technique was used to fabricate W-doped VO$_2$/Ni bilayers. Doping with W allows for the VO$_2$ transition temperature to be lowered in an easily controlled manner, making it more viable for various applications. The effects of this doping technique on the material and magnetic properties of the VO$_2$ layers are investigated. We find a stabilization of the rutile phase of VO$_2$, and formation of V$_2$WO$_6$. VO$_2$/Ni bilayers show a sharp decrease in the coercivity and increase in the magnetic moment at the VO$_2$ SPT. W doping decreases the temperature of these magnetic effects and also decreases their magnitude.
**1:39PM S52.00013: Pulsed-laser epitaxy of metallic delafossite PdCrO₂**  
JONG MOK OK  
(Presenter), MATTHEW BRAHLEK, Materials Science and Technology Division, Oak Ridge National Lab, WOO SEOK CHOI, Department of Physics, Sungkyunkwan University, KEVIN ROCCAPRIORE, MATTHEW F CHISHOLM, Center for Nanophase Materials Sciences, Oak Ridge National Lab, GAURAB RIMAL, Department of Physics and Astronomy, Rutgers University, SOYEUN KIM, CHANGHEE SOHN, Department of Physics, Ulsan National Institute of Science and Technology, ELIZABETH SKOROPATA, Materials Science and Technology Division, Oak Ridge National Lab, SEONGSHIK OH, Department of Physics, Sungkyunkwan University, HO NYUNG LEE, Materials Science and Technology Division, Oak Ridge National Lab — Within the metallic ABO₂ delafossites, the natural heterostructuring among the A-layers, that are highly-conductive and 2-dimensional, with the triangular and localized nature on the BO₂ is a basic platform for many interesting phenomena. Thin film growth of these materials can enable both tuning basic properties as well as giving new insight into the novel phenomena found in this class of materials, yet this has proven extremely challenging. Here, we report the epitaxial growth of the metallic delafossite PdCrO₂ by pulsed laser deposition (PLD) across many different substrates and epitaxial buffer layers and growth conditions. This work has revealed the fundamental role PLD-growth conditions, epitaxial strain, and chemical and structural character of the substrate play in stabilizing the growth of PdCrO₂. It is found that a low-strain delafossite buffer layer is required to stabilize PdCrO₂. The resulting films are commensurately strained, show very narrow rocking curve widths as low as ~0.1°, and show an antiferromagnetic transition at 40 K that persists down to as thin as 3.6 nm. This works provides key insight for the growth of the boarder class of metallic delafossites and will enable tuning the basic properties of these interesting materials.

**1:51PM S52.00014: Growth of metallic delafossite PdCoO₂ by molecular beam epitaxy**  
MATTHEW BRAHLEK (Presenter), Oak Ridge National Lab, GAURAB RIMAL, Physics, Rutgers University, JONG MOK OK, DEBANGSHU MUKHERJEE, ALESSANDRO MAZZA, LU QIYANG, HO NYUNG LEE, THOMAS ZAC WARD, RAYMOND UNOCIC, GYULA ERES, Oak Ridge National Lab, SEONGSHIK OH, Physics, Rutgers University — The ABO₂ delafossite oxides are a unique class of oxides with layered A–BO₂–A–BO₂ structure with inplane trigonal coordination. Here, we report successful growth of the metallic delafossite PdCoO₂ by molecular beam epitaxy (MBE) [1]. The key challenge is controlling the oxidation of Pd in the MBE environment where phase segregation is driven by the reduction of PdCoO₂ to cobalt oxide and metallic palladium. This is overcome by combining low-temperature atomic layer-by-layer MBE growth in the presence of reactive atomic oxygen with a postgrowth high-temperature anneal. Thickness dependence (5-265 nm) reveals that in the thin regime (<75 nm), the resistivity scales inversely with thickness, likely dominated by surface scattering; for thicker films, the resistivity approaches the values reported for the best bulk crystals at room temperature, but the low-temperature resistivity is limited by structural twins. This work shows that the combination of MBE growth and a postgrowth anneal provides a route to creating high-quality films in this interesting family of layered, triangular oxides.  

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.*
Molecular Modeling of the Adsorption-Induced Expansion of Graphene Oxide Frameworks

吸附材料如活性炭（AC）具有潜在的气体存储或分离能力。ACs经常被建模为狭缝形孔：平行的石墨烯状薄片，具有非常高的比表面积。在几乎所有的吸附分析中，吸附剂被假定结构上是惰性的。已知，在液体吸附时，吸附剂会发生结构变形。最近，门控开启转换在金属有机框架（MOF）中被观察到在亚临界气体吸附过程中。这种变形起源于固体-液体相互作用，并取决于吸附剂-吸附质相互作用的性质，有时会收缩或膨胀。最近，苯硼烷酸（DBA）石墨烯氧化物框架（GOF）的d间距的单调增加（大约为4%）在超临界吸附各种气体时被观察到。我们基于第一性原理模型的分子动力学模拟的结果表明，一个随机取向的共价连接DBA链的模型与实验观察结果一致。


Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S53 DMP: Synthesis and Characterizations of Large Scale 2D Materials I Mile High Ballroom 1F - Ismail El Baggari, Cornell University - Tag(s): Focus


In order to build these atomically thin circuits, we developed a series of chemistry-based approaches that are scalable and precise. They include wafer-scale synthesis of three atom thick semiconductors and heterojunctions (Nature, 2015; Science 2018), a wafer-scale patterning method for one-atom-thick lateral heterojunctions (Nature, 2012), and most recently, atomically thin films and devices that are vertically stacked to form more complicated circuitry (Nature, 2017). Once realized, these atomically thin circuits will be foldable and actutable, which will further increase the device density and functionality.
11:51 AM S53.00002: Chirality transfer through multistep reaction processes towards the synthesis of enantiopure chiral graphene nanoribbons*  MOHAMMED SABRI G. MOHAMMED (Presenter), NESTOR MERINO-DÍEZ, Donostia International Physics Center, JESÚS CASTRO-ESTEBAN, University of Santiago de Compostela, LUCIANO COLAZZO, ALEJANDRO BERDONCES, JAMES LAWERENCE, Donostia International Physics Center, JOSÉ IGNACIO PASCUAL, CIC nanogune, DIEGO PEÑA, University of Santiago de Compostela, DIMAS GARCÍA DE OTEYZA, Donostia International Physics Center — Besides its interest for potential optoelectronic devices, molecular chirality is of utmost importance in biology and medicine. Consequently relevant is the selective synthesis of enantiopure molecular compounds, which has been hardly addressed in the growing field of “on-surface synthesis”. In this frame, 2,2'-dibromo-9,9'-bianthracene reactants are known to form chiral graphene nanoribbons (GNR) on coinage metal substrates through a complex multi-step reaction including an initial radical step growth polymerization by Ullmann coupling and following cyclodehydrogenation steps. In this work we show how, starting from enantiopure reactants deposited onto Au(111), their chirality is sequentially transferred to the polymers and finally to the GNRs with an excellent level of selectivity. Unambiguous evidence of this effect is obtained by high-resolution scanning tunneling microscopy images.

*The project leading to this contribution has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 635919), from the Spanish Ministry of Economy, Industry and Competitiveness (MINECO, Grant No. MAT2016-78293-C6).

12:03 PM S53.00003: Narrow optical transition linewidth of MoS2 monolayers grown by chemical vapor deposition: impact of dielectric disorder  SHIVANGI SHREE, CNRS/INSA, ANTONY GEORGE, Friedrich Schiller University Jena, TIBOR LEHNERT, Ulm University, CHRISTOF NEUMANN, Friedrich Schiller University Jena, MERYEM BENELAJLA, CEDRIC ROBERT, XAVIER MARIE, CNRS/INSA, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS Tsukuba, UTE KAISER, Ulm University, ANDREY TURCHANIN, Friedrich Schiller University Jena, BERNHARD URBASZEK (Presenter), CNRS/INSA — Chemical vapor deposition (CVD) allows growing transition metal dichalcogenides (TMDs) over large surface areas on inexpensive substrates, but optical transition linewidth of as-grown monolayers (MLs) is usually tens of meV. We correlate the structural quality of CVD grown MoS2 MLs on SiO2/Si wafers studied by high-resolution transmission electron microscopy (HRTEM) with the optical quality revealed in optical emission and absorption from cryogenic to ambient temperatures. With HRTEM we determine a defect concentration of the order of $10^{13}$/cm$^2$ for our samples, comparable to standard exfoliated flakes from bulk crystals. To have access to the intrinsic optical quality of the CVD grown MLs, we remove the MLs from the SiO2 growth substrate and encapsulate them in hBN flakes with low defect density. In encapsulated MLs we show optical transition linewidth of 5 meV at low temperature T=4 K for the free excitons in emission and absorption. This is comparable to the best ML samples obtained by mechanical exfoliation of bulk material. The CVD grown MoS2 ML shows strong photoluminescence that is dominated by neutral excitons and not by defects even at cryogenic temperatures. We study the valley Zeeman effect in magnetic fields up to 9T accessible thanks to the narrow emission linewidth.
12:15PM S53.00004: Grain rotation and growth in binary hexagonal two-dimensional materials  
BRENDON WATERS (Presenter), ZHI FENG HUANG, Wayne State Univ — Generally polycrystalline structures are formed during large-scale fabrication of 2D materials, with individual crystalline domains separated by grain boundaries. During growth, these grain boundaries move and evolve as neighboring grains interact. We study this dynamic process via Phase Field Crystal (PFC) modeling for 2D hexagonal materials. By tracking the motion of circular grains misoriented with respect to the surrounding crystalline matrix, we analyze the angle dependence of grain boundary dynamics and their implications for grain growth. In particular, due to the continuity of lattice planes across the boundary the grain is expected to rotate towards a larger misorientation angle, as governed by the Cahn-Taylor mechanism for the coupled normal-tangential motion of the boundary. For binary 2D materials like hBN our PFC study indicates a dynamic property beyond this geometrically-controlled effect, particularly for grain misorientations close to 30 degree which show abnormally fast rotation and strong normal-tangential coupling. This behavior can be associated with the change of angle dependence of grain boundary energy in binary materials with lattice inversion symmetry breaking.

12:27PM S53.00005: Van der Waals Epitaxy of the Transition Metal Dichalcogenide WTe₂*  
KEVIN HAUSER (Presenter), CHRISTIAN MATT, JASON HOFFMAN, RUIZHE KANG, Harvard University, JOHAN CHANG, Physics Department, University of Zurich, JENNIFER E. HOFFMAN, Harvard University — Thin film transition metal dichalcogenides (TMD) are strong candidates for future technological application, which require controlled means of ultra-high purity synthesis, as provided by molecular beam epitaxy (MBE). So far, MBE-synthesized TMD monolayers have been limited to islands with lateral sizes on the order of tens of nanometers due to the large difference of surface diffusivity of the transition metals and chalcogen species. Here, we adopt a van der Waals epitaxy method [1], based on the metal-organic precursor W(CO)₆, with the goal to develop a growth recipe for WTe₂ monolayer films. Employing surface-sensitive measurement techniques, we characterized the as-grown films and observed WTeₓ-based, one-dimensional nanostructures at the step edges and two-dimensional islands on the substrate terraces. From these results, we investigate the growth dynamics of WTe₂ few-layer thin films.


* This work was supported by the STC Center for integrated Quantum Materials, NSF Grant. No. DMR-1231319, the Gordon and Betty Moor Foundation’s EPIQS Initiative through Grant No. GBMF4536, the Office of Naval Research, Grants N00014-18-12691 and N00014-19-1-2622, and SNSF under Grant P400P2_183890
12:39PM S53.00006: Synthesis and characterization of large-area single-crystal sheets of borophene on various metal surfaces* RONGTING WU (Presenter), Department of Chemistry and Energy Sciences Institute, Yale University, ADRIAN GOZAR, Energy Sciences Institute, Yale University, IVAN BOZOVIC, Department of Chemistry and Energy Science Institute, Yale University; Bookhaven National Laboratory — Borophene, an atomically thin covalently bonded boron sheet, has attracted great attention as a novel quantum material because of its structural tunability and potential utilization in next-generation electronics. Here, we report the synthesis of borophene on various single-crystal substrates and nanometer-scale thick crystallized metal films on sapphire. With real-time feedback from low-energy electron microscopy and diffraction, we have developed a process of enlarging monocrystal borophene domains, by repeated submersion of boron into substrates at high temperature, resurfacing and re-crystallization at low temperature. We demonstrate the synthesis of borophene as faceted micrometer-size monocrystal islands or as full-monolayer sheets. The process is scalable to wafer size; moreover, metallic buffers could be sacrificed, and sapphire substrate reused. Our work opens the door for new experiments and applications.

R. Wu, A. Gozar, I. Bozovic, “Large-area borophene sheets on sacrificial Cu(111) films promoted by recrystallization from subsurface boron”, *npj Quantum Materials* 4, 40 (2019)

*Gordon and Betty Moore Foundation's EPIQS Initiative through Grant GBMF4410

12:51PM S53.00007: In situ photo-chemical conversion of layered transition metal ditellurides* FLORENCE NUGERA (Presenter), TEPIE MENG, TARIQ AFANEH, NALAKA A KAPURUGE, Physics Department, University of South Florida, YAN XIN, National High Magnetic Field Laboratory, HUMBERTO GUTIERREZ, Physics Department, University of South Florida — WTe$_2$ and MoTe$_2$ are good candidates for spintronics, thermoelectric and piezoelectric applications. In general, the 1T` phase of these 2D materials displays metallic behavior, making them interesting candidates for in-plane interconnects when combined with 2D semiconductors. In this study, we synthesize large-area WTe$_2$ and MoTe$_2$ films using a simple CVD process. Raman spectroscopy and TEM were used to study the crystal quality as well as phase and chemical composition. Subsequently, the as-grown films were chemically modified using an *in situ* laser-assisted method recently developed in our group. The entire process takes place within a home-made mini-chamber with an optical quartz window, were the samples are exposed to a laser beam in the presence of a controlled environment rich in a different chalcogen atom (sulfur in this case). For an optimized set of parameters (e.g. exposure time and laser power), the tellurium atoms are replaced by sulfur atoms and the chemical exchange process is monitored in real time via Raman spectroscopy. The site-selective replacement of the chalcogen atoms generate metal-semiconductor heterojunctions. FET-like devices where fabricated to study the electrical response of these junctions.

*HRG acknowledge support from NSF grant DMR-1557434
Controllable Growth and Electronic Structures of 2D Transition Metal Dichalcogenides Thin Films*  

YI ZHANG (Presenter), Nanjing Univ — The 2D transition metal dichalcogenides (TMDCs) have attracted extensive interest due to their remarkable properties. Using molecular beam epitaxial (MBE) method, we achieved the controllable growth of atomically thin TMDCs MoSe$_2$ and WSe$_2$ films. Combining with the in-situ angle-resolved photoemission spectroscopic (ARPES) measurements, we directly characterized the electronic structures of them and studied the evolution of their electronic structures in 2D limit [1-2]. Moreover, we achieved band structuring engineering in epitaxial TMDCs Mo$_x$W$_{1-x}$Se$_2$ alloy monolayers with controllable stoichiometric ratio x. We also realized the growth of meta-stable 1T'-WSe$_2$ monolayer, and studied its thermo-driven structure phase transition to stable 2H-WSe$_2$ [3]. Our findings not only help understanding of TMDC materials but also enrich the family of epitaxial 2D materials toward a fully MBE grown epitaxial heterostructures for light emission and photon-voltage devices.

References

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Scaling-up atomically thin coplanar semiconductor-metal circuitry via phase engineered chemical assembly  

YU YE (Presenter), Peking Univ — Phase engineered growth of 2H-MoTe$_2$ was understood by a solid-to-solid phase transformation mechanism, enabling the controlled growth of chip-size single-crystalline 2H-MoTe$_2$. Based on that, we report on the large-scale, spatially controlled chemical assembly of the integrated 2H MoTe$_2$ field-effect transistors with coplanar metallic 1T' MoTe$_2$ contacts via phase engineered approaches.
**1:27PM S53.00010: MOCVD Growth of High Quality Large Area WS\textsubscript{2} Films**  
WILLIAM CAMPBELL (Presenter), Univ of Bath, RAVI SUNDARAM, Oxford Instruments, SIMON J BENDING, Univ of Bath — Tungsten disulphide (WS\textsubscript{2}) is of particular interest in optoelectronics because of the band gap transition from indirect to direct as the crystal thickness is reduced from bulk to a single layer [1]. To achieve large area coverage suitable for industrial applications, growth methods such as chemical vapour deposition (CVD) need to be developed. Current powder-based CVD approaches [2] produce crystalline flakes that are useful for fundamental studies but cannot produce continuous wafer scale films [3]. In this work, we produce continuous and uniform thin films of WS\textsubscript{2} via MOCVD techniques at scales up to 200mm wafer sizes.

Our films are deposited at 600C using a tungsten hexachloride precursor gas and a hydrogen sulphide sulphur source. Raman spectroscopy and photoluminescence (PL) measurements demonstrate high quality as-grown WS\textsubscript{2} thin films on sapphire substrates. We further show how a post-growth annealing step in H\textsubscript{2}S quenches sulphur vacancy sites in the WS\textsubscript{2} and dramatically increases the PL intensity.


*This research was supported by the EPSRC and Oxford Instruments (EP/L015544/1)*

**1:39PM S53.00011: Enabling Direct Write Mask Free Fabrication of Low Dimensional Nanoscale Architectures on Different Substrates using Aqueous Inks and CVD synthesis**  
IRMA KULJANISHVILI (Presenter), DHEYAA ALAMERI, DEVON KARBACH, RUI DONG, Saint Louis University, YUZI LIU, RALU DIVAN, Center for Nanoscale Materials, Argonne — Low dimensional materials such as nanowires and 2D films, when assembled in vertical or lateral arrangements, often lead to the largely enhanced properties, and new functionalities. While the preparation of layered architectures usually involves multi-step fabrication processes it also relies on mask assisted lithographic techniques. Here we present methodology for controlled selective preparation of 1D and 2D nanostructures of MoS\textsubscript{2}, WS\textsubscript{2} and ZnO in the variety of geometric assemblies by employing parallel direct write patterning (DWP) of aqueous ink precursors on substrates at predefined locations. In a two-step process (1st patterning and 2nd growth) our unconventional fabrication approach enables simple and flexible production of hetero-structures and other architectures based on “mix and match” principle in precisely controlled fashion. Location specific synthesis of materials provides access to as-grown interfaces and rapid testing of materials’ quality, crystallinity and chemical composition which was confirmed by various characterization methods (Raman Spectroscopy, PL, AFM, XRD etc). Acknowledgement. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Contract No. DE-AC02 06CH11357
**S53.0012: Formation and self-assembly of graphene nanoribbons and nanosheets in metals**

LOURDES SALAMANCA-RIBA (Presenter), XIAOXIAO GE, CHRISTOPHER KLINGSHIRN, MADELINE MORALES, ODED RABIN, MANFRED WUTTIG, University of Maryland, College Park, DANIEL COLE, CHRISTOPHER SHUMEYKO, Aberdeen Proving Ground, MD, U.S. Army Research Laboratory, SHENJIA ZHANG, Indianapolis, IN, General Cable — Composites consisting of carbon nanostructures, such as graphene and carbon nanotubes, and metals are desirable for power transmission lines, interconnects and heat transfer applications due to the combination of excellent charge carrier mobility, thermal conductivity and mechanical strength of the carbon nanostructures and the high density of electrons in the metal. Metal/nanocarbon composites made by chemical vapor deposition, friction stir, ball milling, and plasma spraying have yielded materials with enhanced hardness and tensile strength but their electrical and thermal conductivities usually deteriorate. We use an electrocharging assisted process which consists of the application of a high DC current to a mixture of liquid metal and carbon particles to form crystalline graphitic nanoribbons in the liquid metal. The solid composites have shown 5% higher electrical conductivity and enhanced local stiffness, measured by nanoindentation, compared to the pure Al alloys. Molecular dynamic simulations of nanoindentation tests into the nanocarbon metal composite show how the graphene nanoribbons impede dislocation motion and increase hardness. Conductive AFM shows an increase in the local conductivity from these samples compared to the parent aluminum alloy.

*DOE EERE Award EE0008313

**S53.0013: Growth of 10 × 10 cm² single-crystal hexagonal boron nitride monolayer on the symmetry broken substrate**

LI WANG (Presenter), XUEDONG BAI, Institute of Physics, Chinese Academy of Sciences, DAPENG YU, Shenzhen Key Laboratory of Quantum Science and Engineering, and Department of Physics, South University of Science and Technology, ENGE WANG, KAIHUI LIU, School of Physics, Peking University — The ability to grow high-quality large single crystals of essential 2D materials, is at the heart for the industrial applications of 2D devices. Atom-layered hexagonal boron nitride (hBN), with its excellent stability, flat surface and large bandgap, has been reported to be the best 2D insulator. However, the size of single-crystal 2D hBN is still typically less than the wafer scale, mainly due to the extreme difficulties in its single-crystal growth: the three-fold symmetry of hBN lattice leading to antiparallel domains resulting in twin boundaries on most substrates. Here, we report the first epitaxial growth of a 10 × 10 cm² single-crystal hBN monolayer on a low symmetry Cu(110) “vicinal surface” obtained by annealing an industrial Cu foil. Our experimental and theoretical work indicate that epitaxial growth is made by Cu<211> step-zigzag hBN edge coupling that serves to break the equivalence of antiparallel hBN domains, enabling unidirectional domains alignment of > 99%. The findings in this work can significantly boost the applications of 2D devices, and also pave the way for the epitaxial growth of broad non-centrosymmetric 2D materials, such as various transition metal dichalcogenides, into large-sized single crystals.

Reference:
Li Wang et al., *Nature*, 2019, 570, 9
Session S54 DCMP: Quenches and Transport in Driven Topological Systems  Mile High Ballroom 2A - Lei Wang, Yale University

11:15AM S54.00001: Quantized energy pumping in quasi-periodically driven Nitrogen Vacancy Centres*  ANUSHYA CHANDRAN (Presenter), Boston Univ, IVAR MARTIN, Argonne National Laboratory, PHILIP CROWLEY, Boston Univ — A spin strongly driven by two incommensurate tones can exhibit a topological class of dynamics in which it (i) pumps energy from one drive to the other at a quantized average rate, in precise relationship with the quantum Hall effect, and (ii) exhibits an oscillatory response to a perturbation to the phases of the drives. We show these remarkable signatures to be realized in experiments in Nitrogen Vacancy centres. We further provide an experimental demonstration of half-integer quantization of various responses at the transition between the topological and trivial classes of dynamics.

*This work was supported by NSF DMR- 1752759 and the Sloan Foundation through the Sloan Research Fellowship.

11:27AM S54.00002: Z2 topological quench dynamics  POK-MAN CHIU (Presenter), PO-YAO CHANG, Natl Tsing Hua Univ — In this talk, we present a quench setup for a realization of a Z2 topological quench dynamics in 3+1 dimensions. We show the Z2 feature can be identified from the flow of Berry phase. In addition, the entanglement spectra in both real and frequency space reveal the topological features. Finally, we discuss some possible realizations of our model.

11:39AM S54.00003: Photoinduced interfacial chiral modes in threefold topological semimetal*  SEIKH ISLAM (Presenter), ALEXANDER ZYUZIN, Aalto University — We investigate the chiral electronic modes at the interface between two regions of a threefold topological semimetal, which is illuminated by left and right handed elliptically polarized waves. The radiation effects on the band structure of semimetal is analyzed by using Floquet theory. Two distinct solutions of the interface modes are found with the chirality depending on the phase of the irradiation. We also consider the anomalous Hall response which is attributed to the interband contribution between dispersionless flat band and conic bands.

*This work is supported by the Academy of Finland
11:51AM S54.00004: Space-time group symmetry and response functions Congjun Wu
University of California, San Diego — Congjun Wu (Presenter), University of California, San Diego —
Recently, space-time group was proposed to describe the dynamic crystalline symmetries of a large class of dynamic systems beyond the Floquet system (Xu and Wu, Phys. Rev. Lett. 120, 096401 (2018)), including laser-driven solid crystals, dynamic photonic crystals, and optical lattices. We further study its consequences on physical observables on the response functions by applying the group theory representation analysis. This work will provide useful guidance for studying physical properties in time-dependent systems.

12:03PM S54.00005: Electrons in Narrow-Band Moire Graphene: Electric and Magnetic Two-Dimensional Bloch Oscillations  
Zhiyu Dong, Ali Fahimnia, Leonid Levitov (Presenter), Massachusetts Institute of Technology — Bloch oscillating electrons, moving in a two-dimensional crystal under a DC electric field, are described, in a quasiclassical picture, by trajectories that wind quasiperiodically around the 2D Brillouin zone. The oscillations feature two or more discrete frequencies that depend on the field, but not on individual particle velocities, producing narrow lines in ensemble-averaged noise power spectrum. An externally applied magnetic field alters the dynamics, creating new types of Bloch oscillations that do not exist in one-dimensional solids. The conventional “electric” oscillations persist at weak B fields; above a critical B value a different dynamics sets in that combines Bloch oscillations and Larmor drift. In this “magnetic” regime particle trajectories are extended in position space and confined in momentum space, with a complex chaotic behavior arising at the transition.

12:15PM S54.00006: Energy filtered leads for quantized transport in Floquet systems* 
Netanel Lindner (Presenter), Technion - Israel Institute of Technology, Mads Kruse, Mark Rudner, Niels Bohr Institute —
In equilibrium, robust electronic edge or surface modes play key roles in the fascinating quantized responses exhibited by topological materials. Topological bands and edges states can be induced dynamically even in trivial materials, using a time-periodic drive. In contrast to their equilibrium counterparts, the dynamically induced Floquet topological insulators do not exhibit quantized transport when probed using conventional measurements, such as the differential conductance. This lack of quantization arises due to photon assisted tunneling from the system to the leads and vice versa. We show that quantization of the differential conductance can be restored by connecting the system and the leads via an energy filter. We discuss the utility of this approach for achieving quantization of other responses in topological Floquet systems.

*We acknowledge support from the European Research Council (ERC) under the European Union Horizon 2020 Research and Innovation Programme (Grant Agreements No. 639172 and No.678862), from the Israeli Center of Research Excellence (I-CORE) “Circle of Light”, the Villum Foundation, and CRC 183 of the Deutsche Forschungsgemeinschaft.
Photoinduced Topological Phase Transition and Optical Conductivity of Black Phosphorene

YOUSUNG KANG (Presenter), KYUNGSUN MOON, Yonsei University

We theoretically study the photoinduced topological phase transition of black phosphorene induced by laser light with moderate-intensity, which can satisfy the experimentally realistic requirement to preserve the quality of the sample. By deriving the effective Floquet Hamiltonian in terms of pseudo-spin S=1/2 degrees of freedom, we calculate the Chern number and the optical conductivity of the system with varying laser frequency. As one can expect from the photon-assisted transport, the longitudinal optical conductivity has a threshold frequency at $\Omega=\Delta/h$ with $\Delta$ being the band gap of black phosphorene. Unlike the longitudinal optical conductivity, the optical Hall conductivity sharply increases when $h\Omega$ goes beyond one half of the band gap $\Delta/2$. We also show that the Chern number changes from trivial to non-trivial one upon increasing frequency beyond $h\Omega=\Delta/2$.

This work is supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF-2016R1D1A1B01013756).

Enhancement of High Harmonics Generation by Floquet Engineering

ABHISHEK KUMAR (Presenter), YANTAO LI, BABAK H SERADJEH, Indiana Univ - Bloomington

High harmonic generation (HHG) in gaseous systems and solids is well studied. Since periodically driven systems can produce harmonic response, it is important to study the influence of external driving on the HHG power spectrum. We formulate a theory of high-harmonic current using Floquet theory of periodically driven systems. As an application of our theory, we study HHG in the Su-Schrieffer-Heeger (SSH) model with and without periodic drive. We find that there is a significant enhancement in higher harmonics when the system is driven. Moreover, this enhancement peaks for an optimal harmonic at a value that increases when the intensity of the laser is reduced. This means HHG can be generated even at lower pulse intensities in a Floquet system. We obtain analytical expressions for HHG power spectrum in the high-frequency approximation for driven SSH model. Further, we study the effects of laser polarization and occupation of Floquet bands on HHG in two dimensional systems. We also investigate the consequences of spatiotemporal symmetries and Floquet topology for HHG in Floquet systems.

This work is supported by the NSF CAREER Grant DMR-1350663, DOE grant DE-SC0020343, the College of Arts and Sciences at Indiana University.
12:51PM S54.00009: Correlation-Enhanced Quantized Charge Pumping* JACOB MARKS
(Presenter), Physics Department, Stanford University, MICHAEL SCHÜLER, Stanford Institute for Materials and Energy Science (SIMES), Stanford University, JAN BUDICH, Technical University Dresden, THOMAS DEVEREAUX, Photon Sciences, Stanford Linear Accelerator (SLAC) — We investigate charge pumping in the vicinity of order-obstructed topological phases. To explore this, we study a prototypical Su-Schreiffer-Heefer model with non-local interaction that gives rise to orbital charge density wave order, and characterize the impact of this order on the model's topological properties. In the ordered phase, where the many-body topological invariant loses quantization, we find that not only is quantized charge pumping possible, it is assisted by the collective nature of the orbital charge density wave order.

*Supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract DE-AC02-76SF00515.

1:03PM S54.00010: Stability of dynamical quantum phase transitions in quenched topological insulators: From multi-band to disordered systems CHRISTIAN MENDL (Presenter), TU Munich, JAN BUDICH, Physics, TU Dresden — Dynamical quantum phase transitions (DQPTs) represent a counterpart in non-equilibrium quantum time evolution of thermal phase transitions at equilibrium, where real time becomes analogous to a control parameter such as temperature. In quenched quantum systems, recently the occurrence of DQPTs has been demonstrated to be intimately connected to changes of topological properties. Here, we contribute to broadening the systematic understanding of this relation between topology and DQPTs to multi-orbital and disordered systems. Specifically, we provide a detailed ergodicity analysis to derive criteria for DQPTs in all spatial dimensions, and construct basic counter-examples to the occurrence of DQPTs in multi-band topological insulator models. As a numerical case study illustrating our results, we report on microscopic simulations of the quench dynamics in the Harper-Hofstadter model. Furthermore, going gradually from multi-band to disordered systems, we approach random disorder by increasing the (super) unit cell within which random perturbations are switched on adiabatically. This leads to an intriguing order of limits problem which we address by extensive numerical calculations on quenched one-dimensional topological insulators and superconductors with disorder. (arXiv:1909.01402)

1:15PM S54.00011: Observation of long excitation lifetime in photoexcited Sb-doped Bi$_2$Se$_3$ nanoplatelets* ADAM GROSS (Presenter), YASEN HOU, ANTONIO ROSSI, DONG YU, INNA VISHIK, University of California, Davis — Bi$_2$Se$_3$ is a three-dimensional topological insulator (TI), characterized by a bulk band gap of approximately 0.3 eV and a Dirac-like protected surface state. The material is usually n-type due to selenium vacancies, and chemical substitution, such as Sb-doping, is typically needed to bring the chemical potential into the bulk band gap. We will present ultrafast transient reflectivity measurements on Bi$_2$Se$_3$ and Bi$_{2-x}$Sb$_x$Se$_3$ nanoplatelets which reveal starkly different carrier decay dynamics in n-type vs. insulating samples. This will be discussed in the context of optoelectronic applications of TIs, including as a material for exciton condensation.

*NSF DMR-1838532-0
1:27PM S54.00012: Time-domain anyon interferometry in Kitaev honeycomb spin liquids and beyond  KAI KLOCKE (Presenter), Physics, Caltech, DAVID AASEN, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, ROGER MONG, Physics, University of Pittsburgh, EUGENE DEMLER, Physics, Harvard University, JASON F. ALICEA, Physics, Caltech — Motivated by recent evidence of a non-Abelian spin liquid in α-RuCl₃, we introduce a new experimental method for probing the edge and quasiparticle content of such a phase. Our scheme exploits a pair of ancillary quantum spins that communicate via judicious time-dependent tunneling of energy into and out of the spin liquid's gapless chiral Majorana edge state. We show that the ancillary-spin dynamics not only probes the Majorana edge modes, but in suitable geometries allows one to detect individual non-Abelian anyons and emergent fermions via a time-domain counterpart of anyon interferometry developed in the quantum-Hall context. The tools that we develop are expected to be widely applicable to topological phases both in solid-state and cold-atoms settings.

1:39PM S54.00013: Electron localization in two-dimensional topological and non-topological bands* AKSHAY KRISHNA, Princeton University, MATTEO IPPOLITI, Stanford University, RAVINDRA NAUTAM BHATT (Presenter), Princeton University — Many-body localization (MBL) is a well-established phase present in disordered one-dimensional spin models with short-range interaction. However, the stability of MBL in higher dimensions, in the presence of long range interaction and under the effect of a topologically non-trivial single-particle band structure, is still an area of ongoing research. We demonstrate a method to construct nearly flat subbands with arbitrary Chern numbers, using a weak periodic potential in the lowest Landau level. This two-dimensional system is a novel platform for the detailed study of the interplay between disorder, interaction and topology in a continuum model. Using exact diagonalization, we investigate the localization properties of single-particle eigenstates, as well as the tendency to many-body localize in the presence of interaction, both in the quasi 1-D and 2-D limits. Our results are based on an analysis of both the many-body eigenvalue spacings and the time evolution of an initial charge imbalance [1], [2].


*This work was supported by DoE BES Grant DE-SC0002140.

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S55 DCMP: Topology in Magnetic Systems Mile High Ballroom 2B
11:15AM S55.00001: Infinite Matrix Product States for Spin-Liquid Wavefunctions  GABRIEL PETRICA (Presenter), University of Illinois at Urbana-Champaign, BO-XIAO ZHENG, GARNET CHAN, California Institute of Technology, BRYAN CLARK, University of Illinois at Urbana-Champaign — Quantum spin liquids are disordered ground states of interacting spin systems. As such they cannot be characterized by a local order parameter. Instead, entanglement measures, such as the entanglement spectrum and entanglement entropy, can be used to detect the presence of topological order. We present here a highly parallelizable, efficient method to obtain an infinite matrix product state for Gutzwiller projected mean-field wave-functions, a common variational class of wavefunctions used to study quantum spin liquids. We then extract the entanglement spectrum from the iMPS using it to understand the topological properties of these states.

11:27AM S55.00002: Spinon Fermi surface in the Kitaev model induced by staggered magnetic field  JING-YUN ZHANG (Presenter), HONG YAO, Institute for Advanced Study, Tsinghua University — Kitaev model on the honeycomb lattice is an exactly solvable model of realizing quantum spin liquids which exhibits two distinct spin liquids in the parameter space: a gapped phase 'A' carries $\mathbb{Z}_2$ topological order and a gapless phase 'B' carries gapless fermions and gapped vortices. For the B phase, applying a uniform magnetic field would induce a gapped spin liquid phase with non-Abelian anyons. In this talk, we will discuss the effect of a staggered external magnetic field in the B phase. We show that the original gapless Dirac cone spectra of fermions can be immediately turned into a finite spinon Fermi surface by a weak staggered field. Our analytical perturbative results are further supported by numerical computations.
11:39AM S55.00003: A New Synthetic Quantum Spin Liquid Candidate CCO111*  XIAORAN LIU, SOBHIT SINGH, Physics and Astronomy, Rutgers University, TOMOYA ASABA, Physics, University of Michigan, JESS H BREWER, TRIUMF, QINGHUA ZHANG, CAS, Beijing National Laboratory for Condensed-Matter Physics and Institute of Physics, JOHN WILLIAM FREELAND, Advanced Photon Source, Argonne National Lab, SRIMANTA MIDDEY, Department of Physics, Indian Institute of Science, MIKHAIL KAREEV, Physics and Astronomy, Rutgers University, DIPANKAR DAS SARMA, Department of Physics, Indian Institute of Science, PADRAIC SHAFER, ELKE ARENHOLZ, Advanced Light Source, LBNL, LU LI, Physics, University of Michigan, DAVID VANDERBILT, JAK CHAKHALIAN (Presenter), Physics and Astronomy, Rutgers University — Quantum spin liquid is a new state of quantum strongly correlated topological matter characterized by the presence of a Mott gap, topological order and fictionalized spectrum of spin excitations. Despite the tremendous progress in bulk synthesis of potential QSL candidates the `smoking-gun' compound remains elusive. Here, we present a new synthetic candidate QSL material successfully templated from (111)-oriented CoCr$_2$O$_4$ by pulsed laser deposition. Remarkably, as the thickness is reduced to four Kagome-triangular atomic planes, the magnetic ground state suddenly switches from a spiral order to the quantum paramagnetic regime with no sign of long-range spin ordering down to 30 mK and 9T. At the same time, the frustration factor rises by almost three orders of magnitude indicating the first realization of a quantum spin liquid state on the new artificial lattice. Our findings open the opportunities of achieving novel ultra-quantum states of matter in a broad class of synthetic materials.

*JC and XL acknowledge the support by the Gordon and Betty Moore Foundation EPiQS Initiative through Grant No. GBMF4534, and by the Department of Energy under Grant No. DE-SC0012375.

11:51AM S55.00004: Dynamics of chiral spin liquids in the Kitaev-Yao-Kivelson model  BOHAI LI (Presenter), JING-YUN ZHANG, HONG YAO, Institute for Advanced Study, Tsinghua University — Chiral spin liquid (CSL) is a type of quantum spin liquids which spontaneously break time reversal symmetry (TRS). For the exactly solvable Kitaev-Yao-Kivelson (KYK) model on the star lattice, the ground state is a CSL phase with either Abelian or non-Abelian anyons, depending on the parameters of the KYK model. We perform a theoretical study of the dynamical structure factor in both Abelian and non-Abelian phases of this model. Our result shows direct signatures of the Majorana fermions, vortex excitations, zero-energy modes of vortex excitations in the non-Abelian phase.
**12:03PM S55.00005: Z₂ topological quantum spin liquids with only two-body Ising interactions and transverse fields**  
KAI-HSIN WU (Presenter), CLAUDIO CHAMON, ANDERS W SANDVIK, Physics, Boston University — In the recent study[1], the authors proposed a generalization of the transverse-field Ising model which can realize the $Z₂$ gauge theory with only simple two-body interaction. The deconfined phase in the $Z₂$ gauge model is the topologically ordered phase that is protected against any local perturbation. The model is also interesting in the sense that it can be implemented in the D-Wave Chimera-lattice structure. Here, we study the model using exact diagonalization and stochastic series expansion quantum Monte Carlo. We present our simulation results of the transition between the confined phase and deconfined phase that support the theoretical prediction.  
*This work is supported under NSF Grant No. DMR-1710170, DOE Grant No. DE-FG02-06ER46316 and the Simons Foundation

**12:15PM S55.00006: Numerical evidence of a chiral spin liquid in the spin-1/2 honeycomb XY model**  
YIXUAN HUANG (Presenter), Physics, Univ of Houston, XIAOYU DONG, DONNA SHENG, Physics and Astronomy, California state university, Northridge, CHIN-SEN TING, Physics, Univ of Houston — The frustrated XY model on the honeycomb lattice has received lots of attentions because of the potential chiral spin liquid (CSL) in the intermediate region. Using density matrix renormalization group method on the cylinder system, we study the spin-1/2 XY model with first-neighbor (J₁) and second-neighbor (J₂) interactions, and in the presence of a chiral term. We obtain a quantum phase transition and a non-magnetic phase with finite scalar chiral order when we turn on a small chiral interaction. Further analysis of the entanglement spectrum is consistent with the Kalmeyer-Laughlin CSL in this region.  
*Donna Sheng was supported by National Science Foundation Grants PREM DMR-1828019 and by the Princeton MRSEC through the National Science Foundation Grant DMR-1420541.

**12:27PM S55.00007: Toward Kitaev's Sixteenfold Way in a Honeycomb Lattice Model**  
SHANGSHUN ZHANG, CRISTIAN BATISTA, University of Tennessee, Knoxville, GABOR HALASZ (Presenter), Oak Ridge National Lab — Kitaev's sixteenfold way is a classification of exotic topological orders in which $Z₂$ gauge theory is coupled to Majorana fermions of Chern number C. The 16 distinct topological orders within this class, depending on C mod 16, possess a rich variety of Abelian and non-Abelian anyons. We realize more than half of Kitaev's sixteenfold way, corresponding to Chern numbers 0, ±1, ±2, ±3, ±4, and ±8, in an exactly solvable generalization of the Kitaev honeycomb model. For each topological order, we explicitly identify the anyonic excitations and confirm their topological properties. In doing so, we observe that the interplay between lattice symmetry and anyon permutation symmetry may lead to a "weak supersymmetry" in the anyon spectrum. The topological orders in our honeycomb lattice model could be directly relevant for honeycomb Kitaev materials, such as $\alpha$-RuCl₃, and would be distinguishable by their specific quantized values of the thermal Hall conductivity.
12:39PM S55.00008: Finding the Generalized Gibbs Ensemble in the Real Space Entanglement Spectra of (2+1)-dimensional Chiral Topological Systems  MARK ARILDSEN (Presenter), ANDREAS W LUDWIG, University of California, Santa Barbara — The numerical calculation of entanglement spectra (ES) has become a useful way to diagnose topological properties of interesting many-body ground states. For (2+1)D quantum Hall states a correspondence between the low-lying levels of the ES across a given bipartition and of the physical spectrum of the edge states along the same cut was observed in Ref. [1]. When the ES of a chiral topological state is computed at a (finite) real space entanglement cut, however, we posit that additional physics should be visible in the splitting of the degeneracies of the low-lying energy levels arising from the presence of higher-order conserved quantities (irrelevant in the renormalization group sense) in the generalized Gibbs ensemble (GGE) associated to the theory on the edge. We analyzed the real space ES obtained in several previous numerical studies of (2+1)D chiral spin liquids with edges hosting (1+1)D conformal field theories possessing SU(2)-level-1 and SU(2)-level-2 symmetry. We fitted the splittings in these ES with sets of (irrelevant) conserved quantities and find that for the most part, we confirm their correspondence with the GGE picture outlined above.


12:51PM S55.00009: Exchange Bias and Quantum Anomalous Hall Effect in the MnBi$_2$Te$_4$-CrI$_3$ Heterostructure  HUIXIA FU (Presenter), Department of Condensed Matter Physics, Weizmann Institute of Science, CHAO-XING LIU, Department of Physics, the Pennsylvania State University, BINGHAI YAN, Department of Condensed Matter Physics, Weizmann Institute of Science — The layered antiferromagnetic MnBi$_2$Te$_4$ films have been proposed to be an intrinsic quantum anomalous Hall (QAH) insulator with a large gap. To realize this proposal, it is crucial to open a magnetic gap of surface states. However, recent experiments have observed gapless surface states, indicating the absence of out-of-plane surface magnetism, and thus the quantized Hall resistance can only be achieved at the magnetic field above 6 T. In this work, we propose to induce out-of-plane surface magnetism of MnBi$_2$Te$_4$ films via the magnetic proximity with magnetic insulator CrI$_3$. Our calculations have revealed a strong exchange bias ~40 meV, originating from the long Cr-eg orbital tails that hybridize strongly with Te p-orbitals. By stabilizing surface magnetism, the QAH effect can be realized in the MnBi$_2$Te$_4$/CrI$_3$ heterostructure. Our calculations also demonstrate the high Chern number QAH state can be achieved by controlling external electric gates. Thus, the MnBi$_2$Te$_4$/CrI$_3$ heterostructure provides a promising platform to realize the electrically tunable zero-field QAH effect.
1:03PM S55.00010: ARPES studies on antiferromagnetic topological insulators MnBi$_{2n}$Te$_{3n+1}$

YONG HU (Presenter), University of Science and Technology of China, C.-F. CHEN, ShanghaiTech University, GANG Xu, Huazhong University of Science and Technology, XIANHUI CHEN, JUNFENG HE, University of Science and Technology of China — The intrinsic magnetic topological insulators are believed to be an ideal platform for the study of various topological quantum phenomena, including the quantum anomalous Hall effect and topological magnetoelectric effect. Recently, a van der Waals layered structure, MnBi$_2$Te$_4$, was proposed to be the first intrinsic antiferromagnetic topological insulator. Furthermore, the related MnBi$_{2n}$Te$_{3n+1}$ (n=2,3) heterostructures are considered to be new magnetic topological insulators with weak interlayer magnetic coupling. In this talk, we report angle-resolved photoemission spectroscopy (ARPES) studies on a series of the heterostructures MnBi$_{2n}$Te$_{3n+1}$ (n=1,2,3). Our results reveal that the intrinsic magnetic topological insulators MnBi$_{2n}$Te$_{3n+1}$ host a rich platform to realize various novel topological states.

1:15PM S55.00011: Surface state single Dirac cone in magnetic material Gd$_x$Sb$_{2-x}$Te$_3$.*

FIROZA KABIR (Presenter), M. MOFAZZEL HOSEN, Univ of Central Florida, XIAxin DING, Idaho national lab, GYANENDRA DHAKAL, KLAUSS DIMITRI, CHRISTOPHER SIMS, SABIN REGMI, WILLIAM NEFF, Univ of Central Florida, JIAN-XIN ZHU, Los Alamos National Lab, ARJUN K PATHAK, Ames lab, KRZYSZTOF GOFRYK, Idaho national lab, MADHAB NEUPANE, Univ of Central Florida — Three-dimensional topological insulators (TI) have emerged as novel states in condensed matter physics. The surface states of a 3D TI are composed of odd number of massless Dirac cones in a Brillouin zone. The existence of these Dirac cones on the surface is characterized by the $Z_2$ topological invariant. Strongly spin-orbit coupled material Sb$_2$Te$_3$ and most of its doped materials belong to the $Z_2$ topological-insulator class. Using a combination of first-principles calculations, magneto transport properties and angle resolved photoemission spectroscopy (ARPES), we directly show that Gd$_x$Sb$_{2-x}$Te$_3$ is a large spin-orbit-induced indirect bulk bandgap magnetic material whose surface is characterized by a single topological spin-Dirac cone. We demonstrate that the dynamics of spin Dirac fermions of Sb$_2$Te$_3$ can be controlled through Gd doping, making this magnetic material classes potentially suitable for topological device applications.

*This project is supported by the Center for Thermal Energy Transport under Irradiation, an Energy Frontier Research Center funded by the U.S. DOE, Office of Basic Energy Sciences.
1:27PM S55.00012: Photon energy and polarization dependent electronic structure of Cr doped Bi2Se3 thin films  
TURGUT YILMAZ (Presenter), GENDA GU, ELIO VESCOVO, KONSTANTINE KAZNATCHEEV, Brookhaven National Laboratory, BORIS SINKOVIC, Physics, University of Connecticut — Here, we reported a comparison study of photon energy and photon polarization dependent electronic structure of Cr-doped and pristine Bi2Se3 to reveal the topological phase in transition metal doped topological insulators. Circular dichroism and photon energy dependent angle resolved photoemission experiment strongly confirm that the Cr doped samples have topologically non-trivial band structure. The surface electronic structure measurements with linear and circular polarized light show signature of the hybridization of the surface states and the impurity bands. Our observation not only provide further spectroscopic information about topological materials but also promotes additional experimental pathways to control the spin-orbital texture in topological materials.

1:39PM S55.00013: Electronic structure of topological insulator Bi2Se3 thin films on thulium iron garnet heterostructures  
SHENG-WEN HUANG (Presenter), Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, KENG-YUNG LIN, Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei, Taiwan, CHUN-CHIA CHEN, MENGXIN GUO, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, CHAO-KAI CHENG, Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei, Taiwan, CHENG-MAW CHENG, National Synchrotron Radiation Research Center, Hsinchu, Taiwan, MINGHWEI HONG, Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei, Taiwan, JUEINAI KWO, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan — Breaking time-reversal symmetry (TRS) in topological insulator (TI) leads to exotic phenomena such as quantum anomalous Hall effect (QAHE). The novel phenomena originated from a gap opening at the Dirac surface state by exchange interaction with magnetic elements. Magnetically doped TI was first reported to exhibit such an exchange gap, but the observation temperature of QAHE was less than 2 K. Another way to break TRS is through interfacial magnetic proximity effect (MPE) in TI/ferromagnetic insulator bilayer with a strong ferromagnetism and uniform interfacial magnetization. In this work, TI films Bi2Se3 were grown by molecular beam epitaxy on ferromagnetic thulium iron garnet (TmIG) with perpendicular magnetic anisotropy and high $T_C$ above 500K. The band structures of 2-6 quintuple layer (QL) Bi2Se3/TmIG bilayers were investigated by angle-resolved photoemission spectroscopy. Comparative study in 2-6 QL Bi2Se3/sapphire was also performed. The energy gap opening at the surface state of Bi2Se3/TmIG is larger than that of Bi2Se3/sapphire by about 20 meV. The larger surface state gap of Bi2Se3/TmIG could be induced by MPE, on top of hybridization of top and bottom surfaces. Our study demonstrates the opportunity of probing interfacial band of TI-based heterostructures.
Path to building quantum spin liquids and topological qubits within existing quantum hardware*  ZHICHENG YANG (Presenter), University of Maryland, College Park, DMITRY GREEN, ResearchPULSE LLC, CLAUDIO CHAMON, Boston University — We address a central problem in the creation and manipulation of quantum states: how to build topological quantum spin liquids with physically accessible interactions. Theorists have been studying models of quantum spin liquids that rely on “multi-spin” interactions since the 1970s, and, more recently, have realized that these models can be used for quantum computing. However, nature does not provide such interactions in real materials. We construct a lattice gauge model where the required, fully quantum, multi-spin interactions can in fact be emulated exactly in any system with only two-body Ising interactions plus a uniform transverse field. The latter systems do exist, and we provide an explicit embedding of our model into one such system, the commercially available D-Wave machine. Therefore, our solution is an alternative path to building a workable topological quantum computer within existing hardware. Our bottom-up construction is generalizable to other gauge-like theories, including those with fractonic topological order such as the X-cube model. Taken as a whole, our approach is a blueprint to emulate topologically ordered quantum spin liquids in programmable quantum machines.

*DE-FG02-06ER46316, DE-SC0019275

Thursday, March 5, 2020 11:15 AM - 2:03 PM

Session S56 DCMP: Topology and Correlations  Mile High Ballroom 2C - Narayan Poudel, Idaho National Laboratory

Optical Evidence of an Enhanced Electronic Effective Mass in the Anomalous Pb_{1-x}Tl_{x}Te Superconductor  LEONARDO DEGIORGI, MANUEL CHINOTTI (Presenter), ANIRBAN PAL, ETH Zurich — The narrow band-gap semiconductor PbTe exhibits a number of striking properties upon thallium (Tl)-doping, including the onset of superconductivity at temperatures T_c which are substantially higher than for materials with equivalent charge carrier concentration. Here, we provide a thorough optical investigation of Pb_{1-x}Tl_{x}Te over a very broad spectral range and contrast its normal-state, complete excitation spectrum with the optical response of the non-superconducting analog Na-doped PbTe [1]. We capture the relevant energy scales shaping their electronic structure and uncover the formation of an impurity band upon doping with Tl, which evolves into a resonant state for large doping. This implies a large density of states and an enhancement of the optical effective mass m*/m_e of the itinerant charge carriers, which is stronger for Tl- than for Na-doping. Since the enhancement of m*/m_e particularly occurs upon crossing a critical concentration x_c in Tl-doped PbTe for which T_c≠ 0, we advance its relevance for the onset of superconductivity.

Weyl-Kondo semimetal: controlling the nodes via magnetic field

SARAH GREFE (Presenter), HSIN-HUA LAI, Physics and Astronomy, Rice University, SILKE BUEHLER-PASCHEN, Institute of Solid State Physics, Vienna University of Technology, QIMIAO SI, Physics and Astronomy, Rice University — In the effort to study topological metals in strongly-correlated settings, a Weyl-Kondo semimetal (WKSM) has been concurrently discovered in theoretical\(^1\) and experimental\(^2,3\) studies. This time-reversal-invariant state appears in a non-centrosymmetric Kondo lattice model. The theoretical and experimental signatures of the WKSM phase, include correlations-enhanced specific heat \(C=\Gamma T^3\) and a giant topological Hall response from the Kondo-driven Weyl nodes being pinned near the Fermi energy. Recently, high magnetic field experiments revealed a two-stage quantum phase transition, including a topological transition from the WKSM to a Kondo insulator.\(^4\) To connect with these experiments, we studied an Anderson lattice model with terms that break both time reversal and inversion symmetries.\(^5\) Tuning these terms controls the position and number of Weyl nodes in the Brillouin zone, and several topologically distinct phases emerge in this model.

\(^1\)H.-H. Lai, S. E. Grefe, S. Paschen, and Q. Si, PNAS 115, 93 2018
\(^2\)S. Dzsaber et al., PRL 118, 246601 2017
\(^3\)S. Dzsaber et al., arXiv:1811.02819 2018
\(^4\)S. Dzsaber et al., arXiv:1906.01182 2019
\(^5\)S. E. Grefe, H.-H. Lai, S. Paschen, and Q. Si, Weyl-Kondo semimetal: towards control of Weyl nodes 2019

\(^*\)NSF DMR-1920740
Welch Foundation C-1411
11:39 AM S56.00003: Quasiparticles as Detector of Topological Quantum Phase Transitions*

SOURAV MANNA (Presenter), NAGARA SRINIVASA PRASANNA SRIVATSA, theoretical condensed matter physics, Max Planck Institute for the Physics of Complex Systems, JULIA WILDEBOER, Department of Physics, Arizona State University, ANNE E. B. NIELSEN, theoretical condensed matter physics, Max Planck Institute for the Physics of Complex Systems — Phases and phase transitions provide an important framework to understand the physics of strongly correlated quantum many-body systems. Topologically ordered phases of matter are particularly challenging in this context, because they are characterized by long-range entanglement and go beyond the Landau-Ginzburg theory. A few tools have been developed to study topological phase transitions, but the needed computations are generally demanding, they typically require the system to have particular boundary conditions, and they often provide only partial information. There is hence a high demand for developing further probes. Here, we propose to use the study of quasiparticle properties to detect phase transitions. Topologically ordered states support anyonic quasiparticles with special braiding properties and fractional charge. Being able to generate a given type of anyons in a system is a direct method to detect the topology, and the approach is independent from the choice of boundary conditions. We provide three examples, and for all of them we find that it is sufficient to study the anyon charge to detect the phase transition point. This makes the method numerically cheap.

*NSF Grant No. DMR 1306897 and NSF Grant No. DMR 1056536 for partial support.

11:51 AM S56.00004: Higher-form symmetry perspective on fracton phases*

MARVIN QI (Presenter), LEO RADZIHOVSKY, MICHAEL A HERMELE, University of Colorado, Boulder — Higher form symmetry provides a framework to understand some aspects of topologically ordered phases. Motivated by this, we study the role that higher form symmetry plays in the context of fracton phases. We introduce the notion of a non-faithful higher form symmetry and describe how fractons can arise via condensation of objects charged under such a symmetry. Finally we describe how such a non-faithful higher form symmetry can arise as a quotient of an ordinary higher-form symmetry via gauging certain subgroups.

*This research is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award number DE-SC0014415 prior to September 2019, and by the Department of Defense through the National Defense Science and Engineering Graduate Fellowship (NDSEG) program beginning September 2019.
12:03PM S56.00005: Local and Non-local correlation effects in topological quantum phase transitions  LORENZO CRIPPA (Presenter), ADRIANO AMARICCI, SISSA, GIORGIO SANGIOVANNI, Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, MASSIMO CAPONE, SISSA — The fate of quantum phase transition among different topological states in presence of strong interaction is of primary interest in condensed matter. We study the effects of electronic interactions at the local and non-local level in a paradigmatic model for topological insulator in two dimensions. In the non-interacting regime topological transitions occurs via the continuous closing the energy gap. Using Dynamical Mean-Field Theory and various cluster extensions (Cluster-DMFT, Variational Cluster Approximation, etc.), we show how short-range correlation effects are responsible for the breakdown of the continuous topological transition in favour of a first-order one. The discontinuous transition occurs without the celebrated closing of the energy gap, yet without the breaking of the symmetries which protect the topological state.

References:

12:15PM S56.00006: Anomalous localization at the boundary of an interacting topological insulator  ITAMAR KIMCHI (Presenter), University of Colorado, Boulder, YANG-ZHI CHOU, University of Maryland, RAHUL NANDKISHORE, LEO RADZIHOVSKY, University of Colorado, Boulder — The boundary of a topological insulator (TI) hosts an anomaly restricting its possible phases: e.g. 3D strong and weak TIs maintain surface conductivity at any disorder if symmetry is preserved on-average, at least when electron interactions on the surface are weak. However the interplay of strong interactions and disorder with the boundary anomaly has not been well studied theoretically. Here we present our results on this combination, for the edge of a 2D TI and the surface of a 3D weak TI, showing how it can lead to an "Anomalous Many Body Localized" (AMBL) phase that preserves the anomaly. We discuss its anomaly manifestation, predictions for experimental observations, and theoretical consequences for understanding 3D TIs and anomaly restrictions.
12:27PM S56.00007: Interaction effects on centrosymmetric Bogoliubov Fermi surfaces
HANBIT OH (Presenter), EUN-GOOK MOON, Department of physics, Korea Adv Inst of Sci & Tech —
Exotic quantum phases including topological insulators/semi-metals and non-Fermi liquids may be realized by quantum states with total angular momentum j=3/2 as manifested in HgTe and pyrochlore iridates. Recently, an exotic superconducting state with a finite density of zero energy Bogoliubov quasiparticles, Bogoliubov Fermi-surface, was also proposed in a centrosymmetric j=3/2 system with a Z2 topological invariant. We consider interaction effects of the Bogoliubov Fermi surfaces by using standard renormalization group and mean-field theory and discuss the implication of inversion symmetry breaking. Possible applications of our theory to iron based superconductors and heavy fermion systems including FeSe are also discussed.

12:39PM S56.00008: Twisted dualities and the 2d Majorana checkerboard
MARCUS BINTZ (Presenter), University of California, Berkeley — Large ensembles of bound Majorana modes can form their own strongly-interacting phases of matter. For example, a square lattice of Majoranas coupled purely by four-fermion plaquette terms may be the effective description for the vortex lattice on the surface of certain 3d topological insulators. This talk leverages recently formulated exact dualities to derive novel representations of such a 2d Majorana checkerboard. Some connections to quantum cellular automata (QCA) and subsystem symmetry protected topological order (SSPT) are also discussed.

12:51PM S56.00009: Universal SPT invariants using swap operators*
SHRIYA PAI (Presenter), MICHAEL A HERMELE, University of Colorado, Boulder — We will describe many-body topological invariants/order parameters for SPT phases that involve acting with symmetry operators and a swap operator. To do so, we use the universal notion of distinguishing between different phases of matter: phases are equivalence classes defined in the thermodynamic limit by (i) adiabatic continuity, and (ii) adding trivial degrees of freedom. In the process, we will also formulate gauge-invariant versions of these order parameters. Since our arguments for the universality of such many-body invariants do not depend on the spatial dimension we are working in, this discussion can help serve as a basis for generalizations to higher spatial dimensions. We will also show how to picture the invariant by putting the system on a spacetime manifold and by thinking in terms of TQFT partition functions.

*This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences (BES) under Award number de-sc0014415.
Exceptional-torus in strongly correlated nodal-line semimetals with many-body chiral symmetry

KAZUHIRO KIMURA (Presenter), TSUNEYA YOSHIDA, NORIO KAWAKAMI, Physical Society of Japan — Recent studies have revealed a new type of topological phase described by a non-Hermitian (NH) Hamiltonian. In equilibrium systems, if we describe the energy spectrum of quasiparticles having the complex self-energy in terms of effective Hamiltonian, NH physics naturally shows up because of the life time effects from self-energy. The most important point is the emergence of gapless defective points (DPs), which lead to an open Fermi surface, such as Fermi arcs in the bulk energy spectrum.

In previous studies, it is pointed out that the effect of symmetry leads to the symmetry protected NH band touching, such as the symmetry-protected exceptional torus (SPETs). A typical example is a parity-time reversal (PT) symmetric nodal-line semimetal (NLSM).

In this study, we demonstrate how the SPETs can emerge in strongly correlated systems. We analyze correlated NLSM on a diamond lattice model with a sublattice dependent on-site Hubbard interaction by using the dynamical mean-field theory. First, we reveal the emergence of a SPET unique to NH physics with many-body chiral symmetry, which forms the 3D open Fermi surface locked on the Fermi level. We further elucidate that the static susceptibility for a sublattice with weak interaction is enhanced by the emergence of SPETs.

Realizing the Majorana Quasiparticle fermionic dynamics in (1+1) dimensional Topological Quantum Materials*

SUSHANT KUMAR BEHERA (Presenter), PRITAM DEB, Department of Physics, Tezpur University — A Majorana fermion and its dynamics are determined by the Majorana equation having equal values of spinor and conjugate field, thereby making topological quantum material a technological reality [Phys. Rev. Lett.] 121, 067701, 2018]. It is interesting to study the dynamics of Majorana fermions in presence of external perturbations in (1+1) dimensions, a scalar potential by approaching for the first time implementing the methods of supersymmetric quantum mechanics [Phys. Rev. Lett.] 106, 060503, 2011; Rev. Mod. Phys.] 80, 1083, 2008]. Moreover, the dynamics of two competing effects (i.e. strain and magnetic field) is worth to focus in monolayer quantum material with the aim to explore its impact in various phenomena of quantum field theory, such as induced charge density, magnetic catalysis, symmetry breaking, dynamical mass generation, and magnetization. The combined effect of real and pseudomagnetic fields produces an induced valley polarization creating new platforms to design quantum computers and valleytronics devices.

*Department of Science and Technology, Govt. of India for DST-INSPIRE Fellowship (IF150325).

Tezpur University for providing HPCC Facility to perform simulation work.
1:27PM S56.00012: Crystal-to-Fracton Tensor Gauge Theory Dualities*  ZHENGZHENG ZHAI (Presenter), MICHAEL PRETKO, LEO RADZIHOVSKY, University of Colorado, Boulder — We discuss the duality between elasticity of two-dimensional crystals and fracton tensor gauge theories, developed by two of the authors [1,2,3]. This duality leads to numerous predictions for the phases and phase transitions in fracton systems, such as the existence of gauge theory counterparts to the (commensurate) crystal, supersolid, hexatic, and isotropic fluid phases of elasticity theory, that will be discussed. The classical finite temperature limit, provides a complementary description of the KTHNY theory of 2D melting, formulated in terms of a higher derivative vector sine-Gordon model. Broader implications of this duality, such as the quantum melting transitions and quantum phase diagrams, symmetry enriched fracton order, and connection to the interacting topological crystalline insulators, will be discussed.


*This work was supported by the Simons Investigator Award to L. R. from the Simons Foundation and partially by the NSF Grant 1734006.

1:39PM S56.00013: Interactions in nodal-line semimetals with quadratic band touching*  GEO JOSE (Presenter), BRUNO UCHOA, Univ of Oklahoma — We address the problem of Coloumb interactions in 3D nodal-line semimetals with quadratic band touching using perturbative Wilsonian renormalization group approach. At one loop order, we find that the non-interacting fixed point is unstable and flows to an interacting fixed point. We compute corrections to the dynamical exponent, the screening charge and find corrections to other experimentally measurable quantities such as the specific heat, compressibility, etc. We also consider the emergence of other competing instabilities in the charge sector from short-range interactions.

*We acknowledge the Carl. T. Bush fellowship at the University of Oklahoma.
TIBOR RAKOVSZKY, PABLO SALA DE TORRES-SOLANOT (Presenter), TU Munich, RUBEN VERRESEN, Department of Physics, Harvard university, MICHAEL KNAP, FRANK POLLMANN, TU Munich — Certain disorder-free Hamiltonians can be non-ergodic due to a strong fragmentation of the Hilbert space into disconnected sectors. We show how to characterize such systems by introducing the notion of 'statistically localized integrals of motion' (SLIOM), whose eigenvalues label the connected components of the Hilbert space. SLIOMs are not spatially localized in the operator sense, but appear localized to sub-extensive regions when their expectation value is taken in typical states with a finite density of particles. We will illustrate this general concept on several Hamiltonians, both with and without dipole conservation. For the former we uncover additional SLIOMs due to dipole moment conservation on finite regions of the chain. Moreover, we explain that there exist perturbations which destroy these integrals of motion in the bulk of the system, while keeping them on the boundary. This results in statistically localized strong zero modes, leading to infinitely long-lived edge magnetizations along with a thermalizing bulk. We also show that these edge modes can lead to the appearance of topological string order in a certain subset of highly excited eigenstates, and conclude providing experimental realizations of these models using existing experimental platforms.

WENJIE XI (Presenter), Department of Physics, Southern University of Science and Technology, ZHIHAO ZHANG, School of Mathematical Sciences, University of Science and Technology of China, ZHENGCHENG GU, Department of Physics, The Chinese University of Hong Kong, WEIQIANG CHEN, Department of Physics, Southern University of Science and Technology — Topological phases in non-Hermitian systems became a fascinating subject recently. In this paper, we attempt to classify topological phases in 1D non-Hermitian systems. We begin with the non-Hermitian generalization of Su-Schrieffer-Heeger(SSH) model and discuss its many body topological Berry phase, which is well defined for any quasi hermitian systems(non-Hermitian systems that have real energy spectrum). We then demonstrate that the classifications of topological phases for quasi hermitian systems are exactly the same as their hermitian counterparts. Moreover, we find that unitarity actually can emerge for fixed point partition function describing topological phases in 1D non-Hermitian systems with local interactions. Thus we conjecture that for 1D non-Hermitian system, the classification of topological phases are exactly the same as Hermitian systems.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S57 DMP: Quantum and Ferroelectric Phenomena in Layered Materials Mile High Ballroom 3A - Peter Bøggild - Tag(s): Focus
11:15AM S57.00001: Visualizing and Manipulating Bilayer Graphene Quantum Dot States*

ZHEHAO GE (Presenter), FREDERIC JOUCKEN, EBERTH A QUEZADA, Department of Physics, University of California, Santa Cruz, DIEGO RABELO DA COSTA, Department of Physics, Federal University of Ceará, JOHN DAVENPORT, Department of Physics, University of California, Santa Cruz, BIRAN GIRALDO, NOBUHIKO KOBAYASHI, Department of Electrical and Computer Engineering, University of California, Santa Cruz, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, TONY LOW, Department of Electrical & Computer Engineering, University of Minnesota, JAIRO VELASCO JR., Department of Physics, University of California, Santa Cruz — Quantum confinement enables the control of a material's electronic, spin, and optical properties. A common platform to realize quantum confinement is a quantum dot (QD), which can be achieved through various methods such as electrostatic, self-assembly, and etching. Electrostatically defined monolayer and bilayer graphene QDs are unique compared to lateral semiconductor QDs because the quasi particles in the former possess chirality. As a result, upon normal incidence on a potential barrier monolayer graphene (MLG) features a 100% transmission (Klein tunneling) and bilayer graphene (BLG) features a 100% reflection (anti-Klein tunneling). Recently, several scanning tunneling spectroscopy (STS) studies have been performed on exposed electrostatically defined MLG QDs and have revealed chiral bound states with a tunable Berry phase. However, to date, no STS studies have directly probed the quasi-bound states in BLG QDs. Here we present our latest experimental progress on directly probing and manipulating the quasi-bound states in exposed BLG QDs with a scanning tunneling microscope (STM).

*This research was funded by NSF CAREER award under award number DMR-1753367. We also acknowledge support from the Army Research Office under contract W911NF-17-1-0473.

11:27AM S57.00002: Graphene quantum dot bolometers for high frequency EPR of single molecule magnets

LUKE ST. MARIE (Presenter), A EL FATIMY, Georgetown University, JAKUB HRUBY, IVAN NEMEC, CEITEC, JAMES HUNT, Georgetown University, RACHAEL MYERS-WARD, DAVID KURT GASKILL, Naval Research Laboratory, MATTIAS KRUSKOPF, YANFEI YANG, RANDOLPH ELMQUIST, NIST, RAPHAEL MARX, JORIS VAN SLAGEREN, University of Stuttgart, PETR NEUGEBAUER, CEITEC, PAOLA BARBARA, Georgetown University — Graphene's properties, including broadband absorption and a small heat capacity, make it an ideal material for hot-electron bolometers. By nanostructuring graphene to open a quantum confinement gap, we have fabricated bolometers with extremely high responsivity. We use these graphene quantum bolometers to perform EPR spectroscopy of single molecule magnets (SMMs). We take advantage of the bolometers' extreme sensitivity to conduct these measurements on thin layers of SMMs deposited by sublimation, allowing for the observation of substrate effects not detectable when measuring bulk samples of SMMs using standard techniques.
Manipulation of quantum geometrical properties in Weyl semimetal

JUN XIAO (Presenter), Stanford Univ, YING WANG, University of California Berkeley, HUA WANG, Texas A&M University, SRI CHAITANYA DAS PEMMARAJU, SLAC, SIQI WANG, University of California Berkeley, PHILIPP KARL MUSCHER, EDBERT JARVIS SIE, CLARA M NYBY, THOMAS DEVEREAUX, Stanford Univ, XIAOFENG QIAN, Texas A&M University, XIANG ZHANG, University of California Berkeley, AARON LINDENBERG, Stanford Univ — Quantum materials with novel phases of matter are the key building blocks of energy efficient quantum electronics and powerful quantum computation. Exploiting control of those materials is fascinating to achieve new functionalities and information algorithm in future quantum devices. Quantum nanomaterials like layered materials, has revealed many exotic properties such as extremely large magnetoresistance (MR)\(^1\), type-II Weyl electron transport and diverging Berry curvature\(^2\). On the other hand, the nature of layered materials leads to ultra large tunability of physical properties via external stimuli. Here we report the manipulation of quantum geometrical properties in layered Weyl semimetal devices. With such control and various characterization means, we observed substantial modulation in optical and electrical responses from the device. The observations indicate such changes are closely associated with the variation of topological and geometrical property. Our findings highlight the potential for the realization of topological quantum devices based on layered quantum materials.


Quantum transport of a two-dimensional hole gas in a diamond/h-BN heterostructure

YOSUKE SASAMA (Presenter), KATSUYOSHI KOMATSU, SATOSHI MORIYAMA, MASATAKA IMURA, TOKUYUKI TERAJI, SHIORI SUGIURA, TAICHI TERASHIMA, SHINYA UJI, KENJI WATANABE, TAKASHI TANIGUCHI, TAKASHI UCHIHASHI, YAMAGUCHI TAKAHIDE, National Institute for Materials Science — Diamond attracts increasing attention as a next-generation semiconducting material because of its fascinating properties such as a wide-band gap, high thermal conductivity, high breakdown electric field, and high mobility. In this study, we fabricated a p-type diamond field-effect transistor (FET) using a diamond/hexagonal boron nitride (h-BN) heterostructure. A single-crystalline h-BN was cleaved by the scotch tape method and laminated on a hydrogen-terminated diamond surface. The laminated h-BN flake was used as a gate dielectric. The excellent insulating properties of h-BN enabled the mobilities of holes accumulating at the diamond surface to be higher than 300 cm\(^2\)V\(^{-1}\)s\(^{-1}\) at room temperature for hole densities above 5\times10^{12} cm\(^{-2}\). The high mobility allowed to observe Shubnikov–de Haas oscillations in both the longitudinal and Hall resistivities. The oscillations provided valuable information on the hole transport at the diamond surface, such as the cyclotron effective mass, quantum lifetime, and two dimensionality. The high-quality two-dimensional hole gas demonstrated in this study will lead to new studies of quantum transport in diamond and development of high-performance diamond electric devices. (Y. Sasama et al., APL mater. 6 111105 (2018), arXiv:1907.13500)
12:03PM S57.00005: Electrostatically gated quantum dots in van der Waals materials*
JUSTIN BODDISON-CHOUINARD (Presenter), Univ of Ottawa, ALEXANDER M BOGAN, National Research Council Canada, PAWEL HAWRYLAK, Univ of Ottawa, SERGEI STUDENIKIN, LOUIS GAUDREAU, ANDREW STANISLAW SACHRAJDA, National Research Council Canada, ADINA A LUICAN-MAYER, Univ of Ottawa — Quantum confinement of electrons into quantum dots has been thoroughly explored in materials such as silicon or gallium arsenide showing interesting physical phenomena as well as promise for use in quantum technologies. With rapid advancement in the fabrication of van der Waals heterostructures and their devices, quantum confinement provides a route for harnessing the properties of 2D materials towards building novel quantum computing platforms. Working towards that goal, in this talk we present the design and fabrication of electrostatically gated quantum structures based on monolayer and few atomic layers of molybdenum disulfide (MoS$_2$) and bilayer graphene. Furthermore, we show and discuss our preliminary electron transport results aimed at probing the confined electron states in these structures.

*The authors acknowledge funding from the National Sciences and Engineering Research Council (NSERC) Discovery Grant RGPIN-2016-06717. We also acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC) through Strategic Project STPGP-521420.

12:15PM S57.00006: Transport Properties in Interacting Graphene Quantum Dots*
FILIPÉ MATUSALEM (Presenter), ALEXANDRE R ROCHA, Univ Estadual Paulista-UNESP — Chemically derived graphene quantum dots (QD) hold great promise for applications in electronics, optoelectronics, and bioelectronics. Using a gate electrode, it is possible to control the number of electrons contained in the dot as well as the current flow when electrodes are attached. Experimentally, the fabrication of atomically precise graphene QDs consisting of low-bandgap armchair graphene nanoribbon (AGNR) segments were recently reported [1]. In this work, we apply a combination of dynamic mean field theory [2] and a molecular-based non-equilibrium Green's function technique coupled to DFT [3,4] to tackle the problem of interacting electrons in graphene quantum dots in AGNR including a gate electrode. We observe conductance peaks associated with the localized states related to the graphene QDs presented in the AGNR in a realistic parameters range giving us precise gap tunability. Such device can be used to design a graphene-based single electron transistor.

References:

*Supported by the Brazilian funding agency CNPq.
As transistors continue to scale down in size, physical limitations from nanoscale field-effect operation begin to cause undesirable effects that are detrimental to the further advancement of computing. We explore an alternative to conventional field-effect transistor operation by using dynamic strain engineering on 2D van der Waals materials to induce electronic/structural phase transitions. Strain has been widely popularized in industry in its static form to enhance silicon mobility, but using strain to dynamically control materials properties has been more challenging for 3D bonded systems due to substrate limitations and defect formation. Systems involving 2D materials are freed from substrate constraints and have high elastic limits, but have not been heavily explored for dynamic strain engineering due to the difficulty in transferring strain into a material that is weakly bonded out-of-plane. In this talk, we focus on challenges in achieving dynamically controllable strain in 2D-bonded materials and how these challenges can be overcome in a scalable on-chip device. We introduce one implementation of such a device using both static thin film stress capping layers and ferroelectric oxide gate-dielectrics. Here, MoTe$_2$ can be reversibly switched with electric-field induced strain between the 1T'-MoTe$_2$ (semimetallic) phase and a semiconducting MoTe$_2$ phase in a three-terminal field effect transistor geometry.

Using strain, we achieve large non-volatile changes in channel conductivity ($G_{on}/G_{off}$~$10^7$ vs. $G_{on}/G_{off}$~0.04 in control devices) at room temperature. Using this implementation as a starting point, other phase transitions in 2D materials may be explored using this ‘straintronic’ device concept, which may enable low-power, high-speed, non-volatile, gate-controllability over a wide variety of exotic states of matter.


*This work was supported by the National Science Foundation under Grant No. DMR-1936250.*
1:03PM S57.00008: Imaging Strain-Induced Quantum Emitters* ASHLEY CAVANAGH (Presenter), DYLAN RENAUD, MARKO LONCAR, ROBERT MOORE WESTERVELT, John A. Paulson School of Engineering and Applied Sciences, Harvard University —
Color centers in diamond produce long lived quantum emitters [1]. An alternative approach to creating quantum emitters, as suggested by [2], involves using an array of silica nanopillars to induce strain in a two dimensional Van der Waals material, creating quantum dot-like quantum emitters at each point of strain. This approach is appealing because the locations of the quantum emitters can be controlled and their properties are tunable. Our goal is to electrically characterize these strain-induced quantum emitters using the scanning probe microscope (SPM) technique described in [3]. The cooled SPM tip will be used as a moveable gate to spatially resolve rings of conductance around each point of strain due to the Coulomb-blockade and provide information about the number of electrons at each point.


*Support from STC for Integrated Quantum Materials, NSF DMR 1231319, DOE Basic Energy Sciences DE-FG02-07ER46422, and National Nanotechnology Coordinated Infrastructure (NNCI) NSF ECCS-1541959.

1:15PM S57.00009: Spin-orbit torques in heterostructures of 2D van der Waals magnets* VISHAKHA GUPTA (Presenter), GREGORY M STIEHL, THOW MIN CHAM, JOSEPH MITTELSTAEDT, ARNAB BOSE, KAIFEI KANG, SHENGWEI JIANG, KIN FAI MAK, JIE SHAN, ROBERT BUHRMAN, DANIEL RALPH, Cornell University — The discovery of intrinsic magnetism in 2D materials has opened an exciting new platform for spintronics, allowing fundamental studies of efficient mechanisms for electrically controlling magnetic materials. Here we explore spin-orbit torques in heterostructures of ultrathin single-crystal magnetic insulators and large spin-orbit coupling (SOC) materials: heavy metals and topological insulators. We report current induced switching in insulating ferromagnet \(\text{Cr}_2\text{Ge}_2\text{Te}_6\) at current densities as low as \(10^6 \text{ Acm}^{-2}\) from spin-orbit torques generated in heterostructures with Pt and Ta. We will discuss methods for quantifying the efficiency of these torques using both optical and electrical-transport techniques.

*DOE (DE-SC0017671)
Fabrication of Hall Micromagnetometers for Probing Two-Dimensional Magnets

SEAN NELSON (Presenter), MARC BOCKRATH, JOSHUA GOLDBERGER, DANIEL WEBER, Ohio State Univ - Columbus — Two-dimensional (2D) magnetic materials have emerged as a promising area for both new physics and potential spintronics applications. Recent work has shown the ballistic Hall micromagnetometry using graphene Hall bars can be used to detect the magnetization of atomically thin 2D magnetic materials. We will discuss our approach to the fabrication of such devices on top of 2D magnetic layers. The magnetic layers are first exfoliated onto a clean Si/SiO2 chip. A Hall bar is fabricated using a standard dry transfer technique, layer stacking, and electron beam lithography. The Hall bar is placed so that it half covers the magnetic layer. As in reference 1, the region covering the magnetic material is actively compared to the region not covering the magnetic material, which acts as a control. We perform low temperature magnetoconductance measurements, and the latest results will be discussed.


Effect of Potential Fluctuation on Ferroelectric-Gated Bilayer Graphene*

HANYING CHEN (Presenter), ZHIYONG XIAO, YIFEI HAO, University of Nebraska - Lincoln, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science - Japan, XIA HONG, University of Nebraska - Lincoln — We investigated the effect of a ferroelectric gate on the transport properties of bilayer graphene (BLG). BLG flakes were mechanically exfoliated on epitaxial 300 nm Ba0.6Sr0.4TiO3 (BSTO) thin films grown on Nb-doped SrTiO3 substrates. Selected flakes were fabricated into field-effect transistor devices. At 2 K, the BLG devices exhibit field-effect mobility up to µFE ~ 3,000 cm²/Vs and quantum Hall effect, from which we deduced a dielectric constant of 113 for BSTO. The devices exhibit resistance hysteresis induced by nonvolatile polarization switching at high gate voltage. The temperature dependence of BLG at the charge-neutral point can be well described by thermally activated behavior at high temperature, which evolves to nearest-neighbor hopping below 80 K. We extracted activation energy of ~20 meV and hopping energy of ~0.3 meV. The result indicates that the epitaxial BSTO films yield less potential fluctuation compared with conventional SiO2 substrate. We will also discuss the effects of remote interfacial optical phonon scattering and capping with a top h-BN layer on these ferroelectric-gated BLG devices.

*This work was primarily supported by the U.S. Department of Energy, BES, under Award No. DE-SC0016153.
1:51PM S57.00012: Improved Adhesion of Two-Dimensional Materials to Ferroelectrics from Poling

CARLA WATSON (Presenter), TASNEEM KHAN, TARA PENA, STEPHEN M WU, University of Rochester — Ferroelectric materials can control mechanical strain in coupled 2D materials to induce phase transitions with applied electric field [1]. 2D flake-to-ferroelectric adhesion is crucial to device performance since it affects the efficiency of strain transfer. We discuss a framework to enhance 2D-ferroelectric adhesion through repeated ferroelectric poling. We explore this using exfoliated MoTe$_2$ thin flakes on structurally mixed-phase rhombohedral (R)/tetragonal (T) BiFeO$_3$ (BFO) ferroelectric thin films grown with a metallic La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) bottom counterelectrode for switching. Flakes with less adhesion are less conformal to the underlying R/T-BFO stripe domains due to a competition between strain energy and adhesive force. We quantify adhesion by measuring substrate conformality before and after local out-of-plane electric-field poling with a conductive AFM probe. Local poling causes both ferroelectric switching and structural transformation between R and T phases of BFO, which contribute to enhanced substrate conformality as well as a route to on-demand nanoscale strain engineering.


*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE-1939268.

2:03PM S57.00013: Control of transport properties of hybrid molybdenum disulfide (MoS$_2$) – ferroelectric devices via domain engineering

ALEXEY LIPATOV (Presenter), University of Nebraska - Lincoln, TAO LI, Xi’an Jiaotong University, NATALIIA S. VOROBEVA, ALEXANDER SINITSKII, ALEXEI GRUVERMAN, University of Nebraska - Lincoln — We demonstrate a concept of programmable ferroelectric devices comprised of two-dimensional (2D) and ferroelectric (FE) materials, which enables precise modulation of the in-plane conductivity of a 2D channel material through nanoengineering of FE domains with out-of-plane polarization. The functionality of these new devices has been demonstrated using field-effect transistors (FETs) fabricated with monolayer molybdenum disulfide (MoS$_2$) channels on the Pb(Zr,Ti)O$_3$ substrates. Using piezoresponse force microscopy, we show that local switching of FE polarization by a conductive probe can be used to tune the conductivity of the MoS$_2$ channel. Specifically, patterning of the nanoscale domains with downward polarization creates conductive paths in a resistive MoS$_2$ channel so that the conductivity of an FET is determined by the number and length of the paths connecting source and drain electrodes. In addition to the device programmability, we demonstrate the device ON/OFF cyclic endurance by successive writing and erasing of conductive paths in a MoS$_2$ channel. These findings may inspire the development of advanced energy-efficient programmable synaptic devices based on combination of 2D and FE materials.
11:15AM S58.00001: Theory and implementation of nonlinear X-ray spectroscopies: application to time-resolved diffraction, X-ray chirality and transient grating experiments

[Invited] JEREMY ROUXEL (Presenter), SHAUL MUKAMEL, University of California, Irvine — Thanks to the progresses of X-ray light sources, ultrafast non-linear X-ray experiments are now feasible. We discuss how such spectroscopies can be theoretically described in terms of the minimal coupling Hamiltonian, allowing a unified description of diffraction-detected and resonant techniques. Coherent X-ray sources can access new material quantities such as transition charge densities thanks to their atomic resolution. We present how X-ray experiments can make use of their element selectivity to probe matter chirality with additional structural information. Finally, we present hybrid visible pump - X-ray probe transient grating measurements conducted on Bi4Ge3O12 (BGO). This 3rd order technique allows to probe excited carrier dynamics and propagation at unprecedented time and length scale.

11:51AM S58.00002: Quantum control of high-energy harmonic generation by pulse shaping

GUAN GUI (Presenter), ROBERT M KARL, JEREMY THURSTON, PETER JOHNSEN, CHARLES BEVIS, IONA BINNIE, HENRY KAPTEYN, MARGARET MURNANE, CHEN-TING LIAO, JILA, University of Colorado Boulder — High harmonic generation (HHG) is the most extreme high-order nonlinear optical process, which can be selectively enhanced at lower photon energies around ~40eV by using temporally shaped laser pulses [1]. Here we demonstrate the ability for enhancing the HHG flux and spectrum at higher photon energies around ~100eV, relevant for imaging and magnetic spectroscopies. By changing the spectral phase of the 800nm driving laser pulses using a genetic algorithm, we can enhance the total HHG flux, or selectively enhance individual HHG orders, or spectrally shift the HHG peaks. These control capabilities can be explained by intra-atomic phase matching on attosecond timescales [2]. Here the phase of the driving laser is optimized so that HHG bursts from each half cycle of the laser pulse interfere coherently, leading to enhancement or suppression in HHG spectrum. This demonstrates that we can extend these quantum control capabilities to higher photon energies, to design and tailor HHG sources for applications in ultrafast spectroscopy, resonant magnetic scattering, and hyperspectral imaging.

HANS JAKOB WOERNER (Presenter), ETH Zurich — Attosecond spectroscopy has the potential to address fundamental questions in chemical sciences. A promising approach is offered by the element- and site-sensitivity of X-ray spectroscopy. We have recently demonstrated the potential of table-top X-ray absorption spectroscopy with a water-window high-harmonic source, observing the temporal evolution of unoccupied molecular orbitals and molecular shape resonances during chemical reactions [1]. Compressing the mid-infrared driving pulses to less than 2 optical cycles, we have demonstrated the extension of this light source to fully cover the oxygen K-edge [2]. Using the same technique, we have also demonstrated the generation of isolated attosecond pulses, which have established a new record of the shortest light pulses ever measured (43 attoseconds) [3].

Since the vast majority of chemical processes takes place in the liquid phase, the extension of attosecond spectroscopy to liquids is desirable. I will discuss the first observation of extreme-ultraviolet high-harmomic generation from liquids, achieved through the application of ultrathin (0.6-2 μm) flat microjets [4]. I will also present the extension of attosecond time-resolved spectroscopy from molecules [5] to liquids [6]. The time delays between photoemission from gaseous and liquid water range from 50-70 attoseconds and are shown to mainly originate from the solvation of water molecules, with liquid-phase electron scattering playing a minor role. These developments set the stage for attosecond time-resolved studies of molecular systems of chemical complexity.


*This work has been supported by ETH Zurich, the European Research Council and the Swiss National Science Foundation.*
Fundamental understanding of photo-induced charge generation and charge transfer in organic semiconductors is of crucial importance for understanding the functionality of organic optoelectronics. Transient X-ray absorption spectroscopy (Tr-XAS) offers the opportunity for tracking photo-physical processes at the atomic and molecular scale. Here, using Tr-XAS combined with transient absorption spectroscopy and transient microwave conductivity, we investigate the local structure and time evolution of photoinduced charge-separated species in thin films of molecularly dispersed octabutoxy-Zinc(II) phthalocyanine (OButx-ZnPc) in a matrix of the well-known conjugated polymer poly(3-hexylthiophene) (P3HT). We probed a transient signal associated with OButx-ZnPc charged-species in the host polymer (P3HT). Our findings reveal that the XANES spectra of OButx-ZnPc and the transient signal are largely affected by the degree of order of the host material, which is tuned by the regioregularity of P3HT side chains (an amorphous regiorandom P3HT vs a semicrystalline regioregular P3HT).

*This work was supported by the Department of the Navy, Office of Naval Research (ONR and DOE Office of Basic Energy Science, Chemical Sciences Geosciences and Biosciences, Solar Photochemistry Program.
Enhancement of X-ray image brightness through transient ionic resonances

Most of our high-resolution imaging methods compromise between temporal or spatial resolutions akin to a pinhole camera. This still limits our capabilities to observe fast processes at the nanoscale, especially as the required brightness often damages the sample. Examples of such processes include chemical and catalytic reactions, nucleation dynamics, and growth of nanoparticles, as well as other fragile/intermediate states of matter. One idea to overcome this obstacle is to use Free Electron Lasers (FELs), such as the LCLS at SLAC Nat. Lab., which are capable of producing very bright bursts of coherent X-rays within a few femtoseconds. X-ray FELs help to visualize transient processes in “frozen” time steps via single shot coherent X-ray diffractive imaging (CDI). Currently, the resolution of CDI images is close to tens of nanometers, which is limited by the brightness of the images [1-3]. Our recent study at LCLS suggests that transient ionic resonances (TIR) above an absorption edge can enhance diffraction efficiency before significant structural damage can occur. This is surprising as TIRs are usually regarded as a signature of increased X-ray absorption/damage and thus, detrimental to image quality [4-6].

We recorded a large data set of single exposure diffraction patterns with different FEL pulse durations from Xe nanoparticles by scanning the FEL energy in the vicinity of the 3d absorption edge. TIRs seem to increase the scattering efficiency above the edge even for sub-fs pulses. Our experimental results and a theoretical simulation suggest, that TIRs may provide a pathway to increase the quality of CDI with soft and hard X-ray FELs.

1:27PM S58.00006: Ultrafast X-ray Absorption and Time-Resolved Resonant X-ray Scattering in a Mott Insulator*  BRIAN MORITZ (Presenter), SLAC National Accelerator Laboratory, YAO WANG, Harvard University, YUAN CHEN, Stanford University, CHUNJING JIA, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory — The time-evolution of collective excitations encodes information on photoinduced transient states in correlated systems. The frozen charge degrees of freedom in a Mott insulator can be activated by photodoping, which provides information about the interplay between various intertwined instabilities. Here, we simulate both ultrafast x-ray absorption and time-resolved resonant inelastic x-ray scattering (tr-RIXS) for a Hubbard model under the influence of a strong, transient drive. While absorption primarily provides information on transient photodoping, tr-RIXS allows us to study the evolution of bimagnon, Mott-gap, doublon, and single-particle in-gap excitations, as well as anti-Stokes relaxation following an ultrafast excitation of the system. This work provides a theoretical foundation for existing and future tr-RIXS experiments.

*This work was supported by the U.S. DOE, Office of Science (BES/MSED) under Contract No. DE-AC02-76SF00515 and used the computational resources of NERSC, a U.S. DOE, Office of Science User Facility operated under Contract No. DE-AC02-05CH11231. Yao Wang acknowledges the Postdoctoral Fellowship in Quantum Science (Harvard-MPQ, Center for Quantum Optics/AFOSR-MURI Quantum Phases of Matter) through Grant No. FA9550-14-1-0035.

1:39PM S58.00007: Ultrafast Dynamics and Imaging at the Nanoscale using Tabletop Coherent X-ray Sources* [Invited] HENRY KAPTEYN (Presenter), MARGARET MARY MURNANE, JILA and Department of Physics, University of Colorado, Boulder — Laser-like beams at very short wavelengths (1-50nm) can be routinely generated using high harmonic up-conversion (HHG) of tabletop femtosecond lasers.[1,2] This new quantum light source is both advancing rapidly in fundamental capabilities, and is providing a powerful new tool to understand nanoscale material properties and function. This talk will discuss new capabilities for controlling the polarization, spin and orbital angular momentum of HHG beams by sculpting the driving laser beams, [3,4] and will discuss applications in nanoscale magnetic and thermal dynamics using the short wavelength and element specificity of the EUV light-matter interaction. Highlights include the discovery of a new regime of collective nanoscale heat transport,[5] and work highlighting our current incomplete understanding of dynamic mechanisms in magnetic materials.[6]

References:

*DOE Office of Basic Energy Sciences (AMOS program) (DOE)DE-FG02-99ER14982, National Science Foundation (NSF)DMR 1548924, Gordon and Betty Moore Foundation EPiQS Award GBMF4538, NSF through the JILA Physics Frontiers Center PHY-1125844, Department of Energy Office of Basic Energy Sciences X-Ray Scattering Program DE-SC0002002.
11:15AM S59.00001: Reorientation of antiferromagnetism in Co-doped FeSn and its implications for Dirac electron states*  WILLIAM MEIER (Presenter), JIAQIANG YAN, MICHAEL MCGUIRE, XIAOPING WANG, ANDREW D CHRISTIANSON, BRIAN SALES, Oak Ridge National Lab — FeSn is an itinerant antiferromagnet with an Fe Kagome-lattice that hosts electronic Dirac states[1-2]. I will present magnetization measurements of single crystals of (Fe$_{1-x}$Co$_x$)Sn revealing the evolution and suppression of this magnetic order with Co substitution. We interpret the dramatic changes of the magnetic anisotropy to indicate a reorientation of the magnetic moments from perpendicular to parallel to the hexagonal c-axis and confirm this with neutron diffraction. It has been proposed that the Dirac nodes observed in FeSn should become gapped if the moments rotate as our data suggests[1]. We identify Co-substituted compositions that adopts both antiferromagnetic configurations at different temperatures. This system provides a unique opportunity to study how the details of magnetic order impact Dirac electron states.


*Research supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by Oak Ridge National Laboratory.

11:27AM S59.00002: Above-room-temperature ferromagnetic state in a proximitized topological Dirac semimetal  MASAKI UCHIDA (Presenter), Univ of Tokyo, TAKASHI KORETSUME, Tohoku University, SHIN SATO, Univ of Tokyo, MARKUS KRIENER, RIKEN CEMS, YUSUKE NAKAZAWA, SHINICHI NISHIYAMA, Univ of Tokyo, YASUHIRO TAGUCHI, RIKEN CEMS, RYOTARO ARITA, MASASHI KAWASAKI, Univ of Tokyo — We report an above-room-temperature ferromagnetic state realized in a proximitized Dirac semimetal, which is fabricated by growing typical Dirac semimetal Cd$_3$As$_2$ films on a ferromagnetic garnet with strong perpendicular magnetization. Observed anomalous Hall conductivity with substantially large Hall angles is found to be almost proportional to the separation of the Weyl nodes and opposite in sign to magnetization, in agreement with a minimal model behavior. Theoretical calculations based on first-principles electronic structure of Cd$_3$As$_2$ also demonstrate that the Fermi-level dependent anomalous Hall conductivity reflects the Berry curvature originating in the split Weyl nodes. The present high-mobility Dirac-semimetal/ferromagnetic-insulator heterostructure will provide a novel platform for exploring Weyl-node transport phenomena and spintronic functions lately proposed for topological semimetals.
11:39AM S59.00003: Interplay of magnetic frustration and topology in complex metals*

[Invited] JAMES ANALYTIS (Presenter), ELLA LACHMAN, University of California, Berkeley, ROSS MCDONALD, physics, los alamos national lab, ERAN MANIV, University of California, Berkeley — The interplay of topology and frustration can lead to exotic properties and physical phenomena. We study how signatures of topological transport properties can be affected by complex magnetic textures in Kagome and triangular lattice materials. As an example, we show in the case of Co3Sn2S2 that the presence of frustration leads to coexisting magnetic phases that drive an exchange biased anomalous Hall effect. We also study novel transport anisotropies and magnetoelectric coupling in microstuctured devices.

*We acknowledge support from the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4374 and the National Science Foundation under Grant No. 1607753

12:15PM S59.00004: Introducing ferromagnetism into Dirac semimetal Cd₃As₂ thin films*

RUN XIAO (Presenter), ARPITA MITRA, WILSON YANEZ, Pennsylvania State University, JACOB T HELD, MICHELLE TOMCZYK, University of Minnesota, FAN ZHANG, Pennsylvania State University, YAWEN FANG, Cornell university, K. ANDRE MKHOYAN, University of Minnesota, BRAD J RAMSHAW, Cornell university, NITIN SAMARTH, Pennsylvania State University — Breaking time-reversal symmetry in a Dirac semimetal (DSM) via magnetic doping is expected to create a Weyl semimetal. This motivates us to study the doping of the DSM Cd₃As₂ using transition metals. Here, we attempt to introduce Mn into Cd₃As₂ thin films grown by molecular beam epitaxy on GaAs (111)B substrates with a GaSb buffer layer. Atomic force microscopy and X-ray diffraction show that the films have good crystalline quality (root mean square surface roughness ~ 1.5 nm and full-width half maximum of rocking curves ~ 0.12°). However, cross-sectional scanning transmission electron microscopy indicates constraints on Mn incorporation and the formation of magnetically inhomogeneous films with a near-surface Mn-rich compound. SQUID magnetometry shows the presence of weak ferromagnetism. We use low-temperature transport measurements in patterned devices as a function of gate voltage, temperature, and magnetic field angle to understand Shubnikov-de Haas oscillations and quantum transport in this hybrid Dirac material.

*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331 and by the nCORE/SMART Center.
12:27PM S59.00005: Tunable Berry Curvature Effects Through Volume-wise Magnetic Competition in a Topological Kagome Magnet Co$_3$Sn$_2$S$_2$  ZURAB GUGUCHIA (Presenter), JOEL VEREZHAK, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, DARIUSZ GAWRYLUK, Laboratory for Multiscale Materials Experiments, Paul Scherrer Institute, STEPLAN TSIRKIN, Department of Physics, University of Zurich, JIA XIN YIN, ILYA BELOPOLSKI, Laboratory for Topological Quantum Matter and Spectroscopy, Department of Physics, Princeton University, HUIBIN ZHOU, Peking University, International Center for Quantum Materials, GEDIMINAS SIMUTIS, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, SONGTIAN ZHANG, TYLER COCHRAN, GUOQING CHANG, Laboratory for Topological Quantum Matter and Spectroscopy, Department of Physics, Princeton University, EKATERINA POMJAKUSHINA, Laboratory for Multiscale Materials Experiments, Paul Scherrer Institute, LUKAS KELLER, Laboratory for Neutron Scattering, Paul Scherrer Institute, ZUZANNA SKRZECZKOWSKA, Faculty of Chemistry, Warsaw University of Technology, QI WANG, HECHANG LEI, Department of Physics and Beijing Key Laboratory of Opto-electronic Functional Materials and Micro-nano Devices, Renmin University of China, RUSTEM KHASANOV, ALEX AMATO, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, SHUANG JIA, Peking University, International Center for Quantum Materials, TITUS NEUPERT, Department of Physics, University of Zurich, HUBERTUS LUETKENS, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, ZAHID HASAN, Laboratory for Topological Quantum Matter and Spectroscopy, Department of Physics, Princeton University — Magnetic topological phases of quantum matter are an emerging frontier in physics and material science. Along these lines, several kagome magnets have appeared as the most promising platforms. Here, we explore magnetic correlations in the kagome magnet Co$_3$Sn$_2$S$_2$. Using muon spin-rotation, we present evidence for competing magnetic orders in the kagome lattice of this compound. Our results show that while the sample exhibits an out-of-plane ferromagnetic ground state, an in-plane antiferromagnetic state appears at temperatures above 90 K, eventually attaining a volume fraction of 80% around 170 K, before reaching a non-magnetic state [1]. Strikingly, the reduction of the anomalous Hall conductivity above 90 K linearly follows the disappearance of the volume fraction of the ferromagnetic state. We further show that the competition of these magnetic phases is tunable through applying either an external magnetic field or hydrostatic pressure. Our results taken together suggest the thermal and quantum tuning of Berry curvature field via external tuning of magnetic order. Our study shows that Co$_3$Sn$_2$S$_2$ is a rare example where the magnetic competition drives the thermodynamic evolution of the Berry curvature, thus tuning its topological state.

We report evidences and interpretations for a robust edge supercurrent in type II Weyl semimetal MoTe2 in the superconducting regime, where $T < T_c = 100$ mK at ambient pressure. We fabricated MoTe2 devices (60 – 120 nm thickness) with Au contacts through mechanical exfoliation and nanofabrication. Transport measurements of differential resistance $dV/dI$ versus applied bias and magnetic field $B$ shows a periodic oscillation of critical current $I_c$ with a scalloped profile. The oscillation mode remains coherent and the associated area to its frequency saturates to the physical area of sample with an increasing magnetic field. These observations demonstrate a superconducting edge mode with the width less than 10 nm. We describe the edge condensate with a Ginzburg Landau wave function that is independent from the bulk condensate. Fluxoid quantization causes the edge superfluid velocity to vary, resulting in the scalloped profile. Weak excitations trailing from the scalloped boundaries in $I_c$ vs. $B$ plots exhibit unusual asymmetries.

*This research was supported by the U.S. Army Research Office (W911NF-16-1-0116), the Department of Energy (DESC0017863), and the Gordon and Betty Moore Foundation’s Emergent Phenomena in Quantum Systems Initiative (GBMF4539).
Magnetic Weyl Semimetals* [Invited] CLAUDIA FELSER (Presenter), YAN SUN, KAUSTUV MANNA, Solid State Chemistry, Max Planck Institute Chemical Physics of Solids — Topology a mathematical concept became recently a hot topic in condensed matter physics and materials science. One important criteria for the identification of the topological material is in the language of chemistry the inert pair effect of the s-electrons in heavy elements and the symmetry of the crystal structure [1]. Beside of Weyl and Dirac new fermions can be identified compounds via linear and quadratic 3-, 6- and 8-band crossings stabilized by space group symmetries [2]. In magnetic materials the Berry curvature and the classical AHE helps to identify interesting candidates. Magnetic Heusler compounds were already identified as Weyl semimetals such as Co$_2$YZ [3-6] (Y=Ti, Mn; Z=Ge, Sn, Ga, Al), in Mn$_3$Z [7-9] (Z=Ge, Sn). Co$_3$Sn$_2$S$_2$ is a 2D Weyl semimetal with edge states [11-12].


*Wurzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter (EXC 2147, no. 39085490
ERC Advanced Grant No. 742068 “TOPMAT”

Electronic, magnetic and thermodynamic properties of the Kagome layer metal FeSn* BRIAN SALES (Presenter), JIAQIANG YAN, WILLIAM R MEIER, QIANG ZHENG, ANDREW D CHRISTIANSON, SATOSHI OKAMOTO, MICHAEL MCGUIRE, Oak Ridge National Lab — FeSn is an itinerant antiferromagnet composed of metallic Kagome layers. FeSn single crystals are investigated using x-ray and neutron scattering, magnetic susceptibility and magnetization, heat capacity, resistivity, Hall, Seebeck, thermal expansion, thermal conductivity measurements and density functional theory. In spite of the quasi 2D Kagome layers with Dirac nodal lines along the K-H directions in the magnetic Brillouin zone about 0.3 eV below the Fermi energy, the measured properties strongly suggest that the overall electronic structure is 3D. The magnetism, however, is predicted to be highly 2D with Jin-plane/Jout-of-plane $\approx 10$. The impact of Dirac nodes on the physics on this material will be discussed.

*Research supported by the DOE Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.
1:39PM S59.00009: Low temperature investigation of candidate type-II Weyl semimetal LaAlGe  
MARK ZIC (Presenter), CHRIS ECKBERG, HALYNA HODOVANETS, SEOKJIN BAE, HYUNSOO KIM, TRISTIN METZ, SEAN WINTERS, DANIEL KRAFT, STEVEN ANLAGE, JOHNPIERRE PAGLIONE,  
University of Maryland, College Park — Weyl semimetals continue to be a flourishing topic of research because of their non-trivial surface states and topology [1] and their exciting experimental realizations in magnetotransport [2], thermopower [3], and optical spectroscopy [4]. These unique ground states motivate us to investigate the proposed Weyl semimetal LaAlGe [5], a compound previously only investigated theoretically and with X-ray diffraction. We use a molten flux growth technique to precipitate pristine LaAlGe single crystals that crystallize in the non-centrosymmetric crystal structure required for Weyl points to exist. We will discuss our electrical transport, magnetization, penetration depth, and heat capacity measurements of this topological compound, detailing both our experimental results and the future implications of this work.


1:51PM S59.00010: Magnetostructural instability in Weyl ferromagnet Mn$_3$ZnC*  
SAMUEL TEICHER (Presenter), Materials Research Laboratory and Materials Department, University of California, Santa Barbara, IDA K SVENNINGSSON, Department of Applied Physics, Chalmers Institute of Technology, LESLIE SCHOOP, Department of Chemistry, Princeton University, RAM SESHADRI, Materials Research Laboratory and Materials Department, University of California, Santa Barbara — We present first-principles calculations suggesting that the ferromagnetic phase of cubic antiperovskite Mn$_3$ZnC is a nodal line Weyl semimetal. Electronic structure features that are the hallmark of this nodal line state—a large density of linear band crossing near the Fermi level—can also be interpreted as signatures of structural and magnetic instability. In fact, it is known that Mn$_3$ZnC transitions upon cooling from a paramagnetic to a cubic ferromagnetic state under ambient conditions and then further into a non-collinear tetragonal phase at a temperature between 250 K and 200 K. The existence of Weyl nodes and their destruction via structural and antiferromagnetic ordering is likely relevant to a range of magnetostructurally coupled materials.

*Work at UC Santa Barbara was supported by the National Science Foundation (NSF) through DMR 1710638 and made use of the shared facilities of the UC Santa Barbara MRSEC (DMR 1720256) and Center for Scientific Computing (CNS 1725797, DMR 1720256). LS was supported by the Princeton Center for Complex Materials (DMR 1420541). IKS acknowledges support from NSF-OISE 1827034 and from AoA Materials Science, Chalmers University of Technology. SMLT has been supported by the NSF Graduate Research Fellowship Program under Grant No. DGE 1650114.
2:03PM S59.00011: Ultrasound Studies on the Chiral Antiferromagnet Mn$_3$Ge* FLORIAN THEUSS (Presenter), SAYAK GHOSH, Cornell University, TAISHI CHEN, SATORU NAKATSUJI, Institute for Solid State Physics, University of Tokyo, BRAD J RAMSHAW, Cornell University — The chiral antiferromagnet Mn$_3$Ge is a promising candidate for a magnetic Weyl semimetal, where Weyl nodes arise from broken time reversal symmetry rather than broken inversion symmetry. Recently, Mn$_3$Ge has been shown to exhibit a giant anomalous Hall effect at room temperature, which has been attributed to the presence of Weyl nodes. Given this highly anomalous room-temperature Hall effect, it is natural to ask whether other properties of the Weyl nodes, such as the chiral anomaly, are also present at room temperature. Strong magneto-elastic coupling, known to be present in Mn$_3$Ge, has motivated our investigation of the elastic moduli in this material. We report resonant ultrasound spectroscopy studies of the full elastic tensor of Mn$_3$Ge through the 380 K Néel transition temperature. We investigate how strains of different symmetry couple to the magnetic degrees of freedom on the Kagome lattice formed by manganese ions. We also investigate ultrasonic attenuation - which is predicted to be highly sensitive to chiral charge pumping between Weyl nodes in a magnetic field - both above and below the Néel transition.

*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331.

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S60 DMP: Topological Superconductivity Induced in Spin-Orbit-Coupled Materials Mile High Ballroom 4A - Jay Sau, University of Maryland, College Park - Tag(s): Focus

11:15AM S60.00001: Topological superconductivity in superconductor–semiconductor heterostructures [Invited] ROMAN LUTCHYN (Presenter), Microsoft Corp — Superconductor–semiconductor heterostructures represent a versatile platform for realizing Majorana zero-energy modes. In this talk, I will explain how to engineer topological superconductivity at the interface of a conventional (s-wave) superconductor and a semiconductor with spin-orbit interaction. I will discuss state-of-the-art numerical approaches for modeling realistic devices which take into account proximity-induced superconductivity, orbital and Zeeman effect of an applied magnetic field, spin-orbit coupling as well as the electrostatic environment on equal footing. Finally, I will review recent materials science progress in growing superconductor–semiconductor heterostructures and discuss promising new directions.
11:51AM S60.00002: Josephson controlled topological superconductivity* [Invited] ADY STERN (Presenter), Weizmann Institute of Science — In this talk I will describe how the Josephson effect may be employed to realize one dimensional topological superconductivity, with the Josephson phase difference being a "user-friendly" knob to drive the system to become topological. I will describe the basic idea, the experimental observations, the relation to topological superconductivity based on quantum wires, a surprising effect of disorder, and a scheme for braiding Majorana zero modes in Josephson junctions. I will also describe how this system manifests a first order phase transition into a topological phase.

*This research was supported by ERC projects MUNATOP and LEGOTOP, Microsoft Station Q, and the Israel Science Foundation.

12:27PM S60.00003: Nature of the insulating and superconducting states of monolayer WTe₂* [Invited] DAVID COBDEN (Presenter), University of Washington — Although in the bulk WTe₂ is a semimetal, exfoliated to a monolayer it becomes a topological insulator that undergoes a transition to a metallic state on electron doping of $5 \times 10^{12}$ cm$^{-2}$, and furthermore this metallic state becomes superconducting at temperatures below about 1 K. This proximity, in terms of doping, of a small-gap insulator to a superconductor is surprising, and the insulator exhibits a number of other unusual properties. We will summarize and compare these properties and assess the possibility that the insulating state has a many-body character akin to an excitonic insulator. In addition, we will present and evaluate evidence that the helical edge states remain throughout the insulator to superconductor transition.

*Supported by NSF MRSEC award 1719797 and DMR EAGER award 1936697.
ABHISHEK BANERJEE (Presenter), MD. AHNAF RAHMAN, ANTONIO FORNIERI, ALEXANDER WHITICAR, ASBJORN DRACHMANN, Center for Quantum Devices and Microsoft Quantum Lab Copenhagen, Niels Bohr Institute, University of Copenhagen, TYLER LINDEMAN, SERGEI GRONIN, CANDICE THOMAS, GEOFFREY C. GARDNER, Department of Physics and Astronomy and Station Q Purdue, Birck Nanotechnology Center, Purdue University, MICHAEL MANFRA, Department of Physics and Astronomy and Station Q Purdue, Birck Nanotechnology Center, School of Materials Engineering, School of Electrical and Computer Engineering, Purdue, CHARLES MARCUS, Center for Quantum Devices and Microsoft Quantum Lab Copenhagen, Niels Bohr Institute, University of Copenhagen — Recent works have realized Majorana zero modes in planar Josephson junctions consisting of a semiconductor with strong spin-orbit coupling proximitized by two superconducting leads. Such systems offer the tantalizing possibility of using the phase difference $\Phi$ across the two superconductors as a new experimental knob to tune into and out of the topological regime, possibly at ultra-fast timescales, apart from having advantages such as reduced sensitivity to chemical potential tuning and appearance of Majorana bound states at zero magnetic field. Here, we demonstrate strong phase control of Andreev bound states that emerge from the gap at $\Phi \sim 0$ and coalesce at zero energy at $\Phi \sim \pi$. The zero energy modes at $\Phi \sim \pi$ appear at in-plane magnetic fields as low as $\sim 220$ mT and persist robustly with variations of in-plane Zeeman field and gate voltages in a wide range. At larger in-plane magnetic fields, the zero energy modes become phase independent and stick for all values of $\Phi$. We also study the behavior of the zero energy states with respect to large out-of-plane magnetic fields that can tune the phase texture within the Josephson junction, and possibly result in motion of Majorana zero modes.

*This work was supported by the Danish National Research Foundation and Microsoft.
1:15PM S60.00005: Phase signature of topological transition in Josephson junctions*
MATTIEU DARTIAILH (Presenter), WILLIAM MAYER, JOSEPH YUAN, KAUSHINI S WICKRAMASINGHE, Physics, New York University, ALEX MATOS ABIAGUE, Physics and Astronomy, Wayne State University, IGOR ZUTIC, Physics, Buffalo State University of New York, JAVAD SHABANI, Physics, New York University — Topological transition transforms common superconductivity into an exotic phase of matter, which holds promise for fault-tolerant quantum computing. A hallmark of this transition is the emergence of Majorana states. While two-dimensional semiconductor/superconductor heterostructures are desirable platforms for topological superconductivity, direct phase-measurements as the fingerprint of the underlying topological transition have been missing. On gate tunable Josephson junctions made on epitaxial Al/InAs, we observe a closing and a reopening of the superconducting gap with increasing in-plane magnetic field. Since our junctions are embedded into a phase-sensitive SQUID, we are able to measure a π-jump in the superconducting phase across the junction coincident with the closing and reopening of the superconducting gap. Theoretical simulations confirm this transition is topological and compatible with the emergence of Majorana states while the magnetic field angle dependence of the transition further constrain this scenario. Remarkably, in each junction, this topological transition can be controlled by changing the gate voltage. These findings reveal versatile two-dimensional platforms for scalable topological quantum computing.

*This work was supported by DARPA TEE No. DP18AP90000

1:27PM S60.00006: Signatures of topological superconductivity in Josephson junctions*
ALEX MATOS ABIAGUE (Presenter), Wayne State University, MATTIEU DARTIAILH, WILLIAM MAYER, JOSEPH YUAN, KAUSHINI S WICKRAMASINGHE, New York University, IGOR ZUTIC, University at Buffalo, JAVAD SHABANI, New York University — Topological superconductivity is a phase of matter supporting Majorana bound states, quasiparticles that store information in a nonlocal manner and can be used as qubits that are robust against local perturbations. We theoretically investigate the emergence of topological superconductivity in Josephson junctions with tunable chemical potential and Rashba spin-orbit coupling, subjected to an in-plane magnetic field. As the magnetic field along the junction increases above some critical value the system experiences a transition from the trivial to the topological superconducting phase. Theoretical simulations show that such a transition is accompanied by a minimum in the critical current and a corresponding jump in the phase difference across the junction. The sensitivity of the topological transition to the in-plane magnetization direction provides an additional fingerprint for the emergence of topological superconductivity. The theoretical simulations are in good agreement with the recent experimental detection of topological phase transitions in gate-tunable JJs built on epitaxial Al/InAs [1].


*This work was supported by DARPA Topological Excitations in Electronics, Grant No. DP18AP90000.
1:39PM S60.00007: In-vacuo growth and fabrication of superconductor-semiconductor hybrid heterostructures for topological quantum computation* MIHIR PENDHARKAR (Presenter), Dept. of Electrical Engineering, Univ. of California, Santa Barbara, CA, USA, JOON SUE LEE, California Nano-Systems Institute, Univ. of California, Santa Barbara, CA, USA, ANTHONY P MCFADDEN, Dept. of Electrical Engineering, Univ. of California, Santa Barbara, CA, USA, SASA GAZIBEGOVIC, ROY OP HET VELD, Dept. of Physics, Technical University, Eindhoven, The Netherlands, CONNOR DEMPESEY, Dept. of Electrical Engineering, Univ. of California, Santa Barbara, CA, USA, SEAN HARRINGTON, Dept. of Materials Engineering, Univ. of California, Santa Barbara, CA, USA, ARANYA GOSWAMI, Dept. of Electrical Engineering, Univ. of California, Santa Barbara, CA, USA, MICHAEL A SEAS, Dept. of Materials Engineering, Univ. of California, Santa Barbara, CA, USA, SUKGEUN CHOI, Dept. of Electrical Engineering, Univ. of California, Santa Barbara, CA, USA, GHADA BADAWY, JASON JUNG, Dept. of Physics, Technical University, Eindhoven, The Netherlands, MOIRA HOCEVAR, Institute Neel, CNRS, Grenoble, France, LEO P KOUWENHOVEN, Dept. of Physics, Technical University, Delft, The Netherlands, ROMAN LUTCHYN, MICHAEL H FREEDMAN, Microsoft Quantum, Santa Barbara, CA, USA, SERGEY M FROLOV, Dept. of Physics, Univ. of Pittsburgh, Pittsburgh, PA, USA, ERIK BAKKERS, Dept. of Physics, Technical University, Eindhoven, The Netherlands, CHRIS J PALMSTROM, Dept. of Electrical Engineering, Univ. of California, Santa Barbara, CA, USA — Superconductor-semiconductor heterostructures are the backbone of Majorana Zero Mode (MZM) based topological quantum computing. Magneto-transport in nanowires of InSb with partial shells of aluminum has highlighted the significance of abrupt and epitaxial, in-vacuo growth of superconductors on semiconductors. Going forward, two key challenges need to be addressed. Firstly, the demonstration of in-vacuo, selective area growth of superconductors on wafer-scale semiconductors and, secondly, in-vacuo fabrication of proposed topological qubit devices. This work reports on the Molecular Beam Epitaxy (MBE) of selective area hybrid heterostructures using various approaches with the aim of creating a versatile platform for fabrication of topological qubits in vacuo.

*This work was in part funded by Microsoft Research Station Q at Santa Barbara and NSF-PIRE.

1:51PM S60.00008: Accessing different topological classes and types of Majorana edge states in 1D p-wave superconductors using perturbations* SAYONEE RAY (Presenter), Physics and Astronomy, University of New Mexico, US, SUBROTO MUKERJEE, Department of Physics, Indian Institute of Science, Bangalore, India, NAYANA SHAH, Department of Physics, Washington University, St. Louis, US — Classification and realization of various classes of topological superconductors with different types of Majorana bound states (MBS) is of ongoing interest. The standard platform of these studies have been the conventional 1D Kitaev wire and its realizations. Here, we present the edge states of different types of p-wave SC in 1D in the presence of an additional Zeeman field and s-wave SC component. Within the framework of the tenfold classification scheme, we study the transition between different topological classes caused by such perturbations and analyze the nature of the corresponding MBS. Further, we study the junctions between different classes of topological superconductors and explore transport properties to probe the mid-gap states.

*NSF FRHTP grant
During the main efforts to realize MBS have focused on 1D systems, the onset of topological superconductivity requires delicate parameter tuning and geometric constraints pose significant challenges for their control and demonstration of non-Abelian statistics. To overcome these challenges, building on recent experiments in planar Josephson junctions (JJs) [2-4], we propose a MBS platform of X-shaped JJs. This versatile implementation reveals how external flux control of the superconducting phase difference can generate and manipulate multiple MBS pairs to probe non-Abelian statistics. The underlying topological superconductivity exists over a large parameter space, consistent with materials used in our fabrication of such X junctions, as an important step towards topological quantum computing.

We used Raman light scattering to study the current-stabilized nonequilibrium semimetallic and metallic phases in Ca$_2$RuO$_4$. By determining the local temperature through careful analysis of the Stokes and anti-Stokes intensities, we find that Joule heating can be completely avoided by supplying sufficient cooling power in a helium-flow cryostat and that the current induces the semimetallic state without inducing any significant heating [1]. We further investigate the current-induced semimetallic state as a function of temperature and current. We confirm the absence of long-range antiferromagnetic order [2] and identify a substantial Fano broadening of several phonons, which suggests coupling to charge and orbital fluctuations. Our results demonstrate that the semimetallic state is a genuine effect of the applied electrical current and that the current-induced phases have characteristics distinct from the equilibrium ones.


*We acknowledge support from the European Research Council under Advanced Grant No. 669550 (Com4Com) and from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Projektnummer 107745057 - TRR 80.
Octahedral tilt driven Kondo lattice behavior with orbital-selective Mott transition of 4d Ca$_{2-x}$Sr$_x$RuO$_4$

MINSOO KIM (Presenter), JUNYOUNG KWON, DAUN CHUNG, YOUNSIK KIM, HANYOUNG YOO, JONGKEUN JUNG, BEOM SEO KIM, MI KYUNG KIM, Department of Physics and Astronomy, Seoul Natl Univ; JONATHAN DENLINGER, Advanced Light Source, Lawrence Berkeley National Laboratory; MOONSUP HAN, Department of Physics, University of Seoul; TAKASHI MIZOKAWA, Department of Applied Physics, Waseda University; YOSHIYUKI YOSHIDA, National Institute of Advanced Industrial Science and Technology (AIST); WONSHIK KYUNG, CHANGYOUNG KIM, Department of Physics and Astronomy, Seoul Natl Univ — The physics of heavy fermion (HF) state, which manifests in $f$-electron system [1], begins to germinate in $d$-orbital system, for example, in 3$d$ single-orbital van der Waals ferromagnet, transition metal oxide (TMO) LiV$_2$O$_4$ and multi-orbital Fe based family [2, 3, 4]. However, the existence of the HF state and its underlying mechanism remain to be questionable in 4$d$ multi orbital systems. Using angle-resolved photoemission spectroscopy (ARPES), we observe the HF state in orbital-selective Mott phase (OSMP) of 4$d$ TMO, Ca$_{2-x}$Sr$_x$RuO$_4$. Upon entering OSMP ($x<0.5$), we observe a massive spectral weight transfer, a 100meV-orbital selective gap for $d_{xy}$-originated $\gamma$ and corresponding change in $d_{xz/yz}$-originated $\beta$ band while $d_{xz/yz}$-originated $\alpha$ band remains hardly changed. With the temperature drop across a characteristic temperature $T^*$, spectral weight transfer gradually occurs from lower to higher binding energy in $\beta$ and $\gamma$ bands. This possible Kondo lattice behavior can be well explained by the key role of the octahedral tilt driven $d$-band hybridization. Our work firstly, demonstrates the possible origin of the formation of the HF state from 4$d$ TMOs with structural distortions, which expands the boundary of the HF-candidates to the 4$d$ multi orbital systems.

Electric control of the structural properties of spin-orbit coupled 4$d$ ruthenate Ca$_{2}$Ru$_{0.97}$Mn$_{0.03}$O$_4$

FENG YE (Presenter), CHRISTINA HOFFMANN, Oak Ridge National Lab, HENGDI ZHAO, GANG CAO, Physics Department, University of Colorado Boulder — The unique competition between spin-orbit interaction (SOI) and Coulomb correlation ($U$) in 4$d$/5$d$ oxides drives unusual physical behavior. Novel nonequilibrium phenomena can be further induced by external stimuli including intense synchrotron x-ray or electric current. In this talk, we report neutron diffraction study of the quasi-two-dimensional Mott Ca$_{2}$Ru$_{0.97}$Mn$_{0.03}$O$_4$, which shows dramatic reduction of the electric resistivity, suppression of the antiferromagnetic transition, and induction of new orbital order with critical current density of 0.15 A/cm$^2$. Our in-situ structural characterization implies that the in-plane orthorhombicity diminishes with increasing current density, accompanied by the straightened of the Ru-O-Ru bonding angles. The temperature-current phase diagram establishes an intimate correlation between the lattice and electronic structure in this nonequilibrium, steady state driven by current. Our results shed light to the nature of the Mott-Insulator transition and provide key information for the emerging phenomena near the transition.
11:51AM S61.00004: Metallic and non-metallic duality in the 4d pyrochlore Lu$_2$Rh$_2$O$_7$*

[Invited] ALANNAH HALLAS (Presenter), University of British Columbia — The 4d transition metal oxides exist in an intriguing regime where on-site Coulomb repulsion, the band width, and spin-orbit coupling can all have comparable magnitudes. While spin-orbit coupling for these 4d systems is reduced as compared to their 5d counterparts, it is still strong enough to generate exotic magnetic and electronic states. In this talk, we introduce Lu$_2$Rh$_2$O$_7$, a new cubic pyrochlore oxide based on 4d$^5$ Rh$^{4+}$ with properties that defy simple categorization. Both magnetic susceptibility ($\chi_P = 7.6 \times 10^{-4}$ emu/mol$_{Rh}$) and heat capacity measurements ($\gamma = 21.8(1)$ mJ/mol$_{Rh}$ K$^2$) indicate that this material is a strongly correlated metal and yet electrical resistivity measurements show decidedly non-metallic behavior. Furthermore, although the magnitude of the resistivity is that of a semiconductor (1 $\Omega$-cm), the temperature dependence does not obey any conventional form. The magnetic properties of this material are also enigmatic; if this material is non-metallic, then one would expect 4d$^5$ Rh to carry an $S = \frac{1}{2}$ magnetic moment and yet magnetic susceptibility and muon spin relaxation measurements show no evidence for local moments down to 2 K. We therefore propose that Lu$_2$Rh$_2$O$_7$ may be the prototype for an entirely new class of non-Fermi liquids.

*This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC)

12:27PM S61.00005: Anomalous Hall effect from strained-induced magnetic multipoles in antiferromagnetic material

JEONGKEUN SONG (Presenter), TAEKOO OH, Seoul. Nat. Univ, WOOJIN KIM, Stanford Univ — The origin of anomalous Hall effect (AHE) in magnetic materials has been a central theme of condensed matter physics for a century. In ferromagnetic materials, the origin of AHE is from the magnetization. [1] On the other hand, the large AHE in antiferromagnetic Mn$_3$Sn without large magnetization was observed and its origin remains elusive.[2] Recent theoretical study suggested that the hidden magnetic multipoles formed by the spin clusters can induce the large AHE in antiferromagnet. [3] Here, we establish the comprehensive connection between the large AHE in antiferromagnetic in-situ pyrochlore iridate Nd$_2$Ir$_2$O$_7$ thin film and strain-induced magnetic multipoles, T$_1$-octupole.

Approaching the quantum critical point in a highly-correlated all-in-all-out antiferromagnet  
Yejun Feng (Presenter), Okinawa Inst of Sci & Tech, Yishu Wang, Johns Hopkins University, Dharmalingam Prabhakaran, Andrew T Boothroyd, University of Oxford, Thomas F Rosenbaum, California Institute of Technology — All-in-all-out (AIAO) antiferromagnetic order in strongly spin-orbit-coupled 5d compounds can demonstrate exotic electronic phases and strongly-coupled quantum critical phenomena. Here we experimentally explore this scenario by directly tracing the AIAO spin order in Sm$_2$Ir$_2$O$_7$ using resonant x-ray magnetic diffraction techniques under high pressure. We find that the magnetic order is suppressed at a critical pressure $P_c$=6.30 GPa, while the lattice symmetry remains in the cubic $Fd-3m$ space group across the quantum critical point. Comparing pressure tuning and the chemical series $R_2$Ir$_2$O$_7$ reveals that the suppression of the AIAO order and the approach to the spin-disordered state is characterized by contrasting evolutions of both the pyrochlore lattice parameter $a$ and the trigonal distortion $x$. The former affects the 5d bandwidth, the latter the Ising anisotropy, and so such we posit that the opposite effects of pressure and chemical tuning lead to spin fluctuations with different Ising and Heisenberg character in the quantum critical region. Finally, we compare the iridates to AIAO spin order in osmate analogues, where spin fluctuations, lattice breathing modes, and quasiparticle excitations all interact in the quantum critical region.

Geometric Magnetic Frustration in Y$_{2-x}$Bi$_x$Ru$_2$O$_7$ Pyrochlores across the Metal-Insulator transition  
Sarah Duniger (Presenter), TRIUMF, Sang-Wook Cheong, Physics and Astronomy, Rutgers University, Kim Hooch Chow, Physics, University of Alberta, Martin H Dehn, Physics and Astronomy, University of British Columbia, Shayan Gheidi, Physics, Simon Fraser University, Namjung Hur, Physics, Inha University, Kee Hoon Kim, Physics and Astronomy, Seoul National University, Graeme Luke, Physics and Astronomy, McMaster University, Gerald Morris, TRIUMF, Timothy Munsie, Physics and Astronomy, McMaster University, Jeff Sonier, Shyam Sundar, Physics, Simon Fraser University — Systems based on a triangular or pyrochlore lattice of corner sharing tetrahedra with nearest neighbor antiferromagnetic exchange interactions are the archetypical examples of geometric magnetic frustration, offering a means of accessing novel ground states. Magnetic systems based on 4d and 5d transition metal ions on the pyrochlore lattice offer a unique opportunity to explore the exotic ground states which potentially arise when the electron-electron Coulomb interaction, electronic bandwidth and spin orbit coupling are all of comparable magnitude. I will describe magnetization and muon spin relaxation investigations of a series of 4d Ru4+ based pyrochlores, which may be controllably tuned through a metal insulator transition, providing insight into the magnetic correlations as these finely balanced systems evolve from a localized to itinerant spin character.
Electrically driven inhomogeneous phase transition in $\text{CuIr}_2\text{S}_4$  

AHMED ALI (Presenter), DASHARATH ADHIKARI, ALI M ALSAQQA, COLIN P KILCOYNE, State Univ of NY - Buffalo, NOBUHIRO MATSUMOTO, National Metrology Institute and Chemical Measurement Laboratory, SAMBANDAMURTHY GANAPATHY, State Univ of NY - Buffalo — Comparable energy scales of dominant interactions determining electronic phases and relatively smaller energy barrier separating different phases makes 5d electronic systems sensitive to an external perturbation (e.g. temperature, electric field, strain). $\text{CuIr}_2\text{S}_4$, a 5d transition metal compound with spinel structure, shows a hysteretic metal-insulator transition at $T_c \sim 231$ K (on cooling) accompanied with crystal symmetry lowering from high-temperature cubic (metallic) to low-temperature tetragonal (insulating) phase. The system also exhibits electric field-driven hysteretic switching from insulating to metallic phase below $T_c$. Transport and resistance noise spectroscopy were carried out: at temperatures well below $T_c$, the transition is characterized by a single abrupt switching and the power spectral density (PSD) of the noise varies smoothly across the transition. Approaching $T_c$, on the other hand, switching happens with multiple, step-like jumps and the PSD is found to increase significantly. The melting of long-range charge ordering near $T_c$ likely increases the local inhomogeneity thereby resulting in increased PSD. Results will be discussed in the context of microscopic conduction mechanisms across thermal and electrical driven transitions in strongly correlated systems.

Local orbital degeneracy lifting as a precursor to an orbitalselective Peierls transition* 

EMIL BOZIN (Presenter), WEIGUO YIN, ROBERT KOCH, MILINDA ABEEKOON, Brookhaven National Laboratory, YEW SAN HOR, HONG ZHENG, Argonne National Laboratory, HECHANG LEI, CEDOMIR PETROVIC, Brookhaven National Laboratory, JOHN MITCHELL, Argonne National Laboratory, SIMON J L BILLINGE, Brookhaven National Laboratory — Fundamental electronic principles underlying all transition metal compounds are the symmetry and filling of the $d$-electron orbitals and the influence of this filling on structural configurations and responses. Here we use a sensitive local structural technique, x-ray atomic pair distribution function analysis, to reveal the presence of fluctuating local-structural distortions at high temperature in one such compound, $\text{CuIr}_2\text{S}_4$. We show that this hitherto overlooked fluctuating symmetry-lowering is electronic in origin and will modify the energy-level spectrum and electronic and magnetic properties. The explanation is a local, fluctuating, orbital-degeneracy-lifted state. The natural extension of our result would be that this phenomenon is likely to be widespread amongst diverse classes of partially filled nominally degenerate $d$-electron systems, with potentially broad implications for our understanding of their properties.

*Work at Brookhaven National Laboratory was supported by US DOE, Office of Science, Office of Basic Energy Sciences under contract DE-SC0012704. Work in the Materials Science Division of Argonne National Laboratory, was sponsored by the U.S. Department of Energy Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.
SEVERINO ADLER (Presenter), Institut für Theoretische Physik und Astrophysik, Universität Würzburg, DANIEL SPRINGER, Institute of Solid State Physics, TU Wien, BONGJAE KIM, Department of Physics, Kunsan National University, PEITAO LIU, Faculty of Physics and Center for Computational Materials Science, University of Vienna, ANDREAS HAUSOEL, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, CESARE FRANCHINI, Faculty of Physics and Center for Computational Materials Science, University of Vienna, GIORGIO SANGIOVANNI, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, ALESSANDRO TOSCHI, Institute of Solid State Physics, TU Wien — Experiments on the 5d-Osmium oxide perovskite LiOsO$_3$ have revealed surprising physical properties. In contrast to expectations and to the chemically similar material NaOsO$_3$, LiOsO$_3$ is never magnetic. Further, its optical properties show a bad metallic behaviour, with a quickly decreasing Drude peak as a function of T [1], as in the 3d-oxide V$_2$O$_3$ [2]. A possible origin of this unexpected physics might be the interplay between electronic correlations and spin-orbit coupling (SOC) in this 5d compound. Therefore, we performed a paramagnetic, non SOC dependent DFT and a magnetic DMFT calculation, where we tuned the atomic SOC in the Os t$_{2g}$ manifold. Without atomic SOC, we find a strong long-range G-type antiferromagnetic order. Turning on atomic SOC antiferromagnetism is gradually suppressed, vanishing at a SOC strength of about 600 meV. This strongly suggests that atomic SOC plays a pivotal role in determining the magnetic properties of osmates.


*We acknowledge financial support from the DFG through the Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter – ct.qmat (EXC 2147, project-id 39085490).

MIN YONG JEONG (Presenter), JAE-HOON SIM, Department of Physics, KAIST, HYEONG JUN LEE, ARA GO, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, MYUNG JOON HAN, Department of Physics, KAIST — The lacunar spinel GaTa$_4$Se$_8$ is the first established example of $J_{\text{eff}} = 3/2$ Mott insulator. By applying pressure, it undergoes insulator-to-metal and superconducting transition. In order to understand the nature of this intriguing metallic phase and its possible relation to superconductivity, we performed the LDA+DMFT (local density approximation + dynamical mean-field theory) calculations as a function of pressure and with spin-orbit coupling taken into account. It is found that, even at high pressure corresponding to the metallic and superconducting phase, $J_{\text{eff}} = 3/2$ is well identified, indicating the novel nature of the superconductivity observed in this material. Possibilities of topological superconductivity and the spin-freezing superconductivity will be discussed.

*This work was supported by the National Research Foundation of Korea NRF-2018R1A2B2005204
1:51PM S61.00012: Magnetic impurity behavior in a gapless quantum spin liquid: single-layer 1T-TaSe$_2$  YI CHEN (Presenter), WEI RUAN, University of California, Berkeley, JINWOONG HWANG, Lawrence Berkeley National Lab, MENG WU, University of California, Berkeley, SHUJIE TANG, Stanford University, HYEJIN RYU, Lawrence Berkeley National Lab, STEVEN LOUIE, University of California, Berkeley, PATRICK A LEE, MIT, ZHIXUN SHEN, Stanford University, SUNG-KWAN MO, Lawrence Berkeley National Lab, MICHAEL F CROMMIE, University of California, Berkeley — Quantum spin liquids are a novel state of matter predicted to arise in quantum antiferromagnets where geometric frustration and quantum fluctuations are strong enough to prevent a magnetically ordered ground state. At half filling, fractional spin-carrying excitations termed spinons dominate the low-energy physics. Here we present scanning tunneling microscopy studies of the behavior of magnetic adatoms deposited onto the quantum spin liquid candidate single-layer 1T-TaSe$_2$. Spectroscopic imaging of pristine single-layer 1T-TaSe$_2$ reveals long-wavelength density modulations at the Hubbard band energies consistent with a spinon Fermi surface instability as predicted by theory. Magnetic atoms deposited onto the 1T-TaSe$_2$ surface bind at different sites in the star-of-David unit cell and exhibit distinct spectroscopic features near the Hubbard band edges. One possible explanation for the observed behavior is exchange coupling between magnetic adatoms and itinerant spinons.

2:03PM S61.00013: Spectroscopic signatures of Quasi One-Dimensional Crystallization at Domain Walls in the Mott Insulator TaS$_2$  ANUVA AISHWARYA (Presenter), SEAN HOWARD, BIKASH PADHI, University of Illinois at Urbana-Champaign, LIHAI WANG, Pohang University of Science and Technology, SANG-WOOK CHEONG, Rutgers University, PHILIP PHILLIPS, VIDYA MADHAVAN, University of Illinois at Urbana-Champaign — A tunable Mott state is fortuitous as it is a model system to study emergent phenomena due to broken symmetries like superconductivity, novel magnetic order and charge order, as a Mott band is tuned across Fermi energy ($E_F$). In this work, we use scanning tunneling microscopy at 4K to study the Mott insulator, TaS$_2$. Charge density wave domain walls in TaS$_2$ create band tuning such that part of the lower Hubbard band crosses the $E_F$, creating a mobile pool of charge near the domain walls. STM spectroscopic maps show that these charges crystallize into unexpected 1D patterns. To distinguish the charge patterns from ordinary bound states, we carry out noise spectroscopy measurements and find that the 1D patterns show distinct telegraphic noise signatures indicative of a fragile condensed state. Combined with the large ratio of Coulomb to kinetic energies in this system, our data and calculations are consistent with the formation of a short-range, fragile charge order like an incipient Wigner crystal. The observation of crystallization in a strongly correlated regime makes TaS$_2$ a promising system for exploiting the charge and spin order in quasi 1D systems.

*Supported by U.S. D.O.E., Award # DE-SC0014335 and in part by Gordon and Betty Moore Foundation’s EPiQS Initiative, Grant GBMF4860
11:15AM S62.00001: Thermoelectric Transport in Topological Crystalline Insulator and Topological Semimetal Nanowires* [Invited] SHIXIONG ZHANG (Presenter), Indiana Univ - Bloomington — Many of the topological materials (e.g. Bi$_2$Te$_3$ and Sb$_2$Te$_3$) are also well-known thermoelectric materials with high figures of merit ZTs. This ‘coincidence’ is not accidental but is because the two groups of materials share some similar properties, i.e. they are composed of heavy elements and have small bulk band gaps. Theoretical calculations have suggested the possibility of enhancing thermoelectric properties by utilizing topological non-trivial states. In this talk, I will present our recent experimental studies of thermoelectric transport in some representative topological materials, including SnTe-based topological crystalline insulators (TCIs) and iridium oxide-based topological semimetals (TSMs). Grown by chemical vapor deposition, the TCIs and TSMs are (quasi-)one-dimensional nanowires with large surface-area-to-volume ratios and well-defined facets. Measurements of the Seebeck coefficient, and electrical and thermal conductivities were performed on the same individual nanowires as a function of temperature, allowing for accurate determination of their ZTs. I will discuss the enhancement of Seebeck coefficient and suppression of thermal conductivity in connection with the topological states, doping, alloying, and nanostructuring.

*The author acknowledges support from the LANL-LDRD program and NSF (grant number ECCS-1936406).

11:51AM S62.00002: Tunable Dimensionality Effects on the Thermoelectric Performance of Solution-Processable Hybrid Tellurium Nanowire Composites* MADELEINE GORDON (Presenter), KYLE HAAS, University of California, Berkeley, EDMOND ZAIA, LIN YANG, CHIH-HAO HSU, BORIS RUSS, AYASKANTA SAHU, JEFFREY URBAN, Lawrence Berkeley National Laboratory — Hybrid composite materials have demonstrated a high degree of thermoelectric (TE) performance and manage to leverage positive aspects of both their organic and inorganic counter parts such as ease of solution processability, cost effectiveness, conformal geometries and device printability. To date, there is limited understanding of the physical factors underlying high performance in this class of materials. Here, we investigate the impact of ligand chain length on the physical and TE properties of tellurium nanowires (TeNWs) grown in a simple one-pot synthesis. This work reveals the importance of TeNW dimensionality and polydispersity on TE transport in TeNW systems. Using an aqueous chemical modification technique, conductive polymer ligands are affixed to the surface of the top performing TeNWs, resulting in a p-type hybrid composite TE ink system with an optimized power factor of 130 uW/mK$^2$. This study provides insight into how synthetic chemistry can provide previously unused tools for optimizing performance and understanding transport in such complex hybrid systems.

*Department of Energy BES-LBL Thermoelectrics Program
Molecular Foundry and Advanced Light Source, Lawrence Berkeley National Laboratory
National Science Foundation Graduate Research Fellowship Program.
12:03PM S62.00003: Thermal transport in spin ladder compound Sr$_{14}$Cu$_{24}$O$_{41}$

XI CHEN (Presenter), Department of Electrical and Computer Engineering, University of California, Riverside, JAEHYUN KIM, Department of Mechanical Engineering, The University of Texas at Austin, SEAN E SULLIVAN, KARALEE JARVIS, Materials Science and Engineering Program, Texas Materials Institute, The University of Texas at Austin, JIANSHI ZHOU, LI SHI, Department of Mechanical Engineering, The University of Texas at Austin — Recently, large magnetic contribution to thermal conductivity has been observed in some cuprates with strong antiferromagnetic coupling. One prominent example is the spin ladder compound Sr$_{14}$Cu$_{24}$O$_{41}$ with an incommensurate layered structure. Steady-state thermal transport measurements of single crystals revealed a large anisotropic ratio of thermal conductivity due to the magnons propagating along spin ladders. Previous studies have been devoted to understand the coupling of magnons with phonons and electrons in Sr$_{14}$Cu$_{24}$O$_{41}$ single crystals; however, the effects of boundaries and defects on anisotropic magnon transport have been under-examined. Here, we investigate the thermal transport in Sr$_{14}$Cu$_{24}$O$_{41}$ microrods, which are prepared by co-precipitation synthesis. TEM studies indicate that these microrods are single crystals grown preferentially along the spin ladder axis. The thermal conductivity of Sr$_{14}$Cu$_{24}$O$_{41}$ microrods prepared at different temperatures is measured using a four-probe thermal transport measurement method. The thermal conductivity contribution and mean free paths of magnons are evaluated using a kinetic model of 1D magnon transport. Our results show pronounced effects of defects and boundaries on anisotropic magnon thermal transport in the magnetic microstructures.

12:15PM S62.00004: Probing thermal transport in single-molecule junctions

LONGJI CUI (Presenter), University of Colorado, Boulder — Charge and energy transport in single-molecule junctions is of great interest to reveal exotic quantum transport phenomena at the fundamental size limit, and with potential applications in nanoelectronics and nanophotonics. A key quantity—the thermal conductance of single-molecule junctions—has eluded experimental determination due to challenges in detecting extremely small picowatt-level heat currents that occur in such systems. Here, by employing custom-developed scanning thermal microscopy (SThM) probes that enable picowatt-resolution, we report the quantitative measurement of the thermal conductance of single-molecule junctions and investigate the dependence of thermal transport on molecular length. Our experiments were performed on prototypical Alkanedithiol molecules, revealing that the thermal conductance is approximately independent of the molecular length and is consistent with ab initio simulations. The techniques presented here represent a breakthrough that will enable further studies of thermal transport in many other 1D organic systems, short molecules and polymers, for which interesting thermal transport properties have been theoretically predicted but remain experimentally inaccessible.

12:27PM S62.00005: Photothermoelectric detection of strain variation in gold nanostructure
XIFAN WANG (Presenter), YUNXUAN ZHU, CHARLOTTE EVANS, DOUGLAS NATELSON, Rice Univ — Controlling morphology and composition via nanoscale structuring gives opportunities to improve the thermoelectric properties of materials for energy conversion and photodetection. In this study, we report the detection of the strain variation via open circuit photothermoelectric voltage detection on thin-film Au nanowire devices as a function of the position of an optical heat source. A focused laser beam is used to locally heat the metal nanostructure. The first mapping scan of the photothermoelectric voltage shows a relative high value compare with the second scan on the same device after 12 hours annealing. We also conduct a control experiment to shift the work function of the gold nanowire via self-assembled monolayer. Combining the kelvin probe measurement with the photothermoelectric voltage shows the work function variation of the nanowire doesn't play a key role on the photothermoelectric voltage response. These experiments argue that the strain distribution within the gold nanowire is likely the dominant effect causing the variation of the photothermoelectric voltage. Photothermoelectric voltage measurement provides a sensitive new method to strain distributions within a nanostructured metal.

12:39PM S62.00006: Energy Transport in Extreme Thermal Materials [Invited] YONGJIE HU (Presenter), JOONSANG KANG, MAN LI, HUAN WU, HUU DUY NGUYEN, University of California, Los Angeles — Controlling thermal transport is critical for many applications including electronics and energy technologies. Discovering new materials and nanostructures with extreme conductivity that can efficiently insulate or dissipate heat are in urgent need. In this talk, I will first describe our recent effort in developing emerging high thermal conductivity semiconductors, including boron arsenide (BAs) and boron phosphide (BP) with a room temperature thermal conductivity of 1300 W/mK (Science 361, 575, 2018) and 500 W/mK (Nano Letters 17, 7507, 2017) respectively, beyond most common semiconductors and metals. Ultrafast spectroscopy study in conjunction with atomistic theory reveals that the unique band structure of BAs allows for very long phonon mean free paths and strong high-order anharmonicity through the four-phonon process. Our study establishes BAs and BP as benchmark materials for thermal management, and exemplifies the power of combining experiments and \textit{ab initio} theory in new materials discovery. On the other hand, we investigated ultralow thermal conductivity materials with record-high thermoelectric performance. Examining the intrinsic crystals of tin selenide (Nano Letters 19, 4941, 2019), we observed abnormally strong phonon renormalization at room temperature due to high-order anharmonicity, as well as the failure of widely used quasi-harmonic model in predicting thermophysical properties. In addition, I will briefly describe our effort in developing in-situ techniques to characterize electrochemical materials (Nano Letters 17, 1431, 2017) and quantifying interface energy transport (Advanced Materials 31, 1901021, 2019) that enable better fundamental understanding of phonon spectra and defect scattering for electronics, sensors, batteries, and quantum information.
1:15PM S62.00007: Super Compliant and Soft \((\text{CH}_3\text{NH}_3)_3\text{Bi}_2\text{I}_9\) Crystals with Ultralow Thermal Conductivity*  
HAO MA, CHEN LI, Cornell University, YUNWEI MA, Virginia Tech, HENG WANG, Illinois Institute of Technology, ZACHARY ROUSE, Cornell University, ZHUOLEI ZHANG, Lawrence Berkeley National Laboratory, CARLA SLEBODNICK, Virginia Tech, AHMET ALATAS, Argonne National Laboratory, SHEFFORD BAKER, Cornell University, JEFFREY URBAN, Lawrence Berkeley National Laboratory, ZHITING TIAN (Presenter), Cornell University — In this work, we show the phonon dispersion of \((\text{CH}_3\text{NH}_3)_3\text{Bi}_2\text{I}_9\) single crystals at 300 K measured by inelastic x-ray scattering. The frequencies of acoustic phonons are among the lowest of crystals. Nanoindentation measurements verified that these crystals are very compliant and considerably soft. The frequency overlap between acoustic and optical phonons results in strong acoustic-optical scattering. All these features lead to an ultralow thermal conductivity, as validated by the laser flash method. The fundamental knowledge obtained from this study will accelerate the design of novel hybrid materials for energy applications. This work has been published in Phys. Rev. Lett. 123, 155901 (2019).

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1:27PM S62.00008: Photothermoelectric detection of local strain variations in gold single-crystal and bicrystal stripes*  
CHARLOTTE EVANS (Presenter), Physics and Astronomy, Rice University, RUI YANG, Electrical Engineering, UM-SJTU Joint Institute, Shanghai Jiao Tong University, LUCIA GAN, Electrical Engineering, Stanford University, MAHDIYEH ABBASI, Electrical and Computer Engineering, Rice University, XIFAN WANG, Materials Science and NanoEngineering, Rice University, JONATHAN FAN, Electrical Engineering, Stanford University, DOUGLAS NATELSON, Physics and Astronomy, Rice University — Nanoscale manipulation of the thermoelectric effect has recently been used in photodetection and energy conversion applications. In metals, the electronic Seebeck coefficient depends on the energy-dependent electrical conductivity. At the nanoscale, single metal thermocouples are created by modifying the conductivity via nanostructuring, changing the energy-dependent mean free path of the charge carriers. Here, we present scanning photothermoelectric measurements of gold single crystal devices and compare the photovoltages with electron back-scatter diffraction measurements, which provide insight on the local strain variation in the device. The good correlation between these measurements show that photovoltage measurements are sensitive to local variation in strain. Finite-element modeling suggests that these results are consistent with long-scale gradients in the Seebeck coefficient, which yield reasonable estimates of local strain. Extending these measurements to devices with individual grain boundaries demonstrate that local strain has a larger effect than simple changes in crystallographic orientation. These measurements show that residual strain gradients in nanostructures can dominate thermoelectric response.

*Robert A. Welch Foundation grant C-1636 and NSF No. ECCS-1704625.
1:39PM S62.00009: Modeling quasiballistic phonon transport from a cylindrical electron beam heat source* GEOFF WEHMEYER (Presenter), Mechanical Engineering, Rice University — Electron microscopy experiments use focused electron beams as nanoscale heat sources or thermometers. However, when the electron beam radius is smaller than the heat carrier mean free path, Fourier's law will underpredict the electron-beam induced heating. Here, beam heating in nonmetallic samples is modeled by applying a general solution of the Boltzmann Transport Equation (BTE) under the relaxation time approximation [Hua and Minnich, PRB 90.21 (2014): 214306]. BTE results show that ballistic phonon effects in this radial heat spreading scenario are conveniently represented using a ballistic thermal resistance. Calculations of this ballistic resistance for Si, GaAs, and 3C-SiC show that ballistic effects dominate the total thermal resistance for typical beam radii (<10 nm), indicating that the ballistic resistance could be measured using electron beam heating experiments. However, the magnitude of the temperature rise remains small (<1 K), even when considering these ballistic effects. These BTE modeling results can be used to quantify electron-beam induced heating or to design experiments probing ballistic phonon transport using electron beam heat sources.


*Welch Foundation (Grant #C-2023)

1:51PM S62.00010: Nondestructive probing of the transport and elastic properties of nanostructured metalattices using coherent EUV beams JOSHUA KNOBLOCH (Presenter), BEGOÑA ABAD, TRAVIS D FRAZER, BRENDAN MCBENNETT, STROBE and JILA, University of Colorado, Boulder, WEINAN CHEN, HIU CHENG, ALEX GREDE, NABILA NOVA, Pennsylvania State University, JORGE HERNÁNDEZ-CHARPAK, STROBE and JILA, University of Colorado, Boulder, PRATIBHA MAHALE, DISHA TALREJA, YIHUANG XIONG, TOM MALLOUK, NOEL C GIEBINK, VENKATRAMAN GOPALAN, ISMAILA DABO, VINCENT CRESPI, JOHN BADDING, Pennsylvania State University, HENRY KAPTEYN, MARGARET MURNANE, STROBE and JILA, University of Colorado, Boulder — Nanoscale metamaterials exhibit engineered thermal, magnetic, and electronic properties, which are essential for nanoelectronics, thermoelectrics, and ultralight media. Nanostructured metalattices are artificial 3D solids, periodic on length scales 1-100nm, that enable the functional properties of materials to be tuned. However, characterizing such materials is extremely challenging. Here we overcome this challenge by using tabletop high harmonic extreme ultraviolet (EUV) beams, with wavelengths (∼30nm) and pulse durations (∼10fs) that are well-matched for probing nanoscale structure and function. We demonstrate nondestructive measurements of the mechanical, structural, and transport properties of complex 3D nanostructured media—specifically in metalattices made from 14-30nm silica nanosphere templates infiltrated with silicon. We extract the mechanical and structural properties from the measured acoustic dispersion, which agrees with continuum models. In contrast, the heat flow through the metalattices deviates from macroscopic models due to the nanoscale structure. These samples have not only a lower thermal conductivity than expected, but also exhibit transport properties that depend on the heat source geometry. We support these findings with advanced atomistic models.
The composite material: a gold nanoparticle array embedded in a hydrogel polymer with a fluorinated surface layer; combines length scales from atomistic to microscale. When a laser excites the array local heating occurs, causing the polymer to shrink and the surface to wrinkle. The wrinkles deflect lasing and allow the system to relax. Using FTDT, the array geometry has been designed to maximize temperate change. The alteration of the mechanical properties of the hydrogel polymer due to the temperature change is essential to reproduce the wrinkling. When heated, the concentration of water in the polymer layer changes, altering the thermal and mechanical properties explored via molecular dynamics. Thermal transport is modeled using Reverse Non-Equilibrium Molecular Dynamics. A pure water/polymer system is compared to a system with different salts. This atomistic information feeds into finite element mechanics calculations, where previous studies have displayed wrinkling in similar systems. All these pieces help to create an autoregulatory humidity sensor.

1. S. Kuang, J.D. Gezelter. *Molecular Physics* 2012 110(9-10), 691-701

**Thursday, March 5, 2020 11:15 AM - 2:03 PM**

**Session S63 DCMP: Twisted 2D Heterostructures: Computational and Theoretical Studies I** Mile High Ballroom 4D - Nicolas Leconte
11:15AM S63.00001: Exploring van der Waals Heterostructures behavior: Stability vs.
Twisting  ANDREA SILVA (Presenter), Univ of Southampton, VICTOR P. E. CLAERBOUT, TOMAS
POLCAR, Advanced Materials Group, CVUT, DENIS KRAMER, Univ of Southampton, PAOLO NICOLINI,
Advanced Materials Group, CVUT — While the outstanding properties of van der Waals 2D materials
are widely known, recent efforts have been focusing on the physics emerging from the stacking
and rotational degrees of freedom of these lamellar compounds. Notable examples are
unconventional superconductivity in twisted bilayer graphene\(^1\) and frictionless dynamics
obtained by switching from commensurate to incommensurate orientation in graphitic systems\(^2\).

In this study we focus on an often overlooked question: are twisted geometries
thermodynamically stable and what defines the energy landscape induced by the rotation? We
answer this question in the MoS\(_2\)/Graphene system, as the pristine components are widely
known and experimental data on this heterostructure is contradictory.

We use a refined classical potential to simulate edge-free rotated heterostructure and obtain the
energy behavior as a function of the imposed angle in the thermodynamic limit. Our work shows
the breakdown of a known theory of 2D incommensurate interfaces\(^3\) and offers new insights
about the microscopic mechanism governing the stability of this class of materials.


11:27AM S63.00002: Structural and electronic properties of twisted bilayer transition metal
dichalcogenides from linear-scaling DFT\(^*\)  VALERIO VITALE (Presenter), JOHANNES LISCHNER,
ARASH A MOSTOFI, Imperial College London — Recently, it has been proposed that Moiré
superlattices of twisted homobilayer transition metal dichalcogenides (TMDs) exhibit many
interesting structural and electronic properties, including shear solitons, phasons, topological
point defects and ultraflatbands close to the Fermi level \([1,2]\). For small twist angles the unit cells
of these systems contain thousands of atoms rendering first-principles investigations of their
structural and electronic properties numerically challenging. To overcome this obstacle, we
employ the linear-scaling DFT code ONETEP \([3]\) and present results for relaxed geometries and
band structures for both homo- and heterobilayers of transition metal dichalcogenides as
function of twist angle.


\(^*\)V.V., J.L. and A.A.M. acknowledge support from EPSRC (Grant no: EP/S025324/1)
11:39AM S63.00003: Moire quasicrystals in graphene encapsulated by hexagonal boron nitride
NICOLAS LECONTE (Presenter), JEIL JUNG, University of Seoul — Interference of double moire patterns of graphene (G) encapsulated by hexagonal boron nitride (BN) can alter the electronic structure features near the primary/secondary Dirac points and the electron-hole symmetry introduced by a single G/BN moire pattern depending on the relative stacking arrangements of the top/bottom BN layers. For equal moire periods and commensurate patterns with Δφ = 60° angle differences, the patterns can add up constructively or cancel out destructively depending on their relative sliding, while moire quasicrystals are expected for Δφ = 30° differences. We present calculations on the double moire interference effects in the density of states and magnetic oscillations in nearly aligned BN/G/BN systems giving rise to moire quasicrystals and their evolution as a function of moire superlattice twist angles.

*N.L. acknowledges grants KRF-2016H1D3A1023826 and 2018R1C1B6004437 from the Korean National Research Foundation, and J. J acknowledges SSTF-BA1802-06 from Samsung Science and Technology Foundation.

11:51AM S63.00004: Modeling mechanical relaxation and electronic states of incommensurate trilayer van der Waals heterostructures
ZIYAN ZHU (Presenter), STEPHEN CARR, Harvard University, PAUL CAZEAUX, University of Kansas, MITCHELL LUSKIN, University of Minnesota, Twin Cities, EFTHIMIOS KAXIRAS, Harvard University — Incommensurate stacking provides an intriguing avenue for manipulating the physical properties of layered two-dimensional materials, but is a challenging problem from a theoretical perspective. Here, we present a multiscale model to obtain the mechanical relaxation pattern and electronic structure of twisted trilayer van der Waals heterostructures with two independent twist angles. This serves as a prototype system of a generally incommensurate system without a supercell description.

To study mechanical properties, we adopt configuration space as a natural description of incommensurate layers, which describes the local environment of each atomic position. We minimize the total energy, parameterized using Density Functional Theory calculations, to obtain the relaxation pattern. For the electronic properties, we focus on twisted trilayer graphene. We adopt a \( k.p \) effective theory derived from a low-energy expansion around the Dirac point. Our results suggest that the twisted trilayer systems are interesting from theoretical and mathematical points of view, as well as a promising platform to study correlated physics.

*This work was supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319.
12:03PM S63.00005: First-principles calculation of gate-tunable magnetism in twisted bilayer graphene under pressure*

XIAO CHEN (Presenter), SHUANGLONG LIU, HAI-PING CHENG, University of Florida — Magic angle twisted bilayer graphene (MAtBLG) is believed to be a highly tunable platform for investigating strongly correlated phenomena such as high-$T_c$ superconductors and quantum spin liquids, due to easy control of doping level through gating and sensitive dependence of the magic angle on hydrostatic pressure. Experimental observations of correlated insulating states, unconventional superconductivity and ferromagnetism in MAtBLG indicate that rich exotic phases exist in this system, which is also suggested by various theoretical works. In this work, with a combination of density functional theory and effective screening medium method, we systematically study the ground state of twisted bilayer graphene at magic twist angle $2.88^\circ$ under pressure and simulate how the ground state evolves when doping level is gate-tuned. We find that at zero doping, a ferromagnetic solution showing half-metallic behavior with spin density localized at AA stacking sites is lower in energy than the trivial spin non-polarized solution. Interestingly, the magnetic moment per moiré unit cell of this ferromagnetic state decreases upon both electron and hole doping and vanishes at four electrons/holes doped per moiré unit cell.

*This work is supported by the US DOE/BES DE-FG02-02ER45995.

12:15PM S63.00006: Origin and Evolution of Ultraflatbands in Twisted Bilayer Transition Metal Dichalcogenides: Realization of Triangular Quantum Dots

MIT H. NAIK (Presenter), University of California at Berkeley and Lawrence Berkeley National Lab, SUDIPTA KUNDU, INDRAJIT MAITY, MANISH JAIN, Indian Institute of Science — Using a multiscale computational approach, we probe the origin and evolution of ultraflatbands in moiré superlattices of twisted bilayer MoS$_2$ (TBLM), a prototypical transition metal dichalcogenide. Unlike twisted bilayer graphene, we find no special magic angles in TBLM. Ultraflatbands, which form at the valence band edge for twist angles ($\theta$) close to $0^\circ$ and at both the valence and conduction band edges for $\theta$ close to $60^\circ$, have distinct origins. For $\theta$ close to $0^\circ$, inhomogeneous hybridization in the relaxed moiré superlattice is sufficient to explain the formation of flatbands. For $\theta$ close to $60^\circ$, apart from the inhomogeneous hybridisation, local strains cause the formation of modulating triangular potential wells such that electrons and holes are spatially separated. This leads to multiple energy-separated ultraflatbands closely resembling eigenfunctions of a quantum particle in an equilateral triangle well.
**12:27PM S63.00007: Correlated states in transition metal dichalcogenide heterobilayer moiré superlattices** – NAICHAO HU (Presenter), AJESH KUMAR, ALLAN MACDONALD, Department of Physics, University of Texas at Austin — 2D van der Waals moiré superlattices have attracted much attention recently as highly tunable platforms to study strong correlation phenomena. In particular, transition metal dichalcogenide (TMD) heterobilayers at small twist angles develop isolated flat moiré bands that are accurately described [1] by triangular lattice (generalized) Hubbard models. Using a fully self-consistent mean-field-theory, we investigate the competing correlated phases at various fractional filling factors and twist angle, and identify metal-Mott insulator phase transition at 1/2 band filling and Wigner crystal phases at 1/6 band filling. We will discuss the relationship between our calculations and recent related experiments.


*Work supported by DOE grant DE- FG02-02ER45958.

**12:39PM S63.00008: Spontaneous symmetry breaking and topology in twisted bilayer graphene: the nature of the correlated insulating states and the quantum anomalous Hall effect** – JIANPENG LIU (Presenter), XI DAI, Hong Kong University of Science and Technology — We theoretically study the nature of the correlated insulating states and the quantum anomalous Hall (QAH) effect in twisted bilayer graphene (TBG) at the magic angle. Using a generic Hartree-Fock theory applied to all the energy bands, both the experimentally observed correlated insulating states at +/-1/2 filling and the quantum anomalous Hall effect at 3/4 filling of the flat bands near magic angle can be successfully explained. Our results indicate that the correlated insulating states at +/-1/2 filling are states with co-existing valley coherent order and valley polarized order. When a hexagonal boron nitride (hBN) substrate is aligned with the TBG, the valley polarized states are energetically favored over the valley coherent states at +/-1/2 filling, giving rise to QAH insulating states with Chern numbers (C) +/-2 by virtue of the C2z symmetry breaking induced by the substrate. We propose that such valley polarized QAH states would be strongly suppressed by weak in-plane magnetic fields. We further predict that, for the same valley polarization, the anomalous Hall conductivities are opposite for +/- p (p=1/2 or 3/4) fillings, which implies opposite hysteresis behaviors for the QAH states at the electron and hole fillings.
**12:51PM S63.00009: Quasiperiodicity induced eigenstate criticality and flat $\mathbb{Z}_2$ bands in a topological insulator**  
YIXING FU (Presenter), JED PIXLEY, JUSTIN WILSON, Rutgers University, New Brunswick — Flat topological bands have been sought after as a route to the fascinating phenomena of topology with strong correlations. The discovery of correlated insulator and superconductivity in various twisted multilayer graphene systems has shown that the superlattice pattern generated in van der Waals heterostructure, or more generally incommensurate effects, provides an ample playground for generating flat bands. We demonstrate that perturbing topological insulators with a quasiperiodic potential creates flat topological bands in a controllable fashion as well as induces non-trivial quantum phase transitions that are beyond the Landau-Ginzburg paradigm. Using a combination of analytic and numeric calculations, including a Convolutionary Neural Network classification of wavefunctions, we reveal the rich phase diagram induced by quasiperiodicity and topology. We show that quasiperiodicity can make a trivial insulator topological through a topological eigenstate phase transition that represent a unique universality class, and in the process creates essentially flat topological bands.

**1:03PM S63.00010: Modelling realistic Hamiltonians for moire lattices**  
ARKADIY DAVYDOV (Presenter), ALEXEY SOLUYANOV, physics, Univ of Zurich — The tight-binding (TB) approximation to the Hamiltonian of the Twisted Bilayer Graphene (TBG) is considered in the Slater-Koster (SK) form. Instead of taking the commonly-accepted parametrization, we generate a new one by fitting the data obtained in the *ab-initio* Density Functional Based (DFT) calculations. The resulting Hamiltonian is further projected to a smaller twelve-band tight-binding model, giving a systematic way to reduce the dimensionality of the problem. Finally, the localization of the Wannier orbitals and the symmetry of the final Hamiltonian is considered in this work.

**1:15PM S63.00011: Electronic properties of twisted transition metal dichalcogenide bilayers**  
MADELEINE PHILLIPS (Presenter), C STEPHEN HELLBERG, United States Naval Research Laboratory — The electronic properties of transition metal dichalcogenide (TMD) bilayers vary according to the local atomic structure [1]. In minimally twisted bilayers, there is significant atomic reconstruction away from the rigid moire pattern [2]. We present the results of density functional theory (DFT) calculations that model the electronic properties of MoSe$_2$/WSe$_2$ bilayers with a small (~1 degree) twist away from commensurate 180-degree stacking. We consider how the local density of states and charge density vary with atomic reconstruction and compare our results to recent experiments.


*M.P. holds a National Research Council fellowship at NRL.*
1:27PM S63.00012: Structure of twisted transition metal dichalcogenide bilayers  
STEPHEN HELLBERG (Presenter), MADELEINE PHILLIPS, U.S. Naval Research Lab — We present density functional (DFT) calculations of the reconstruction in transition metal dichalcogenide (TMD) hetero-bilayers twisted a small angle from from commensurate 180-degree stacking [1]. In both MoS$_2$/WS$_2$ and MoSe$_2$/WSe$_2$, the bilayer untwists and reconstructs to increase the area of the domains with the lowest energy stacking [2]. The overall twist is concentrated in the domain walls and vertices, where the energetic cost of twisting away from 180 degrees is reduced.

*M.P. holds a National Research Council fellowship at NRL.

1:39PM S63.00013: Surface States and Arcless Angles in Twisted Weyl Semimetals*
HERBERT FERTIG (Presenter), Indiana Univ - Bloomington, GANPATHY MURTHY, Physics and Astronomy, University of Kentucky, EFRAT SHIMSHONI, Physics, Bar Ilan University — Fermi arc states are features of Weyl semimetal (WSM) surfaces which are robust due to the topological character of the bulk band structure. We demonstrate that Fermi arcs may undergo profound restructurings when surfaces of different systems with a well-defined twist angle are tunnel-coupled. The twisted WSM interface supports a moiré pattern which may be approximated as a periodic system with large real-space unit cell. States bound to the interface emerge, with interesting consequences for the magneto-oscillations expected when a magnetic field is applied perpendicular to the system surfaces. As the twist angle passes through special “arcless angles”, for which open Fermi arc states are absent at the interface, Fermi loops of states confined to the interface may break off, without connecting to bulk states of the WSM. We argue that such states have interesting resonance signatures in the optical conductivity of the system in a magnetic field perpendicular to the interface.

*US-Israel Binational Science Foundation; NSF; Research Corporation

1:51PM S63.00014: Open Momentum Space Method for Hofstadter Butterfly: Application in Moire Models  
BIAO LIAN (Presenter), FANG XIE, ANDREI BERNEVIG, Princeton University — We develop a generic open momentum space method for calculating the Hofstadter butterfly of both continuum models (for Moire superlattices, etc) and tight-binding models, where the quasimomentum is directly substituted by the Landau level (LL) operators. By taking a LL cutoff (and a reciprocal lattice cutoff for continuum models), one obtains the Hofstadter butterfly with in-gap spectral flows. For continuum models such as the model for twisted bilayer graphene, our method gives a sparse Hamiltonian, making it much more efficient to calculate the spectrum. The spectral flows can be understood as edge states on a momentum space boundary, from which one can determine the two integers $(tv, sv)$ of a gap $v$ satisfying the Diophantine equation. The spectral flows can also be removed to plot a clear Hofstadter butterfly. While $tv$ is known as the Chern number, our picture identifies $sv$ as a dual Chern number in the momentum space, which corresponds to a quantized Lorentz susceptibility $\gamma_{xy} = eBsv$. 
11:15AM S64.00001: Low-Voltage Control of Magnetism in Fe$_{0.49}$Rh$_{0.51}$/0.68PbMg$_{1/3}$Nb$_{2/3}$O$_3$-0.32PbTiO$_3$ Thin Films Heterostructures  WENBO ZHAO (Presenter), LEI ZHANG, JIEUN KIM, DAVID PESQUERA, GABRIEL VELARDE, LANE WYATT MARTIN, Department of Materials Science and Engineering, University of California, Berkeley — With the rapid development of computing applications, researchers are motivated to develop novel low-energy consumption devices for information processing. Amongst candidate technology for such devices are low-power spin logics. Therein, magnetoelectric heterostructures remain a promising route to address the rising need of processing power. Previous research, however, has mainly utilized piezo-strains from piezoelectric bulk or thick films which require high voltages and energies due to their size.[1] Here, using 100 nm-thick 0.68PbMg$_{1/3}$Nb$_{2/3}$O$_3$-0.32PbTiO$_3$ thin-films as actuator layers, we discuss the potential for ultra-low-voltage control of magnetism in Fe$_{0.49}$Rh$_{0.51}$ thin-films via strain. Leveraging routes for epitaxial integration of metallic ferromagnets on oxide thin films, initial studies have demonstrated reversible changes in anomalous Hall resistivity with small voltages applied to the 0.68PbMg$_{1/3}$Nb$_{2/3}$O$_3$-0.32PbTiO$_3$ at room temperature which are attributed to the strain induced ferromagnetic and antiferromagnetic phase transition in Fe$_{0.49}$Rh$_{0.51}$. Our findings reveal the feasibility of voltage control of magnetism with piezoelectric thin-films and can be used in low-voltage/energy computing.

Recent observations of domain wall conductivity in the LiNbO$_3$ thin films may facilitate the development of electrically-tunable resistive switching devices employing conductive domain walls as functional elements. In LiNbO$_3$ capacitors, several orders of magnitude modulation of resistance can be achieved by systematically changing the density of injected domain walls using voltage pulse amplitude above the coercive bias. However, a deleterious characteristic of this approach is a high-energy cost of polarization reversal due to high leakage current. Here, we demonstrate a new approach for tuning the device resistance by modulating the conductivity of domain walls rather than changing the domain configuration. Using the LiNbO$_3$ thin film capacitors with graphene top electrodes, we show that once the device is set to a specific polydomain state, its resistance can be continuously tuned by application of sub-coercive voltage. The tuning mechanism is based on reversible transition between the conducting and insulating states of the domain walls due to the electrically-induced wall bending near the sample surface. The developed approach provides an energy-efficient way to realize resistive functionality without the need of the domain structure modification by high voltage pulses.
Most modern computing is built upon the von Neumann architecture composed of the data storage and data operation in a central processing unit. However, as Moore’s law made exponential gains over the decades, a memory bottleneck emerged, also known as the von Neumann bottleneck. This memory bottleneck can often degrade computing by orders of magnitude below the maximum potential of the computer especially for applications with large data sets. Hence it is of great interest to develop new energy-efficient memory technologies. Spintronic memory based on spin-transfer torque has emerged as a potential on-chip memory but it suffers from high energy dissipation (due to the requirement for a large current) and high voltages (due to the use of tunnel junctions). In contrast, a magneto-electric memory can operate with a capacitive displacement charge and potentially reach a $1-10 \text{ aJ/switching operation}$. Here we show magneto-electric switching of a memory element with a giant magnetoresistance (GMR) readout, operating at $\sim200 \text{ mV}$. We utilize a combination of phase detuning via isovalent substitution, thickness scaling, and conductive oxide electrode choice to scale the switching energy density to $20 \text{ µJ/cm}^2$. To the best of our knowledge, this is among the lowest voltage and energy density demonstrated in a spintronic memory element, thus presenting an attractive pathway to ultralow-power electronics.

*U.S. Department of Energy Advanced Manufacturing Office, and the support of Intel Corp. through the FEINMAN program
12:27PM S64.00005: Magnetocapacitance Effect and Magnetoelectric Coupling in Type-II Multiferroics RFeWO\textsubscript{6} (R=Ho, Dy and Tb)* MOEIN ADNANI TAKANTAPEH (Presenter), MELISSA GOOCH, NARAYAN POUDEL, HUNG-CHENG WU, LIANGZI DENG, ZHENG WU, Texas Center for Superconductivity, University of Houston, CHUNG-KAI CHANG, National Synchrotron Radiation Research Center, Taiwan, TAHA SALAVATI-FARD, Department of Chemical and Biomolecular Engineering, University of Houston, YEN-CHUNG LAI, National Synchrotron Radiation Research Center, Taiwan, HUNG-DUEN YANG, Department of Physics, National Sun Yat-sen University, LARS C. GRABOW, Department of Chemical and Biomolecular Engineering, University of Houston, PAUL C. W. CHU, Texas Center for Superconductivity, University of Houston — In this work, we investigated the multiferroic property and magnetoelectric (ME) coupling in HoFeWO\textsubscript{6} with a noncentrosymmetric polar structure (space group Pna\textsubscript{2}1). Low temperature XRD measurements down to 8 K did not show a structural phase transition and our DFT calculations reveal a stable structure. With an antiferromagnetic transition at T\textsubscript{N}=17.8 K and a ferroelectric transition with the onset at the same temperature, this compound is a type-II multiferroic which shows magnetoelectric (ME) coupling. Field-dependent dielectric measurements show magnetocapacitance (MC) effect with double hysteresis loop at low temperature, which is directly related to its metamagnetic behavior. We further studied the MC effect in other members of this family, in particular, DyFeWO\textsubscript{6} and TbFeWO\textsubscript{6} and compared the results with HoFeWO\textsubscript{6}. The observed MC effect and its direct correspondence with magnetization further confirm the ME coupling in these compounds.

*The work performed at Houston is supported by USAFOSR Grant FA9550-15-1-0236, TLL Temple Foundation, JJ&R Moores Endowment, and State of Texas through TCSUH.

12:39PM S64.00006: Negative capacitance in the hexagonal-YbFeO\textsubscript{3} epitaxial thin films* YU YUN (Presenter), XIAOSHAN XU, University of Nebraska - Lincoln —
The management of the heat generation and the power dissipation during information processing are very import issues in highly integrated electronic circuits. The ferroelectric negative capacitance (NC) effects, which was proposed to overcome the fundamental limit posed by the Boltzmann distribution of electrons, are attracting a great deal of interests. This work, we designed a heterostructure based on the hexagonal-YbFeO\textsubscript{3} (h-YbFO) multiferroic thin films to study the transient NC effects. For the first time, room-temperature ferroelectric properties in the epitaxial h-YbFO thin films and a direct observation of NC effects of h-YbFO thin films are reported. The transient NC effects as a function of the load resistance and applied source voltage are systematically investigated, which qualitatively follow the theoretical prediction. The structural requirements for the NC effects have been discussed, e.g. domain structure correlation with dielectric layers, grain size effects, microscopy mechanisms of ferroelectric switching. This work provides a new platform for the study of NC effects, and opens new horizons for understanding and improving the NC effects.

*This work was supported by the NSF DMR-1454618
12:51PM S64.00007: Stability of the magnetoelectric state in Y-type hexaferrite single crystals  
VILMOS KOCSIS (Presenter), TARO NAKAJIMA, RIKEN, MASAAKI MATSUDA, Oak Ridge National Laboratory, AKIKO KIKKAWA, YOSHIO KANEKO, JUNYA TAKASHIMA, RIKEN, KAZUHISAKAKURAI, Comprehensive Research Organization for Science and Society (CROSS), TAKA-HISA ARIMA, YUSUKE TOKUNAGA, Department of Advanced Materials Science, University of Tokyo, YOSHINORI TOKURA, YASUJIRO TAGUCHI, RIKEN — The magnetoelectric (ME) properties of the trigonal Y-type hexaferrites, $\text{Ba}_{2-y}\text{Sr}_y\text{Co}_2\text{Fe}_{12-x}\text{Al}_x\text{O}_{22}$, are related to the multiferroic FE3 phase [1,2]. Although this phase has been observed both as a metastable and as a stable phase [3,4,5], stable control over magnetization by electric field has not yet been achieved close to room temperature. This indicates that for applications, the stability of the multiferroic phase as well as the ME state are crucial issues, which are hard to investigate using conventional approaches.

In this presentation, we report the results of the direct ($P-H$) and inverse ($M-E$) magnetoelectric effects in Y-type hexaferrites with different Sr doping levels. Using the combination of high electric and magnetic fields, we investigate the isothermal switching between two ME states. We discuss these new findings in terms of a possible way to evaluate the stability of the ME state in multiferroic materials.


1:03PM S64.00008: Local probing of jerky switching dynamics in Pb(Zr0.2Ti0.8)O3 thin films  
PHILIPPE TUCKMANTEL (Presenter), IAROSLAV GAPONENKO, STEFANO GARIGLIO, DQMP, University of Geneva, JOSHUA AGAR, MSE, Lehigh University, LANE WYATT MARTIN, DMSE, University of California, Berkeley, PATRYCJA PARUCH, DQMP, University of Geneva — Polarisation switching in ferroelectric materials is governed by the same competition between elasticity and disorder, which describes many systems from earthquake statistics to magnetic domain walls. The movement of the interface follows nonlinear creep and (de)pinning dynamics, with jerky individual events whose energy and size distributions are characterised by universal power laws. In ferroelectrics, domain nucleation and growth can be observed from nano to macroscale, providing a useful system in which this complex fundamental behaviour can be explored.

While past measurements have focused on average responses at the level of the whole sample, recent theoretical studies suggest that spatial resolution of the switching event distribution can provide important new information about the dynamic regime under observation.

Here, using piezoresponse force microscopy to follow polarisation reversal at the nanoscale in two epitaxially grown Pb(Zr0.2Ti0.8)O3 thin films, we show that the probability distribution of switching event sizes follows a power law with different exponents in samples with different disorder landscapes. Furthermore, we show how individual jerks attributed to domain wall motion and domain merging events contribute differently to the global switching dynamics.
1:15PM S64.00009: 2D Semiconductor Transistors using Layered van der Waals Oxide MoO$_3$ as High-$K$ Gate Dielectric*  
BRIAN HOLLER (Presenter), KYLE CROWLEY, Case Western Reserve University, HALYNA VOLKOVA, MARIE-HELENE BERGER, MINES Paris Tech, XUAN GAO, Case Western Reserve University — The search for smaller field effect transistors is leading research towards atomically thin 2D semiconductor materials. Due to the decreasing size of these transistors, there must be an emphasis on finding compatible gate dielectrics that can be equally effective in the 2D regime. MoO$_3$ is an attractive multi-functional transition metal oxide replacement for gate dielectrics in field effect transistors due to its exfoliatable van der Waals structure in addition to its high dielectric constant. This study demonstrates that as-grown MoO$_3$ has a high dielectric constant, $K$, of approximately 35 at room temperature at low frequencies by fabricating parallel plate capacitors from these thin flakes. Mechanically exfoliated MoO$_3$ flakes are used to create 2D heterostructures with WSe$_2$, demonstrating that MoO$_3$ also induces holes in the WSe$_2$ layer. Most importantly, MoO$_3$ proves to be a strong gate dielectric when used as a top-gate material for WSe$_2$ heterostructure devices.

*Work at CWRU is supported by Air Force Office of Scientific Research (AFOSR) Grant FA 9550-18-1-0030.

1:27PM S64.00010: First-principles investigations of ferroelectric and pyroelectric properties of HfO$_2$*  
SHI LIU (Presenter), School of Science, Westlake University, JIAN LIU, Optics and Thermal Radiation Research Center, Shandong University, BRENDAN HANRAHAN, Sensors & Electron Devices Directorate, U.S. Army Research Laboratory — The presence of ferroelectricity in HfO$_2$-based thin films have revitalized the interests in using ferroelectrics at the nanoscale. To understand the origin of ferroelectricity in this silicon-compatible ferroelectric, we investigated the kinetic effects of phase transitions in HfO$_2$ thin films by quantifying the transition barriers between different polymorphs of hafnia with density-functional-theory calculations and variable-cell nudged elastic band technique. We found that the transition from the tetragonal phase to the polar orthorhombic phase is a fast process kinetically under clamping. We further explored the pyroelectricity in HfO$_2$ with both first-principles lattice dynamics and ab initio molecular dynamics calculations. Unlike most conventional pyroelectrics, the large pyroelectricity of HfO$_2$ results from the secondary effect which is intimately related to the negative longitudinal piezoelectric effect.

*J.L. acknowledges the support from the NSFC (No. 11904202) and Qilu Young Scholar Program of Shandong University.
S.L. acknowledges the support of SEDD Distinguished Fellowship from ARL and the support from Westlake University.
Ferroelectricity in [111]-oriented epitaxially strained HfO$_2$ from first principles* SEBASTIAN REYES-LILLO (Presenter), Andres Bello University — First principles calculations are used to investigate the effect of (111) epitaxial strain in the structural and ferroelectric properties of Hafnia (HfO$_2$), a silicon compatible high-k dielectric that is already used in high volume semiconductor manufacturing applications. We find that [111]-oriented epitaxial strain lowers the symmetry of the bulk cubic Fm-3m and tetragonal P4$_2$/nmc phases of HfO$_2$ to rhombohedral R-3m and monoclinic P2$_1$/m, respectively. The polar orthorhombic Pca$_2_1$ phase stabilizes a ferroelectric monoclinic P1 structure above -2% (111)-strain, not present in either bulk or (001)-strained form. Under (111)-strain, ferroelectricity displays an out of plane polarization component P~ 35μC/cm$^2$. At large compressive strain (>2%), [111]-oriented thin films are paraelectric. We further explore the energy landscape of (111) strained HfO$_2$ and possible pathways for the stabilization of ferroelectricity.

*This work is supported by FONDECYT Iniciacion en la Investigacion under grant N° 11180590.

Thursday, March 5, 2020 11:15 AM - 1:27 PM

Session S65 DCMP: Superlattices and Nanostructures II: Transport and Electronic Phenomena Mile High Ballroom 4F - Simone Assali, Ecole Polytechnique de Montreal

Classical diffusion anomalies in two-dimensional Lorentz gases THOMAS HEINZEL (Presenter), BEATE HORN-COSFELD, JÜRGEN HORBACH, NIMA SIBONI, RENE LOHMANN, JAKOB SCHLUCK, University of Dusseldorf — The magnetoresistivity of two-dimensional Lorentz gases, formed by a free electron gas exposed to sparse, strong scatterers of identical shape at random positions, shows strong deviations from the Drude-Boltzmann model due to classical memory effects. At intermediate magnetic fields where the cyclotron radius is similar to the obstacle size, a conductance peak is observed which originates from transient superdiffusive motion along, and across, the obstacle clusters. [1] On the other hand, for strongly retroreflective [2] obstacles of sufficiently large number density, transient subdiffusive motion of the electrons is found in molecular dynamics simulations, which increases as the magnetic field approaches zero, and an anomaly is observed for $B=0$ where the diffusion constant cannot be defined, similar to earlier kinetic studies at low obstacle densities.[3] A suppression of the longitudinal conductivity around zero magnetic field is measured at sub-Kelvin temperatures and interpreted as an experimental signature of this transport anomaly.

11:27AM S65.00002: Kondo effect in Aharonov-Casher spin field-effect transistor  ANTON
PARAFILO (Presenter), Center for Theoretical Physics of Complex Systems, Institute for Basic Science,
LEONID GORELIK, Chalmers University of Technology, MIKHAIL KISELEV, The Abdus Salam International
Centre for Theoretical Physics, HEE CHUL PARK, Center for Theoretical Physics of Complex Systems,
Institute for Basic Science, ROBERT SHEKHTER, University of Gothenburg — We address the question
how Coulomb blockade in the nanowire affects the transport in Datta-Das transistor with anti-
collinear partially magnetized electrodes in the regime when Kondo phenomena is reached. We
use non-equilibrium Keldysh Green function technique at weak coupling regime to obtain first
two non-vanishing contribution to the charge current. It is predicted that the effects of spin-orbit
interaction result in a non-vanishing current for any spin polarization of the leads including the
case of fully polarized anti-collinear contacts.
The dependence of the Kondo temperature on the Aharonov-Casher phase and degree of
polarization in the leads is determined by the solution of the system of coupled Renormalization
Group equations. Analysis of the Kondo temperature shows that it decays with increasing of the
Aharonov-Casher phase and decreasing of the degree of polarization in the leads.

11:39AM S65.00003: Control of Resonant Tunneling transport in III-Nitride Double-Barrier
Heterostructures by δ-doping engineering*  JIMY ENCOMENDERO (Presenter), VLADIMIR
PROTASENKO, DEBDEEP JENA, HUILI GRACE XING, Cornell University — The spontaneous and
piezoelectric polarization fields in III-Nitride semiconductors control their electronic, optical, and
piezoelectric properties. Accordingly, the fundamental physics of resonant tunneling transport
through nitride resonant tunneling diodes (RTDs) is also dominated by the built-in polarization
fields. We have recently elucidated this connection by developing a transport model which
reproduces the measured tunneling currents in multiple RTD designs. Using this model and the
exponential dependence of the currents on the electric fields, we measured the polarization
fields with unprecedented precision.

III-Nitride RTDs are also of interest in practical applications since they provide electronic and
optical gain within the THz band. However, because of the internal fields, the resonant levels shift
toward higher energies due to the electrostatic polarization of the barriers and quantum-
confined Stark effect in the well. Thus, the resonant voltages exhibit values > 4 V, for multiple RTD
designs. Here, we present a new δ-doped GaN/AlN RTD which enables control over the resonant
voltages, making them independent of the built-in fields. We demonstrate devices with resonant
voltages ~1 V, while maintaining a high current density and peak-to-valley current ratio.

*CNF, CCMR
11:51AM S65.00004: Wentzel-Kramers-Brillouin (WKB) analysis and resonant electron tunneling in \(\alpha\)-T\(_3\) lattices

LIUBOV ZHEMCHUZHNA (Presenter), Hunter college, ANDRII IUROV, Medgar Evers college, GODFREY GUMBS, Hunter college, DANHONG HUANG, Air Force Research Lab — We have adopted the Wentzel-Kramers-Brillouin (WKB) theory for investigating pseudospin-1 \(\alpha\)-T\(_3\) materials for arbitrary hopping parameter \(0 < \alpha < 1\), including the extreme case when \(\alpha=1\) for the dice lattice. It has been revealed that the solution for this stationary eigenvalue problem has a power series depending on the Planck constant and we also obtained the corresponding semi-classical wave function. Using these results, we investigated the tunneling of pseudospin-1 Dirac electrons impinging various non-rectangular electrostatic potential barriers. We will present results for tunneling when optical dressed states arising from an electron interacting with a non-resonant dressing field with chosen polarization.

12:03PM S65.00005: Electron tunneling and transport in \(\alpha\)-T\(_3\) lattices under linearly polarized irradiation

PAULA FEKETE (Presenter), US Military Academy at West Point, ANDRII IUROV, Medgar Evers College of City University of New York, GODFREY GUMBS, Hunter College of the City University of New York, DANHONG HUANG, Air Force Research Laboratory, Kirtland Air Force Base, Albuquerque, NM — We have considered electron tunneling through a square electrostatic potential barrier for Floquet states, i.e., pseudospin-1 Dirac electrons coupled to a dressing, off-resonant field which is linearly polarized. While for the dice lattice we can still observe an asymmetric Klein tunneling, i.e., perfect transmission for electrons colliding with the barrier that is different from the head-on case, the Klein paradox is completely suppressed for the \(\alpha\)-T\(_3\) lattice in general with \(\alpha \neq 1\). We have also calculated electron transmission for finite incidence angles and the tunneling conductance corresponding to these transmission amplitudes.
12:15PM S65.00006: Incoherent Effects in Hot-Electron Quantum Optics*  CLARISSA BARRATT (Presenter), LEWIS CLARK, CLIVE EMARY, Univ of Newcastle — Using dynamical quantum dot single electron pumps, high-energy (“hot”) single electrons may be injected into semiconductor systems both reliably and at a high rate. When combined with energy and time-resolved detection, electrons from these sources provide us with a new platform to probe fundamental semiconductor physics in unprecedented detail.

In this contribution, we discuss coupling single-electron sources into interferometer geometries, such as the Mach-Zehnder interferometer, where the visibility of the quantum interference acts as a sensitive probe of the properties both of the emitted electrons and their environment. We investigate the effect of the uncertainty in injection energy on the phase contributions of the path lengths and quantum point contacts.

We also present theoretical calculations of the decay rate of a hot electron subject to phonon scattering, and determine how these rates are affected by parameters such as the electron injection energy and the magnetic field. Using our calculations for both phase averaging and phonon rates, we derive strategies for minimising the effects of these processes, thus maximising the quantum-coherent properties of the electrons.

*This research was supported by EPSRC Grant EP/P034012/1

12:27PM S65.00007: Photoconductivity of DNA-Porphyrin Complexes*  DANIEL VAN BEVEREN (Presenter), PECO MYINT, STEFANOS LOGOTHETIS, Haverford College, ZHENQING JOHN QI, CARL NAYLOR, MENGQIANG ZHAO, QICHENG ZHANG, ALAN T JOHNSON, Physics, University of Pennsylvania, WALTER FOX SMITH, Haverford College — DNA has attracted attention for potential use in nanocircuitry largely due to its pattern-recognition and self-assembly characteristics, but low electrical conductivity limits its potential usefulness for these applications. We attempt to address these issues by modifying DNA with meso-tetrakis(N-methyl-4-pyridiniumyl)porphyrin (TMPyP) intercalated between the base pairs. By measuring the electrical characteristics of these DNA-porphyring complexes deposited on a SiO2 under nitrogen gas, we show that this alteration increases the DNA strand conductivity and leads to significant photoconductive behavior at 445 nm, a wavelength strongly absorbed by the TMPyP-DNA complex. We also find a strong dependence on humidity, as photoconductive effects were only observed above 30% relative humidity, and increased both with the humidity in the chamber and with the length of exposure to the humid environment. A significant hysteresis is also observed, as the increased conductivity observed at higher humidity persists even after the humidity is lowered.

*NSF grants DMR 1306170 and BMAT 1306170
Thermal conductivity of thermally annealed nanocrystalline silicon film grown by PECVD technique*  

BATOOGTOKH JUGDERSUREN (Presenter), KeyW Corporation, XIAO LIU, United States Naval Research Laboratory, BRIAN T KEARNEY, National Research Council, JAMES CLIFFORD CULBERTSON, CHRISTOPHER N CHERVIN, RHONDA MICHELE STROUD, United States Naval Research Laboratory — Nanocrystalline silicon films (nc-Si) have been shown to have significantly lower lattice thermal conductivity than its micro-polycrystalline counterparts. However, it is essential for high temperature applications, such as thermoelectrics, to maintain their low thermal conductivity characteristics upon annealing, which may depend on the details of film preparation techniques. We investigate the effect of postdeposition thermal annealing on the thermal conductivity of nc-Si films prepared by plasma-enhanced chemical vapor deposition (PECVD). After annealing the PECVD nc-Si at 600°C for two hours, its thermal conductivity is increased two-fold, reaching 1.86 W/mK at 300K, however this value is lower than similarly annealed nc-Si films prepared by the hot-wire chemical vapor deposition technique by a factor of 2.5. Our structural characterizations reveal that after annealing, the average crystalline grain size of PECVD nc-Si is increased to ~4.6 nm from the as-grown value of 3 nm. We discuss the possible cause of the low lattice thermal conductivity of PECVD nc-samples in terms of grain boundary scattering.

*Work supported by the Office of Naval Research

Strain Controlled Modulations and Anomalies in the Thermopower of Si/Ge Superlattices: A First-Principles Study*  

MANOJ SETTIPALLI (Presenter), SANGHAMITRA NEOGI, University of Colorado, Boulder — The thermopower/Seebeck coefficient (S) of metals and heavily doped semiconductors usually decreases monotonically with increasing carrier concentration, n_e, following the Pisarenko relation (PR). Heterostructures, such as III-V semiconductor superlattices (SLs), have been shown to display oscillatory S, deviating from the PR. Interestingly, this behavior has not been observed in highly technologically relevant n-doped Si/Ge SLs. Here, we demonstrate a strong oscillatory behavior of the cross-plane S of n-doped Si/Ge SLs with n_e, deviating from the PR, using symmetry, composition, and strain engineering. We use the density functional theory (DFT) and the effective mass approximation, independently, in combination with the Boltzmann transport equation framework, to establish the results. We predict 5.4- and 1.8-fold enhancements in the cross-plane S and the power factor of Si/Ge SLs, respectively, in the high doping regime, compared to bulk Si. In addition, our DFT study shows that cross-plane S displays anomalous sign-changing nature within the conduction miniband regime. This study will open up research directions to use strain-engineered bands to control electronic properties for various heterostructures.

*The project is funded by DARPA (DSO) [Agreement No.: HR0011-16-2-0043].
1:03PM S65.00010: Prediction of large Seebeck coefficient in ferroelectric domain walls of GeTe*  
DORDE DANGIC (Presenter), University College Cork, EAMONN D MURRAY, Imperial College London, STEPHEN B FAHY, University College Cork, IVANA SAVIC, Tyndall National Institute — Domain walls in ferroelectric materials can have significantly different properties than their bulk counterparts, which creates new opportunities for the manipulation of material properties. GeTe is a ferroelectric material that is also an excellent thermoelectric, exhibiting relatively high electrical conductivity and Seebeck coefficient, as well as low lattice thermal conductivity. In this work, we present a first principles study indicating that ferroelectric domain walls in GeTe have a considerably larger Seebeck coefficient than bulk GeTe. Polarization discontinuity at domain walls gives rise to bound charge that localizes free charge carriers on the domain walls. We find that the two-dimensional electron gas confined to domain walls can exhibit large peaks in the local density of states near the Fermi level due to Van Hove singularities, resulting in an enhanced Seebeck coefficient. Van der Waals gaps along domain walls cause additional confinement of carriers within the domain walls that further increases the in-plane Seebeck coefficient perpendicular to the van der Waals gaps. The out-of-plane Seebeck coefficient is also significantly enhanced due to the charge localization on domain walls.

*This work is supported by Science Foundation Ireland PI Award 15/IA/3160.

1:15PM S65.00011: Visualizing Electronic Inhomogeneity in CsPbBr₃ Perovskite Nanorods  
YIZE LI (Presenter), California State University, Bakersfield, SHUANG LIANG, School of Materials Science and Engineering, Georgia Institute of Technology, TUONG TRIEU, TYLER STABILE, California State University, Bakersfield, ZHIQUN LIN, School of Materials Science and Engineering, Georgia Institute of Technology — Abstract: All-inorganic perovskite nanocrystals (NCs), such as CsPbBr₃ NCs, have demonstrated promising applications in solar cells, light-emitting diodes (LEDs), electroluminescence devices, and lasing. Grain boundaries and point defects influence carrier transport in perovskite NCs, thereby impacting the device performance. We use contactless dielectric force microscopy (DFM), a novel scanning probe microscopy (SPM)-based imaging technique, to probe local electronic inhomogeneity in CsPbBr₃ nanorods (NRs). We find that while some NRs exhibit nearly homogeneous DFM responses, others behave as p-n junctions with well-defined grain boundaries. Moreover, point defects are observed in some CsPbBr₃ NRs. It is thus feasible to identify CsPbBr₃ NRs that are suitable for device fabrications based on their DFM responses.
Quantum mirage is a fascinating phenomenon in fundamental physics. Landmark experiment on quantum mirage reveals novel information transport at the atomic scale and exhibits great potentials for remotely probing atoms or molecules with minimized perturbation. Previous experimental investigations are Kondo effect based and quantum mirages only appear near Fermi energy. This strongly limits the exploration of the mechanism and potential application. Here we demonstrate a Kondo-free quantum mirage, which can operate in a wide energy range beyond Fermi energy. Together with an analytical model, our systematic investigations identify that quantum mirage is the result of quantum interference of the onsite electronic states with those scattered by the adatom at the focus of elliptical quantum corrals, where two kinds of scattering paths are of critical importance. Moreover, we also demonstrate the manipulation of quantum mirage with pseudo logic operations, such as NOT, FANOUT and OR gates.

*This work was supported by National Key R&D Program of China (Grant No. 2017YFA0303202, No. 2018YFA0306004), National Natural Science Foundation of China (Grants No. 11974165, No. 51971110, No. 11734006), Natural Science Foundation of Jiangsu Province (Grant No. BK20190057).

Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S66 DCMP: Strongly Correlated Topological Metals

Subir Sachdev, Harvard University - Tag(s): Invited
The interplay of topology and strong electron correlations is emerging as a new frontier in quantum science; it is expected to bring forth exotic phases and excitations, as epitomized by the example of the fractional quantum Hall effect. Indeed, (weakly interacting) topological semimetals—featuring states with Dirac or Weyl dispersion in the bulk—were discovered when their correlation-driven counterparts were pursued. Heavy fermion systems provide an ideal setting because the Kondo interaction implements extreme correlation strength and representatives with strong spin-orbit coupling exist. A joint effort of experiments and theory has recently led to the discovery of a Weyl-Kondo semimetal phase [1-3]. Experimentally, it is realized in the noncentrosymmetric time reversal symmetry preserving heavy fermion semimetal Ce\(_3\)Bi\(_4\)Pd\(_3\) [1,3]. This material has a Kondo temperature of 13 K [1] and remains paramagnetic down to at least 250 mK [3]. Our most striking observation is a giant spontaneous (zero-field) Hall effect, and an associated even-in-field Hall component, which provide direct evidence of Berry curvature singularities in close vicinity to the Fermi level [3]. These characteristics of Weyl physics develop only in the Kondo coherent state, and are thus manifestly correlation driven. The application of large magnetic fields leads to an annihilation of the Weyl nodes at a first critical field, and to the metallization of the system at a second one, featuring quantum criticality [4].


*We acknowledge financial support from the Austrian Science Fund (FWF grants No. P29279-N27, P29296-N27, and DK W1243) and the European Union’s Horizon 2020 Research and Innovation Programme, under Grant Agreement no EMP-824109.
There is considerable current interest to explore electronic topology in strongly correlated metals. A promising setting arises in heavy fermion systems, which may feature not only strong correlations but also a large spin-orbit coupling. Recently, a Weyl-Kondo semimetal phase has been concurrently discovered in theoretical [1] and experimental [2] studies. The theoretical work was carried out in a Kondo lattice model that is time-reversal invariant but inversion-symmetry breaking. The defining characteristics of the Weyl-Kondo semimetal include linearly-dispersing Weyl nodal excitations with highly reduced velocity and the Weyl nodes being pinned to the Fermi energy. In this talk, I will summarize the theoretical developments, with a focus on the effect of non-symmorphic space-group symmetry in conjunction with strong correlations [1,3], the transitions to nearby quantum phases, as well as the efficient control of the Weyl nodes including their annihilation by a magnetic field [4,5]. The enrichment of these results for the global phase diagram of heavy fermion metals, reflecting on the role of spin-orbit coupling in the competition of quantum phases that develop out of the spin degrees of freedom [6], will be discussed.


*Work at Rice University was done in collaboration with Sarah Grefe and Hsin-Hua Lai. Supported by the NSF grant DMR-1920740, ARO grant W911NF-14-1-0525 and Robert A. Welch Foundation grant C-1411
From Trivial Kondo Insulator Ce$_3$Pt$_3$Bi$_4$ to Topological Nodal-line Semimetal Ce$_3$Pd$_3$Bi$_4$ [Invited]  CHAO CAO (Presenter), Department of Physics, Hangzhou Normal University, GUOXIANG ZHI, Department of Physics, Zhejiang University, JIAN-XIN ZHU, Los Alamos National Lab — Using the density functional theory combined with dynamical mean-field theory, we have performed systematic study of the electronic structure and its band topology properties of Ce$_3$Pt$_3$Bi$_4$ and Ce$_3$Pd$_3$Bi$_4$. At high temperatures (~290K), the electronic structures of both compounds resemble the open-core 4f density functional calculation results. For Ce$_3$Pt$_3$Bi$_4$, clear hybridization gap can be observed below 72K, and its coherent momentum-resolved spectral function below 18K exhibits an topologically trivial indirect gap of ~6 meV and resembles density functional band structure with itinerant 4f state. For Ce$_3$Pd$_3$Bi$_4$, no clear hybridization gap can be observed down to 4K, and its momentum-resolved spectral function resembles electron-doped open-core 4f density functional calculations. The band nodal points of Ce$_3$Pd$_3$Bi$_4$ at 4K are protected by the gliding-mirror symmetry and form ring-like structure. Therefore, the Ce$_3$Pt$_3$Bi$_4$ compound is topologically trivial Kondo insulator while the Ce$_3$Pd$_3$Bi$_4$ compound is topological nodal-line semimetal.

*This work was support by NSFC 11874137 and 973 Project 2014CB648400 and U.S. Office of Basic Energy Sciences under LANL-E3B5.

Evidence for Undoped Weyl Semimetal Charge Transport in a bad Weyl Semi-Metal: Y2Ir2O7* [Invited]  ARTHUR RAMIREZ (Presenter), University of California, Santa Cruz — Most Weyl semimetals studied to date either have a chemical potential not situated at the nodal point, or multiple nodal points at different energies, thus leading to metallic behavior in resistivity versus temperature. Undoped Weyl semimetals, in which the chemical potential is exactly at the nodal point will exhibit characteristic non-metallic behavior in transport that should reveal the density of electronic states as well as the dominant scattering mechanisms. We discuss the various types of transport for both doped and undoped Weyl systems. We show that one candidate, Y2Ir2O7, predicted to display a spectrum of an undoped Weyl semimetal, exhibits behavior of a system with the expected quadratic density of states and scattering from charged impurities, namely resistivity varying as 1/T^4 over a large temperature range. We discuss the implications of these results in light of exciting theories, as well as prospects for future work.

*NSF DMR 1534741 and 1534818 and NSF DGE-1339067
STM studies of candidate topological Kondo insulator SmB$_6^*$ [Invited]

STEFFEN WIRTH (Presenter), LIN JIAO, SAHANA RÖSSLER, DEEPA KASINATHAN, Max Planck Institute for Chemical Physics of Solids, PRISCILA ROSA, Los Alamos National Laboratory, USA, CHAO-XING LIU, Department of Physics, Pennsylvania State University, ZACHARY FISK, University of California, Irvine, USA, FRANK STEGLICH, Max Planck Institute for Chemical Physics of Solids — SmB$_6$ has been proposed a topological Kondo insulator with nontrivial surface states inside a bulk hybridization gap. Experimentally, hybridization between localized 4$f$ and conduction band states at low temperatures is well established [1]. Using STM, we performed local measurements on well identified, atomically flat, unreconstructed surfaces [2]. Tunneling spectroscopy down to 0.35 K revealed sharp peak-like features with a strong temperature dependence within the hybridization gap. The features around −6 mV and −2 mV are dominated by surface contributions to the local density of states [3]. These surface states are robust in the vicinity of randomly occurring non-magnetic impurities, while introducing magnetic impurities in samples (Sm$_{1-x}$R$_x$)B$_6$ with $R$ = Gd influences the surface states on a much larger length scale compared to non-magnetic impurities [4]. Another material of topical interest is the magnetic Kagome lattice Weyl semimetal Co$_3$Sn$_2$S$_2$ in which time-reversal symmetry breaking causes fascinating physics [5]. The measured local density of states reveals a semimetallic gap of −300 mV, verified as the gap in the spin-minority band using spin-resolved tunneling spectra [6].

Work conducted in collaboration with Y. Cheon, C. Felser, C. Guo, G. Li, E. Liu, Y. Sun, L. H. Tjeng, Q. Xu, and H. Yuan.


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Thursday, March 5, 2020 11:15 AM - 2:15 PM

Session S67 DCMP: Recent Experimental Surprises in Strongly Correlated Superconductors Four Seasons 2-3 - Richard Greene, University of Maryland, College Park

- Tag(s): Invited
11:15AM S67.00001: Unconventional superconductivity in Sr$_2$RuO$_4$ probed under stressed conditions* [Invited] STUART BROWN (Presenter), University of California, Los Angeles — The stoichiometric transition metal oxide Sr$_2$RuO$_4$ is widely considered a model unconventional superconductor, owing to experimental evidence for strong correlations, and to the emergence of an odd-parity superconducting ground state with transition temperature near 1 K. With additional evidence for time-reversal symmetry breaking came the proposal for a two-component chiral $p$-wave order parameter, for which there is an expectation for a split superconducting transition when subjected to in-plane uniaxial stress. Recent studies instead revealed a factor 2.5 increase in the transition temperature of stressed samples, motivating us to probe the evolution of the normal and superconducting states using $^{17}$O NMR. Under stressed conditions, the normal state Knight shifts are consistent with tuning the Fermi surface through a van Hove singularity, along with an associated Stoner factor enhancement [1]. Over a broad temperature range, the magnetic response implies a dominant influence of the small energy difference between $E_F$ and that of the van Hove singularity, which can be controlled by strain, and independently by the Zeeman interaction. A reduced superconducting state spin polarization for in-plane magnetic fields, for all strain values studied, rules out the long-considered chiral $p$-wave state [2]. Although the helical state is an unlikely possibility under stressed conditions, further tightening of constraints on the superconducting state is a priority.


*Support from the National Science Foundation (DMR-1709304) and by the Laboratory Directed Research and Development (LDRD) programme of Los Alamos National Laboratory (20170204ER) is acknowledged.
KENJI ISHIDA (Presenter), KATSUKI KINJO, MASAHIRO MANAGO, SHUNSAKU KITAGAWA, YOSHITERU MAENO, Kyoto Univ — NMR experiments have been done in various unconventional superconductors, and gave information about superconducting (SC) pairing state and SC gap structure. We reported that the Knight shift at the Ru and O sites in Sr$_2$RuO$_4$ is invariant on passing through $T_c$[1,2]. Quite recently, Pustogow and Luo et al. reported a reduction of the Knight shift at the O site measured with a small-energy RF pulse[3]. We reexamined $^{17}$O-NMR on our sample with similar small-energy RF pulses and reproduced their results[4]. Furthermore, we measured the temperature variation of the Knight shift by a standard spin-echo method with small-power RF pulses, and found that the spin susceptibility decreases in the SC state. We conclude that our previous results of the invariance of the Knight shift in the SC state were due to instantaneous destruction of superconductivity by the RF pulses. The heat-up effect was characterized by the temperature variation of the Knight shift under various measurement conditions. In the presentation, we will also present new results obtained near $H_{c2}$ along the $ab$ plane.


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ANNA TAMAI (Presenter), Departement of Quantum Matter Physics, University of Geneva — We used laser-based angle-resolved photoemission spectroscopy to explore the interplay of electron-electron correlations and spin-orbit coupling in the model Fermi liquid Sr$_2$RuO$_4$. Our precise measurement of the Fermi surface confirms the importance of spin-orbit coupling in this material and reveals that its effective value is enhanced by a factor of about 2 due to electronic correlations. The self-energies for the $\beta$ and $\gamma$ sheets are found to display significant angular dependence. We demonstrate that this behavior does not imply momentum-dependent many-body effects, but arises from a substantial orbital mixing induced by spin-orbit coupling. A comparison to single-site dynamical mean-field theory further supports the notion of dominantly local orbital self-energies and provides strong evidence for an electronic origin of the observed nonlinear frequency dependence of the self-energies, leading to “kinks” in the quasiparticle dispersion of Sr$_2$RuO$_4$. 
Magnetic excitations and their possible role in the superconducting pairing in \( \text{Sr}_2\text{RuO}_4 \)^{*} [Invited]  
MARKUS BRADEN (Presenter), STEFAN KUNKEMÖLLER, KEVIN JENNI, II. Physics Institute, University of Cologne, PAUL STEFFENS, Univ. of Cologne; Institut Laue Langevin, YVAN SIDIS, Laboratoire Leon Brillouin, ZHIQIANG MAO, Tulane University, IGOR MAZIN, Naval Research Laboratory, YOSHITERU MAENO, Kyoto University — The magnetic excitations in the unconventional superconductor \( \text{Sr}_2\text{RuO}_4 \) consist of several contributions, an incommensurate signal arising from nesting and quasiferromagnetic fluctuations. We were able to follow the nesting signal of the quasi-one-dimensional bands across the superconducting transition down to very low energies. Even at \( E=0.325 \) meV, which lies well below the superconducting gap 2D values reported from tunneling experiments or deduced from BCS theory, there is no change in the magnetic response [1], which seems incompatible with the picture of a large gap on these Fermi-surface sheets. The quantitative analysis of the quasiferromagnetic fluctuations in \( \text{Sr}_2\text{RuO}_4 \) is hampered by the smaller amplitude and the little structure in \( Q \) space of this signal. Only by use of polarized neutron scattering we can determine the strength and characteristics of the ferromagnetic response, which agrees with reports of specific heat, magnetic susceptibility and NMR. Incorporating this ferromagnetic response into the gap equation, however, does not stabilize a triplet pairing state [2]. Furthermore, the quasiferromagnetic response in \( \text{Sr}_2\text{RuO}_4 \) does not resemble the paramagnon scattering expected for a nearly ferromagnetic material, but it seems to arise from broad instabilities at low propagation vectors. In contrast recent INS on the ferromagnetic perovskite \( \text{SrRuO}_3 \) find the typical ferromagnetic magnon and paramagnon scattering below and above the Curie temperature [3]. The magnon stiffness and gap in \( \text{SrRuO}_3 \) is found to anomalously soften upon cooling well below the Curie temperature, which can be attributed to the impact of Weyl points [3].


*This work was funded by the Deutsche Forschungsgemeinschaft — Project No. 277146847 — CRC 1238, project A02 and B04.
11:15AM S68.00001: Sandwich Layering in Binary Colloidal Films During Evaporative Drying* [Invited]
WEIPING LIU, AMANDA CARR, State Univ of NY - Stony Brook, ALEXANDER ROUTH, University of Cambridge, KEVIN YAGER, Brookhaven National Laboratory, SURITA BHATIA (Presenter), State Univ of NY - Stony Brook — Multicomponent films based on colloidal dispersions have a wide range of applications, including antimicrobial coatings for medical instruments, conductive textiles for flexible electronics, anti-reflective coatings for optical devices, paints for humid environments that are resistant to mold growth, and drug-loaded coatings for medical implants. Often, there is a need to spatially control location of certain components in the film. In this talk, I will present our recent results from microbeam small-angle X-ray scattering (SAXS) on films prepared from binary colloidal dispersions containing large and small particles of varying size and initial volume fraction. Our results show evidence of different types of stratification behavior, including large-on-top (e.g., large particles migrating to the top surface of the film), small-on-top, and “sandwich”-like layering. Additionally, I will present recent modeling results with different forms of the interaction potential, some of which qualitatively capture formation of "sandwich" structures.

*National Science Foundation CBET-1335787 and CBET-1903189
Illuminating the dynamics of drying suspensions in droplets and films

JORIS SPRAKEL (Presenter), Wageningen University — The drying of a suspension, e.g. in an inkjet printed droplet or a coating film, driven by evaporation or capillary imbibition into the substrate, leads to complex changes in the internal dynamics and mechanics of the system. As the particle concentration increases, diffusivities decrease, collective phenomena emerge, particle begin to interact, aggregate and coalesce. Often, these phenomena occur simultaneously without clear temporal separation, at a wide range of characteristic time scales, and in a spatially-inhomogeneous manner. Here we give an overview of recent advances in the development of an experimental tool, Laser Speckle Imaging, that can unravel many of these phenomena across a wide range of time scales, and in a spatially-resolved manner, even in complex and realistic coating formulations. We show how LSI can be used to pinpoint the coating open time and moment of film formation, give insight into subsurface transport and the emergence and propagation of cracks.

Drying Process in Films of Nanoparticle Suspensions and Polymer Solutions

SHENGFENG CHENG (Presenter), Virginia Tech — The drying process of polymer solutions or nanoparticle suspensions provides an excellent playground to explore nonequilibrium physics. For example, novel stratification phenomena have recently been discovered in polydisperse particle suspension films that undergo rapid drying. In these systems, the complex interplay of solvent evaporation, fluid dynamics, diffusion, phoresis, and capillarity leads to rich, far-from-equilibrium phenomena. I will describe our efforts using large scale molecular dynamics (MD) simulations to study the drying process of colloid suspensions, polymer solutions, and their mixtures. For bidisperse particle suspensions, a state diagram of stratification is determined and the counterintuitive "small-on-top" stratification, with an enrichment of the smaller particles at the receding liquid-vapor interface during fast drying, is observed. Results are compared to the predictions of several theoretical models based on diffusiophoresis. We show that the temperature gradient induced by evaporative cooling can lead to size-dependent thermophoretic responses of nanoparticles, which compete with diffusiophoresis and suppress the “small-on-top” stratification. On the basis of this observation, an approach to control stratification using various externally imposed thermal gradients is suggested and validated with MD simulations. We further show that a mixture of two liquids stratifies when rapidly dried with the less volatile component concentrated near the evaporating interface. This phenomenon can be used to separate and stratify particles which have different couplings to the components of a liquid mixture. Finally, we demonstrate a new strategy of unfirmly dispersing nanoparticles into a polymer matrix using fast solvent evaporation, based on the stratification behavior of polymer-particle mixtures in a far-from-equilibrium situation induced by rapid drying.

*Computational hours are provided through a DOE ALCC award.
Stratification in Drying Colloidal Films: A competition between diffusion, evaporation and diffusiophoresis* [Invited] CLARE REES-ZIMMERMAN, ALEXANDER ROUTH (Presenter), Chemical Engineering and Biotechnology, University of Cambridge — Waterborne dispersions are an environmentally friendly formulation for coatings. There are a number of issues associated with drying such coatings such as reduced open time and crack formation. Blending dispersions with hard and soft components has been shown to allow better film formation; however, stratification of components can lead to regions of cracking. Alternatively stratification can be beneficial and used to place different components at desired regions within the film. This could be used for expensive anti-fungal agents in bathroom coatings or catalysts in the walls of tubular reactors.

To understand stratification in drying coatings, one dimensional drying of bi-disperse mixtures has recently been the subject of intense theoretical and experimental study. The experimental observation is of accumulation of smaller particles at the top surface of drying films. The physics driving such stratification is still being debated and the competing theories of cross interactions, diffusiophoresis and a surface interaction will be explored. We have written transport equations for an evaporating film containing a bi-disperse mixture of particles and examine the contribution from different terms.

*The Oppenheimer fund of Cambridge University for a PhD studentship for CRZ
The role of hydrodynamic interactions in models and simulations of drying*

MICHAEL P HOWARD (Presenter), Chemical Engineering, University of Texas at Austin, ANTONIA STATT, ATHANASSIOS PANAGIOTOPoulos, Princeton University — Nonequilibrium molecular modeling is valuable for predicting the microstructure of drying films. For example, simulations were recently key to uncovering the “small-on-top” stratification of binary colloidal mixtures. In the absence of solvent effects, drying can be well-described using implicit models without hydrodynamic interactions; however, these models tend to overestimate the solute migration speeds and stratification observed in experiments. Here, I will highlight two examples from our recent work that clearly demonstrate the important role of hydrodynamic interactions in nonequilibrium models of drying. I will first discuss the evaporation-induced crystallization of a colloidal dispersion, where we found that the crystal nucleation and growth depended sensitively on the hydrodynamic interactions because of the colloid distribution in the drying film. I will then discuss the stratification of a mixture of two differently sized polymers; the mixture stratified without hydrodynamic interactions, as predicted, but did not stratify when they were included. Our work shows that although implicit-solvent models neglecting hydrodynamic interactions are computationally efficient, the corresponding sacrifice in accuracy may not be acceptable for faithfully predicting structure in drying films.

*Financial support for this work was provided by the Princeton Center for Complex Materials (PCCM), a U.S. National Science Foundation Materials Research Science and Engineering Center (grant DMR-1420541). Additionally, M.P.H. received Government support under Contract FA9550-11-C-0028 and awarded by the Department of Defense, Air Force Office of Scientific Research, National Defense Science and Engineering Graduate (NDSEG) Fellowship, 32 FR 168a, and the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (Awards OCI-0725070 and ACI-1238993) and the state of Illinois.

Thursday, March 5, 2020 12:00 PM - 1:30 PM

Session T01 APS: Young Physicists Lunch with APS Human Rights Leaders
Hyatt Mineral ABC

12:00PM T01.00001: Young Physicists Lunch with APS Human Rights Leaders —

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U01 GERA: Miscellaneous Energy-related Materials, Concepts and Phenomena 103
2:30PM U01.00001: Improved light outcoupling by spontaneously formed nanostructured micro-islands in perovskite films

JITENDRA KUMAR (Presenter), RAMESH KUMAR, Indian Inst of Technology Roorkee, KYLE FROHNA, Department of Chemical Engineering and Biotechnology, University of Cambridge, DHANASHREE MOGHE, DINESH KABRA, Department of Physics, Indian Institute of Technology Bombay, SAM STRANKS, Department of Chemical Engineering and Biotechnology, University of Cambridge, MONOJIT BAG, Indian Inst of Technology Roorkee — Halide perovskites have been the hot topic of research for their unprecedented optoelectronic properties such as high photoluminescence quantum yield (PLQY)\(^1\) and ambipolar charge transport. These properties are generally measured at the macroscopic level, but they differ significantly at micro to nano-scale. Here, we have fabricated CH\(_3\)NH\(_3\)PbBr\(_3\) films containing nanostructured micro-islands (MIs). We have observed that the presence of MIs shows 7 fold increased photoluminescence (PL). This enhancement is due to nanostructured morphology that can also improve the outcoupling. As seen from the fluorescence microscope, PL is mostly coming from MIs. These films were characterized by hyperspectral microscopy. The PL spectrum shows \(\sim\)10 nm blue shift as compared to that of untreated films. The blue shift is attributed to the increased octahedral tilting, because the MIs consists of 20-40nm sized crystals, whereas the background has \(\sim\)300 nm feature size. PL spectrum can be fitted with two Gaussian functions centered at 533 nm and 540 nm respectively, which shows the inefficient funneling of excitons. However, we have seen that the MIs show photodegradation whereas background and untreated films show photoactivation.

Reference

2:42PM U01.00002: Optimized fabrication of nanoporous membranes for osmotic power generation

KHADIJA YAZDA (Presenter), YUNING ZHANG, PETER H GRUTTER, WALTER W REISNER, McGill Univ — Osmotic energy, the energy extracted by mixing two solutions with different salinities, has been receiving significant attention in the scientific community as a potential source of clean and renewable energy (so called “Blue Energy”). A major impediment to exploiting osmotic energy is the poor efficiency of commercially available membranes for osmotic energy conversion. Nanoscale membranes with pores at or below 10 nm in diameter may provide sufficient power generation to make osmotic energy viable. Yet, currently no technology exists that can produce such membranes with sufficient control and scale. Here, leveraging our breakthrough tip-controlled local breakdown (TCLB) pore fabrication approach, we demonstrate high osmotic power density comparable to the density obtained with atomically thin 2D materials, yet with a scalable hybrid hBN/SiN membrane. In particular, the TCLB technique can produce pore arrays with a controlled spacing that yields optimum performance. Our work shows that the optimum membrane selectivity and overall power density is obtained with a pore spacing that balances the need for high pore density while maintaining a large extent of charged surface surrounding each pore.
Toward understanding of a mechanism for electrical current generation from ionic water flow using metal nanofilms

JEONGMIN KIM (Presenter), Division of Chemistry and Chemical Engineering, Caltech, DAVIS D. BOAMAH, EMILIE H. LOZIER, CATHERINE E. WALKER, FRANZ M. GEIGER, Department of Chemistry, Northwestern University, THOMAS MILLER, Division of Chemistry and Chemical Engineering, Caltech — “Hydrovoltaic” technologies convert energy from flowing water to electricity via a mechanism that primarily relies on ion adsorption and desorption at water-solid interfaces. Recently, we found metal/metal-oxide nanofilms that generate electrical current from aqueous flow of alternating salinity gradients. Atom probe tomography revealed the 10 nm thick nanofilms are composed of a thermal oxide overlayer about 2-4 nm thick and a lower layer of metal about 6-8 nm thick. Experiments suggested the following design rules for the nanofilms: (i) the metal oxide needs to be redox-active, containing several metal-oxidation states, and (ii) there is an optimal thickness for the nanofilms, comparable to electron mean-free path. For example, 10 nm thick Fe:FeOx films with an alternating flow of sea water and de-ionized water produce current-densities of several microA cm⁻² at the flow rate of a few cm s⁻¹, where iron oxide (FeOx) has iron in both the Fe²⁺ and Fe³⁺ oxidation states. In this poster, we present simulation and theoretical approaches to understand and design the connections between microscopic variables and device-level observables.

A theoretical upper bound on gas deliverable capacity via pressure-swing adsorption in nanoporous materials

JORDAN POMMERENCK (Presenter), Department of Physics, Oregon State University, CORY M SIMON, School of Chemical, Biological, and Environmental Engineering, Oregon State University, DAVID J ROUNDY, Department of Physics, Oregon State University — Due to their low volumetric energy density at ambient conditions, both hydrogen and natural gas are challenging to commercially store onboard environmentally sustainable vehicles. One strategy to densify these gases is to pack the fuel tank with a porous material. Metal-organic frameworks are tunable, nanoporous materials with large internal surface areas and show considerable promise for densifying gases. The US Department of Energy (DOE) has set volumetric deliverable capacity targets which, if met, would help to enable commercial adoption of hydrogen/natural gas as transportation fuels. Here, we present a theoretical upper bound on the deliverable capacity via an isothermal pressure-swing storage. The goals set by DOE for natural gas and hydrogen storage are theoretically possible, but sufficiently close to the upper bound as to be impractical for any real porous material. However, this upper bound directly leads to important realizations which should guide future development. Firstly, one could extract the gas at a higher temperature than that used while filling. Secondly, the fundamental physics of our upper bound do not rule out any material that changes its structure due to the presence of gas, suggesting that flexible materials could still satisfy the DOE target.
3:18PM U01.00005: Effective electrical conductivity of nanocarbon-metal composites made by the electrocharging assisted process*  
CHRISTOPHER KLINGSHIRN (Presenter), Materials Science and Engineering, University of Maryland, College Park, ANDREW PALUGHI, Materials Science and Engineering, Texas A&M University, XIAOXIAO GE, MADELINE MORALES, JESSICA YE, Materials Science and Engineering, University of Maryland, College Park, CHRISTOPHER SHUMEYKO, Aberdeen Proving Ground, U.S. Army Research Laboratory, TAHIR ÇAĞIN, Materials Science and Engineering, Texas A&M University, LOURDES SALAMANCA-RIBA, Materials Science and Engineering, University of Maryland, College Park — Robust materials with high conductivity are essential to electronic devices and systems. Novel composites called “covetics” have the potential to improve upon the electrical conductivity of established metals and alloys, including Al and Cu, by incorporating carbon nanostructures known for their superior electrical properties. During fabrication, electric current applied to the melt containing a C precursor is believed to ionize carbon atoms and cause nanoscale graphitic ribbons and chains to form within the metal lattice. This work combines fundamental assumptions about the nature of covetics, specifically a tightly bound metal-carbon interface, with a simple effective-medium model to estimate the bulk conductivity of ideal Al and Cu covetics with randomly distributed graphene nanoribbons. Density-functional theory estimates of charge transfer at the graphene-metal interface, local electrical conductivity measurements, and transmission electron microscopy investigation of the interface region provide inputs to the model. We find potential for improvements on the order of 10% under ideal conditions, but substantial processing challenges remain before these gains may be realized on an industrial scale.

*Supported by the U.S. Department of Energy under Award No. DE-EE0008313.

3:30PM U01.00006: Optimizing the role of impact ionization in conventional insulators*  
EFSTRATIOS MANOUSAKIS (Presenter), Physics, Florida State University and University of Athens — A mechanism for multiple carrier generation through impact ionization (IA) proposed earlier for bulk systems of strongly correlated insulators is generalized to the case of conventional insulators that contain localized bands a few eV above and below the highest occupied band. Specifically, we study the case of hybridization of localized orbitals with more dispersive bands near the Fermi level, where the generated multiple carriers, which ultimately decay to the edges of the dispersive bands by means of IA processes, acquire lighter mass and this could allow their more efficient separation before recombination. We argue that this may be applicable to the case of halide perovskites and it could be one of the reasons for their observed photovoltaic efficiency. We discuss the criteria one should use to uncover the appropriate material in order to harvest the optimum effect of IA for the spectrum of the solar photon energy distribution.

*This work was supported in part by the U.S. National High Magnetic Field Laboratory, which is funded by NSF DMR-1157490 and the State of Florida.
3:42PM U01.00007: A Molecular Dynamics Study of Silicon Nanowire/Silica Aerogel Nanocomposite Thermal Conductivity  MITRA SEDEEQI (Presenter), BRUCE EDWARD WHITE, Binghamton University — Growing demand for waste heat recycling technology have accelerated research in efficient thermoelectric materials. Because silicon has a large Seebeck coefficient, can be easily doped to be both n-type and p-type and has high Earth abundance, research has focused on methods for reducing the lattice thermal conductivity of this material through nanostructuring techniques. In this work, Reverse Non-Equilibrium Molecular Dynamics (RNEMD) is applied to study the thermal conductivity of silicon-silica aerogel nanocomposites. Embedding the silicon nanowire in an aerogel is found to result in significant reductions to the lattice thermal conductivity of the nanowire when the surface of the nanowire is a major source of phonon scattering. These results can be explained based on the diffuse mismatch model of phonon transport at interfaces and point to a possible path to independently optimize the electronic components of a thermoelectric material from that of its lattice vibration components.

3:54PM U01.00008: Brownian Ratchets as Non-Traditional Energy Harvesters  ANTHONY CHO (Presenter), ARJENDU KISHORE PATTANAYAK, Carleton College — We seek to harness non-traditional forms of energy such as vibrations and blackbody radiation via Brownian ratchets. We have simulated particle diffusion in a thermal bath subject to an asymmetric (ratchet) potential. The potential has been studied using both white and colored noise to incur net directed transport. We find a minimum temperature for the thermal bath to obtain a maximum transport velocity dependent on the level of asymmetry and the diffusion constant. We also find that the transport velocity was equivalent regardless if the particle traveled in the direction of or against the bias.

4:06PM U01.00009: Elemental Additions to Enhance Precipitate Formation in Superalloys*  TYLER WHITAKER (Presenter), BRAYDEN BEKKER, HAYDEN S OLIVER, GUS HART, Physics and Astronomy, Brigham Young University — Recent discoveries of cobalt-based superalloys has sparked interest in finding new ternary alloy systems that exhibit the essential L1_2 precipitate hardening mechanism. The higher operating temperature of cobalt-based alloys translates to increases in fuel efficiency for energy applications. One recent high-throughput search identified six new potential superalloys, two of which were confirmed to be at least metastable. Using the Moment Tensor Potential (MTP) framework, we explore fourth element additions to these new ternary systems. Several elements lower the formation enthalpy of the L1_2 phase, possibly enhancing its stability. These elemental additions offer a promising direction in designing new superalloys.

*We acknowledge funding from ONR (MURI N00014-13-1-0635).
4:18PM U01.00010: Proficient quantum energy storage for in-plane microsupercapacitor using hybrid nanocomposite*  MEENAKSHI TALUKDAR (Presenter), SUSHANT KUMAR BEHERA, PRITAM DEB, Tezpur University — Planar micro-supercapacitors with innovative characteristics are recognized as one of the most feasible next generation power source for incorporation in electronics devices. Microsupercapacitor (MSCs), in the world of microelectronics have engrossed more and more attention due to its power and energy storage capacity but achieving desired electrode structure design is still an open challenge. Our study has reported a novel concept of achieving synergic effect of both EDLC and pseudocapacitive in 2D architecture with ultra-high energy density and high capacitive retention, catering the need of fast growing energy demands in portable miniaturized storage device. This miniaturized micro-supercapacitor can offer a nano/micro-scale power source apposite to meet the applications which require higher operating currents and voltages in a short time-frame [DOI: 10.1039/C9DT02423A].


4:30PM U01.00011: Control of Quantum Energy Transport by Environmental Engineering*  CHIKAKO UCHIYAMA (Presenter), Yamanashi Univ — The energy transport in the light harvesting mechanisms of photosynthetic bacteria has attracted intensive attentions. Especially, the model proposed to describe the mechanism which shows that environmental noises can assist the energy transport[1] has been intensively studied, since the model has opened a way for biomimetic studies. However, the complexities of biological molecules have been obstacles to reproduce the mechanism of energy transport. To overcome the difficulty, we propose another way to control energy transport by an active control on environment. In this presentation, we show that we can accelerate an energy transport through a linear chain model by applying stochastic noises with spatial-temporal correlations[2]. Especially, we show that anti-spatial correlation and optimum correlation time can accelerate energy transport. We believe that the results show new possibilities to improve energy transport. [1] P. Rebentrost, et al., New J. Phys. 11, 033003 (2009); M. B. Plenio, and S. F. Huelga, New J. Phys. 10, 113019 (2008).[2] C. Uchiyama, W. J. Munro, and K. Nemoto, npj Quantum Information vol.4, 33 (2018).

*This study was supported by JSPS KAKENHI Grant Numbers 15K05200, 18H04290 and a grant from the John Templeton Foundation(JTF #60478).
**4:42PM U01.00012: Stability of dynamically disordered materials from ab initio molecular dynamics**  
SERGEI SIMAK (Presenter), JOHAN KLARBRING, Linkoping University — Large atomic displacements and atoms vibrating without well-defined equilibrium positions are the signatures of dynamically disordered materials. These materials show immense potential in applications, such as superionic conductors, solid-state batteries, and fuel cells. The biggest obstacle in living up to this potential is the limited stability of the dynamically disordered phases. To predict it, the free energies have to be calculated. That has long been a challenge. We have introduced a method that offers a solution [1]. It relies on a density functional theory (DFT), ab initio molecular dynamics (AIMD), and stress-strain thermodynamic integration between the dynamically disordered phase and its metastable ordered variant. The successful application of the method to the stability of notorious cubic bismuth oxide and lithium carbide [2] will be discussed.


*Swedish Research Council (VR), the Swedish Government Strategic Research Area in Materials Science on Advanced Functional Materials at Linköping University (Faculty Grant SFO-Mat-LiU No. 2009-00971), and Swedish National Infrastructure for Computing (SNIC).*

**4:54PM U01.00013: Framework Materials as Porous Liquids**  
RACHEL MOW (Presenter), Materials Science, Colorado School of Mines, WADE BRAUNECKER, THOMAS GENNETT, National Renewable Energy Laboratory — Porous liquids have recently been introduced as a new class of material with great potential for gas storage and purification. The permanent porosity and fluid properties of porous liquids provide an avenue for gas storage and transportation that avoids the processing restrictions of solid porous materials. Despite the promise of porous liquids, only a handful of these materials have been realized to date. This work develops porous liquids from covalent organic frameworks (COFs). Colloidal 3D imine-based COFs are synthesized with particle size control down to 60 nm. The colloidal COFs are suspended in a bulky ionic liquid solvent that is size-excluded from entering the COF pore, demonstrating a Type 3 porous liquid. Gas sorption studies are used to determine the gas uptake and adsorption enthalpy of hydrogen and other gases in the porous liquid. This work presents a new type of tunable organic porous liquid that can be used for gas storage and separation.

*The authors gratefully acknowledge research support from the Hydrogen Materials - Advanced Research Consortium (HyMARC), established as part of the Energy Materials Network under the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Fuel Cell Technologies Office, under Contract Number DEAC36-08-G028308*
5:06PM U01.00014: Order in the ground state of a simple cubic dipole lattice in an external field  
SAHEL ASHHAB (Presenter), MARCELO CARIGNANO, MOHAMED EL-AMINE MADJET, Qatar Environment & Energy Research Institute — Motivated by the presence of a lattice of rotating molecular dipoles in the high-temperature phase of methylammonium lead iodide, we investigate the ground state of a simple cubic lattice of dipoles interacting with each other via the dipole-dipole interaction and with an external field via the standard, linear dipole-field interaction. In the absence of an external field, the ground state is infinitely degenerate, and all the configurations in the ground state manifold are periodic along the three lattice axes with a period of two lattice sites. Using a 1000-dipole lattice as a unit cell in numerical simulations of an infinite simple cubic lattice, we determine the ground state dipole configurations in the presence of an external field. We then analyze the polarization, dipole orientation statistics and correlations in these configurations. Our calculations show that for some special directions of the external field the two-site periodicity in the dipole configurations is preserved, while in the general case this periodicity is lost and complex dipole configurations form under the influence of the external field. More specifically, a sudden transition from two-site periodic configurations to irregular configurations occurs at a finite value of the applied field strength.

5:18PM U01.00015: Kepler's Laws and Elliptic path might suggest that nature uses the function of TIME to provide needed energy for its accelerated motion*  
IBRAHIM HANNA (Presenter), Self — Classical physics correctly calculate planetary positions, and energy conservation as a function of position, however using Kepler's laws as a function of time, may conclude that potential energy available for a planet's motion, is bigger than kinetic energy used at the actual path, and have the path was to be circular, such energy difference would not exist. Keplers equation A^3/T^2 =Constant, as a function of time, may also explain how nature chooses the elliptic path, to gain such energy difference, from time, to maintain and finance its accelerated motion, where Time is a form of energy, and where the expansion of universe, is not measured by coordinates of positions, but by positive coordinates of time while black holes can be identified by negative coordinates of time.

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Thursday, March 5, 2020 2:30 PM - 5:06 PM

Session U02 GSCCM: Materials in Extremes: Dynamic Compression III

105 - Richard Briggs, Lawrence Livermore Natl Lab - Tag(s): Focus
2:30PM U02.00001: Shockwave diode: A new direction in shock physics

BRITTANY BRANCH (Presenter), Dynamic Material Properties, Sandia National Laboratories, JONATHAN SPOWART, ANDREW ABBOTT, GEOFFREY FRANK, DAVID LACINA, CHRISTOPHER NEEL, Air Force Research Laboratory — With the advent of additive manufacturing techniques, a new class of shockwave mitigation and structural supports have been realized through the hierarchical assembly of material. To date, there have been a limited number of studies investigating the role of structure on shockwave localization and whether AM offers a means to tailor shockwave behavior. Of particular interest is whether the mesoscopic structure can be tailored to achieve shockwave properties in one direction of impact versus the other. Here, we illustrate, for the first time, directional response in polymer-based foams that act as a one-way switch. In-situ time-resolved x-ray phase contrast imaging at the Advanced Photon Source was used to characterize these diode-like structures. This work offers a breakthrough in materials technology for the development of protection structures that are important for a broad range of applications and have been a long sought-after goal in shock research.

*Sandia National Laboratories a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2019-12278 A

2:42PM U02.00002: Iron Response in Extreme Compression and Tension Regimes: Complementary NIF and Janus Experiments

GAIA RIGHI (Presenter), University of California, San Diego — Iron is the major component of the Earth’s solid inner core, so determining its strength under extreme conditions is crucial to understanding the rheology of Earth’s core and interpreting geophysical observations. Although it has been widely accepted that body centered cubic Fe will go through at least one, possibly more, phase transitions at high pressures, the influence of such a reversible phase transition on the strength of Fe is still unknown. Molecular dynamics simulations of shock-compressed single crystal bcc iron show that the newly formed epsilon phase is nanocrystalline. Strength dependence on grain size and strain rate has been investigated through campaigns at NIF and JLF. Preliminary results show that at ultra-high strain rates, initial grain size has no effect on material strength while at lower strain rate, minor effects can still be seen. The strength of iron at Earth core conditions achievable with NIF was found to be approximately 16 GPa, which is remarkably high. These results will lead to an improved understanding of asteroid impact dynamics, planetary formation dynamics, and interior structures of the earth, planets and exoplanets.
Particle-based studies in support of high-power laser experiments to study metal ejecta interactions

TOMORR HAXHIMALI (Presenter), Lawrence Livermore Natl Lab, MARCO J ECHEVERRIA, University of Connecticut, FADY MICHEL NAJJAR, Lawrence Livermore Natl Lab, PETROS TZEFERACOS, university of Chicago, SUZANNE J ALI, HYE-SOOK PARK, JON HENRY EGGERT, BRANDON E MORGAN, YUAN PING, Lawrence Livermore Natl Lab, HANS RINDERKNECHT, University of Rochester, ALISON SAUNDERS, Lawrence Livermore Natl Lab — Shock-driven material can emit a fine spray of ejecta from its free surface. Understanding the dynamic and interaction of the metal ejecta is important to areas of study as diverse as industrial safety, astrophysics, spacecraft shielding, and inertial confinement fusion.

We present results from particle-based dynamics at atomistic as well as macro-scale simulation studies of the ejecta formation in the presence of grooves at the free surface as a result of a shock wave created at the ablator-metal interface. At the atomistic level, we use large scale simulations, ~ $10^9$ atoms, to extract values of pressure breakout and release, as well as ejecta mass and velocity density. The fractality of the ejecta ligaments is also being investigated.

At the macro-scale, we use Smooth Particle Hydrodynamics for the same conditions. This provides valuable information to the experimental campaign on the OMEGA and OMEGA-EP lasers platforms for studying the ejecta formation. The metals studied are pure Cu and Sn. Time permitting, initial investigation of the effect of alloying will also be presented.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC.
Lattice dynamics of laser-driven compressed Al studied with ultrafast electron diffraction

MIAZHEN MO (Presenter), SLAC - Natl Accelerator Lab, MINXUE TANG, The Peac Institute of Multiscale Sciences, ZHIJIANG CHEN, XIAOZHE SHEN, JOHN RYAN PETERSON, MUNG FROST, MICHAEL EDMUND KOZINA, ALEX REID, ADRIEN DESCAMPS, SLAC - Natl Accelerator Lab, JUNCHENG E, The Peac Institute of Multiscale Sciences, RENKAI LI, SLAC - Natl Accelerator Lab, SHENG-NIAN LUO, The Peac Institute of Multiscale Sciences, XIJIE WANG, SIEGFRIED GLENZER, SLAC - Natl Accelerator Lab — Understanding the lattice dynamics of shock-compressed materials is of great interest to many areas including planetary formation, aeronautics and spacecraft. Here we report the study on elastic-to-plastic strain transition in dynamically compressed Al using the technique of ultrafast-electron-diffraction (UED). The targets employed in our experiments are 200-nm-thick free-standing single-crystal Al thin films. The compression wave was launched normal to the sample surface by ablating the sample with a focused 800nm, 20ps, <12 mJ laser pulse. The lattice response of the sample was probed by MeV electrons coming from the opposite side at 45° incident angle. As the sample is compressed, we first observed the elastic response and then the plastic relaxation, indicated by shifts of the Laue peaks reflected from the normal and transverse lattice planes respectively. The dependence of this elastic-plastic transition on the pump fluence and crystal orientation were studied and the results will be presented. We also performed Molecular Dynamics simulations incorporated with hydrodynamics simulations to understand the underlying physics of the experimental observations and the results will be presented.

This work is supported by DOE Office of Science, Fusion Energy Science under FWP100182.

Modeling High Strain Rate Plasticity in BCC Lead

ROBERT RUDD (Presenter), LIN H YANG, ANDREW KRYGIER, PHILIP POWELL, DAMIAN SWIFT, CHRISTOPHER WEHRENBERG, JAMES M MCVaney, HYE-SOOK PARK, Lawrence Livermore Natl Lab, PETER GRAHAM, AWE — High-energy lasers enable determination of metal strength at very high pressures. Here we consider the strength (flow stress) of lead in the high-pressure body-centered cubic (bcc) phase at a peak pressure of ~400 GPa. Two previous models of Pb strength were built from the low-pressure fcc phase. Plasticity in bcc and fcc crystals can be very different. Experiments conducted at the National Ignition Facility have used ramp-compression to drive Rayleigh-Taylor instability and measured the ripple growth to infer strength in the bcc phase of lead and lead alloy [1]. We have developed an Improved Steinberg-Guinan model for bcc lead strength [2] using ab initio calculations of the shear modulus at pressure that agrees well with those experiments. The alloying, which increases strength 4x at ambient conditions, has no measurable effect at high-pressure.


This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.
3:30PM U02.00006: Effect of peak stress on spall in copper and a copper-lead alloy*  DAVID ROBERT JONES (Presenter), SARYU FENSIN, MST-8, Los Alamos National Laboratory — Spall fracture is often seen in shock loaded materials. It has been shown extensively that spall is a weak-link driven event, with microstructural features such as grain boundaries, impurities, porosity etc. acting as nucleation sites for voids and cracks. Here, we present results studying spall fracture in a two-phase material, copper-lead. The alloy contains approximately 1% lead, which is contained as precipitates primarily at the copper grain boundaries. The effect of the peak compressive stress prior to spall is investigated, with a pure copper target also included as a control. It is shown that this small amount of lead drastically reduces the spall strength. Further, the spall strength of the copper-lead alloy begins to decrease at a far lower peak stress than the pure copper. Modeling efforts, at both continuum and molecular dynamics length scales, are used to elucidate the reasons behind these results. Initial conclusions are based on the slow wave velocities in the lead compared to the copper leading to a ‘shock-focusing’ in the lead precipitates, causing thermal softening and even melt, producing weak points and lowering the spall strength.

*DOE Science Campaign 2

3:42PM U02.00007: Towards a Dynamic Thermal Conductivity Measurement: Temperature Convergence of Iron Coatings to a Bulk Temperature Source*  DAVID BRANTLEY (Presenter), MARKUS DAENE, RYAN CRUM, HANNAH SHELTON, MINTA C AKIN, Lawrence Livermore Natl Lab — The thermal conductivity of iron under Earth’s core temperatures and pressures is a critical parameter in models of the geophysical history of Earth's core. Recent DAC measurements and first principles calculations have presented conflicting trends in the thermal conductivity as a function of temperature and pressure, leading to large uncertainties in the predicted age of Earth's solid inner core. Confidently resolving this discrepancy requires corroborative conductivity measurements using multiple experimental methodologies, however dynamic compression experiments have so far suffered from uncontrolled systematics. We present the results of gas gun experiments testing the convergence of coating temperatures to a bulk temperature source. A series of experiments were performed at 50 and 120 GPa, where Fe and Sn were used as coating and temperature source materials. Temperature of the coating material was measured using optical pyrometry, and simulations were performed which show matching trends in the observed temperature data for a range of input thermal conductivity values.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 LLNL-ABS-795546
3:54PM U02.00008: “Reflectance Thermometry for Time-Resolved Measurements of Low-Temperature Compression on Sandia’s Z Machine”* KALEB BURRAGE (Presenter), PATRICIA KALITA, RICHARD HACKING, CHRISTOPHER T SEAGLE, Sandia National Labs, YOGESH VOHRA, Univ of Alabama - Birmingham, DAN DOLAN, Sandia National Labs — Pulsed current from Sandia’s Z machine compresses samples to 10-1000 GPa pressures on nanosecond time scales. Such rapid compression results in 10-100,000 K temperature (T) changes, depending on how loading is applied. Shock compression of solids leads to T above 2000 K, whereas ramp compression to the same pressure leads to T below 1000 K. Optical pyrometry is well-suited for the former but impractical for the latter—samples do not emit enough photons for such high-speed measurements. To fill this gap, we are investigating the thermo-reflectance of aluminum as an optical thermometer. Aluminum has an absorption feature at 1.5 eV that shifts to higher energy under static compression and in the opposite direction upon heating. We carried out static compression of Al in diamond anvil cell at high T, coupled with reflectivity measurements. The distinction between absorption energies at higher T for any given pressure is promising for the calibration of an optical thermometer for Z.

*Math Physics, Sandia National Laboratories, is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

4:06PM U02.00009: Single ultrafast x-ray pulse imaging and diffraction of mesoscale shockwave dynamics* RICHARD SANDBERG (Presenter), Brigham Young Univ - Provo, CYNTHIA BOLME, Los Alamos National Laboratory, ARIANNA E GLEASON, SLAC National Accelerator Laboratory, KYLE RAMOS, QUINN MCCULLOCH, SHAWN DAVID MCGRANE, MARC CAWKWELL, DARBY J LUSCHER, Los Alamos National Laboratory, BOB NAGLER, ERIC GALTIER, SLAC National Accelerator Laboratory, PHILIP HEIMANN, HAEJA LEE, Los Alamos National Laboratory — The revolution in accelerator based x-ray sources known as x-ray free electron lasers are drastically changing the way we understand materials, especially in extreme conditions. With the intense, ultrafast, and coherent x-ray pulses provided by these new sources, we are now able to probe inside materials under extreme conditions at unprecedented temporal and spatial resolutions. In this talk, I will review work on understanding materials strength, damage, and failure mechanisms under shock loading conditions using x-ray diffraction and coherent diffraction imaging at the world's first hard x-ray free electron laser, the Linac Coherent Light Source. We study materials in such condition as the effect of pore collapse in the high explosive PETN and Richtmyer–Meshkov Instabilities off of copper samples that have been shocked by a high energy laser.

*We acknowledge use of the Linac Coherent Light Source, a DOE Office of Science User Facility. This work was supported by Los Alamos Laboratory Research and Development (LRDR) program and the Dynamic Materials Properties Campaign (C2) at Los Alamos National Laboratory, an affirmative action equal opportunity employer, managed by Triad National Security, LLC for the U.S. DOE NNSA, under contract 89233218CNA000001.
4:18PM U02.00010: Role of Heterogeneities in Ejecta via MD Simulation* RACHEL FLANAGAN (Presenter), Department of Mechanical and Aerospace Engineering, University of California, San Diego, TIMOTHY GERMANN, Theoretical Division, Los Alamos National Laboratory, MARC A MEYERS, Department of Mechanical and Aerospace Engineering, University of California, San Diego, SARYU FENSIN, Materials Science & Technology, Los Alamos National Laboratory — We investigate the shock behavior of copper seeded with heterogeneities via molecular dynamics simulations. Specifically, we aim to understand the influence of heterogeneities such as atomic defects and bubbles on ejecta production in copper. Since shock melting plays a key role in ejecta production, microstructure was previously thought to not matter, but recent results suggest that different microstructures alter the mechanism through which ejecta is produced. For example, the presence of helium bubbles near the free surface of copper has been shown to nearly triple ejecta production due to a loss of planarity at the shock front. We analyze the size and velocity distributions to understand the mechanisms of ejecta production and the influence of heterogeneities on material strength. The ultimate goal of this work is to inform and elucidate upon parallel experiments, where data collection presents a significant challenge. LA-UR-19-26660

*RF and MM gratefully acknowledge support from the Center for Matter in Extreme Conditions (award number DE-NA0003842.) This work was supported by the U.S. Department of Energy (DOE) through Los Alamos National Laboratory, operated by Triad National Security, LLC, for the National Nuclear Security Administration (Contract No. 89233218CNA000001).

4:30PM U02.00011: Shock-induced consolidation of tungsten nanoparticles - a molecular dynamics approach* JIANRUI FENG (Presenter), CHEN PENGWAN, Beijing Institute of Technology — Shock-induced consolidation of tungsten nanoparticles to form a bulk material is modeled through molecular dynamics simulation. By arranging the nanoparticles in a three-dimensional model of BCC super-lattice, the calculated shock velocity-particle velocity Hugoniot data is in good agreement with the experiment. Three states, including solid-undensified, solid-densified and liquid-densified can be sequentially obtained with the increase of impact velocity. It is the flow deformation at the particle surface that densifies the cavity, and the high pressure and temperature that join the particles together. Melting is not a necessary factor for shock consolidation. Based on whether melting takes place, the consolidation mechanism can be considered as solid-pressure welding or liquid-diffusion welding.

*China Postdoctoral Science Foundation funded project under grant No. 2019M650504.
4:42PM U02.00012: Particle breakage of granular materials subject to explosion  KUN XUE (Presenter), CHUANSHAN ZHANG, Beijing Institute of Technology — Unconfined granular medium subjected to central explosion experiences transient stresses and strains which are distributed heterogeneously. The particle breakage are markedly different from the fractal fracture of granular materials under confined comminution which are typical in the quasi-static and dynamic compression experiments. The particle size distribution of shocked particles recovered from the explosive dispersal of particle shells consisting of glass spheres reveal varying breakage modes depending on the mass ratio of payload and charge, M/C. When M/C is small, the particle size distributions of blasted materials shows three regimes, and the second regime satisfies fractal distribution. The fractal dimension of the second regime ranges from 2.9 to 2.5 with increasing M/C. With M/C beyond a threshold, an increasing amount of particles remains intact, the particle size distributions of fractured materials transitions to a two-regime mode, in which the fractal dimensions are well below 2 and progressively decreases with increasing M/C. The distinct behaviors of particle breakage are a result of the compound and transient loadings due to a sequence of incident shock, unloading and reshock as revealed by grain scale investigations using FDEM.

4:54PM U02.00013: SHOCK COMPRESSIBILITY AND SPALL STRENGTH OF TWO COMPOSITE MATERIALS BASED ON ARAMID FIBERS* VALENTINA MOCHALOVA (Presenter), ALEXANDER UTKIN, Institute of Problems of Chemical Physics RAS — Using a VISAR laser interferometer, the experiments on investigation of the shock wave structure, spall strength and determination of Hugoniot were performed for two composites based on aramid fibers - textolite and kevlar. They have the same compound, but different structure. The density is 1.27 g/cc. To study the shock wave compressibility of composites under extreme conditions, the explosive propellant charges were used. On the velocity profiles with transverse fiber orientation, for both materials after the initial shock jump, oscillations are observed due to the heterogeneous structure. When a shock wave propagates along the fibers, a two-wave configuration is recorded, which is due to the anisotropic structure. For each composite, Hugoniot data were obtained for two orientations. It was found that Hugoniots for transverse orientation of the fibers are parallel to each other and differ only in the first coefficient determined by the sound speed of the material. For both materials, the value of spall strength along the fibers is several times higher than that for the transverse direction. It was found that shock wave properties of textolite and kevlar were strongly dependent on the orientation and structure of the fibers.

*The work was supported by FAIR-Russia Research Center

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U07 DQI: Hybrid Systems - Diamond Color Centers, Magnonics
102 - Dolev Bluvstein, Harvard University - Tag(s): Focus
Coherent storage of microwave photons over 100ms in an ensemble of electron spins. EMMANUEL FLURIN (Presenter), VISHAL RAJAN, EMANUELE ALBERTINALE, DANIEL ESTEVE, PATRICE BERTET, CEA Saclay — Electron and nuclear spins in crystals are attractive for storing quantum information due to their long coherence times in pure matrices. Bismuth donors in silicon have the particular appeal to possess special biasing points (the so-called “clock transitions”) at which the electron spin becomes insensitive to first-order to magnetic field noise, yielding long coherence times [1]. Here we report the coupling of a small ensemble of \( \approx 10^4 \) Bismuth donors in silicon to a superconducting micro-resonator at a clock-transition, at millikelvin temperatures. At this point, we measure a Hahn-echo coherence time of up to \( T_2=300 \text{ms} \). This makes it possible to store coherently a train of weak microwave pulses of \( \approx 10 \) photons over 100ms. [2]


Optomechanically induced selective emitter—emitter interactions for control of quantum networks* TOMAS NEUMAN (Presenter), MATTHEW TRUSHEIM, DEREK WANG, ISAAC HARRIS, PRINEHA NARANG, SEAS, Harvard University — Quantum emitters such as point-defects (artificial atoms) in diamond [1] can be used as elementary building blocks (qubits) of quantum information systems. The function of a a quantum network, however, also relies on efficient qubit-qubit interactions and thus allowing for practical implementation of quantum gates. Here we suggest a coupling scheme where optically active qubits (e.g. artificial atoms in diamond) of different excitation frequencies are dispersively coupled to a shared mode of an optical cavity. The cavity induces an effective generally off-resonant qubit-qubit interaction [2] prohibiting direct exchange of information among these qubits. By applying coherent acoustical driving [3] to modulate the qubit frequencies it is possible to bring to resonance a desired subset of qubits and thus selectively open an inter-qubit communication channel. We theoretically demonstrate this principle by solving the quantum master equation both numerically and analytically and suggest practical experimental scenarios to test our predictions.


*US DOE PTL EFRC Grant # DE-SC0019140
ARO MURI Grant # W911NF-18-1-0431
2:54PM U07.00003: Optically hyperpolarized nanodiamonds: quantum control and avenues for signal-enhanced NMR  ASHOK AJoy (Presenter), EMANUEL DRUGA, XUDONG LV, University of California, Berkeley, CARLOS MERILES, City College of New York, JEFFREY A REIMER, ALEXANDER PINES, University of California, Berkeley — I will describe quantum-assisted modalities to deliver signal enhancements in conventional MRI and NMR mediated by quantum defects in nanodiamond powder. This relies on the use of Nitrogen-Vacancy (NV) center spins within the diamond particles that can be optically polarized at room temperature with modest laser powers. This polarization can be transferred to nuclei surrounding the NV spins to hyperpolarize them to levels far above Boltzmann levels, manifesting in a highly enhanced NMR signature. Nanodiamonds are particularly suited for this task, given their large surface areas, and the ability to arrange for close physical contact between the polarized NVs and analyte molecules of interest.

I will discuss our experimental effort in this direction, particularly focusing on new results, including in the prolongation of relaxation and coherence times of hyperpolarized spins, as well as materials advances that yield substantial improvements in $^{13}$C lattice hyperpolarization levels, and new applications in dual-mode (optical and NMR) hybrid electron-nuclear magnetometers constructed out of hyperpolarized nanoparticles.

3:06PM U07.00004: Design and fabrication of large-scale diamond quantum memories in hybrid photonic circuits*  TSUNG-JU LU (Presenter), NOEL WAN, KEVIN CHEN, MICHAEL P WALSH, MATTHEW TRUSHEIM, LORENZO DE SANTIS, ERIC A BERSIN, ISAAC HARRIS, SARA MOURADIAN, Massachusetts Institute of Technology MIT, EDWARD S BIELEJEC, Sandia National Laboratories, DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — A central goal in quantum information processing is the development of scalable quantum processors and quantum networks. Towards this end, solid-state “artificial atoms” such as color centers in diamond are especially promising because they combine efficient optical interfaces, minutes of spin coherence, and potentially very-large-scale fabrication. Here, we describe the design, fabrication, and integration of diamond quantum micro-chiplets containing single SiV and GeV centers with photonic integrated circuits (PICs). A near-deterministic photonic nanofabrication produces unity coupling of emitters to single-mode diamond waveguide arrays, which are subsequently assembled on an aluminum nitride PIC for on-chip routing and manipulation of photons. The combination of these advances allows the construction of a 72-channel quantum memory microphotonic chip. The ability to assemble large numbers of quantum memories with phase-stable PICs enables an architecture for high-efficiency, multiplexed quantum repeaters on a chip.

*We acknowledge support from ARL CDQI, NSF EFRI ACQUIRE, NSF CUA, NSF CIQM, DoD NDSEG, NSF GRFP, IC Postdoctoral Fellowship, MIT Lincoln Lab, NASA Space Technology Research Fellowship
3:18PM U07.00005: Characterizing a 72-channel defect-free array of diamond quantum memories in a photonic integrated circuit*

NOEL WAN (Presenter), TSUNG-JU LU, KEVIN CHEN, MICHAEL P WALSH, MATTHEW TRUSHEIM, LORENZO DE SANTIS, ERIC A BERSIN, ISAAC HARRIS, SARA MOURADIAN, Massachusetts Institute of Technology MIT, EDWARD S BIELEJEC, Sandia National Laboratories, DIRK R. ENGLUND, Massachusetts Institute of Technology MIT — In a previous abstract, we described the unity creation, coupling and integration of diamond "artificial atoms" of silicon vacancy (SiV) and germanium vacancy (GeV) centers with a large-scale photonic integrated circuit (PIC) in aluminum nitride. Here, we present the characterization of our 72-channel quantum memory chip. First, we demonstrate the routing of single-photon emission from 72 distinct optical channels in a fiber-coupled PIC. We performed low-temperature spectroscopy of the emitters, finding near-lifetime-limited optical transitions from both SiV and GeV centers following nanofabrication, micromanipulation, and heterogeneous integration. Additionally, we demonstrate the tuning of optical transitions with the same integrated system, overcoming the spectral inhomogeneities between separate emitter-waveguide systems. These advances set the stage for high-rate, multi-channel photon-mediated entanglement for quantum repeaters and computers.

*We acknowledge support from ARL CDQI, NSF EFRI ACQUIRE, NSF CUA, NSF CIQM, DoD NDSEG, NSF GRFP, IC Postdoctoral Fellowship, MIT Lincoln Lab, NASA Space Technology Research Fellowship

3:30PM U07.00006: Nanophotonic Quantum Registers based on Silicon Vacancy Centers in Diamond*

ERIK KNALL (Presenter), MIHIR K BHASKAR, CHRISTIAN NGUYEN, RALF RIEDINGER, BARTHOLOMEUS J MACHIELSE, DAVID LEVONIAN, PAVEL STROGANOV, DENIS D SUKACHEV, HONGKUN PARK, MARKO LONCAR, MIKHAIL LUKIN, Harvard University — The development of scalable quantum technologies requires robust and well controlled quantum systems. Integrated solid-state devices are particularly promising because lithographically defined systems offer a route toward mass production. Recent progress in diamond nanofabrication has opened the door to unprecedented control of an optically accessible solid-state quantum memory, the silicon vacancy center in diamond. Integration of this point defect into a nanophotonic cavity combined with efficient photon detection recently enabled a proof-of-principle demonstration of memory enhanced quantum communication. In this talk, I will discuss how interfacing with nearby nuclear spins as well as improved device design and fabrication continue to push this system’s capabilities as a platform for foundational demonstrations of memory based quantum communication.

*This work was supported by the NSF, CUA, DoD/ARO DURIP, AFOSR MURI, ONR MURI, ARL, and a Vannevar Bush Faculty Fellowship. Devices were fabricated at Harvard CNS, NSF award no. 1541959. E.N.K. is supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE1745303.
Coupling an Inverted Spin Ensemble to a Microwave Resonator

JASON BALL (Presenter), PETER MOROSHKIN, SHOTA NORIMOTO, DENIS KONSTANTINOV, YUIMARU KUBO, Quantum Dynamics Unit, Okinawa Inst of Sci & Tech — Using an ensemble of nitrogen (P1) centers in diamond placed inside a 3-D loop-gap resonator, we observe population inversion of a satellite P1 transition when a microwave pump tone is applied to the central P1 transition. This inversion is manifested by amplification of the probe tone applied to the satellite transition. A mechanism for generating this inversion is proposed, involving higher-order cross relaxations within the P1 centers [1] and spin flip-flops with nearby nitrogen-vacancy (NV) centers that are also present in the diamond sample.

We also observe a splitting of this amplifying peak due to coupling with the microwave resonator. The polariton modes created by this coupling differ qualitatively from the standard, non-inverted case, in particular lacking an avoided crossing [2]. We modeled this “abnormal” anticrossing by assuming a “negative ensemble coupling constant,” and find that the model is consistent with the observed experimental data.


Coherent coupling of V[TCNE]x≈2 magnons to NV center spins

DENIS CANDIDO (Presenter), University of Iowa, GREGORY FUCHS, Cornell University, MICHAEL FLATTÉ, University of Iowa — The application of a rf magnetic field in magnetic materials yield the creation of magnons (spin waves) [1]. For the organic V[TCNE]x≈2 ferrimagnetic material [2], those magnons are found to have very long spin lifetime, thus enhancing the practical chances for applications. In our work, these excitations are coherent coupled – through the magnon fringe fields – to the spin of a Nitrogen-Vacancy (NV) center within a diamond substrate, placed below our magnetic structure. Interestingly, this coherent coupling has the potential to solve the problem of the communication between local qubits at low temperatures and optical photons, a necessary ingredient for networking and quantum communication. Here, we calculate the magnon spectrum, fringe fields and magnetizations profiles for V[TCNE]x≈2 disks. In addition, we also derive an effective Hamiltonian describing the coupling between NV center spins and magnons. We calculate the realistic effective Hamiltonian parameters, e.g., the spin-magnon coupling, for different physical setups.


*The material is based on work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Award Number DE-SC0019250.
4:06PM U07.00009: Cavity mediated interactions and strong entanglement between YIG samples without using intrinsic nonlinearities.*  JAYAKRISHNAN MUTTATHIL
PRABHAKARAPADA NAIR (Presenter), GIRISH AGARWAL, Texas A&M University — A question attracting great attention is the possibility of quantum entanglement between macroscopic systems. Several systems like cold atomic ensembles; opto and electromechanical systems have been reported. It turns out that the magnetic systems like the excitations in YIG spheres in cavities could be excellent candidates for the quantum information tasks.
We study this new platform for producing quantum characteristics. In particular we present a novel scheme to generate an entangled pair of yttrium iron garnet (YIG) samples in a cavity system. A novel aspect of our proposal is that it does not involve any nonlinearities which are typically very weak. This is against the conventional wisdom which necessarily requires strong Kerr like nonlinearity. Our key idea, which leads to entanglement, is to drive the cavity by a weak strictly quantum field like squeezed vacuum field which can be generated by a flux-driven Josephson parametric amplifier (JPA). The two YIG samples interact via the cavity. We demonstrate a high degree of macroscopic entanglement that can survive up to temperatures like 300-500mK. The entanglement is tested using several different quantitative criteria. We also find the optimal parameter regime for entanglement.

*Thank the support of the HEEP fellowship

4:18PM U07.00010: Improving coupling strengths and lifetimes in quantum magnonics*
DANY LACHANCE-QUIRION (Presenter), SAMUEL PIOTR WOLSKI, YUTAKA TABUCHI, Research Center for Advanced Science and Technology, The University of Tokyo, SHINGO KONO, Center for Emergent Matter Science, RIKEN, YOSHIKI SUNADA, KOJI USAMI, YASUNOBU NAKAMURA, Research Center for Advanced Science and Technology, The University of Tokyo — Quantum magnonics is an architecture in which collective modes of spin excitations in magnetically-ordered systems interact coherently with superconducting qubits. One of the main milestones to be demonstrated in quantum magnonics is the creation and observation of macroscopic quantum states of magnons. This task is challenging due to (i) the second-order nature of the effective interaction between magnetostatic modes and superconducting qubits and (ii) the relatively high relaxation rate of magnons. The first challenge is tackled by using a three-dimensional lumped-element microwave cavity designed to optimally enhance the effective coupling strength up to a few tens of MHz. Furthermore, we have observed that two-level systems (TLSs) in yttrium iron garnet at millikelvin temperatures have lifetimes much longer than the magnon lifetime. The long lifetime of the TLSs could potentially enable us to perform quantum magnonics experiments in an out-of-equilibrium situation where magnon decay is partially suppressed. Both advances are important steps towards the observation of quantum states of magnons.

*This work is partly supported by JSPS KAKENHI (26220601, 18F18015), JST ERATO (JPMJER1601), JSPS and FRQNT Postdoctoral Fellowships, and the MEXT Monbukagakusho Scholarship.
4:30PM U07.00011: High frequency ferromagnetic spectroscopy enabled by coupling pairs of magnons to NV spins*  BRENDA MCCULLIAN (Presenter), AHMED THABT, Ohio State Univ - Columbus, BENJAMIN GRAY, Materials and Manufacturing Directorate, Air Force Research Laboratory, ALEX MELENDEZ, Ohio State Univ - Columbus, MICHAEL WOLF, VLADIMIR L SAFONOV, Materials and Manufacturing Directorate, Air Force Research Laboratory, DENIS PELEKHOV, Ohio State Univ - Columbus, VIDYA P BHALLAMUDI, Indian Institute of Technology Madras, MICHAEL PAGE, Materials and Manufacturing Directorate, Air Force Research Laboratory, P CHRIS HAMMEL, Ohio State Univ - Columbus — Coupling NV center defects in diamond to ferromagnetic dynamics is of interest for both quantum sensing and for NV spin manipulation. We have used NV relaxometry to detect driven ferromagnetic dynamics in a low-damping insulating ferrimagnet, nickel zinc aluminum ferrite. We determine that NV coupling to driven magnetization has two regimes: first, when the uniform mode FMR frequency is less than the NV spin resonance frequency, and the converse. A driven spinwave instability in the nickel ferrite populates the magnons far above thermal levels. The spectral response of NV-ferromagnet coupling in the first regime can be understood from the spinwave instability physics. The second regime of NV-ferromagnet coupling can be understood via a two-magnon relaxation process. These results further the understanding of how driven ferromagnetic dynamics lead to NV spin relaxation, and demonstrate the potential to detect magnons with frequencies well above the NV frequency.

*Funding was provided primarily by the Center for Emergent Materials at The Ohio State University, an NSF MRSEC through Award No. DMR-1420451, with partial support from ARO through Award No. W911NF-16-1-0547 and by the AFOSR through Award No. FA9550-15RXCOR198.

4:42PM U07.00012: Electrical switching of spin-magnon interaction*  ABHISHEK SOLANKI (Presenter), SIMEON BOGDANOV, AVINASH RUSTAGI, NEIL ROSS DILLEY, TINGTING SHEN, PUNYASHLOKA DEBASHIS, ZHIHONG CHEN, JOERG APPENZELLER, YONG CHEN, VLADIMIR SHALAEV, PRAMEY UPADHYAYA, Purdue Univ — In recent years, strong interaction between surface confined propagating spin waves in ferromagnetic materials and single spins in color centers of diamond has been utilized for applications like quantum sensing and coherent driving of spins. The ability to switch this interaction electrically is essential to deterministically couple two spins via spin waves. In this work, we demonstrate electrical tuning of the coupling between spin waves and electron spins of nitrogen-vacancy centers (NV) in diamond. We electrically tune the magnon dispersion in thin CoFeB films, putting them in and out of resonance with the NV spin levels. The room-temperature magnetic noise of spin-waves affects the spin relaxation rate in NVs, in good quantitative agreement with analytical calculations. Our work opens up considerable opportunities for utilizing hybrid platforms combining quantum degree of freedom spins with macroscopic spin-waves in spin-based information and nanoscale sensing.

*We acknowledge NSF grant DMR-1838513

4:54PM U07.00013: Optical quantum nondemolition measurement of a solid-state spin without a cycling transition [Invited]  JEFF THOMPSON (Presenter), Princeton University — Jeff Thompson has led the development of a new platform for hybrid systems, coupling a solid state system - implanted erbium ions - with a silicon nanophotonic resonator.
2:30PM U08.00001: Two-qubit coupler with exponential suppression of virtual interactions*

CATHERINE LEROUX (Presenter), AGUSTIN DI PAOLO, ALEXANDRE BLAIS, Universite de Sherbrooke
— We present a superconducting two-qubit coupler where a tunable bus interacts with a driven mode such as to, on demand, exponentially suppress the qubit-qubit virtual interactions with respect to the amplitude of the external control field. The proposed mechanism can be combined with tuning the bus frequency, which is the standard approach to suppress dispersive interactions, thus making current tunable bus designs more efficient.

*This work was undertaken thanks in part to funding from NSERC and the Canada First Research Excellence Fund.

2:42PM U08.00002: Suppression of Qubit Crosstalk between Transmons and Capacitively Shunted Flux Qubits : Part1, Experiment

JASEUNG KU (Presenter), BRITTON L PLOURDE, Syracuse University, JARED HERTZBERG, MARKUS BRINK, DAVID MCKAY, JERRY M. CHOW, IBM Thomas J. Watson Research Center, XUEXIN XU, MOHAMMAD ANSARI, Forschungszentrum Julich — In multi-qubit cQED systems, the static ZZ crosstalk can be a limiting factor for high-fidelity two-qubit gates. Thus, mitigating such ZZ interactions becomes critically important for achieving high-fidelity entangling gates as the number of qubits increases. One potential way to suppress the static ZZ interaction involves combining different types of qubits. Capacitively shunted flux qubits (CSFQs), in contrast to transmon qubits, possess relatively large and positive anharmonicity. When they are paired with an appropriate detuning, the static ZZ term can be significantly suppressed for two-qubit gates based on the cross resonance interaction. We fabricated a two-qubit system consisting of a CSFQ and a fixed-frequency transmon coupled via a bus cavity. In this talk, we will present experimental results from these measurements, including the ZZ crosstalk and two-qubit gate fidelity versus detuning between the two qubits.
2:54PM U08.00003: Suppression of Qubit Crosstalk between Transmons and Capacitively Shunted Flux Qubits: Part 2, Theory  
XUEXIN XU (Presenter), MOHAMMAD ANSARI, Forschungszentrum Juelich, JASEUNG KU, BRITTON L PLOURDE, Syracuse University, JARED HERTZBERG, MARKUS BRINK, DAVID MCKAY, JERRY M. CHOW, IBM Thomas J. Watson Research Center — We compare two-qubit superconducting circuits composed of either different-species qubits or all-transmon qubits. In the different-species case, we use qubits with the opposite sign of anharmonicity, while for the all-transmon circuit, both qubits have a negative anharmonicity. We show that there are unique features in the different-species approach that makes it attractive for use in near-term quantum computers. Circuits with different-species qubits are capable of fast two-qubit gates and they allow for complete cancellation of ZZ crosstalk interactions. Our theoretical results are in agreement with an experiment on a two-qubit device consisting of a capacitively shunted flux qubit and a transmon and show a promising way to improve two-qubit gate operations.

*Support from Intelligence Advanced Research Projects Activity (IARPA) under Contract No. W911NF-16-0114 is gratefully acknowledged

3:06PM U08.00004: High fidelity encoded gate operations for composite superconducting qubit  
YUN-PIL SHIM (Presenter), Laboratory for Physical Sciences, DANIEL L CAMPBELL, BHARATH KANNAN, RONI WINIK, Research Laboratory of Electronics, Massachusetts Institute of Technology, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, JONILYN YODER, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, WILLIAM OLIVER, Research Laboratory of Electronics, Massachusetts Institute of Technology, CHARLES TAHAN, Laboratory for Physical Sciences — Our encoded qubit scheme for superconducting transmon qubits explores a non-traditional architecture where the computational states are encoded by the hybridized states formed by a pair of capacitively coupled degenerate transmons. Gate operations can be implemented on the encoded qubit using non-adiabatic Landau-Zener control at the small avoided crossing and requiring only baseband control, without individual microwave control for each transmon. Even with frequencies far below the effective temperature, high fidelity encoded gates can be achieved utilizing the sweet spot (optimal operating point) and dynamical sweet spot (optimal pulse shape). Further, these composite qubits show immunity to photon noise in readout resonators, which can be a limiting factor in many transmon-based quantum computing systems, often requiring special attenuators to mitigate. We also discuss the leakage errors due to relaxation to the physical ground state which is outside of the encoded qubit's computational subspace.

3:18PM U08.00005: A multi-qubit gate for non-interacting qubits in circuit-QED using the Zeno effect  
CHEN MOR, BOAZ KOREN, ASAF DIRINGER, SHAY HACOHEN-GOURGY (Presenter), Physics, Technion - Israel Institute of technology — The quantum Zeno effect is known for freezing dynamics due to observation. The observation can also confine the evolution to an unobserved subspace of the system. This confinement can lead to non-trivial evolution. We show that using a single qubit drive, and a strong continuous observation that blocks part of the evolution, we can create a multi-qubit entangling gate between non-interacting qubits. We use transmon qubits coupled to a 3D cavity. The qubits are far detuned from each other, such that they are effectively non-interacting. We present the experimental results and discuss the fidelity and limitations of this gate.
**3:30PM U08.00006: Cross-resonance Dynamics with Tunable Transmon Qubits**

BRADLEY MITCHELL (Presenter), RAVI KAUSHIK NAIK, AKEL HASHIM, JOHN MARK KREIKEBAUM, IRFAN SIDDIQI, University of California, Berkeley — The cross-resonance gate is a widely-utilized entangling gate in modern superconducting quantum processors. Recent theoretical work [1] has illustrated that the dynamics of the cross-resonance interaction depend strongly on circuit and control parameters, such as frequency detuning and the effective coupling rate. We experimentally investigate the dynamics of the cross-resonance gate across a range of qubit detuning, intrinsic coupling strength, drive frequency, and compare our findings with the model.

https://doi.org/10.1103/PhysRevA.100.012301.

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**3:42PM U08.00007: Density Matrix Exponentiation on a Superconducting Quantum Processor (Part 1): Introduction and construction**

MORTEN KJAERGAARD (Presenter), Massachusetts Institute of Technology MIT, MOLLIE SCHWARTZ, MIT Lincoln Laboratory, AMY GREENE, GABRIEL SAMACH, Massachusetts Institute of Technology MIT, ANDREAS BENGTTSSON, Chalmers University of Technology, MICHAEL O'KEEFFE, MIT Lincoln Laboratory, CHRIS MCNALLY, YOUNGKYU SUNG, MILAD MARVIAN, Massachusetts Institute of Technology MIT, PHILIP KRANTZ, Chalmers University of Technology, JOCHEN BRAUMUELLER, RONI WINIK, Massachusetts Institute of Technology MIT, DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, JONILYN YODER, DANNA ROSENBERG, KEVIN OBENLAND, TERRY PHILIP ORLANDO, MIT Lincoln Laboratory, IMAN MARVIAN, Duke University, SIMON GUSTAVSSON, SETH LLOYD, WILLIAM OLIVER, Massachusetts Institute of Technology MIT — In conventional quantum processors, the parameters of the unitary operators to be implemented as part of a quantum circuit are controlled using classical hardware. Here we experimentally demonstrate a two-qubit implementation of the Density Matrix Exponentiation (DME) algorithm, in which the unitary operators of a quantum circuit are programmed by other quantum states. By using multiple copies of a quantum state, the DME algorithm efficiently implements a unitary operator with that state acting as a Hamiltonian. In Part 1 of this talk, we will introduce the DME algorithm, its uses, and our experimental implementation on a small quantum processor using a 99.7% fidelity CPHASE gate between two superconducting transmons.

*This research was funded in part by the ARO grant No. W911NF-18-1-0411; and was funded in part by the Assistant Secretary of Defense for Research & Engineering via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.
Density Matrix Exponentiation on a Superconducting Quantum Processor (Part 2): Demonstration and Characterization*  

MOLLIE SCHWARTZ (Presenter), MIT Lincoln Laboratory, MORTEN KJAERGAARD, AMY GREENE, GABRIEL SAMACH, Massachusetts Institute of Technology, ANDREAS BENGTSSON, Chalmers University of Technology, MICHAEL O’KEEFFE, MIT Lincoln Laboratory, CHRIS MCNALLY, YOUNGKYU SUNG, MILAD MARVIAN, Massachusetts Institute of Technology, PHILIP KRANTZ, Chalmers University of Technology, JOCHEN BRAUMUELLER, RONI WINIK, Massachusetts Institute of Technology, DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, JONILYN YODER, DANNA ROSENBERG, KEVIN OBENLAND, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, Massachusetts Institute of Technology, IMAN MARVIAN, Duke University, SIMON GUSTAVSSON, SETH LLOYD, WILLIAM OLIVER, Massachusetts Institute of Technology — Density matrix exponentiation (DME) represents a unique style of quantum operation, in which many copies of a quantum state $\rho$ are used to perform a unitary operation $U(\rho, \theta) = e^{i\rho\theta}$ on a second quantum system $\sigma$. Traditionally, changing an operation on $\sigma$ requires changing a sequence of classically-defined gates; in DME, a fixed gate sequence performs a range of operations simply by varying the quantum input. DME is a Trotter-style algorithm, in which the total angle of rotation $\theta$ is built up by performing $N$ rotations of $\theta/N$ with algorithmic error $\theta^2/N$. In Part 2 of this talk, we benchmark an implementation of the DME algorithm in a two-qubit system. We characterize $U(\rho, \theta)$ via process tomography, and demonstrate that the unitary depends on the input quantum state. We also explore tradeoffs between algorithmic error at small $N$ and noise/loss limits at large $N$.

*This research was funded in part by the ARO grant No. W911NF-18-1-0411 and by the Assistant Secretary of Defense for Research & Engineering via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.

Experimental considerations for zero noise extrapolation  

ABHINAV KANDALA (Presenter), KRISTAN TEMME, SETH MERKEL, DAVID MCKAY, EASWAR M MAGESAN, JAY M GAMBETTA, IBM TJ Watson Research Center — While decoherence and control errors limit the size of quantum computation in the absence of fault tolerance, a number of error mitigation techniques have been developed to access noise free estimates of expectation values. In particular, the zero-noise extrapolation technique was shown to extend the computational reach of a noisy superconducting processor. Here, quantum circuits are run at amplified noise rates, to extrapolate the results of these runs to the zero noise limit. Under the assumption of time invariant noise, such noise amplification may be achieved by stretching in time the gates employed in the circuit. We test these assumptions for superconducting processors with all-microwave drives and also consider the effect of errors in the gate rescaling on the extrapolation.
4:18PM U08.00010: Realizing giant artificial atoms in superconducting waveguide QED  A.M. VADIRAJ (Presenter), Electrical and Computer Engineering, Institute for Quantum Computing, University of Waterloo, ANDREAS ASK, Department of Microtechnology and Nanoscience, Chalmers University of Technology, IBRAHIM NSANZINEZA, CHUNG WAI SANDBO CHANG, Electrical and Computer Engineering, Institute for Quantum Computing, University of Waterloo, ANTON FRISK KOCKUM, Department of Microtechnology and Nanoscience, Chalmers University of Technology, C.M. WILSON, Electrical and Computer Engineering, Institute for Quantum Computing, University of Waterloo — In most studies of light-matter interaction, the atoms, either natural or artificial, are approximated as featureless dipoles, since the atomic dimension is much smaller than the wavelength of light. However, a new regime in waveguide QED, first proposed by Kockum et al, can realize a “giant” artificial atom by coupling to light at multiple points along a waveguide. As a result, the atom interacts with itself, resulting in a range of phenomena including non-Markovian dynamics and frequency-dependent coupling. The same proposal also discussed possibilities to extend this architecture to multiple giant atoms with interesting new physics. Motivated by this, we experimentally investigate circuits with one and two giant transmon qubits which are coupled to propagating microwaves at multiple points separated by wavelength-scale distances. For one qubit circuit, we demonstrate that we can enhance or suppress the relaxation rate of the 1-2 transition relative to the 0-1 transition by more than an order of magnitude. Using this capability, we show that we can engineer the giant transmon into an effective lambda system, including demonstrating EIT. We will also present preliminary measurements of a circuit with two giant qubits coupled in a braided geometry.


*This work was supported by Department of Energy grant DE-SC0019461.
4:42PM U08.00012: A novel bus design for a highly connected multi-qubit processor in 3D cQED architecture

SUMERU HAZRA (Presenter), ANIRBAN BHATTACHARJEE, KISHOR V SALUNKHE, SANSKRITI CHITRANSH, MEGHAN P. PATANKAR, R VIJAY, Tata Inst of Fundamental Res — Highly connected qubit networks offer efficient implementation of quantum algorithms by requiring fewer gates to implement a given circuit. While not considered to be highly scalable, the 3D cQED architecture offers a cleaner microwave environment and modular design which can be used effectively to build small to intermediate scale processors. We will present a novel bus design to couple multiple qubits in 3D cQED with high inter-qubit connectivity and sufficient spatial separation to minimize cross-talk effects. We will show preliminary experimental data to demonstrate qubit interactions using the cross-resonance gate but will also explain how it can be integrated with multiple gate schemes to build scalable multi-qubit processor in 3D architecture.

*Department of Atomic Energy, Government of India

4:54PM U08.00013: Waveguide-mediated Interactions Between Giant Superconducting Artificial Atoms

BHARATH KANNAN (Presenter), MAX RUCKREIGEL, DANIEL L CAMPBELL, Research Laboratory of Electronics, Massachusetts Institute of Technology, ANTON FRISK KOCKUM, Department of Microtechnology and Nanoscience, Chalmers University of Technology, JOCHEN BRAUMUELLER, RONI WINIK, MORTEN KJAERGAARD, Research Laboratory of Electronics, Massachusetts Institute of Technology, DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, JONILYN YODER, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, WILLIAM OLIVER, Department of Electrical Engineering and Computer Science, Department of Physics, MIT Lincoln Laboratory, Massachusetts Institute of Technology — In quantum optics experiments, atoms are typically treated as small point-like objects compared to the wavelength of the modes they interact with. Superconducting circuits offer a platform to study the physics of systems where this approximation no longer holds. Here, we realize a “giant” artificial atom by coupling a transmon qubit to multiple positions along a superconducting waveguide with separation on the order of the qubit wavelength. We show that the coupling between the qubits and the waveguide can be strongly tuned with the qubit frequency. Furthermore, we demonstrate waveguide-mediated exchange interactions between two giant atoms that can be tuned to be “decoherence-free” with respect to the waveguide. Finally, we show how varying the number of and distance between coupling points can be used to engineer exotic decay and coupling spectra, with applications to quantum information and simulation.

*This research was funded in part by an NDSEG Fellowship and by the Department of Defense via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.
5:06PM U08.00014: Building and benchmarking diabatic entangling gates for frequency-tunable qubits, part I  ANDRE PETUKHOV (Presenter), RAMI BARENDS, CHRIS QUINTANA, YU CHEN, VADIM SMELYANSKIY, Google Inc - Santa Barbara — One of the key needs in quantum computing are gates that are fast and precise, requiring minimization of the control errors and the suppression of leakage out of the computational states. We present a non-adiabatic protocol for iSWAP-like gates with minimal leakage and duration close to the speed limit. The key notion behind our approach is minimizing the gate error by synchronizing the Rabi clocks in the one- and two-excitation channels in a pair of transmon qubits to align minima of the leakage and residual swap population. This, in turn, can be accomplished by utilizing limited but sufficient tunability of the “fixed” interqubit coupling via a proper choice of the three key parameters such as interaction frequency, hold time and overshoot between the qubit frequencies near the avoided crossing. We show that our approach can be extended to other gate operations and discuss pulse-shape optimization suitable for particular gates and architectures.

5:18PM U08.00015: Building and benchmarking diabatic entangling gates for frequency-tunable qubits, part II  RAMI BARENDS (Presenter), CHRIS QUINTANA, ANDRE PETUKHOV, YU CHEN, VADIM SMELYANSKIY, Google Inc - Santa Barbara — One of the key needs in quantum computing are gates that are fast and precise, requiring precision control and the minimization of leakage out of the computational states. We present the experimental implementation of a synchronization protocol for constructing gates that have minimal leakage and a duration close to the speed limit. Using this method we achieve diabatic iSWAP-like and CPHASE gates with Pauli error rates down to $4.3(2) \times 10^{-3}$ in as fast as 18 ns with frequency-tunable superconducting qubits. In addition, we show how we use cross-entropy benchmarking (XEB) for quantifying the gates and error budgets.

Thursday, March 5, 2020 2:30 PM - 5:06 PM

Session U09 DQI: Quantum Foundations III  106 - Flaminia Giacomini, Perimeter Inst for Theo Phys - Tag(s): Focus
**2:30PM U09.00001: Time in Quantum Information**  
MOHAMMAD ANSARI (Presenter), ALWIN VAN STEENSEL, Forschungszentrum Julich, YULI NAZAROV, Department of Quantum Nanoscience, Kavli Institute of Nanoscience, TU Delft — Currently 'time' does not play any essential role in quantum information theory. In this sense, the theory is underdeveloped, similarly to how quantum physics was before Erwin Schrodinger introduced his famous evolution of wave functions. I will describe the problem of defining time-evolution in quantum information theory, specially for a central measures in the theory, i.e. Renyi entropy. I use a newly-developed replica trick formalism, namely 'Multiparallel World (MW)' formalism, that revolutionizes the theory. This formalism is one of the first attempts to introduce 'time evolution' for information transfer. With the total entropy being conserved in a closed system, entropy can flow internally between subsystems and I show that this flow is not limited to physical correlations as literature suggests, in fact information correlations are also involved. The mere existence of this new class of correlations allows for faster and slower information transfer.

References:

**2:42PM U09.00002: Violations of macroscopic local reality, time and the Q-function**
MARGARET REID (Presenter), MANUSHAN THENABADU, PETER DRUMMOND, Swinburne Univ of Tech — A macroscopic superposition state would appear to be inconsistent with the classical concept of macroscopic realism. Leggett and Garg proposed tests of macroscopic realism based on the validity of a second premise: (macroscopic) noninvasive measureability. Here, we consider tests of macroscopic realism where the second premise is replaced by that of macroscopic locality. Extending results obtained for NOON states [1], we show how one can falsify macroscopic local realism, by using Bell inequalities for cat-states where the choice of polarizer setting is replaced with a choice of time-of-evolution through a nonlinear medium. Different to the original Bell tests, here the outcomes of all relevant measurements are distinct by N bosons at each site, or else are well-separated in phase space. This motivates us to consider a model of reality based on the Q function. In that model, measurement is described by a dynamical interaction where sharp eigenvalues emerge for sufficient amplification, and Bell violations arise, there being backwards-in-time effects arising through negative diffusion terms [2].

References:
How can we observe an asymmetry in the temporal order of events when physics at the quantum level is time-symmetric? The source of time's barbed arrow is a longstanding puzzle. Causal asymmetry offers a provocative perspective. It asks how Occam's razor can privilege one temporal direction over another. That is, if we want to make statistically correct future predictions then what is the minimum past information we must store? Are we forced to store more data if we model events in one particular temporal order over the other?

Take a glass shattering upon impacting the floor. In one direction, the future distribution of shards depends only on the glass's initial position, velocity and orientation. In the opposite, we may need to track relevant information regarding each shard to infer the prior trajectory. Does this require more or less information? For stochastic processes, this potential divergence is quantified in the theory of computational mechanics. It is not only generally non-zero, but can also be unbounded. This phenomenon implies a simulator operating in the 'less natural' temporal direction is penalized with potentially unbounded memory overhead, and is cited as a candidate source of time's barbed arrow. However these studies assumed models were implemented via classical physics. Could the observed causal asymmetry have been a consequence of this classicality constraint?

In this presentation, we answer this question in the affirmative, by directly constructing a process where there is a classical arrow of time, but at the quantum level this arrow vanishes [1], and reporting on the experimental observation of this effect in a photonic quantum processor [2]. Our work suggests that causal asymmetry could be an artefact of forcing classical causal explanations in a fundamentally quantum world.


*FQXi grant: "Are quantum agents more energetically efficient at making predictions?"
3:30PM U09.00004: Time operators and time crystals: self-adjointness by topology change
KEIJI NAKATSUGAWA (Presenter), Applied Physics, Hokkaido University, TOSHIYUKI FUJII, Physics, Asahikawa Medical University, AVADH SAXENA, Center for Nonlinear Studies, Los Alamos National Laboratory, SATOSHI TANDA, Applied Physics, Hokkaido University — In the standard formulation of quantum mechanics and quantum field theory, time is not an observable but merely a parameter. There are two open problems which can promote time to an observable, namely 1) how to define self-adjoint time operators and 2) how to obtain systems called quantum time crystals.

In this presentation, we investigate time operators in the context of quantum time crystals in ring systems [1,2]. A generalized commutation relation called the generalized weak Weyl relation [3] is used to derive a class of self-adjoint time operators for ring systems. The conventional Aharonov-Bohm time operator, which describes the time of arrival of a particle on a one-dimensional line, is obtained by taking the infinite-radius limit. We also reveal the relationship between our time operators and a PT-symmetric time operator. These time operators are then used to derive several energy-time uncertainty relations.

We surmise that time operators and time crystals are closely related and also that topology change is important when time promotes from a parameter to an observable.


3:42PM U09.00005: Classically-forbidden probability flow in the quantum reentry problem
ARSENI GOUSSEV (Presenter), University of Portsmouth — The laws of quantum mechanics allow for a moving particle to temporarily reverse the direction of its motion even in the absence of any external force. A well-known manifestation of this counterintuitive phenomenon is the so-called quantum backflow effect, whereby the probability of finding a particle "on the left" increases with time despite the particle velocity pointing "to the right". In my talk, I will provide another clear-cut demonstration of nonconstancy of the direction of motion of a free particle. I will show that the free-space expansion of a quantum wave packet, initially confined to an interval, may be nonmonotonous: The probability density may sometimes flow back into (or reenter) the interval. The supremum of the classically-forbidden probability flow in this reentry problem appears to be the same as in the case of quantum backflow.

Indefinite Causal Orderings for Quantum Depolarizing Channel Identification

MICHAEL FREY (Presenter), National Institute of Standards and Technology Boulder —

Quantum channel identification (QCI) is the statistical estimation of channel parameters, accomplished by passing probe systems in prepared states through the quantum channel. Indefinite causal ordering (ICO) is a channel probing scheme in which copies of a quantum channel are physically or logically arranged so that the path through them is a superposition of different possible paths. Channel probing is known to be aided in a strong sense by ICO in the case of the qudit (d-dimensional) depolarizing channel. Specifically, ICO-assisted probing increases the quantum Fisher information (QFI) in the processed probe state about the unknown parameter(s), with increasing order indefiniteness yielding correspondingly greater QFI.

Investigations up until now have involved just superpositions of forward and reverse channel orderings; for example, three channel copies, A, B, and C, in a superposition of orderings A-B-C and C-B-A. Alternatively, these channels copies can be cyclically indefinitely ordered: a superposition of A-B-C, B-C-A, and C-A-B. The present work compares the effectiveness (QFI) of disparate competing ICOs for probing the qudit depolarizing channel. The QFIs associated with these competing ICOs are expressed analytically.

Contextuality in non-interacting measurement

SACHA GREENFIELD (Presenter), MORDECAI WAEGELL, JUSTIN DRESSEL, Chapman Univ — Non-interacting measurement is a phenomenon of seemingly non-local information transfer that arises for a single photon in a cascade of two-arm interferometers. Since contextuality has been identified as a resource for quantum informational tasks, it is reasonable to posit that non-interacting measurement requires contextuality in some form. We confirm this suspicion for the case of imbalanced beam splitters and discuss the exception that admits a noncontextual model. In contrast to existing proofs of contextuality for a single qubit, this scenario involves only pure states and sharp measurements.

A tight quantum speed limit for open quantum dynamics

YUSEF MALEKI (Presenter), Texas A&M Univ —

Determining the speed of the quantum dynamics of a system is significantly important in many physical studies. The faster dynamics in quantum gates can escalate the speed of computation. In condensed matter physics, determining how fast correlations can be spread in many-body systems, relies on the dynamical speed of the system. Finally, in black hole physics, the entropy change rate of the system is limited by the speed of quantum dynamics.

Quantum Speed Limit imposes a bound on the speed of evolution of all quantum processes. However, in spite of their significant importance, the existing bounds are usually not tight, which underestimate the best possible speedup, and they usually are difficult to compute. Overcoming these issues becomes even more challenging when we deal with open quantum systems. In this work, we present a new quantum speed limit, which resolves both tightness and computability issues. Unlike most of speed limits, this limit is applicable to any open or closed quantum dynamics.
**4:30PM U09.00009: The Heisenberg Interpretation of Quantum Mechanics**  ARMIN NIKKHAH SHIRAZI (Presenter), Univ of Michigan - Ann Arbor — In his book `Physics and Philosophy', Werner Heisenberg posited a distinction between the quantum and the classical worlds, which he characterized in terms of "potentialities or possibilities" versus "things and facts". However, the standard quantum formalism does not express such distinctions.

In this talk, we present a concrete implementation of this distinction into the quantum formalism, resulting in what will be called the Heisenberg interpretation of quantum mechanics. The modification of the formalism mainly involves replacing state reduction by a composition of two maps between the Hilbert space and a set of corresponding classical states. These maps represent the emergence and submergence of a classical state from a quantum state from interactions currently labeled as "measurements". This modified formalism has a number of advantages over the Copenhagen interpretation and sets the stage for experimental predictions which are not obvious under the standard formalism.

**4:42PM U09.00010: Experimental Comparison of Bohm-like Theories with Different Ontologies**  ARTHUR OU TEEN PANG (Presenter), HUGO FERRETTI, NOAH LUPU-GLADSTEIN, WENG-KIAN THAM, AHARON BRODUTCH, KENT AG BONSMA-FISHER, JOHN EDWARD SIPE, AEPHRAIM M STEINBERG, Univ of Toronto — The de Broglie-Bohm theory is a hidden variable interpretation of quantum mechanics which involves particles moving through space with definite trajectories. This theory singles out position as the primary ontological variable. Mathematically, it is possible to construct a similar theory where particles are moving through momentum space, and momentum is singled out as the primary ontological variable. In this paper we experimentally show how the two theories lead to different ontological descriptions. We construct the putative particle trajectories for a two-slit experiment in both the position and momentum space theories by simulating particle dynamics with coherent light. Using a method for constructing trajectories through the primary and derived (i.e. non-primary) spaces, we compare the ontological pictures offered by the two theories and show that they do not agree. This contradictory behaviour brings into question which ontology for Bohmian mechanics is to be preferred.

*This work was supported by NSERC and the Fetzer Franklin Fund of the John E. Fetzer Memorial Trust. Aephraim M. Steinberg is a fellow of CIFAR.*
Quantum Mechanical Reset-Observer Reset, not Observation, results in QM Wave-Particle Duality in Multi-Slit experiments  

MARTIN ALPERT (Presenter), President, Universal Empowering Technologies — A quantum mechanical mechanism based on statistical mechanics is proposed. It is based on corresponding and reciprocal changes in the number of states with associated energy changes at the observer and observed at reset and observation of the observer. The change in the number of states is different than the value of the observation. Each state is a possible input to the system. Bits, as a measure of information content, are considered the discrete cell size of a state. An experiment is proposed to determine where and when energy changes occur and how they are related to the observer and observed during the entire measurement process. A related experiment is proposed to determine timing between changes in the number of states. No time delay would indicate this is an entangled process and explain delayed choice observations. Bits not stored are lost, so when the number of inputs is greater than the number of outputs, an energy change occurs, and interference is observed (wave characteristics). If the number of inputs equals the number of outputs, no energy change occurs, and no interference is observed (particle characteristics). The theory, if verified, would further the understanding of the measurement process and entanglement’s involvement in the process.

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U16 DQI: Characterizing Quantum Computing Systems and Components III

2:30PM U16.00001: Understanding Crosstalk in Quantum Processors*  
ROBIN BLUME-KOHOUT (Presenter), MOHAN SAROVAR, ERIK NIELSEN, KENNETH RUDINGER, KEVIN YOUNG, TIMOTHY PROCTOR, Sandia National Laboratories — Multi-qubit quantum processors fail – i.e., deviate from ideal behavior – in many ways. One of the most important, especially as the number of qubits grows, is crosstalk. But “crosstalk” refers to a wide range of distinct phenomena. In this talk, I will present a precise and rigorous framework that we have developed for defining and classifying crosstalk errors, and compare it to existing ad hoc definitions. Then, I will present two protocols that we are deploying to detect and characterize crosstalk, and show how we are using them to break down and demystify the error behavior of testbed-class quantum processors in the wild.

*This material was funded in part by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research Quantum Testbed Program, and also by IARPA’s LogiQ program. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
**2:42PM U16.00002: Hold the onion: using fewer circuits to characterize your qubits.** ERIK NIELSEN (Presenter), TIMOTHY PROCTOR, KENNETH RUDINGER, MOHAN SAROVAR, KEVIN YOUNG, ROBIN BLUME-KOHOUT, Quantum Performance Lab, Sandia National Laboratories — A common complaint about qubit characterization protocols - especially tomographic protocols – is that they require running a ridiculously large number of circuits (experiments). In this talk, we compare the resources required by several QCVV protocols, including gate set tomography (GST) and randomized benchmarking (RB). We show how resources, primarily the number and type of circuits, depend on desired accuracy and on noise model. In particular, we show how QCVV techniques can capitalize on one's ability to simplify the relevant noise model – i.e. the types of noise being probed - and, for example, utilize an experimentalist's physical intuition to perform targeted characterization with significantly fewer circuits. We conclude by considering how existing QCVV techniques may be used in complementary ways during the holistic characterization of a quantum processor. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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**2:54PM U16.00003: Filter Function Formalism for Unitary Quantum Operations** TOBIAS HANGLEITER (Presenter), PASCAL CERFONTAINE, HENDRIK BLUHM, JARA-FIT Institute for Quantum Information, RWTH Aachen University — While the quantum process formalism provides a natural framework for describing the concatenation of quantum operations, it is of limited use when describing the effects of non-Markovian noise. In my talk, I will first present an extension of the filter function formalism, which so far has mostly been used to model gate fidelities and the effects of dynamical decoupling sequences. Our extension facilitates the efficient, perturbative calculation of full quantum processes in the presence of correlated noise, e.g. the 1/f-like noise found in many solid-state qubit systems. I will then show that a simple composition rule arises for the filter functions of gate sequences. This enables the investigation of quantum algorithms in the presence of correlated noise with moderate computational resources. Lastly, we present a fast and easy-to-use open source software framework (quantuminfo.physik.rwth-aachen.de/code) which facilitates the calculation of (first order) quantum processes and fidelities for arbitrary system dimensions. Other features include the efficient concatenation of several operations, and an optimized treatment of periodic Hamiltonians.
3:06PM U16.00004: Detection of coherent noise through the output of random quantum circuits* JIN-SUNG KIM (Presenter), LEV S BISHOP, ANTONIO D CORCOLES, JAY M GAMBETTA, DAVID MCKAY, SETH MERKEL, JOHN A SMOLIN, SARAH SHELDON, IBM TJ Watson Research Center — As quantum systems with increasing numbers of qubits emerge, new methods of characterizing and mitigating noise sources are required in the multi-qubit regime. While methods like randomized benchmarking (RB) and its variations are widely used in single and few-qubit systems to characterize coherent and incoherent noise sources, multi-qubit RB quickly becomes prohibitive at current coherence and control limits. In addition, it has been shown in recent experiments with three qubit RB that single and two-qubit RB fail to capture error sources present in larger qubit systems. On the other end of the spectrum, system-level metrics like quantum volume and other methods exist, but lump coherent and incoherent errors together in their output. We present here a method, based on the output of random quantum circuits, capable of quantitatively discriminating coherent noise from incoherent noise in multi-qubit systems.

*This work was supported by ARO under Contract No. W911NF-14-1-012.

3:18PM U16.00005: Investigating widespread correlated errors in superconducting qubit arrays MATTHEW MCEWEN (Presenter), University of California, Santa Barbara; Google Inc, RAMI BARENDS, Google Inc, JOHN M MARTINIS, University of California, Santa Barbara; Google Inc — With the advent of large arrays of superconducting qubits, such as Google's Sycamore processor, it is now possible to investigate the prevalence of correlated decoherence mechanisms that affect large numbers of qubits. Correlated errors are of particular importance with regard to implementing surface code error correction schemes, as errors are assumed to be independent or only weakly correlated. Control crosstalk and stray couplings are known to generate errors that are correlated, but the correlation is limited to a relatively small number of qubits. However, error mechanisms that affect large numbers of qubits simultaneously are problematic for error correction. In order to quantify the prevalence of such errors, we take rapid, simultaneous time-resolved measurements of error rates across large numbers of qubits on a single chip.
**3:30PM U16.00006: Renyi Entropy Benchmarking of Superconducting Qubits**

XIAO MI (Presenter), Google Inc - Santa Barbara, BENOIT VERMERSCH, ANDREAS ELBEN, University of Innsbruck, PEDRAM ROUSHAN, YU CHEN, Google Inc - Santa Barbara, PETER ZOLLER, University of Innsbruck, VADIM SMELYANSKIY, Google Inc — The ever-growing size of superconducting processors in recent years has significantly elevated the demand to efficiently benchmark the performance of large quantum circuits. Traditional methods such as state or process tomography suffer from a measurement overhead that scales double-exponentially with the number of qubits. Motivated by recent progress in trapped ion systems [1], we use sets of random gate unitaries to scramble many-body quantum states and infer their Renyi entropies, which reveal the rate of purity loss of the quantum system. The protocol is applied to benchmark the coherence of large quantum circuits run on the Google quantum processor. The scaling behavior of the randomized measurement protocol over system size is investigated in detail.


**3:42PM U16.00007: Demonstrating Scalable Benchmarking of Quantum Computers**

TIMOTHY PROCTOR (Presenter), KENNETH RUDINGER, KEVIN YOUNG, ERIK NIELSEN, ROBIN BLUME-KOHOUT, Sandia National Laboratories — Reliably testing multi-qubit quantum computers is notoriously challenging, but it is vital for measuring and aiding experimental progress, as well as for quantifying the capabilities of available processors. In this talk, I will present experimental results demonstrating simple, fast and scalable methods for benchmarking quantum computers. Our methods will work on essentially all current and near-term quantum computers, and they can be applied to hundreds of qubits with moderate error rates (around 0.1-1%) and thousands of high-quality qubits. Our core method is based on a class of randomized circuits, and it can be used to estimate the rate of errors in an average many-qubit circuit layer, using an analysis that will be familiar from randomized benchmarking. Our experiments reveal noise phenomena that only emerge at scale (e.g., crosstalk), quantify the divergence between the predictions of one- and two-qubit performance data and the actual behavior of many-qubit circuits, and provide high-level summaries of device performance versus circuit width and depth.

*This material was funded in part by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research Quantum Testbed Program, and the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
4:18PM U16.00008: Qutrit randomized benchmarking*  ALEXIS MORVAN (Presenter), Lawrence Berkeley National Laboratory, MACHIEL S BLOK, VINAY RAMASESH, LARRY CHEN, IRFAN SIDDIQI, Univ of California - Berkeley — Qutrits are an alternative to qubits to implement quantum computers by using three-, rather than two-level systems, and have proved useful to explore connections between high-energy physics and quantum information science. A standard measure of the performance of qubit-based processors would be to use randomized benchmarking and its derivatives as these techniques allows scalable characterization of the processor. In this talk, we present an experimental implementation of qutrit randomized benchmarking on a 5-qutrit processor. This gives us a measure of the overall performance of our processor, as well as a tool to diagnose specific gate fidelity and cross-talk error.

*This work was supported by the testbed program of the Advanced Scientific Computing Research for Basic Energy Sciences program, Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

4:30PM U16.00009: Effect of Imperfections on the Cross Entropy Benchmark Fidelity of Random Circuit Sampling  YIMU BAO, SOONWON CHOI (Presenter), EHUD ALTMAN, University of California, Berkeley — Random circuit sampling (RCS) is a computationally intractable task for exact classical simulations, and thus proposed as a way to demonstrate quantum supremacy. The fidelity of RCS from a realistic quantum device with respect to its ideal case can be quantified by so-called (linear) cross entropy benchmark, which is inevitably reduced by the presence of various imperfections. Here, we present an efficient method to evaluate the amount of average fidelity reduction originating from various kinds of imperfections without any simplifying assumptions. More specifically, we develop an exact relation between the linear cross entropy averaged over random circuit realizations and the partition function of a classical spin model, which allows efficient classical simulations. Using Monte-Carlo algorithms, we quantitatively analyze the average cross entropy in the presence of imperfections for both 1D and 2D systems with various layouts of circuits for reasonably large system sizes.

4:42PM U16.00010: Engineering Quantum Process Fidelity via Generalized Markovian Noise*  EVANGELOS VLACHOS (Presenter), HAIMENG ZHANG, JAMES FARMER, DARIAN HARTSELL, ELI M LEVENSON-FALK, Univ of Southern California — Markovian noise causes errors in quantum processes in ways that are difficult to correct. Surprisingly, theoretical studies have recently proposed that short-memory (generalized Markovian) noise can be used as a resource to mitigate the effects of Markovian noise. We have investigated the efficacy of adding generalized Markovian noisy signals, with various types of memory kernels, at improving fidelity and reducing decoherence in superconducting qubits, using both computational and experimental methods. We present quantum trajectory simulations and experimental tests of different corrective noise schemes, and discuss paths forward for optimizing quantum process fidelity.

*This work was supported by the ARO STIR program grant W911NF-19-1-0070 and by NSF QAA-TAQS grant OMA-1936388.
4:54PM U16.00011: Characterizing the performance of NISQ devices with random Clifford circuits*  
SETH MERKEL (Presenter), ANTONIO D CORCOLES, IBM Tj Watson Research Center,  
ANIMESH DATTA, SAMUELE FERRACIN, University of Warwick, JIN-SUNG KIM, DAVID MCKAY, SARAH SHELDON, IBM Tj Watson Research Center — There has been recent interest in sampling the output distributions of pseudo-random quantum circuits as a benchmark for large quantum systems [1,2]. However, based on the work of the Datta group on circuit accreditation [3] we suggest that for characterizing device performance, it is sufficient to measure the outputs of only pseudo-random Clifford circuits, a classically-simulatable subset of all quantum circuits. We require a few reasonable assumptions about our devices at IBM, namely that both Clifford and non-Clifford Z-rotations are done in software and therefore have the same error rates. Given this result, we note that a) all of the classical pre/post-processing is efficient and b) we can deal with the variational distance of the output distributions directly without proxies such as the cross entropy or heavy output generation.


*This work was supported by ARO under Contract No. W911NF-14-1-012

5:06PM U16.00012: Effects of qubit frequency crowding on scalable quantum processors*  
JARED HERTZBERG (Presenter), SAMI ROSENBLATT, JOSE M CHAVEZ, EASWAR M MAGESAN, JOHN A SMOLIN, JENG-BANG YAU, VIVEKANANDA ADIGA, MARKUS BRINK, ERIC J ZHANG, JASON ORCUTT, JERRY M. CHOW, IBM Tj Watson Research Center — Lattices of transmon qubits offer a scalable architecture to build quantum processors. Long qubit coherence times and hardware-efficient cross-resonance gates enable low gate error rates. However, frequency-crowding among the qubits can increase gate errors. Neighboring qubits must have similar but non-degenerate excitation energies. In this talk we will quantify the effects of frequency crowding and consider how this behavior scales with device size for 50-qubit and larger systems. We will also discuss strategies to mitigate or eliminate frequency crowding during device fabrication.

*We acknowledge support from IARPA under Contract No. W911NF-16-0114
Entanglement of Microwave-Optical Modes in a Strongly Coupled Electro-Optomechanical System

XU HAN (Presenter), Argonne Natl Lab, CHANGCHUN ZHONG, LIANG JIANG, University of Chicago — Quantum transduction between microwave and optics can be realized by quantum teleportation if given reliable entanglement between microwave and optical modes, namely entanglement-based quantum transduction. To realize this protocol, an entangled source with high-fidelity is necessary. Based on a generic strongly coupled cavity electro-optomechanical system, we study the microwave-optical entanglement generation and quantify the frequency entanglement between the two modes. The entanglement can be straightforwardly encoded in the frequency-bin degree of freedom with a feasible experiment to verify entangled photon pairs. The experimental implementation is systematically analyzed, and the preferable parameter regime for entanglement verification is identified. An inequality is given as a criterion for good entanglement verification, including practical imperfections.

In Part A: We introduce frequency entanglement in the strongly coupled electro-optomechanical system and discuss the experimental detection scheme.

Part B: we theoretically evaluate the entanglement of formation rate, analyze Bell state violation and estimate the coincidence rate.

2:54PM U17.00003: Ground state cooling and high-fidelity quantum transduction via parametrically-driven bad-cavity optomechanics*

HOI-KWAN LAU (Presenter), AASHISH CLERK, University of Chicago — In optomechanical systems, the beam-splitter interaction underlies the utility of many applications, but the two-mode-squeezing interaction creates unwanted excitations and is usually detrimental. In this work, we propose a simple but powerful method based on cavity parametric driving to suppress the unwanted excitation that does not require working with a deeply sideband-resolved cavity. Our approach is based on a simple observation: as both the optomechanical two-mode-squeezing interaction and the cavity parametric drive induce squeezing transformations of the relevant photonic bath modes, they can be made to cancel one another. We illustrate how our method can cool a mechanical oscillator below the quantum back-action limit, and significantly suppress the output noise of a sideband-unresolved optomechanical transducer.

*This work is supported by the AFOSR MURI FA9550-15-1-0029 on quantum transduction.

3:06PM U17.00004: Mechanical Purcell Filter for Microwave Quantum Machines*

AGNETTA CLELAND (Presenter), MAREK PECHAL, PIETER-JAN C. STAS, CHRISTOPHER J SARABALIS, PATRICIO ARRANGOIZ-ARRIOLA, EDWARD A WOLLACK, WENTAO JIANG, TIMOTHY MCKENNA, AMIR SAFAVI-NAEINI, Stanford Univ — Measuring the state of a superconducting qubit introduces a loss channel which can enhance spontaneous emission through the Purcell effect. This can be mitigated by implementing a Purcell filter which strongly suppresses signal propagation at the qubit frequency. If the filter is well-matched at the readout cavity frequency, it will protect the qubit from decoherence channels without sacrificing measurement bandwidth. In this talk, we propose and analyze design for a mechanical Purcell filter, composed of an array of nanomechanical resonators in thin-film lithium niobate, whose frequencies are chosen to produce a bandpass response. A modest footprint, steep band edges, and lack of cross-talk make these filters a novel and appealing alternative to electromagnetic versions currently used in microwave quantum machines. We will present a circuit model depiction of this filter, as well as design, fabrication, and characterization results. Our filters achieve over 200 MHz bandwidth at 3.5 GHz, with over 50 dB out-of-band suppression, while occupying less than 0.3 square mm on-chip in a qubit-compatible material platform.

*This work is supported by the U.S. government through the Department of Energy Grant No. DE-SC0019174 and the National Science Foundation Grant No. ECCS-1808100.
3:18PM U17.00005: Microwave-frequency acoustic resonators with high quality factors*
MING-HAN CHOU (Presenter), University of Chicago, ETIENNE DUMUR, Argonne National Laboratory; University of Chicago, GREGORY PEAIRS, University of California, Santa Barbara; University of Chicago, AUDREY BIENFAIT, HUNG-SHEN CHANG, CHRISTOPHER R CONNER, JOEL GREBEL, RHYS G POVEY, University of Chicago, KEVIN SATZINGER, University of California, Santa Barbara; University of Chicago(present in Google Inc), AUDREY BIENFAIT, HUNG-SHEN CHANG, CHRISTOPHER R CONNER, JOEL GREBEL, RHYS G POVEY, University of Chicago, KEVIN SATZINGER, University of California, Santa Barbara; University of Chicago(present in Google Inc), YOUPENG ZHONG, University of Chicago, ANDREW CLELAND, Argonne National Laboratory; University of Chicago — We are pursuing the development of microwave-frequency acoustic resonators that can be integrated with superconducting circuits. By combining the mechanical properties of single crystal silicon with the mechanical isolation provided by phononic crystals, high quality factors at GHz frequencies should become achievable. In this talk, we describe the design and fabrication of mechanical resonators comprising suspended hybrid structures combining aluminum nitride and silicon supported by a phononic crystal, providing mechanical isolation with an integrated piezoelectric transduction mechanism. Measurements at low temperatures indicate this type of mechanical device can achieve quality factors approaching those of coplanar waveguide resonators, providing interesting potential for use in quantum information applications.

*This work supported by AFOSR MURI (FA9550-15-1-0029), UChicago MRSEC (NSF DMR-1420709), DOE, UChicago PNF via SHyNE (NNCI NSF -1542205), ARL (W911NF-15-2-0058), and ANL

3:30PM U17.00006: A multimode nonlinear resonator for quantum acoustics  GUSTAV ANDERSSON (Presenter), Chalmers Univ of Tech, SHAN WILLIAMS JOLIN, KTH Royal Institute of Technology, MARCO SCIGLIUZZO, PER DELSING, Chalmers Univ of Tech — Exploiting multiple modes in a quantum acoustic device could enable applications in quantum information in a hardware-minimal setup. Surface Acoustic Wave (SAW) resonators in the quantum regime support high Q-factors (>10^5) and dense mode spectra. We introduce a Kerr nonlinearity to a SAW resonator by integrating a SQUID (Superconducting QUantum Interference Device) into one of the Bragg reflectors. The SQUID inductance modulates the reflectivity of each unit cell in the mirror and hence the effective length of the resonator. Due to the narrow free spectral range, this gives rise to a cross-Kerr coupling between the more than 20 accessible modes. We attempt to exploit this nonlinear coupling to generate multimode non-classical states that could potentially provide a resource for quantum computation. Avenues towards quantum simulation using the coupled modes as lattice sites occupied by SAW phonons are further explored.
3:42PM U17.00007: Existence of a new surface mode with transverse electric field*
ZONGYE WANG (Presenter), XUEDONG HU, State Univ of NY - Buffalo — Surface acoustic waves, in particular Rayleigh waves near the surface of a piezoelectric material, have attracted a lot of attention lately through their abilities to carry electrons and to couple strongly with superconducting qubits. Here we report the study of a surface mode in a piezoelectric material with transverse electric field, which has not been explored in previous studies of surface acoustic waves. This transverse mode is different from both the well-understood Rayleigh wave that contains a longitudinal component, and the Bleustein-Gulyaev wave, which has been actively studied recently. In order to describe surface modes with transverse electric field, we develop a theory of elastic waves coupled with electromagnetic field, and find among its solutions the Rayleigh wave, the Bleustein-Gulyaev wave, and the new transverse mode. We clarify properties of this mode, such as its polarization, dispersion, and speed of sound. While this surface mode cannot be used to carry an electron, it could play an important role when surface acoustic phonons are used as quantum bus to convey information between quantum dots.

* We thank support by US ARO.

3:54PM U17.00008: Optimal control of nanomechanical quantum memory coupled to superconducting qubit  
MINGYU KANG (Presenter), ZHAOYOU WANG, EDWARD A WOLLACK, AGNETTA CLELAND, RACHEL GRUENKE, NATHAN LEE, KEVIN MULTANI, MAREK PECHAL, PATRICIO ARRANGOIZ-ARRIOLA, AMIR SAFAVI-NAEINI, Stanford Univ — Quantum memory coupled to a single non-linear element such as superconducting qubit can serve as a promising quantum information processing platform with advantages in lifetime and hardware-efficiency. However, naïve implementation of this quantum computing architecture requires two additional SWAP gates between the memory resonator and the processing qubit per each gate operation, which can cause longer gate time and larger error. In this work we explore the optimal control for performing high-fidelity state preparation and unitary gates on quantum memory by using a power- and bandwidth-limited pulse optimization method. Specifically, we apply our method to a hybrid system of nanomechanical resonators coupled to tunable-frequency transmon qubit and find the optimal pulse for generating entangled states of mechanical resonators as well as implementing phonon-phonon CNOT gate. We test the pulse's robustness to experimental imperfections, such as pulse noise, parameter uncertainties, and decoherence. Finally, we find the optimal pulse length and gate fidelity as a function of the qubit-resonator coupling strength and frequency spacing of resonators, suggesting the experimental parameter regime for achieving scalable quantum computing.
4:06PM U17.00009: Synthesizing multi-phonon quantum superposition states using three-body interactions with transmon qubits*  MARIOS KOUNALAKIS (Presenter), YAROSLAV M. BLANTER, GARY STEELE, Delft University of Technology — We propose a scheme for controlling a radio-frequency mechanical resonator at the quantum scale using two superconducting transmon qubits. The qubits are coupled via a capacitor in parallel to a superconducting quantum interference device (SQUID), which has a suspended mechanical beam embedded in one of its arms. Following a theoretical analysis of the quantum system, we find that this configuration, in combination with an in-plane magnetic field, can give rise to a tuneable three-body interaction in the single-photon strong-coupling regime, while enabling suppression of the stray qubit-qubit coupling. Using state-of-the-art parameters and qubit operations at single-excitation levels, we numerically demonstrate the possibility of ground-state cooling as well as high-fidelity preparation of multi-phonon quantum states and qubit-phonon entanglement. Our work significantly extends the quantum control toolbox of radio-frequency mechanical resonators and may serve as a promising architecture for integrating such mechanical elements with transmon-based quantum processors.

*This work was supported by the Netherlands Organisation for Scientific Research (NWO/OCW), as part of the Frontiers of Nanoscience program.

4:18PM U17.00010: Nonclassical energy squeezing with quadratic electromechanics
XIZHENG MA (Presenter), University of Colorado, Boulder, JEREMIE VIENNOT, Univ. Grenoble Alpes, CNRS, Institut Néel, SHLOMI KOTLER, JOHN TEUFEL, National Institute of Standards and Technology Boulder, KONRAD LEHNERT, University of Colorado, Boulder — The ability to access a broad range of quantum state of motion with massive mechanical oscillators has been an enduring ambition in the field of opto- and electromechanics. Despite achieving many landmarks, the often exploited radiation pressure coupling between these mechanical oscillators and microwave or optical light relies on a linearized interaction that limits possible quantum effects. To go beyond this limitation, we quadratically couple the displacement of a mechanical oscillator to the energy levels of a superconducting charge qubit[1]. Through microwave frequency drives that change both the state of the oscillator and the qubit, we dissipatively stabilize the oscillator in a non-classical state with a large mean phonon number of 43 and sub-Poissonian number fluctuations of approximately 3. In this number squeezed state, we observe a striking feature of the quadratic coupling, the two phonon recoils of the mechanical oscillator due to qubit transitions. These are closely analogous to the vibronic transitions in molecules, heralding entry into a new regime of artificial systems with fast electrons coupled strongly to slow vibrations.

Recent progress in the design and realization of phononic structures has resulted in a number of quantum analogues. Elastic waves in one-dimensional waveguides with broken time-reversal or parity symmetry obey Dirac-like equations and possess spin-like topology. Of particular interest for quantum computing is the design, construction, and demonstration of coherent superpositions of elastic waves in waveguides and coupled waveguides. These coherent superpositions can be characterized by the phase of the elastic wavefunction and are called phase-bits or phi-bits. The construction of non-separable (i.e., ‘classically entangled’) superpositions has been achieved using phi-bits comprised of coupled waveguides. These phononic structures allow accessing quantum analogue computing at room temperatures and long coherence times.

2 P. A. Deymier and K. Runge, Crystals 6, 44 (2016).

*W. M. Keck Foundation

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U18 GSNP: Glassy Dynamics: From Simple Models to Biological Tissues II 205 - Grzegorz Szamel, Colorado State University - Tag(s): Invited
Dense assemblies of particles are prototypes of structurally disordered systems, such as amorphous solids or yield stress fluids. In infinite dimension their mean-field description becomes exact, and solving their equilibrium dynamics in this limit has been remarkably fruitful in capturing static properties of finite-dimensional systems as well. Here we address their out-of-equilibrium dynamics, paving the way to obtaining a similar infinite-dimensional benchmark for the mechanical or rheological properties of structurally disordered systems.

More specifically, we derive the mean-field dynamical equations that describe a system of pairwise interacting particles, in infinite dimension and in the thermodynamic limit, in a generic setting with arbitrary noise and friction kernels, and possibly under a global shear. We show that the complex many-body dynamics can then be exactly reduced to a single one-dimensional stochastic process, with three effective kernels that have to be determined self-consistently.

In this talk, I will sketch the derivation of this effective dynamics, highlighting in particular the few key ingredients of the high-dimensional physics and their possible relevance for finite-dimensional systems. Since we consider a very general setting, we can model a broad range of situations — equilibrium, quasi-statics, transients or steady-states — such as liquid and glass rheology or active self-propelled particles.


*This project has received funding from the European Research Council (ERC) under the European Union Horizon 2020 research and innovation programme (grant agreement n. 723955 - Glas- sUniversality). This research was supported in part by the National Science Foundation under Grant No. NSF PHY-1748958. E.A. acknowledges support from the SNSF Ambizione Grant PZ00P2_173962. T.M. acknowledges funding from the Grant ANR-16-CE30-0023-01 (THERMOLOC).

3:06PM U18.00002: Beyond mean-field theories of glassy dynamics* [Invited] GIULIO BIROLI (Presenter), LPENS, Ecole Normale Superieure — I will present new theoretical frameworks that allow to go beyond the mean-field theory of glassy dynamics. I will present the state of the art and the central directions for future works. The main aim and outcome of our approaches is a theory of activated dynamics of glassy systems.

*Simons Foundation collaboration Cracking the Glass Problem (No. 454935 to G. Biroli)
To understand the origin of universal low-temperature properties of glasses, which differ dramatically from those of their crystalline counterparts, it is paramount to understand what controls the low frequency vibrational modes of glasses. Numerical methods generally create glasses by quenching mildly supercooled liquids, which limits the variation of glasses' vibrational spectra and the ability to examine correlations between the properties and the vibrational spectra. Due to a combination of advances in simulation techniques and the formulation of new glass forming models, we are now able to study glasses with a wide range of stabilities. Here we study vibrational modes, sound attenuation, and energy transport in simulated glasses with stabilities that range from very poorly annealed to very stable. Our most stable glass is comparable to exceptionally-stable, vapor-deposited laboratory glasses. We find that the density of the localized, low-frequency modes decreases quickly with increasing stability. This decrease is accompanied by a a large decrease in sound attenuation. We find that at low-frequencies, in the harmonic approximation, sound attenuation follows Rayleigh scattering scaling with wave-vector. We examined energy transport by exciting a wave packet and determined the energy diffusivity. For a low frequency excitation, the decrease in sound attenuation is mirrored by an increase in the energy diffusivity. However, for a high frequency excitation, the diffusivity is nearly constant and independent of stability.

*National Science Foundation DMR-1608086
Simons Foundation
**4:18PM U18.00004: Gelation in Soft Matter: from Colloids to Decorated Protein Networks**

[Invited] PADDY ROYALL (Presenter), Physics, University of Bristol, IOATZIN RIOS DE ANDA, Mathematics, University of Bristol, ANGELIQUE COUTABLE-PENNARUN, Biochemistry, University of Bristol, CHRISTOPHER BRASNETT, Physics, University of Bristol, STEPHEN WHITElam, Molecular Foundry, Berkeley, ANNELA SEDDON, Physics, University of Bristol, JOHN RUSSO, Physics, La Sapienza, ROSS ANDERSON, Biochemistry, University of Bristol — Gelation unites many central issues in soft matter: phase transitions, dynamical arrest and self-assembly. *Spinodal* Gelation the formation of a network during spinodal decomposition has been recognized in colloids and proteins [1,2]. The competition between dynamical arrest and self-assembly has also been exploited in critical soft matter, where fluctuations associated with a non-equilibrium critical point introduce an additional tunable lengthscale [3]. Here we extend these concepts to a new system of fluorescent proteins, to produce multicomponent networks. We tune the structural properties and functional behavior of these decorated protein networks with a variety of soft matter and biochemical techniques [4].


*European Research Council
Leverhulme Trust
Biotechnology and Biological Sciences Research Council
Engineering and Physical Sciences Research Council
4:54PM U18.00005: Rigidity and glass transitions in collections of cells and fiber networks*

[Invited] M. LISA MANNING (Presenter), Syracuse University — In biological processes like embryonic development and in cancer metastasis, collective groups of cells must dramatically reorganize and move over substantial distances like a fluid. In other cases, such as the mature lining of the human lung, it is functionally important for the cells to behave as an intact solid, and still other tissues appear to straddle a disordered fluid-solid transition. First, I will discuss a theory for the origin of rigidity and the scaling laws that occur in a broad class of models for biological tissues (including vertex models for confluent cell aggregates and spring network models for extracellular matrix), and then I will discuss the anomalous glassy behavior that arises in such models in the presence of thermal or active fluctuations.

*This work is funded supported by grants #454947, and #446222 from the Simons Foundation.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U19 DAMOP: Quantum Simulators for Quantum Complex Network Science 207 - Tag(s): Invited

2:30PM U19.00001: Hyperbolic Lattices in Circuit QED* [Invited] ALICIA KOLLAR (Presenter), University of Maryland, College Park — After two decades of development, superconducting circuits have emerged as a rich platform for quantum computation and simulation. Lattices of coplanar waveguide (CPW) resonators have been shown to produce artificial materials for microwave photons, where interactions can be introduced either via non-linear resonator materials or qubit-resonator coupling. Here, we highlight the previously-overlooked property that these lattice sites are deformable and permit tight-binding lattices which are unattainable, even in solid-state systems. Networks of CPW resonators can create a new class of materials, including lattices in an effective hyperbolic space with constant negative curvature. We will discuss the mathematical tools needed to study the spectra of such structures and present experimental data showing that hyperbolic analogs of the kagome lattice in which photons in this lattice propagate along geodesics of the hyperbolic metric, rather than along the standard straight lines of flat Euclidean, space can be produced in the lab. Additionally, we will highlight the prospects for studies of information and entanglement propagation in hyperbolic geometries, as well as realization of other non-flat structures, such as trees or models with varying curvature.

*This work was supported by the NSF, the Princeton Center for Complex Materials DMR-1420541, and by the MURI W911NF-15-1-0397.
3:06PM U19.00002: Optically networked color centers* [Invited] JELENA VUCKOVIC (Presenter), Stanford Univ — Most quantum technologies rely on homogeneous, long lived qubits which are efficiently optically interconnected. To achieve this goal, we have been studying color centers in diamond and silicon carbide, in combination with novel fabrication techniques, and our photonics inverse design approach.

*DOE, ARO, NSF

3:42PM U19.00003: Entangled Radiofrequency-Photonic Sensor Network* [Invited] ZHESHEN ZHANG (Presenter), YI XIA, WEI LI, Univ of Arizona, WILLIAM CLARK, DARLENE HART, General Dynamics Mission Systems, QUNTAO ZHUANG, Univ of Arizona — Quantum metrology enables a measurement sensitivity below the standard quantum limit (SQL), as demonstrated in the Laser Interferometer Gravitational-wave Observatory (LIGO). As a unique quantum resource, entanglement has been utilized to enhance the performance of, e.g., microscopy, target detection, and phase estimation. To date, almost all existing entanglement-enhanced sensing demonstrations are restricted to improving the performance of probing optical parameters at a single sensor, but a multitude of applications rely on an array of sensors that work collectively to undertake sensing tasks in the radiofrequency (RF) and microwave spectral ranges. Here, we propose and experimentally demonstrate a reconfigurable RF-photonic sensor network comprised of three entangled sensor nodes. We show that the entanglement shared by the sensors can be tailored to substantially increase the precision of parameter estimation in networked sensing tasks, such as estimating the angle of arrival (AoA) of an RF field. The entangled RF-photonic sensor network achieves an estimation variance 3.2 dB below the SQL in measuring the average field amplitudes and an estimation variance 3.5 dB (3.2 dB) below the SQL in measuring the AoA at a central (edge) node. Our work would open a new avenue toward utilizing quantum metrology for ultrasensitive positioning, navigation, and timing.

*General Dynamics Mission Systems
4:18PM U19.00004: Quantum Optical Neural Network with Multimode Cavity QED* [Invited]
YUDAN GUO (Presenter), BRENDA MARSH, RONEN KROEZE, SURYA GANGULI, Stanford Univ, JONATHAN KEELING, University of St Andrews, BENJAMIN L LEV, Stanford Univ — The ability to engineer inter-particle interaction is at the heart of quantum simulation of many-body systems. However, the necessary nonlocal interaction in complex neural networks poses challenges to traditional implementation of ultracold atoms quantum simulators. We present our theoretical and experimental studies of photon-mediated interactions with atoms trapped inside a multimode confocal cavity. Superposition of different photon modes with incommensurate spatial profiles gives rise to a sign-changing and non-local interaction. Through numerical simulations, we show that the connectivity resulting from such non-local interaction will allow us to explore spin models featuring an associative memory to spin glass transition. In addition, the dissipative cavity photon dynamics facilitate more efficient spin relaxation to low energy states than the textbook Glauber dynamics. Combined with our recent experimental demonstration of cavity-mediated spin-spin interaction and characterization of the non-local interaction, a quantum optical neural network is within our reach.

*We acknowledge funding support from the Army Research Office, the National Science Foundation under Grant No. CCF-1640075, the Semiconductor Research Corporation under Grant No. 2016-EP-2693-C.

4:54PM U19.00005: Complex Networks in Multimode Continuous Variable Quantum Optics* [Invited] VALENTINA PARIGI (Presenter), Laboratoire Kastler Brossel, Sorbonne Université — The study of quantum complex structures is crucial for choosing the best strategies to use in future multi-scales complex quantum technologies. Multimode quantum optics processes offer scalable platforms for implementing large networks of continuous variables entanglement correlation and emulating networks of harmonic oscillators with physical interactions. The strategy offers totally reconfigurable topology from regular to complex shapes. In particular, I’m going to discuss continuous variables entangled networks for quantum routing protocols, the emergence of complex network structures in quantum networks under non-Gaussian operations, and machine learning techniques for their experimental characterization.

*The author acknowledge financial support from the European Research Council under the Consolidator Grant COQCOoN (Grant No. 820079).

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U20 DBIO: Physics of the Cytoskeleton Across Scales III: Transport 301 - Jing Xu, University of California, Merced - Tag(s): Focus
2:30PM U20.00001: Microtubules Regulate Localization and Availability of Insulin Granules in Pancreatic Beta Cells*

WILLIAM HOLMES (Presenter), Vanderbilt Univ — Two key prerequisites for glucose stimulated insulin secretion (GSIS) in beta cells are the proximity of insulin granules to the plasma membrane and their anchoring or docking to the plasma membrane (PM). To this point, it is unclear what regulates localization of insulin granules and their interactions with the PM within single cells. We demonstrate that microtubule (MT) motor transport dynamics have a critical role in regulating both factors. Super-resolution imaging shows that while the MT cytoskeleton resembles a random meshwork in the cells’ interior, MTs near the cell surface are aligned with the PM. Computational modeling suggests two consequences of this. First, this structured MT network withdraws granules from the PM. Second, the binding and transport of insulin granules by MT motors prevents their stable anchoring to the PM. These findings suggest the MT cytoskeleton may negatively regulate GSIS by both limiting the amount of insulin proximal to the PM and preventing stable docking of insulin granules to the PM. These results predict that altering MT network structure in beta cells can be used to tune GSIS. Thus, our study points to a potential of an alternative therapeutic strategy for diabetes by targeting specific MT regulators.

*Supported by NSF DMS1562078.

2:42PM U20.00002: Anomalous transport across scales in crosslinked actin-microtubule composites*

SYLAS ANDERSON (Presenter), JONATHAN GARAMELLA, RYAN J. MCGORTY, RAE M ROBERTSON-ANDERSON, Univ of San Diego — The diffusion of microscopic particles through the cell is largely controlled by the cytoskeletal network, comprised of semiflexible actin filaments, rigid microtubules, and crosslinking proteins. Yet, how the interactions between actin and microtubules and the various types of filament crosslinking affect particle transport remain unresolved. In our experiments, we couple single-particle tracking (SPT) with differential dynamic microscopy (DDM) to characterize the transport of micron-sized particles diffusing through crosslinked composite networks of actin filaments and microtubules. Specifically, we investigate the impact of permanently crosslinking actin to actin, microtubules to microtubules, and actin to microtubules. By combining SPT and DDM, we are able to couple single-particle dynamics to ensemble transport phenomena, and link particle diffusion to the viscoelastic characteristics of the networks. We find that subtle changes to the crosslinking interactions between cytoskeleton filaments play surprisingly important roles in the anomalous subdiffusion that particles exhibit within a composite cytoskeletal system.

*NIH Award #R15GM123420
ELENA KOSLOVER (Presenter), University of California, San Diego — Cells rely on a variety of mechanisms for delivering particles ranging from small molecules to micron-sized organelles to their various destinations. We use physical modeling coupled with live-cell imaging data from collaborating groups to explore the interplay of different transport modes in distributing particles through the complex intracellular environment. This talk will focus on two examples of multi-modal transport: combining motor-driven motion, diffusion, and fluid flow for efficient dispersion of particles within the cell.

Organelle hitchhiking is a non-canonical form of transport, which relies on a cargo organelle attaching to a motor-driven "carrier" with the aid of linker proteins. We quantify the effect of physical parameters on hitchhiking efficiency, demonstrating an insensitivity to linker density and a substantial benefit from tethering of cargo organelles to microtubule tracks. Our model is parameterized and validated against dynamic imaging data in fungal hyphae.

In addition, we investigate the role of advective transport for proteins and ions within the endoplasmic reticulum (ER). Capitalizing on recent experimental evidence of contraction-driven uncoordinated flow within ER tubules, we show that rapid flow combine with mobile calcium-binding buffer proteins can substantially enhance the distribution of calcium ions within the active network structure of the ER.

*This work was supported by grants from the Alfred P. Sloan Foundation, a CAREER award from the National Science Foundation, and a graduate research fellowship from the Visible Molecular Cell Consortium / Center for Trans-scale Structural Biology and Biophysics.
3:30PM U20.00004: MEMBRANE CHOLESTEROL IS A NOVEL CONTROL FOR KINESIN-BASED TRANSPORT* QIAOCHU LI, JOHN WILSON, University of California, Merced, KUO-FU TSENG, WEIHONG QIU, Oregon State University, MICHAEL VERSHININ, University of Utah, STEPHEN KING, University of Central Florida, JING XU (Presenter), University of California, Merced — Motor protein-based transport in cells underlies all eukaryotic cell function and survival; dysfunctions in this transport are implicated in many diseases, including neurodegeneration. While the properties of motor proteins have been extensively studied both in vivo and in vitro, many important questions remain, including how the properties of the cargo itself impact motor function. In cells, cargos are often membrane-bound; the composition of the cargo membrane has long been hypothesized to impact motor protein-based transport. Here we combined advances in membrane biophysics with single-molecule optical-trap experiments to characterize the transport of membrane-enclosed cargos in vitro. We found that coupling motors via a biomimetic membrane significantly enhanced the transport of cargos along tau-decorated microtubules. This effect diminished when we added cholesterol to our model membrane. To our knowledge, our study uncovers the first direct link between cargo-membrane composition and kinesin function. The experimental approach employed here is generally applicable as a controlled experimental platform for interrogating the control of motor proteins in a context directly relevant to in vivo scenarios.

*National Institutes of Health R15 GM120682 (J.X.) and R01 NS048501 (S.J.K.)

3:42PM U20.00005: Effect of membrane fluidity on the multi-motor transport of intracellular cargoes* NIRANJAN SARPANGALA (Presenter), AJAY GOPINATHAN, University of California, Merced — In eukaryotic cells, membrane-bound cargoes are transported by teams of molecular motors that diffuse on the lipid membrane. The effect of the cargo fluidity on transport properties is unclear. In particular, it's unknown whether the motor diffusivity helps cargoes navigate the crowded cellular environment especially in the presence of heterogeneity in motor properties. We developed a stochastic dynamical simulation of kinesin-based cargo transport along microtubules that explicitly considers the Langevin dynamics of motors on the cargo surface to answer these questions. Our previous work showed that motor diffusivity reduces inter-motor interference and enhances cargo runlength even in the absence of crowding and heterogeneity. Here we study the effect of motor diffusivity on multi-motor transport when the motor population has a distribution of velocities and also explore how cargoes navigate roadblocks (like Microtubule Associated Proteins) that are typically present on microtubules in vivo.

*We acknowledge support from National Science Foundation NSF grant DMS-1616926, NSF-CREST:Center for Cellular and Bio-molecular Machines at UC Merced(NSF-HRD-1547848) and computing time on the MERCED cluster at UC Merced(NSF-ACI-1429783). NS acknowledges the GSOP Fellowship from UC Merced.
**3:54PM U20.00006: The Dynein Catch Bond: Implications for cooperative transport**

MITHUN MITRA (Presenter), Indian Inst of Tech-Bombay, PALKA PURI, University of California San Diego, ABHISHEK CHAUDHURI, IISER Mohali, SUDIPTO MUHURI, Savitribai Phule Pune University — Intracellular bidirectional transport of cargo on microtubule filaments is achieved by the collective action of oppositely directed dynein and kinesin motors. Recent experiments have demonstrated that unlike kinesin, dynein motor exhibits catch bonding behaviour, in which the unbinding rate of a single dynein decreases with increasing force, for a certain range of force. Motivated by these experiments, we propose a phenomenological model for catch bonding in dynein. We study the implications of the dynein catch bond for unidirectional and bidirectional cargo transport. We show that the functional divergence of the two motor species manifests itself as an internal regulatory mechanism, and can lead to codependent transport behavior in biologically relevant regimes.


*Financial support is acknowledged from the Ramanujan Fellowship, DST, India and IIT Bombay.

**4:06PM U20.00007: Tracking Down the Fast and Superprocessive KIF1A with Gold Scattering Microscopy** [Invited] ALLISON GICKING (Presenter), TAYLOR M ZANIEWSKI, WILLIAM O. HANCOCK, Pennsylvania State University — The kinesin-3 family member KIF1A is a neuronal kinesin that performs long-distance anterograde vesicle transport in axons and dendrites. Single molecule studies observe KIF1A velocities > 1 mm/s and average run lengths > 5 mm, making KIF1A one of the fastest and most processive members of the kinesin superfamily; however, the mechanistic basis of these high speeds and long run lengths is unknown. One prevailing model for superprocessivity holds that the positively-charged “K-loop” in the KIF1A motor domain diffusively tethers the motor to the negatively-charged microtubule, which prevents complete dissociation of the motor and effectively links together short runs. However, this model does not account for how KIF1A reaches such high speeds, or what role the K-loop plays in the ATP-driven stepping mechanism. To address these questions, we used biochemical assays in conjunction with direct observations of stepping of wild type KIF1A and k-loop mutants. We captured the transient states of the stepping cycle by tracking a 30-nm gold nanoparticle-functionalized motor domain via interferometric scattering microscopy (iSCAT), which enables fast acquisition of gold particles < 40 nm and simultaneous visualization of the microtubule tracks. We find that the chemomechanical cycle of KIF1A is distinct from other neuronal transport kinesins.
Investigating the Effect of Cargo-Motor Linkage Stiffness on Cellular Functions of Myosin VI* RACHIT SHRIVASTAVA (Presenter), ASHIM RAI, MURTI SALAPAKA, SIVARAJ SIVARAMAKRISHNAN, University of Minnesota — We examine the effect of cargo-motor linkage stiffness on the mechanobiological properties of the molecular motor Myosin VI. We use the programmability of DNA nanostructures to systematically modulate cargo-motor linkage stiffness and combine it with high precision optical trapping measurements to measure the effect of linkage stiffness on motile properties of Myosin VI. Our single molecule experiments reveal that a stiff cargo-motor linkage leads to shorter step sizes and load-induced anchoring of Myosin VI, while a flexible linkage results in longer steps with frequent detachments from the actin filament under load. These findings suggest a novel regulatory mechanism for tuning the dual cellular roles of anchor and transporter ascribed to Myosin VI [1]. We further make an attempt to investigate the physical basis of our findings using simulations and thermodynamics principles.


*Research was supported by the NIH (1R35GM126940-01) and NSF (CNS 1544721)

Deviations from Arrhenius behavior of Kinesin-1 at low temperatures* FLORENCE DOVAL (Presenter), University of Utah, KASSANDRA M ORI-MCKENNEY, RICHARD J MCKENNEY, University of California Davis, MICHAEL VERSHININ, University of Utah — Kinesin-1 is a mechanochemical enzyme that is essential for executing long-distance transport of cargos in eukaryotic cells via processive motility along the microtubule network. KIF5A is a conventional kinesin in the Kinesin-1 family. The temperature dependence of enzymatic activity for several kinesin-1 motors has been reported to follow a simple Arrhenius trend. The range for this observation has been gradually extended to higher temperatures, as it became possible to circumvent and more recently control kinesin degradation. However, both biophysical and biochemical measurements to date have been limited down to ~5 °C. We investigated the enzymatic activity of KIF5A at even lower temperatures and have observed a break in the Arrhenius trend, corresponding to higher activation energy at lower temperature. We will report our investigations of this phenomenon in different biochemical backgrounds and discuss its cause as it relates to the nature of the rate-limiting step of kinesin's enzymatic cycle.

*This research was funded by NSF ENG-1563280
Cargo diffusion shortens single-kinesin runs at low viscous drag*  

JOHN WILSON (Presenter), JING XU, DAVID QUINT, AJAY GOPINATHAN, University of California, Merced — Molecular motors such as kinesin-1 drive active, long-range transport of cargos along microtubules in cells. Thermal diffusion of the cargo can impose a randomly directed, fluctuating mechanical load on the motor carrying the cargo. Recent experiments highlighted a strong asymmetry in the sensitivity of single-kinesin run length to load direction, raising the intriguing possibility that cargo diffusion may non-trivially influence kinesin. To test this possibility, here we employed Monte Carlo-based simulations to evaluate the transport of cargo by a single kinesin. Our simulations included physiologically relevant viscous drag on the cargo and interrogated a large parameter space of cytoplasmic viscosities, cargo sizes, and motor velocities that captures their respective ranges in living cells. We found that cargo diffusion significantly shortens single-kinesin runs. This diffusion-based shortening is countered by viscous drag, leading to an unexpected, non-monotonic variation in run length as viscous drag increases. Our study highlights the importance of cargo diffusion and load-detachment kinetics on single-motor function.

*NIH R15 GM120682  
NSF HRD-1547848  
ACI-1429783

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U21 FED: Jonathan F. Reichert and Barbara Wolff-Reichert Award for Excellence in Advanced Laboratory Instruction

Award for Excellence in Advanced Laboratory Instruction 302 - Gerald Feldman, George Washington Univ - Tag(s): Education, Focus

2:30PM U21.00001: From Cool Research to Cool Teaching Labs* [Invited]  
ENRIQUE GALVEZ (Presenter), Colgate University — Physicists are often drawn into research when the physical world offers phenomena that show uncanny symmetry or elegant mathematical structure; a puzzling intricacy that is irresistible not to figure out; or even just plain awe at “cool” phenomena that display the beauty of the natural world. These are compelling factors that motivate investigation. Why not have instructional labs with such motivating factors? In this talk I will present some of my efforts to convert the investigation of a motivating physical problems into curricular offerings. It includes optical beams that carry puzzling structures, such as mathematical singularities, symmetrical shapes and puzzling mechanisms. Another initiative that we have worked on involves labs on the quantum mechanics of entangled photons. We have developed a suite of experiments that explore the quantum mechanics of situations involving this source of light. They let students confront counterintuitive but real manifestations of quantum physics. More recently we have been exploring a problem that hopefully will become a new lab: using light to simulate the quantum mechanics of the simple pendulum.

*This work received funding from the National Science Foundation.
3:06PM U21.00002: The “Compleat Physicist” seen through the lens of experiments [Invited]
RANDALL TAGG (Presenter), University of Colorado, Denver — In 1653, thirty-four years before the appearance of Newton’s ‘Principia’, Isaak Walton published “The Compleat Angler”...a book that is still in print! Now in the 21st Century, how might we view the activities of the Compleat Physicist in the context of physics experiments and laboratory skills? If we look at what physicists ultimately do in life, many work in basic research but a far greater number apply physics to a wide range of human needs. How do the knowledge and skills of physics experimentation manifest themselves in these applications? Circling back to fundamental physics, what sort of versatile foundation does a broad experience in the physics laboratory provide so that an emerging professional physicist has a rich conceptual repertoire with which to approach real-world problems? And finally, how can this conceptual repertoire be matched with the nuts-and-bolts technical and computational skills needed to create actual prototypes of new devices and processes?

3:42PM U21.00003: Advanced Labs in the Small Liberal Arts College Environment [Invited]
NICOLE ACKERMAN (Presenter), Physics and Astronomy, Agnes Scott College — The Advanced Lab course is critical for teaching many important skills to physics majors, regardless of their career trajectory. At a small liberal arts college, this course may be run with few pre-requisites, no dedicated funds, limited equipment, no support staff, and as one of many classes a single professor is teaching. While this necessitates certain changes from how the course might be structured at a large research university, the course is nonetheless an invaluable experience for students. I will present my strategies for maintaining an Advanced Lab course at my college, where our department serves a diverse student population and graduates about 6 majors (including Astrophysics) a year. My experiences shows that it is key to focus on learning outcomes and leverage the resources in the broader advanced lab instructor community.
Developing and teaching both Intermediate and Advanced Lab courses contain benefits and challenges in the undergraduate program of study. An Intermediate lab provides requisite skills for students to transition from introductory lab experiences to more rigorous experiments appropriate for advanced/capstone lab courses. The *AAPT Recommendations for the Undergraduate Laboratory Curriculum*\(^1\) and *Phys21: Preparing Physics Students for 21\(^{st}\)-Century Careers*\(^2\) reports provide learning outcomes for physics majors beyond the first year laboratory experience. While no one lab course can prepare majors for post-graduate life, be it teaching, industry, or graduate study, efforts at Appalachian State University (and elsewhere) could serve as a guide to other institutions interested in increasing laboratory experiences in their programs of study. An overview of the Intermediate and Advanced lab courses at Appalachian will be presented, along with how effective these courses are in preparing majors for their future careers, including interviews with former students.


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**Thursday, March 5, 2020 2:30 PM - 5:30 PM**

**Session U22 DBIO: Robophysics II**

303 - Shai Revzen, University of Michigan - Tag(s): Focus
2:30PM U22.00001: Centipede locomotion in varying terrains  ALEXANDRA CARRUTHERS FERRERO (Presenter), KELIMAR DIAZ, YASEMIN OZKAN-AYDIN, JOSEPH MENDELSON, DANIEL I GOLDMAN, Georgia Institute of Technology — Animals which move via waves of body undulation and/or few numbers of limbs have been extensively studied. Limited progress has been made studying animals with many degrees of freedom in their bodies in coordination with numerous limbs (i.e. myriapods like centipedes). To discover principles by which body undulation and limb dynamics in concert with body mechanics leads to high performance in diverse environments, we challenged Scolopocryptops sexspinous (body length of ~4.5 cm, 23 pairs of legs) to traverse both a flat terrain and a Gaussian distributed rough terrain (12 x 12 cm with variable height of blocks). On flat terrain, centipedes maintain a constant out of phase traveling wave along their limbs during locomotion. In contrast, on rough terrain, centipedes will symmetrically use their limbs when their various segments are at different heights. We hypothesize that the centipedes will modulate the use of their limbs in order to overcome heterogeneities. Insight from a robophysical model suggests centipede limbs integrate passive dynamics allowing the locomotorto traverse myriad environments.

2:42PM U22.00002: Modeling Locomotion in a Segmented Soft Robot using Planar Discrete Elastic Rods*  NATHANIEL GOLDBERG, University Of California At Berkeley, XIAONAN HUANG, CARMELO MAJIDI, Carnegie Mellon University, ALYSSA NOVELIA, OLIVER M. O’REILLY, University Of California At Berkeley, DEREK A. PALEY, WILLIAM SCOTT (Presenter), University of Maryland, College Park — Modeling soft robots that move on surfaces is challenging from a variety of perspectives. Recently Bergou, et al. introduced a numerically efficient formulation of Discrete Elastic Rods (DER) based on discrete differential geometry. In this talk, we describe a simplified planar version of Bergou et al.’s theory and show how it can be used to model soft robots that are composed of segments of soft material folded and bonded together. To show the efficacy of DER, the formulation is used to describe and analyze the dynamics of a prototype caterpillar-inspired soft robot. The robot consists of six segments of a shape memory alloy actuated soft material. By controlling the timing and sequencing of the actuators, locomotion can be achieved by exploiting stick-slip friction and the variation in the normal force exerted by the ground plane on each contacting actuator. Successful modeling of the robot also entailed the development and implementation of procedures to prescribe the parameters for components of the soft robot. After describing these procedures, we discuss the comparison of our calibrated model to the experimental behavior of the caterpillar-inspired soft robot. The extension of the DER modeling to other soft robot designs will be discussed.

*ARO Grant No. W911NF1610244
2:54PM U22.00003: Geometric mechanics reveals optimal coordination of limb and body waves during centipede locomotion  BAXI CHONG (Presenter), PERRIN E SCHIEBEL, YASEMIN OZKAN-AYDIN, MALCOLM BROWN, ALEXANDRA C CARRUTHERS, JENNIFER RIESER, SIMON SPONBERG, DANIEL I GOLDMAN, Georgia Inst of Tech — Running epimorphic centipedes display a characteristic body undulation. Elucidating the role of body-leg coordination is difficult because of the many degrees of freedom in the flexible body and numerous limbs. We decomposed the centipede locomotion into body undulation and leg stepping waves, and used the mathematical framework of geometric mechanics to study body-leg coordination. We characterized the body-leg coordination by the phase offset between two waves. We recorded high-speed video and tracked the motion of a centipede (*Scolopendra polymorpha*, 5 trials) running on a treadmill. Our theory predicted that the speed (in body lengths per cycle, BLC) was maximized when the body undulation (1.6 spatial waves) had a phase of 2.50 rad leading that of the leg wave (2 spatial waves). The theoretical prediction of centipede speed was 0.40 BLC, 0.10 BLC and 0.25 BLC with best, worst and no body undulation respectively. Experiments revealed that the centipede moved at 0.41±0.05 BLC with the phase offset 2.51±0.71 rad, in good agreement with our theoretical prediction. Our preliminary results suggest that the geometric approach captures centipede locomotion dynamics without including inertial effects.

3:06PM U22.00004: Geometric Gait Optimization with a five-link wheeled snake*  BRIAN BITTNER (Presenter), SHAI REVZEN, Univ of Michigan - Ann Arbor — Geometric mechanics offers a powerful set of tools for understanding locomotion. In past work we used data-driven oscillator theory to design a sample efficient method for modeling geometric systems such as the Purcell swimmer. We extended this method to include the modeling of highly damped systems inhabiting the perturbed Stokes dynamical regime. Here, we present a case study on a physical five-link wheeled snake robot. Under each link, a pair of wheels were co-aligned to decrease friction in the direction along the link. We seeded the geometric gait optimizer with a zero displacement gait. After 9 iterations of 80 cycles, we produced a motion that achieved 45% body length per cycle translation motion, while optimizing over 84 parameters. Running the system at 0.5 Hz, this took 24 minutes. We noticed the final gait changes combinations of wheels that are contacting and not contacting the ground, a feature not observed in the first gait, suggesting that the optimizer successfully exploited hybrid features of the dynamics.

*NSF CMMI 1825918
3:18PM U22.00005: Directional Compliance in Snake Robot Obstacle-Aided Locomotion
TIANYU WANG (Presenter), JULIAN WHITMAN, MATTHEW TRAVERS, HOWIE CHOSSET, Carnegie Mellon Univ — This work investigates the role of compliance in high-degree-of-freedom snake robots. Prior work used geometric methods to reduce the dimension of the robot’s state space to efficiently control the robot; instead of controlling all of the robot’s degrees-of-freedom, we need only control two for meaningful motions. Recently, we adapted this technique to handle unmodeled terrain irregularities. We defined a compliant controller on the reduced state space, which used torque information measured at the robot’s joints. This improved the robot’s performance, but still the robot arrived at stuck configurations. To address this problem, we introduce a biologically inspired strategy called directional compliance, which selectively allows some portions of the robot to comply to the environment, while others remain stiff to push off for forward progression. Unfortunately, with pure directional compliance method, the robot can still get stuck. Therefore, we develop an estimator to determine the state of the robot and a controller that switches between compliance and directional compliance modes to help the robot get unstuck. We experimentally find that our method enables the snake robot to locomote more consistently than the pure compliant controller in obstacle-rich environments.

3:30PM U22.00006: Body compliance helps oscillating snake robots reduce roll instability to traverse large steps
QIYUAN FU, CHEN LI (Presenter), Johns Hopkins University — Snakes traverse a diversity of complex terrain at ease, an ability that snake robots still aspire to achieve. Despite progress in arboreal (or similar) and granular environments, a major knowledge gap is how to maintain stability on large, smooth obstacles like large rocks or steps that lack “push points” to grip or brace against. Our previous study (Gart et al 2019 JEB) discovered that kingsnakes traverse large steps stably by combining lateral oscillation for propulsion with cantilevering for bridging height change. Here, to understand stability principles, we developed a snake robot as a physical model and tested two hypotheses: (1) roll stability diminishes as step becomes higher; and (2) body compliance helps maintain contact and reduce roll instability. With similar gait as the animal, the rigid body robot was able to traverse steps as high as 40% body length, but traversal probability quickly diminished with increasing step height. A locomotor transition analysis revealed that this was mainly due to an increase in roll instability. Adding body compliance improved contact, reduced roll instability, and increased traversal probability by up to 40% while maintaining speeds. Our study demonstrated that maintaining contact is important for stable locomotion in complex terrain.
Exploring the role of passive mechanics in limbless locomotors via a novel robophysical snake. MARINE C MAISONNEUVE (Presenter), PERRIN E SCHIEBEL, DANIEL I GOLDMAN, Georgia Inst of Tech — Animals like snakes use traveling body bends to move in terrestrial terrain. Previously, we discovered that passive body buckling, facilitated by unilateral muscle activation, allowed negotiation of sparse obstacles without additional control input in the snake (C. occipitalis) [Schiebel et al., 2019]. To explore the implications of this scheme we developed a robophysical model with passive mechanical flexibility. Most snake robots precisely control the position of each joint with a single actuator. In contrast, the actuation in our robot is modeled after biological snakes, in which pairs of muscles, one on each side of the spine, create body bends by contracting unilaterally. The robot has 8 joints and 16 motors, each joint has two motor-driven pulleys on opposite sides of the body. The pulleys increase curvature by shortening a wire attached to the adjacent joint. Opposite an active motor, the pulley is completely unspooled; pairs of motors can resist forces which would lengthen active wires but not those pushing them shorter, allowing the body to passively buckle during certain obstacle collisions. Preliminary tests demonstrate that a travelling sinusoidal wave of joint angles allows locomotion using wheels (which provide directional friction).

Amplitude modulation enhances obstacle negotiation for sidewinders ABDUL KABA (Presenter), JENNIFER RIESER, VERONICA M PAEZ, Georgia Tech, HENRY ASTLEY, Akron University, JOSEPH MENDELSON, Atlanta Zoo, DANIEL I GOLDMAN, Georgia Tech — Sidewinding snakes cyclically lift portions of their body as they move. This gait can be modeled as two coupled head-to-tail traveling waves: a horizontal wave of body undulation and a vertical wave controlling substrate contact. The changing contact pattern introduces a lateral component to movement that creates a large projection of the body onto the direction of motion and makes obstacle negotiation challenging. Biological experiments revealed that the sidewinder moves through a row rigidly-anchored vertical posts by squeezing parts of its body, which we hypothesized was achieved by increasing the amplitude of the horizontal wave. To test this, we created a sidewinding robot from a chain of 14 servo motors with alternating direction of actuation. Horizontally and vertically oriented sets of motors were each driven sinusoidally in time and position along the body. When in contact with a rigid post (detected via capacitive touch sensors), the robot either increased its horizontal amplitude for one full cycle or continued with its nominal waveform. The robot successfully moved beyond the post in 80% of the trials with increased amplitude, compared to never succeeding when maintaining the nominal waveform.
Springs and Wings: Elastic Energy Exchange in Insect Flight

JEFFREY GAU (Presenter), Interdisciplinary Bioengineering Graduate Program & Woodruff School of Mechanical Engineering, Georgia Institute of Technology, JAMES LYNCH, NICK GRAVISH, Mechanical and Aerospace Engineering Department, University of California, San Diego, SIMON SPONBERG, School of Physics & School of Biological Sciences, Georgia Institute of Technology — In many insects, wing movements are generated indirectly via deformations of an exoskeletal shell. Estimates of power expenditure suggest that elastic energy recovery between wingstrokes may reduce flight power requirements. We tested three questions: 1) Can the thoracic shell provide significant energy return? 2) Does a simple damped elastic model describe bulk mechanical behavior? and 3) Are different thorax regions specialized for elastic energy exchange? We measured deformation mechanics by recording the force required to sinusoidally deform the exoskeleton over a wide frequency range. Elastic energy storage in the exoskeleton is sufficient to minimize power requirements and a structural (frequency-independent) damping model, not a viscoelastic one, describes bulk mechanical properties. We next performed complementary experiments on a structurally damped hemispherical shell. In contrast to the hemispherical shell, mechanical coupling between exoskeleton regions improved spring performance and local properties depended on global strain patterns. We found regions specialized for energy recovery with low dissipation, highlighting the specificity of exoskeleton regions for flight energetics. Finally, we consider the implications of resonance mechanics on flapping wing flight.

Springs and Wings: Robophysical investigation of unsteady flapping wing dynamics

JAMES LYNCH (Presenter), Department of Mechanical and Aerospace Engineering, University of California, San Diego, JEFFREY GAU, Interdisciplinary Bioengineering Graduate Program & Woodruff School of Mechanical Engineering, Georgia Institute of Technology, SIMON SPONBERG, School of Physics & School of Biological Sciences, Georgia Institute of Technology, NICK GRAVISH, Department of Mechanical and Aerospace Engineering, University of California, San Diego — Flying insects are thought to achieve energy-efficient flapping flight by storing and releasing elastic energy in their muscles, tendons, and thorax. However, the dynamics of even simple elastic elements coupled to nonlinear, unsteady aerodynamic forces may make controlling flapping motions via muscle force inputs challenging. In previous work, we examined the resonance properties of a dynamically-scaled robophysical system consisting of a rigid wing actuated by a motor in series with a spring. In this talk, we describe experiments to study the control implications of operating spring-wing transmissions on and off resonance. We consider the response of systems to changing control inputs and external perturbations. We conduct robophysical experiments and model simulations measuring the response of elastic flapping wing systems to realistic control inputs and external perturbations that simulate environmental interactions like wind gusts or collisions. We vary mechanical parameters of the system and track results across a non-dimensional parameter space, enabling comparisons across length scales. The results suggest that series-elastic flapping wings designed for maximum efficiency experience commensurate losses to control authority but may be more robust to external perturbations.
4:30PM U22.00011: Springs and wings: robophysical and biological investigations inform the design, energetics, and control space for effective flapping wing flight  JAMES LYNCH, University of California, San Diego, JEFFREY GAU, SIMON SPONBERG, Physics, Georgia Institute of Technology, NICK GRAVISH (Presenter), University of California, San Diego — Flying insects and robots possess a wide range of elastic structures that may enable energy saving in flapping wing flight. However, there is little direct experimental evidence of flight energy reduction through spring-like elements. Furthermore, the implications of a resonant flight system, such as the material and mechanical demands of the thorax, and the control and perturbation responses, are poorly understood. Here we present an overview of how elastic structures in flapping wing flight can improve flight energetics while at the same time altering control capabilities. We present these arguments through a non-dimensional representation of flapping-wing systems, supported by biological and robophysical experiments. This approach enables us to compare the energetic and control implications for flapping wing systems with elastic structures across the relevant spatial scales of flying insects and robots.

4:42PM U22.00012: Biologically inspired vision based aerial robot perching*  HAIJIE ZHANG (Presenter), JIANGUO ZHAO, Colorado State University — Limited flight time has constrained the application of the aerial robot. One possible solution is to learn from biological flyers (i.e. birds, flies) to perch on the desired objects. During perching, the aerial robots can still do surveillance related tasks with the desired height and orientation instead of hovering. Research results have shown that visual information named time-to-contact is used for biological flyers perching guidance. And this information can be extracted from consecutive images. It is widely used for robot motion control for autonomous braking and landing since it can realize zero contact velocity. However, for aerial robot perching, a non-zero contact velocity is usually required to make the perching mechanism functionalize. In this research, we propose an optimized two-stage time-to-contact based guidance law. With a properly designed time-to-contact controller, we finally realize the fastest perching with desired contact velocity. The research presented in this paper can be readily applied to the control of the aerial robot for perching with visual feedback, and can inspire more alternative forms of time-to-contact based planning and control for robotic applications.

*National Science Foundation under Grant IIS-1815476 and IIS-1815519
Robophysics is an indispensable approach to discovering general principles of robots operating in complex environments. Fortunately, physics principles governing non-equilibrium processes where motion emerges by internal actuation in synergy with robotic physical models meeting real world environments can generate quantifiable, testable hypotheses of complex biological systems not otherwise possible. In biology, robophysics has led to simple system-level models (templates) that collapse staggering complexity, while exploring how behavior emerges from more representative models (anchors). A next step is to examine the parallel and serial composition of templates and their dynamic reconfiguration. Robophysics provides the opportunity to determine how: biologically embodied mechanical computation works with neural computation; stability occurs in complex environments using soft-matter physics; performance of multiple tasks results without change in structure; multifunctional hierarchical and heterarchical control networks emerge; properties of fail-safe and fault tolerant performance evolve; and how learning can occur using a reduced set of control modules. In turn, robophysics approach to biological locomotion can inspire the design of novel robots and applied mathematics.

*Supported by ARO Grants W911NF1810327, W911NF-17-S-0002, W911NF1710229, and past award ARL W911NF-08-2-0004.

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U23 DBIO DSOFT DPOLY GSNP: Macromolecular Phase Separation in Biology II 304 - Patrick McCall, Max Planck Institute for the Physics of Complex Systems - Tag(s): Focus
2:30PM U23.00001: Pollen cell walls form from modulated phases [Invited]  ASJA RADJA
(Presenter), Harvard University, ALISON SWEENY, Physics and Ecology & Evolutionary Biology, Yale
University, MAXIM O LAVRENTOVICH, Physics and Astronomy, University of Tennessee — Pollen cell
walls exhibit a huge diversity of morphologies including ordered and disordered arrangements of
spikes, stripes, and holes. Electron microscopy images of pollen wall development across the
spermatophyte tree reveal that a ubiquitous material called primexine, thought to be made of a
mixture of polysaccharides, lipoproteins and glycoproteins, templates these morphologies.
Recently, our imaging studies identified that a phase separation of primexine coupled to the cell
membrane induces a phase transition to modulated phases which pattern the pollen wall. We
formulated a Landau-Ginzburg free energy description of this process in which we treat the
primexine concentration as a scalar field coupled to the cell membrane and calculated the
equilibrium states. We also studied the dynamics of our model and found that together
kinetically-arrested and equilibrium states recapitulate most extant cell morphologies. Further
imaging studies indicate that nanoscale patterns form within the phase-separated domains, thus
we additionally model the lyotropic liquid crystalline-like phases employing self-consistent field
theory simulations. Finally, we completed an evolutionary analysis in which character traits are
defined by parameters of our model that reveals while equilibrium patterns have appeared
multiple times during evolution, selection does not favor these states.

3:06PM U23.00002: Designing morphology of separated phases in multicomponent liquid
mixtures*  MILENA S CHAKRAVERTI-WUERTHWEIN, SHENG MAO, Princeton University, HUNTER
GAUDIO, Villanova University, MIKKO HAATAJA, ANDREJ KOSMRLJ (Presenter), Princeton University —
Morphology of multiphase membraneless organelles formed via intracellular phase separation
plays an important role for their functionality. Yet, very little is known how intermolecular
interactions can be tuned to achieve target microstructures of separated phases. To address this,
we systematically investigate morphologies of coexisting phases obtained via phase separation in
Flory-Huggins liquid mixtures with 4 or more components. We demonstrate that the topology of
separated phases is completely determined by their surface tensions, while their volume
fractions dictate the geometry of microstructure (e.g. droplets, percolated structure). We
developed a novel method based on graphs that enabled us to enumerate all topologically
distinct morphologies of separated phases. Each graph is associated with a set of inequalities for
surface tensions and this enabled us to reverse engineered intermolecular interaction
parameters to realize all topologically distinct morphologies for 4 coexisting phases. The
developed approach is general and can be applied to design morphologies with an arbitrary
number of coexisting phases.

*This work was supported by the NSF through the Princeton Center for Complex Materials DMR-
1420541.
3:18PM U23.00003: Microscopic Model of a Biological Condensate  SWAN HTUN (Presenter), HAN-YI CHOU, KUMAR SARTHAK, ALEKSEI AKSIMENTIEV, University of Illinois at Urbana-Champaign — Liquid-liquid phase separation governs the intracellular organization of biological molecules into membraneless organelles also known as biological condensates. Fused in Sarcoma (FUS), an RNA-binding protein, is the principle component of a biological condensate involved in DNA repair. The intrinsically disordered nature of FUS eludes structural characterization using conventional methods. Here, we report a fully-atomistic structure of a FUS condensate obtained through a combination of coarse-grained and all-atom simulations. Using existing structural and biochemical information, we constructed a coarse-grained model of the FUS protein. An ensemble of such proteins was found to undergo phase separation into a liquid-like condensate in a temperature and composition-dependent manner. The final configurations obtained through the coarse-grained simulations were used to construct an all-atom model of the condensate, including the surrounding solvent. The microscopic structure was refined using atomistic simulations and used to probe the condensate's viscoelastic behavior and identify specific interactions that control its viscosity. The resulting structural model sets the stage for subsequent systematic inquiry into the sequence-structure-function relationship of the condensate.

3:30PM U23.00004: Microstructure in biological phase transition  KAMAL BHANDARI (Presenter), JEREMY SCHMIT, Kansas State Univ — Many cellular structures are formed by the spontaneous condensation of biomolecules into liquid states. Biological condensed states may contain hundreds of different molecules, but only a few of them are necessary to form a condensates. These are called “Scaffolds” while other non-essential molecules, called “Clients”, provide the unique biochemical properties of droplets. We study a synthetic system of phase separating molecules designed by Rosen and co-workers. There are two types of scaffolds (poly-SUMO/poly-SIM) and two types of clients (SUMO/SIM). Mixture of multivalent scaffolds gives condensates which can recruit monovalent clients. Since the condensed phase has a low density, we propose that molecules are highly aligned to form zipper structures. These zippers have defects in the bonding structure that will allow for the subsequent formation of a network. We employ a transfer matrix formalism to compute the grand partition function of the zipper structures and to explain the curious non-monotonic client binding behavior observed in experiments. We find that the 1D nature of the scaffold assembly has important consequence for client recruitment.
Experimental determination of binodal compositions of protein and peptide solutions  
EMMANOUELA FILIPPIDI (Presenter), Max Planck Institute for Molecular Cell Biology and Genetics, FRANK JULICHER, Max Planck Institute for the Physics of Complex Systems, ANTHONY HYMAN, Max Planck Institute for Molecular Cell Biology and Genetics — Biomacromolecules such as proteins are known to undergo liquid-liquid phase separation to a dense phase and a dilute phase under certain conditions of temperature, pH, salt and protein concentrations. As the study of proteins is complex due to their zwitterionic nature, hydrogen bonding, inclusion of hydrophobic side chains, pi-cation interactions and presence of metal binding and folded domains, we will study in parallel both a protein, FUS, and simplified peptides of known sequences.

We will present quantitative measurements of both branches of the binodal curves of the phase diagrams obtained via quantitative phase imaging microscopy for the protein FUS and simpler peptide sequences. As the tyrosine-arginine interactions are believed to play a significant role in inter-molecular association, we shall examine the variation of the branches as FUS tyrosines are alterned to phenylalanines and 3,4-dihydroxy-L-phenylalanines imparting changes in hydrogen bonding and pi-cation interaction strength. In the case of peptides, we will examine how multiplicity of pi-cation interactions at constant density of tyrosines and arginines affects the associations and thus the phase diagram.

Spinodal Dynamics in Non-Equilibrium Compression of Two Self-Avoiding Polymer Chains  
LILI ZENG (Presenter), RABEA SEYBOLDT, ZEZHOU LIU, XAVIER CAPALDI, AHMED KHORSHID, PAUL FRANCOIS, NIKOLAS PROVATAS, WALTER W REISNER, Physics, McGill University — Two polymers under 1D confinement can phase separate as a consequence of chain interconnectivity and entropy maximization, and this demixing may be one mechanism leading to bulk chromosomal segregation in bacteria. While there has been considerable theoretical effort to explore this problem, few experiments have attempted to directly investigate segregation/mixing behaviour of two self-avoiding chains in model geometries. In this experiment, two differentially labeled nanochannel confined DNA molecules are compressed against a barrier using hydrodynamic flow. The differential labeling enables us to quantify the concentration profile of each chain along the channel independently. The two DNA molecules will mix given that the applied forcing is strong enough, but instead of simple mixing, we observe a complex phenomena whereby the chains interpenetrate but form alternating, fluctuating bands in which one chain has higher concentration relative to the other. We interpret this phenomenon as a spinodal decomposition of the two polymers and rationalize it using a model based on a 1D convective Cahn-Hilliard equation, a classic model describing spinodal decomposition in driven binary systems. Simulations for such a model yield striking similarity to the experimental observations.
4:06PM U23.00007: Relating chemical and physical properties controlling oligonucleotide polyelectrolyte complex phase separation* ALEXANDER E. MARRAS (Presenter), JEFFREY VIEREGG, Pritzker School of Molecular Engineering, University of Chicago, MICHAEL LUECKHEIDE, Polymers and Complex Fluids Group, National Institute of Standards and Technology, MATTHEW TIRRELL, Pritzker School of Molecular Engineering, University of Chicago — Nucleic acids are some of the most highly-charged molecules known, and interact strongly with charged molecules in the cell. Condensation of long double-stranded DNA is a classic problem of biophysics, but the polyelectrolyte behavior of short and/or single-stranded nucleic acids is far less studied despite its importance for both biological and engineered systems. Homopolycations and neutral-cationic block copolymers condense nucleic acids driving macro- or nanoscale phase separation, respectively. Here, we present an investigation of the impact of physical and chemical properties of each polyelectrolyte on complex and micelle assembly. We find molecular details including hybridization, charge density, and chemical structure strongly influence complexation behavior and stability. These observations narrow the design space for optimizing therapeutic micelles and provide new insights into the physics of polyelectrolyte self-assembly.

*National Institute of Standards and Technology, Center for Hierarchical Materials Design (CHiMaD) award 70NANB14H012. Advanced Photon Source, Department of Energy Office of Science User Facility Contract No. DE-AC02-06CH11357.

4:18PM U23.00008: Entropic localization of plasmids in nanofluidic compartments ZEZHOU LIU (Presenter), XAVIER CAPALDI, LILI ZENG, RODRIGO REYES LAMOTHE, WALTER W REISNER, McGill Univ — Bacteria must stably partition their plasmids to their daughter cells upon division. While purely random partitioning can theoretically ensure stable transmission of plasmids to daughter cells, it is not clear that plasmid partitioning is random. Studies tracking plasmids in vivo show that multi-plasmid clusters present at the cell poles, but the roles played by the cell geometry and chromosome-plasmid interactions are still unclear. Here, we present a nanofluidic device with compartments simulating the confinement induced by a cell membrane. The compartments can be opened and closed by pneumatically actuating the thin membrane lid. The cavities are elliptical with a width varying from around 200 nm to 2 um. A differentially stained T4 DNA molecule and one plasmid molecule are introduced inside the compartment and monitored in real time from their fluorescence signals. We find that the plasmid prefers the peripheral of the cavity as has been observed in in vivo measurements in E. Coli, forming a ring shape distribution. In addition, as the cavity aspect ratio increases, the plasmid shows a preference for the cavity poles. Our results suggest that the free energy landscape formed by chain-chain interaction and the confinement geometry helps promote plasmid localization.
4:30PM U23.00009: Computational Insights into Phase Separation of Multivalent Polymers*
EMIKO ZUMBRO (Presenter), ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology MIT — Liquid-liquid phase separation has emerged as an important biological process. In membraneless organelles, phase separation in solution is often controlled by weak multivalent interactions between polymers using a variety of bond types. How to control phase compositions and specificity in biological contexts is still not well understood. In this work we compare phase separation of multivalent polymers through non-specific Van der Waals interactions to phase separation through specific reactive-binding interactions. We use a coarse-grain, reactive-binding, Brownian dynamics simulation to investigate the transition dynamics, resulting compositions, and specificity of polymer phase separation. Our results provide insights on how multivalently binding polymers control phase separation in synthetic and biological systems.

*The authors were supported by the Department of Defense through the National Defense Science & Engineering Graduate Fellowship Program.

4:42PM U23.00010: Stable drops: the Gibbs-Thomson condition and drop dynamics
ANDREW RUTENBERG (Presenter), SAMUEL CAMERON, Dalhousie Univ — In standard phase separated binary liquids, larger droplets grow while small droplets shrink due to the Gibbs-Thomson condition at droplet boundaries. As a result, the liquid reduces its overall interfacial area between the two phases. The dynamics of these systems can be described by Lifshitz-Slyozov-Wagner theory, and ultimately only one large (bulk) drop will survive in equilibrium. However, some binary liquid-like systems have a preferred, stable droplet size, and their final steady states have multiple microphase-separated droplets. This phenomena not well described by the standard Gibbs-Thomson condition or the standard Lifshitz-Slyozov-Wagner dynamics. This talk addresses three questions for systems with small stable droplets: how does the Gibbs-Thomson condition generalize, how does Lifshitz-Slyozov-Wagner dynamics generalize, and how much of this should apply when stable drops arise from non-equilibrium processes?

4:54PM U23.00011: Simulation Informed Thermodynamic Model for Polyampholyte Self-Coacervation with Heterogeneous Charge Distribution*
JASON MADINYA (Presenter), CHARLES SING, University of Illinois at Urbana-Champaign — Living cells rely on phase separation to achieve many of its critical functions such as organelle formation and signaling and regulatory complexation. Intrinsically disordered proteins (IDPs) often play a role in intracellular liquid-liquid phase separation. IDPs are frequently ampholytic and they can be driven to phase separation through electrostatic interactions. The solution behavior and properties are encoded in the peptide sequence of the proteins, particularly the distribution of the charged residues. Previous work from the authors introduced a Transfer Matrix model for charge-driven polyampholyte phase separation, which resolved the impact of charge sequence on phase separation. This model was limited to looking at homogenous sequences made up of repeating blocks of charge patterns. In this work we present a coarse-grained simulation model to resolve phase separation in polyampholytes with any arbitrary charge sequence. Of particular interest is characterizing the inhomogeneity of the sequence and quantifying the impact on solution behavior.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE-1746047.
5:06 PM U23.00012: Nematic transition and liquid-liquid phase separation in semiflexible polymers – nanoparticle mixtures* SUPRIYA ROY (Presenter), YENG-LONG CHEN, Institute of Physics, Academia Sinica, Taiwan — Adding nanoparticles (NPs) to a polymer matrix may significantly modify its glass transition temperature, dielectric constant, isotropic-nematic phase transition behavior, etc. In the present study, we used GPU-accelerated Langevin dynamics simulation to explore how polymer-NP interaction affect the isotropic-nematic (I-N) transition and microstructural modifications of a matrix of semi-flexible polymers with persistence length \( P = 20 \) and contour length \( L = 25 \). The mixture is confined under slit. Polymers are modeled as semi-flexible chains with beads of diameter \( \sigma_m = 1 \), and NPs are spheres with \( \sigma_p = 2.5 \).

Two limits of NP-polymer interactions - hard NPs that repel, and ideal NPs do not interact with other NPs are explored. Adding low volume fraction \( \Phi_p \) of hard NPs disperse the NPs in the polymer matrix, which disrupt the polymer nematic ordering and upshifts the I-N transition. In contrast, ideal NP additives induce depletion attraction between polymers, which enhances polymer alignment and downshifts the I-N transition. For moderate or high \( \Phi_p \), hard NPs would crystalize and discrete nematic polymer micro-domains are formed. On the other hand, ideal NPs forms a liquid micro-domain that decreases in size as the monomer volume fraction \( \Phi_m \) increases.

*Ministry of Science and Technology, ROC

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U24 GSNP GDS: Statistical Physics Meets Machine Learning

2:30PM U24.00001: A nonlinear and statistical physics approach to machine learning electronic hardware* DANIEL LATHROP (Presenter), LIAM SHAUGHNESSY, BRIAN HUNT, HEIDI KOMKOV, ALESSANDRO RESTELLI, University of Maryland, College Park — As the uses of machine learning continue to grow in science and industry, there is a need to reduce power and increase processing speed. As has been done before, hardware co-processors can take over some tasks. We present research developing novel machine learning hardware that relies on a large network of nonlinear electronic nodes to instantiate a reservoir computer. We characterize the behaviors of these networks and find a critical point as we adjust their sensitivity. Moreover, we find that their machine learning performance, in terms of accuracy, depends on the sensitivity of the network.

*This material is based in part upon work supported by the National Science Foundation (EAR 1417148 and 1909055), as well as the NSF Graduate Research Fellowship Program under Grant No. 1322106. Our research was partially supported through a DoD contract under the Laboratory of Telecommunication Sciences Partnership with the University of Maryland. We would also like to thank the Maryland Innovation Initiate for their support.
2:42PM U24.00002: Reservoir Computer Optimization for Parity Checking*  
WENDSON BARBOSA (Presenter), Department of Physics, The Ohio State University, GUILHEM RIBEILL, MINH-HAI NGUYEN, THOMAS A OHKI, GRAHAM E ROWLANDS, Raytheon BBN Technologies, DANIEL J GAUTHIER, Department of Physics, The Ohio State University — In recent years, the Reservoir Computing (RC) approach, a recurrent-neural-network-based scheme for Machine Learning (ML), has been used extensively for solving different tasks such as time-series prediction, nonlinear system control and classification tasks. A benchmark problem regarding the latter is the parity check of a random sequence of bits. Although at a first look it seems to be a simple problem, it is known to be a very difficult task to be solved using ML techniques. We shall discuss the reservoir computer hyper-parameters optimization and exploration of different architectures for inputting data to the reservoir to improve the parity classification performance as well as paths toward high-speed hardware implementation.

*This work was funded by Raytheon BBN Technologies Corp.

2:54PM U24.00003: Using Machine Learning to Infer Composition of Complex Chemical Mixtures  
UNAB JAVED (Presenter), Rutgers University, New Brunswick, KANNAN P RAMAIYAN, CORTNEY R KRELLER, ERIC L BROSHA, RANGACHARY MUKUNDAN, Los Alamos National Laboratory, ALEXANDRE MOROZOV, Rutgers University, New Brunswick — Predicting the concentration of each constituent in a complex gas or liquid mixture is an important challenge in many fields of science and technology, ranging from real-time monitoring of automotive exhaust to detecting potentially toxic substances in the air. We employ an array of solid-state sensors to test gas mixtures in a controlled laboratory environment, recording voltage responses from the sensor array. The sensors in the array typically react to more than one gas in the mixture and their voltage responses are non-linear, making the task of decoding compositions of gas mixtures highly non-trivial. We have developed a Bayesian algorithm which, given a set of readings from the array, identifies and quantifies all gases present in the system. The Bayesian nature of our approach allows us to estimate the uncertainty of the predictions in a rigorous manner and to carry out model selection. Our machine learning framework can be used to model any non-linear system with correlations between inputs and has applications in a wide variety of settings.

3:06PM U24.00004: Deep generative spin-glass models with normalizing flows  
MASOUD MOHSENI (Presenter), Google Inc., GAVIN HARTNETT, Rand Cooperation — We develop and train a novel universal class of deep spin-glass models that can learn to represent multiscale phenomena in physics and computer science including critical phenomena, discrete optimization, and probabilistic inference in graphical models. To this end, we first provide a continuous formulation of spin-glasses and convert the discrete Boltzmann distributions into physically equivalent continuous distributions. We then use recent techniques in deep learning known as “Normalizing Flows” to generate new low-energy states of such complex systems below spin-glass phase transitions. In particular, we demonstrate that the real non-volume preserving flows can be successfully trained to generate complex spin-glass distributions. We explore two alternative methods for training the normalizing flow based on minimizing reverse and forward Kullback-Leibler divergence. Moreover, we show how the problem of mode collapse for such deep generative models can be overcome at or below a critical point.
3:18 PM U24.00005: A Continuous Formulation of Discrete Spin-Glass Systems

GAVIN HARTNETT (Presenter), Engineering and Applied Sciences, RAND Corporation, MASOUD MOHSENI, Google Inc — We introduce a new, continuous formulation of discrete spin-glasses in which the discrete Boltzmann distribution is replaced by a continuous probability density over the real numbers. This formulation applies for any discrete spin-glass with Ising spins coupled through 2-body interaction terms. A major benefit of working with such a continuous formulation is that the energy landscape may be studied directly using tools from differential geometry and topology. In particular, we show that for a given set of couplings there is a critical temperature above which the energy landscape is convex. Below this temperature the landscape becomes non-convex due to the appearance of multiple critical points. In general, this convex/non-convex transition is distinct from phase transitions to the spin-glass or ferromagnetic phases. In this talk, we introduce our general formalism and theoretically establish the similarities and differences with the mean-field models and the Thouless-Anderson-Palmer equation. We then provide details for a few specific cases including the Sherrington-Kirkpatrick model and random restricted Boltzmann machines.

3:30 PM U24.00006: Machine-learning the DFT of a classical statistical-mechanical system*

PETR YATSYSHIN (Presenter), ANDREW DUNCAN, SERAFIM KALLIADASIS, Imperial College London — We apply machine-learning (ML) to the construction of mean-field theories of classical statistical-mechanical systems. In the density functional formulation of classical statistical physics, the Helmholtz free energy generates a hierarchy of many-body direct correlation functions, and the one-body density is its first member. In equilibrium, the latter minimises the free energy functional of the system. Thus, knowing the free energy functional allows one to solve classical statistical mechanics. In this talk, we address the inverse problem of finding the free energy functional, given the particle data corresponding to the system in equilibrium. Introducing an adversarial ML methodology, we reformulate the learning problem as a two-player game, with the best fitting parameters obtained as the solution of a minimax problem. As proof of concept, we consider the Percus’ model of a 1D fluid, consisting of hard rods on a line, for which the exact functional is known. We emphasize the physics-informed aspect of ML, where the physical constraints, including the “physical intuition”, are combined with ML methods to obtain meaningful results.

*We acknowledge support from European Research Council via Advanced Grant No. 247031 and EPSRC via Grant Nos. EP/L020564, EP/L027186/1 and EP/K503733
Dynamical loss functions for Machine Learning

MIGUEL RUIZ GARCIA
(Presenter), GE ZHANG, Univ of Pennsylvania,
SAMUEL SCHOENHOLZ, Google Brain,
ANDREA JO-WEI LIU, Univ of Pennsylvania — Current deep learning approaches usually rely on very diverse architectures, stemming from trial and error design. This has triggered great interest in improving the theoretical understanding of machine learning. The structure of the loss function landscape and the way it affects the performance of the algorithm have received recent interest. Loss functions penalize incorrect identifications and the focus has largely been on optimizing algorithms (e.g. stochastic gradient descent) within the landscapes defined by the loss functions. We take a different approach by exploring new loss functions. In particular, we explore the effect of dynamical loss functions, where weights on each training example change during training. Preliminary results show that this new approach can outperform the results obtained with static loss functions for particular cases.

A mechanical model for supervised learning

MENACHEM STERN
(Presenter), CHUKWUNONSO ARINZE, LERON PEREZ, STEPHANIE PALMER, ARVIND MURUGAN,
University of Chicago — A broad goal of engineering is to make functional machines with specific, programmed input-output responses. When inputs are specified in advance and few in number, this goal is sought through rational design, changing the system elements to obtain desired responses. In the supervised learning framework of computer science, system parameters (synapses) are modified in response to observed examples of the correct input-output mapping (classification). In this work, we apply the supervised learning framework to self-folding sheets, using a physically motivated learning rule. The trained sheet classifies labeled forces by folding into discrete folded states. These sheets succeed in classifying real-world data like Iris flowers, and also generalize, similar to other learning algorithms. As learning provides a straightforward framework to programming complex input-output relationships, we hope that implementing these ideas in engineering could usher in new classes of machines, that have so far eluded design.

*We acknowledge NSF-MRSEC 1420709 for funding and the University of Chicago Research Computing Center for computing resources.
Quantifying statistical mechanical learning in a many-body system with machine learning

WEISHUN ZHONG (Presenter), JACOB M GOLD, Massachusetts Institute of Technology, SARAH MARZEN, Massachusetts Institute of Technology and the Claremont Colleges, JEREMY L ENGLAND, Massachusetts Institute of Technology and GlaxoSmithKline, NICOLE YUNGER HALPERN, Harvard University and Massachusetts Institute of Technology — Far-from-equilibrium many-body systems, from soap bubbles to suspensions to polymers, learn the drives that push them. This learning has been characterized with thermodynamic properties, such as work dissipation and strain. We move beyond these macroscopic properties first defined for equilibrium contexts: We quantify statistical mechanical learning with machine learning. Our strategy relies on a parallel that we identify between representation learning and statistical mechanics in the presence of a drive. We apply this parallel to measure novelty detection, classification, and memory capacity. Numerical simulations of a spin glass illustrate our technique. This toolkit exposes self-organization that eludes detection by thermodynamic measures. Our toolkit more reliably and precisely identifies and quantifies learning by matter.


Information-bottleneck renormalization group for self-supervised representation learning*

VUDTIWAT NGAMPRUETIKORN (Presenter), Initiative for the Theoretical Sciences, The Graduate Center, City University of New York, WILLIAM S BIALEK, Department of Physics, Princeton University, DAVID J. SCHWAB, Initiative for the Theoretical Sciences, The Graduate Center, City University of New York — While highly successful, most deep learning applications rely on supervised learning which requires a large set of manually labelled data. But labelled data are not always available, and effective learning from unlabelled datasets - self-supervised learning - has the potential to greatly expand the scope of deep learning applications. Here we propose a self-supervised learning method that combines the concepts of the information bottleneck and the renormalization group. More specifically we use the information bottleneck to regularize a coarse-graining procedure by encouraging a representation to discard locally specific information (bottleneck) while retaining the long-wavelength features (implicitly assumed to be relevant for downstream tasks). We use variational and noise contrastive approaches to scale up our method for large systems, and we demonstrate our implementation on datasets from machine learning.

*We acknowledge support from the National Institutes of Health under Grant R01 EB026943-01.
4:30PM U24.00011: On matching symmetries and information between training time series and machine dynamics.*  JAN ENGELBRECHT (Presenter), OWEN TONG YANG, RENATO MIROLLO, Boston College — Recurrent networks and some deep feed-forward networks in machine learning effectively construct a very high-dimensional dynamical system that classifies objects through its asymptotic dynamics. Many training inputs of the same class are used to construct a machine with similar trajectories flowing to the same fixed point attractor. The attractor itself carries no information/entropy. A specific example in reservoir computing is to train a single-layer machine using a trajectory of a known chaotic dynamical system and construct a linear projection from machine variables back to the chaotic system that reproduces the training chaotic trajectory (validation) and "predicts" a bit into the future (testing). Our perspective is to go beyond validation/testing of a particular trajectory and analyze the symmetry and information in the general asymptotic dynamics of the trained machine. For well trained machines we can get the information and symmetries of the machine dynamics to approximately match that of the training dynamical system. The machine’s dynamics then has its own strange attractor and the machine can generate new time series of the same class, i.e. that are different but equivalent to the training data.

*This work was funded by NSF grants DMS 1413020 and DMS 1910303

4:42PM U24.00012: Deep Learning on the 2-Dimensional Ising Model to Extract the Crossover Region*  NICHOLAS WALKER (Presenter), KA-MING TAM, MARK JARRELL, Louisiana State University, Baton Rouge — The 2-dimensional square Ising model is investigated with a variational autoencoder in the non-vanishing field case for the purpose of extracting the crossover region between the ferromagnetic and paramagnetic phases. The encoded latent variable space is found to provide suitable metrics for tracking the order and disorder in the Ising configurations that extends to the extraction of a crossover region in a way that is consistent with expectations. The extracted results achieve an exceptional prediction for the critical point as well as favorable comparison to the configurational energetics of the model and agreement with previously published results on the configurational magnetizations of the model. The performance of this method provides encouragement for the use of machine learning to extract meaningful structural information from complex physical systems with no known order parameters.

*This work is funded by the NSF EPSCoR CIMM project under award OIA-1541079. Additional support (MJ) was provided by NSF Materials Theory grant DMR-1728457. An award of computer time was provided by the INCITE program. This research also used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.
Training and classification using Restricted Boltzmann Machine (RBM) on the D-Wave 2000Q

Training and classification of a restricted Boltzmann machine (RBM) has been performed using D-Wave system. RBM is an energy-based model, which assigns low energy values to the configurations of interest. The D-Wave 2000Q is an adiabatic quantum computer which has been used to obtain samples for the gradient learning. Two datasets namely ‘bars and stripes (BAS)’ and ‘solar farm (PV)’ have been used. For BAS dataset, objective is to classify a given pattern as bars or stripes, while for PV dataset the goal is to predict “efficiency degradation” based on some model parameters. Results are compared with RBM trained using standard contrastive divergence. Classification and data reconstruction are also presented. Estimated classification accuracies indicate comparable performance of the both methods. D-Wave training seems to result in smaller weights, thus reduces overfitting problems.

Statistical Physics Analysis of Training of Restricted Boltzmann Machines

A restricted Boltzmann machine is a generative probabilistic graphic network. A probability of finding the network in a certain configuration is given by the Boltzmann distribution. It has wide applications from the image generation to the neural network representation of quantum many-body states. We analyze the training process of the restricted Boltzmann machine in the context of statistical physics. For the Bar-and-Stripe pattern as a small size restricted Boltzmann machine, thermodynamic quantities such as free energy, internal energy, work, and entropy are calculated as a function of training epochs. We also investigate the Jarzynski equality that connects the work done during training and the difference in free energies before and after training. It is found that, even after long training, the probabilities of possible outcomes are not even. Some possible sources that cause imperfect training are discussed.
5:18PM U24.00015: Mode-Assisted Unsupervised Learning of Restricted Boltzmann Machines*  HAIK MANUKIAN (Presenter), YAN RU PEI, SEAN BEARDEN, MASSIMILIANO DI VENTRA, University of California, San Diego — Restricted Boltzmann Machines (RBMs) are a powerful class of unsupervised models well known in machine learning. However, unlike their more popular supervised counterparts, their training requires computing a gradient that is notoriously difficult even to approximate. In this work we show that properly combining standard gradient approximations with an off-gradient direction, constructed from samples of the RBM ground state (mode), improves their training dramatically over the standard methods. This approach, which we call "mode training", promotes faster training and stability, in addition to lowering the converged relative entropy (KL divergence). We report promising preliminary results with small models on synthetic data sets and discuss extensions to more realistic scenarios, where a physics-based approach, memcomputing [1], is used to sample the mode efficiently. The mode training we suggest is versatile, as it can be applied with any given gradient method, and is easily extended to more general energy-based neural network structures such as deep, convolutional and unrestricted Boltzmann machines. [1] M. Di Ventra and F.L. Traversa, J. Appl. Phys. 123, 180901 (2018). Work supported in part by CMRR and DARPA.

*Work supported in part by CMRR and DARPA.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U25 GSNP: Pattern Formation, Chaos, Nonlinear Dynamics I 402
- Michel Pleimling

2:30PM U25.00001: Creating novel patterns with localized control in non-linear reaction-diffusion systems*  JASON CZAK (Presenter), MICHEL PLEIMLING, Virginia Tech — The Gray-Scott model has been subject of numerous investigations. Due to the nonlinear nature of the coupled reaction-diffusion equations, the system exhibits interesting behavior for certain parameter sets. In many previous studies of this system investigators have used a limited range of parameter values dictated by neglecting diffusion effects. Through systematic parameter adjustment we are able to observe and characterize novel system patterns that were previously overlooked. Localized control routines are applied to the system creating long range periodic order from a chaotic parameter space region. We present a comprehensive view of the effects of control routines applied to this system.

*This research is supported by the Army Research Office under the Grant Number W911NF-17-1-0156.
2:42PM U25.00002: Motion and Chain formation of Conductive Spheres on a Horizontal Insulator Surface Immersed in Dielectric Liquids XUEWEI ZHANG (Presenter), Texas A&M University — This work presents an analysis of the dynamics of conductive, possibly charged spheres resting on the horizontal surface of an ideal insulator, both immersed in dielectric liquids. The system is subject to a uniform background field with components normal and parallel to the surface. The inclusion of dielectric liquids complicates the problem by adding the induced charge electrophoresis effect. In this work, for individual sphere, the dependence of the total force that drives its motion on the properties of the dielectric liquid is shown. For a pair of spheres, the conditions under which they can be pulled together to form a chain are derived. Experimental results are presented to qualitatively verify the theoretical analysis. This is a complex electromechanical system that has been studied for branched pattern formation. However, no detailed analysis of the sphere motion and chain formation has been conducted. This work will bridge this gap, as well as inform some sensor designs for engineering applications.

2:54PM U25.00003: Classical many-body chaos across Kosterlitz-Thouless and Ising transitions in two dimensions* SIBARAM RUIDAS (Presenter), SUMILAN BANERJEE, Indian Institute of Science - Dept of Physics — Chaos, the sensitivity to the initial condition, lies at the foundation of statistical mechanics. Chaotic systems are characterized by a growth rate, the Lyapunov exponent $\lambda_L$, and a velocity for ballistic spread, the butterfly velocity $v_B$, of local perturbation. Here we study the temperature dependence of the chaotic behavior across thermal phase transitions in a well-known classical spin system, the XXZ model on a square lattice. We tune the finite-temperature phase transition from the Kosterlitz-Thouless (KT) to Ising universality class by changing the anisotropy and find the temperature ($T$) dependence of $\lambda_L$, $v_B$ and the diffusion coefficient $D$ across these transitions. For both the KT and Ising cases, we find a crossover in $\lambda_L(T)$ across the transitions. On the contrary, a naive extraction of $v_B(T)$ assuming a ballistic spread of perturbation leads to a non-monotonic temperature dependence of $v_B$ across the transitions. In the KT case, we show that even though the systems show subdiffusive behaviors at intermediate times below transitions due to spin-waves, the spread of perturbation is actually superballistic due to algebraic decay of spatial correlations in KT phase.

*SB is supported by SERB, DST, India and The Infosys Foundation, India through Infosys Young Investigator Award
**3:06PM U25.00004: New parameters for an alternative characterization of the nematic transition for rods deposition on 2D lattices**  

EUGENIO VOGEL (Presenter), GONZALO SARAVIA, Univ de La Frontera, ANTONIO RAMIREZ-PASTOR, MARCELO PASINETTI, Univ. Nacional de San Luis — The problem of excluded volume deposition of rigid rods of length k unit cells over square lattices is revisited. Two new features are introduced: a) two new short-distance complementary order parameters (called \( \Pi \) and \( \Sigma \)) are defined, calculated and discussed to deal with the phases present as coverage increases; b) the interpretation is now done beginning at the high-coverage locally ordered phase (present regardless of the k value) which allows to interpret the low coverage nematic phase as an ergodicity breakdown present for \( k \geq 7 \). In addition data analysis offers also some novelty as both mutability (dynamical information theory method) and Shannon entropy (static distribution analysis) will be invoked to further characterize the phases. Moreover, mutability and Shannon entropy are compared between themselves reporting their advantages and disadvantages for dealing with this problem. The advantages of parameter \( \Pi \) over any other parameter is also established.

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**3:18PM U25.00005: Deterministic Phase Transitions and Self-Organization in Logistic Cellular Automata**  

MUHAMED IBRAHIMI, OGUZ GULSEREN (Presenter), Physics, Bilkent University, SEYMUR JAHANGIROV, Institute of Material Science and Nanotechnology, Bilkent University - UNAM — We present a simple extension in which a single parameter tunes the dynamics of Cellular Automata by consequently expanding their discrete state space into a Cantor Set. Such an implementation serves as a potent platform for further investigation of several emergent phenomena, including deterministic phase transitions, pattern formation, autocatalysis and self-organization. We first apply this approach to Conway's Game of Life and observe sudden changes in asymptotic dynamics of the system accompanied by emergence of complex propagators. Incorporation of the new state space with system features is used to explain the transitions and formulate the tuning parameter range where the propagators adaptively survive by investigating their autocatalytic local interactions. Similar behavior is present when the same recipe is applied to Rule 90, an outer totalistic elementary one-dimensional CA. The latter case shows that deterministic transitions between classes of CA can be achieved by tuning a single parameter continuously.

*S. J. acknowledges support from The Turkish Academy of Sciences, Outstanding Young Scientists Award Program (TUBA-GEBIP). Part of the computational resources is provided by the National Center for High Performance Computing of Turkey (UHeM) under Grant No. 5003622015.*
3:30PM U25.00006: New type of oscillation death in coupled counter-rotating identical nonlinear oscillators*  JUNG-WAN RYU (Presenter), Institute for Basic Science, WOO-SIK SON, DONG-UK HWANG, National Institute for Mathematical Sciences — We study oscillatory and oscillation suppressed phases in coupled counter-rotating nonlinear oscillators. We demonstrate the existence of limit cycle, amplitude death, and oscillation death, and also clarify the Hopf, pitchfork, and infinite period bifurcations between them. Especially, the oscillation death is a new type of oscillation suppressions of which the inhomogeneous steady states are neutrally stable. We discuss the robust neutral stability of the oscillation death in non-conservative systems via the anti-PT-symmetric phase transitions at exceptional points in terms of non-Hermitian systems.

*This research was supported by Project Code (IBS-R024- D1).

3:42PM U25.00007: Effects of the fluid flows on the stability of enzymatic chemical oscillations  OLEG SHKLYAEV (Presenter), VICTOR V YASHIN, ANNA BALAZS, Univ of Pittsburgh — Chemical oscillations are ubiquitous in nature and have a variety of promising applications. Chemical oscillations are usually analyzed within the context of a reaction-diffusion model framework. In real systems, the fluid flux modifies the chemical diffusion transport. To examine this effect, we consider a flow of chemical solution confined between two parallel walls forming a channel. The solution contains two reactants, A and B, which undergo transformations catalyzed by enzymes immobilized on the channel walls. Mutual transformations of the reactants provide a positive-negative feedback loop, which enables oscillations. We study the effect of the flow velocity on the stability boundary separating oscillating regimes from stationary distributions of chemicals in the channel. We show that the flow promotes the chemical transport in the system and, thereby, increases the amplitude and frequency of the oscillations. We support the predictions of the stability theory by the relevant numerical simulations. The findings can improve functionalities of micro-scale chemical reactors.

3:54PM U25.00008: Spatiotemporal dynamics of flame front instability described by an extended Kuramoto-Sivashinsky equation  YUJI NOMI, HIROSHI GOTODA (Presenter), Tokyo University of Science, CHRISTOPHE ALMARCHA, Aix-Marseille University — We numerically study the spatiotemporal dynamics in an extended Kuramoto-Sivashinsky equation describing a freely propagating flame in a Hele-Shaw cell. The spatiotemporal dynamics of flame front undergoes a significant transition from low-dimensional to high-dimensional deterministic chaos with increasing the Rayleigh number. This is clearly identified by the permutation spectrum and the multiscale complexity-entropy causality plane. The Shannon entropy incorporating the probability of the degree in the interface network is useful for capturing the significant changes in randomness in the spatiotemporal dynamics.
4:06PM U25.00009: Dendritic crystal growth of ammonium nitrate and ammonium chloride
ANDREW DOUGHERTY (Presenter), Lafayette College — Dendritic crystal growth is an important example of nonequilibrium pattern formation that involves both nonlinear and noise-driven effects. The resulting large-scale structures are sensitively dependent on relatively small effects, such as surface tension, and on small anisotropies in those quantities. In this work, we present results for ammonium chloride dendrites, and compare them with new results for ammonium nitrate dendrites grown from supersaturated aqueous solution. This new system has been studied previously by van Driel et al.[1] and shown to exhibit several different morphologies, including both steady state dendritic growth and a state with persistent tip-splitting behavior. Specifically, we present new measurements of the tip radius $\rho$, growth speed $v$, and sidebranch spacing $\lambda$, along with initial estimates of the product $Dd_0$, where $D$ is the chemical diffusion constant and $d_0$ is the capillary length, as well as the stability constant $\sigma^*=-\frac{2d_0D}{v\rho^2}$. We discuss important similarities and differences between the two materials.

https://doi.org/10.1016/0022-0248(93)90324-P

4:18PM U25.00010: Emergent Bose-Einstein statistics in classical non-equilibrium systems with scale selection
VILI HEINONEN (Presenter), Department of Mathematics, Massachusetts Institute of Technology, PEDRO J SAENZ, Department of Mathematics, University of North Carolina at Chapel Hill, JONASZ J SLOMKA, Department of Civil, Environmental, and Geomatic Engineering, ETH Zurich, KEATON BURNS, JÖRN DUNKEL, Department of Mathematics, Massachusetts Institute of Technology — Non-equilibrium systems are ubiquitous in nature, from driven quantum matter and biological life forms to atmospheric and interstellar gases. Identifying and characterizing universal aspects of their dynamics continues to pose major conceptual challenges due to the absence of conserved quantities like energy. Here, we investigate the statistics of a broad class of non-equilibrium systems in which an intrinsic length-scale selection mechanism effectively constrains the dynamics of the microscopic degrees of freedom. As specific examples, we compare experimental observations of chaotic Faraday surface waves on water with simulations of a generalized Navier-Stokes equation for active fluids and quantum particle simulations in a random potential. Strikingly, we find that in all three cases the Fourier amplitudes of the energy density follow Bose-Einstein statistics. Furthermore, we show that the time evolution of these systems can be approximated by a sequence of randomly sampled monochromatic Gaussian fields, suggesting a unified view of non-equilibrium and equilibrium systems with length scale selection.
4:30PM U25.00011: Coarse-Graining and Renormalization without Locality*  JOSEPH NATALE (Presenter), K. MICHAEL MARTINI, ILYA M NEMENMAN, Emory University — The renormalization group (RG) describes how to systematically coarse-grain physical models and calculate their scaling behavior near a critical point. This approach has been immensely successful for systems where interactions are local, with a high degree of symmetry that effectively reduces the number of parameters that can contribute to the behavior in the ultraviolet limit. Here, we introduce a scheme inspired by the recent work on coarse-graining neural dynamics [1], which is capable of detecting infra-red behavior directly from experimental data without explicit reference to locality or symmetry. Specifically, our approach selects maximally correlated pairs of system elements, taking the correlations themselves as a proxy for local interaction, and compresses their activity using the Information Bottleneck method, while preserving the information that the compressed variables contain about the next-closest scale. Repeatedly applying such transformations recovers the renormalization group flow for the coupling strengths and variation of nearest-neighbor correlations with length scale for data taken from a 2D Ising system on the square lattice, showing the viability of this data-driven approach.


*NIH, NSF, JSMF support

4:42PM U25.00012: Statistics of coherent subsets in the Kuramoto model for uniform distributions  TAYLOR A GURREITHUN (Presenter), DAVID MERTENS, Physics, Eckerd College — Experiments in synchronization and simulations of the Kuramoto model reveal that small subsets of oscillators tend to synchronize into coherent clumps at moderate coupling strengths below the critical coupling strength. Such clumps are not present in the thermodynamic limit, and so are intrinsically a finite size effect. We develop a theory that predicts the critical coupling for the formation of individual coherent subsets. Applying these new conditions to a finite population sampled from a uniform distribution, we obtain known results, such as a discontinuous transition to synchrony. We also obtain a lower estimate for the critical coupling of this transition that is consistent with simulation and previous results for uniformly sampled oscillators. This opens a new route for computing finite size effects, which we will present.
4:54PM U25.00013: Emergence of Complexity in Self-Limited Assemblies of Nanoparticles*
NICHOLAS KOTOV (Presenter), Univ of Michigan - Ann Arbor — Inorganic nanoparticles (NPs) have the ability to self-organize into variety of structures with sophisticated and dynamic geometries. Many of them are self-limited due to repulsive electrostatic interactions, which manifests in monodispersity of mesoscale superstructures formed from hundreds of polydispersed NPs. Remarkably, the organization of self-assembled NP systems can rival in complexity to those found in biology which reflects the biomimetic behavior of nanoscale inorganic matter. In this talk, I will address the mechanism and variety of self-limited assemblies of NPs and mechanisms of emergent complexity especially for chiral NPs. Self-limited assemblies of the latter will illustrate the importance of subtle anisotropic effects stemming from collective behavior of NPs and non-additivity of their interactions. While these phenomena present obvious fundamental significance for instance as a path to spontaneous compartmentalization and protocells, the practicality of self-organization of nanoparticles will be discussed in relation to charge polarization-based optoelectronics, quantum optics, and chiral catalysis.

*National Sciences Foundation, Vannevar Bush Fellowship

5:06PM U25.00014: Topological Control of Synchronization Patterns: Trading Symmetry for Stability*
JOSEPH HART, Naval Research Laboratory, YUANZHAO ZHANG (Presenter), Northwestern University, RAJARSHI ROY, University of Maryland, College Park, ADILSON E MOTTER, Northwestern University — Symmetries are ubiquitous in network systems and have profound impacts on the observable dynamics. At the most fundamental level, many synchronization patterns are induced by underlying network symmetry, and a high degree of symmetry is believed to enhance the stability of identical synchronization. Yet, here we show that the synchronizability of almost any symmetry cluster in a network of identical nodes can be enhanced precisely by breaking its structural symmetry. This counterintuitive effect holds for generic node dynamics and arbitrary network structure and is, moreover, robust against noise and imperfections typical of real systems, which we demonstrate by implementing a state-of-the-art optoelectronic experiment. These results lead to new possibilities for the topological control of synchronization patterns, which we substantiate by presenting an algorithm that optimizes the structure of individual clusters under various constraints

*This work was supported by ONR Grant No. N000141612481 (J.D.H. and R.R.) and ARO Grant No. W911NF-15-1-0272 (Y.Z. and A.E.M.).
Phase Synchronization in 2D Kuramoto Model

MRINAL SARKAR (Presenter), NEELIMA M GUPTE, Indian Inst of Tech-Madras — We study a system of identical Kuramoto oscillators in the presence of Gaussian white noise. The oscillators are arranged on a two-dimensional periodic lattice and interact with their nearest neighbors only [1-2]. In the thermodynamic limit, the stationary states at very low temperatures (limit $T \to 0$) are well described by the presence of topological defects (vortices and anti-vortices) in the phase-field of the oscillators. We apply duality transformation on a Hamiltonian [3] to explore the underlying vortex structure.

The system exhibits a phase transition from stochastic synchronization to de-synchronization as temperature varies. We investigate the nature of the phase transition and calculate the critical temperature numerically. The relaxation dynamics is also studied. In the low-temperature regime, the system relaxes to equilibrium algebraically whereas, at high temperature, the decay is exponential. Moreover, the system, at very low temperature belongs to the EW universality class yielding the dynamic exponent $z=2$ [4].


Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U26 DBIO: Physics in Synthetic Biology 403 - Gabor Balazsi, State Univ of NY - Stony Brook - Tag(s): Focus

Spatiotemporal dynamics in synthetic microbial consortia [Invited]
MATTHEW BENNETT (Presenter), Rice Univ — Synthetic microbial consortia have an advantage over isogenic synthetic microbes because they can apportion biochemical and regulatory tasks among the strains. However, it is difficult to coordinate gene expression in spatially extended consortia because the range of signaling molecules is limited by diffusion. In this talk I will discuss how spatiotemporal coordination of gene expression can be achieved even when the spatial extent of the consortium is much greater than the diffusion distance of the signaling molecules. To do this, we examined the dynamics of a two-strain synthetic microbial consortium that generates coherent oscillations in small colonies. In large colonies, we found that temporally coordinated oscillations across the population depend on the presence of an intrinsic positive feedback loop that amplifies and propagates intercellular signals. These results demonstrate that synthetic multi-cellular systems can be engineered to exhibit coordinated gene expression using only transient, short-range coupling among constituent cells.
3:06PM U26.00002: Synthetic genetic circuits using plant protoplasts* KATHERINE KIWIMAGI, MIT, MAURICIO ANTUNES, University of North Texas, WENLONG XU, MIT, TESSEMA KASSAW, Colorado State University, CHRISTOPHER ZALEWSKI, Front Range Biosciences, JUNE MEDFORD, ASHOK PRASAD (Presenter), Colorado State University — The complexity of plant biology has slowed the development of synthetic gene circuits in plants. However plant synthetic biology can form the basis for sustainable green technologies. The rational design of synthetic networks requires quantitative characterization of components for predictive modeling. This poses special difficulties for plants, since stably transforming plants is time consuming. We developed an experimental system for rapid quantitative measurements of synthetically designed repressors using plant protoplasts but found that protoplast assays show significant experimental batch effects that lead to incorrect quantitative results. With the help of a mathematical model coupled with stochastic simulations, we were successful in explaining and normalizing the batch effects to make quantitative comparisons between different inducible repressors, and approximately predict quantitative properties of synthetic circuits in stably transformed plants. We tested hundreds of repressible promoters, and carried out a statistical analysis of the quantitative data to uncover design principles for building synthetic inducible repressors in plants (*Nature Methods, v13, pp94–100, (2016)). Our mathematical model may be broadly applicable to a wider class of cells and assays.

*DOE-ARPAE

3:18PM U26.00003: Construction and Characterization of a Tunable Plasmid Copy Number System MILES ROUCHES (Presenter), GUILLAUME LAMBERT, Cornell University — Plasmids have evolved elegant mechanisms to ensure stable replication which balance the probability of plasmid loss with their metabolic burden on host cells. The pUC19 plasmid controls its copy number through a replication priming RNA (RNAII) and an inhibitory antisense RNA (RNAI). Through randomized mutagenesis of the promoters controlling these RNAs, we have created a library of over 1000 plasmids with copy numbers spanning a range greater than 2 orders of magnitude, allowing plasmid copy number to be used as a tunable parameter in several systems. We demonstrate the broad applicability of this system by using it to tune the behavior of simple genetic circuit elements and determine the fitness cost of green fluorescent protein and several CRISPR proteins. We additionally infer transcription rates for over 1000 different promoters of both RNAI and RNAII by combining our copy number measurements with the results of stochastic molecular simulations.
3:30PM U26.00004: Engineering Transcriptional Interference for Genetic Logic Gates
NOLAN O'CONNOR (Presenter), ANTONI ESCALAS BORDOY, ANUSHREE CHATTERJEE, Chemical and Biological Engineering, University of Colorado, Boulder — Transcriptional Interference (TI) is widespread in the genomes in all kingdoms of life and serves to regulate important cellular decisions. TI can occur through the collisions of RNA Polymerases (RNAPs) in tandem or in convergent orientation, and through the collision of RNAPs with protein roadblocks. Mathematical modeling and experiments have characterized several naturally occurring TI systems, but the design rules for constructing TI-based genetic devices are not yet well-defined. Here, we show that rationally controlling RNAP traffic on DNA through TI can lead to diverse gene expression profiles and facilitate the construction of TI-based logic gates. We demonstrate that tuning the dissociation constant of a protein roadblock enables optimized AND and OR logic gates, and that gate behavior can be predicted and validated through mathematical modeling. We then show that protein roadblocks coupled with RNAP collisions can produce NAND and NOR gates, and that the magnitude of gene repression from RNAP collisions can be tuned through inhibition of Rho-dependent transcription termination. These results expand the potential for TI as a novel tool for synthetic biology and offer insights into an important but relatively unexplored gene regulatory mechanism.

3:42PM U26.00005: Multicellular Drug Resistance from Synthetic Mitosis Control in Budding Yeast*
OLEKSANDRA ROMANYSYN (Presenter), GABOR BALAZSI, Biomedical Engineering, Stony Brook University — Experimental modeling plays a vital role in understanding microbial drug resistance. Multicellular, biofilm- or clump-forming microbes encounter smaller local antibiotic concentrations and can survive harsher drug treatment than unicellular populations. However, how drug resistance depends on specific characteristics of multicellular populations, such as gene expression, and clump size distribution, is poorly understood. By deleting the $AMN1$ (antagonist of mitotic exit network) gene from multicellular $S.~cerevisiae$, we obtained a drug-sensitive unicellular yeast strain. Assuming that AMN1 levels control clumping, we implemented a negative feedback-based gene circuit to control a synthetic copy of $AMN1$, mitotic progression, and consequently, clump sizes and drug resistance. This technology can be applied to extract parameters for computational models of multicellular drug resistance in yeast and has potential for testing the effect of novel drugs on a custom range of discrete multicellular yeast phenotypes.

*Work supported by NIH MIRA grant #R35GM122561 and Laufer Center for Physical & Quantitative Biology
University of Colorado, Boulder — The rapid rise of multidrug-resistant (MDR) superbugs and the declining antibiotic pipeline are serious challenges to global health. Rational design of therapeutics can accelerate development of effective therapies against MDR bacteria. In this talk, I will describe multi-pronged systems, synthetic biology, and nano-biotechnology based approaches being devised in our lab to rationally engineer therapeutics that can overcome antimicrobial resistance. We have developed Synthetic biology-based approach dubbed “Controlled Hindrance of Adaptation of OrganismS” or “CHAOS” to slow the evolution of antibiotic resistance by interfering with the processes involved in adaptive resistance. To translate our findings into the clinical setting, we have engineered antisense therapeutics that can block translation or increase transcription of any desired gene in a species-specific manner for targeted inhibition. Using this approach we have built a Facile Accelerated Specific Therapeutic (FAST) platform for the accelerated therapeutics in less than a week. Finally, I will also present a nano-biotechnology based approach involving development of a unique semiconductor material based quantum dot-antibiotic (QD ABx) which, when activated by stimuli, release reactive oxygen species to eliminate a broad range of MDR bacterial clinical isolates. The CHAOS, FAST and QD Abx platforms and inter-disciplinary approaches presented in this talk offer novel methods for rationally engineering new therapeutics to combat disease challenges.

*National Science Foundation
Defense Advanced Research Projects Agency
National Aeronautics and Space Administration
Translational Research Institute for Space Health

Indian Inst of Tech-Bombay, Centre for Theoretical Studies, Indian Institute of Science, MITHUN KUMAR MITRA, Indian Inst of Tech-Bombay, BUDDHAPRIYA CHAKRABARTI, Dept of physics and astronomy, The University of Sheffield — Recent advances in reprogramming a differentiated cell back to a pluripotent cell fate has rekindled interest in a quantitative understanding of the epigenetic landscape describing cellular differentiation. Reprogramming is a multistep process, involving multiple feedback loops. While the importance of feedback loops is well appreciated, most models assume instantaneous feedback, while biological feedback often involves a time delay between the signal and the response. In the present work, we propose a theoretical model based on a two-gene regulatory motif to investigate the role of time delay in the regulation of gene expression level. In particular, we focus on the interplay between time delayed feedback loops and time-dependent external chemical drive and their effect on dynamics. We observed that the concentration of the two transcription factors can undergo sustained oscillations and we speculate that this oscillatory state may provide an explanation of certain puzzling experiments on the reprogramming process. We also observe transdifferentiation-like behavior, where one differentiated state transitions to another without passing through an intermediate stem cell state.
**4:42PM U26.00008: Synthetic gene circuits enable quantitative comparison of proteosynthesis rates in mammalian cells**

YIMING WAN (Presenter), JOSEPH COHEN, ALEX SMASHNOV, GABOR BALAZSI, Stony Brook University — Transcription and translation may vary significantly among mammalian cell types. Such differences may be important for comprehensively understanding cellular homeostasis and responses in various conditions. Here, we establish a synthetic biological framework to enable such comparisons. To minimize the random effects of genomic integration, we performed site-specific recombination (SSR) by applying FLPe recombinase-mediated cassette exchange (RMCE) to integrate single genes or gene circuits into the same “genomic safe harbor” locus AAVS1 in multiple mammalian cell lines. Upon establishing stable cell lines, we charted and compared the constitutive and inducer-dependent proteosynthesis levels using the eGFP reporter, and characterized the fold change, coefficient of variation (CV), expression kinetics based on the proliferation rate of each cell type. Overall, our study provided a systematic approach to quantify the variation of proteosynthesis due to the activity of the transcription and translation machinery in various mammalian cell types, allowing a better understanding of cell state diversity, which may be useful in mammalian biosystem modeling.

*We acknowledge the NIH MIRA grant #R35GM122561, Laufer Center for Physical & Quantitative Biology*

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**4:54PM U26.00009: Synthetic Gene Circuits Reveal how KRAS(G12V) Affects Cell Proliferation & Migration Patterns**

TYLER GUINN (Presenter), DAMIANO CORACI, KARTHIK LEDALLA, GABOR BALAZSI, State Univ of NY - Stony Brook — Small chemicals and light can serve as stimuli for controlling synthetic gene circuits to probe biological networks relevant to systems biology and biological physics. We previously developed Light-Inducible Tuner (LITer) gene circuits that have a wide dynamic range of gene expression, low gene expression noise, and an ability to respond with gene expression changes to both chemicals and light. As a foundation for exploring gene regulatory networks, we have created LITer variants controlling half-a-dozen functional genes. Here we present results from perturbing the levels of proto-oncogene KRAS(G12V). We explore a range of cellular features including cellular distance travelled, velocity, acceleration, proliferation, and invasion versus KRAS(G12V) levels. This study reveals that functional genes can have nontrivial effects at intermediate levels of activity, illustrating the utility of analog synthetic gene circuits to complement existing knock-out and overexpression genetic approaches. Furthermore, these tools may reveal quantitatively biological thresholds for functional genes to produce cellular phenotypes.

*We acknowledge the NIH MIRA grant #R35GM122561, Laufer Center for Physical & Quantitative Biology, & the National Defense Science and Engineering Fellowship for funding.*
5:06PM U26.00010: Improved CRISPRi gene circuit function via antisense RNA sequestration
DAVID SPECHT (Presenter), GUILLAUME LAMBERT, Cornell University — By using the binding of the catalytically-dead CRISPR protein dCas12a, we can create programmable gene circuit elements in E. coli. These ‘CRISPRgates’ are simple NOT gate elements which can target genes or other CRISPRgate elements and in principle can be combined to create complex genetic circuits, a fundamental goal of synthetic biology. While natural transcription factors have built-in advantages for transcriptional regulation (e.g. cooperativity), they are not programmable or individually orthogonal and a limited number of them exist. Repression with CRISPR is advantageous because we can in principle repress many different targets simultaneously without crosstalk. However, such gene circuit elements behave poorly when placed in series due to signal loss that occurs due to leaky repression (e.g. NOT NOT NOT != NOT) and retroactivity effects due to a shared pool of Cas proteins. By utilizing antisense RNAs to sequester guide RNA transcripts, we demonstrate a mechanism to suppress leaky CRISPRi repression and restore logical gene circuit function when elements are used in series. Further, we explore utilizing this system to enhance cooperativity in CRISPR-based gene circuits to create better dynamic gene circuit elements such as oscillators and toggle switches.

5:18PM U26.00011: Uncovering thermodynamic determinants of CRISPR-Cas gene circuit design. GUILLAUME LAMBERT (Presenter), DAVID SPECHT, YASU XU, Cornell University — The versatility of CRISPR-Cas endonucleases as a tool for synthetic biology has lead to diverse applications in gene editing, programmable transcriptional control, and nucleic acid detection. Most CRISPR-Cas systems, however, suffer from off-target effects and unpredictable non-specific binding that negatively impact their reliability and broader applicability. To better evaluate the impact of mismatches on DNA target recognition and binding, we develop a massively parallel CRISPR interference assay to measure the binding energy between tens of thousands of CRISPR RNA and target DNA sequences. By developing a general thermodynamic model of CRISPR-Cas binding dynamics, our results unravel a comprehensive map of the energetic landscape of CRISPR-Cas as it searches for its DNA target. Our generalizable approach provides a mechanistic understanding of target recognition and DNA binding by CRISPR-Cas variants, which should contribute to the advancement of recent synthetic biology efforts to repurpose dCas as gene circuit elements that behave orthogonally and operate independently without crosstalk.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U27 DBIO GSNP: Population Dynamics in Antibiotics and Time-Varying Environments 404 - Arvind Murugan, University of Chicago - Tag(s): Focus
2:30PM U27.00001: Immune repertoire dynamics out of steady state* [Invited] MARIO UDO GAIMANN, Ludwig-Maximilians-Universität München, JONATHAN J DESPONDS, University of California San Diego, ANDREAS MAYER (Presenter), Princeton University — Over the last ten years high-throughput sequencing has enabled increasingly quantitative measurements of the diversity of lymphocyte receptor repertoires. A striking finding of these sequencing efforts has been that the clone sizes of cells sharing the same receptor are heavy-tail distributed. Here, we show how such long tails can emerge out of steady state from a simple neutral model for immune repertoire formation. In our theory homeostatic proliferation leads to a founder effect, which produces transient but long-lived power-law scaling of clone sizes. In a human cohort study we find evidence for the prediction that early founded clones are overrepresented among the largest clones. We show how the slow multidecadal decay of this overrepresentation suggests a dynamical model of immune aging in which peripheral selection only slowly reshapes the initially established repertoire. Overall, our work suggests a mechanism through which dynamical processes early in life can have a strong and long-lasting influence on the adaptive immune system with potential implications for pathogen defense and autoimmunity.

*DAAD RISE Worldwide fellowship (MUG), Lewis–Sigler fellowship (AM)

3:06PM U27.00002: The role of drug kinetics on the evolution of resistance. ANJALIKA NANDE (Presenter), MARTIN NOWAK, ALISON LYNN HILL, Harvard University — Emergence of drug resistance due to treatment non-adherence is a problem especially in chronic prolonged viral infections like the Human Immunodeficiency virus (HIV) and Hepatitis B (HBV) and C (HCV) viruses. Long acting drugs are being developed as one way to address this problem. Though this promises to be useful in the context of treatment adherence, we do not yet know how this would affect resistance.

With this in mind, we analyze the effect of dosing intervals on the establishment of drug resistance due to mutants existing prior to treatment (pre-existing) and those that are produced during treatment (rescue) in the presence of time-dependent drug profiles.

We find that there exists an initial time-frame after treatment initiation that has the most influence on the establishment probability of the drug resistant strain. Depending upon the nature of the drug kinetics during this time as well as infection parameters, increasing the dosing interval might be better or worse for the establishment of resistance. Our results suggest that drug kinetics affect selection and competition in the system in a complicated manner and should be factored in while designing new treatment strategies.
3:18PM U27.00003: The Dynamics of Human Society Evolution: An Energetics Approach*
RAM POUDEL (Presenter), Institute of Engineering, Tribhuvan University, JON MCGOWAN, University of Massachusetts — Human society is an open system that evolves by coupling with various known and unknown (energy) fluxes. How do these dynamics precisely unfold? Energetics may provide further insights. We expand on Navier-Stokes’ approach to study non-equilibrium dynamics in a field that evolves with time. Based on the ‘social field theory’, an induction of the classical field theories, we define social force, social energy and Hamiltonian of an individual in a society. The equations for the evolution of an individual and society are sketched based on the time-dependent Hamiltonian that includes power dynamics. In this paper, we will demonstrate that Lotka-Volterra type equations can be derived from the Hamiltonian equation in the social field.

*We did not seek any funding for this research. RP acknowledges a sabbatical granted by the Institute of Engineering, Tribhuvan University.

3:30PM U27.00004: Understanding the Dynamics of Antibiotic Resistance in Microbial Communities using Tensor Methods  MAX DE JONG (Presenter), KEVIN WOOD, Univ of Michigan - Ann Arbor — Spatial heterogeneity plays an important role in the evolution of drug resistance, but relatively little is known about resistance in complex spatial profiles of selection pressure. We have developed a toy model of stochastic microbial dynamics to investigate how different spatial profiles of selection pressure impact the time to fixation of a resistant allele using mean first passage time calculations. While our previous results established that spatial profiles can dramatically speed or slow the emergence of resistance, they provide little information about the trajectory taken by the system to reach fixation. We now expand our analysis to consider the third-order tensor composed of the time to fixation from all possible intermediate states of the system. We develop several methods to deconstruct this tensor into quantities that allow us to gain insight into the evolutionary dynamics of the system as it reaches fixation. We use a 3-D convolution to relate fixation times of neighboring states and a modified CP decomposition to reduce the fixation time tensor into single-microhabitat fixation profiles lacking spatial structure. We demonstrate that these tools allow us to intuitively understand the emergence of fixation in spatially-structured systems.
Evolving generalists in optimal cycling environments

SHENSHEN WANG (Presenter), Department of Physics and Astronomy, University of California, Los Angeles — To persist and thrive in ever changing conditions, living organisms must adapt to new challenges while maintaining performance to prior related tasks. How this ability to generalize evolves remains a puzzle. To evolve a proper defense against rapidly adapting pathogens, vertebrates’ adaptive immune system searches for broadly neutralizing antibodies through B cell affinity maturation. However, these generalist antibodies are hard to evolve and often outcompeted by specialists fitter in any particular environment. Using a generative approach, we find that switching between environments neither too similar nor too different can efficiently evolve fit generalists, via dynamically enlarging their attractor basins in sequence space. We further demonstrate that changing environments before populations reach a steady state can mobilize specialists but leave generalists undisturbed, thereby allowing specialists to evolve into generalists and not specialize again. Our framework predicts optimal correlations between vaccine antigens to be cycled at intermediate timescales for reliably evolving generalists. These design principles exploit nonequilibrium fitness ‘seascapes’ to drive populations into genotypes unevolvable in static environments.

Search strategies that find generalists in time varying environments

JONATHAN KUTASOV (Presenter), Physics, Princeton University, KABIR HUSAIN, University of Chicago, SHENSHEN WANG, UCLA, ARVIND MURUGAN, University of Chicago — Many evolutionary and ecological processes can be seen as a search process for fitter genotypes or spatial regions with more resources. Time varying environments are often thought to naturally bias such search processes towards generalists, i.e., regions with relatively smaller changes in fitness or resources over time. But it is not clear what underlying characteristics of a search process lead to this effect.

Here we consider several search processes in biology such as foraging in real space, growth of microtubules towards chromosomes, and evolution towards fitter genotypes in sequence space. We find that a class of biased random walks that we call ‘directed’ are naturally driven towards generalists by time varying environments at intermediate timescales; this class includes classic E. coli chemotaxis with run times modulated by food availability and constant tumble times. However, closely related ‘undirected’ biased walks are not driven towards generalists, such as chemotaxis with constant run times but modulated tumble times. The distinction between directed and undirected walks corresponds to the Ito and Stratonovich ambiguity in stochastic calculus. Our work provides examples where the microscopic details of biological search have macroscopic consequences.
4:30PM U27.00007: Time-Dependent Effective Sampling Bias in Populations with Broad Offspring Numbers  TAKASHI OKADA (Presenter), RIKEN, University of California, Berkeley, OSKAR HALLATSCHEK, University of California, Berkeley — It has been increasingly recognized that natural populations exhibit broad family size distributions, either because offspring numbers are strongly variable or because range expansion processes generate jackpot events. Despite recent progress in the neutral dynamics induced by broad offspring numbers, our knowledge of their interactions with selection remains limited, except for certain special cases. Here, we establish a number of new scaling relations about the fixation probability, the extinction time and the site frequency spectrum that arise when offspring numbers are distributed according to a power law with divergent variance. Finally, we validate the new findings within semi-pushed traveling waves, which are microscopic models that give rise to the power law of offspring numbers.

4:42PM U27.00008: Using environmental noise to hedge one's evolutionary bets  BINGKAN XUE (Presenter), University of Florida, PABLO SARTORI, STANISLAS LEIBLER, The Rockefeller University — Bet-hedging is an adaptation strategy commonly used by organisms living in unpredictable environments: Each individual randomly expresses one of many possible phenotypes so that a subset of the population may survive. The random choice of phenotypes is usually attributed to stochastic biochemical processes internal to the organism, such as multi-stable dynamics of the gene regulatory network. Alternatively, the organism may rely on randomness that is present (and probably abundant) in the external environment. We illustrate the latter possibility using a model of "environment-to-phenotype mapping". That is, we let the organism's phenotype depend on an environmental signal, and numerically evolve such dependence to maximize the population growth rate. We show that, even when the signal is extremely noisy and uninformative of the true environment, the organism can still benefit from the signal by using it as a source of randomness for bet-hedging.

4:54PM U27.00009: Clocks, Anticipation, and Growth in Bacteria  MICHELE MONTI, Centre for Genomic Regulation (CRG), The Barcelona Institute for Science and Technology, PIETER REIN TEN WOLDE, AMOLF, DAVID LUBENSKY (Presenter), Univ of Michigan - Ann Arbor — Circadian rhythms are widespread across all kingdoms of life, and they are frequently assumed to provide an adaptive benefit by allowing organisms to anticipate diel cycles in their environment. Yet it has proven extremely difficult to determine precisely how such anticipation confers a fitness advantage. Here, we use mathematical modeling to address this question for nitrogen-fixing cyanobacteria.\(^1\) By extending recent work on growth laws in \textit{E. coli},\(^2\) we show that it is difficult to change the composition of the proteome when the growth rate is small, and thus that the average growth rate can be increased by using a clock to anticipate the onset of darkness by switching to a dark-adapted proteome late in the day, when growth rates are still large.

5:06PM U27.00010: Minimal model reveals key features of vaccination protocols that optimally elicit broadly neutralizing antibodies*  RAMAN GANTI (Presenter), MEHRAN KARDAR, ARUP K CHAKRABORTY, Massachusetts Institute of Technology MIT — During affinity maturation, B cell populations evolve in response to time-varying environments within germinal centers (GC). Recent simulations and experiments have shown that controlling the temporal application and degree of “frustration” (i.e. conflicting selection forces) within the GC crucially determines the successful production of broadly neutralizing antibodies (bnAbs). A one-dimensional fitness landscape enables us to quantify frustration as the change in entropy of the imposed fitness distribution as the selection forces change with time. Using a simple birth-death model, we then find that an optimal temporal profile of frustration maximizes bnAb production and determines the mechanisms underlying this result. The vaccination protocol requires a relatively low optimal level of frustration during GC priming to maintain the correct level of B cell diversity so that the surviving B cells have a high chance of evolving into bnAbs upon subsequently increasing the frustration by choosing appropriately designed vaccine immunogens. Our results also illustrate the importance of clonal interference in bnAb evolution due to time-varying environments.

*The work was supported by the NIH, NIAID P01 AI091580-06.

5:18PM U27.00011: Predicting antibiotic resistance evolution  FERNANDA PINHEIRO (Presenter), Institute for Biological Physics, University of Cologne, OMAR WARSII, DAN ANDERSSON, Department of Medical Biochemistry and Microbiology, Uppsala University, MICHAEL LÄSSIG, Institute for Biological Physics, University of Cologne — Bacteria can rapidly evolve resistance to antibiotics. Resistance mutations confer a fitness advantage in the presence of the drug, which is frequently coupled to a fitness cost in drug-free environments. But how do these effects set the strength of resistance elicited by a given drug dosage and the resulting cell growth? Here we develop a fitness model that predicts dosage-dependent growth rates of common resistance mutations. Selection experiments in E. coli populations at moderate drug levels reveal multiple resistance mutations of different strength, most of which affect membrane genes. By reducing both drug and nutrient uptake, these mutations cause antagonistic effects on cell metabolism and growth. Our fitness model maps this tradeoff and defines a Pareto surface of resistance evolution. We show that optimal mutants elicited at a given drug level occur at a specific point on this surface, leading to predictable dosage-dependent growth. Our analysis delineates the dosage regime where broad, membrane-mediated resistance evolution is prevalent compared to mere physiological response and drug-specific target mutations. These results show that drug resistance evolution, by coupling major metabolic pathways, is strongly intertwined with the systems biology of the cell.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U28 FIAP: Innovations from Industry 405-407 - Steven Lambert, American Physical Society - Tag(s): Industry, Invited, Undergrad Friendly
2:30PM U28.00001: From Innovation to the Marketplace: The Role of a Physicist [Invited]  
SCOTT DAVIS (Presenter), Vescent Photonics — Science has and continues to change the world. The process through which this happens is varied, complex, and fascinating. I believe that a physics education equips one to navigate and expedite this process, from innovation, to technology maturation, and ultimately to production and commercialization. Furthermore, I feel that this is especially true in an entrepreneurial, small business setting. As a physics Ph.D., then co-founder and now CEO of Vescent Photonics, I have been a part of each step. I will share examples from my personal professional journey that illustrate this progression. Examples will include non-mechanical laser beamsteerers, first invented in my garage and then sold to a large public company for automotive markets, laser systems for quantum systems such as clocks and computers, and a variety of electronic and electro-optic technologies. I will highlight examples where my physics training proved invaluable in both obvious but also less obvious ways. Participating in the journey from the spark of an idea to a manufacturing line could not be more meaningful. I continue to rely on the physics training of both myself and my employees to play and profit in this process.

ERIC OSTBY (Presenter), Google — TBD

3:42PM U28.00003: Pake Prize: A Physics Career in Industry [Invited]  
JAMES BRAY (Presenter), General Electric Research — I speak about my own experiences as a physicist in industry (GE) for 45 years. I begin with a general look at US R&D expenditures in industry compared to academia and government in the recent past and how these expenditures divide among basic research, applied research, and development. I then focus down to physics: recent US expenditures and how physicists have chosen and think about their career in the recent past. Then I focus further to my own career in industry and my learnings. Finally, I use superconductivity and MRI (magnetic resonance imaging) to illustrate examples of my learnings as a physicist in industry.

4:18PM U28.00004: Academia to Entrepreneurship- Who is this for? [Invited]  
THIRUMALAI VENKATESAN (Presenter), Natl Univ of Singapore —
There has been a sea change over the last few decades in the way academic institutions view entrepreneurial activities of the faculty and the role of the Institution in fostering an ecosystem conducive to such activities. This has become a global phenomenon and many of the leading Institutions in Europe and Asia are also beginning to replicate the model of the Boston or Silicon Valley academic Institutions. This clearly presents a wonderful opportunity for those who want to strike out on their own as opposed to waiting for someone else to offer them a job. This is the transition from a job seeker to a job creator. Are entrepreneurs born or made? In my observation, a much higher proportion of graduate students/ post docs ought to become entrepreneurs as the qualities required for a successful entrepreneur are possessed by a fairly large proportion of students than they realize. In my talk I will discuss a variety of models that are available to the academic entrepreneur, their pluses and minuses and also some of the critical knowledge one needs to understand about the world of entrepreneurship in general. I will use examples from several of my students and colleagues’ startups and my own experience in running a company for over three decades amidst an academic career.
4:54PM U28.00005: Rocket Science is Just Cool [Invited] JANICA CHENEY (Presenter), Lockheed Martin Space Systems — Why yes, this is rocket science...

How do astronauts, satellites, and payloads get into space? What does NASA's mission to Mars look like? What does a rocket scientist really do? This presentation will provide a behind the scenes look at the engineering and physics of past and current space missions using solid rocket motors from the perspective of a rocket scientist. Learn about the ins and outs of her career path and discover what it really takes to be a rocket scientist. The foundation developed in an academic career in physics or engineering will provide a strong background required for launching your career as a rocket scientist.

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U29 DSOFT DPOLY DBIO DFD: Electrostatic Manipulation of Fluids and Soft Matter I: Electrohydrodynamics 501 - Jonathan Singer, Rutgers University, New Brunswick

2:30PM U29.00001: Control and characterization of thin film formation by electrospray deposition techniques* KRISTOF TOTH (Presenter), Yale University, GREGORY DOERK, KEVIN YAGER, Brookhaven National Laboratory, CHINEDUM OSUJI, University of Pennsylvania — Electrospray deposition (ESD) offers a precise and continuous manner by which to deliver sub-micron sized droplets of soft matter in dilute solution to a substrate. Preparation of thin films by ESD have offered advantages of making sequentially deposited, continually equilibrated or even compositionally varying systems on a single substrate for high-throughput characterization. However, understanding and control of the thin film formation are important to limit the Marangoni effects of the droplets on the surface to ensure uniform deposition and coverage. We describe a simple feedback control for visual analysis of various electrospray modes and their corresponding film formation. We also model the surface coverage of the films as a function of deposition time of varying molecular weight homopolymer and block copolymer systems. Furthermore, by changing the geometry of the ESD setup, the area of deposition can be tuned to fit the needs of transmission or reflection X-ray scattering experiments.

*Research perfumed at the CFN and NSLS-II, U.S. DOE Office of Science Facilities at BNL under Contract No. DE-SC0012704. NSF support through DGE-1122492, INTERN supplement to CBET-1703494, and DMR-1410568.
2:42PM U29.00002: Morphological Control of Multifunctional Melting Gel Coatings via Electrospray Deposition* ARIELLE MARIE GAMBOA (Presenter), LIN LEI, Department of Mechanical and Aerospace Engineering, Rutgers University, New Brunswick, JAMES MERCADO, JENNIFER GUZMAN, Department of Chemistry, Lehman College - CUNY, LISA C KLEIN, Department of Materials Science Engineering, Rutgers University, New Brunswick, ANDREI JITIANU, Department of Chemistry, Lehman College - CUNY, JONATHAN SINGER, Department of Mechanical and Aerospace Engineering, Rutgers University, New Brunswick — Melting gels (MG) are hybrid organic-inorganic gels with glass transition temperatures ~28°C and consolidation temperatures ~150°C. They exhibit thermoplastic behavior below their consolidation temperature and undergo complete cross-linking to form organically modified silica networks upon consolidation. By tuning surface properties, these glass sprays can be used as protective coatings in electronics and anti-corrosion coatings in metals. Electrospray deposition was used to spray solutions of 1wt% MG in 2-butanone. The high voltage produces charged, monodisperse droplets that, due to the low solid content of solutions, deliver small amounts of MG at a continuous rate. The pH of MG synthesis, solution viscosity, and spray polarity were varied to study the effects of charge injection on the consolidation of MG into hybrid glasses. The low MG content of solutions allows for the addition of viscosity modifiers such as terpineol which alter the ability of the spray to dissipate charge. Optical images, film measurements, and FT-IR were used to evaluate the effects of these variables on both the physical morphology along with the chemical structure of the final coatings.

*This work is supported by the Advanced Manufacturing Program of the National Science Foundation, Award No. 1911518.

2:54PM U29.00003: Using Multiplexed Electrosprays to Manipulate Fluids and (Soft) Materials [Invited] ALESSANDRO GOMEZ (Presenter), Mechanical Engineering and Materials Science, Yale University — The cone-jet electrospray has revolutionized the field of mass spectrometry but, despite the unique ability of this device to produce quasi-monodispersed particles in a phenomenal size range down to the nanoscale, it has not been applied to other fields, except for small scale proof-of-concept demonstrations. The primary reason for the lack of widespread use is the low flow rate at which the spray is dispersed. Using fluid mechanics and electrostatics, we a) developed criteria for compact multiplexing to increase flow rate drastically, b) microfabricated systems with high packing densities (1.1 104 sources/cm2), reducing the cost per electrospray source, and c) demonstrated successful operation of these devices in the synthesis of (soft) materials (e.g., polymer nanoparticles of controlled shape for drug delivery and battery materials) and in microchip cooling. I will review design criteria and applications.
3:30PM U29.00004: Self-Limiting Electrospray Deposition for the Surface Modification of Additively Manufactured Parts
DYLAN KOVACEVICH, LIN LEI, DAEHOON HAN, CHRISTIANNA KUZNETSOVA, STEVEN E KOOI, HOWON LEE, JONATHAN SINGER (Presenter), Rutgers University, New Brunswick — Electrospray deposition utilizes a high voltage to atomize a flowing solution into charged microdroplets loaded with solute. Our previous research investigated the conditions necessary to minimize charge dissipation and deposit a thickness-limited film through self-limiting electrospray deposition (SLED). Such sprays possess the ability to conformally-coat complex three-dimensional objects without changing the location of the spray needle or orientation of the object. This makes them ideally suited for the post-processing of materials fabricated through additive manufacturing (AM), opening a paradigm of independent bulk and surface functionality. Having demonstrated three-dimensional coating with film thickness in the range of 1-50 µm on a variety of conductive objects, in this study we employed model substrates and finite element method simulations to quantitatively study the technique's limits with regard to geometry and scale. Specifically, we examined recessed features with gaps ranging from 50 µm to 1 cm, as well as the ability to coat surfaces hidden from the line-of-sight of the spray needle. This was then extended to the coating of hydrogel structures printed by AM, as a means to create hydrophobic surfaces without affecting the absorption-driven humidity response.

3:42PM U29.00005: The Role of Surface Charging in Electrospray Printing of Thin Films*
YAQUN ZHU (Presenter), PAUL CHIAROT, Binghamton University — We report on the use of electrospray printing to create thin continuous multiscale films from nanoparticle aggregates. Nanomaterials are delivered to the target substrate in a dry state with an excess electric charge. The charge accumulates on the target and its decay rate plays a significant role in the film formation. Films printed on conductive substrates are thick and exhibit a periodic island structure, while films on insulating substrates are thickness-limited and more uniform. We leveraged the surface charging from electrospray to direct the assembly of nanoparticles using electrostatic focusing. This was achieved by patterning a photoresist layer on the target substrate. Charge accumulates on this layer and electrostatic forces direct the emitted material to the exposed parts of the substrate, which created high aspect ratio porous structures when the target substrate was silicon. The deposit growth was inhibited on glass substrates. To quantify the accumulated electric charge and its decay rate, we measured the spray and image charging for nylon and glass substrates. A scaling analysis revealed the importance of the processing conditions in determining the maximum accumulated charge and its decay rate.

*Funded by the National Science Foundation (CAREER Award #1554038).
Effect of Processing Conditions on the Formation and Microstructure of Electrospray Printed Polymer Films

BRYCE KINGSLEY (Presenter), PAUL CHIAROT, Binghamton University — An electrospray uses high electric potential to atomize a liquid suspension. The droplets evaporate in-flight, leaving behind dry solute particles that can be printed on a target substrate. We report on the use of electrospray to print thin films of polytetrafluoroethylene (PTFE) on silicon substrates. The coupled effects of ambient humidity (50%, 10%), suspension conductivity (9, 25, 85 μS/cm), suspension volatility (20%, 60%; alcohol in suspension), and flow rate (0.5, 1 μL/min) on the growth and microstructure of the films is reported. The suspension conductivity governed the net electric charge of the emitted droplets and particles, while humidity and volatility influenced the in-flight droplet dynamics. Films printed in dry air were denser with a well-defined boundary compared to films printed in humid air. Semi-spherical polymer aggregates were delivered to the substrate when the suspension conductivity was low. Suspensions with higher conductivity produced films with a woven structure of interconnected particle groups. Similarly, sprays utilizing a more volatile suspension produced films with a woven structure, with strands of solute linking groups of aggregates. The use of higher flow rates increased the particle packing density in the printed film.

Electrospray deposition of nanowire forests through spinodal gellation

LIN LEI (Presenter), CATHARINE NACHTIGAL, New Brunswick, Rutgers University, SHENSHENG CHEN, TYLER MOY, XIN YONG, Mechanical Engineering, Binghamton University, JONATHAN SINGER, New Brunswick, Rutgers University — The morphology of coatings created by electrostatic deposition can be generally divided into three categories: wire mats (electrospinning), particles (electrostatic spray, electrospray deposition), and films (all low-viscosity applications). There should exist nanowire forests as a mixture of wire and particulate deposition. Such a morphology has yet to be observed experimentally, which we propose is the result of spatially-varying viscosity in sprayed droplets. We utilized electrospray deposition (ESD) to explore the spray of methylcellulose (MC) in water:ethanol mixtures. MC possesses a lower critical solution temperature (LCST) in water and water:ethanol blends. Above the LCST, MC and water phase separate concurrently with the rapid evaporation of ethanol, forming a shear-thickening, homogeneous gel phase. This gel can undergo the elongation of electrospinning on a drop-by-drop basis to create forests of individual nanowires. Our study indicates that the homogenous evolution of viscosity is necessary for nanowire forest formation and that the specific viscosity (along with droplet size) further controls the morphology of the forests.
**4:18PM U29.00008: Modelling Nanowire Formation in Electrospray Deposition of Polymeric Droplets**  SHENSHENG CHEN (Presenter), XIN YONG, Binghamton University — The formation of nanowire forests was recently reported for the first time in electrospray deposition (ESD) of methylcellulose solutions. This novel morphology provides new opportunities for nanomaterial processing. The atypical nanowire geometry is a result of complex interplay among electrostatic interaction, solvent evaporation and polymer rheology. We conducted computer simulations to uncover the physics underpinning the morphological evolution of a highly charged polymeric droplets in ESD. We utilize electrostatic dissipative particle dynamics (EDPD) to simulate a model system that captures electrostatic interaction, evaporation, and polymer dynamics. We explored droplet morphological development under different evaporation conditions, which results in distinct modes of viscosity evolution. Our results show that the nanowire formation is a result of spinodal phase separation between polymers and solvents that homogeneously increases viscosity within the droplet. In contrast, a steep viscosity gradient formed leads to a bead-strings morphology. The coupling between electrostatically-driven deformation and evaporation-driven viscosity change in polymeric droplets can result in new and beautiful morphological evolution.

**4:30PM U29.00009: Influence of ionic conductivity on unconfined melt electrospinning of thermoplastics**  NEELAM SHEORAN (Presenter), BRENTON BOLAND, Elnaz Shabani, Russell Gorga, Jason R Bochinski, Laura Clarke, North Carolina State University — Ionic additives incorporated into thermoplastics melts can influence both viscoelastic properties and ionic conductivity. Such effects can be used to manipulate the process of melt electrospinning. In particular, fiber diameter is impacted by the melt viscosity as well as ionic motion within the melt under the influence of an applied electric field. Decreased fiber diameter could open pathways for fabrication of high strength mesoscale thermoplastic nanofibers, which have significant importance for filtration and biological applications. My talk will focus on how altered melt ionic conductivity due to commercial additives affects an unconfined melt electrospinning process. I will report ionic conductivity measurements obtained using broad-band impedance spectroscopy for two different grades of commercial linear low-density polyethylene with varying viscosities as a function of melt temperature and additive concentration. Corresponding viscosity measurements were performed by means of rotational plate rheometry. The rate of jet formation, the number of jets in steady-state, and the resulting fiber diameters were determined to characterize the effects of additive-doping of melts on the unconfined melt electrospinning process.

*Support from National Science Foundation CMMI-1635113*
Unconfined melt electrospinning from molten polymer experiencing an electric discharge to manipulate ion density and ionic conductivity* BRENTON BOLAND (Presenter), NEELAM SHEORAN, LAURA CLARKE, JASON R BOCHINSKI, North Carolina State University — Melt electrospinning is a promising way of achieving solvent-free mesoscale fibers for applications in tissue scaffolding, water filtration, and wound dressing; however, large fiber diameters is a persistent problem that must be understood. To address this, we are interested in the role of ionic conductivity in determining fiber diameter in melt electrospinning. We utilize an unconfined geometry where jets spontaneously form and organize on the edge of a melt-covered plate under the influence of the applied electrospinning electric field. Inspired by recent results from our group that show enhancement of ionic conductivity by additives resulted in reduced fiber diameter and by historical work on corona-assisted electrospraying, we controllably create a discharge near the plate edge to manipulate local ion density and alter the electrospinning process. This manipulation of local ion density by pulsed Dielectric Barrier Discharge (DBD) altered the electrospinning process in a way similar to the addition of ionic additives, suggesting a temporary enhancement of ionic conductivity.

*Support from National Science Foundation CMMI-1635113

Liquid Selection for Electrohydrodynamic Capillary Thermal Switches* TIANXING MA (Presenter), DARREL DSOUZA, Rutgers University, New Brunswick, KYRSTEN MCKENZIE RYERSON, Biola University, MATTHEW SIGNORELLI, Rutgers University, New Brunswick, YANG ZHAO, CHINEDUM OSUJI, University of Pennsylvania, JONATHAN SINGER, Rutgers University, New Brunswick — The deformation of sessile droplets and capillary bridging in a parallel-plate capacitor under DC field has been the subject of several scientific studies. Coaxially located droplets on opposing electrodes experience an attraction in the presence of an electric field. Application of a suitably large field will lead to either the droplets forming a liquid bridge or oscillation between bridged and de-bridged (i.e. droplet) states. We explored the bridging behavior of a variety of liquids in air. Among the liquids that could form a stable field-induced bridge, only a limited set could reversibly make and break the capillary bridge by switching the electric field on and off. The ability to form a switchable liquid bridge is a function of both the liquid's properties, including surface tension, electric conductivity, and dielectric constant, and external conditions such as electrode separation, droplet volume, and the substrate selection. Taking advantage of this phenomenon, through periodically forming and breaking the capillary bridge, we demonstrate the realization of a planar thermal switch that can control the flow of heat.

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5:06PM U29.00012: Dielectric modulation of two-dimensional dipolar materials  ZIWEI WANG (Presenter), ERIK LUIJ TEN, Northwestern University — Spontaneous pattern formation plays an important role in a wide variety of natural phenomena and materials systems. A key ingredient for the occurrence of modulated phases is the presence of competing interactions, generally of different physical origins. We demonstrate that in dipolar films, a prototypical system for pattern formation, patterns can be induced by dielectric effects alone [1]. A rich phase diagram arises, where striped and circular morphologies emerge with geometric properties that can be controlled through variation of particle shape and substrate permittivity or permeability. These effects are particularly enhanced by metamaterial substrates.


Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U30 DSOFT GSNP: Programmable Matter

2:30PM U30.00001: Mechanical Metamaterials You Can Count On  MATHIS MUNCK, HADRIEN BENSE, Designer Matter, AMOLF Amsterdam, MARTIN VAN HECKE (Presenter), Leiden University and AMOLF Amsterdam — Most mechanical metamaterials perform a single-step function, such as shape-morphing under pressure. However, nonlinearities in mechanical building blocks - buckling, snapping, self-contacts - open a route towards multi-step metamaterials, crucial for storing and processing information. Here we present a class of structures whose state depends on a sequence of identical input cycles: these metamaterials count.

2:42PM U30.00002: Multifunctional Combinatorial Metamaterials [Invited]  CORENTIN COULAIS (Presenter), Univ of Amsterdam — We introduce a novel class of combinatorial metamaterials that are multifunctional. We first define a combinatorial design space and find a rich phenomenology, ranging from disordered, to periodic and quasicrystalline tilings, who can host multiple yet a sub-extensive number of soft deformation modes. We then demonstrate the multifunctional nature of such metamaterials using both boundary textures and viscoelasticity. In particular, we realize a metamaterial that has a negative (positive) Poisson's ratio for low (high) compression rate. Their ability our metamaterials to host multiple mechanical responses makes them an early example of multi-functional matter, thus paving the way for robust and adaptable devices.
A truly-programmable mechanical metamaterial using magnetic actuation  TIAN CHEN (Presenter), School of Engineering, and School of Computer and Communication Sciences, Ecole polytechnique federale de Lausanne, MARK PAULY, School of Computer and Communication Sciences, Ecole polytechnique federale de Lausanne, PEDRO REIS, School of Engineering, Ecole polytechnique federale de Lausanne — Mechanical metamaterials are engineered systems with a sub-structure that, when tiled, exhibits physical properties that may not exist in conventional bulk materials. While disrupting the definition of a ‘material’, the periodicity or the internal unit structure of a metamaterial is often optimized to target a specific (set of) function(s) or mechanical behavior. As such, upon fabrication, standard metamaterials are effectively “programmed”, once and for all, and their functionality cannot be altered a posteriori. Here, we show a truly-programmable metamaterial where both the periodicity and the internal structure are preserved during fabrication but each unit cell can be independently programmed and reprogrammed, reversely and on-demand. Programming of individual cells is achieved by switching between the equilibrium states of a multi-stable elastic shell using magnetic actuation. When tiled into sheets or columns, we are able to tune the effective mechanical properties of our system including its stiffness, strength, and localization strain. Through a combination of quasi-static compression of experimental fabricated prototypes and finite element simulations, we demonstrate both the programming and the range of the exhibited mechanical response of our designs.

One Dimensional Mechanical Memory  AUSTIN REID (Presenter), Indiana Univ - Bloomington, KAREN DANIELS, Physics, North Carolina State University, THÉO JULES, FREDERIC LECHENAULT, Laboratoire de Physique Statistique, Ecole Normale Superieure, MUHITTIN MUNGAN, University of Bonn — Some bellows-like origami folded cylinders have bistable configurations, and the energy barriers between these bistable states are tunable with geometry. Stacked Kresling (twisted triangular tessellations) patterns on a cylinder can be can be tuned to collapse or deploy incrementally. If these folded cells are allowed to interact, the interaction energy can shift transition barriers such that the bellows achieves geometrically suppressed configurations. We have developed laser-cut and folded cylinders where adjacent unit cells can either be elastically connected or completely decoupled. For cylinders where cells are non-interacting, these unit cells function as "bits" with perfect return-point memory. In experimental tests, we find that a cylinder-based memory unit of 4 bits can be predictably driven to any of its 16 allowable states with a prescribed sequence of compression and extension.
Muscle-inspired flexible mechanical logic architecture for miniature robotics

MAYANK AGRAWAL (Presenter), SHARON C GLOTZER, Chemical Engineering, Univ of Michigan - Ann Arbor — Miniature robots (~10nm-100micron) that morph in response to external stimuli such as light or chemicals in their local environment have the potential to perform non-invasive treatments inside the body, clean up oil spills, or be embedded in textiles to intelligently tune fabric properties. Such robots can now be realized due to advancements in materials offering, e.g., stimuli-responsive polymers that actuate like artificial muscles. For maximum control using global triggers (stimuli), computation ability needs to be incorporated within these robots. The challenge is to design an architecture that is compact, material agnostic, stable under stochastic forces, and employs stimuli-responsive materials. Here we demonstrate such an architecture, which computes combinatorial logic via mechanical gates that use linear actuation (expansion and contraction). Additionally, the logic circuitry is physically flexible. We mathematically analyze gate geometry and discuss tuning it for the given signal requirements. We validate the design at colloidal scales using Brownian dynamics simulations. Finally, we simulate a complete robot that folds into Tetris shapes.

*This work was supported as part of the Center for Bio-Inspired Energy Science, funded by the U.S. D.O.E. under Award #DE-SC0000989.

Active stabilisation of patterned robotic swarms

PANKAJ POPLI (Presenter), PRASAD PERLEKAR, SURAJIT SENGUPTA, TIFR Centre for Interdisciplinary Sciences — Flocks of birds naturally order as a result of active forces which counteract destabilisation by random noise. Ordered patterns of drones or robotic agents are useful for many purposes such as surveying unknown territory, taking measurements of scientifically or economically important quantities over a large area, drone shows etc. Disruption of this pattern may occur due to many factors for e.g. atmospheric or ocean turbulence. Stabilising any given pattern in such a swarm is energy expensive and requires extensive computation and communication overheads. We propose an algorithm where one can achieve this in an energy efficient way. The strategy involves suppressing a class of fluctuations viz. non-affine displacements away from the given reference pattern while allowing affine deformations such as translations and rotations. The agents are not forced to sense, difficult to measure, environmental parameters such as local velocity of air or water in order to stabilise the swarm. Additionally, we show that by maintaining the structure/pattern of robotic swarms the statistics of the underlying flow field can be determined solely from "non-affine" forces. As the knowledge of these forces is a priori known, no extra measurement on the turbulent field is needed.
4:06PM U30.00007: Assembly by Solvent Evaporation: Equilibrium Clusters and Relaxation Times
ELIZABETH MACIAS (Presenter), ALEX TRAVESSET, Iowa State University, THOMAS R WALTMANN, Physics, University of Michigan — We present a theoretical and computational description of equilibrium clusters of alkylthiolated gold nanocrystals assembled by solvent evaporation. We consider N nanocrystals in an octane or nonane liquid droplet. Equilibrium structures consist of Tetrahedron (N=4), Square pyramid (N=5), Octahedron (N=6), Pentagonal bipyrimad (N=7), Biaugmented triangular prism (N=8), Gyroelongated square pyramid (N=9), Sphenocorona (N=10), Icosahedron (N=13). We also characterize the relaxation times of the system and show that they increase linearly with N, thus deviating from the classical Maxwell theory of solvent evaporation. Implications for self-assembly of superlattices will also be discussed.

*This work is funded by NSF, DMR-CMMT 1606336 "CDS&E: Design Principles for Ordering Nanoparticles into Super-crystals". This work used the Extreme Science and Engineering Discovery Environment(XSEDE), which is supported by National Science Foundation grant number ACI-1548562. Our project within XSEDE is supported by grant TG-MCB140071.

4:18PM U30.00008: Reprogrammable phononic metasurfaces
OSAMA BILAL (Presenter), Univ of Connecticut - Storrs — Mechanical metamaterials are materials with tailored, architectured geometry, designed to retain properties that do not exist or rare in nature. Most of these mechanical properties are inscribed in the material's frequency dispersion spectrum, ranging form its stiffness at zero frequency to its wave attenuation capacity at finite frequencies. These materials usually feature a structural pattern that repeats spatially (i.e., unit cell). A special class of these metamaterials can manipulate elastic waves (i.e., phonons). Most of the existing design frameworks for phononic metamaterials capitalize only one of there mechanisms; scattering, resonance or inertia amplification. In addition, once these designs are realized, their operational frequencies cannot be altered, limiting their potential for practical applications. Here, we present a reporprogrammable metamterial platform for manipulating phonons utilizing all the aforementioned wave manipulation mechanisms [Foehr and Bilal et al.,PRL, 2018]. We program our nonlinear metamaterial to redirect stress waves, in real-time, in an element-wise fashion [Bilal et al., Adv. Mater. 2017]. Moreover, we use it to realize the first purely acoustic transistor (switching and cascading sound with sound) [Bilal et al., PNAS 2017].
**4:30PM U30.00009: Synthetic Mechanoreceptors with Collocated Logic**

JANAV P. UDANI, ANDRES ARRIETA (Presenter), Mechanical Engineering, Purdue University — We present a new class of synthetic mechanoreceptor exhibiting large changes in conductivity as a function of their shape. Concretely, such mechanoreceptors consist of a mechanical bistable structure showing shape-dependent electrical conductivity. The electromechanical response is designed such that on one state the unit shows large resistance, while on the second state the conductivity increases significantly. The bistable nature of such units and their ability to switch conductivity in response to external forcing allows our mechanoreceptors to serve as sensors with collocated input dependent memory. Specifically, the amplitude and frequency of the pressure/force inputs activating our mechanoreceptors change of shape (snap-through) result in distinct dynamical signatures, which are transduced by adding a voltage bias and reading current time histories. This allows to interpret specific external inputs into electrical output signatures that can be feed into an artificial neural network. We demonstrate this by subjecting a network of such mechanoreceptors to different force inputs resulting in recognizable electrical signatures which correlate to specific patterns of local states.

*This work is supported by DARPA under agreement No. HR00112090010.

**4:42PM U30.00010: Sending Signals Through Mechanical Wiring**

MICHELLE BERRY (Presenter), RYAN HAYWARD, University of Massachusetts Amherst, CHRISTIAN SANTANGELO, Syracuse University — Some progress has been made in the development of logic gates from mechanical systems, but in order to realize fully functioning devices, we need a reliable way to transmit a mechanical signal between logic gates. We consider a mechanical “wire”, a series of bistable units that interact with each other, as a way to connect the output of one logic gate to the input of another logic gate. Using both computer simulations and analytical calculation to analyze the propagation of a signal through the wire, we have determined how parameters such as the number of bistable units and the signal strength affect how far a signal can propagate through the wire. We determine whether and to what degree signals can propagate based on the shape of the bistable potential.

*ARMY W911NF-19-1-0348

**4:54PM U30.00011: Training for desired Folding Pathways in Self Folding Origami**

CHUKWUNONSO ARINZE (Presenter), MENACHEM STERN, SIDNEY ROBERT NAGEL, ARVIND MURUGAN, University of Chicago — Creased sheets can possess an exponential number of folding pathways accessible from the flat state. This property poses an engineering challenge in the design of specialized self-folding origami patterns with one or a few prescribed folding pathways. We seek an alternative means to eliminating undesired folding pathways via physical training. We fold creased sheets along desired folding pathways and allow the initially equal crease stiffnesses to dynamically evolve according to a local rule dependent on folding strain. We find that undesired folding pathways are eliminated in saddle-node bifurcations, leaving behind only one or two desired folded pathways. In this way, we find that physical folding, combined with a plasticity rule for crease stiffness, can naturally arrive at design parameters needed for non-linear behaviors that are hard to predict otherwise.
5:06PM U30.00012: Computational wrapping: A novel method for wrapping 3D-curved surfaces with brittle, nonstretchable materials for conformable devices  YU-KI LEE, Department of Materials Science and Engineering, Seoul National University, JYH-MING LIEN, Department of computer science, George Mason University, IN-SUK CHOI (Presenter), Department of Materials Science and Engineering, Seoul National University — In this talk, we propose a novel method to make conformable devices on non-zero Gaussian surfaces, i.e. flexible devices that can be transformed into any complex 3-dimensional shape. We used computational polyhedral edge unfolding methods to obtain planar figures of arbitrary complex 3-dimensional shapes. It is well-known that 2-dimensional substrates cannot be attached on the non-zero surfaces without stretching, however, by computational approximation of 3-D surface and making it flat by algorithmic method, we could convert any 3-D shapes into a 2-D sheet. We can make devices having the programmed unfolded figures and return it to the original 3D shape. In this way, we could make electroluminescent lighting and primary battery which can conformably wrap diverse 3-D surfaces without failure. Shape programmable devices with computational wrapping design can cover anywhere on the 3-dimensional shapes including human skin and are able to be applied not only personalized wearable or skin attachable devices but also various industries, such as automotive design, clothing, and fashion accessories, medical services and so on.

5:18PM U30.00013: How to weave a perfect sphere with curved strips  CHANGYEOB BAEK (Presenter), Department of Mechanical Engineering, Massachusetts Institute of Technology, ALISON G MARTIN, Italy, Independent artist, TIAN CHEN, SAMUEL POINCLOUX, Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, YINGYING REN, JULIAN PANETTA, MARK PAULY, School of Computer and Communication Sciences, École Polytechnique Fédérale de Lausanne, PEDRO REIS, Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne — Triaxial weaving, a craft technique that enables the generation of surfaces with tri-directional arrays of initially straight elastic strips, has long been loved by basket makers and artists seeking a combination of practical and aesthetically-pleasing structures. The design principles of traditional weaving are based on the observation that the non-hexagonal topology of unit cells imparts out-of-plane shapes. In the realm of differential geometry, the weaving tradition is rooted in the concept of Euler characteristics through the Gauss-Bonnet theorem, with discrete topological defects being used as building blocks. Taking an alternative point of departure, we introduce a novel approach for triaxial weaving that enables us to continuously span a variety of 3D shapes of the weave by tuning the natural in-plane curvature of the strips. We systematically explore the validity of the new strategy by quantifying the shape of experimental specimens with X-ray tomography in combination with continuum-based simulations. To demonstrate the potential of our design scheme, and as a canonical example, we present a fullerene-like weave that is perfectly spherical, which cannot be readily achieved using straight strips. Ellipsoidal and toroidal structures are also explored.
2:30PM U31.00001: Collective behavior of platelets in blood clotting*  YUEYI SUN (Presenter), Mechanical Engineering, Georgia Institution of Technology, DAVID MYERS, Biomedical Engineering, Georgia Institute of Technology, WILBUR LAM, Wallace H. Coulter Department of Biomedical Engineering, Georgia Institution of Technology, ALEXANDER ALEXEEV, Mechanical Engineering, Georgia Institute of Technology — Blood clotting disorders prevent the body’s natural ability to achieve hemostasis and lead to bleeding, stroke or heart attack. Understanding the underlying physics behind the clotting process is essential to developing treatment of these disorders. Interaction between platelet and fibrin network leads to blood clotting, a highly complex multiscale mechanism taking place in blood flow. With experimental insights, we develop a mesoscale computational approach based on dissipative particle dynamics to examine the biophysics of clot contraction. The model contains platelets seeded in polymerized fibrin mesh. With platelets contracting surrounding fibrin, the model predicts bulk clot volume contraction and kinetics. The model shows that the heterogeneities involved in platelet contraction behavior enhance both clot volume contraction efficiency and clot force efficiency.

*Financial support from the National Science Foundation (CAREER Award DMR-1255288) is gratefully acknowledged.

2:42PM U31.00002: Living oil-water interfaces: Buckling of droplets by cell growth at finite liquid interfaces  GABRIEL JUAREZ (Presenter), University of Illinois at Urbana-Champaign — Cell growth on solid substrates confined by rigid boundaries has been shown to influence cell morphology and lead to the emergence of collective behavior. Here, through microfluidic experiments and time-lapse microscopy, we demonstrate that the colonization of oil droplets by the growth and division of rod-shaped bacteria depends strongly on the droplet diameter, or the interfacial curvature. For droplets larger than a critical diameter, bacteria grow and divide at the oil-water interface, leading to the self-assembly of a densely packed monolayer of bacteria that eventually encapsulates the droplet. The stress from cell growth exerted at the oil-water interface causes the droplet to buckle and the fluid interface to undergo large deformations, including wrinkling and tubulation. For droplets smaller than a critical diameter, the formation of a self-assembled monolayer is not observed and no interfacial deformations occur. A simple energetic argument, comparing the attachment energy and bending energy due to elastocapillarity of a rod-shaped bacterium at curved oil-water interfaces, is able to determine the critical diameter, or interfacial curvature, for colonization and may provide insight on the hydrophobicity of the cell wall.
2:54PM U31.00003: A trace amount of surfactants enable diffusiophoretic swimming of bacteria

VIET SANG DOAN, Department of Mechanical Engineering, University of Hawaii at Manoa, PRAKIT SAINGAM, TAO YAN, Department of Civil and Environmental Engineering, University of Hawaii at Manoa, SANGWOO SHIN (Presenter), Department of Mechanical Engineering, University of Hawaii at Manoa — From birth to health, from personal care products to pharmaceutical and petroleum industries, surfactants are all around us. Due to the importance, their environmental impacts are extensively studied and well understood. One of the aspects that have been studied in recent years is their impact on bacteria, particularly the swimming behavior of motile bacteria. Here, we uncover an alternate chemotactic strategy triggered by the presence of surfactants, namely diffusiophoresis. We show that even a trace amount of ionic surfactants, down to a single ppm level, can impact the bacteria diffusiophoresis by boosting the surface charge of the cells. Because diffusiophoresis is driven by the surface-solute interactions, the surfactant-enhanced diffusiophoresis is observed regardless of the types of bacteria. Whether gram-positive or -negative, motile or non-motile, the surfactants enable fast migration of bacteria even under non-swimming conditions, suggesting a ubiquitous mechanism that has been largely overlooked.

*This material is based upon work supported by the National Science Foundation under Grant No. CBET-1930691.

3:06PM U31.00004: Bridging Scales to Model Emergent Collective Oscillations in Social Amoeba

CHUQIAO HUYAN (Presenter), ALEXANDER GOLDEN, XINWEN ZHU, PANKAJ MEHTA, ALLYSON SGRO, Boston Univ — A key challenge in modeling emergent biological behaviors such as collective oscillations is identifying what dynamical features are important to capture at the level of individuals to recapitulate group-wide phenomena. To address this, we conducted a case study on five major existing models that describe intracellular collective cyclic AMP (cAMP) oscillations in the social amoeba, Dictostelium discoideum. We compared each model to published experimental findings about how amoeba cells modulate internal cAMP dynamics in response to external changes in cAMP. By doing so we evaluated how well these models recapitulate the observed behaviors. All models reproduce group-wide signaling oscillations and a majority are able to reproduce some single cell observations. Our main observation is models that do a good job recapitulating single cell dynamics are better at reproducing a critical feature of group oscillations: tuning their group oscillation rate in response to changes in cell density and the cAMP dilution rate. Overall, we find that accurate recapitulation of single cell dynamics and noise are important for modeling qualitative group oscillations.
3:18PM U31.00005: Pattern engineering of living bacterial colonies using meniscus-driven fluidic channels  
VASILY KANTSLER, Physics, University of Warwick, UK, ELENA ONTAÑÓN-MCDONALD, CANSU KUEY, MANJARI J GHANSHYAM, School of Life Sciences, University of Warwick, UK, MARIA CHIARA ROFFIN (Presenter), Physics, University of Warwick, UK, MUNEHIRO ASALLY, School of Life Sciences, University of Warwick, UK — Engineering spatially organized biofilms for creating adaptive and sustainable biomaterials is a forthcoming mission of synthetic biology. Existing technologies of patterning biofilm materials suffer limitations associated with the high technical barrier and the requirements of special equipment. Here we present controlled meniscus-driven fluidics, MeniFluidics; an easily implementable technique for patterning living bacterial populations. We demonstrate multiscale patterning of living-colony and biofilm formation with submillimetre resolution. Relying on fast bacterial spreading in liquid channels, MeniFluidics allows controlled anisotropic bacterial colonies expansion both in space and time. The technique has also been applied for studying collective phenomena in confined bacterial swarming and organizing different fluorescently labelled *Bacillus subtilis* strains into a converged pattern. We believe that the robustness and low technical barrier of MeniFluidics offer a tool for developing living functional materials, bioengineering and bio-art, and adding to fundamental research of microbial interactions.

3:30PM U31.00006: Control of patterning in human pluripotent stem cell colonies via a Turing system with reactive boundaries  
BENJAMIN MCMASTER, HIMANSHU KAUL, DANIEL AGUILAR-HIDALGO (Presenter), PETER ZANDSTRA, School of Biomedical Engineering, University of British Columbia — During early stages of gastrulation, cells differentiate and organize into well-defined structures that lead to the emergence of the 3-germ layers, which represent early progenitors of precursor tissues for all the body organs. Recently, in-vitro studies using human pluripotent stem cells (hPSC) in confined environments have shown the emergence of spatially organized markers of an early gastrulation-like state following induction by the *bone morphogenetic protein 4* (BMP4), thus providing a framework to understand, and ultimately control, collective self-organization and pattern formation in hPSC. We present minimal Turing system that is consistent with hPSC patterns observed in 2- and 3-D structures. Our approach considers that the morphogen flux at the colony boundaries is morphogen-concentration dependent (a so-called reactive boundary). Using this framework, we have quantified the effective transport dynamics of the morphogen BMP4 in hPSC colonies, and defined conditions that predict pattern properties such as marker spatial order, domain size and thresholds for symmetry-breaking events. This work presents a general framework for self-organized pattern formation that explain observed patterns in hPSC colonies, leading to a design-based specification of collective cell behavior.
3:42PM U31.00007: Cellular integration of physical and biochemical damage signals in the generation of tissue-level wound responses*  AARON STEVENS (Presenter), KAZI TASNEEM, JAMES OCONNOR, SHANE HUTSON, ANDREA PAGE-MCCAW, Vanderbilt Univ — Laser wounds in Drosophila epithelia trigger calcium signaling – an early and conserved sign of wound detection – that includes an initial calcium influx into damaged cells within 0.1 s, a first expansion into adjacent cells over ~20 s, and a delayed second expansion to a much larger set of surrounding cells between 40-300 s. We have developed a computational model to test the plausibility of multiple hypothesized mechanisms driving these calcium signals and to further understand the underlying biology. The model includes calcium currents between each cell's cytosol and its endoplasmic reticulum (ER), the extracellular space, and neighboring cells. These calcium currents are initiated in the model by cavitation-induced microtears in the plasma membranes of cells near the wound (initial influx), flow through gap junctions into adjacent cells (first expansion), and by the activation of G-protein coupled receptors via a wound-induced diffusible ligand (second expansion). The production, processing and propagation of the ligand is modeled using reaction-diffusion equations on a continuous, two-dimensional space. We will discuss how the model matches experimental observations and makes experimentally testable predictions.

*Supported by NIH Grant 1R01GM130130.

3:54PM U31.00008: Dorsal closure in numbers: quantification of epithelial cell oscillations using machine learning  DANIEL HAERTTER (Presenter), Department of Physics, Duke University, DANTE RHODES, JANICE CRAWFORD, DANIEL P KIEHART, Department of Biology, Duke University, CHRISTOPH F. SCHMIDT, Department of Physics, Duke University — Dorsal closure in Drosophila melanogaster embryos is a key model system for cell sheet morphogenesis and wound healing. Multiple sub-systems are involved in the mechanical closing of the dorsal opening. Understanding system dynamics, regulation and causal relations requires a quantitative understanding of the mesoscopic mechanical and dynamic properties of this “active soft material”. Individual cells in the amnioserosa, a one-cell-thick sheet of epithelial cells filling the dorsal opening, show sustained oscillations of apical cell area. These oscillations exhibit large variations from cell to cell and during the course of closure. Past studies of epithelial dynamics were restricted to semi-manual segmentation of cell shapes and thus suffered from relatively low statistics. We present a novel analysis pipeline, based on a convolutional neural network (machine learning), that allows an automated and robust segmentation of large numbers of video recordings. We further employ statistical approaches to analyze spatial-temporal dynamics and quantify embryo-to-embryo variability. We observe emerging long-range dynamical patterns providing clues about possible communication mechanisms between cells.
**4:06PM U31.00009: Signatures of tissue surface tension in 3D models with two tissue types**

PREETI SAHU (Presenter), J M SCHWARZ, M. LISA MANNING, Syracuse University — Dense biological tissues maintain sharp surfaces between cell types performing different roles. For example, in multi-layered epithelia, the bottom-most basal layer remains distinctly compartmentalized from the supra-basal layer above, in spite of newly born basal cells being pushed upwards. Similarly, in experimental co-cultures of healthy (MCF10A) and invasive (MDA-MB-231) breast cell lines, initially MCF10A forms a distinct inner core leaving the MDA231 exposed, although that structure inverts on longer timescales. To better understand the mechanisms for such sharp compartmentalization, we study the effect of an imposed heterotypic tension at the interface between two distinct cell types in a fully 3D model for confluent tissues. We find that cells rapidly sort to generate a tissue-scale interface between cell types, and cells adjacent to this interface exhibit signature geometric features including nematic-like ordering and bimodal facet areas along the surface. The magnitude of these features scale directly with the magnitude of imposed tension, suggesting that experiments might estimate the magnitude of tissue surface tension simply by segmenting a 3D tissue.

*This work is funded by NSF-POLS-1607416.

**4:18PM U31.00010: Defect Driven Morphogenesis: Active Cell Division Generates Four-Fold Order**

DILLON CISLO (Presenter), HAODONG QIN, MARK J BOWICK, SEBASTIAN STREICHAN, University of California, Santa Barbara — The generation of 2D hexagon-dominated topologies has been well studied in thermally equilibrated systems. Six-fold coordinated patterns also frequently arise in living matter far from equilibrium as a result of cell proliferation. We present a quantitative profile of exotic non-equilibrium pattern formation in the crustacean *Parhyale hawaiensis*. Active orchestration of cell proliferation transforms an initially disordered epithelial tissue into a regular rectangular lattice that cannot be explained by cell packing or randomly oriented divisions. Using light-sheet microscopy and computer vision techniques, we extract the dynamics of cell proliferation in the growing *Parhyale* embryo and quantify the spatiotemporal dependence of orientational order. *In vivo* cell tracking and lineage reconstruction together with simulation and theoretical modeling reveal the relationship between division axis orientation and both the emergence and preservation of order. Disorder introduced into the lattice by divisions must be mitigated by the active control of subsequent divisions in order to maintain the lattice structure in a program we call defect driven morphogenesis.

*National Institutes of Health (NIH)
National Science Foundation (NSF)*
4:30PM U31.00011: Quantifying mechanics in non-confluent tissues using an extended vertex model*  
ELIZABETH LAWSON-KEISTER (Presenter), AMANDA PARKER, JENNIFER SCHWARZ, M. LISA MANNING, Syracuse University — Vertex models for tissues have correctly predicted cell shapes and fluid-solid transitions in confluent epithelial monolayers where there are no gaps between cells and negligible curvature along cell-cell boundaries. However, in many situations of interest, such as in the development of the zebrafish tailbud, epithelial sheets transition from non-confluent layers with significant gaps between cells to confluent configurations with no gaps. Therefore, we develop simple extensions of vertex models that are able continuously transition between these two states, and demonstrate that there is a reasonable parameter regime in which the minimum energy state of this extended vertex model has gaps between cells. We study the mechanical behavior of these non-confluent models to understand how such gaps alter tissue mechanics and collective cell motility.

*This work is funded by NSF-PHY-1607416 and NSF-DMR-1352184.

4:42PM U31.00012: The branched architecture of the airway is physically shaped by the extracellular matrix and contractile airway smooth muscle during lung development*  
[Invited] JAMES SPURLIN (Presenter), RAWLISON ZHANG, CELESTE NELSON, Princeton University — The lung possesses a highly branched airway epithelial network, which is required for rapid gas exchange. To build the network of branches in the lung, airway morphogenesis requires three critical steps including branch site specification, branch elongation, and mesenchymal remodeling. Using comparative embryology, we have found several novel mechanisms of how airway branches are physically shaped. During airway morphogenesis, epithelial branches are wrapped by a sheath of extracellular matrix (ECM), known as the basement membrane (BM), and a layer of contractile airway smooth muscle (ASM). We hypothesized these tissue layers direct airway branching morphogenesis by constraining the growth of the airway epithelium. In the bird lung, early stages of branching morphogenesis occurs in the absence of ASM, permitting the investigation of how ECM remodeling influences branch shape. In birds, we found branch elongation rate and surface area expansion requires proteolytic turnover of the BM. As branches elongate, mesenchymal cells surrounding the tips of the airway branches become elongated and the mesenchyme begins to rearrange fluidly, resembling a mesenchymal unjamming transition. This facilitates the transport and assembly of new ECM components ahead of the growing branch, which may also influence growth and shaping of the extending branch. In the mammalian lung, ASM wraps the airway epithelium and is critical for specifying the location of newly formed branches. We found mechanotransduction signaling through focal adhesion kinase (FAK) controls the distribution of ASM wrapping around the growing airway epithelium. Inhibiting of FAK signaling results in altered ASM contractility, leading to changes in the branched architecture of the airway. Taken together, the ECM and ASM shape airways of the developing lung by constraining the growth of the epithelium to build a functional branched airway network.

*This work was supported by the NIH (HL118532, HL120142 and CA187692).

Thursday, March 5, 2020 2:30 PM - 5:30 PM
2:30PM U32.00001: Effect of Molecular Architecture on the Conformational Relaxation for Interfacial Polymer Chains* HUNG K. NGUYEN, DAISUKE KAWAGUCHI, KEIJI TANAKA (Presenter), Kyushu Univ — Conformational relaxation processes of polymer chains trapped in a metastable state in close proximity to a solid interface can strongly affect the physical properties of polymer nanocomposites. Using sum-frequency generation spectroscopy, we here report the thermal annealing effect on chain conformations of polystyrene (PS) with different molecular architecture near at the quartz interface. Relaxation dynamics for PS chains strongly adsorbed at the outermost substrate interface and those located next to the adsorbed layer were characterized. PS chains exhibited much slower relaxation dynamics with a star-shaped architecture than with a linear one. This finding is in consistent with a scenario that the entropic interaction with the solid surface is stronger for a star-shaped macromolecule than for a linear one.

*This research was partially supported by the JST-Mirai Program (JPMJMI18A2).

2:42PM U32.00002: In Situ Synchrotron Radiation X-ray Scattering Evaluation of Domain Size and Spacing of Thermoplastic Elastomer under Elongation NATTANEE DECHNARONG (Presenter), Graduate School of Engineering, Kyushu University, KAZUTAKA KAMITANI, Institute for Materials Chemistry and Engineering, Kyushu University, CHAO-HUNG CHENG, SHIORI MASUDA, SHUHEI NOZAKI, CHIGUSA NAGANO, Graduate School of Engineering, Kyushu University, YOSHIFUMI AMAMOTO, KEN KOJIO, ATSUSHI TAKAHARA, Kyushu Univ — Microphase separation occurs in polystyrene (PS)-b-poly(ethylene-co-butylene)-b-PS (SEBS), leading PS domains to serve as physical crosslinking points. To improve mechanical strength of SEBS, mechanical stability of PS needs to be clarified. Here, the molecular aggregation structure of SEBS films containing spherical PS domains packed in b.c.c. lattice was measured during stretching using in situ SAXS. During uniaxial stretching, a shift of structure factor reveals an increase in domain spacing in parallel to stretching direction while it decreased in the perpendicular direction. Affine deformation of all diffraction planes was observed, while they deviated from the trend above strain 5 equally. In the case of biaxial stretching, an increase in the domain spacing was observed in both stretching directions, indicating an isotropic deformation. Deviation from affine deformation of each diffraction plane was observed above strain 1.5, referring to the difficulty of maintaining the paracrystalline structures during biaxial stretching. Domain size of PS domains with polydispersity was determined from form factor using model calculation. From the change of radius, PS domains were proposed to deform to prolate and oblate spheroids during uniaxial and biaxial elongation, respectively.
Structure and Physical Properties of Zwitter Ionic Polyelectrolyte Brushes at Aqueous Interface

ATSUSHI TAKAHARA (Presenter), Kyushu Univ — Polymers chemically grafted to the surface of substrates are typical soft interfaces known as polymer brushes. Surfaces covered with polyelectrolyte brushes are attractive because of their potential applications including adhesion, antifouling, biocompatibility and water lubrication systems. In this presentation, our recent researches on control of wettability and adhesion through precise design of polyelectrolyte brush surfaces are presented. We started from fundamental science including precise polyelectrolyte synthesis and solution characterization of polyelectrolytes, characterization of polymer brush at water interfaces, and water structure in polymer brushes. On the basis of these fundamental studies, we have achieved 1) superhydrophilicity, 2) antifouling properties, 3) super-lubricant behavior, 4) intelligent adhesion and 5) cell-surface interaction control.

*This work was supported by the Photon and Quantum Basic Research Coordinated Development Program of the Ministry of Education, Culture, Sports, Science and Technology, Japan.

Highly Branched Polymers with High Ether Oxygen Content for Membrane CO₂/N₂ Separation

HAIQING LIN (Presenter), State Univ of NY - Buffalo — Membrane technology has emerged as a potentially economically viable alternative for CO₂ captures from fossil fuel-fired powers, enabled by advanced membrane materials with high CO₂ permeability and high CO₂/N₂ selectivity. Current leading membrane materials usually contain poly(ethylene oxide) (PEO) because the ether oxygen in PEO interacts favorably with CO₂, resulting in high CO₂/N₂ selectivity. Herein we prepare a series of highly branched amorphous polymers containing poly(1,3-dioxolane), which has an O:C ratio of 0.67, higher than 0.5 in PEO. The length of the poly(1,3-dioxolane)-based branches are tuned to yield amorphous nature, and mobile ethoxyl chain end groups are introduced to provide high free volume and gas diffusivity. These ether oxygen-rich polymers exhibit more superior CO₂/N₂ separation properties than the PEO-based materials at practical conditions for flue gas processing, and above the Robeson’s upper bound. This work demonstrates that harnessing the interactions between polymers and CO₂ may provide unprecedented opportunities in designing gas separation membranes with robust performance under practical conditions.

*DOE NETL and NSF
3:18PM U32.00005: Protein Resistant Property of Nanometer-Scale Architecture of Polymer Chains

MAYA ENDOH (Presenter), DANIEL SALATTO, ZHIXING HUANG, State Univ of NY - Stony Brook, YUTO KOGA, Cornell University, YASHASVI BAJAJ, BENJAMIN YAVITT, State Univ of NY - Stony Brook, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory, DMYTRO NYKYPANCHUK, Brookhaven National Laboratory, TAD KOGA, State Univ of NY - Stony Brook — We recently reported that a few nanometer-thick polymer layer formed on a solid, which consists of physisorbed non-charged homopolymer chains, exhibits anti-fouling properties against a model protein, bovine serum albumin (BSA), independent of polymer hydrophilicity/hydrophobicity[1]. We revealed that the highly packed chain architecture plays a crucial role in its protein resistant property over surface chemistry. Here, we further illuminate how this nanometer-scale chain structure impacts the protein adsorption on ultrathin polymer films. Polymer films with different thicknesses ranging from 2 nm to 200 nm of polystyrene, poly(2-vinyl pyridine), polybutadiene, poly(methyl methacrylate), and polypropylene were prepared. Adsorption of fluorescein labeled BSA and fibrinogen on these thin films were studied as a function of film thickness using photon counting spectrofluorometry. We observe that the critical thickness of the adsorption transition from anti-fouling to fouling appeared irrespective of the type of polymers and proteins. In addition, molecular dynamics simulations were performed to mimic the protein adsorption process. We will discuss the mechanism behind the phenomenon.


3:30PM U32.00006: Linear vs Star polymers in Hydrogen-Bonded Assemblies

ALIAKSEI ALIAKSEYEU (Presenter), Materials Science and Engineering, Texas A&M University, JOHN F ANKNER, Spallation Neutron Source, Oak Ridge National Laboratory, SVETLANA SUKHISHVILI, Materials Science and Engineering, Texas A&M University — We report on the effect of the molecular architecture of poly(ethylene oxide), PEO (linear vs. 6-arm polymer, /PEO and sPEO, respectively) and molecular weight of poly(methacrylic acid) (PMAA) on hydrogen-bonding assembly of these polymers. Isothermal titration calorimetry studies (ITC) revealed the entropic nature of complex formation and complex strengthening with the increase of molecular weight of PMAA. At the same time, /PEO-containing and sPEO-containing complexes had a different stoichiometry of PMAA-to-PEO repeat units of 1 and 1.5 for PMAA/PEO and PMAA/sPEO, respectively, suggesting possible formation of necklace-like complexes on a PMAA string. When the assembly was performed at surfaces, layer-by-layer (LbL) PMAA/PEO films constructed with linear PEO exhibited faster deposition of polymer mass as compared to films built with sPEO. Consistent with these results, neutron reflectometry revealed stronger molecular intermixing within films containing /PEO, suggesting faster diffusion of /PEO in LbL films as compared to the necklace-included sPEO polymer.
The dynamics of the thermally stimulated surface height fluctuations in a polymer melt dictate wetting, adhesion, and tribology at that surface. These surface fluctuations can be profoundly altered by tethering of the chains. One type of tethering is the tethering of one part of a molecule to another part of the same molecule. This tethering is found in both long chain branched polymers and in macrocycles. We have studied the surface fluctuations with X-ray Photon Correlation Spectroscopy for melts of well-defined, anionically polymerized polystyrenes of various architectures, including linear, 6 arm star, pom-pom, comb and cyclic architectures. For linear chains, the variation of surface relaxation time with in-plane scattering vector can be fit using a hydrodynamic continuum theory (HCT) of thermally stimulated capillary waves that knows nothing of the chain architecture. Assuming the theory is applicable, apparent viscosities of the films may then be inferred from the XPCS data. For unentangled linear chains, the viscosity inferred from XPCS data for sufficiently thick films is the same as that measured by conventional bulk rheometry. For star-branched chains the film thickness relative to chain size must be much larger to obtain this agreement. Densely branched combs, cyclic and bicyclic chains show yet another behavior. It appears these differences are related to the manner in which the chains organize at the substrate interface.

4:18PM U32.00008: Dilute solution structure of bottlebrush polymers  SARIT DUTTA (Presenter), TIANYUAN PAN, MATTHEW AARON WADE, DYLAN J WALSH, SIMON A ROGERS, DAMIEN S GUIRONNET, CHARLES SING, University of Illinois at Urbana-Champaign — Bottlebrush polymers are the canonical example of hyperbranched polymers, consisting of a central backbone chain with numerous side chains densely grafted onto it. This architecture lends additional thickness to the molecule as well as enhancing its stiffness due to steric interaction between the side chains. The side chain length and grafting density can be used as control parameters for tuning the material properties, as leveraged in recent applications to photonic crystals and soft elastomers.

We present results from Brownian Dynamics and Monte Carlo simulations on bottlebrush conformations in dilute solution, emphasizing the role of side chain length and grafting density on the size, shape, and intramolecular structure of a bottlebrush molecule. These simulations are based on bead-spring models, with suitably chosen potentials. We find good agreement between our simulation results and viscometric studies on well-characterized samples of polynorbornene-polylactic acid bottlebrushes. We coarse-grain the above bead-spring model as a wormlike cylinder, where the side-chains are treated in an implicit fashion. Furthermore, we discuss the elastic response of bottlebrush polymers to a pulling force and contextualize this behavior with respect to classical entropy elasticity of linear polymers.

4:30PM U32.00009: Morphology and Dynamics of Catenanes in Dilute Solutions and at Liquid/Liquid Interface  SAEED AKBARI (Presenter), SHAGHAYEGH KHANI, JOAO M MAIA, Macromolecular Science & Engineering, Case Western Reserve University, MESFIN TSIGE, Polymer Science, University of Akron — Molecular Dynamics simulations are performed with all-atom poly (ethylene oxide) (PEO) and polystyrene (PS) structures in water and in toluene and at the water/toluene interface and the dynamics and structural properties of PEO and PS chains with different topologies such as linear, isolated rings and interlocked rings (homo and hetero catenation) are studied. This includes the comprehensive study of the effect of chain flexibility, solvent quality and interface as deterministic factors that influence the morphology and dynamics of the catenanes. The results can be exploited to design and fabricate molecules with desired dynamics and will be of particular significance for drug delivery applications. Our simulations predict larger radius of gyration and faster dynamics for flexible topologies in a good solvent. In a poor solvent, they shrink to smaller size and again diffuse faster compared to the rigid counterparts. Moreover, hydrogen bonding significantly affects the dynamics of the molecules in water both in bulk and at the interface. At the water/toluene interface, molecules develop a flat morphology and thus have larger size as compared to their coil structures in the bulk of a good solvent and are found to show faster diffusion.
4:42PM U32.00010: Bottlebrush Polymers in the Melt and Polyelectrolytes in Solution Share Common Structural Features

JOEL SARAPAS, TYLER MARTIN, National Institute of Standards and Technology, ALEXANDROS CHREMOS, National Institutes of Health, JACK DOUGLAS, KATHRYN BEERS (Presenter), National Institute of Standards and Technology — Uncharged bottlebrush polymer melts and highly charged polyelectrolytes in solution exhibit correlation peaks in scattering measurements and simulations. Given the striking superficial similarities of these scattering features, there may be a deeper structural interrelationship in these chemically different classes of materials. Correspondingly, we constructed a library of isotopically labeled bottlebrush molecules and measured the bottlebrush correlation peak position $q^* = 2\pi / \xi$ by neutron scattering and simulations. We find that the correlation length scales with the backbone concentration, $\xi \sim c_{BB}^{-0.47}$, in striking accord with the scaling of $\xi$ with polymer concentration $c_p$ in semi-dilute polyelectrolyte solutions ($\xi \sim c_p^{-1/2}$). The bottlebrush correlation peak broadens with decreasing grafting density, similar to increasing salt concentration in polyelectrolyte solutions. $\xi$ also scales with sidechain length to a power in the range of 0.35 to 0.44, suggesting that the sidechains are relatively collapsed in comparison to the bristle-like configurations often imagined for bottlebrush polymers.

4:54PM U32.00011: Effect of Chain Architecture on the Structure, Diffusion, and Swelling in Thin Polymer Films*

BULENT AKGUN (Presenter), MAKBULE GIZEM KIREVIYASI, AYSE CAGLAYAN, Bogazici University, KUNLUN HONG, DAVID UHRIG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, TADANORI KOGA, Department of Materials Science and Chemical Engineering, Stony Brook University, GUANGCUI YUAN, SUSHIL K SATIJA, NIST Center for Neutron Research, National Institute of Standards and Technology — Polymers with special architectures are utilized in wide variety of technologies such as in pressure sensitive adhesives, biomedical coatings, photoresists, targeting multi-drug resistant gram-negative bacteria, and electrochromic displays. Being able to control the chain architecture opens new pathways to tune physical properties of the polymer thin films through alterations in the entropic contribution. In this work, we have investigated the role of chain architecture on the adsorption, diffusion and swelling in supercritical carbon dioxide (ScCO$_2$) using well-defined linear, star, centipede and comb polystyrene (PS). Structure of irreversibly adsorbed layers are determined using ellipsometry and X-ray reflectivity. Vertical diffusion in bilayer films and ScCO$_2$ swelling in single layer films were determined using in-situ neutron reflectivity measurements. Our results indicated that the normalized equilibrium thickness of the adsorbed layer increases as the number of branches increases and the length of the branches decreases. Independent of the architecture the films are consistently fit using a single layer of uniform density. For the same total molecular weight, thin films composed of more branched polymers have larger diffusion constants than that are made of linear chains. Increase in the fraction of adsorbed chains in a thin film causes a decrease in the vertical diffusion and ScCO$_2$ swelling.

*BA acknowledges the support provided by TUBITAK 215Z334, TUBA- GEBIP and BAGEP Young Investigator Award.

Thursday, March 5, 2020 2:30 PM - 5:30 PM
2:30PM U33.00001: Formation of Pickering Emulsions Using Nanodiamonds  BARBARA V FARIAS, DEREK BROWN, ALLISON HEARN, SAAD KHAN (Presenter), North Carolina State University — Pickering emulsions are used over surfactant stabilized emulsions in a wide range of applications including personal care products, pharmaceuticals, and oil recovery because of their enhanced stability and lower toxicity. We examine here the use of nanodiamonds (ND), a relatively novel carbonaceous filler with high adsorption activity, small size, and large surface area to create solid stabilized emulsions. Using a system consisting of isopropyl palmitate and water, stabilized by hydroxylated NDs, we investigate the stability, rheology and frictional behavior of these emulsions as a function of ND concentration. Optical microscopy reveals increasing ND concentration results in smaller droplet sizes, due to the greater availability of particles that can be adsorbed on the oil-water interface. This behavior is consistent with our rheological results of higher G’ and yield stress with increased ND, as the presence of smaller droplets facilitate the formation of a densely packed network. Microstructure recovery after breakdown at different stress levels correlate with the ratio of applied stress to the yield stress for each ND concentration. Tribological behavior of ND emulsions was also investigated using a soft model contact and the data related to the rheological characteristics.

2:42PM U33.00002: Utilizing Inorganic Nanoadditives to Influence the Surface Properties of Polymer Films*  SPIROS H. ANASTASIADIS (Presenter), FANOURIOS KRASANAKIS, ANTIGONOS THEODORAKIS, KIRIAKI CHRISSOPOULOU, Foundation for Research and Technology-Hellas and Univ. of Crete — Addition of nanosized inorganic materials to a polymer matrix results in nanohybrids with optimized properties. In this work, we report on the development of superhydrophobic and water repellent polymer coatings by utilizing nanoadditives of different geometries and size. The nanocomposite coatings were deposited either on a soft polyethylene, PE, substrate or on a hard silicon wafer. The coating morphology and effective roughness were studied with Scanning Electron Microscopy and profilometry, respectively, as a function of the nanoadditive content. In the case of PE substrates, the optical clarity of the original film was preserved following the nanohybrid coating, as verified by UV-Vis spectroscopy. The surface properties of all films were investigated by contact angle measurements; the water contact angle showed a non-monotonic dependence on the coating composition and depended strongly on the kind of nanoadditive whereas the contact angle hysteresis was significantly affected by its presence.

*This research has been co-financed by EU and Greek national funds (Action RESEARCH – CREATE - INNOVATE, project INGRECO, MIS: 5030174).
2:54PM U33.00003: Interfacial Dynamics of Confined Microgel Liquids on Soft Surfaces
KEHUA LIN (Presenter), YINGXI ELAINE ZHU, Wayne State Univ — While much research has strived to understanding the dynamics of confined liquids on a hard solid surface, the dynamics of liquids confined on a soft and deformable surface remains unclear. In this work, we employed poly(N-isopropylacrylamide) (PNIPAM) microgels of varied crosslinking density as the confined liquids as well as confining surface coatings. We analyzed the mean-squared-displacement (MSD) of confined PNIPAM microgel particles in the first 1-2 particle layers immediately adjacent to PNIPAM coated surface of varied particle-to-surface elasticity ratios. We observed that soft surface of low elasticity show little impact on the interfacial dynamics of confined microgel particles of varied elasticity, where the MSD of confined microgels exhibits little deviation from their bulk behaviors. Such interfacial behavior is in sharp contrast to the dynamic arrest of microgels confined on hard surface of high elasticity. Furthermore, we found that the dynamic heterogeneity in confined glass-like microgel liquids could diminish with decreasing the elasticity of confining surface, which gives insight to design low-friction and lubrious coatings and surfaces.

3:06PM U33.00004: How osmotic pressure governs sliding and surface structures of swollen crosslinked hydrogels* [Invited] SHABNAM Z BONYADI, CHRISTOPHER L JOHNSON, JIHO KIM, ERIK R REALE, MICHAEL ATTEN, ALISON C DUNN (Presenter), University of Illinois at Urbana-Champaign — High-water-content hydrogels are being increasingly explored for applications in biomedicine, water filtration, and hybrid materials. As these materials slide against hard, impermeable countersurfaces, they exhibit time-dependent and history-dependent friction related to their response under stress. Here I present two vignettes of the role of osmotic pressure in understanding hydrogel lubrication. The first considers the competitive rates of surface slip and pressure-driven dehydration due to applied loads. Given initial measurements of friction at very low and very high speeds, the ratio of the timescales of these effects can predict friction along the intermediate spectrum. The second vignette describes the inherent generation of less-dense surface layers (~single microns) that arise from the bulk due to the discontinuity of osmotic pressure between the bulk and the open bath submerging a crosslinked hydrogel. These layers are confirmed with multiscale indentation techniques and material creep localized to the near-surface region.

*This work is supported by NSF awards 1563087 and 1751945.
3:42PM U33.00005: Bio-inspired surface modification of PDMS to reduce dry friction
MENGYUAN WANG, University of Colorado, Boulder, SUJAN GHOSH, University of Arkansas, ADRIENNE BLEVINS, University of Colorado, Boulder, CHRISTOPHER M STAFFORD, JASON KILGORE, National Institute of Standards and Technology, SIJIA HUANG, University of Colorado, Boulder, MIN ZOU, University of Arkansas, YIFU DING (Presenter), University of Colorado, Boulder — Reducing friction and associated energy dissipation in mechanical systems is critical for a broad range of applications. Under dry condition, soft elastomers are inherently adhesive and display high friction coefficient, which leads to severe wear and damage during contact. The skin structure and the scales geometry of some squamate reptiles, especially snakes and lizards, offers a potential way for friction reduction under extremely dry conditions. The stiff keratin-based epidermis on soft dermic tissue helps snakes reduce friction in forward locomotion. This study aims to mimic such functional skins by modifying both the stiffness and topography of the elastomeric surfaces. Using a photoinitiated infiltration polymerization, glassy polyHEMA is formed within the skin of PDMS, in the presence of water. The as-prepared surface displays a integrated skin layer possessing fold-like structure, with stiffness increasing from glassy to rubbery with the increase of load. Under dry condition, the friction coefficient of the PDMS reduces from 1.6 to 0.14 with the modification.

3:54PM U33.00006: Friction and wear of polyzwitterionic brush-grafted surfaces*
CHRISTOPHER SERFASS (Presenter), Department of Chemical and Biomolecular Engineering, North Carolina State University, EMILY F ROE, Department of Materials Science and Engineering, North Carolina State University, LILIAN C HSIAO, Department of Chemical and Biomolecular Engineering, North Carolina State University — Inspired by the hydrophilic biomacromolecules adsorbed to the surface of articular cartilage, we investigate the tribology of betainized poly(2-(dimethylamino)ethyl methacrylate) (PDMAEMA) brushes grafted on soft poly(dimethyl siloxane) (PDMS) and hard silicon substrates. These polyzwitterions are known to provide excellent lubricity due to their ability to retain water in their side groups. Surfaces are hydrolyzed to introduce surface silanol groups which serve as an attachment point for a trichlorosilane initiator. After initiator deposition, PDMAEMA is grown from the surface via atom transfer radical polymerization (ATRP) and then betainized to render it zwitterionic. We measure the steady state and transient friction coefficients of the substrates as a function of brush film thickness and substrate elasticity. Our initial results suggest that use of soft, deformable substrates such as PDMS yields increased wear resistance for brush films due to a reduction in the contact pressure below the yield point of the polymer brushes. Furthermore, repetitive transient contact appears to result in increased wear resistance, with the total shearing time required for noticeable wear to occur increasing by an order of magnitude.

*NC State CBE Startup Funds
AAAS Marion Milligan Mason Award
4:06PM U33.00007: Surface Forces Apparatus Measurements Between Oppositely Charged Polyelectrolyte Brushes as a Function of Ionic Strength  DEAN MASTROPIETRO (Presenter), MATTHEW TIRRELL, Argonne National Laboratory — Interactions between polyanions and polycations result in polyelectrolyte complexation and the formation of polymer dilute (aqueous) and polymer rich (coacervate) phases. Understanding the forces governing the formation and stability of these complexes as well as their dependence on solution conditions is of great interest. We directly measure the interactions between densely grafted, apposing polycationic and polyanionic brushes as a function of ionic strength using the surface forces apparatus (SFA). Additionally, we compare these force profiles with SFA measurements between apposing polyanionic brushes and between apposing polycationic brushes.

4:18PM U33.00008: Tribology of soft colloidal microgels: An oral perspective*  [Invited] ANWESHA SARKAR (Presenter), Univ of Leeds — Oral tribology is emerging as a new paradigm in the tribology field to quantify friction in soft sliding contact surfaces\(^1\). Using a combination of experimental techniques and theoretical considerations, this talk will cover three case studies\(^2\)\(^-\)\(^4\) on tribology of soft elastomeric surfaces (with different wetting properties) in the presence of biopolymeric microgels with well-defined deformability, designed using variable cross-linking densities and particle sizes. Some of these microgels show aqueous ‘ball-bearing’ abilities depending upon their volume fraction\(^2\). A case study\(^4\) will be presented on how these microgels can act as viscosity modifiers of the continuum, where the lubrication performance can be quantitatively described using the Newtonian plateau value ($\eta_\infty$). Finally, ongoing research on development of novel soft tribo-surfaces to emulate the highly sophisticated oral mucosal surfaces engineered by the nature will be highlighted \(^1\).

References

*The European Research Council (ERC) is acknowledged for its financial support (757993).
Pore-size dependence and glassy behavior of hydrogel friction on smooth surfaces

**NICHOLAS CUCCIA, SURAJ POTHINENI, BRADY WU, JUSTIN BURTON**
(Presenter), Physics, Emory University — Hydrogels are important in many scientific and engineering applications due to their tunable physiochemical properties and bio-compatibility. Bulk hydrogels consist of a crosslinked polymer matrix imbibed with water or a similar solvent at volume fractions that can exceed 90%, leading to a rich spectrum of interfacial rheological behaviors. Using a custom-built, continuous pin-on-disc tribometer, here we identify three distinct regimes of frictional behavior for both polyacrylamide (PAAm) and agarose hydrogel spheres on smooth surfaces. At low velocities, friction is controlled by hydrodynamic flow through the porous hydrogel network, and is inversely proportional to the characteristic pore size. At high velocities, a mesoscopic, lubricating liquid film forms obeying elastohydrodynamic theory. In between these regimes, the frictional force sharply decreases with velocity and simultaneously displays time-dependent behavior characteristic of glassy, slow relaxation over several minutes. This relaxation strongly depends on the fluid shear rate, and the transition can be tuned by varying the solvent salt concentration, solvent viscosity, and sliding geometry at the interface.

*This work was funded by NSF DMR 1455086.*

Study of the tribological behavior of hydrogel-like materials with an extended Surface Forces Apparatus

**ROSA M. ESPINOSA-MARZAL** (Presenter), TOOBA SHOAIB, University of Illinois at Urbana-Champaign — Biological tribosystems are excellent examples of nature leveraging material properties to achieve exceptional lubrication for prolonged periods of activity. In these systems, lubrication is provided by hydrogel-like surface layers and an aqueous lubricant. Our research aims to advance the knowledge about the relation between frictional dissipation and hydrogel's microstructure. In this talk, we will present steady and dynamic shear measurements with an extended surface forces apparatus (eSFA) on hydrogel thin films under modulated compression. Complimentary quasi-equilibrium compression measurements with the eSFA can be performed during tribological measurements; this is a unique capability of the SFA and enables to detect polymer rearrangements upon shear. This type of experiments provides new insight into the influence of hydrogel's microstructure on dissipative mechanisms that dictate lubrication with special emphasis on the influence of hydrogel's microstructure.

*National Science Foundation Grant No. 17-61696.*
5:18PM U33.00011: Indentation of a microparticle into an oil-coated, soft silicone surface
JUSTIN GLOVER, JONATHAN PHAM (Presenter), Univ of Kentucky — Small scale contact between a
soft, liquid-coated layer and a stiff surface is found in many situations, from synovial fluid on
articular cartilage to adhesives in humid environments. Moreover, many model studies on soft
adhesive contacts are conducted with soft silicone elastomers, which usually possess
uncrosslinked molecules (i.e. liquid silicone oil) when the modulus is low. The presence of liquid
near the contact line can cause capillary forces on the particle. We consider a similar situation in
which uncrosslinked liquid molecules are already placed at a surface prior to contact. More
specifically, we investigate how the thickness of an oil layer relates to the indentation depth of a
glass microsphere into a lightly crosslinked PDMS network. A simple model that balances the
capillary force of the oil layer with the elastic force from the substrate is proposed to predict the
position of the particle. Interestingly, the vertical force associated with a thin layer of liquid on a
soft substrate appears to govern the indentation depth of a microsphere into the polymer
network.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U34 DPOLY FIAP DMP: Organic Electronics II: Charge Transport
and Theory 506 - Stephanie Lee, Stevens Inst of Tech - Tag(s): Focus

2:30PM U34.00001: Electro-reflectance study of low-voltage turn-on in triplet fusion OLED
materials  SEBASTIAN ENGMANN (Presenter), Theiss Research, EMILY BITTLE, LEE RICHTER, DAVID
JAMES GUNDLACH, National Institute of Standards and Technology — Coherent spin processes like
singlet-fission (SF) and triplet fusion (TF) are gaining in interest to the scientific community, as SF
could lead to an increase in performance of organic photovoltaics and TF in the emission
efficiency of OLED devices. Recently reported results have suggested that higher order effects
such as TF lead to a reduction of the luminescence turn-on voltage and is necessary for what was
referred to as “sub-band gap turn-on”. However, we have shown that heterojunction band
alignment can describe the low voltage turn-on. In this presentation we will present electro-
reflection (ER) studies that elucidate the built-in potentials in 2 prototypical OLED devices based
on Rubrene and DiFTES-ADT as the emitting layer. The results are put into context of the low
luminescence turn-on, which is observed in both cases, and potential higher order effects.
Furthermore, differences in the luminescence - current density-voltage-characteristics, L-J-V and
magneto-electro-luminescence, MEL, between the two systems will be presented. A kinetic model
captures zero field splitting and various exciton and charge carrier recombination pathways.
**2:42PM U34.00002: The rationale behind the acceptor-donor-acceptor chemical design of non-fullerene acceptors**

ANASTASIA MARKINA (Presenter), Theory Group, Max Planck Institute for Polymer Research, FREDERIC LAQUAI, Solar Center, King Abdullah University of Science and Technology, DENIS ANDRIENKO, Theory Group, Max Planck Institute for Polymer Research — Efficiencies of organic solar cells have seen a rapid increase due to the development of non-fullerene acceptors (NFAs). We explain why excitons dissociation into charge-transfer (CT) states, and the subsequent CT state splitting into charge-separated (CS) states, are efficient in NFAs-based solar cells. We show that the driving force of the excited-to-CT state transition comes from a stronger dielectric stabilization of charges compared to the localized excited state. CT-to-CS transition is driven by the gradient of the acceptor concentration, which bends the electrostatic potential, helping to overcome the Coulomb binding of the CT state. Both effects depend on the related molecular quadrupole moments and their long-range contribution to the solid-state ionization energies and electron affinities.

The results are supported by simple lattice models, as well as atomistic-level descriptions performed for a number of solar cells based on the polymer donor PCE10 and small molecule NFAs. These include IEICO, IEICO-4F, IEICO-4Cl, O-IDTBR, O-IDTBCN, ITIC, ITIC-4F, ITIC-4Cl. The present study suggests several design rules for NFAs with efficient charge separation in photovoltaic applications.

*AM acknowledges support from the Alexander von Humboldt foundation.

**2:54PM U34.00003: Engineering Diffusion of Charge-Transfer States at Organic Semiconductor Heterojunctions**

NOLAN CONCANNON (Presenter), TAO ZHANG, RUSSELL J HOLMES, University of Minnesota — Interfacial excited states formed at electron donor-acceptor heterojunctions, called charge-transfer (CT) states, are essential intermediates for organic photovoltaic and light-emitting devices. While CT states are known to diffuse, questions remain around the underlying transport mechanism and the materials parameters that determine the diffusion length. In this work, we examine CT state diffusion in donor-acceptor mixtures via photoluminescence quenching methods. The diffusion length is extracted across donor and acceptor type as well as relative composition. In general, we find that CT states are at least as mobile as their bulk counterparts, despite being confined to an interface. Further, the energy of the CT state, and the presence of low-lying triplet states do not strongly determine the scale of the diffusion length. We instead find a correlation between the diffusion length and the mobility of the slowest component charge carrier. The connection between charge carrier transport and CT state diffusion suggests strategies to engineer CT state migration in various devices. These conclusions may also elucidate CT state transport at hybrid interfaces of organic and inorganic semiconductors.
First-Principles Theory for Understanding Excitons in Stacked Organic Assemblies* [Invited] SAHAR SHARIFZADEH (Presenter), Boston University — Organic semiconductors are tunable light absorbers with promise as solar energy conversion materials, with their efficiency highly dependent on the nature and energy of electron-hole pairs or excitons formed upon light absorption. Excitons in these materials are controlled by the interplay between inter- and intra-molecular electronic as well as vibrational interactions, which is not yet well-controlled in devices. Here, we utilize first-principles theory to investigate the optoelectronic and vibrational properties of stacks of functionalized PTCDI DNA base surrogates as a model system to study inter- and intra-molecular interactions. We apply time-dependent density functional theory, along with a Franck-Condon analysis of vibronic effects, to finite stacks of molecules that have been recently synthesized. We determine that the intra- and inter-molecular interactions result in distinct vibrational, electronic, and optical properties. For a periodic assembly of PTCDI, many-body perturbation theory predicts a bandstructure with significant bandwidth (~0.8 eV), consistent with strong inter-molecular electronic interactions, and several spatially delocalized low-energy optically excited-states. By incorporating electron-phonon interactions, we find that at T = 300K, the optical absorption is altered from T = 0 K due to allowed indirect transitions, while exciton delocalization and binding energy, a measure of intermolecular electronic interactions, remains constant. Overall, this work demonstrates that excitonic properties can be modified via inter-molecular electronic and vibrational interactions.

*The author acknowledges financial support from the National Science Foundation (DMR-1610031, DMR-1847774).

Quantum Yield Enhancement of BDMO-PPV During Photo-Degradation MATTHEW DEUTSCH (Presenter), HEUNGMAN PARK, Texas A&M University, Commerce — Poly-2,5-bis(3',7'-dimethyloctyloxy)-1,4-phenylenevinylene (BDMO-PPV) is a photoluminescent semiconducting polymer similar to other well-studied polyphenylene vinylenes such as MEH-PPV and MDMO-PPV. This family of organic semiconductors has similar emission spectra and absorption spectra due to their backbone structure. However, side-chain structures between different polyphenylene vinylene (PPV) derivatives can result in different optoelectrical and material properties. PPVs are known for their instability, degradation, and low efficiency - a barrier for use in organic electronic devices. BDMO-PPV exhibits enhanced internal and external quantum yield while degrading in organic solvents such as chloroform and toluene. A proposed highly emissive intermediate state during photodegradation is responsible for an increase in internal and external quantum yield. Using photoluminescence spectroscopy, infrared spectroscopy, and light scattering measurements we intend to define the physical and chemical processes behind the photo-degradation of BDMO-PPV.
Photospintronics- Light-controlled spin transport in hybrid chiral oligopeptide-nanoparticle structures*  RUPSHALI ROY (Presenter), Indian Institute of Engineering Science and Technology, Shibpur — It has been found the transmission of electrons through chiral molecules depends on their spin orientation; this is known as chiral induced spin selectivity. This effect makes it feasible to build spintronic devices without ferromagnetic spin injectors since the chiral molecules themselves serve to choose a specific spin to transfer across the molecules. We began building a device which would aid in furthering research on spintronics. It consists of an Si substrate, plated with a layer of Ni, a ferromagnetic material, further coated by a layer of gold, as the base layer. In the hybrid system studied therein. Helical chiral molecules of cysteine hydrochloride were attached on one end to the base layer mentioned above, and on the other end to a MoS$_2$ thin film.

The chiral molecules taken in this case were right helical structures. When right circularly polarized light is shined on the device, electron hole pairs are generated and those electrons with right handed spin are excited and are selected to move through the chiral molecules. Vice versa occurs when the chirality or polarisation is reversed.

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Collaborated with A. Singha and S. Masanta from the Bose Inst.

Morphology-Dependent Triplet Exciton Diffusion in Vapor Deposited Pentacene Thin Films  KAICHENG SHI (Presenter), IAN CURTIN, ANDREW HEALY, TAO ZHANG, DAVID BLANK, RUSSELL J HOLMES, University of Minnesota — Singlet exciton fission is among the most efficient multiexciton-generation process reported to date. Materials exhibiting singlet fission can potentially generate two triplets for each photogenerated singlet, and are of interest for a variety of applications in photoconversion and light-emission. While the kinetics of fission have been previously examined, fewer works have sought to probe the diffusion length of the resulting non-luminescent triplet state. Here, we probe triplet exciton diffusion in thin films of the archetypical singlet fission material pentacene using a device-based methodology capable of extracting the intrinsic, materials-relevant exciton diffusion length. The dependence of triplet exciton diffusion on morphology and crystalline grain size is probed by varying thin film deposition rate. Increased grain size leads to an increase in exciton lifetime, and a commensurate improvement in the triplet diffusion length. For a change in growth rate from 10 Å/s to 0.05 Å/s, the triplet diffusion length increases from 16.3 nm to 22.0 nm. These results offer an additional handle on how to maximize the triplet exciton diffusion length with optimization of thin film processing conditions.
4:18PM U34.00008: Polaronic effects and charge transport in donor-acceptor semiconducting polymers*  XIAO WANG (Presenter), LEONARD F REGISTER, ANANTH DODABALAPUR, University of Texas at Austin — Molecular polaron theories, when applied to high mobility donor-acceptor semiconducting polymers along the chain, indicate that polaronic effects can be very small. These effects include changes to the electronic bandwidth and effective mass resulting from the strong coupling of phonons with charge carriers.\(^1\) The bandwidth and effective mass remain essentially unchanged with increasing temperature and are adequate for band transport to take place along the chain. However, the small mean free path obtained from the polymer mobility is still an obstacle in understanding band transport in polymers. We invoke the statistical distribution of carrier free paths and consider the carriers with small free paths as effectively localized due to strong scattering. Only carriers with adequately large free paths can participate in band transport.\(^2\) For such carriers, we are able to apply the Boltzmann Transport Equation with appropriate scattering mechanisms to calculate band mobility and the results are in good agreement with experimental data.


*The authors acknowledge partial financial support from the National Science Foundation under Grant No. EEC-1160494

4:30PM U34.00009: Switching dynamics in Croconic Acid thin film*  XUANYUAN JIANG (Presenter), PRATYUSH P BURAGOHAIN, SHASHI PODDAR, HAIDONG LU, ALEXEI GRUVERMAN, XIAOSHAN XU, University of Nebraska - Lincoln — Croconic Acid (CA) exhibits ferroelectricity due to proton displacement between molecules. The voltage and pulse duration dependence of polarization switching in CA thin film are studied using piezoresponse force microscopy (PFM). From this study, the microscopic mechanism of CA polarization switching is revealed. And the KAI domain growth model is used to fit with this switching dynamic behavior. From the fitting, the dimensionality of domain wall, the nucleation activation energy and other structural parameters are obtained. Also, the dependence of film thickness and substrate effect for CA switching are investigated. This study should be helpful for the control experiments in the ferroelectric devices and organic spin-valves using CA as the spacer.

*This work is primarily funded by the U.S. Department of Energy, Office of Science. (Grant DE-SC0019173)
4:42PM U34.00010: Self-assembled monolayer formation of linear molecules onto a FCC(111) surface*  EDUARDO CISTERNAS (Presenter), Univ de La Frontera, GONZALO DOS SANTOS, Facultad de Ingeniería, Universidad de Mendoza, MARCOS FLORES, Physics, Universidad de Chile, EUGENIO VOGEL, Univ de La Frontera, ANTONIO JOSE RAMIREZ-PASTOR, Physics, Univ. Nac. San Luis, Argentina — The self-organization of molecules deposited over different surfaces have interesting technological applications. The adsorption of linear molecules as well the formation of self-assembled monolayers are considered in response to the experimental evidence for curcuminoids over gold surfaces. These processes are mainly controlled by the surface-molecule and molecule-molecule interactions. By performing computational calculations based on the density functional theory, we have obtained interaction energies for different configurations of two adsorbed molecules over a Au(111) surface. Such molecules were approximated to linear pentamers while the gold surface corresponds to a triangular lattice. This model system was investigated under the framework of Grand Canonical Monte Carlo simulations paying special attention to two quantities: the surface coverage and an order parameter reflecting the molecular alignment over the surface. As expected, the surface coverage is directly proportional to the system pressure (chemical potential). However, for critical values of the chemical potential the molecules present patterns evidencing nematic transitions.

*The following Chilean sources partially funded this work: Fondecyt (1190036 and 1197799), Millenium Nucleus Multimat and Cedenna.

4:54PM U34.00011: Controlling energy levels and Fermi level en route to fully tailored energetics in organic semiconductors [Invited]  ROSS WARREN, ALBERTO PRIVITERA, PASCAL KAIENBURG, ANDREAS EJDRUP LAURITZEN, Department of Physics, University of Oxford, OLIVER THIMM, IEK5-Photovoltaics, Forschungszentrum Jülich, JENNY NELSON, Department of Physics, Imperial College London, MORITZ RIEDE (Presenter), Department of Physics, University of Oxford — Organic semiconductors have yet to achieve simultaneous control over both the energy levels and Fermi level, which was a key breakthrough for inorganic electronics. Here, we combine two approaches from band engineering and molecular doping to demonstrate controlled shifts in ionisation potential and Fermi level of an organic thin film. We experimentally investigate the doping efficiency of a ternary blend system consisting of two host molecules, ZnPc and F8-ZnPc, and the p-dopant F6–TCNNQ. We explain the observed doping behaviour with a statistical model based on energy level shifts of both host and dopant materials, resulting from the quadrupole moments of all involved molecules. We thereby demonstrate that band tuning crucially affects the doping process in organic semiconductors. The practice of comparing host and dopant energy levels must consider the long-range electrostatic shifts, arising from the quadrupole interactions to consistently explain the doping mechanism in organic semiconductors.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U35 DPOLY DSOFT GSOFP DBIO: Rheology and Dynamics of Polymers and Polyelectrolytes 507 - Vivek Sharma, Univ of Illinois - Chicago - Tag(s): Focus
2:30PM U35.00001: Polyelectrolyte solutions in complex macro- and micro-scale flows
[Invited] ATHENA E METAXAS, VISHAL PANWAR, CARI DUTCHER (Presenter), University of Minnesota — Studying the behavior of polymer and polyelectrolyte solutions under complex hydrodynamic flow conditions is of interest to a variety of processes, such as extrusion, coating, and flocculation. Often these flow fields include combinations of both shear and extension flows, requiring characterization of the shear and extensional rheology for optimized materials processing. Here, the behavior of polymer solutions in two flow fields will be discussed: Taylor-Couette flows and microfluidic flow-focusing. First, in Taylor-Couette flow, which is flow between two concentric, rotating cylinders, the complex solutions are subjected to a wide variation of hydrodynamic flow states. The addition of non-Newtonian polymer solutions increases the solution's elasticity, which in turn can modify flow states that are typically dominated by inertial forces. In this study, a cationic polyacrylamide was used to modify the elasticity of the solution, and with varying concentrations of NaCl to alter the ionic strength of the solution. The coil conformation and relaxation times of charged polymers changes depending on the ionic strength, from a more rigid conformation at low ionic strengths to a more flexible conformation at high ionic strengths, resulting in different non-Newtonian responses to shear. The effect of polymer conformation as a result of varying solution ionic strength on TC flows with co- and counter-rotation of the cylinders will be discussed. Second, microfluidic geometries will be used to characterize the extensional properties of low molecular weight, low viscosity polymer and polyelectrolyte solutions. Specifically, filament stretching using a cross-slot microfluidic channel will be used to resolve extensional properties of polyelectrolyte solutions at varying NaCl concentrations.

3:06PM U35.00002: Measuring packing length in simulations for different polymer architectures*
SAI VINEETH BOBBILI (Presenter), SCOTT MILNER, Pennsylvania State University — The packing length \( p \) is the range over which the density near a given monomer is dominated by monomers from the same chain. Bulky, flexible polymers have larger \( p \) while thin, stiff polymers have smaller \( p \). The packing length figures prominently in scaling predictions of the entanglement length and bulk modulus for polymer melts and solutions. \( p \) has been argued to scale as the ratio \( V/R^2 \) of chain displaced volume \( V \) and mean-square end-to-end distance \( R^2 \). This scaling works for several cases, but it is not obvious how to apply it to chains with side groups, in particular how to estimate the diameter of such a chain.

In this work, we measure the packing length, as the typical distance of closest approach of two polymer strands in a simulated bead-spring melt. We use the intermolecular correlation function to measure the distance up to which a given polymer strand dominates the volume fraction. We compare this measured packing length to our recent measurements of the entanglement length in simulations. Using our measured packing length, we find good agreement of entanglement properties with the Lin-Noolandi ansatz for flexible polymers of different architectures, which we explore by varying chain stiffness and sidegroup lengths.

*We acknowledge funding from NSF grant no. DMR1507980
3:18PM U35.00003: Influence of Sodium Salts on the Swelling and Rheology of Hydrophobically Crosslinked Hydrogels Determined by QCM-D*  
BRYAN VOGT (Presenter), Pennsylvania State University, MENGXUE ZHANG, University of Akron, JACK DOUGLAS, NIST — Hydrophobically modified copolymers provide a versatile platform of hydrogel materials for diverse applications, but the influence of salts on the swelling and material properties of this class of hydrogels has not been extensively studied. Here, we investigate model hydrogels with three different sodium salts with anions chosen from the classic Hofmeister series to determine how these counterions influence the swelling and mechanical properties of neutral hydrogels. Our measurements utilize a quartz crystal microbalance with dissipation (QCM-D) to quantify both swelling and rheological properties of these gels. Overall, the observed trends are broadly consistent with more kosmotropic ions causing diminished solubility (‘salting out’) and strongly chaotropic ions causing improved solubility (‘salting in’), a trend characteristic of the Hoffmeister series governing the solubility of many proteins and synthetic water soluble polymers, but trends in the shear stiffness with gel swelling are clearly different from those normally observed in chemically cross-linked gels.

*This work was supported by a grant from the National Science Foundation (CBET-1606685).

3:30PM U35.00004: Effects of humidity on the rheology of supramolecular organogels  
DIMITRIS VLASSOPOULOS (Presenter), EMMANOUIL VEREROUDAKIS, Institute of Electronic Structure & Laser — It is known that organic oils typically contain tiny amounts of water (0.01% by weight) which can influence the self-assembly as well as the macroscopic properties of supramolecular gelators. We explore here the rheological consequences of this phenomenon which has been overlooked. Specifically, we investigate the properties of biphenyl tricarboxamides (BPTA) in dodecane which exhibit structural transitions with varying temperature. The driving force behind these transitions is the fact that the humidity content of the supramolecular polymer changes with temperature. We perform shear rheological measurements under controlled humidity conditions in both humid (~60% relative humidity) and dry (~5% relative humidity) conditions and observe that in a humid environment the linear and nonlinear rheological properties are substantially affected by the temperature. At temperatures where the systems strongly interacts with water the plateau modulus is lower, the relaxation faster and there is absolutely no sign of strain hardening behaviour. These findings are discussed in the context of existing theories of living polymers. It is concluded that humidity effects cannot be ignored when working in oily environments.

Rheology of Jammed Silicone Microgels

SENTHILKUMAR DURAIVEL (Presenter), Department of Materials Science and Engineering, University of Florida, THOMAS ANGELINI, Department of Mechanical and Aerospace Engineering, University of Florida — Colloidal and granular-scale hydrogel particles have been widely used to study jammed and glassy matter in systems with soft inter-particle potentials. Aqueous microgels are most commonly used for these investigations and a diversity of chemical formulations have been developed for controlling inter-particle interactions, microgel size, and particle stiffness. However, there are numerous industrial applications of non-aqueous microgels, creating the need for the fundamental understanding of the rheology of jammed non-aqueous microgels. In this presentation, we will describe our investigations of polydimethylsiloxane (PDMS) microgels. We synthesize PDMS microgels using several different silicone formulations and swell them to a jammed state in silicone oil. The size and the shape of the microgels are varied during synthesis and the resulting effect on the rheological properties of the microgels are studied. By independently varying microgel composition and solvent viscosity, we can independently tune the yield stress and flow characteristics of this jammed system.

Predicting the plateau modulus from molecular parameters of conjugated polymers

ABIGAIL FENTON (Presenter), RALPH H COLBY, ENRIQUE D GOMEZ, Pennsylvania State University — The relationship between Kuhn length $b$, packing length $p$, and plateau modulus $G_N^0$ initially proposed by Graessley and Edwards and experimentally investigated by Everaers, while well-studied for flexible and stiff polymers, has a large gap in experimental data between the flexible and stiff regimes. This gap prevents the validation of theoretical models of the crossover between flexible and stiff polymers and therefore, the prediction of mechanical properties from chain structure of any polymer in this region. Given the chain architecture, including a semiflexible backbone and side chains, conjugated polymers are an ideal class of material to study this cross-over region. Using small angle neutron scattering (SANS), static light scattering (SLS), and oscillatory shear rheology along with the freely rotating chain model we have shown that nine non-crystalline conjugated polymers and three aromatic polymers not only populate a large part of this gap, but that they follow the proposed relationship between $b$, $p$, and $G_N^0$ as well. We have also experimentally validated the freely rotating chain model for various conjugated polymers using SANS and SLS and find good agreement in Kuhn length values from 1.7 nm in aromatic polymers up to 23.2 nm in conjugated polymers.

*NSF DMREF, NIST NCNR
4:06PM U35.00007: Accessing Viscoelasticity of PDMS at MHz Frequencies: Physically Intuitive Continuum Mechanics Model for QCM Able to Treat Film Resonance Region
YANNIC GAGNON (Presenter), JUSTIN BURTON, CONNIE ROTH, Emory University — Quartz crystal microbalance (QCM) is increasingly applied as a MHz-rheometer to measure viscoelastic properties of films beyond the simple Sauerbrey equation relating frequency shifts to mass loading of the crystal. For films, the range of harmonics available is often limited by needing higher harmonics to access where frequency shifts become sensitive to the film’s viscoelasticity, while avoiding the film resonance region where shifts and dissipation become large. Film resonance corresponds to the harmonics that form standing acoustic waves in the film. Most QCM modeling applies simplifications assuming small resonance shifts, like the small load approximation, which are not valid under film resonance. This limits the range of film thicknesses whose viscoelasticity can be accurately measured, especially for rubbery films where film resonance occurs at lower harmonics. We present a physically intuitive continuum mechanics model with no small frequency-shift approximations that can numerically treat film resonance, accessing a wider range of film thicknesses. Fits for polydimethylsiloxane (PDMS) films, including film resonance conditions, give shear modulus values in good agreement with interpolated literature values from kHz and GHz frequencies.

4:18PM U35.00008: Viscoelastic properties of tightly entangled polymeric systems*
TADASHI INOUE (Presenter), Osaka Univ — The rheology of semiflexible polymer solutions has attracted much attention now because it provides a basis for fundamental understanding the physical properties of cellulose nanofibers, which have been considered to be a new material for sustainable society. This talk describes recent experimental findings on the rheology of semiflexible polymers including cellulose derivatives and DNA. In addition to the orientational stress of the viscoelastic segment, the bending and tension modes of the segment contribute to the viscoelasticity of the semiflexible polymer solution. In particular, in tightly entangled systems, where the entanglement length is shorter than the persistent length, the bending mode significantly contributes to the viscoelasticity of the rubbery plateau region. In this talk, by combining simultaneous measurement of strain-induced birefringence, the mode separation of orientation, bending, and tension is carried out on on the linear viscoelasticity of the model materials, and the contribution of each mode is quantitatively discussed.

*This research was financially supported by JSPS KAKENHI (Grant Number JP19H02777).
Recent NEMD simulations of an entangled polyethylene melt revealed that within intermediate extensional rates, entangled melts could undergo a coil-stretch transition, and exhibit bimodal configurational distributions with peaks corresponding to coiled and stretched configurations. Furthermore, it was shown that through a configurational microphase separation, the coiled molecules develop distinct domains surrounded by stretched molecules. On the other hand, various experimental studies have shown that the response of entangled polymeric melts to elongational flow fields could be very different from those of entangled solutions depending on the solvent molecule architecture. Such complexities bring up many questions about the coil-stretch transition in entangled polymeric liquids. Do entangled solutions undergo a coil-stretch transition? Do they experience any configurational or chemical microphase separation?

To address these questions, we performed a series of NEMD simulations for entangled \( C_{1000}H_{2002} \) polyethylene solutions in oligomeric \( C_{16}H_{32} \) and benzene solvents. The solutions were subject to planar elongational flows within a wide range of extension rates. The simulations revealed both similarities and differences between entangled melts and solutions that will be discussed.

**Predicting the Microstructure of Bottlebrush Copolymers**

- **CHRISTIAN TABEDZKI** (Presenter), **ROBERT RIGGLEMAN**, University of Pennsylvania — The unique structure of bottlebrush polymers, a typically linear polymer backbone with densely grafted polymer side-chains, allows for the creation of interesting and unique morphologies. By combining structurally dissimilar backbone and grafts, copolymer bottlebrushes serve as candidates for materials with unique combinations of properties. An example includes polymers with a mechanically rigid backbone and conductive grafts, which can be useful as membranes in battery applications. In this talk, we present a field-theoretic model for the structure of bottlebrush copolymers. We systematically explore the transition from the comb to the bottlebrush regime and show how this modulates the phase diagram of the bottlebrush copolymers. Finally, we show how the chain conformations change in the various microphases in the comb and bottlebrush limits. We accomplish this via our recently developed theoretically informed Langevin dynamics (TILD) package for LAMMPS, in which field-based self-consistent forces are calculated in lieu of pair-wise interactions.

*NSF GIRE #1829436, NSF PIRE #1545884*
4:54PM U35.00011: Interactions between two knots in a stretched DNA molecule
ALEXANDER KLOTZ (Presenter), California State University, Long Beach, BEATRICE SOH, PATRICK DOYLE, Massachusetts Institute of Technology — Knots in DNA serve as a model system with which to study the physics of polymer entanglement, and are known to affect the function of genomic sequencing devices. We use microfluidic devices to stretch viral genomic DNA molecules in an elongational electric field, and observe the molecules using fluorescence microscopy. Previously, we have reported the effects that knots have on the relaxation and elasticity of single molecules, as well as the mechanisms by which knots translate along molecules and untie. Here, we discuss molecules that have two knots, and the interactions between the knots. It has been predicted computationally that in a doubly-knotted molecule an attraction exists between the knots, with a minimum in the free energy occurring when the two knots are intertwined. We see long range attraction of knots towards each other from opposite ends of the molecule over tens of seconds, in contrast to the end-migrating behavior of single knots. At short distances, pairs of knots fluctuate in and out of visual contact, remaining in proximity for tens of seconds to minutes. The distribution of intraknot distances can be used to measure free energy landscapes for the knot-knot interactions, which are qualitatively and quantitatively similar to previous computational studies.

5:06PM U35.00012: Diffusion of knots in DNA molecules confined in nanochannels
ZIXUE MA (Presenter), KEVIN D DORFMAN, University of Minnesota — Knots formed in DNA influence biological processes (e.g., DNA replication) and the accuracy of genomics technologies. Knot diffusion, which destroys knots in linear DNA molecules when the knot reaches the chain end, is a key step to understanding these processes. We present experimental data on the diffusion of knots in single DNA molecules via a combination of a nanofluidic "knot factory" device and fluorescence microscopy. Knots are first generated using pressure-driven flow, which compresses single DNA molecules against slit barriers in nanochannels. The knots are identified as bright spikes in intensity profiles of DNA backbone and their motions are tracked for 8 minutes. The ensembled-averaged data for the mean-squared displacement produce a scaling exponent that indicates that confined knots undergo subdiffusion. This result supports the theory that the knot breathing mechanism, where knot diffusion originates from a local motion of knot region, dominates knot diffusion in long polymer chains.
5:18PM U35.00013: Dynamics of DNA-bridged particle dumbbells in well-entangled, shear-banding polymer solutions under large amplitude oscillatory shear (LAOS)* SEUNGHWAN SHIN (Presenter), KEVIN D DORFMAN, XIANG CHENG, Chemical Engineering and Materials Science, University of Minnesota — Despite accumulation of experimental evidence for shear-banding flows in highly entangled polymer solutions over the last two decades, the current understanding of the conformational changes that induce shear banding remains incomplete. To elucidate the microscopic dynamics of entangled chains in shear-banding flows, we study the dynamics of DNA-bridged particle dumbbells in the shear-banding flow of well-entangled double-stranded DNA (dsDNA) solutions under LAOS using a rheo-confocal shear cell. First, we confirm that the velocity profiles of the entangled dsDNA solutions become inhomogeneous and strong shear-banding flows arise at high Weissenberg number. We then analyze the translation and orientation of particle dumbbells in the co-existing high- and low-shear rate bands. The orientational distribution of dumbbells exhibits clear difference in the co-existing bands. Moreover, we find that the coupling between sudden reorientation and rapid translational motion of dumbbells occurs exclusively in the high-shear rate band. Quantitative investigation of the spatially distinct dynamics of such dsDNA-bridged dumbbells provides new insights into the microscopic structural origin of shear-banding flows in entangled polymer solutions.

*This research is supported by NSF CBET-1700771.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U36 DMP: Physics For Everyone 601/603 - Rachel Goldman, Univ of Michigan - Ann Arbor - Tag(s): Invited, Outreach, Undergrad Friendly

2:30PM U36.00001: Using Superheroes to Engage the Public [Invited] JAMES KAKALIOS (Presenter), University of Minnesota — Costumed superheroes seem to dominate our movie and television screens, making them an excellent delivery system to bring real physics to the general public. While the super powers these characters possess clearly violate the laws of nature, often times how the super-heroes and super-villains utilize their powers is consistent with known physical laws. One can therefore leverage the public's interest in these characters to illustrate and explain the physics principles that underlie their fantastic adventures. A discussion of the strength of Spider-Man's webbing can lead to the real physics of carbon nanotubes. What metal would be strong enough for Wonder Woman's bullet deflecting bracelets? One can draw the connection between the Black Panther's vibranium suit and conservation of energy, while the Infinity Stones (the MacGuffin of the last 22 Marvel Cinematic Universe films) can be related to Emmy Noether and her theorem explicating a deep connection between all conservation principles and symmetries in the laws of physics. People come for the superhero ice cream sundae, and stay for the real science. If superheroes can help explain physics and the benefits of research to the general public – well, it wouldn't be the first time these heroes have saved the day!
3:06PM U36.00002: Physics of Star Wars [Invited]  PATRICK JOHNSON (Presenter), Georgetown University — Since he was young, Patrick has loved both science and Star Wars. As an adult, he wrote a book that tries to explain different theories as to how scenes and devices in the Star Wars universe work. Have you ever wondered how the Death Star works? How shields can stop catapults, but droids can walk right through? This talk will offer possible explanations of these scenes and more. This will be an enjoyable talk for anybody who is a fan of Star Wars, physics, or both.

3:42PM U36.00003: Science and Cooking: Making Physics Fun (and Tasty!) [Invited]  DAVID A WEITZ (Presenter), Harvard University — This talk will describe the experiences of physics course for non-scientists that makes physics fun. It uses the science of food and cooking to motivate students to learn physics. A feature of the class is a weekly guest lecture by a famous chef about cooking. In addition the course includes a lab, where you can eat your experiment. The lab consists of the recipe of the week, where students, cook, do physics experiments and plate and eat their creations. It also includes an equation of the week to teach students how to calculate results without being afraid of equations. The class has several traditions: You have to clap when you see an equation, and you have to clap when you see a cool dessert. Remember!

4:18PM U36.00004: Bringing Science to the Public Using Popular Culture [Invited]  ANISSA RAMIREZ (Presenter), Science Underground — In our modern age when many of the key issues have an underlying science component, it is critical that the general public become more comfortable with science. This talk describes the use of popular culture as a way to bring scientific ideas to life. The examples that will be highlighted show how physics and other science fields can be embedded into discussions about American football. This talk will also showcase how science can be stealthily encased in a historical context in stories about inventions. Using a forthcoming book called The Alchemy of Us as a model, this talk will show how concepts of physics, materials science, and electrical engineering can be displayed in an engaging way for a general readership. Overall, this presentation makes a case for scientists to instill a new habit of sharing their knowledge with the public by connecting on a human level.
4:54PM U36.00005: The Physics of NASCAR: How March Meeting Physicists Have Unique Opportunities to Share Physics with the Public [Invited]  DIANDRA LESLIE-PELECKY (Presenter), Trivalent Productions — Ask the average person on the street about physics and you'll probably hear about black holes, astronomy, quarks, or gravitational waves. Anyone attending the March Meeting, however, knows that most of the physics presented here has significantly more impact on the average person's life than any black hole.

Most physics outreach is aimed at a smal elite group of college-degreed, already science-interested people. But there are millions more who want -- who need -- to know about science, scientists, and how science is done. Drawing on my decade of experience sharing the science of motorsport through television, books, blogs and a regular spot on SiriusXM Satellite radio, I'll share ideas for how you can not only reach this underserved audience, but also broaden the public's perception of what physics really is. I'll also share a few things I've learned along the way: why there are lots of engineers, but few physicists, in NASCAR; the NASA technology in every NASCAR racecar; the move toward electric vehicles and sustainability; safety innovations that started on the track and moved to the interstate, and the cheap polymer component used on racecars that the military now uses on their helicopters.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U37 APS: Careers in Physics Workshop: Putting Your Science to WORK 605 - Tag(s): Careers, Undergrad Friendly

2:30PM U37.00001: Careers in Physics Workshop: Putting Your Science to WORK — In this informative workshop, celebrated career coach and author Peter Fiske provides advice and strategies for taking your physics job search to the next level, including tips for self-assessment, network building, resume writing, interviewing, and salary negotiation. Don't miss this great opportunity to get some great help on taking your next steps. This workshop is free.

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U38 DQI: Landauer and Bennett Award Session: Quantum Resource Theories and Thermodynamics 607 - Todd Brun, Univ of Southern California

2:30PM U38.00001: Rolf Landauer and Charles H. Bennett Award in Quantum Computing talk [Invited]  FERNANDO BRANDÃO (Presenter), Caltech — tbd
3:06PM U38.00002: Resource theory of asymmetric distinguishability*  XIN WANG, Institute for Quantum Computing, Baidu Research, MARK WILDE (Presenter), Louisiana State University, Baton Rouge — We systematically develop the resource-theoretic perspective on distinguishability. The theory is a resource theory of asymmetric distinguishability, given that approximation is allowed for the first quantum state in general transformation tasks. We introduce bits of asymmetric distinguishability as the basic currency in this resource theory, and we prove that it is a reversible resource theory in the asymptotic limit, with the quantum relative entropy being the fundamental rate of resource interconversion. We formally define the distillation and dilution tasks, and we find that the exact one-shot distillable distinguishability is equal to the min-relative entropy, the exact one-shot distinguishability cost is equal to the max-relative entropy, the approximate one-shot distillable distinguishability is equal to the smooth min-relative entropy, and the approximate one-shot distinguishability cost is equal to the smooth max-relative entropy. We also develop the resource theory of asymmetric distinguishability for quantum channels. For this setting, we prove that the exact distinguishability cost is equal to channel max-relative entropy and the distillable distinguishability is equal to the amortized channel relative entropy.

*XW acknowledges DoD, & MMW NSF grant 1907615.

3:18PM U38.00003: Quantifying non-Markovianity: a quantum resource-theoretic approach*  NAMIT ANAND (Presenter), TODD BRUN, Univ of Southern California — We study quantum non-Markovianity as a resource theory and introduce the robustness of non-Markovianity: an operationally-motivated, optimization-free measure that quantifies the minimum amount of Markovian noise that can be mixed with a non-Markovian evolution before it becomes Markovian. We show that this quantity is a bonafide non-Markovianity measure since it is faithful, convex, and monotonic under composition with Markovian maps. A two-fold operational interpretation of this measure is provided, with the robustness measure quantifying an advantage in both state and channel discrimination tasks. Moreover, we connect the robustness measure to single-shot information theory by using it to upper bound the min-accessible information of a non-Markovian map. Furthermore, we provide a closed-form analytical expression for this measure and show that, quite remarkably, the robustness measure is exactly equal to half the Rivas-Huelga-Plenio (RHP) measure [Phys. Rev. Lett. 105, 050403 (2010)]. As a result, we provide a direct operational meaning to the RHP measure while endowing the robustness measure with the physical characterizations of the RHP measure.

*This work was supported in part by NSF Grant No. QIS-1719778.
3:30PM U38.00004: log singularities in studying quantum capacities  VIKESH SIDDHU
(Presenter), Carnegie Mellon University — Understanding the quantum capacity of a quantum channel is a long standing issue which lies at the center of quantum information theory. Determining the quantum capacity of a general channel or checking that it is positive is difficult. A major source of this difficulty arises due to non-additivity of the one-shot quantum capacity. In this work, we present a new method for checking positivity and non-additivity of the one-shot quantum capacity. This method is based on logarithmic singularities of the von-Neumann entropy. Using this log singularity method, we find a new type of non-additivity where using two very simple channels in parallel, one that doesn't have quantum capacity and a second that has positive one-shot quantum capacity, produces a channel whose one-shot quantum capacity exceeds that of the second channel.

3:42PM U38.00005: Quuantum Simplicity: Complexity Science in a Quantum World* MILE GU (Presenter), School of Physical and Mathematical Sciences, Nanyang Technological University — Complexity and quantum science appear at first to be two fields that bear little relation. One deals with the science of the very large – seeking the understand how unexpected phenomena can emerge in vast systems consisting of many interacting components. Quantum theory, on the other hand, deals with particles at the microscopic level and is usually considered limited to the domain of individual photons and atoms. Yet, different as they appear, there is growing evidence that in interfacing ideas from quantum and complexity science, we may unveil new perspective in either both fields.

Here, I introduce computational mechanics, a branch of complexity science captures structure by building the simplest causal models of natural observations. I illustrate how many processes that require complex classical models may be simulated by remarkably simple quantum devices, and describe recent experiments to test this laboratory conditions [1-3]. I survey the potential consequences these developments, highlighting how the indicate that fundamental notions of structure, complexity and causality [4]

References:
[1] Nature Communications 3, 762

*Singapore National Research Foundation Fellowship NRFNRFF2016-02.
Coherence cost for measurement and computation under conservation laws

HIROYASU TAJIMA (Presenter), Kyoto Univ, NAOTO SHIRAISHI, Gakushuin university, KEIJI SAITO, Keio university, HIROSHI NAGAOKA, The University of Electro-Communications — Nature imposes many restrictions on the operations that we perform. Among such restrictions, the restriction imposed by conservation laws on two types of the basic operations of quantum information processing, i.e. measurements and unitary operations, has been studied for a particularly long time.

One of the open problems in this field is to clarify the amount of required resource for implementing unitary operations and measurements under conservation laws. Here, we provide a solution to this open problem.

We derive two asymptotically exact equalities that clarify the necessary and sufficient amount of quantum coherence as a resource to implement an arbitrary unitary operation and a measurement for arbitrary physical quantities within a desired error, respectively. This work provides an optimal improvement of the Wigner-Araki-Yanase-Ozawa theorem and a proof of the long standing conjecture that WAY-type tradeoff relation holds for the implementation of an arbitrary unitary channel under conservation laws.

It also clarifies the key question of the resource theory of the quantum channels in the region of resource theory of asymmetry, for the case of unitary channels.

The technical details of this work are in [PRL \textbf{121}, 110403], [arXiv:1906.04076] and [arXiv:1909.02904].

Fusion rules from entanglement*

BOWEN SHI (Presenter), Ohio State Univ - Columbus, KOHTARO KATO, IQIM, Caltech, ISAAC H KIM, Physics, Stanford University — We derive some of the axioms of the algebraic theory of anyon [A. Kitaev, Ann. Phys., 321, 2 (2006)] from a conjectured form of entanglement area law for two-dimensional gapped systems. We derive the fusion rules of topological charges and show that the multiplicities of the fusion rules satisfy these axioms. Moreover, even though we make no assumption about the exact value of the constant sub-leading term of the entanglement entropy, this term is shown to be equal to the logarithm of the total quantum dimension of the underlying anyon theory. These derivations are rigorous and follow from the entanglement area law alone. More precisely, our framework starts from two local entropic constraints, which are implied by the area law. They allow us to prove what we refer to as the isomorphism theorem, which enables us to define superselection sectors and fusion multiplicities without a Hamiltonian. These objects and the axioms of the anyon theory are shown to emerge from the structure and the internal self-consistency relations of an object known as the information convex.

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The Government of Canada.
IBM T. J. Watson research center.
Simons Foundation.
NSF PHY-1733907.
4:18PM U38.00008: Nonequilibrium work relations of open quantum systems in one-time measurement scheme*  AKIRA SONE (Presenter), Los Alamos National Laboratory, YI-XIANG LIU, PAOLA CAPPELLARO, Massachusetts Institute of Technology — Because of the ambiguity in defining work and heat in open quantum systems, it is challenging to formulate non-equilibrium work relations for general quantum channels, beyond the unital case. To overcome this challenge, here we introduce well-defined notions of quantum heat and work in open quantum systems, based on the notion of guessed state defined by the one-time measurement scheme, as developed in [Phys. Rev. E 94, 010103(R)]. This allows us to derive non-equilibrium work relations for general quantum channels, and formulate a modified maximum work theorem with respect to the defined “guessed” quantum work.

*This work is in part supported by ARO MURI W911NF-11-1-0400 and MIT MIST-FVG. AS acknowledges Thomas G. Stockham Jr. Fellowship from MIT, and he is currently supported by the U.S. Department of Energy and by the Center for Nonlinear Studies at Los Alamos National Laboratory.

4:30PM U38.00009: An ergodic theorem for homogeneously distributed quantum channels with applications to matrix product states*  RAMIS MOVASSAGH, IBM TJ Watson Research Center, JEFFREY SCHENKER (Presenter), Michigan State Univ — Quantum channels represent the most general physical changes of a quantum system. We consider ergodic sequences of channels, obtained by sampling channel valued maps along the trajectories of an ergodic dynamical system. Such maps vastly generalize stochastically independent maps (e.g., random independence) or equality of the channel maps (i.e., translation invariance). The repeated composition of an ergodic sequence of maps could represent the effect of repeated application of a given quantum channel subject to arbitrary correlated noise or decoherence. Under such a hypothesis, we obtain a general ergodic theorem showing that the composition of maps converges exponentially fast to a rank-one -- entanglement breaking-- channel. As an application, we describe the thermodynamic limit of ergodic Matrix Product States and derive a formula for the expectation value of a local observable and prove that the 2-point correlations of local observables in such states decay exponentially in the bulk with their distance.

*National Science Foundation #1900015
4:42PM U38.00010: Quantifying Structure and Information Processing in One-Dimensional Quantum Systems* DAVID GIER (Presenter), JAMES P CRUTCHFIELD, University of California, Davis — We develop a framework for studying one-dimensional quantum systems with stationary, ergodic dynamics and introduce quantum information properties related to the von Neumann entropies of blocks of qubits within a structured chain. Some of the resulting statistical features are unique to quantum systems and others can be recreated with purely classical ensembles. Applying sequential measurements on these quantum states yields classical stochastic processes whose information properties are determined by the structure of the initial quantum state and the measurement protocol. Examples states with short- and long-range entanglement, as well as specific Hamiltonian ground states are analyzed within this framework.

*This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. 1650042.

4:54PM U38.00011: Measurement-Induced Randomness and Structure in Controlled Qubit Processes ARIADNA VENEGAS-LI (Presenter), ALEXANDRA JURGENS, JAMES P CRUTCHFIELD, Physics Department, University of California, Davis — When an observer measures a time series of qubits, the outcomes generate a classical stochastic process. We present a model family of classically controlled qubit time series and show that measurement induces high complexity in these processes in two specific senses: they are inherently unpredictable (positive Shannon entropy rate) and they require an infinite number of features for optimal prediction (divergent statistical complexity). We argue that nonunifilarity is the mechanism underlying the resulting complexities and identify the different contributions to the randomness of the observed process. We examine the influence that the choice of measurement has on the randomness and structure of the measured qubit process and discuss measurement choices of potential interest in obtaining information about the underlying time series of qubits.

5:06PM U38.00012: A study about complete cohering/decohering power with ancillary system. MASAYA TAKAHASHI (Presenter), Southern Illinois University Carbondale, ALEXANDER STRELTSOV, Centre of New Technologies, University of Warsaw — In this talk we will discuss the cohering/decohering power of a quantum operation which quantifies the maximum amount of coherence which can be generated/eliminated through that operation taken over all input states. Complete cohering/decohering power (CCP and CDP respectively) of an operation is defined as cohering power of the product of the original operation and an identical operation on ancillary system. In our talk we will compare the properties of CCP and CDP with the general cohering/decohering power when only one system is considered.

We first observe that the CCP with L1 measure is not the same with general cohering power, or even not bounded. Taking dimension to be a large number, CCP increases unboundedly too. In contrast, for the relative entropy measure, the two cohering powers have the same value. Then we consider the decohering power. Here we will have an unexpected result. For L1 measure, CDP does not have a boundary again. On the other hand, CDP with the relative entropy measure is larger than the general decohering power which can be seen with an entangled input state. This result strongly implies that entanglement helps CDP exceed the general cohering power. We will conclude with some open problems.
Session U39 DCOMP GDS DMP: Machine learning for quantum matter

V 703 - Isaac Tamblyn, Natl Res Council - Tag(s): Focus

2:30PM U39.00001: Nicholas Metropolis Award Talk: Enhancing Quantum Simulators with Neural Networks*

GIACOMO TORLAI (Presenter), Center for Computational Quantum Physics, Flatiron Institute — Machine learning offers a set of flexible and powerful algorithms to enhance the capabilities of quantum simulation platforms. Artificial neural networks trained on measurement data can be integrated in the experimental stack for a variety of tasks, such as error mitigation, detecting quantum phase transitions and improving the measurement precision. I will review a data-driven framework for reconstructing quantum states prepared by experimental quantum hardware. Once trained, the neural networks can be used to deliver precise measurements of specialized observables that are either costly or not accessible in the original experimental setup. I will present results for a cold Rydberg-atom quantum simulator and quantum chemistry calculations on a superconducting quantum hardware.

*The Flatiron Institute is supported by the Simons Foundation.

3:06PM U39.00002: Topological codes revisited: Hamiltonian learning and topological phase transitions*

ELISKA GREPLOVA (Presenter), AGNES VALENTI, ETH Zurich, EVERT VAN NIEUWENBURG, Caltech, GREGOR BOSCHUNG, ETH Zurich, FRANK SCHÄFER, NIELS LOERCH, University of Basel, SEBASTIAN HUBER, ETH Zurich — The efficient validation of quantum devices is critical for emerging technological applications. The precise engineering of a Hamiltonian is required both for the implementation of quantum information processing as well as for quantum memories. Inferring the experimentally realized Hamiltonian through a scalable number of measurements constitutes the challenging task of Hamiltonian learning. In particular, assessing the quality of the implementation of topological codes is essential for quantum error correction. We introduce a neural net based approach to this challenge. We capitalize on a family of exactly solvable models to train our algorithm and generalize to a broad class of experimentally relevant sources of errors. We discuss how our algorithm scales with system size and analyze its resilience towards noise. A related issue regarding topological codes is to ensure that the system does not leave the topological manifold due to experimental noise. We present an unsupervised machine learning technique that is able to detect topological order from experimentally accessible data.

*Swiss National Science Foundation, the NCCR QSIT and Grant No. 183945, European Research Council Grant no. 771503, National Science Foundation Grant No. NSF PHY-1748958.
3:18PM U39.00003: Real time evolution with neural network quantum states  IRENE LOPEZ GUTIERREZ (Presenter), CHRISTIAN MENDL, TU Munich — The Hilbert space of a quantum system grows exponentially with system size, which makes many-body quantum systems challenging to simulate on a classical computer. One approach is to use tensor network methods, but these require an increasing bond dimension to capture the growth in entanglement during real time evolution, which limits their application to short time intervals. An alternative method proposed recently uses a neural network as a variational Ansatz to describe the quantum wave function. However, its application for real time evolution has not been extensively explored. In this work, we propose the use of standard machine learning optimization techniques, combined with a modified backpropagation for a neural network with complex parameters, to tackle the time evolution of an example system: the Ising model in 1 and 2-D. Our preliminary results show that our method performs comparably as well as stochastic reconfiguration, while avoiding a sensitivity issue related to the pseudo-inverse of the covariance matrix.

3:30PM U39.00004: Hunting for Hamiltonians with a General-Purpose Symmetry-to-Hamiltonian Approach  ELI CHERTKOV (Presenter), BENJAMIN VILLALONGA, BRYAN CLARK, University of Illinois at Urbana-Champaign — Inverse methods that learn models from data are widely used in the field of machine learning to solve difficult engineering tasks. Recently, inverse methods have been applied in the context of quantum physics to engineer quantum models, i.e., Hamiltonians, with targeted properties, such as targeted eigenstates or reduced density matrices. Here we present a new efficient and general-purpose inverse method approach, the symmetric Hamiltonian construction (SHC), for engineering Hamiltonians with particular symmetries, such as integrals of motion or discrete symmetries [1]. This method extends on ideas developed in the slow operator method [2]. Using the SHC inverse method, we design new Hamiltonians with topological properties: superconducting Hamiltonians with Majorana zero modes and $Z_2$ quantum spin liquid Hamiltonians. In this talk, we will introduce the SHC method and discuss the topological Hamiltonians that we find. Our open-source numerical implementation of the SHC method is available at github.com/ClarkResearchGroup/qosy.


3:42PM U39.00005: Studying inhomogeneous quantum many-body problems using neural networks  ALEXANDER BLANIA (Presenter), Max Planck Inst for Sci Light, EVERT VAN NIEUWENBURG, IQIM, Caltech, FLORIAN MARQUARDT, Max Planck Inst for Sci Light — We show how convolutional neural networks can be employed to learn the mapping from arbitrary potential landscapes to observables in quantum many-body systems. While following the general spirit of density-functional theory, our approach can easily be applied without modification to a wide variety of settings, effectively learning the significant underlying physical principles from raw training data. We verify the performance of this framework for a number of examples such as the prediction of Friedel oscillations and level spacing statistics. Our network architecture allows us to predict on system sizes larger than seen in the training data, and we analyze its scaling performance.
3:54PM U39.00006: Calculating Wannier functions via basis pursuit using a machine learned dictionary  
BRADLEY MAGNETTA (Presenter), VIDVUDS OZOLINS, Yale University — One of the earliest methods for calculating Wannier functions enforced localization by maximizing their projection onto a carefully chosen set of localized functions. Eventually use of this method faded with the emergence of more systematic approaches such as maximal localization. In this work we provide a modern method for calculating Wannier functions via projection by incorporating basis pursuit into the quantum variational method to automatically generate a set of localized functions needed to enforce localization while obtaining the ground state. We determine the dictionary to use for basis pursuit by performing sparse coding on a set of known Wannier functions. The algorithmic simplicity of our method suggests that it may be suited for automated calculation of Wannier functions. Other applications in physics that involve the variational principle could benefit from the inclusion of basis pursuit and sparse coding.

4:06PM U39.00007: Classical Quantum Optimization with Neural Network Quantum States*  
JOSEPH GOMES (Presenter), The University of Iowa — The classical simulation of quantum systems typically requires exponential resources. Recently, the introduction of a machine learning-based wavefunction ansatz has led to the ability to solve the quantum many-body problem in regimes that had previously been intractable for existing exact numerical methods. Here, we demonstrate the utility of the variational representation of quantum states based on artificial neural networks for performing quantum optimization. We show empirically that this methodology achieves high approximation ratio solutions with polynomial classical computing resources for a range of instances of the Maximum Cut (MaxCut) problem whose solutions have been encoded into the ground state of quantum many-body systems up to and including 256 qubits.

*J.G acknowledges start up funding from the University of Iowa. This research was supported in part through computational resources provided by The University of Iowa.

4:18PM U39.00008: Solving frustrated quantum many-particle models with convolutional neural networks  
XIAO LIANG (Presenter), Institute for Advanced Study, Tsinghua University — Recently, there has been significant progress in solving quantum many-particle problems via machine learning based on the restricted Boltzmann machine. However, it is still highly challenging to solve frustrated models via machine learning, which has not been demonstrated so far. In this paper, we design a brand new convolutional neural network (CNN) to solve such quantum many-particle problems. We demonstrate, for the first time, solving the highly frustrated spin-1/2 $J_1 - J_2$ antiferromagnetic Heisenberg model on square lattices via CNN. The energy per site achieved by the CNN is even better than previous string-bond-state calculations. Our work therefore opens up a new routine to solve challenging frustrated quantum many-particle problems using machine learning.
4:30PM U39.00009: Quantum dynamics in driven spin systems with neural-network quantum states

DAMIAN HOFMANN (Presenter), Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany, GIUSEPPE CARLEO, Center for Computational Quantum Physics, Flatiron Institute, New York, NY, USA, ANGEL RUBIO, MICHAEL SENTEF, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — Neural-network quantum states (NQS) provide an effective variational representation of quantum states, which can be used for the study of many-body quantum systems [1]. NQS can be time-propagated using time-dependent variational Monte Carlo (tVMC) [1,2], making it possible to simulate non-equilibrium phenomena. In particular, this approach can be used to compute dynamical properties of two-dimensional spin systems [3], a setting that has proven to be challenging for established numerical techniques. In this talk, we study magnetic excitations in a driven two-dimensional Heisenberg antiferromagnet. Further, we provide benchmarks of time-dependent NQS against results obtained from exact calculations for small systems as well as results obtained using a time-dependent matrix product state (t-MPS) approach.


*We acknowledge support from Flatiron Institute, a division of the Simons Foundation. M.S. acknowledges funding from the DFG through the Emmy Noether program (SE 2558/2-1).

4:42PM U39.00010: Study of phi-4 theories with deep learning methods

ZHONG YUAN LAI (Presenter), Fudan Univ, FRANCISCO COSTA MEIRINHOS, Department of Physics, University of Bonn, XIAOPENG LI, Fudan Univ — Field theories find wide applications from characterization of scattering processes in particle physics, to analysis of statistical models, to description of critical phenomena in condensed matter. One key problem in using field theories is to perform non-perturbative calculations, which is crucial in various places, but has remained an open question. In this talk I will present our recent work combining field theoretical and deep learning methods to systematically account for non-perturbative aspects. In calculating Green’s functions, nonperturbative Feynmann diagrams are automatically taken into account in our approach. I will present applications of this new approach to phi-4 field theories in one and two dimensions. Our approach potentially offers a generic solver for nonperturbative field theory calculations, of relevance to a broad context.

*This work is supported by National Program on Key Basic Research Project of China under Grant No. 2017YFA0304204, National Natural Science Foundation of China under Grants No. 117740067, 11934002, and the Thousand-Youth-Talent Program of China.
Unsupervised machine learning for accelerating discoveries from temperature dependent X-ray data*  JORDAN VENDERLEY (Presenter), MICHAEL MATTY, VARSHA KISHORE, GEOFF PLEISS, KILIAN WEINBERGER, EUN-AH KIM, Cornell University — Data analysis is becoming an increasingly prominent bottleneck for many experimental fronts of quantum matter research. In particular, advancements in detector capabilities for X-ray and neutron scattering have enabled researchers to rapidly collect hundreds of GB of data. Here, we present a novel unsupervised machine learning approach for accelerating the analysis of temperature dependent single crystal X-ray diffraction data. Our method employs a mixture model to cluster over the temperature dependence of scattering intensities and readily identify phase transitions. It is capable of analyzing hundreds of GBs of data in the span of minutes, offering the tantalizing possibility of real time analysis. Applications to several materials are discussed.

*This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-SC0018946.

Machine learning effective models for quantum systems*  ANDREW MITCHELL (Presenter), JONAS RIGO, Univ Coll Dublin — The construction of good effective models is an essential part of understanding and simulating complex systems in many areas of science. It is a particular challenge for correlated many body quantum systems displaying emergent physics. Using information theoretic techniques, we propose a model machine learning approach that optimizes an effective model based on an estimation of its partition function. The success of the method is exemplified by application to the single impurity Anderson model and double quantum dots, with new non-perturbative results obtained for the old problem of mapping to effective Kondo models. We also show that the correct effective model is not in general obtained by attempting to match observables to those of its parent Hamiltonian, due to information monotonicity along RG flow.


Thursday, March 5, 2020 2:30 PM - 4:06 PM

Session U40 DCOMP DCP DMP: Physics and effects on transport of ion-ion correlation in electrolyte materials II 705 - Arthur France-Lanord, Massachusetts Institute of Technology MIT - Tag(s): Focus
2:30PM U40.00001: Ion-ion correlations across and between micropores in carbon electrodes* [Invited] TRINIDAD MÉNDEZ-MORALES (Presenter), MATHIEU SALANNE, Laboratoire PHENIX, Sorbonne Université — Graphene nanostructures can be the solution for maximizing the capacitance and improving the performance of electrical double-layer capacitors [1]. Also, ionic liquids (IL) can be considered for optimizing these devices owing to some of their unique properties [2]. The combination of both is expected to be key for the development of supercapacitors with high energy density and long cycling life [3].

In this work, we performed MD simulations of a common IL confined between two types of nanoporous carbons with very different features. This IL was represented by a coarse-grained model with reduced charges [4], and the electrodes were maintained at constant potential. The first type of electrode consists in a carbide-derived carbon with a highly disordered structure [5], whereas the second one is a highly-ordered nanoporous electrode consisting of 6 graphene planes that are randomly perforated and separated by an interlayer distance which was systematically varied between 7 and 10 Å [6, 7]. The former was observed to be a better candidate for supercapacitor applications. In particular, we show that disordered materials are needed to mitigate the importance of the ion-ion correlations between the pores that arise when the IL is strongly confined between highly-ordered electrodes, which has important consequences for the performance of supercapacitors.


*This project has received funding from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme (grant agreement no. 771294).
3:06PM U40.00002: Ion and solvent dynamics in ‘solvent-in-salt’ electrolytes*

Presented by: IVAN POPOV

*Work was supported by the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

3:18PM U40.00003: Electroneutrality Breakdown in Nanoporous Membranes*

Presented by: PEDRO DE SOUZA

*We acknowledge support from CENT, a DOE EFRC under award # DE-SC0019112.
3:30PM U40.00004: Atomic Scale Characterization of the Voltage-Dependent Electrical Double Layer Structure*  KATHERINE HARMON (Presenter), FELIPE JIMENEZ-ANGELES, Northwestern University, SANG SOO LEE, Argonne National Lab, MICHAEL J BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University, PAUL FENTER, Argonne National Lab — The adsorption of ions at charged surfaces into an electrical double layer (EDL) is a driving factor in many phenomena including energy storage, nanoparticle stabilization, and biomolecule transport. The ability to control these processes relies on a detailed understanding of the atomic-scale interactions at play. Several EDL models with different assumptions have been proposed, including the diffuse ion cloud of Gouy-Chapman (GC) theory and complex ion-ion correlation phenomena. However, significant debate persists over the accuracy and limitations of these theories. Direct experimental probes of the structures at different surface charges can help to elucidate many open questions. Here, we use in situ resonant anomalous X-ray reflectivity (RAXR) to study the EDL structure of Rb$^+$ at a graphene/SiC electrode in aqueous 0.1 M RbCl as a function of applied potential. The results are compared to molecular dynamics (MD) predictions. Differences in RAXR and MD results are evaluated in the context of GC and ion-ion correlation theories with an eye on the possibility of overcharging at the most negative potentials.

*KH gratefully acknowledges support from DoD NDSEG and the Ryan Fellowship, Northwestern IIN. XR measurements were performed at the Advanced Photon Source at ANL (DOE/BES).

3:42PM U40.00005: Ionic liquid dynamics measured with implanted-ion β-NMR  DEREK FUJIMOTO (Presenter), RYAN M. L. MCFADDEN, MARTIN H DEHN, YAEL PETEL, ARIS CHATZICHRISTOS, University of British Columbia, LARS HEMMINGSEN, University of Copenhagen, VICTORIA L. KARNER, ROBERT F KIEFL, University of British Columbia, PHILIP C. P. LEVY, IAIN MCKENZIE, TRIUMF, CARL MICHAL, University of British Columbia, GERALD MORRIS, MATT PEARSON, TRIUMF, DANIEL SZUNYOGH, University of Copenhagen, JOHN TICKNOR, University of British Columbia, MONIKA K STACHURA, TRIUMF, W ANDREW MACFARLANE, University of British Columbia — Ionic liquids (ILs) not only found in a wide range of potential applications, spanning energy storage to space travel, but the constituent ions have fascinating dynamics and structure. In this study, we use implanted-ion $^8$Li β-NMR to probe these dynamics in the IL 1-ethyl-3-methylimidazolium acetate. Sensitivity to nanosecond $^8$Li$^+$ solvation dynamics is inferred from the motional narrowing of the resonance and the local maxima in the $^8$Li relaxation rate. We show that the activation energy and Vogel-Fulcher-Tammann temperature associated with the relaxation process agree with the dynamic viscosity. Near the melting point, the lineshape is broad and intense, and the form of the relaxation is non-exponential, reflective of heterogeneous dynamics. This demonstration establishes the feasibility of studying the local structure and dynamics of IL thin films and interfaces using β-NMR$^1$.

3:54PM U40.00006: Fundamental Studies of Tritium Diffusivity in Irradiation Defective LiAlO$_2$ and Li$_2$ZrO$_3$: A First Principles Density Function Theory Study*  
HARI PAUDEL (Presenter), YUHUA DUAN, National Energy Technology Laboratory — The thermal neutron irradiation of lithium isotope (\(^6\)Li) in tritium (\(^3\)H)-producing burnable absorber rods (TPBARS) of LiAlO$_2$ and Li$_2$ZrO$_3$ crystal produces vacancies, defects of its constituent elements, and several different trapping sites which hinder tritium diffusion process and releasing behavior. Here we investigate the diffusion mechanisms of tritium and O\(^3\)H species in LiAlO$_2$ and Li$_2$ZrO$_3$ ceramic pellet in order to understand and quantify the effects on diffusion barriers and diffusion coefficients due to the presence of interstitial and substitutional Li defects, hydroxide (O-\(^3\)H) vacancy defect, and the interactions of \(^3\)H with O-vacancies in Li$_2$ZrO$_3$. We find the smallest activation energy barriers of 0.63 and 0.3 eV in LiAlO$_2$ and Li$_2$ZrO$_3$, respectively. The obtained results indicate that the performance of Li$_2$ZrO$_3$ could be better than a widely used ceramic in TPBAR, \(\gamma\)-LiAlO$_2$.

*This research was supported by the National Nuclear Security Administration (NNSA) of the U.S. Department of Energy (DOE) through the Tritium Science Research Supporting the Tritium Sustainment Program (TSP) managed by Pacific Northwest National Laboratory (PNNL).

Thursday, March 5, 2020 2:30 PM - 5:06 PM

Session U41 GMAG DMP FIAP DCOMP: Quantum Spins in Semiconductors 707 - Denis Candido, Univ of Iowa - Tag(s): Focus

2:30PM U41.00001: Spatiotemporal mapping of photocurrent in 2D materials using diamond quantum sensors* [Invited]  
BRIAN ZHOU (Presenter), Boston College — Photocurrents are conventionally detected by counting the charge that flows between two contacts, but electrical detection cannot resolve the path that photocurrents travel within a material. Here, we leverage nitrogen-vacancy (NV) center magnetometers to resolve the spatial distribution of photocurrent flow in a 2D material by measuring the magnetic field profile produced by the photocurrents [1]. We reveal that photocurrent in monolayer MoS$_2$ circulates as a micron-scale vortex under an external magnetic field due to a strong photo-Nernst effect. By synchronizing dynamical decoupling of the sensor spin with pulsed photoexcitation, we significantly enhance sensitivity and resolve current densities as small as 20 nA/\(\mu\)m. Importantly, our pulsed approach allows probing of the temporal dynamics of photocurrent generation with sub-microsecond resolution. This combined spatiotemporal resolution is invaluable for understanding how novel photocurrent generation mechanisms and local variations control the flow of photocurrent in next-generation optoelectronic devices.


*This work is supported by the AFOSR, ARO, ONR, NSF, and UChicago and Cornell MRSECs.
3:06PM U41.00002: Optically pumped spin polarization as a probe of many-body thermalization

DANIELA PAGLIERO, The City College of New York, PABLO ZANGARA, Physics Department, Universidad Nacional de Cordoba, JACOB HENSHAW (Presenter), The City College of New York, ASHOK AJOY, Chemistry Department, University of California, Berkeley, RODOLFO ACOSTA, Physics Department, Universidad Nacional de Cordoba, JEFFREY A REIMER, Department of Chemical Engineering, University of California, Berkeley, ALEXANDER PINES, Chemistry Department, University of California, Berkeley, CARLOS MERILES, The City College of New York — The interplay between disorder and transport is a problem central to the understanding of thermalization. Disorder and many-body interactions are known to compete, with the dominance of one or the other giving rise to fundamentally different dynamical phases. Here we investigate the spin diffusion dynamics of $^{13}$C in diamond, which we dynamically polarize at room temperature via optical spin pumping of engineered color centers. We focus on low-abundance, strongly hyperfine-coupled nuclei, whose role in the polarization transport we expose through the integrated impact of variable radio-frequency excitation on the observable bulk $^{13}$C magnetic resonance signal. Unexpectedly, we find excellent thermal contact throughout the nuclear spin bath, regardless the hyperfine coupling strength, which we attribute to effective carbon-carbon interactions mediated by the electronic spin ensemble. In particular, observations across the full range of hyperfine couplings suggest the nuclear spin diffusion constant is approximately uniform, taking values up to two orders of magnitude greater than that expected from homo-nuclear spin couplings. Our results open intriguing opportunities to study the onset of thermalization in a system by controlling the internal interactions within the bath.

3:18PM U41.00003: Nanoscale structure of the orbital magnetic moment of a single dopant spin in a semiconductor*

ADONAI RODRIGUES DA CRUZ (Presenter), Applied Physics, Eindhoven University of Technology, MICHAEL FLATTÉ, Department of Physics and Astronomy, University of Iowa — The localized electron spin of a single impurity in a semiconductor is a promising system to realize quantum information schemes. In this work we investigate the orbital contribution to the magnetic moment originated from the spin-orbit induced circulating current [1] associated with the ground state of a single magnetic impurity in III-V semiconductors. In this project we developed a formalism employing Green's functions obtained by the Koster-Slater technique [2] with a sp$^3$d$^5$s* empirical tight-binding Hamiltonian [3] to describe the host material. We calculated the circulating current and orbital moments of a single Mn dopant in GaAs. The spin-correlated orbital moments originates from the hybridization between the Mn(d$^5$) spin-polarized electrons and the As dangling bonds leading to $t_2$-symmetric triplet acceptor states in the bandgap above the valence band edge.


*This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 721394
3:30PM U41.00004: Pulsed Electrically Detected Magnetic Resonance (pEDMR) at Low Magnetic Fields using an Arbitrary Wave Form Generator (AWG)*

TANIYA TENNAHEWA (Presenter), HANS MALISSA, HENNA POPLI, SABASTIAN ATWOOD, SANAZ HOSSEINZADEH, Physics And Astronomy, University of Utah, JOHN M LUPTON, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, CHRISTOPH M BOEHME, Physics And Astronomy, University of Utah — We use pulsed electrically detected magnetic resonance (pEDMR) in order to observe the coherent propagation of electron spins under strong drive magnetic resonance conditions in organic materials, where excitation frequencies (~100 MHz) and Zeeman fields (~3 mT) are low. In these materials, transverse relaxation times of electron spins are known to be in the on the order to 1µs [1], requiring the bandwidths of the pulse experiments to be in the 10-100 MHz range in order to accommodate effective pulse sequences. Thus, at low excitation frequencies [2,3], the duration of spin manipulation pulsed becomes comparable to the carrier-wave frequency, and conventional methods for generating RF pulses become impossible. We therefore utilize an arbitrary waveform generator (AWG) to directly synthesize RF pulses with a shape derived directly from the desired excitation spectrum. We evaluate the fidelity of such pulsed low-frequency excitation and conduct experiments that demonstrate electrically detected coherent spin motion under the given low-field conditions.[1] R. Miller, et al., Phys. Rev. B, 94, 214202 (2016); [2] S. Jamali et al., Nano Lett. 4648 (2017); [3] D. P. Waters et al., Nature Physics 11, 910 (2015).

*This work is supported by the Department of Energy DE-SC0000909.

3:42PM U41.00005: Detection of electron spin resonance in the strong, non-linear drive regime using spin-dependent charge carrier recombination currents and an amplitude-modulated continuous wave electrically detected magnetic resonance scheme*

SABASTIAN ATWOOD (Presenter), ADNAN NAHLAWI, SANAZ HOSSEINZADEH, TANIYA TENNAHEWA, HENNA POPLI, HANS MALISSA, Department of Physics and Astronomy, University of Utah, JOHN M LUPTON, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, CHRISTOPH M BOEHME, Department of Physics and Astronomy, University of Utah — Electrically detected magnetic resonance spectroscopy of organic light-emitting diodes with conductive polymers as active layers allows for the study of high-magnetic resonance drive regimes of electron spins in which Zeeman fields are on the same magnitude as drive field amplitudes [1, 2]. Drive amplitude limits of such non-linear magnetic resonance experiments are posed by the superposition of the studied spin-dependent electric currents with other, randomly occurring, radiation-induced artifact signals, possibly due to electric dipole transitions in lowest unoccupied molecular orbitals. Here, we demonstrate the use of amplitude-modulated lock-in detection for the isolation of these two electric current signatures, taking advantage of their different dynamic natures. We validate this approach by analyzing the dependence of the lock-in detected signals on modulation phase and frequency and demonstrate a significant signal improvement allowing for the detection of multi-photon magnetic dipole transitions and the Bloch-Siegert shift. [1] S. Jamali et. al., Nano Lett., 17, 4648 (2017), [2] S. Jamali et al. (unpublished).

*Supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0000909.
Probing spin-dependent electronic transitions in a conjugated polymer using electrically detected magnetic resonance (EDMR) under hole injection with MoO$_3$ electrodes

SANAZ HOSSEINZADEH (Presenter), HANS MALISSA, ADNAN NAHLAWI, CHRISTOPH M BOEHME, The University of Utah — Spin-dependent recombination in organic light emitting diodes (OLEDs) occurs when an active polymer layer is sandwiched between an electron and hole charge carrier injection layers. As spin-dependent electronic transitions rates change under magnetic resonant excitation, spin-dependent recombination can be studied using a method called electrically detected magnetic resonance spectroscopy (EDMR) [1-2]. Most past EDMR studies used the copolymer blend poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT: PSS) as hole injector layer. Here, we report EDMR spectroscopy of OLEDs based on various π-conjugated poly-phenylenevinlenes as active materials and the Ca and MoO$_3$ layers as electron and hole injectors, respectively, in order to test whether Mo, (atomic number Z=42) is able to affect the charge carrier spin-orbit coupling (SOC) in the active layer, e.g. by suppression of spin-dependent processes. Our results indicate that no SOC effects can be observed and, thus, that SOC in hole injection layers does not affect pEDMR signals in OLEDs. [1] D. McCamey et al., Nature Materials, 7 (9), 723 (2008); [2] H. Malissa et al., Science 345 (6203), 1487 (2014).

*This work is supported by the DOE, award #DE-SC000909.

Manipulation of Dynamic Nuclear Polarization in Gallium Arsenide under periodic optical electron spin pumping

MICHAEL DOMINGUEZ (Presenter), JOSEPH IAFRATE, VANESSA A SIH, Univ of Michigan - Ann Arbor — Optically oriented electron spins in gallium arsenide polarize the nuclear spin system through a process called dynamic nuclear polarization. The polarized nuclear system will create an effective magnetic field back onto the electron spin system and affect the Larmor precession frequency. The nuclear polarization can be calculated from the change in electron spin polarization using periodic optical pump probe Kerr rotation measurements[1]. We demonstrate that the coupled electron-nuclear spin systems can be manipulated by varying the excitation energy and sweeping an external magnetic field. These dependencies are corroborated by numerical calculations from a model incorporating optical orientation and the optical Stark effect. This model is justified by its correspondence to our experimental observations and can be used to predict the behavior of the nuclear spin polarization.


*This work was supported in part by NSF and by the U.S. Department of Defense NDSEG program
The impact of dynamic nuclear polarization on non-local spin valve and inverse spin Hall Hanle measurements in n-GaAs

ZHENG JIANG (Presenter), School of Physics and Astronomy, University of Minnesota, Twin Cities, SAHIL PATEL, Departments of Electrical and Computer Engineering and Materials, University of California, Santa Barbara, PAUL CROWELL, School of Physics and Astronomy, University of Minnesota, Twin Cities, CHRIS J PALMSTROM, Departments of Electrical and Computer Engineering and Materials, University of California, Santa Barbara — Non-local spin valve (NLSV) and inverse spin Hall (ISHE) Hanle measurements are important tools to probe spin-transport parameters such as the spin lifetime and spin Hall angle. We carried out such measurements on Fe/n-GaAs heterostructure samples with varying doping (3x10^{16} to 7x10^{16} cm^{-3}) and at temperatures from 2 K to 110 K. The Hanle curves are very sensitive to the hyperfine field generated by dynamic nuclear polarization (DNP). Below a threshold temperature that depends on doping, the hyperfine field leads to distortion of the Hanle line-shapes for both NLSV and ISHE measurements and can enhance the ISHE signal by one order of magnitude. We have developed a pulsed-current technique which utilizes the vast difference between electron and nuclear spin relaxation time scales (about ns and s respectively) to eliminate the impact of the steady-state hyperfine field, and the obtained Hanle curves then match expectations based on simple drift-diffusion models. We will discuss the extracted spin lifetime and spin Hall angle, numerical modeling of the Hanle curves and the role of the hyperfine field in enhancing the apparent spin Hall signal.

*This work was supported by NSF DMR-1708287 and the NSF National Nano Coordinated Infrastructure Network (NNCI) under Award Number ECCS-1542202

Magnetic properties of a single micrometer-sized YIG/FGT multilayer heterostructure revealed by ferromagnetic resonance

BASSIM ARKOOK (Presenter), MOHAMMED ALGHAMDI, VICTOR ORTIZ, JING SHI, IGOR BARSUKOV, Physics and Astronomy, University of California, Riverside — Multilayer heterostructures consisting of a magnetic insulator and 2D spin system offer a promising platform for next-generation spintronic applications. Understanding interfacial spin coupling and transport in such heterostructures require a local microwave spectroscopy technique since the flakes of 2D materials obtained by exfoliation are limited to micrometers in size. Here, we fabricate disks of 20um diameter from epitaxial ferrimagnetic insulator, yttrium iron garnet (YIG), thin-film using pulsed laser deposition, e-beam lithography, and lift-off. We place few-nm thick flakes of van-der-Waals material Fe3GeTe2 (FGT) on the pre-patterned YIG disks and transfer a single disk onto a planar microwave resonator. Using angle-dependent ferromagnetic resonance, we find low-energy spin-wave modes in YIG at several microwave frequencies, allowing for the evaluation of magnetic anisotropy and damping. Using cryogenic measurements, we observe an anomalous temperature dependence of effective magnetic anisotropy. The results shed light on spin phenomena at YIG/FGT interfaces and present an experimental approach for studies of micro-scale magnetic insulator/2D heterostructures.

*This work was supported by NSF under Grant No. ECCS-1810541 and by DoE EFRC SHINES under Award DE-SC0012670.
**4:42PM U41.00010: Dynamics of Spin Waves in 1D and 2D Magnonic Crystals of V[TCNE]_{x-2} with YIG or Cobalt**

KWANGYUL HU (Presenter), MICHAEL FLATTÉ, Optical Science and Technology Center and Department of Physics, The University of Iowa — A semiconducting organic ferrimagnet V[TCNE]_{x-2} is a newly emerging magnonic material. Recent studies have revealed that V[TCNE]_{x-2} has narrow linewidth, long spin lifetime and high Q factor[1-3]. In addition, deposition of high quality V[TCNE]_{x-2} does not require specific substrates or high temperature which is a significant advantage compared to YIG[1]. These properties of V[TCNE]_{x-2} indicate that it is attractive magnonic media. Here, we calculate and present the magnonic dispersions and linewidths of quasi one-dimensional and two-dimensional magnonic crystals consisting of V[TCNE]_{x-2} with YIG or cobalt. In each case, we consider infinitely periodic lattice structures with a finite thickness. For the calculation, the linearized Landau-Lifshitz-Gilbert equation with the plane-wave method is used[4]. We anticipate that these results will provide fundamental understanding of how to design magnonic devices based on V[TCNE]_{x-2}.


*We acknowledge support from NSF EFRI NewLAW under Award No. EFMA-1741666.

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**4:54PM U41.00011: Impact of hidden structural order on low temperature magnetic resonance in V[TCNE]_{x}**

HUMA YUSUF (Presenter), ANDREW FRANSON, SETH KURFMAN, EZEKIEL JOHNSTON-HALPERIN, Physics, Ohio State Univ - Columbus — The coordination compound V[TCNE]_{x} is a promising magnetic material for integration into solid-state quantum information systems due to its low damping (α = (3.98 ± 0.22) × 10^{-5}), high quality factor (Q up to 8,000) microwave resonance, ease of patterning, and compatibility with a wide variety of substrates. Since current quantum information systems require low temperature operation, a comprehensive study of the low temperature magnetic behavior of V[TCNE]_{x} is essential for realizing this promise. Here we report the observation of anomalous temperature dependent anisotropy in thin films of V[TCNE]_{x} at temperatures down to 5 K. The resonance linewidth at 5K is larger by a factor of 3 than at room temperature, competitive with the very best liquid phase epitaxy (LPE) yittrium iron garnet (YIG) films. Further, we observe temperature-dependent changes in the magnetic anisotropy that suggest that this modest increase in linewidth may in fact arise from inhomogeneous thermally-induced strain in the thin film. This result promises further reductions in the low temperature linewidth in structures engineered to minimize differences in thermal contraction between the sample and the substrate.

*This work is supported by DOE Project No. 60072770
2:30PM U42.00001: Time-resolved ultrafast oscillation of octupole polarization in a chiral antiferromagnet Mn$_3$Sn$^*$ [Invited] SHINJI MIWA (Presenter), The Institute for Solid State Physics, The University of Tokyo — Understanding of spin-precession dynamics forms the basis of spintronic application. For the ultrafast THz control of staggered moments in antiferromagnets, the time-resolved observation of spin precession is essential for developing the associated technology. However, such observation has been limited to insulators to date [1]. Recently, the metallic antiferromagnets Mn$_3$X have attracted significant attention for its strong response (e.g. anomalous Hall effect) comparable to ferromagnets owing to the hidden ferroic order, which configures large Berry curvature originated from Weyl points in momentum space [2]. Such ferroic order can be characterized by cluster octupoles based on neighboring magnetic moments [3], and thus it is highly important to clarify the dynamics of cluster octupole for designing the spintronic application.

In this talk, we report our time-resolved observation of spin precession in a metallic chiral antiferromagnet Mn$_3$Sn [4]. In particular, we find that the dynamics of the cluster octupole is enhanced by exchange interaction, and it is feasible to conduct an ultrafast switching at $< 10$ ps, a hundred times faster than the case of spin-magnetization in a ferromagnet. Moreover, our theoretical study demonstrates that the domain wall velocity of the cluster octupole could reach as high as 10 km/s. Our work paves the path towards realizing ultrafast electronic devices.


*This is a work in collaboration with T. Nomoto, T. Tomita, T. Higo, M. Ikhlas, S. Sakamoto, Y. Otani, R. Arita, and S. Nakatsuji of The University of Tokyo, S. Iihama and S. Mizukami of Tohoku University, T. Nakano, and K. Yakushiji of AIST. This work was partially supported by JST-CREST (No. JPMJCR18T3) and JSPS-KAKENHI (No. 18H03880), Japan.
3:06PM U42.00002: Evidence of Electrical Switching of the Antiferromagnetic Néel Vector*

CHIH-CHIEH CHIANG (Presenter), SSU YEN HUANG, Department of Physics, National Taiwan University, DANRU QU, Institute of Physics, Academia Sinica, PO-HSUN WU, Department of Physics, National Taiwan University, CHIA-LING CHIEN, Department of Physics and Astronomy, Johns Hopkins University —

Recently, field-free switching of antiferromagnetic (AFM) Néel vector via spin-orbit torque (SOT) attracting worldwide attention. By applying a writing current in the AFM or the normal metal (NM)/AFM bilayer, in a patterned multi-terminal structures, the measured resistance shows recurring signals due to supposedly electrical switching of the AFM Néel vector. However, in this work, we demonstrate that similar signals can be observed in such patterned structures, with and without the AFM layer [1]. The strength of the signal is also greatly affected by different metals and substrates. We show that under a large writing current density beyond the Ohmic regime, the multi-terminal devices can generate unintended anisotropic thermal gradient and voltages. Therefore, this switching signal may not be the conclusive evidence of the SOT switching of AFM, but the thermal artifacts of patterned metal structures on substrate.


*This work was supported by the Ministry of Science and Technology of Taiwan (Grant No. MOST 106-2628-M-002-015-MY3). Work at JHU was supported by KAUST (Grant No. OSR2017-CRG6-3427.01) and the U.S. Department of Energy (Award No. DE-SC0009390 and No. SC0012670).

3:18PM U42.00003: Spin-torque control of the noncollinear antiferromagnetic order in antiperovskites

GAUTAM GURUNG (Presenter), DING-FU SHAO, EVGENY Y TSYMBAL, University of Nebraska - Lincoln —

Antiferromagnetic (AFM) spintronics exploits the AFM order to control the spin-dependent transport properties. Recent theoretical studies suggest that the AFM order parameter can be switched by a spin torque, while the related experimental realizations are limited to a few collinear antiferromagnets. There is, however, a large group of high temperature noncollinear antiferromagnets, which are suitable for such switching. Here, we predict that the spin torque can be efficiently used to control the noncollinear AFM order in antiperovskite materials. Based on first-principles calculations and atomistic spin model simulations, we show that in antiperovskites ANMn$_3$ (A = Ga, Ni, etc) with the $\Gamma_{4g}$ AFM ground state, the AFM order parameter can be switched on the picosecond scale by a spin-transfer torque generated by a spin polarized current. The threshold switching current density can be tuned by the ANMn$_3$ stoichiometry engineering, changing the magnetocrystalline anisotropy. The $\Gamma_{4g}$ AFM phase supports the anomalous Hall effect, which can be used to detect the spin-torque switching of the AFM order. The predicted ultrafast switching dynamics and the efficient detection of AFM order parameter make noncollinear AFM antiperovskites promising material platforms for AFM spintronics.
3:30PM U42.00004: Nonlinear anomalous Hall effect for Néel vector detection  DING-FU SHAO (Presenter), Department of Physics and Astronomy, University of Nebraska - Lincoln, SHUHUI ZHANG, College of Science, Beijing University of Chemical Technology, GAUTAM GURUNG, Department of Physics and Astronomy, University of Nebraska - Lincoln, WEN YANG, Beijing Computational Science Research Center, EVGENY Y TSYMBAL, Department of Physics and Astronomy, University of Nebraska - Lincoln — The manipulation and detection of the Néel vector are cores of antiferromagnetic (AFM) spintronics. Recent studies have shown that the field-like and antidamping spin-orbit torques (SOT) can be used to switch the Néel vector in antiferromagnets with proper symmetries. On the other hand, the efficient detection of the AFM order parameter remains a challenging problem. Here, we predict that the nonlinear anomalous Hall effect (AHE) can be used to detect the Néel vector in most compensated antiferromagnets supporting the antidamping SOT. The magnetic crystal group symmetry of these antiferromagnets combined with spin-orbit coupling results in a sizable Berry curvature dipole and hence the nonlinear AHE. As a specific example, we consider half Heusler alloy CuMnSb, which Néel vector can be switched by the antidamping SOT. Based on density functional theory calculations, we show that the nonlinear AHE in CuMnSb produces a measurable Hall voltage under conventional experimental conditions. The strong dependence of the Berry curvature dipole on the Néel vector orientation provides a new detection scheme of the AFM order parameter based on the nonlinear AHE.

3:42PM U42.00005: Rotating Néel Order to Probe Crystalline and Non-Crystalline AMR in FeRh  JOSEPH SKLENAR (Presenter), Wayne State Univ, SOHO SHIM, University of Illinois Urbana-Champaign, HILAL SAGLAM, Argonne National Laboratory, KISUNG KANG, JUNSEOK OH, GREG A HAMILTON, University of Illinois Urbana-Champaign, WEI ZHANG, Oakland University, MATTHEW GILBERT, ANDRE SCHLEIFE, AXEL HOFFMANN, NADYA MASON, University of Illinois Urbana-Champaign — Anisotropic magnetoresistance (AMR) effects are a promising starting point for the electrical readout of antiferromagnetic memory in a spintronic device. We characterized both crystalline and non-crystalline AMR in thin films of FeRh, a material which undergoes a ferro- to antiferromagnetic transition near room temperature. The resistance is measured as an external field is rotated in the sample plane. In the antiferromagnetic phase we observe a striking dependence of the AMR signal on both field magnitude, and current orientation relative to the FeRh [100] crystalline axis. We confirm that AMR arises from rotating Neel order two ways: 1) We developed a procedure combining rotating and linearly swept fields to demonstrate an angular hysteresis effect; 2) We use density functional theory for a first-principles description of the evolution of the AMR signal, representing the external magnetic field by canted spins and the sweeping field by Néel vector rotation from the [100] direction.

*This work was undertaken as part of the Illinois Materials Research Science and Engineering Center, supported by the NSF MRSEC program under NSF award number DMR-1720633. Sample growth was supported by the DoE, Office of Science, Materials Science and Engineering Division.
3:54PM U42.00006: Nonvolatile control of long-distance spin transport in an easy-plane antiferromagnetic insulator

JIAHAO HAN (Presenter), PENGXIANG ZHANG, YABIN FAN, T AQIYYAH S SAFI, JUNXIANG XIA N, Massachusetts Institute of Technology MIT, RAN CHENG, University of California, Riverside, LUQIAO LIU, Massachusetts Institute of Technology MIT — Transmission of spin angular momentum can be implemented by the quanta of spin-wave excitations, viz. magnons, without dissipative electron flows. Therefore, spin information can be transported over long distances in insulating materials devoid of Joule heating. Antiferromagnetic insulators with vanishingly small magnetization and high operating frequency are promising candidates for high-density and ultrafast magnonic devices. It is generally believed that easy-axis anisotropy is essential for long-distance spin transport in antiferromagnets, while easy-plane anisotropy suppresses spin transmission due to the vanished angular momentum carried by the magnon eigenmodes. Here we show that efficient spin transport over micrometer distance indeed happens in an easy-plane antiferromagnetic insulator, α-Fe$_2$O$_3$ thin film. The amplitude of spin transmission can be easily manipulated by a magnetic field much weaker than those in previous studies, making our systems more practical for applications. Moreover, the stable magnetic orientation enables control of spin transport under zero remnant field, realizing a nonvolatile spin-current switch with a 100% on/off ratio.

*NSF, NIST

4:06PM U42.00007: Intrinsic spin Nernst effect of magnons in a noncollinear antiferromagnet

BO LI (Presenter), SHANE SANDHOEFNER, ALEXEY KOVALEV, University of Nebraska - Lincoln — We investigate the intrinsic magnon spin current in a noncollinear antiferromagnetic insulator. To this end, we derive a magnon spin current in a noncollinear antiferromagnet from continuity equation and find that in general it is not conserved, but for certain symmetries and spin polarizations, the averaged effect of non-conserving terms can vanish. We formulate a general linear response theory for magnons in noncollinear antiferromagnets subject to a temperature gradient and analyze the effect of symmetries on the response tensor. We apply this theory to single-layer potassium iron jarosite KFe$_3$(OH)$_6$(SO$_4$)$_2$ and predict a measurable spin current response. According to the symmetry analysis, many other material candidates should exhibit the spin Nernst effect, including quasi-two- and three-dimensional noncollinear antiferromagnets and antiferromagnets with magnetic textures such as skyrmions. Our proposal can be useful for spin generation in spintronics applications. Furthermore, this effect can also serve as a probe for the materials that can hold multiple noncollinear states.
4:18PM U42.00008: Electric-field control of magnon spin current in an antiferromagnetic insulator*  
CHANGJIANG LIU (Presenter), YONGMING LUO, DESHUN HONG, SHULEI ZHANG, JOHN PEARSON, BRANDON FISHER, AXEL HOFFMANN, ANAND BHATTACHARYA, Argonne National Laboratory — A fundamental challenge in the development of spintronics is the effective control of spin currents by electrical means. This is because the spin degree of freedom is often decoupled from external electric fields, making its control difficult. Over the last few years, the spin Seebeck effect has shown its versatility in generating pure spin currents in a diverse class of magnetic systems. Here we first show how a magnon spin current can be produced in an antiferromagnetic insulator by means of the spin Seebeck effect. The polarity of the spin current is determined by the orientation of the magnetic sublattice in this antiferromagnet. Owning to the response of the magnetic ions to an external electric field, the anisotropy energy of this material may be effectively tuned. As a result, we show that the spin-flop transition in this material can be switched on or off by varying only an electrical voltage. Furthermore, we demonstrate how thermally generated spin currents in this antiferromagnet can be effectively controlled by sweeping the control voltage.

*Supported by the US DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. The use of facilities at the CNM was supported by the DOE, Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

4:30PM U42.00009: Phenomenological theory of coherent and incoherent spin currents in antiferromagnetic spin pumping  
RAN CHENG (Presenter), University of California, Riverside — Magnetic resonance driven by coherent microwaves can pump spin currents into a neighboring nonmagnetic system. Owing to non-linear effects, however, coherently driven spin dynamics inevitably generates incoherent magnons through thermalization, which makes it complicated to distinguish between coherent and incoherent contributions in real experiments. Recent measurements have demonstrated spin pumping effects in antiferromagnets at the sub-THz frequency, where coherent and incoherent magnons contribute oppositely to the spin current and are thus distinguishable. We formulate a phenomenological theory to capture the coupled dynamics of coherent and incoherent magnons in collinear antiferromagnets driven by sub-THz sources, which can fit very well with the experimental observation and explain why the competition between coherent and incoherent magnons leads to a sign change in the spin current at a turning temperature. Our phenomenological theory predicts that using magnetic thin films can substantially suppress the undesirable incoherent contribution and magnify coherent spin pumping.
4:42PM U42.00010: Coherent ac spin current transmission across an antiferromagnetic CoO insulator  QIAN LI (Presenter), MENGMENG YANG, University of California, Berkeley, CHRISTOPH KLEWE, PADRAIC SHAFER, ALPHA T. N’DIAYE, Lawrence Berkeley National Lab, DAZHI HOU, Tohoku University, TIANYE WANG, NAN GAO, University of California, Berkeley, EIJJI SAITOH, Tohoku University, CHANYONG HWANG, Korea Research Institute of Standards and Science, ROBERT J HICKEN, University of Exeter, JIA LI, Peking University, ELKE ARENHOLZ, Lawrence Berkeley National Lab, ZI Q. QIU, University of California, Berkeley — The recent discovery of spin-current transmission through antiferromagnetic insulating materials opens up vast opportunities for fundamental physics and spintronics applications. The question currently surrounding this topic is: whether and how could THz antiferromagnetic magnons mediate a GHz spin current? This mis-match of frequencies becomes particularly critical for the case of coherent ac spin-current, raising the fundamental question of whether a GHz ac spin-current can ever keep its coherence inside an antiferromagnetic insulator and so drive the spin precession of another ferromagnet layer coherently? Utilizing element- and time-resolved x-ray pump-probe measurements on Py/Ag/CoO/Ag/Fe$_{75}$Co$_{25}$/MgO(001) heterostructures, here we demonstrate that a coherent GHz ac spin current pumped by the Py ferromagnetic resonance can transmit coherently across an antiferromagnetic CoO insulating layer to drive a coherent spin precession of the Fe$_{75}$Co$_{25}$ layer. Further measurement results favor thermal magnons rather than evanescent spin waves as the mediator of the coherent ac spin current in CoO.

4:54PM U42.00011: Spin Current from sub-Terahertz-generated Antiferromagnetic Magnons*  JUNXUE LI, University of California, Riverside, BLAKE WILSON, Physics Department and Institute for Terahertz Science and Technology, University of California, Santa Barbara, RAN CHENG, MARK I LOHMANN, University of California, Riverside, MARZIEH KAVAND, Physics Department and Institute for Terahertz Science and Technology, University of California, Santa Barbara, WEI YUAN, MOHAMMED ALDOSARY, University of California, Riverside, NIKOLAY I AGLADZE, Physics Department and Institute for Terahertz Science and Technology, University of California, Santa Barbara, PENG WEI, University of California, Riverside, MARK S SHERWIN, Physics Department and Institute for Terahertz Science and Technology, University of California, Santa Barbara, JING SHI (Presenter), University of California, Riverside — Spin dynamics in antiferromagnets offers attractive benefits for potential ultrafast device applications. To date, spin current generation via antiferromagnetic resonance and simultaneous electrical detection by the inverse spin Hall effect in heavy metals have not been explicitly demonstrated. Here we report sub-terahertz spin pumping in heterostructures of a uniaxial antiferromagnetic Cr$_2$O$_3$ crystal and a heavy metal of Pt or Ta (Beta-phase). The magnetic resonances in Cr$_2$O$_3$ are excited both below and above spin flop transitions. Both resonances generate pure spin currents in the heterostructures, which are detected by the heavy metal as an open-circuit voltage peak or dip. The pure spin current nature of the electrically detected signals is unambiguously confirmed by the reversal of voltage polarity under two circumstances: one when switching the detector metal from Pt to Ta which reverses the sign of spin Hall angle, and the other when flipping the magnetic field direction which reverses the magnon chirality.

*Work at UC Riverside was supported as part of the Spins and Heat in Nanoscale Electronic Systems, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under award no. SC0012670 (JXL, ML, WY, MA, and JS).
5:06PM U42.00012: Quantitative Study on Current-Induced Effects in an Antiferromagnet Insulator/Pt Bilayer Film*  

PENGXUANG ZHANG (Presenter), LUQIAO LIU, Electrical Engineering and Computer Science, Massachusetts Institute of Technology — Quantitative investigation on the current-induced torque in antiferromagnets represents a great challenge, due to the lack of an independent method for controlling Néel vectors. Here by utilizing an antiferromagnetic insulator with Dzyaloshinskii-Moriya interaction, α-Fe2O3, we show that the Néel vector can be controlled with a moderate external field, which is further utilized to calibrate the current-induced magnetic dynamics. In a Pt/α-Fe2O3(0001) bilayer film, we see that the current-induced magnetoresistance change in antiferromagnets can be complicated by resistive switching that is non-magnetic. By excluding non-magnetic switching, we reveal two significant magnetic contributions, the magnetoelastic effect and the field-like spin-orbit torque, and quantify their magnitudes. Our approach in principle is applicable to many other easy plane antiferromagnets, and would be beneficial for future systematic studies of current-induced antiferromagnetic dynamics.

*This work is supported in part by National Science foundation under award ECCS-1808826 and DMR 14-19807, and by SMART, one of seven centers of nCORE, a Semiconductor Research Corporation program, sponsored by National Institute of Standards and Technology (NIST).

5:18PM U42.00013: Resonant ultrasound studies of Fe$_{x=0.33}$NbS$_2$*  

SYLVIA LEWIN (Presenter), VIKRAM NAGARAJAN, GABRIEL PERKO-ENGEL, ERAN MANIV, SHANNON HALEY, JAMES ANALYTIS, University of California, Berkeley — The intercalated transition metal dichalcogenide Fe$_{x=0.33}$NbS$_2$ appears to exhibit frustrated antiferromagnetism. The orientation of its antiferromagnetic order can be switched by the application of electrical currents [1]. Similar behavior at room temperature could form the basis of a new generation of magnetic memory storage. However, the specific magnetic order of Fe$_{x=0.33}$NbS$_2$ and how it evolves with temperature have not been exactly determined, leaving open questions about the microscopic mechanism of switching. Resonant Ultrasound Spectroscopy—a study of the material’s mechanical resonances—can shed light on the magnetic order in Fe$_{x=0.33}$NbS$_2$.

1. N. L. Nair et al., arxiv:1907.11698.

*This work was supported by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4374. S.K.L. also acknowledges support from the AAUW American Dissertation Fellowship. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U43 DCOMP DMP: Computational design and discovery of novel materials V: Electronic structure  

Tag(s): Focus
Towards ideal topological materials: Comprehensive database searches using symmetry indicators

FENG TANG, Nanjing Univ, HOI CHUN PO, MIT, ASHVIN VISHWANATH, Harvard University, XIANGANG WAN (Presenter), Nanjing Univ — Although the richness of spatial symmetries has led to a rapidly expanding inventory of possible topological crystalline (TC) phases of electrons, physical realizations have been slow to materialize due to the practical difficulty to ascertaining band topology in realistic calculations. Here, we integrate the recently established theory of symmetry indicators of band topology into first-principle band-structure calculations and apply it to all non-magnetic compounds in the 230 space groups. An exhaustive database search reveals thousands of TM candidates. Of these, we highlight the excellent TMs, the 258 topological insulators and 165 topological crystalline insulators which have either noticeable full band gap or a considerable direct gap together with small trivial Fermi pockets. We also give a list of 489 topological semimetals with the band crossing points located near the Fermi level. All predictions obtained through standard generalized gradient approximation (GGA) calculations were cross-checked with the modified Becke-Johnson (MBJ) potential calculations, appropriate for narrow gap materials. With the electronic and optical behavior around the Fermi level dominated by the topologically non-trivial bands, these newly found TMs candidates open wide possibilities for realizing the promise of TMs in next-generation electronic devices.

First principle study of structural, electronic and magnetic properties of layer-structured MnSb

BIPIN LAMICHHANE (Presenter), DINESH THAPA, CHANDANI NANDADASA, Physics and Astronomy, Mississippi State University, JUNSEONG SONG, SUNG WNG KIM, Energy Science, Sungkyunkwan University, SEONG-GON KIM, Physics and Astronomy, Mississippi State University — Manganese antimonide (MnSb) as a half-metallic ferromagnets can be used as a spin injector in semiconductor to develop spintronic devices. We performed ab initio total-energy calculations and geometry optimizations within Density Functional Theory (DFT) using the generalized gradient approximation (GGA) Perdew–Burke–Ernzerhof (PBE) functional and the projected augmented wave (PAW) method to investigate the structural, electronic, and bonding properties of layer-structured MnSb. We found a metallic density of states (DOS) in one spin channel (majority spin) and a band energy gap at the Fermi level in another (minority spin), which presents MnSb to have a half metallic character. Furthermore, atom projected band structure was used to investigate the electronic contributions from Mn and Sb atoms.

This work was supported by a National Research Foundation of Korea (NRF) grant funded by the Korean government (Ministry of Science, ICT & Future Planning) (No.2015M3D1A1070639) and in part by the Center for Computational Sciences (CCS) at Mississippi State University.
3:18PM U43.00003: Near-Fermi-level electronic states in hexagonal ABC compounds from first principles* KONRAD GENSER (Presenter), KARIN M RABE, Rutgers University, New Brunswick — Ternary ABC intermetallic compounds exhibit a rich variety of crystal structures and electronic properties. In this work, we study the band structures of real and hypothetical ABC intermetallic phases with structures obtained by stacking binary honeycomb layers with single layers of interstitial atoms in various ways, using first principles calculations to determine the structural parameters and the bands in each phase. We use this dataset to analyze and model the bands near the Fermi level to classify the systems considered and to extract a set of rules that allows us to predict and design hexagonal ABC intermetallic materials with targeted transport and optical properties, connecting to experimental measurements on known hexagonal ABC phases.

*This work is supported by ONR N00014-17-1-2770 and NSF-DMR 1629346.

3:30PM U43.00004: A symmetry-based approach to reciprocal space path selection in band structure calculations JASON MUNRO (Presenter), Energy Technologies Area, Lawrence Berkeley National Laboratory, KATHERINE LATIMER, Department of Physics, University of California, Berkeley, SHYAM DWARAKNATH, KRISTIN PERSSON, Energy Technologies Area, Lawrence Berkeley National Laboratory — The calculation of band structures is a critical step in describing many different properties of crystalline solids such as optical absorption, and both thermal and electronic transport. Most commonly, these are computed along a one-dimensional path in reciprocal space, which is presumed to capture important features of the entire dispersion landscape. However, conventions for choosing this path rely on data for high-symmetry points and lines in the first Brillouin zone, defined using different arbitrary criteria and an inflexible predefined unit cell. Furthermore, this data is contained in hard-coded lookup tables for different crystal classes and lattice vector lengths. To address these issues, a new “on-the-fly” symmetry based algorithm and utility for obtaining paths in reciprocal space is presented. For an arbitrary input cell, the site-symmetries of points and lines in the first Brillouin zone are determined and used to define the high-symmetry criteria. A smooth path connecting them is then obtained using graph theory based tools. This new framework not only allows for increased flexibility, but is also shown for a general high-symmetry criteria to provide new notable features in the electronic band structure for systems with both magnetic and nonmagnetic symmetry.
Recently, the nonsymmorphic compound CeSbTe was studied experimentally and computationally to determine its crystal structure and its electronic structure, due to the interest in topological semimetals [1]. The material was found to contain several four-fold degenerate points, including a Dirac crossing near the Fermi level, which are topologically protected. A similar, as-yet unstudied material, SmSbTe, has recently been synthesized, and initial experiments show that it has the same space group as CeSbTe. The calculated band structures show the same topologically protected crossings near the Fermi level. This means that SmSbTe could be another candidate to study exotic magnetic phases. We present calculated band structures for SmSbTe in different magnetic phases with spin-orbit coupling and LDA+U corrections [2,3] included.

References

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This work is funded by the Department of Energy, Grant DE-SC0019467. Calculations were performed at Cori at NERSC, a U.S. DOE Office of Science User Facility operated under Contract DE-AC02-05CH11231.

3:54PM U43.00006: Atomic-Level Insight into Oxygen Adsorption on (hkl) Platinum Surfaces and Implications for the Reactivity in the Oxygen Reduction Reaction  SHIYI WANG (Presenter), Department of Chemical and Biological Engineering, University of Colorado Boulder, ENBO ZHU, YU HUANG, Department of Materials Science and Engineering, University of California, Los Angeles, HENDRIK HEINZ, Department of Chemical and Biological Engineering, University of Colorado Boulder — Understanding of the oxygen reduction reaction (ORR) on nanometal catalysts and specific rate predictions remain a major challenge. We quantified adsorption of molecular oxygen on Pt (100), (111), and (110) surfaces in common electrolytes and for a range of applied potentials in several times higher accuracy than feasible before using molecular dynamics simulations, and explore the following covalent bond formation using density functional theory calculations. A direct correlation between the oxygen affinity to Pt (hkl) surfaces and the experimentally measured ORR activity in the order Pt(100) < Pt(111) < Pt(110) in HClO₄ solution and Pt(111) < Pt(100) < Pt(110) in H₂SO₄ and H₃PO₄ solutions is discovered. The adsorption energies are in a range to explain specific rate differences. Experimental data for the time scale of events support that the ORR activity is driven by O₂ adsorption and initial chemisorption. The methods can be potentially applied to metal and alloy surfaces of any regularity, shape, and composition to provide quantitative insights into metal-electrolyte-gas interfaces, and promote the rational design of more effective catalysts for ORR, OER, and other electrode reactions to the large nanometer scale.
4:06PM U43.00007: Novel fundamental bounds in photovoltaic materials*  ELLA BANYAS (Presenter), University of California, Berkeley, LIANG TAN, Lawrence Berkeley National Laboratory — Effective photovoltaic materials require not only an ideal band gap, but a high carrier mobility. Identifying new candidate photovoltaics can be challenging, as generalized methods for predicting materials with the requisite properties do not yet exist. Here we use a local orbital-based approach and the nearsightedness principle to derive novel analytic bounds on effective masses, which are inversely proportional to carrier mobility in the Boltzmann transport limit. These bounds explicitly depend on both the electronic band structure (e.g. the band gap) and the physical structure of the crystalline material itself, thereby enhancing our ability to identify materials classes that have both small band gaps and high mobilities. We present the methodology used for generating these “structure-informed” fundamental bounds and compare current results to a high-throughput survey of Materials Project data.

*This work was supported by the Heising-Simons Foundation.

4:18PM U43.00008: Catalytic properties of one-dimensional electrides: A first-principles study  JINSEON PARK (Presenter), Department of Physics and Astronomy, University of Tennessee, Knoxville, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Electrides are ionic compounds in which “free” electrons (anionic electrons) are confined in a low-dimensional cavity space. The characteristic features of electrides—the existence of large void spaces and non-nucleus-bound anionic electrons—make them attractive for various applications, such as gas storage, electron/ion transport, and electrocatalytic processes. Recently, we identified Cs$_3$O as a new type of one-dimensional (1D) electride with nontrivial band topology. The compound Y$_5$Si$_3$ also was recently discovered, another 1D electride that exhibits excellent durability and catalytic efficiency. We demonstrate that hexagonal Y$_5$X$_3$ (X = Ge, Sn, and Pb) also can be classified as a 1D electride with different lattice parameters. A global structure search confirms that these compounds are thermodynamically stable. To understand the catalytic properties of Y$_5$X$_3$ as a reducing agent, the interaction between a Y$_3$X$_3$(001) surface and a Cu adsorbate is investigated, and the ability of the Y$_5$X$_3$ to donate electrons to Cu is quantitatively analyzed in terms of charge transfer. We further shed light on the role of anionic electrons in the electrochemical corrosion of Cu atoms. Our results are expected to provide a better understanding of catalytic properties of 1D electrides.
4:30PM U43.00009: Predicting 2D Materials with Machine Learning*  
GABRIEL SCHLEDER (Presenter), CARLOS MERA, Universidade Federal do ABC, ADALBERTO FAZZIO, Brazilian Nanotechnology National Laboratory — The increasing interest and research on two-dimensional materials has not yet translated into a reality of diverse materials applications. To go beyond graphene and transition metal dichalcogenides for several applications, candidates with desirable properties must be proposed. We use machine learning techniques to identify thermodynamically stable 2D materials, which is the first essential requirement for any application.

According to the formation energy and energy above the convex-hull, we classify materials as having low, medium, or high stability. The proposed approach enables the stability evaluation of novel 2D compounds for further investigation of promising candidates, using only composition properties and structural symmetry, without the need for information about atomic positions. We demonstrate the usefulness of the model generating more than a thousand novel compounds, corroborating with DFT calculations the classification for five of these materials. To illustrate the applicability we perform a screening of materials suitable for photoelectrocatalytic water splitting, identifying the potential candidate Sn$_2$SeTe generated by our model and PbTe, both not yet reported for this application.

*The authors acknowledge support from FAPESP (17/18139-6, 18/11856-7, 17/02317-2).

4:42PM U43.00010: Predicting band alignments and structural interdependence in 2D hybrid organic inorganic halide lead perovskites from First-Principles Calculations*  
SAMPREETI BHATTACHARYA (Presenter), YOSUKE KANAI, Univ of NC - Chapel Hill — Authors: Sampreeti Bhattacharya, Yosuke Kanai

2D Hybrid organic inorganic perovskites (HOIP) have emerged as a promising class of materials for various optoelectronic and electronic devices. Using first-principles density functional theory calculations based on hybrid exchange-correlation functional with spin-orbit-coupling (SOC) and with van der Waals correction, we study structural and electronic/optical properties of these materials. We discuss the effects of spatial orientation of the organic layer (Phenyl ethyl ammonium- PEA) and of the inorganic layer on the band structure alignment. In particular, we will discuss the structural stability and the SOC induced band splitting and their interdependence at the molecular level.

*This work was financially supported by the NSF under Awards No. DMR-1728921.
4:54PM U43.00011: A tunable and unidirectional one-dimensional electronic system

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\text{Nb}_{2n+1}\text{Si}_n\text{Te}_{4n+2}
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ZHENG ZHU (Presenter), HAO ZHENG, JINFENG JIA, Shanghai Jiao Tong Univ — One dimensional (1D) electronic system is a versatile platform hosting novel physics, such as charge density wave, Su-Schrieffer-Heeger (SSH) topological state and solitons, Tomonaga-Luttinger Liquid etc. However, since real 1D materials do not exist in nature, quasi-1D structures in 3D crystals become a practical substitute. Here, we systemically study the surface electronic properties on layered composition-tunable compounds \(\text{Nb}_{2n+1}\text{Si}_n\text{Te}_{4n+2}\) (\(n=1\text{~}5\)), which is predicted to be a nodal-line semimetal when \(n=1\) (\(\text{Nb}_3\text{SiTe}_6\)). Via scanning tunneling microscopy/spectroscopy, we observe 1D chains spontaneous formed on the surface of the compounds. We uncover that with the increasing of \(n\), the distance between the chains becomes larger, and the 1D electronic state is developed in the compounds with \(n \geq 3\). Our first-principle calculations reveal that the nodal-line in \(\text{Nb}_3\text{SiTe}_6\) and the 1D electronic state in the crystals with higher \(n\) in fact arise from the same bands, which are protected by the same nonsymmorphic symmetry. Furthermore, we can understand the evolution of the electronic states based on a simple SSH type picture. Our experiment demonstrates the first tunable 1D electronic system, which offers a concrete platform for the exploration of intriguing 1D electron physics.

5:06PM U43.00012: An ab-initio study of structural, electronic, and bonding properties of layer-structured ZnSb

DINESH THAPA (Presenter), BIPIN LAMICHHANE, CHANDANI NANDADASA, Physics and Astronomy, Mississippi State University, JUNSEONG SONG, SUNG WNG KIM, Department of Energy Science, Sungkyunkwan University, SEONG-GON KIM, Physics and Astronomy, Mississippi State University — The orthorhombic structure of Zinc Antimonide (ZnSb) that belongs to the space group Pbca has been extensively studied because of its promising thermoelectric properties. It is of great interest to study the different phases of ZnSb in order to figure out the inherent possibilities of electronic properties. We performed ab initio total-energy calculations and geometry optimizations within Density Functional Theory (DFT) using the generalized gradient approximation (GGA) Perdew–Burke–Ernzerhof (PBE) functional and the projected augmented wave (PAW) method to investigate the structural, electronic, and bonding properties of tetragonal (P4/nmm) and wurzite (P63mc) phases of layer-structured ZnSb. We calculated the charge density, electron localization function (ELF), Bader charge analysis, density of states (DOS), and band Structures of these materials. The energy barrier between tetragonal and wurzite phases has been calculated using the climbing image Nudged Elastic Band (CI-NEB) method. The screened Heyd-Scuseria-Ernzerhof (HSE) hybrid functional within the PBE functional was also applied to improve the band gap and compared to the experiment.

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5:18PM U43.00013: Unraveling the thermodynamic stability, catalytic activity and electronic structure of bimetallic clusters at realistic conditions*  SHIKHA SAINI (Presenter), SASWATA BHATTACHARYA, Department of Physics, Indian Institute of Technology Delhi — Cluster is considered as the prototypical system to gain a better understanding of active sites and the elementary steps of reaction mechanism at the atomistic level. Aiming toward catalytic applications, a large data set is generated on \([\text{TM}_x\text{Mg}_y\text{O}_z]^{+/0/-}\) clusters (TM = Cr, Fe, Co, Ni, \(x + y \leq 5\)) using a massively parallel cascade genetic algorithm (cGA) at the hybrid density functional level of theory. The low-energy isomers are further analyzed via \textit{ab initio} atomistic thermodynamics to estimate their free energy of formation at a realistic temperature \(T\) and partial pressure of oxygen \(p_O\). A thermodynamic phase diagram is drawn by minimizing the free energy of formation to identify the stable phases of \([\text{TM}_x\text{Mg}_y\text{O}_z]^{+/0/-}\) clusters. From this analysis, we notice that neutral and negatively charged clusters are stable in the wide range of \((T, p_O)\). The negatively charged clusters are more effective as a catalyst to lower the C–H bond activation barrier of methane. We find that the nature of TM atoms toward controlling the activation barrier is less important. However, TM gives rise to different structural motifs in the cluster, which may act as active centers for catalysis.

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Thursday, March 5, 2020 2:30 PM - 5:06 PM

Session U44 DCOMP DMP: Electrons, Phonons, Electron Phonon Scattering, and Phononics VI  704 - Hans Braun, University of Bayreuth - Tag(s): Focus
2:30PM U44.00001: Phonons in van der Waals materials and heterostructures: New probes & novel applications [Invited]  ADITYA SOOD (Presenter), Stanford University — Van der Waals (vdW) layered 2D materials and heterostructures are exciting candidates for applications in electronics and photonics. Heat dissipation presents a significant bottleneck that limits device performance. What determines the intrinsic limits of thermal transport in vdW materials? How do phonons transmit at interfaces between individual 2D layers? Can we create active thermal devices by manipulating phonon scattering rates in real time? I will present experiments designed to answer these questions, using new probes such as spatially-resolved ultrafast microscopy, femtosecond electron diffraction, and picosecond X-ray diffraction. First, I will discuss measurements of the out-of-plane thermal conductivity in thin layered crystals. Contrary to what is generally expected, we uncover evidence of propagating phonons with long mean-free-paths spanning 100s of layers. Next, to break the coherence of these vibrational modes, we use electrochemical ion insertion and achieve large reversible modulation (~10x) of thermal conductance in a nm scale device. Such thermal transistors could have interesting applications for the dynamic routing of heat. Finally, I will discuss experiments designed to elucidate interfacial energy transport at 2D heterojunctions. By addressing basic questions about the role of vibrational mismatch, we create synthetic solids with ultralow thermal conductivity. Using a new femtosecond electron diffraction technique, we probe strong coupling between photoexcited electrons and lattice vibrations in a type-II heterostructure, and directly visualize energy transport across a single vdW junction.


I gratefully acknowledge collaborations with the groups of Ken Goodson, Eric Pop, Aaron Lindenberg, Yi Cui, & Tony Heinz (Stanford University), Archana Raja (Molecular Foundry), Davide Donadio (UC Davis) & Xijie Wang (SLAC), and funding from NSF, AFOSR & DOE.

3:06PM U44.00002: Ab Initio Electron-Defect Interactions Using Wannier Functions  I-TE LU (Presenter), JINSOO PARK, JIN-JIAN ZHOU, MARCO BERNARDI, Caltech — The interactions between electrons and crystallographic defects control electron scattering and transport at low temperature. Electron-defect (e-d) interactions and the associated matrix elements can be computed from first principles using density functional theory through a method we recently developed. However, relevant quantities such as the e-d relaxation times (RTs) and carrier mobility require integrals over very fine Brillouin zone grids. Since computing a large number of e-d matrix elements is expensive, convergence and accuracy at a reasonable computational cost are challenging to achieve. In this talk, we present a Wannier interpolation scheme for e-d matrix elements and apply it to example calculations of vacancy defects in semiconductors and metals. We discuss the accuracy and versatility of the interpolation scheme, which can correctly reproduce the matrix elements computed directly, and apply it to compute and systematically converge e-d RTs and defect-limited charge transport properties at low temperature. We outline how our Wannier interpolation scheme for e-d interactions can serve as a powerful ab initio tool for studying a wide range of low-temperature transport phenomena and e-d interactions in materials.
3:18PM U44.00003: Capturing non-perturbative electron-phonon effects in real materials using DMFT  ADAM DENCHFIELD (Presenter), HYOWON PARK, Physics, University of Illinois-Chicago, PETER B LITTLEWOOD, Condensed Matter Theory, Argonne National Laboratory — Dynamical Mean Field Theory (DMFT) can capture dynamical correlation effects on real materials by combining with Density Functional Theory (DFT) and solving the DMFT equation self-consistently within the multi-orbital Hubbard model extracted from DFT. Using a similar philosophy, we show that a multi-orbital Hubbard-Holstein model can be constructed from DFT electron-phonon calculations. We then derive an effective Hubbard model with a frequency-dependent electron-electron interaction $U(\omega)$ by integrating out the phonon degrees of freedom. This model can be solved using DMFT to capture the non-perturbative electron-phonon and electron-electron interaction effects. As a proof of the concept, we calculate phase diagrams of the two-orbital Hubbard-Holstein model as functions of the Coulomb interaction, the electron-phonon coupling, and temperature. We use Niobium to illustrate the process on a real material by obtaining model parameters from DFT, obtaining new insights on the effect of electron-phonon interactions in Niobium.

3:30PM U44.00004: Computation of Phonon-Mediated Resistivity in Sr2RuO4*  FELIX ANTOINE GOUDREAULT (Presenter), MICHEL COTE, Universite de Montreal, FELICIANO GIUSTINO, University of Texas at Austin, SAMUEL PONCE, University of Oxford — Because of its strong structural similarities to some high-Tc cuprates, Sr2RuO4 (SRO), a supposedly correlated superconductor, is attracting a lot of attention recently. Even though the discovery of superconductivity in SRO happened more than 20 years ago, the nature of the superconducting gap symmetry is still debated today. SRO also bears other unconventional properties like the strong anisotropy of the temperature dependence of its resistivity. Indeed, at low temperature, resistivity behaves like a highly anisotropic 3D Fermi-liquid, but low metallic transport has been reported for the in-plane resistivity at high temperature while the out-of-plane resistivity possesses a transition from metallic to incoherent transport mechanism around 130K which remains unexplained. In order to shed light on these phenomena, we carried out ab initio calculations to compute the electron-phonon coupling in SRO in the framework of density functional theory as implemented in the Quantum ESPRESSO software. Then, using the EPW code of the Quantum ESPRESSO suite, we report the temperature dependent phonon-mediated resistivity of SRO as computed from the Iterative Boltzmann Transport Equation scheme.

*We acknowledge the support of the NSERC, scholarships and grant No. RGPIN-2016-06666.
3:42PM U44.00005: Ab initio study of spin and momentum relaxation in Elliott-Yafet spin decoherence  JINSOO PARK (Presenter), JIN-JIAN ZHOU, MARCO BERNARDI, Caltech — In the Elliott-Yafet (EY) theory, spin decoherence near room temperature is mainly mediated by electron-phonon (e-ph) interactions. The conventional wisdom is that the EY spin and momentum relaxation times are directly proportional. This proportionality has been widely used to analyze spin relaxation mechanisms in many different materials, although it is justified only for simple model systems. Here, we use our recently developed first-principles method [1] to compute independently and analyze the e-ph spin-flip and momentum-scattering interactions. We reveal stark differences between the two, and show that the EY spin and momentum relaxation mechanisms are governed by distinct microscopic processes, both in simple materials such as silicon and diamond and in complex topological semimetals. We demonstrate that the widely used proportionality between EY spin and momentum relaxation times is inaccurate, and so is the Elliott approximation relating the two. Our results highlight the need for atomistic spin relaxation calculations that take into account the electronic wave function, spin texture, phonon modes and their mode-dependent spin-phonon interactions.


3:54PM U44.00006: Ab Initio Approach for Exciton Dynamics  HSIAO-YI CHEN (Presenter), MARCO BERNARDI, Caltech — We investigate exciton dynamics from first principles by combining our recently developed formalism to compute exciton-phonon (ex-ph) interactions with the Boltzmann transport equation (BTE) to simulate the exciton non-equilibrium dynamics. The computations are challenging – the ex-ph interactions require solving the finite-momentum Bethe Salpeter equation and density functional perturbation theory on fine Brillouin zone grids, and time-stepping the exciton BTE requires a parallel algorithm to explicitly time-step the exciton occupations. We apply our approach to transition metal dichalcogenides, focusing on the time scale for exciton valley decoherence and on exciton transport and relaxation. Our work provides a rigorous framework for computing exciton dynamics in materials from first principles, advancing the understanding of ultrafast excited state dynamics in materials.
4:06PM U44.00007: Phonon-limited carrier mobility in semiconductors: importance of the dynamical quadrupoles GUILLAUME BRUNIN, HENRIQUE MIRANDA, MATTEO GIANTOMASSI, Université catholique de Louvain, MIQUEL ROYO, MASSIMILIANO STENGEL, Institute of Materials Science, Autonomous University of Barcelona, XAVIER GONZE, GIAM-MARCO RIGNANESE (Presenter), GEOFFROY HAUTIER, Université catholique de Louvain — First-principles computations of phonon-limited carrier mobilities in semiconductors have recently gained popularity. Such calculations are indeed crucial for the discovery and development of new functional materials. In state-of-the-art approaches, Fourier-based interpolation schemes are used to obtain the electron-phonon matrix elements on the very dense wavevector grids needed to converge carrier lifetimes and mobilities. In polar semiconductors, the long-range electrostatic interactions lead to a divergence of the matrix elements, rendering their interpolation unstable. For this reason, *ab initio* methods have been recently developed to model the non-analytical behavior of the matrix elements for $q \to 0$ [1]. Most of the studies performed so far have focused on this Fröhlich divergence generated by dynamical dipoles. However, additional non-analytical terms are present in the $q \to 0$ limit [2]. In this work, we analyze the role played by the dynamical quadrupoles and show that an accurate interpolation is obtained only when both dipolar and quadrupolar fields are taken into account. We discuss their impact on the accuracy and on the convergence of carrier mobilities both in polar and non-polar semiconductors.


4:18PM U44.00008: First-principles charge transport including electron-two-phonon scattering processes NIEN-EN LEE (Presenter), JIN-JIAN ZHOU, HSIAO-YI CHEN, MARCO BERNARDI, Caltech — Predicting charge transport in materials from first principles is an open challenge. Although much progress has been made recently, nearly all work to date has relied on electron-phonon (e-ph) interactions obtained from lowest-order perturbation theory. However, in materials with polar bonds, the e-ph interactions are long-ranged, so assuming that higher-order e-ph processes are negligible is not justified. We recently investigated electron-two-phonon (e-2ph) scattering processes, and showed that these higher-order contributions are substantial even in a weakly polar material like GaAs [N.-E. Lee et. al., arxiv 1903.08261]. In this talk, we address the question of how the e-2ph processes affect transport. We derive a Boltzmann transport equation (BTE) that incorporates both one-phonon and two-phonon scattering, and solve it both within the relaxation time approximation and with an iterative approach (ITA). We compute the mobility in GaAs at 200-400 K, and show that the BTE-ITA with e-2ph processes gives a mobility in excellent agreement with experiments, resolving the known mobility overestimate in the BTE-ITA with one-phonon processes only. Future extensions to strongly polar materials will also be discussed.
4:30PM U44.00009: Ab Initio Study of Impurity and Defect Scattering of Electrons in Nb and Nb₃Sn

NATHAN SITARAMAN (Presenter), TOMAS ALBERTO ARIAS, Cornell University — This talk will present ab initio density functional theory results on the effect of defects and impurities in Nb and Nb₃Sn on electron mean free path at cryogenic temperatures. The mean free path is a key quantity of interest for scientists studying the properties of superconducting radiofrequency (SRF) cavities used in particle accelerators. Using a Wannier-function based approach, we calculate electron velocities and scattering lifetimes for dense samples of states near the complex Fermi surfaces of these materials. We compare the resulting mean free path estimates to experimental measurements, and present insights into the relative importance of different impurities and defects. We discuss other potential applications of the Wannier-function method to the study of impurities and defects, such as the calculation of inelastic scattering amplitudes.

*Funded by the Center for Bright Beams.

4:42PM U44.00010: Anharmonicity and Ultra-Low Thermal Conductivity in Lead-Free Halide Double Perovskites

JOHAN KLARBRING (Presenter), OLLE HELLMAN, IGOR ABRIKOSOV, SERGEI SIMAK, Linkoping University — The lead-free halide double perovskite class of materials offers a promising venue for resolving issues related to the presence of toxic Pb and long-term stability of the very intensively studied class of single lead halide single perovskites.

The single lead halide perovskites are well known to be very anharmonic materials. In particular, the atomistic dynamics relating to distortions and tilting of octahedral units and movement of the A site is highly complex. Anharmonicity in the lead-free halide double perovskites are comparatively much less studied.

In this talk I present our first-principles study of the lattice vibrations in Cs₂AgBiBr₆, the prototypical lead-free halide double perovskite, and show that it is very soft and highly anharmonic, in particular in regards to tilting of AgBr₆ and BiBr₆ octahedra and for motion along the Ag-Br-Bi bond. Using an energy and temperature dependent phonon spectral function derived from ab initio molecular dynamics we then show how the experimentally observed cubic-to-tetragonal phase transformation can be related to the collapse of a soft phonon branch. We finally reveal that the softness and anharmonic features of Cs₂AgBiBr₆ yield an ultra-low thermal conductivity with a non standard ~T⁻⁰.⁵ temperature dependence.
Interfacial thermal transport between large lattice mismatch materials enhanced by atomic defects

ZEXI LU (Presenter), PETR SUSHKO, AMRA PELES, ANNE CHAKA, Pacific Northwest National Laboratory — Control of interfacial thermal transport across complex interfaces is predicated on our ability to identify and (de-)couple contributions associated with low-dimensional interfacial features and structural and compositional inhomogeneities. In this study, we aim to reveal the relationship between interfacial thermal transport and defects, and establish its connection with underlying phonon-interfacial defect scattering mechanisms. We combine classical non-equilibrium molecular dynamics (MD) simulations with normal mode analysis (NMA) to investigate thermal transport across Cu/Si interface as a function of defect concentration in the interfacial region. We find that vacancies have a dramatic effect: interfacial thermal conductance increases by as much as 76% for the surface vacancy concentration of only 3%. NMA decomposition of the spectral phonon heat flux suggests that interfacial defects strongly affect inelastic phonon transmission. Our results establish relationships among the distribution of near interface defects, the extent of intermixing, thermal conductance and phonon scattering.

*PNNL Chemical Dynamics Initiative LDRD

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U45 DCOMP GSNP: Computational Methods for Statistical Mechanics: Advances and Applications III 706 - Ying Wai Li, Los Alamos National Laboratory

- Tag(s): Focus
2:30PM U45.00001: Clusters and Surfaces in Reactive Atmospheres at Realistic Conditions: Beyond the Static, Monostructure Description [Invited] LUCA GHIRINGHELLI (Presenter), Fritz-Haber Institute — The processes occurring at surfaces play a critical role in the manufacture and performance of advanced materials, e.g., electronic, magnetic, and optical devices, sensors, and catalysts. A prerequisite for analyzing and understanding the electronic properties and the function of surfaces is detailed knowledge of the atomic structure, i.e., the surface composition and geometry under realistic gas-phase conditions. The key quantity for studying the structure and function of surfaces/clusters in reactive atmospheres is the Gibbs free energy, as function of number of particles, pressure, and temperature. Here, I present a set of methods for the sampling of the configurational space of (nano)clusters and surfaces in reactive (e.g., O2, H2) atmosphere, in the canonical and grand-canonical ensembles, aiming at the unbiased determination of the phase diagrams as function of temperature and partial pressure of the reactive gas. A common trait of the analysis of the different systems is the description of ensembles of structures as function of environmental variables, i.e., the identification of the invariant, permanent features, within the "noise" of continuously transforming ones. Applications to gold and metal-oxide nanoclusters, and silicon surfaces, described with first-principles potential-energy surfaces, will demonstrate the insight gained by the direct access to observables at finite temperature and pressure.

*European Unions Horizon 2020 research and innovation program (No. 676580: the NOMAD Laboratory and European Center of Excellence and No. 740233: TEC1p) and the Leibniz ScienceCampus GraFOx.

3:06PM U45.00002: Langevin dynamics for linear scaling quantum Monte Carlo [Invited] KIPTON BARROS (Presenter), Los Alamos Natl Lab, BENJAMIN COHEN-STEAD, Physics, UC Davis, GEORGE BATROUNI, Université Côte d'Azur, CNRS, RICHARD THEODORE SCALETTAR, Physics, UC Davis — We discuss recent advances in quantum Monte Carlo (QMC) sampling for models of interacting electrons. A shortcoming of traditional determinant QMC is its cubic scaling with system size. The alternative Langevin approach offers, in principle, linear scaling. With some new tricks, the Langevin method can be very competitive with determinant QMC. Applications to the Holstein model of electron-phonon interactions will be presented.

*Support was provided by the LANL LDRD program and the DOE/BES COMSCOPE project.
3:18PM U45.00003: Assessing the Quality of Approximate Quantum Dynamics in Condensed Phase via Sum Rules*  LISANDRO HERNANDEZ DE LA PENA (Presenter), Kettering University — In this work, we discuss a general protocol for analyzing the quality of approximate quantum time correlation functions of non-trivial systems in many dimensions. This approach is based on the generalized deconvolution of the Kubo transformed quantum time correlation function onto an ensemble averaged quantum correlation function, at a given value $\tau$ in imaginary time ($0 \leq \tau \leq \beta$), which leads to a series of sum rules linking derivatives of different order in the corresponding pair of convoluted correlation functions. We focus on the case when $\tau = \beta/2$ for which all deconvolution kernels become real valued functions and their asymptotic behavior at long times exhibit a polynomial divergence. It is then shown that thermally symmetrized static averages, and the static averages of the corresponding time derivatives, are ideally suited to investigate the quality of approximate quantum time correlation functions at successively larger, and up to arbitrarily long, times. This overall strategy is illustrated analytically for a harmonic system, and numerically for a multidimensional double-well potential and a Lennard-Jones fluid representing liquid neon at 30 K.

* Kettering University

3:30PM U45.00004: Ground State Properties of the Diluted Sherrington-Kirkpatrick Spin Glass  STEFAN BOETTCHER (Presenter), Physics, Emory University — In a numerical study of dilute versions of the Sherrington-Kirkpatrick mean-field spin glass at temperature $T=0$, we approximate the energies of ground states of ensembles at variable dilution with high accuracy using the Extremal Optimization heuristic [1,2]. We find that the scaling properties of such systems possess exponents that are parametrized by the degree of dilution [3,4]. This is a surprising result, as one would not expect that gradual bond-dilution would continuously change the universality class of a statistical model. (There is no evidence of a percolation transition separating a trivially disconnected regime from a percolation regime, as one might expect.) It may open the door to a perturbative study of finite-size corrections in replica symmetry breaking.

Evidence of Information Limitations in Bottom-Up Coarse-Graining Models

ADITI KHOT (Presenter), STEPHEN SHIRING, BRETT SAVOIE, Purdue Univ — Chemically specific coarse-grained (CG) models exhibit simplified configurational phase spaces and hence, can potentially capture processes that occur on time and length scales that are too costly for direct atomistic simulation. However, there are fundamental and practical problems associated with coarse-graining, such as the incomplete understanding of CG errors in comparison with atomistic simulations, the lack of transferability of typical CG models to new chemistries, and the costly bespoke approach to developing new CG models from scratch. In this talk, I will present recent results on an automated methodology to parameterize CG models from quantum chemistry calculations. Using the throughput of this methodology, we have systematically characterized the sources of error in common bottom-up parameterization methods as a function of dimension reduction for over 50 independently trained CG models. We find clear evidence that these models are systematically information limited, rather than representability limited, which suggests further improvement is obtainable without resorting to more complex functional forms. Additional implications of these findings, as well as the conditions under which representability related errors arise will also be discussed.

Hilbert Entropy for the Simple and Precise Measurement of Complexity of Two or Higher Dimensional Arrays*

SEOK JOON KWON (Presenter), KIST — Measuring complexity of higher dimensional arrays has been an important way of quantifying information. For the measurement of complexity of 1D vectors, there are a variety of methods of calculating entropies such as sample, permutation, or Lempel-Ziv entropy. Unfortunately, for higher dimensional arrays, it is not possible to employ these entropies. This is due mainly to the information loss in the course of dimension reduction. To address this problem, we introduce space-filling curve (SFC)-based approach. Thanks to the fact that SFC allows information loss-free dimension reduction, we successfully measured complexity by calculating sample entropy of higher dimensional arrays. We found that developed algorithm precisely measured the complexity of higher dimensional arrays as well as detected the critical points in the cases of various phase transition experiments. We also observed that the developed algorithm (Hilbert entropy) can measure scale-invariance and fractal dimension of higher dimensional arrays. We proved that the Hilbert entropy for higher dimensional arrays exhibits power law dependence for arrays with self-similarity.

*This work is supported by KIST (2E29300, 2V07560) and the National Research Foundation of Korea (2017R1A2B3006469).
4:06PM U45.00007: Computation of correlation functions and various statistical quantities of different types of Random Matrix Ensembles  KAZI ALAM (Presenter), SWAPNIL YADAV, KHANDKER A MUTTALIB, University of Florida — We propose a method to compute correlation functions for biorthogonal random matrix ensembles with arbitrary confining potential, by inverting the associated Hankel moment-matrix. We show that using this method it is possible to calculate eigenvalue density, two-point correlation functions, gap functions and other statistical quantities of interest for a wide class of log-gas models. The method allows one to calculate such statistical quantities numerically without evaluating the relevant polynomials or generating explicit matrices. We reproduce standard results for a variety of well-known ensembles and show some new results for Muttalib-Borodin ensembles for which analytic or numerical results have not yet been obtained.

4:18PM U45.00008: A Parameter Free Genetic Algorithm for Estimating the Dynamic Structure Factor at Zero and Finite Temperature*  NATHAN NICHOLS (Presenter), ADRIAN DEL MAESTRO, University of Vermont, TIMOTHY PRISK, National Institute of Standards and Technology, GARFIELD T WARREN, PAUL E SOKOL, Indiana University Bloomington — We report on a self adaptive Differential Evolution for Analytic Continuation (DEAC) algorithm that can be used to reconstruct the dynamic structure factor from imaginary time density-density correlations. Our approach to this long-standing problem in quantum many-body physics achieves improved resolution of spectral features over earlier methods based on genetic algorithms. The need for fine-tuning of algorithmic control parameters is reduced by embedding them within the genome to be optimized. Benchmarks are presented for models where the dynamic structure factor is known exactly and we report new results for quantum Monte Carlo simulations of confined superfluid helium at low temperatures.

*This work was supported by the NSF through grants DMR-1809027 and DMR-1808440. Simulations performed on the Vermont Advanced Computing Core were partially supported by NSF grant OAC-1827314.

4:30PM U45.00009: Study of strongly correlated materials at finite temperature with density matrix embedding theory*  CHONG SUN (Presenter), GARNET CHAN, Caltech — Density matrix embedding theory (DMET) is a wavefunction-in-wavefuction embedding scheme, aimed at describing the ground state of large strongly correlated systems. In this talk, the finite temperature extension of ground state DMET, i.e., FT-DMET, is introduced. We show its performance in both model systems such as 2D Hubbard model and realistic materials such as the hydrogen chain and transition metal oxides. The thermal averages of physical observables such as energy are calculated. The Néel transition is also studied and the Néel temperature is approximated for both 2D Hubbard model and transition metal oxides.

*Simons Foundation Burger Fellowship
Two-dimensional translation-invariant probability distributions: approximations, characterizations and no-go theorems  

4:42PM U45.00010: Two-dimensional translation-invariant probability distributions: approximations, characterizations and no-go theorems  
ZIZHU WANG (Presenter), University of Electronic Science and Technology of China, MIGUEL NAVASCUÉS, Institute of Quantum Optics and Quantum Information - Vienna, Austrian Academy of Sciences — We study the properties of the set of marginal distributions of infinite translation-invariant systems in the 2D square lattice. In cases where the local variables can only take a small number $d$ of possible values, we completely solve the marginal or membership problem for nearest-neighbors distributions ($d=2,3$) and nearest and next-to-nearest neighbors distributions ($d=2$). All these sets form convex polytopes in probability space. This allows us to devise an algorithm to compute the minimum energy per site of any TI Hamiltonian in these scenarios exactly. We also devise a simple algorithm to approximate the minimum energy per site up to arbitrary accuracy for the cases not covered. For variables of a higher (but finite) dimensionality, we prove two no-go results. The exact computation of the energy per site of arbitrary TI Hamiltonians with only nearest-neighbor interactions is undecidable. In addition, in scenarios with $d\geq 2947$, the boundary of the set of nearest-neighbor marginal distributions contains both flat and smoothly curved surfaces and the set itself is not semi-algebraic. This implies, in particular, that it cannot be characterized via semidefinite programming, even if we allow the input of the program to include polynomials of nearest-neighbor probabilities.

Stars & Bars: A Compact Representation for Bosonic Occupation States

4:54PM U45.00011: Stars & Bars: A Compact Representation for Bosonic Occupation States*  
CALEB USADI (Presenter), HATEM BARGHATHI, ADRIAN DEL MAESTRO, Univ of Vermont — An efficient representation of bosonic occupation states is a critical tool for the exact diagonalization of bosonic Hamiltonians. The memory demands of the traditional method of representing such systems, as lexicographically ordered arrays of integers, increases rapidly as system size grows, limiting current studies to approximately 16 particles at unit filling. Representing basis vectors using the combinatoric stars and bars method allows each basis state to be stored as a single 64 bit integer. This optimally compact representation will enable the analysis of new properties of larger bosonic Hamiltonians, including accessible entanglement, which may be useful in evaluating many-body phases as potential candidate quantum resource states.

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**5:06PM U45.00012: Telediagnostics of Heterogeneous Plasma properties of combustion products according to the characteristics of its braking radiation.** MYKOLA POTOMKIN (Presenter), Taras Shevchenko National University of Kyiv, VOLODYMYR MARENKOV, Odessa I.I. Mechnikov National University — An important applied aspect of the statistical theory of electronic properties of heterogeneous plasma (HP) formations for determining the amplitude-frequency intensity of its braking radiation is considered. New physical model for braking radiation of HP formations, based on the statistical approach of quasi-neutral cell for the description of electron-ion processes in the HP formations is proposed. Stochastic motion of charged plasma particles is presented in sequence of stages of anharmonic oscillations in effective electrostatic field of cells perturbed by particle displacements relative to the electrical centers of the cells of quasi-neutrality in HP formations.

The integral power of the braking radiation of HP formations in the radio band is determined in the approximation of chaotic phases using the statistical distribution of the individual cells of HP formations by correlation energy. Results of computer simulation in comparison to full-scale experiment for plasma model combustion products of the fuel, based on aluminum powder are presented.

The problems of telediagnoistics of the HP formations with cylindrical nanoparticles of condensed dispersed phase and contribution of its rotational modes to the integral intensity of the braking radiation are discussed.

**5:18PM U45.00013: Bosonic entanglement crossover from groundstate scaling to volume laws** * QIANG MIAO (Presenter), THOMAS BARTHEL, Duke University — The crossover behavior of eigenstate entanglement entropies from an area law or log-area law for low energies and small subsystem sizes to volume laws for high energies and large subsystems can be described by scaling functions. We demonstrate this for two bosonic systems. The harmonic lattice model describes a system of coupled harmonic oscillators and is a lattice regularization for free scalar field theories. For dimensions $d \geq 2$, the ground state of this model displays an entanglement area law, even at criticality, because excitation energies vanish only at a single point in momentum space. In contrast, Bose metals feature a finite Bose surface with zero excitation energy. One hence finds log-area laws for the groundstate entanglement. For both models, we sample excited states. The distributions of their entanglement entropies are sharply peaked around subsystem entropies of corresponding thermodynamic ensembles in accordance with the eigenstate thermalization hypothesis. In this way, we determine the scaling functions numerically. Eigenstates for quasi-free bosonic systems are not Gaussian. We resolve this problem by considering appropriate squeezed states instead, for which entanglement entropies can be evaluated efficiently.

*Research supported by DOE grant DE-SC0019449

**Thursday, March 5, 2020 2:30 PM - 5:30 PM**

**Session U46 GMAG DMP: Spin Ice: Classical, Quantum, and Artificial** 708

- Christopher Wiebe, Univ of Edinburgh - Tag(s): Focus
2:30PM U46.00001: Application of machine learning to frustrated magnets [Invited]  ANJANA SAMARAKOON (Presenter), DAVID TENNANT, Oak Ridge National Lab — Understanding complex phases in materials showing glassy, or highly correlated liquid states is extremely challenging. Conventional simulation approaches struggle to deal with the need to account for multiple and competing interactions, as well as relate models and data together. At the heart of the problem is the difficulty in extracting accurate models from experimental data. Further, the scale and complexity of data, such as from neutron scattering on frustrated magnets, has made any form of quantitative analysis very demanding. By training neural nets over large numbers of models, machine learning techniques discriminate between different models and identify different physical regimes including formation of spin liquids and unusual broken symmetries. The neural nets can for example learn diffuse scattering directly in three-dimensional reciprocal space and can extract the most relevant information, denoise, and remove background by projecting the experimental neutron data on a finite dimensional space that is determined by an autoencoder. Machine learning outputs the potential models, quantifies their uncertainty and identifies and classifies different regimes that could be reached by modifying or applying external forces/fields to the material under consideration. This approach is shown to provide better understanding of the formation of a glass on cooling the spin liquid Dy2Ti2O7, quantum spin liquids on honeycomb lattices, and understanding the interactions and phases in RuCl3. Examples of them as well as powder scattering data are shown.

3:06PM U46.00002: Spin dynamics in stoichiometric Ho2Ti2O7 probed by neutrons in the time domain and magnetometry in the frequency domain*  YISHU WANG (Presenter), TIMOTHY REEDER, JONAS KINDERVATER, Johns Hopkins University, YOSHITOMO KARAKI, University of the Ryukyus, NICHOLAS MALISZEWSKYJ, SERGIY GLADCHENKO, National Institute of Standards and Technology, SEYED KOOHPAYEH, Johns Hopkins University, SATORU NAKATSUJI, University of Tokyo, COLLIN LESLIE BROHOLM, Johns Hopkins University — We describe an experimental investigation of classical spin ice dynamics in a new class of high quality Ho2Ti2O7 single crystals. Employing a pump-probe method with microsecond time resolution, we have tracked neutrons diffracted from the (002) pinch point in response to an Oe range step changes in field applied along <110>. The relaxation time rises acutely from 10ms to over 10 ks upon cooling from 1.3K to 0.6K. Similar characteristic timescales were obtained from SQUID-based AC susceptibility measurements down to 1mHz on similar crystals. There are major quantitative differences between the present result and previously published works that we ascribe to our ultra-pure crystals. In addition, our simultaneous study of the Fourier-transform-related responses in time and frequency allows detailed mathematical scrutiny of the non-Debye relaxation process in spin ice.

*This work is supported by Gordon and Betty Moore Foundation under the EPIQS program GBMF no. 4532, and the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331.
3:18PM U46.00003: Frequency Dependent Susceptibility Measurements of Dilute Spin Ice.*
SEAN GIBLIN (Presenter), DAVID BILLINGTON, EDWARD RIORDAN, School of Physics and Astronomy, Cardiff University, ELSA LHOTEL, CARLEY PAULSEN, CNRS, Grenoble, STEVEN BRAMWELL, UCL — We have recently demonstrated in the classical spin ice materials Dy2Ti2O7 and Ho2Ti2O7 that the magnetic relaxation below the spin freezing transition is dominated by nuclear assisted tunnelling. Indeed, this is likely a mechanism for monopole separation and dynamics under an applied potential at temperature below ~0.65K. Given this surprising result, we have simplified the system further to isolate possible dynamical processes driven by the nuclear moments. We have considered samples with non-magnetic ion dilution, namely HoₓY₂₋ₓTiO₇ at the 1 and 0.25% level. We have investigated the samples as a function of frequency up 5 MHz and see clear evidence of evolving single ion dynamics within distinct frequency response time windows strongly suggesting other mechanisms of spin dynamics in the dilute spin ice system. The properties of these dynamics will be explained in detail.

*EPSRC

3:30PM U46.00004: Fluence Dependent Modification of Spin Ice Physics in Ho₂Ti₂O₇ Thin Films* KEVIN BARRY, Florida State Univ, NAWEEN ANAND, YAN XIN, National High Magnetic Field Laboratory, JENNIFER NEU, THEO SIEGRIST, CHRISTIANNE BEEKMAN (Presenter), Florida State Univ — We investigate the effects of strain, substrate orientation, and disorder on spin ice physics in Ho₂Ti₂O₇ thin films grown on yttria-stabilized-zirconia substrates via pulsed laser deposition. Regardless of growth orientation, all films exhibit an inflated unit cell that is larger than the one previously identified for bulk. Transmission electron microscopy has revealed the presence of anti-disorder and growth defects within the films, with the (110) oriented films showing the least number of defects. Magnetization measurements show the expected anisotropy and saturation values associated with spin ice physics. Interestingly, only the (110) oriented films show the hallmark spin ice plateau in magnetization, and the strength of this plateau shows a clear trend with the laser fluence used during growth. This study demonstrates the importance of disorder in the modification of spin ice physics in thin films.

*C.B. acknowledges support from the National Research Foundation, under Grant No. NSF DMR-1847887. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreements No. DMR-1157490 and No. DMR-1644779, and the State of Florida. JN and TS acknowledge support from NSF/DMR-1606952.
Spin ice compounds are exemplar frustrated magnetic systems that realize a classical spin liquid phase at low temperature described by an emergent gauge field with fractionalized magnetic monopole excitations. This emergent gauge structure manifests in polarized neutron scattering experiments as the characteristic pinch point singularities which have been clearly observed in the spin-flip (SF) channel. On the other hand, the non-spin-flip (NSF) channel generally lacks such striking features. In fact, within an extended model of spin ice, the NSF channel is found to be completely dispersionless, and we explore this utilizing both Monte Carlo and Large-N techniques. At the level of the Large-N approximation, this flatness is inherited directly from the flat bands of the adjacency matrix, and the temperature-dependent intensity of the featureless NSF channel is inversely proportional to the stiffness of the emergent gauge fields. We show how the SF and NSF channels can be understood as direct probes of the emergent gauge field correlations and explore the implications of this finding. This work lays the groundwork for a deeper understanding of NSF scattering in spin ice compounds, and could potentially lead to new experimental insights.
3:54PM U46.00006: Anomalous magnetic behaviour of the mixed b-site pyrochlore

Dy$_2$ScNbO$_7^*$

MEGAN RUTHERFORD (Presenter), McMaster Univ, COLE D MAUWS, Chemistry, University of Manitoba, ADAM ACZEL, Oakridge National Lab, JAMES W BEARE, GRAEME LUKE, CASEY MARJERRISON, McMaster Univ, SARA HARAVIFARD, Duke University, HAIDONG ZHOU, University of Knoxville, Tennessee, CHRISTOPHER WIEBE, The University of Winnipeg — The spin ice state, a magnetic ground state exhibiting Pauling entropy analogous to water ice, has been well characterized in the rare-earth pyrochlores Dy$_2$Ti$_2$O$_7$, and Dy$_2$Sn$_2$O$_7$. To explore the response of the spin ice state to non-magnetic perturbation in dysprosium based pyrochlores, we present here a new species Dy$_2$ScNbO$_7$, which we have synthesized as both powder and single crystal. Our physical characterization has shown unexpected behaviour arising from the disordered b-site, with increased spin dynamics and an anomalously low spin-freezing temperature. We performed heat capacity measurements with an applied magnetic field along the [111] direction, notable in pyrochlores for its alternating Kagomé-Triangular layers, and the [110] direction, a bond direction between magnetic species. The phase diagrams we have constructed from these measurements and other recent physical characterization results show a divergence from spin ice behaviour but recent neutron scattering data lead us to believe that the novel physics in our system is not entirely due to the disordered B-site. We will present these results to this meeting for discussion.

*I would like to thank the following funding agencies:

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4:06PM U46.00007: Long-range Coulomb interactions and nonhydrodynamic behavior in thermal quenches in spin ice*

OLIVER HART (Presenter), MARIANNE HAROCHE, CLAUDIO CASTELNOVO, University of Cambridge — When spin ice systems undergo a sudden thermal quench, they have been shown to enter long-lived metastable states where the monopole excitations form so-called noncontractible pairs [Phys. Rev. Lett. 104, 107201 (2010)]. While the nature of these states is well understood, the dynamical mechanisms underpinning their formation remain largely unexplored. We find that the long-range tail of the Coulomb interactions between monopoles plays a central role by suppressing the monopole-assisted decay of noncontractible pairs with respect to monopole–antimonopole annihilation. The existence of a transient, nonhydrodynamic regime allows the system to enter a metastable state whose lifetime can easily be astronomically large at low temperatures. We demonstrate this using Monte Carlo simulations and mean field population dynamics theory, and we provide an analytical understanding of the mechanisms at play. We derive the finite size scaling behavior of the density of noncontractible pairs in the plateau for both short- and long-range interactions and discuss the experimental implications of our results.

*This work was supported in part by the Engineering and Physical Sciences Research Council (EPSRC) Grants No. EP/K028960/1, No. EP/M007065/1, and No. EP/P034616/1.
4:18PM U46.00008: Peering into the darkness: vison-generated photon mass in quantum spin ice

MICHAL KWASIGROCH (Presenter), London Centre for Nanotechnology, University College London — Describing experimenetal signatures of quantum spin ice has been the focus of many theoretical efforts, as its definitive experimental verification is yet to be achieved. Gapped excitations known as visons have largely eluded those efforts. We provide a theoretical framework, which captures their dynamics and predicts new experimental signatures in the magnetic response. We achieve this by studying the ring-exchange Hamiltonian of quantum spin ice in the large-s approximation, taking into account the compact nature of the emergent U(1) gauge theory. We find the stationary solutions of the action - the instantons - which correspond to visons tunneling between lattice sites. By integrating out the instantons, we calculate the effective vison Hamiltonian, including their mass. We show that in the ground state virtual vison pairs simply renormalise the speed of light. At low temperatures, however, thermally activated visons form a Debye plasma and introduce a mass gap in the photon spectrum, equal to the plasma frequency, which we calculate as a function of temperature. We demonstrate that this dynamical mass gap should be visible in energy-resolved neutron scattering spectra but not in the energy-integrated ones. We show that it does not lead to confinement of static spinons.

4:30PM U46.00009: Broadband Spectroscopy of Magnetic Monopole Noise in Artificial Spin Ice

MATEUSZ GORYCA (Presenter), CRISTIANO NISOLI, Los Alamos National Laboratory, XIAOYU ZHANG, Yale University, CRIS LEIGHTON, University of Minnesota, JING LI, ANDREW L BALK, Los Alamos National Laboratory, PETER E SCHIFFER, Yale University, SCOTT CROOKER, Los Alamos National Laboratory — Arrays of lithographically-patterned interacting nanomagnets known as Artificial Spin Ice (ASI) have allowed the design of geometrically-frustrated collective states not found in natural magnets, as well as the ability to characterize the magnetic state at the level of the individual elements. Particularly for thermally-active ASIs, real-time studies of magnetization dynamics over a wide frequency range are highly desirable to reveal the underlying dynamics and to test theoretical models of the kinetics. Here we present an all-optical method to study the spontaneous magnetization fluctuations in ASIs over a broad frequency range (1 Hz - 1 MHz), which allows us to investigate magnetization dynamics through temperature- and field-dependent phase transitions. We focus first on the simple case of thermally-active square ASIs (using ~3 nm thick permalloy), to develop and benchmark tools for future investigations of more complex topologies. The field- and temperature-dependent total activity of the material follows theoretical models describing the creation, annihilation, and motion of ‘magnetic monopoles’ in the square ASI lattice. However, more subtle quantities such as correlation/relaxation rates deviate from widely-accepted theoretical paradigms.
4:42PM U46.00010: New Vertex Type to Study Phase Transition in Artificial Spin Ices  ALI FROTANPOUR (Presenter), Physics Department, University of Kentucky — Artificial spin ices are frustrated magnetic nanostructures constructed based on single domain segments [1]. A new type of vertex with five segments is engineered to generate eight degenerate ground states. The vertex is like the square ice vertex but one the segments split into two parallel segments creating a magnetic quadrupole. The distance between the parallel segments \(d\) determines ground state configuration. Micromagnetic simulation, OOMMF has been used to sweep \(d\), and the results show that eight configurations have the same energy at a specific distance, \(d_0\). A two-atom rectangular lattice has been made using this vertex. Stimulated annealing with Monte Carlo assistance along with magnetic field sweeping has been performed looking for phase transition behaviour of the lattice (Different antiferroquadrupolar and ferroquadrupolar ordering [2]).


4:54PM U46.00011: Hall Responses in Larger Spin Quantum Magnets* [Invited] JUDIT ROMHANYI (Presenter), University of California, Irvine, KARLO PENC, Wigner Research Centre, Budapest — Phenomena related to nontrivial band topology and transverse transports have recently gained enormous interest. Including spin degrees of freedom, a new branch of Hall responses has been proposed and observed. The concept of (anomalous/spin) Hall and (anomalous/spin) Nernst effects spread quickly from the electronic systems to magnetic excitations, leading to magnon-mediated Hall responses [1-7].

We consider magnetic insulators characterized by a larger spin and therefore by spin-multipolar degrees of freedom. We investigate the topology of the multipolar excitations and discuss the spin Nernst and thermal Hall effects arising for the nontrivial magnon modes.

Furthermore, we address the multipole character of the nontrivial bands with focus on possible new experimental detection of nontrivial magnon-band topology due to these additional degrees of freedom.


*This work was supported by the Department of Physics and Astronomy, University of California Irvine (UCI) and the Hungarian NKFIH Grant No. K 124176.

Thursday, March 5, 2020 2:30 PM - 5:30 PM
2:30PM U47.00001: The Case for Octupolar Order in Cubic 5d2 Double Perovskites* [Invited]
BRUCE D. GAULIN (Presenter), McMaster Univ — We have carried out neutron spectroscopic and diffraction studies on powder samples of the cubic 5d2 family of double perovskites, Ba2ZnOsO6, Ba2MgOsO6, and Ba2CaOsO6. These materials all display thermodynamic phase transitions at T*=30 K, 49 K, and 50 K, respectively, where ~ R ln(2) in entropy is released on passing through T*. All three display Curie-Weiss susceptibilities with antiferromagnetic Curie-Weiss constants of ~ -150 K, and show oscillations in low temperature zero longitudinal μSR, indicating time reversal symmetry breaking. Our inelastic neutron scattering shows the development of a gapped spin excitation spectrum, where a gap of ~ 15 meV develops below T*. This spectral weight is centred at wavevectors typical of type I AF order, however no magnetic Bragg diffraction is observed at low temperatures. Our neutron powder diffraction measurements place an upper limit on any possible ordered dipole moment of ~ 0.1 μB. To understand these results, we introduce a model for orbital repulsion between the two 5d electrons in Os6+ in these materials. This results in a non-Kramer's doublet and excited triplet of states for the ion, and ferro-octupolar order below T*, consistent with the full set of experimental observations. We believe this likely constitutes the first compelling case for octupolar order in a d-orbital Mott insulators.

*This work was funded by NSERC of Canada. It employed neutron scattering facilities at the Spallation Neutron Source of Oak Ridge National Laboratory and the Institut Laue Langevin, as well as synchrtron x-ray diffraction facilities at ALBA.

3:06PM U47.00002: Octupolar order in d-orbital Mott insulators.* ARUN PARAMEKANTI (Presenter), Univ of Toronto, DALINI D MAHARAJ, BRUCE D. GAULIN, Physics, McMaster University — We discuss the quantum magnetism of J = 2 ions which can be realized in spin-orbit coupled oxides with 5d2 transition metal ions. We discuss a microscopic mechanism where the combination of orbital repulsion and antiferromagnetic spin interactions leads to ferro-octupolar coupling, potentially stabilizing ferro-octupolar order. We discuss experimental signatures of octupolar order. We uncover a a gapped and dispersive magnetic exciton in the ferro-octupolar state using a slave-boson approach, which can be observed in neutron scattering. For sufficiently strong magnetic exchange, this dispersive exciton can condense, leading to conventional type-I antiferromagnetic order which can coexist with or even preempt octupolar order. Our proposal for ferrooctupolar order provides a comprehensive understanding of thermodynamics, μSR, X-ray diffraction, and inelastic neutron scattering measurements on a range of cubic 5d2 double perovskite materials including Ba2ZnOsO6, Ba2CaOsO6, and Ba2MgOsO6. Our proposal for exciton condensation leading to type-I magnetic ordering is potentially relevant to materials such as Sr2MgOsO6.

*NSERC of Canada
3:18PM U47.00003: Neutron scattering study of magnetic excitation in spinel structure spin-orbital coupling compound CuGa2O4  ZHIJUN XU (Presenter), NIST and University of Maryland, GUANGYONG XU, NIST, AASHISH SAPKOTA, Brookhaven national lab, YIMIN QIU, NIST, GENDA GU, JOHN TRANQUADA, Brookhaven national lab — We report neutron scattering measurements on a single crystal CuGa2O4 sample. The spinel structure of CuGa2O4 can cause strong spin-orbit coupling in this compound. From DC susceptibility and elastic neutron measurements, we found no sign of long- or short-range magnetic order down to 0.1K. Measurements on low energy magnetic excitations show ring shape intensity distribution in momentum space from this sample at low temperature. With increasing temperature, the magnetic excitation intensity gradually goes away.

3:30PM U47.00004: d-Orbital Occupancy Systematics of 4d/5d Row Transition Metal Oxides by X-Ray Absorption Near Edge Spectra (XANES)*  ERIC KURYWCZAK (Presenter), MEHMET ALPER SAHINER, Physics, Seton Hall University, MARK CLYDE CROFT, Physics, Rutgers University — XANES L₂ and L₃ edge X-Ray Absorption Near Edge Spectra (XANES) for 4d and 5d row transition metals (TM) oxides are assumed to be directly reflecting unoccupied d-orbitals influenced by the local symmetry of the metal ion¹. XANES L₂ and L₃ edge data analysis through non-linear curve fitting allows for a unique, efficient look at the structural eccentricities of transition metal oxides. In this way it is possible to determine the oxidation state of a material as well as its site symmetry. We have used non-linear least-squares fitting across the near-edge region of the various 4d row and 5d row TM oxides in order to investigate the systematics of the d-orbital occupancy and the XANES white line features for t²g and e₈ symmetry orbitals. The statistics have already shown promising trends to be expected in 4d and 5d row level transition metal oxides. The systematics obtained by these results provide crucial information for the synthesis of the new materials with specific electronic structures and crystal symmetries.

¹ Megan E. Fieser et al., Chem. Sci., 2017, 8, 6076–6091

*NSF-DMI 0420952

3:42PM U47.00005: From multipolar to spin-lattice disordered states in Mott insulators [Invited]  GEORGE JACKELI (Presenter), Max Planck Institute for Solid State Research, Stuttgart, Germany — We theoretically explore how in the Mott insulating compounds the spin-orbit coupling could give rise to unusual disordered (glass or liquid) states of spin-orbital or spin-lattice degrees of freedom depending on the local d-electron counting. We discuss d¹ and d² transition metal compounds, such as molybdenum oxides with fcc and pyrochlore lattices, as candidate materials and consider experimental results from this perspective.
**4:18PM U47.00006: Observation of Spin Glassy Behavior in Sr$_3$(Ru$_{0.64}$Mn$_{0.36}$)$_2$O$_7$**

ROSHAN NEPAL (Presenter), LINGYI XING, RONGYING JIN, Louisiana State University, Baton Rouge — One of the most accessible knobs to tune the ground state properties of a material system is chemical doping. Double-layered Ruddlesden-Popper ruthenate Sr$_3$Ru$_2$O$_7$ is known to respond dramatically to the substitution of Ru by Mn leading to a rich phase diagram. We report the magnetic properties of 36% Mn doped single-crystalline Sr$_3$(Ru$_{1-x}$Mn$_x$)$_2$O$_7$ (x = 0.36). The temperature dependence of the zero-field cooled magnetic susceptibility shows a significant downturn akin to the collective freezing of the spins below a freezing temperature $T_f$, which is suppressed by the applied magnetic field. The onset of the spin freezing is accompanied by the development of large magnetic memory, magnetic relaxation, and exchange bias effects, which suggests Sr$_3$(Ru$_{0.64}$Mn$_{0.36}$)$_2$O$_7$ has the spin glass (SG) ground state. Further analysis reveals the presence of de Almeida-Thouless phase line separating the high temperature paramagnetic (PM) and low temperature SG phases with $T_{SG} \sim 32$ K. The nature of the SG state and its implication will be discussed.

*This work was supported by DoE through DE-SC0016315.

**4:30PM U47.00007: A muSR study of current-induced destruction of order in Ca$_2$RuO$_4**

MATTHEW NUGENT (Presenter), GRAEME LUKE, JAMES W BEARE, McMaster Univ, MARKUS BRADEN, KEVIN JENNI, University of Cologne, SUDARSHAN SHARMA, MEGAN RUTHERFORD, McMaster Univ, QI SHENG, Columbia University — Past work has shown that Ca$_2$RuO$_4$ is a Mott insulator, but can be switched to a semimetallic state with the application of a reasonable amount of current. The material is an antiferromagnet below 113K in the insulating state, but achieving the semimetallic state causes a destruction of order, instead giving a diamagnetic response [1]. For this muSR study on the material, we used a 1% Ti doped Ca$_2$RuO$_4$ sample, which provided improved structural stability without significantly impacting magnetic ordering temperature [1]. We measured the sample under 0mA, 30mA, and 100mA of current, demonstrating both the presence of an antiferromagnetic ordering and its destruction in the semimetallic state when a current is applied down to 15K.


4:42PM U47.00008: Electronic and magnetic properties in barium iridium oxides*  Xiang Chen (Presenter), Dongsheng Yuan, Edith Bourret-Courchesne, Lawrence Berkeley National Laboratory, Robert J Birgeneau, University of California, Berkeley — The strongly spin orbit coupled Jeff = 1/2 spin residing on various lattice motifs are promising playgrounds for realizing assorted unusual ground states, such as Kitaev quantum spin liquid in frustrated Kagome lattice, proximity to unconventional superconducting state in layered square lattice. The recently proposed exotic quantum liquid state in facing sharing spin chain Ba4Ir3O10 might offer another platform for novel frustration. Here we introduce detailed experimental studies on those spin chain barium iridium oxides, which might be another intriguing system for engineering unusual electronic and magnetic ground states.

*Department of energy

4:54PM U47.00009: First-Principles Calculations of the atomic and magnetic structure of perovskite oxides SrMoO3, PbMoO3 and LaMoO3  Jeremy Lee-Hand (Presenter), Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York, 11794-3800, USA, Cyrus Dreyer, Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York, 11794-3800, USA and Center for Computational Quantum Physics, Flatiron Institute, 162 5th — Perovskite oxides have a characteristic ABO3 structure that is able to accommodate a large number of different cations in the A and B locations. In particular, perovskites with Mo on the B site, including SrMoO3 and PbMoO3 have recently been fabricated. SrMoO3 has been shown to have high electron mobility, and PbMoO3 exhibits metallic behavior to low temperatures with a resistivity displaying a sublinear dependence on temperature. We use first-principles calculations based on density-functional theory (DFT) plus Hubbard U to investigate the family of perovskite molybdenates: SrMoO3, PbMoO3, and LaMoO3 in order to determine their ground-state atomic and magnetic structures. We determine the dependence with the choice of U, exchange-correlation functional, and implementation with respect to DFT code. Finally, we interpret the ground-state structures in terms of unstable phonons of higher symmetry structures including cubic Pm-3m.
5:06PM U47.00010: Random singlet state in the spin liquid candidate $\text{Ba}_5\text{CuIr}_3\text{O}_{12}$*  DENIS GORBUNOV (Presenter), Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany, PAVEL VOLKOV, Department of Physics and Astronomy, Center for Materials Theory, Rutgers University, CHOONG-JAE WON, Max Planck POSTECH/Korea Research Initiative, Pohang University of Science and Technology and Laboratory of Pohang Emergent Materials, Pohang Accelerator Laboratory, Korea, JAEWOOK KIM, Department of Physics and Astronomy, Center for Emergent Materials, Rutgers University, MAI YE, Department of Physics and Astronomy, Rutgers University, HEUNG-SIK KIM, Department of Physics and Astronomy, Rutgers University; Kangwon National University, Chuncheon, Korea, JED PIXLEY, Department of Physics and Astronomy, Center for Materials Theory, Rutgers University, SANG-WOOK CHEONG, Department of Physics and Astronomy, Center for Emergent Materials, Rutgers University; Max Planck POSTECH/Korea Research Initiative, Pohang University of Science and Technol, GIRSH BLUMBERG, Department of Physics and Astronomy, Rutgers University — Understanding the role of disorder is crucial for the realization of quantum spin liquid (QSL) states in frustrated magnets, as it can lead to states mimicking QSL, but devoid of long-range entanglement. We study the thermodynamic and high magnetic field properties of the magnetic insulator $\text{Ba}_5\text{CuIr}_3\text{O}_{12}$, a QSL candidate showing no magnetic order down to 2 K. The temperature dependencies of the magnetic susceptibility and the specific heat suggest weak antiferromagnetic correlations, in stark contrast to the magnetization that does not saturate up to a field of 59 Tesla. We show that these results can be reconciled only within the framework of a disorder-dominated random singlet state. The obtained exchange coupling distribution $P(J)$ is found to be consistent with the power-law form $P(J) \sim J^{-\alpha}$ with $\alpha \approx 0.6$. Our work highlights the use of high magnetic field measurements for distinguishing QSL candidates from disorder-dominated states and characterizing the latter.

*The work was supported by the NSF Grant No. DMR-1629059; HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL); National Research Foundation of Korea, Ministry of Science and ICT (No. 2016K1A4A4A01922028); NSF Grant No. DMR-1709161 (M.Y. and G.B); P. V. is supported by the Rutgers CMT Postdoc fellowship.

5:18PM U47.00011: Valence bond solids and hidden order phases in a pyrochlore $U(1)$ quantum spin liquid  HYEOK-JUN YANG (Presenter), SUNGBIN LEE, KAIST — Antiferromagnetic spin-1/2 system on a pyrochlore lattice has been extensively studied as a host of the exotic phase of matter, $U(1)$ quantum spin liquid (QSL). In a low-energy sector, the spin degrees of freedom are mapped to the emergent $U(1)$ gauge fields and fractionalized excitations. As the kinematics of the fractionalized excitations dominates the system, the emergent gauge structure is broken and the QSL encounters the magnetic instability. Beyond the $U(1)$ QSL and the conventional orderings, the realization of unconventional phases such as the spin nematic, multiple order etc., in frustrated magnet opens an interesting question. Here, we study the pyrochlore XXZ model with farther and competing exchange interactions. Analyzing the effective spinon actions, we schematically depict the richer phase diagram exhibiting the valence bond solids, spin nematic, and inversion breaking hidden orders.

Thursday, March 5, 2020 2:30 PM - 4:54 PM
Nickelate superconductivity --Formation of self-doped 2D single-orbital correlated electron systems in NdNiO$_2$

YUSUKE NOMURA (Presenter), MOTOAKI HIRAYAMA, RIKEN, TERUMASA TADANO, National Institute for Materials Science (NIMS), YOSHIHIDE YOSHIMOTO, University of Tokyo, KAZUMA NAKAMURA, Kyushu Institute of Technology, RYOTARO ARITA, University of Tokyo — The recent discovery of superconductivity in the doped nickelate Nd$_{0.8}$Sr$_{0.2}$NiO$_2$ has opened up a great opportunity to unravel the mystery of superconductivity in correlated materials. While the electronic structure of the nickelate is similar to that of the celebrated cuprates, there is one distinct difference: not only the Ni $3d_{x^2-y^2}$ electrons but electrons in the Nd layer also form the Fermi surface. The electronic structure around the Fermi level is well described by the Ni $3d_{x^2-y^2}$, Nd $5d_{3z^2-r^2}$, and a bonding orbital made from the interstitial $s$ and Nd $5d_{xy}$ orbitals. The hybridization between the Ni $3d_{x^2-y^2}$ and Nd-layer states is small, so that the screening effect of the Nd-layer states is less effective, which leaves the Ni $3d_{x^2-y^2}$ electrons strongly correlated. On the other hand, the electron-phonon coupling constant is not strong enough to mediate superconductivity of $T_c \approx 10$ K. These results indicate that NdNiO$_2$ hosts an almost isolated correlated Ni $3d_{x^2-y^2}$ orbital system with a self-doping due to the Nd-layer-state Fermi pockets [1]. Furthermore, we provide a useful guideline to eliminate the complication due to the self-doping and realize prototypical $d^9$ nickelates [2].

Nickelate superconductivity — A systematic computational design of dynamically stable $d^9$ nickelates

MOTOAKI HIRAYAMA, RIKEN, TERUMASA TADANO (Presenter), National Institute for Materials Science (NIMS), YUSUKE NOMURA, RIKEN, RYOTARO ARITA, University of Tokyo — The origin of superconductivity in the Sr-doped layered nickelate NdNiO$_2$ has been studied actively since its recent discovery [1]. Several theoretical studies, including our own [2], have shown that the electronic structure of NdNiO$_2$ is quite similar to that of the cuprates near the Fermi level, but they are different in that the Ni $3d_{x^2-y^2}$ orbital is self-doped due to the presence of Fermi pockets formed by the states originating from the Nd block layer (BL).

In this talk, we show that more ideal $d^9$ nickelates can be realized by adopting different types of BLs. By systematically generating new potential nickelate structures and then performing ab initio phonon calculations, we theoretically propose more than 10 new compounds that are dynamically stable and whose electronic structures better mimic that of the cuprates. We demonstrate that the newly proposed layered nickelates are in the strongly-correlated regime without forming an extra Fermi pocket as large as that of NdNiO$_2$. We also discuss the possibility of palladate analogues of high-$T_c$ cuprates briefly. This presentation is based on Ref. [3].


Superconductivity in infinite-layer nickelates: similarities and differences from cuprates

ANTIA BOTANA (Presenter), Arizona State University, MICHAEL NORMAN, Argonne Natl Lab — The electronic structure of infinite-layer nickelates RNiO$_2$ (R= La, Nd) is revisited in light of the discovery of superconductivity in Sr-doped NdNiO$_2$. From a comparison to their cuprate counterpart CaCuO$_2$, we derive essential facts related to their electronic structures, in particular, the values for hopping parameters and energy splittings, and the influence of the spacer cation. From this detailed comparison, we comment on expectations in regards to superconductivity. In particular, both materials exhibit a large ratio of longer-range hopping to nearest-neighbor hopping which should be conducive for superconductivity.

*U.S. Dept. of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division
Two-band model for magnetism and superconductivity in nickelates

Nd$_{1-x}$Sr$_x$NiO$_2$ LUN-HUI HU (Presenter), CONGJUN WU, University of California, San Diego — The recently discovered superconductivity in Nd$_{1-x}$Sr$_x$NiO$_2$ provides a new opportunity for studying strongly correlated unconventional superconductivity.

The single-hole Ni$^+$ (3d$^9$) configuration in the parent compound NdNiO$_2$ is similar to that of Cu$^{2+}$ in cuprates.

We suggest that after doping, the intra-orbital spin-singlet and inter-orbital spin-triplet double-hole (doublon) configurations of Ni$^{2+}$ are competing, and we construct a two-band Hubbard model by including both the 3d$_{x^2-y^2}$ and 3d$_{xy}$ orbitals.

The effective spin-orbital super-exchange model in the undoped case is a variant of the SU(4) Kugel-Khomskii model augmented by symmetry breaking terms.

Upon doping, the effective exchange interactions between spin-1/2 single-holes, spin-1 (triplet) doublons, and singlet doublons are derived.

Possible superconducting pairing symmetries are classified in accordance to the D$_{4h}$ crystalline symmetry, and their connections to the superexchange interactions are analyzed.

D-wave superconductivity in the t−J model with spin one holes: possible applications to the nickelate superconductor Nd$_{1-x}$Sr$_x$NiO$_2$

YAHUI ZHANG (Presenter), ASHVIN VISHWANATH, Harvard University — The recent observation of superconductivity at relatively high temperatures in hole doped NdNiO$_2$ has generated considerable interest, particularly due to its similarity with the infinite layer cuprates. Building on the observation that the Ni$^{2+}$ ions resulting from hole doping are commonly found in the spin-triplet state, we introduce and study a variant of the t−J model in which the holes carry S=1. We find two distinct mechanisms for d wave superconductivity. In both scenarios the pairing is driven by the spin coupling J. However, coherence is gained in distinct ways in these two scenarios. In the first case, the spin-one holes condense leading to a d wave superconductor along with spin-symmetry breaking. In the second scenario, a coherent and symmetric d wave superconductor is achieved from "Kondo resonance": spin one holes contribute two electrons to form large Fermi surface together with the spin 1/2 singly occupied sites. The large Fermi surface then undergoes d wave pairing because of spin coupling J, similar to heavy fermion superconductor. Our study shows that a combination of "cuprate physics" and "heavy fermion physics" may emerge in this novel t−J model.

*This work was supported by a Simons Investigator Grant (A.V.).
Superconductivity in trilayer Nickelates

EMILIAN NICA (Presenter), JYOTI KRISHNA, Department of Physics, Arizona State Univ, RONG YU, Department of Physics and Beijing Key Laboratory of Opto-electronic Functional Materials and Micro-nano Devices, Renmin University of China, QIMIAO SI, Department of Physics and Astronomy, Rice University, ANTIA S. BOTANA, ONUR ERTEN, Department of Physics, Arizona State Univ — Infinite-layer NdNiO$_2$ has recently been shown to exhibit superconductivity upon Sr-doping [1].

For doped NdNiO$_2$, it is believed that pairing in the superconducting phase occurs mainly in the Ni $d_{x^2-y^2}$ band [2]. In contrast to the Cu-based high-$T_c$ superconductors, the parent RNiO$_2$ (R=La, Nd) phases are not insulating-in spite of containing Ni$^{1+}$: $d^9$ ions-due to the appearance of rare-earth 5d-bands in the Fermi surface (FS) [2]. RNiO$_2$ materials are members of a larger family of layered nickelates R$_{n+1}$(NiO$_2$)$_n$O$_2$ with $n= 2, 3, ... \infty$ determining the number of NiO$_2$ planes along the c-axis. Here, we consider alternate trilayer compounds [3] where the rare-earth bands are pushed away from the FS which only includes three Ni- $d_{x^2-y^2}$ sheets. We study superconductivity in these compounds in several doping regimes using a t-J model. We compare and contrast the pairing instabilities in the tri- and infinite-layer cases.


Understanding magnetism in infinite-layer nickelates ab initio

VICTOR PARDO (Presenter), ADOLFO O. FUMEGA, University of Santiago de Compostela, ANTIA S. BOTANA, Arizona State University — Since the discovery of superconductivity in Sr-doped NdNiO$_2$ [1], magnetism has been ruled out [2] as being part of the equation in superconducting layered nickelates. Even though NdNiO$_2$ (containing NiO$_2$ layers with Ni$^{1+}$:d$^9$ cations) should be magnetically similar to the cuprates, it turns out to be drastically different [3]. In this talk, we will analyze the underlying electronic-structure mechanisms that lead to such different behavior in infinite-layer nickelates. In particular, we will describe the tendency towards magnetic order in a series of DFT-based ab initio calculations carried out on RNiO$_2$ (R:Nd, La).


*We acknowledge support of the MINECO through the Project No. PGC2018-101334-B-C21 and FPU grant FPU16/02572.
4:06PM U48.00009: Robust $d_{x^2-y^2}$ wave superconductivity of infinite-layer nickelates\footnote{The work in Würzburg is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through Project-ID 258499086 - SFB 1170 and through the Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter – ct.qmat Project-ID 39085490 - EXC 2147. H.Y.H. and S.R. are supported by the DOE Office of Basic Energy Sciences, contract DEAC02-76SF00515.}

XIANXIN WU, DOMENICO DI SANTE, TILMAN SCHWEMMER (Presenter), WERNER R HANKE, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, HAROLD HWANG, SRINIVAS RAGHU, Institute for Materials and Energy Sciences, Stanford University, RONNY THOMALE, Institut für Theoretische Physik und Astrophysik, Universität Würzburg — Motivated by the recent observation of superconductivity in strontium doped NdNiO$_2$, we study the superconducting instabilities in this system from various vantage points. Starting with first principles calculations, we construct two distinct tight-binding models, a simpler single-orbital as well as a three-orbital model, both of which capture the key low energy degrees of freedom to varying degree of accuracy. We study superconductivity in both models using the random phase approximation (RPA). We then analyze the problem at stronger coupling, and study the dominant pairing instability in the associated t-J model limits. In all instances, the dominant pairing tendency is in the $d_{x^2-y^2}$ channel, analogous to the cuprate superconductors.

4:18PM U48.00010: Ground States of Infinite-Layer Nickelates at Strong Coupling: A Variational Study\footnote{VBS and DC thank the visitor program at MPIPKS, Dresden, where part of this work was carried out.}

AMAL MEDHI (Presenter), Indian Institute of Science Education and Research Thiruvananthapuram, CHUAN CHEN, MPIPKS, Dresden, VIJAY SHENOY, Indian Institute of Science, Bangalore, DEBANJAN CHOWDHURY, Cornell University, Ithaca — Motivated by the recent discovery of superconductivity in infinite-layer nickelates, we study a two orbital model, including both nickel 3d and the rare-earth 5d orbitals, in the regime of strong local repulsive interactions. Using variational Monte-Carlo calculations which treat strong correlations via suitable projection techniques, we investigate superconductivity and study its dependence on the hole and electron doping, three-dimensionality, and the energetics of the rare-earth 5d orbital. We report a ground state phase diagram of this system, and provide complementary insights using a parton mean-field theory.
4:30PM U48.00011: Hole superconductivity in infinite-layer nickelates  
FRANK MARSIGLIO  
(Presenter), Physics, University of Alberta, JORGE HIRSCH, University of California, San Diego — We propose that the superconductivity recently observed in Nd$_{0.8}$Sr$_{0.2}$NiO$_2$ with critical temperature in the range 9 K to 15 K results from the same charge carriers and the same mechanism that we have proposed give rise to superconductivity in both hole-doped and electron-doped cuprates: pairing of hole carriers in oxygen $p\pi$ orbitals, driven by a correlated hopping term in the effective Hamiltonian that lowers the kinetic energy, as described by the theory of hole superconductivity. We predict a large increase in $T_c$ with compressive epitaxial strain.

*This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC)

4:42PM U48.00012: A Determinant Quantum Monte Carlo Study of an Effective Low Energy Model for Infinite-layer Nickelates  
FANGZE LIU (Presenter), XUXIN HUANG, Stanford University, BRIAN MORITZ, SLAC National Accelerator Laboratory, EDWIN HUANG, University of Illinois at Urbana-Champaign, THOMAS DEVEREAUX, Stanford University — Our study was motivated by the recent experimental observation of superconductivity in layered nickelate heterostructures with Tc of about 9K to 15K (D Li, et al. 2019). Here, we use determinant quantum Monte Carlo (DQMC) simulations of a composite system, consisting of Hubbard-like Ni, or NiO$_2$, layers coupled to metallic rare-earth layers, to investigate the physics associated with nickelate superconductors. We study the doping-dependent magnetic and electronic properties, such as spin and charge correlations, the single-particle spectral function, interlayer pair correlations, and even superfluid stiffness.

Reference:

Thursday, March 5, 2020 2:30 PM - 5:06 PM

Session U49 DCMP: Superconductivity: Response to Electromagnetic Fields (Optical and Raman Spectroscopy, Surface Impedance, Etc.)

Mile High Ballroom 1B - Richard Klemm, Univ of Central Florida
2:30PM U49.00001: Effects of Forward Scattering from Dopant Impurities in Overdoped Cuprates*  
PETER HIRSCHFELD (Presenter), University of Florida, VIVEK MISHRA, Kavli Institute for Theoretical Sciences, Chinese Academy of Sciences, NICHOLAS LEE-HONE, ULAS OZDEMIR, DAVID BROUN, Physics, Simon Fraser U. — Many properties of overdoped cuprate superconductors can be explained by simple BCS and Landau Fermi liquid theory, supplemented by an appropriate description of disorder from dopant impurities. In addition to simply providing weaker scattering, out-of-plane dopants give rise to extended impurity potentials that scatter preferentially in the forward direction. Here we investigate the effects of such forward scattering on the optical conductivity and the penetration depth, and make specific quantitative comparisons with both LSCO and Ti-2201. We discuss previous work on forward scattering in ARPES in the same context.

*PJH was partially supported by NSF-DMR-1849751. DB, NL-H and UO acknowledge support from Natural Science and Engineering Research Council of Canada, the Canadian Institute for Advanced Research, and the Canadian Foundation for Innovation.

2:42PM U49.00002: Gauge-invariant microscopic kinetic theory of superconductivity in response to electromagnetic fields I: Application to current excitation   
FEI YANG, MING-WEI WU (Presenter), University of Science and Technology of China — Within a gauge-invariant microscopic kinetic theory, we study the electromagnetic response in the superconducting states. Both superfluid and normal-fluid dynamics are involved. We predict that the normal fluid is present only when the excited superconducting velocity is larger than a threshold. Interestingly, with the normal fluid, we find that there exists friction between the normal-fluid and superfluid currents. Due to this friction, part of the superfluid becomes viscous. Therefore a three-fluid model, normal fluid and nonviscous and viscous superfluids, is proposed to capture both the magnetic and optical responses. Moreover, an exotic phase in which both the resistivity and superconducting gap are finite is predicted.

2:54PM U49.00003: Phase-sensitive analysis of Higgs oscillations in quenched superconductors with time- and angle-resolved photo emission spectroscopy  
LUKAS SCHWARZ (Presenter), DIRK MANSKE, Max Planck Institute for Solid State Research — Higgs oscillations in nonequilibrium superconductors provide a unique tool to obtain information about the underlying order parameter. Several quantities like the absolute value, existence of multiple gaps and the symmetry of the order parameter can be encoded in the Higgs oscillation frequency. Most works so far concentrate on experiments, where momentum averaged quantities like the optical conductivity or third-harmonic effects in the transmitted light field are investigated, which does not allow to access all possible information contained in the Higgs oscillations. Here, we study the time-resolved spectral function measured in angle-resolved photo emission spectroscopy after quenching the system using a general approach. We analyze the induced oscillations all over momentum space to study the creation process of collective Higgs oscillations and we extract phase information of the order parameter from the oscillations of the spectral function.
**3:06PM U49.00004: Driving the Higgs oscillation in cuprates: unveiling collective modes or interactions coupled to Cooper pairs**  
HAO CHU (Presenter), MIN-JAE KIM, Max Planck Institute for Solid State Research, KOTA KATSUMI, Physics, University of Tokyo, SERGEY KOVALEV, Helmholtz-Zentrum Dresden-Rossendorf, ROBERT DAWSON, LUKAS SCHWARZ, Max Planck Institute for Solid State Research, NAOTAKA YOSHIKAWA, Physics, University of Tokyo, GIDEOK KIM, DANIEL PUTZKY, Max Planck Institute for Solid State Research, JAN-CHRISTOPH DEINERT, NILESH AWARI, MIN CHEN, Helmholtz-Zentrum Dresden-Rossendorf, GEORG CHRISTIANI, GENNADY LOGVENOV, Max Planck Institute for Solid State Research, YANN GALLAIS, University Paris Diderot, ALEXANDER BORIS, BERNHARD KEIMER, ANDREAS P SCHNYDER, DIRK MANSKE, Max Planck Institute for Solid State Research, MICHAEL GENSC, ZHE WANG, Helmholtz-Zentrum Dresden-Rossendorf, RYO SHIMANO, Physics, University of Tokyo, STEFAN KAISER, Max Planck Institute for Solid State Research — The Higgs mode of a superconductor is a collective excitation of the amplitude of the superconducting order parameter. It can be coherently driven at a frequency $2\omega$ by a multicycle terahertz pulse of frequency $\omega$. This then leads to third harmonic generation (THG) as a result of sum frequency generation between the oscillating condensate and the terahertz driving pulse. We applied such experimental scheme to different families of cuprate high-Tc superconductors. By phase-resolving the THG response with respect to the terahertz drive, we uncover the universal anti-resonance of the driven Higgs oscillation in all samples. This may be understood in terms of an additional collective mode coupled to the Higgs mode. Careful analysis of the anti-resonance feature as a function of hole doping with the help of a coupled oscillators model suggests that the coupled mode could be the magnetic resonant mode. Our findings may shed light on the pairing mechanism in d-wave superconductors.

*Hao Chu acknowledges support from the Max Planck-UBC-UTokyo Centre for Quantum Materials

**3:18PM U49.00005: Spectroscopic and optical response of odd-frequency Berezinskii superconductors**  
PAVLO SUKHACHOV (Presenter), ALEXANDER BALATSKY, Nordita — By using a simple model with a parabolic dispersion law and a non-magnetic disorder, the spectral function, the electron density of states, and the optical conductivity are calculated in clean and disordered Berezinskii superconductors for a few gap ansatzes. The strong dependence of the spectral function and the electron DOS on the frequency profile of the gap is rather unusual and could explain why it is experimentally hard to identify the Berezinskii state. It is found also that the OF pairing allows for peaks in the real part of the optical conductivity, whose form and position depend on the specific frequency profiles of the gap. For the frequencies that correspond to these peaks, sharp cusps appear in the imaginary part. The form of these cusps is nontrivial for the OF pairing. In particular, the imaginary part of the optical conductivity can become negative allowing for the optical transparency windows.

*POS and AVB acknowledge support from VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744), the European Research Council under the European Unions Seventh Framework ERS-2018-SYG 810451 HERO, and the Knut and Alice Wallenberg Foundation KAW 2018.0104.
3:30PM U49.00006: Control of Supercurrents and Collective Modes in Superconductors by Terahertz Lightwave Propagation*  MARTIN MOOTZ (Presenter), ILIAS PERAKIS, Univ of Alabama - Birmingham, JIGANG WANG, Physics and Astronomy, Ames Laboratory, Iowa State University — Terahertz (THz) lightwave driving of supercurrents as a dynamical symmetry-breaking principle in superconductors allows for control of collective modes and excitation of non-equilibrium phases such as gapless superconductivity. Here we demonstrate that THz light-induced nonlinear response together with THz lightwave propagation can induce an unipolar ac electric field pulse inside the superconductor for sufficiently weak current relaxation. The resulting dynamical inversion symmetry breaking in form of the induced Cooper-pair condensate flow manifests itself by high harmonic generation at equilibrium-symmetry forbidden frequencies and allows for control of collective modes by THz-pulse shaping. To systematically describe the dynamic interplay of THz lightwave acceleration of Cooper-pair condensate and THz lightwave propagation inside the superconductor, we solve full nonlinear gauge-invariant Maxwell-Bloch equations beyond the Anderson pseudo-spin precession model that we derived by using a gauge-invariant non-equilibrium density matrix approach.

*The work at the University of Alabama, Birmingham acknowledges support by the U.S. Department of Energy, Office of Science, Basic Energy Sciences DoE under award DE-SC0019137

3:42PM U49.00007: Giant Microwave Absorption in d-Wave Superconductors*  MICHAEL SMITH (Presenter), ANTON ANDREEV, BORIS SPIVAK, University of Washington — We discuss a new mechanism of microwave absorption in d-wave superconductors which arises in the presence of a dc supercurrent. This mechanism produces a contribution to the ac conductivity that is proportional to the inelastic quasiparticle relaxation time and determines the supercurrent dependence of the conductivity. This new contribution may also be much larger than the conventional contribution because, in superconductors, the inelastic relaxation time typically exceeds the elastic one by several orders of magnitude. We show that the calculation of the aforementioned contribution to the conductivity can be reduced to the calculation of the single particle density of states in the presence of a dc supercurrent. Our results may enable determination of the inelastic relaxation time in superconductors from microwave absorption measurements.

*The work of A.A. and M.S. was supported by the U.S. Department of Energy Office of Science, Basic Energy Sciences under Award No. DE-FG02-07ER46452 and by the NSF grant MRSEC DMR-1719797. The work of B.S. was funded in part by the Gordon and Betty Moore Foundation’s EPIQS Initiative through Grant GBMF4302 and GBMF8686.
3:54PM U49.00008: High-Frequency Nonlinear Response of Superconducting Cavity-Grade Surfaces

BAKHROM ORIPOV (Presenter), STEVEN ANLAGE, University of Maryland, College Park — Superconducting Radio Frequency (SRF) cavities are used to accelerate charged particles to high energies, but their performance is limited by surface defects which lead to cavity breakdown at high accelerating gradients. A novel near-field magnetic microwave microscope that can study these defects was successfully built using a magnetic writer from a conventional magnetic recording hard-disk drive. We study the 3rd harmonic response $V_{3f}$ as a function of rf field amplitude ($H_{rf}$) and temperature ($T$). In our experiments on bulk and thin-film Nb surfaces, we observed 2 different classes of nonlinearity, which we call Low-field and Periodic. The low-field response is the intrinsic response of the sample due to the dynamics of vortex semiloops created by the magnetic writer (arXiv:1909.02714). In the periodic case there exists a relatively strong onset nonlinear response signal with periodic dips at $H_{rf} = H_1(T), H_2(T), H_3(T)$. This response can be linked to the Josephson effect at or near the surface and is in good agreement with the nonlinear response expected from rf-current-biased RCSJ model (PRApplied 11, 064030 (2019)). Efforts to image third harmonic response across Nb surfaces will be presented.

*This work is funded by US DOE, HEP through grant #DESC0017931 and CNAM.

4:06PM U49.00009: 2D THz spectroscopy and anomalous non-linear response of La$_{2-x}$Sr$_x$CuO$_4$

DIPANJAN CHAUDHURI (Presenter), Johns Hopkins University, FAHAD MAHMOOD, Department of Physics, University of Illinois Urbana-Champaign, DAVID BARBALAS, Johns Hopkins University, XI HE, IVAN BOZOVIC, Brookhaven National Laboratory, PETER ARMITAGE, Johns Hopkins University — La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) is a prototypical example of hole-doped single layer cuprate superconductor. Here we investigate the low frequency broadband non-linear optical response of LSCO across a wide range of doping as a function of temperature. In addition to the large optical non-linearities that is expected in the superconducting state, we find anomalous non-linear response even in the normal state, well above the superconducting critical temperature. This is in sharp contrast to the clean BCS type superconductors where the strong non-linear response at low temperatures promptly disappear at the critical temperature. Furthermore, we perform 2D THz spectroscopy on these samples to identify the different underlying non-linear processes that give rise to the overall response. We compare our results to existing theories on the superconductivity in this class of materials.

*DARPA DRINQS project FP-017, “Long-term High Temperature Coherence in Driven Superconductors”
4:18PM U49.00010: Terahertz conductivity of superconducting Beta-tungsten thin films*

PETER ARMITAGE, PRASHANT CHAUHAN (Presenter), Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, RAMESH BUDHANI, Department of Physics, Morgan State University, 1700E Cold Spring Lane, Baltimore MD -21251 — Ultrathin films of β-tungsten host superconductivity with strong spin-orbit coupling (SOC). This non-equilibrium phase of tungsten has attracted considerable attention in recent years for spintronic applications due to its giant spin Hall effect and the potential promise of exotic superconductivity. After more than 60 years of its discovery, the superconductivity in this material is still not well understood. We investigate the superconducting order in β-Tungsten using high precision time-domain THz transmission spectroscopy. Superconductivity is exhibited below 4.2 K for 70 nm film and the transition temperature reduces with increasing thickness. We study the frequency response of the complex conductivity of a thin film with a Tc of 4.2 K. In the superconducting state down to 1.6 K, the superfluid spectral weight developed is much less than the expected spectral weight for a BCS-type superconductor. This anomalous spectral weight is a possible indication of unconventional superconductivity in this system. The magnetic field response of the optical conductivity that can give additional information about the superconducting order parameter of this system, is currently under investigation.

*Work at MSU was supported through the Office of Naval Research – Grant No. N00014-17-1-2794

4:30PM U49.00011: Thickness dependence of superfluid density scaling in DyBa$_2$Cu$_3$O$_{7-x}$ thin films

ROBERT DAWSON (Presenter), DANIEL PUTZKY, GEORG CHRISTIANI, GENNADY LOGVENOV, BERNHARD KEIMER, ALEXANDER BORIS, Max Planck Institute for Solid State Research — Understanding the nature of the pseudogap phase and the relationship between charge order and superconductivity (SC) in the cuprates remains an outstanding challenge [1]. Recently, 2D SC has gained much interest due to its discovery in a variety of unconventional materials, and advancements in MBE growth of thin films have shown that 2D SC can also exist in the cuprates [2]. One interesting approach, therefore, is to investigate the evolution of cuprate physics in the ultra-thin film limit where only a few superconducting CuO$_2$ planes are present. Here, we report a study of the temperature dependence of the superfluid density as a function of thickness as well as measurements of the terahertz and infrared optical conductivity in a series of DyBa$_2$Cu$_3$O$_{7-x}$ SC thin films. We find that in the ultra-thin film limit the temperature scaling rapidly approaches that expected for dirty s-wave SC, while with decreasing oxygen content the scaling shows the opposite trend. These results suggest an increasing isotropic order parameter component below a threshold thickness due to distortions of the Fermi surface in the 2D limit.

4:42PM U49.00012: Non-linear Vortex Dynamics and Dissipation at High-amplitude Microwave Drive
MATTIA CHECCHIN (Presenter), ANNA GRASSELLINO, ALEXANDER ROMANENKO, Fermilab — In this talk, the description of the vortex dynamics and dissipation at arbitrary value of microwave field amplitude is discussed. Experimental data of vortex surface resistance in bulk niobium elliptical cavities as a function of frequency, trapped magnetic field value and field amplitude will be presented. Numerical calculations of non-linear vortex dynamics under microwave drive for different pinning landscapes allows to describe the mechanism underneath the electromagnetic field amplitude dependence of the surface resistance due to trapped vortices, pointing to the progressive microwave depinning as the most likely mechanism capable to generate such non-linearities.

4:54PM U49.00013: Optical properties of severely overdoped La$_{1.75}$Sr$_{0.25}$CuO$_4$*
CHRISTOPHER HOMES (Presenter), GENDA GU, P. M. LOZANO, QIANG LI, Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory — The temperature dependence of the optical properties of the severely overdoped cuprate La$_{1.75}$Sr$_{0.25}$CuO$_4$ have been determined above and below the critical temperature $T_c \sim 16$ K over a wide frequency range for light polarized in the $a$-$b$ plane. The real part of the optical conductivity can be reproduced reasonably well at low frequency using a simple Drude model, yielding an estimate for the plasma frequency $\omega_{pD} \sim 9300$ cm$^{-1}$. Below $T_c$ the superconducting plasma frequency $\omega_{ps} \sim 2700$ cm$^{-1}$ is determined from the Ferrell-Glover-Tinkham sum rule, indicating that less than 8% of the free carriers collapse into the superconducting condensate, in agreement with a recent study [1]. However, there is unusual structure below $\sim 0.1$ eV that suggests that the free-carrier scattering rate is strongly renormalized with frequency. In addition, the nature of the magnetic susceptibility through the superconducting transition suggests that this compound may not be homogeneous.


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Doping-dependent phonon anomaly and charge order in Hg-family of high-$T_c$ cuprates

* LICHEN WANG, Peking University, China, BIQIONG YU, University of Minnesota, RAN JING, XIANGPENG LUO, JUNBANG ZENG, JIARUI LI, Peking University, China, IZABELA BIALO, AGH University of Science and Technology, Poland, MARTIN BLUSCHKE, Max Planck Institute for Solid State Research, Germany, YANG TANG, JACOB FREYERMUTH, GUICHUAN YU, University of Minnesota, RONNY SUTARTO, FEIZHOU HE, Canadian Light Source, EUGEN WESCHKE, HZB, Germany, WOJCIECH TABIS, MARTIN GREVEN, University of Minnesota, YUAN LI (Presenter), Peking University, China — Charge order is ubiquitously found in high-$T_c$ cuprate superconductors, yet their microscopic origin has been elusive. The Hg-family of cuprates are known for their high $T_c$ and relatively simple structure, and are therefore promising systems for avoiding material-specific complexity in experimental studies. Using resonant X-ray diffraction and Raman spectroscopy to study high-quality single crystals [1,2] of the first two members of the family, Hg1201 and Hg1212, we establish universal existence of charge order in these compounds. The most robust charge order is found in underdoped samples near a hole-carrier concentration of 0.09. Interestingly, we observe concomitant anomalies in the lattice dynamics that involve the motion of atoms in and/or adjacent to the CuO2 layers, around the same doping in both materials. As these anomalies are already present at room temperature, before the formation of charge order, we attribute them to a doping-dependent instability of the CuO2 layers that drives the formation of charge order as an emergent phenomenon [3].


*Work at PKU and UMN is supported by NSFC and MOST of China and by DoE of the US, respectively.
U49.00015: Gauge-invariant microscopic kinetic theory of superconductivity in response to electromagnetic fields II: Application to collective modes  FEI YANG (Presenter), MING-WEI WU, University of Science and Technology of China — We show that the gauge-invariant kinetic equation of superconductivity provides an efficient approach to study the electromagnetic response of the gapless Nambu-Goldstone and gapful Higgs modes on an equal footing. We prove that the Fock energy in the kinetic equation is equivalent to the generalized Ward's identity. Hence, the gauge invariance directly leads to the charge conservation. Both linear and second-order responses are investigated. The linear response of the Higgs mode vanishes in the long-wave limit. The linear response of the Nambu-Goldstone mode is in consistency with the previous works. Whereas the second-order response exhibits interesting physics. On one hand, a finite second-order response of the Higgs mode is obtained in the long-wave limit. We reveal that this response, which has been experimentally observed, is attributed solely to the drive effect rather than the widely considered Anderson-pump effect. On the other hand, the second-order response of the Nambu-Goldstone mode, free from the influence of the long-range Coulomb interaction and hence the Anderson-Higgs mechanism, is predicted. We find that both Anderson-pump and drive effects play important role in this response. A tentative scheme to detect this second-order response is proposed.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U50 DCMP: Metal Insulator Transition Theory  Mile High Ballroom 1C - Yan Wang, Oak Ridge National Laboratory

2:30PM U50.00001: Avalanche induced co-existing localised and thermal regions in disordered spin chains  PHILIP CROWLEY (Presenter), ANUSHYA CHANDRAN, Boston Univ — We investigate the stability of an Anderson localised chain to the inclusion of a single finite interacting thermal seed. This system models the effects of rare low-disorder regions on many-body localised chains. Above a threshold value of the mean localisation length, the seed causes runaway thermalisation in which a finite fraction of the orbitals are absorbed into a thermal bubble. This 'partially avalanched' regime provides a simple example of a delocalised, non-ergodic dynamical phase. We derive the hierarchy of length scales necessary for typical samples to exhibit the avalanche stability, and show that the required seed size diverges at the avalanche threshold. We introduce a new dimensionless statistic that measures the effective size of the thermal bubble, and use it to numerically confirm the predictions of avalanche theory in the Anderson chain at infinite temperature.
2:42PM U50.00002: Oxygen vacancy effect on the electronic structure of LaNiO3 using first-principles  XINGYU LIAO (Presenter), HYOWON PARK, VIJAY SINGH, Univ of Illinois - Chicago — While bulk LaNiO3 remains metallic at all temperatures, many experiments show that LaNiO3-x exhibits the metal-insulator transition as the oxygen vacancy level x goes from 0 to 0.5. In addition to the resistivity data, both photoelectron and X-ray absorption spectroscopy works show some intriguing features that cannot be explained based on density functional theory (DFT). In this talk, I will present DFT plus dynamical mean field theory (DMFT) calculations of LaNiO3-x for x=0, 0.25, and 0.5 in different magnetic states. Our DFT+DMFT method was implemented using the maximally localized Wannier function as local orbitals for the correlated subspace. While the DFT density of states (DOS) is similar to experimental spectroscopy data for LaNiO3, it failed to describe the insulating ground state and the peak splitting of unoccupied DOS as x increases to 0.5. Our DFT+DMFT calculations can capture both the resistivity change as well as the spectral features arising from the oxygen vacancy. We find that both the crystal splitting and the Ni d valence changes due to the oxygen vacancy play important roles in explaining the electronic structure. We will also discuss both similarity and difference of vacancy effects between the bulk and ultra-thin film structures.

2:54PM U50.00003: The metal-to-insulator transition in polar metals  EVAN SHERIDAN (Presenter), University of California, Berkeley, CEDRIC WEBER, Physics Department, King's College London, SINÉAD GRIFFIN, Lawrence Berkeley National Laboratory, JEFFREY NEATON, University of California, Berkeley — The fundamental design principles that drive a switchable polarity in oxide-based electronics whilst preserving a metallic state are not well understood. This is partly because it requires the coexistence of two seemingly incompatible properties: ferroelectric polar distortions and metallic conductivity. We study the prototypical polar metal LiOsO3 as a function of strain, which acts as a benchmark to further elucidate the role of electronic correlations in the alkali osmate perovskite-based series. Building on these results, we report a fully correlated DFT+DMFT approach to search and design new polar metals.

3:06PM U50.00004: Phase transition and instability in dimensionality-controlled artificial oxide crystals  TAEWON MIN (Presenter), Department of Physics, Pusan Natl Univ, SEUNGGYO JEONG, WOO SEOK CHOI, Department of Physics, Sungkyunkwan University, JAEKWANG LEE, Department of Physics, Pusan Natl Univ — The metal-insulator transition (MIT) is one of the fascinating physical phenomena in complex oxide system, and that has inspired the physics community during the last 20th century. In particular, recent advances in atomically controlled growth of oxide material have enabled the realization of artificial crystals with customized dimensions. Herein, by combining density functional theory calculations with optical and electrical measurements, we investigate dimensionality-induced MIT in atomically well-defined SrRuO3/SrTiO3 (SRO/STO) superlattices. We note that SRO/STO superlattices favor an antiferromagnetic insulating state as the SRO layers are getting thinner, which indicates that MIT is strongly coupled with magnetic ordering. Furthermore, we find that electronic and magnetic instabilities in the two SRO unit cell induce thermally-driven MIT along with magnetic transition. Novel theoretical finding will be presented along with transport and optical observations.
3:18PM U50.00005: Theory of Dipole Insulators*  OLEG DUBINKIN (Presenter), JULIAN MAY-MANN, TAYLOR L HUGHES, University of Illinois at Urbana-Champaign — Insulating systems are characterized by their insensitivity to twisted boundary conditions as quantified by the charge stiffness and charge localization length. The latter quantity serves as a universal criterion to distinguish between metals and insulators. In this work we extend these concepts to a new class of quantum systems having conserved charge and dipole moments. We refine the concept of a charge insulator by introducing notions of multipolar insulators, e.g., a charge insulator could be a dipole insulator or dipole metal. We develop a universal criterion to distinguish between these phases by extending the concept of charge stiffness and localization to analogous versions for multipole moments, but with our focus on dipoles. This refined structure allows for the identification of phase transitions where charge remains localized but, e.g., dipoles delocalize. We illustrate the proposed criterion using several exactly solvable models that exemplify these concepts.

*OD and TLH thank the US NSF under grant DMR 1351895-CAR, and the MRSEC program under NSF Award Number DMR-1720633 (SuperSEED) for support JM is supported by the NSF Graduate Research Fellowship Program under Grant No. DGE 1746047. TLH also thanks the NSF under Grant No.NSF PHY- 1748958(KITP) for partial support.

3:30PM U50.00006: Disorder in the one-dimensional half-filled extended Hubbard model
JON SPALDING (Presenter), University of California, Riverside, KA-MING TAM, Physics and Astronomy, Louisiana State University, DAVID K CAMPBELL, Physics, Boston University, SHAN-WEN TSAI, University of California, Riverside — The addition of disorder to interacting electron systems presents a challenging theoretical problem. In this talk, I will describe the effects of disorder on the phase diagram of the extended Hubbard model in one spatial dimension. Our theoretical analysis is possible in the weak coupling and weak disorder case due to the low dimensionality.

3:42PM U50.00007: Electronic and Lattice Dynamical Properties of MgTa$_2$O$_6$*  KYLE MILLER (Presenter), JAMES RONDINELLI, Northwestern University — Materials exhibiting metal-insulator transitions (MIT) are proposed platforms for next-generation low-power electronics. In addition, most of these materials exhibit strong coupling between the electronic and lattice degrees-of-freedom, which makes them ideal systems to examine the interplay between lattice dynamics, electronic structure, and magnetic order. Well-studied rutile-structured MIT oxides, such as VO$_2$ and NbO$_2$, exhibit dimerized cations within the edge-connected octahedra along the c axis in the insulating state. Analogous compounds with the related trirutile superstructure, e.g., V$_2$WO$_6$ and CuSb$_2$O$_6$, exhibit a similar dimerization. Here we investigate the propensity for MIT in MgTa$_2$O$_6$, a $d^0$ insulator, upon electron doping. Our calculations suggest that MgTa$_2$O$_6$ remains metallic for electron doping configurations within the $d^{0.25}$-$d^{0.5}$ range, whereas Ta-Ta dimerization occurs for higher electron concentrations. Overall, these results indicate that trirutile oxides may be a promising materials class for which to functionalize MITs.

*This work was supported by the NSF DMREF program under grant numbers DMR-1729303 and DMR-1729489.
3:54PM U50.00008: Theoretical study of electronic and structural phase transitions in MPS$_3$ with M = (Fe, Ni, Mn, Co)∗ MINSUNG KIM (Presenter), Department of Physics & Astronomy, Rutgers University, HEUNG-SIK KIM, Department of Physics, Kangwon National University, KRISTJAN HAULE, DAVID VANDERBILT, Department of Physics & Astronomy, Rutgers University — Metal phosphorus trisulfides (MPS$_3$ with M = Fe, Ni, Mn, Co) are layered materials which show Mott-insulator-to-metal transitions under the application of pressure. In addition, some of the compounds are reported to undergo structural phase transitions, making the theoretical description of the phase transitions more complicated. Here, we investigate the electronic and structural phase transitions of representative MPS$_3$ compounds using first-principles methods based on density functional theory and dynamical mean-field theory. We discuss the origin and the relation of the two types of phase transitions and clarify the role of the electron correlation and interlayer stacking configurations. We also examine how different metal species change the evolution of the phases under pressure. Our results provide needed theoretical understanding of these tunable Mott insulators.

∗This work has been supported by NSF DMREF grant DMR-1629059.

4:06PM U50.00009: Insight into the insulator-to-metal transition in ruthenium A$_2$Ru$_2$O$_7$ pyrochlores∗ DANILO PUGGIONI (Presenter), Department of Materials Science and Engineering, Northwestern University, GENEVA LAURITA, Department of Chemistry and Biochemistry, Bates College, RAM SESHADRI, Materials Department and Materials Research Laboratory, University of California, JAMES RONDINELLI, Department of Materials Science and Engineering, Northwestern University — The study of insulator-to-metal transitions (IMT) is of interest from the viewpoint of fundamental understanding of the underlying physics, and that materials at such a brink often can be harnessed for useful functionality. Here, using first principle calculations, we study the role of disorder, in the form of cation off-centering, on the compositionally-controlled IMT in the oxide pyrochlore (Pr$_{1-x}$Bi$_x$)$_2$Ru$_2$O$_7$. Our results suggest the combination of primary and secondary (due to size) electronic effects of the lone pair-driven incoherent cation displacements are responsible for the metallic state of pyrochlores with Bi substitution.

∗Support from Army Research Office under grant no. W911NF-15-1-0017.

4:18PM U50.00010: Metal-insulator transition in a Hubbard model with random and all-to-all hopping and exchange∗ GRIGORY TARNOPOLSKY, SUBIR SACHDEV (Presenter), Harvard University — We examine a $N$ site Hubbard model with an on-site repulsion $U$, and random and all-to-all hopping, $t$, and exchange $J$. In the large $N$ limit, the problem reduces to a single site symmetric Anderson impurity coupled to self-consistent bosonic and fermionic baths. We present large $M$ (for a model with SU($M$) spin symmetry) and renormalization group analyses of a metal-insulator transition in this model.

∗National Science Foundation Grant No. DMR-1664842
4:30PM U50.00011: Many Body Localization Due to Correlated Disorder in Fock Space
SOUMI GHOSH, Indian Institute of Science, ATITHI ACHARYA, Physics, Rutgers University, SUBHAYAN SAHU, Physics, University of Maryland, SUBROTO MUKERJEE (Presenter), Indian Institute of Science — The Hamiltonian of an interacting system of spinless fermions looks like that of a single particle hopping on a Fock graph in the presence of a random disordered potential. The coordination number of the Fock graph increases linearly with the system size L in 1D. Thus, in the thermodynamic limit, the disordered interacting problem in 1D maps on to an Anderson model with infinite coordination number. Despite this, this system displays localization which appears counterintuitive. The resolution lies in the on-site disorder on the Fock graph being highly correlated as they are derived from an exponentially smaller number of on-site disorder potentials in real space. Thus, such correlations have a strong effect on the localization properties of the corresponding many-body system. In this work we perform a systematic quantitative exploration of the nature of correlations of the Fock space potential required for localization. We show that changing the correlation strength can induce thermalization or localization in systems. We find that a linear variation of correlations with Hamming distance in Fock space is drives a thermal-MBL phase transition where the transition is driven by the correlation strength. Systems with the other forms of correlations we study are found to be ergodic.

4:42PM U50.00012: Current driven first order metal-metal martensitic phase transitions in correlated electron systems
STEWART BARNES (Presenter), Univ of Miami — As a function of temperature and pressure, a number elemental 3d metals such as Fe or V undergo first order martensitic phase transitions between bcc and fcc structures. Similar metal to metal first order phase transitions occur in other transition metals and alloys including most famously shape memory alloys. In analogy with the spin Berry phase, defined is an electro-mechanical such phase defined by the four connection $A_\mu$ that couples to the conduction electron charge current. It is implied that, for highly pure wires of such materials, an electronic charge current can drive say the bcc to fcc martensitic phase transition of a suitable metrial well below the strain, temperature and/or pressure that which this usually occurs. This leaves the material in a higher energy state thereby converting electrical to lattice energy in much the same manner as currents can drive a magnetic state to higher energy. The theory also applies to domain walls in conducting ferro and antiferroelectric materials.
4:54PM U50.00013: Theoretical phase diagram of unconventional alkali-doped fullerides*
THEJA DE SILVA (Presenter), Augusta University — By constructing an effective model based on recently calculated *ab initio* bare interaction parameters, we study the phase diagram of alkali-doped fullerides as a function of temperature and internal pressure. While we use a slave-rotor mean-field theory to determine the metal-insulator-superconductor phase boundaries, we use a variational mean-field approach to detect the magnetic phase transitions. We find a good agreement with experimental phase diagram in both weak and strong coupling limits. We explain the unified description of the phase diagram including the proximity of s-wave superconducting state and the Mott-insulating state, and the existence of Jahn-Teller distorted metallic state using orbital selective physics. We argue that the double electronic occupation of two degenerate orbitals triggers both s-wave superconductivity and Jahn-Teller distortion. While the orbital ordering of two electrons causes the distortion, the remaining single electron in the third orbital causes the metal-insulator transition.

*Augusta University and KITP at UC-Santa Barbara.

5:06PM U50.00014: Operator growth in disordered systems, a translation invariant approach*
XIANGYU CAO (Presenter), University of California, Berkeley — Operator growth in disordered systems, a translation invariant approach

Recently, we proposed [1] a general framework to study operator growth and complexity, using the Lanczos algorithm (aka Krylov subspace or recursion method). Here, we apply the framework to disordered systems, especially random spin chains and many-body localization (MBL). An argument based on l-bits shows that in MBL phases, the Krylov-complexity [1] grows polynomially in time (as opposed to exponentially in chaotic systems). An equivalence between quenched disorder and static ancilla allows us to carry out numerical study to in a translation invariant systems, bypassing finite size effects and statistical fluctuations of disorder averaging. Under strong disorder, the Lanczos coefficients define a quasi-random Krylov chain with multiple bound states, which we identify as local integral of motions and long-lived oscillating modes. We propose to study the MBL transition as the divergence of localization length on the Krylov chain. Finally, we apply the disorder-free method to a mean-field random magnet realized in a recent cold-atom experiment [2].


*This work is supported by ERC synergy Grant UQUAM and DOE grant de-sc0019380.
Electrostatic gating Effects on the Metal to Mott Insulator Transition of NiS$_2$: a DFT+DMFT study* EZRA DAY-ROBERTS (Presenter), TURAN BIROL, RAFAEL FERNANDES, University of Minnesota — Electrostatic gating provides a convenient way to manipulate carrier densities without introducing defects that lead to impurity scattering as in chemical doping. Recent advances, including those in ionic liquid and gel gating, have allowed experimental access to a much larger range of added carrier concentrations. NiS$_2$, in the pyrite structure, is a Mott insulator that has previously been found to undergo a metal-to-insulator transition (MIT) as function of isovalent selenium substitution as well as pressure. This suggests that NiS$_2$ is near the edge of the MIT, making it a good candidate material to be electrostatically driven across the MIT. Here, we present results of a first-principles study of this material using fully charge self-consistent Dynamical Mean Field Theory (DFT+DMFT). We explore the properties of NiS$_2$ across the MIT as a function of temperature and added carrier concentration, contrasting the cases of electrostatic gating and chemical doping.

*This work was supported by the National Science Foundation through the UMN MRSEC under DMR-1420013

Thursday, March 5, 2020 2:30 PM - 5:06 PM

Session U51 DCP: Graphene: Imaging and Spectroscopy Mile High Ballroom 1D - Jennifer DeMell, Laboratory for Physical Sciences

Imaging magnon transport in a quantum Hall ferromagnet: Part 1 SEUNG HWAN LEE (Presenter), ANDREW PIERCE, YONGLONG XIE, PATRICK R FORRESTER, Department of Physics, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, AMIR YACOBY, Department of Physics, Harvard University — Graphene exhibits quantum Hall ferromagnetism at partial fillings in the N=0 Landau level where its SU(4) isospin symmetry is spontaneously broken due to strong electron-electron interactions. It has been demonstrated that it is possible to generate and detect magnons, collective excitations of spins, in the ν= ±1 quantum Hall ferromagnets by exploiting equilibration of spin-polarized edge states. However, the nature of magnon transport in the system is still under active investigation. In this two-part talk, we will discuss scanning gate microscopy (SGM) of magnon transport in the graphene quantum Hall ferromagnet. Using a metallic scanning tip, a small region of graphene can be gated away from integer filling, effectively acting as a barrier for magnon transport inside the system. In this talk, we present a general scheme of performing SGM of magnon transport, and report observation of localized response in transport as we place the local barrier near the magnon generation and absorption sites.
Imaging magnon transport in a quantum Hall ferromagnet: Part 2

ANDREW PIERCE (Presenter), SEUNG HWAN LEE, YONGLONG XIE, PATRICK R FORRESTER, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, AMIR YACOBY, Harvard University — The spin-polarized ν=1 quantum Hall state of monolayer graphene constitutes a unique laboratory for studying mesoscopic magnetic phenomena. Among many interesting properties, the system supports magnons which can be generated and detected electrically. Here we study the ν=1 state of graphene using a scanning single-electron transistor (SET) operated simultaneously as a local gate and electrometer. Processes involving localized states near device contacts are shown to strongly influence transport response, suggesting a microscopic mechanism for magnon generation and absorption. Moreover, operating the SET as an electrometer enables us to perform local compressibility measurements which further clarify the effects of magnon generation on the system.

*This work was supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program.

Visualizing unexpected magnetic field-tuned electron flow through ballistic channels

JOSEPH SULPIZIO (Presenter), LIOR ELLA, ASAF ROZEN, Weizmann Institute of Science, JOHN BIRKBECK, DAVID PERELLO, University of Manchester, DEBARGHYA DUTTA, Weizmann Institute of Science, MOSHE BEN-SHALOM, Tel Aviv University, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, ANDRE GEIM, University of Manchester, SHAHAL ILANI, Weizmann Institute of Science — The advent of ultra-clean materials has enabled the exploration of ballistic flow, where electrons traverse a sample unperturbed before colliding with the walls. We have developed a nanoscale probe based on a scanning nanotube single electron transistor that is sufficiently sensitive to image the electrostatic potential of ballistic electrons in such materials for the first time. We apply this probe to high-mobility graphene channel devices, and image how the potential of the flowing electrons drops sharply at the contacts while remaining constant along the bulk, which is the textbook picture of ballistic electron flow. We then image how the Hall voltage profiles of the flowing electrons develop a rich set of patterns as the cyclotron radius is tuned by varying the perpendicular magnetic field. Contrary to the expectation that the electron current primarily flows along the edges in magnetic field, our results reveal that the current varies considerably across the bulk of the channel, and can even concentrate near the center. These results open the path for visualizing other ballistic electron flow phenomena that previously could only be studied via transport, including electron optics.
3:06PM U51.00004: Realization of Nanoscale Mapping of Noise Source Activities on Graphene Domains* JEEHYE PARK (Presenter), HYUNGWOO LEE, DUCKHYUNG CHO, SHASHANK SHEKHAR, JEONGSU KIM, Department of Physics and Astronomy, and Institute of Applied Physics, Seoul National University, Seoul, 08826, Korea, JAESUNG PARK, Center for Electricity & Magnetism, Korea Research Institute of Standards and Science, Daejeon, 34125, Korea, BYUNG HEE HONG, Department of Chemistry, Seoul National University, Seoul, 08826, Korea, SEUNGHUN HONG, Department of Physics and Astronomy, and Institute of Applied Physics, Seoul National University, Seoul, 08826, Korea — We report a “noise spectral imaging” strategy to directly map the noise source activities in graphene domains. Here, the lateral current and noise maps were measured by scanning a conductive contact probe on the graphene surface. The measured data were analyzed by using a two-dimensional network model to obtain the sheet resistance and charge trap density maps inside graphene domains, on domain boundaries, and on the edge of graphene. The results showed high activities of noise sources and large sheet resistance values at the domain boundary and edge of graphene. Furthermore, the top layer of double-layer graphene was found to have lower noises than those of single-layer graphene, as predicted previously. Our method allows one to image the localized noise source distribution in two-dimensional electronic channels such as graphene, and thus it can be a powerful tool for the basic research and applications about two-dimensional transports in nanostructures.

*This work was supported by the National Research Foundation(NRF) Grant (No. 2013M3A6B2078961). B.H.H. thanks Graphene Resesarch Center at Advanced Institute of Convergence Technology. S.H. also acknowledges support from the NRF Grant (Nos. 2014M3A7B4051591 and 2015M3C1A3002152).

3:18PM U51.00005: Photothermal nanoimaging of dissipative surface polaritons* HONGHUA U YANG, LIANG-CHUN LIN, TAO JIANG, University of Colorado, Boulder, SAMUEL BERWEGGER, NIST Boulder, FABIAN MENGES (Presenter), MARKUS B. RASCHKE, University of Colorado, Boulder — Controlling the functionalities of 2D material structures via strong light-matter coupling requires understanding of the dissipation and thermalization dynamics of surface polaritons. However, the intricate details of polaritonic decay processes are rooted in a plethora of physical mechanism spanning widely separated length and time scales, even down to regimes where dissipation is no longer a readily measurable quantity. Here, we introduce photothermal force microscopy as a nanoimaging modality to visualize energy dissipation via surface plasmon polaritons (SPPs). Studying graphene on silicon dioxide, we perform real-space imaging of SPPs via photothermal force detection (AFM-IR) with contrast interpreted due to thermal substrate expansion induced by the local SPP decay. Complementary to previous studies, reporting the optical characterization of SPPs via IR-sSNOM, we will show that photothermal expansion forces facilitate the direct mechanical detection of the non-radiative SPP decay process. Our observations reveal that dissipative surface polariton modes might enable to control the spatio-temporal dynamics of thermal nanosystems.

*F. Menges gratefully acknowledges funding support by The Branco Weiss Fellowship - Society in Science, administered by the ETH Zurich.

We investigate the optical response of graphene and graphene nanoribbons using the broadband nonlinear generation and detection capabilities of nanoscale junctions created at the LaAlO$_3$/SrTiO$_3$ interface [1]. Using the large third-order nonlinear susceptibility in SrTiO$_3$, strong difference frequency mixing occurs when the junction is biased, leading to induced polarization that can also be detected at the junction [2,3]. Here we discuss the results of experiments which interrogate the relationship between the THz signal and the gate location with respect to the Dirac point in devices where graphene is coupled to the LaAlO$_3$/SrTiO$_3$ interface. Results show near-100% extinction of VIS-NIR light in graphene, and suggest we may be detecting a surface plasmon resonance. Additional results on individual graphene nanoribbons reinforce this interpretation.


*J. Levy acknowledges a Vannevar Bush Faculty Fellowship (ONR N00014-15-1-2847), and the Office of Naval Research (N00014-16-1-3152). C-BE acknowledges support from AFOSR (FA9550-15-1-0334), NSF DMREF (DMR-1629270), and NSF MRSEC (DMR-1420645) (C-BE). ES acknowledges support from NSF GRFP (1747452).

3:42PM U51.00007: Lattice vibrations of single and multi-layer isotopologic graphene HWANSOO JEON (Presenter), Pohang Univ of Sci & Tech, TOKUYUKI TERAJI, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, SUNMIN RYU, Pohang Univ of Sci & Tech — Isotope-substituted materials, isotopologues, have been crucial in understanding various scientific problems. In this work, we report full Raman spectroscopic investigation of $^{13}$C graphene, its multilayers, and isotopologic bilayers. All samples were prepared using $^{13}$C-enriched bulk crystals that were grown by the high-pressure and high-temperature method. Frequencies of G, 2D, and combination peaks showed a linear relation between two isotopologues of $^{12}$C and $^{13}$C, which led to a precise optical determination of isotopic purity in agreement with mass spectrometric results. Single to eight-layered graphene exhibited correspondence in spectral features between isotopologues: thickness-dependent progressions of intensities and line shapes, and excitation energy-dependent dispersion of 2D frequency. Line shape analyses of stacking-sensitive 2D revealed the spatial distribution of stacking domains and dominance of ABC-polytype unlike natural or kish graphite. Using isotopologic bilayers of $^{12}$C/$^{13}$C, we quantified the change in Fermi velocity induced by vdW interlayer interactions separately from strain and charge density. This work also presents direct evidence that the puzzling thermally activated doping is induced by hole dopants located at the graphene-substrate interface.
Detecting Photo-Induced Topological Edge States in a Graphene Nanoribbon Using Pump-Probe Spectroscopies

YUAN CHEN (Presenter), Stanford University, YAO WANG, Harvard University, MARTIN CLAASSEN, Simons Foundation Flatiron Institute, BRIAN MORITZ, SLAC National Accelerator Laboratory, THOMAS DEVEREAUX, Stanford University — Recently, photo-induced topological edge states in low dimensional materials have attracted considerable attention due to the tunability of dispersion and topological properties using light. Here, we present a numerical study of various pump-probe spectroscopies for a graphene nanoribbon subject to circularly polarized pump light. In particular, we calculate time-resolved resonant inelastic x-ray scattering (tr-RIXS) for the graphene nanoribbon, which clearly resolves the pump-induced band gap and the edge states. These tr-RIXS features have a direct correspondence with Floquet states and the calculated time-resolved ARPES spectra. We also calculate the pump-probe optical conductivity and nonresonant Raman scattering, demonstrating that the signatures from the pump-induced gap and edge states also should be visible, especially at low energy. These pump-probe techniques provide powerful tools for detecting photo-induced topological states in low dimensional materials.

Graphene Conductivity and Dielectric Response at THz frequencies

DAVID CAREY (Presenter), University of Surrey — The calculations of the dynamical conductivity of graphene allows further determination of the high frequency, from dc to optical frequencies, response of the real and imaginary parts of the dielectric constant of graphene. In this study we explore how the dynamical conductivity, dielectric properties and refractive index of single layer graphene vary as a function of frequency for different carrier concentrations and scattering times. We play particular attention to the differing roles of the intra- and interband transitions and explore the THz response of graphene as a possible functional material to bridge the so-called THz gap between electronics and optics. We find in the 1-10 THz frequency region that for moderately doped graphene (i) $\varepsilon_1$ is negative and approaches values in the mid $10^5$ but does not vary strongly at lower frequencies and (ii) $\varepsilon_2$ is positive for all THz frequencies explored but is one to two orders lower in magnitude; comparisons are made with noble metals. We also calculate the variation of real and imaginary components of the refractive index with wavelength. Potential applications in graphene based antennas and metamaterials are discussed.
4:18PM U51.00010: Strong magnetophonon oscillations induced by Dirac fermion - transverse acoustic phonon scattering in graphene  
PIRANAVAN KUMARAVADIVEL (Presenter), School of Physics and Astronomy, University of Manchester, MARK GREENAWAY, Department of Physics, Loughborough University, DAVID PERELLO, ALEXEY BERDYUGIN, JOHN BIRKBECK, JOSHUA WENGRAF, School of Physics and Astronomy, University of Manchester, SONG LIU, JAMES H. EDGAR, Department of Chemical Engineering, Kansas State University, ANDRE GEIM, LAURENCE EAVES, ROSHAN KRISHNA KUMAR, School of Physics and Astronomy, University of Manchester — Two dimensional electron gas systems exhibit a plethora of quantum phenomena. Graphene has not only provided a versatile platform for studying many of these phenomena but also revealed new effects. However one of the first discoveries in quantum transport, well known for fifty years has remained conspicuously absent in graphene: magnetophonon oscillations. Here we present our recent work on magnetotransport in boron nitride encapsulated graphene devices of different widths [1] and show that the magnetoresistance of wider graphene devices reveal this hitherto elusive quantum phenomenon. In devices of channel width greater than ten micrometres we observe pronounced magnetophonon oscillations caused by resonant scattering of Landau quantised Dirac quasiparticles with acoustic phonons in graphene. Using this we determine graphene’s low energy phonon dispersion and also find that transverse acoustic modes are the dominant source of phonon scattering. The results highlight the importance of device size in studying new quantum phenomena and demonstrates a spectroscopic technique for studying the nature of electron-phonon interactions in van der Waals heterostructures.  
TIANHAO ZHAO (Presenter), Georgia Inst of Tech, YUXUAN JIANG, National High Magnetic Field Lab, YIRAN HU, YUE HU, GRANT H NUNN, Georgia Inst of Tech, MYKHAYLO OZEROV, DMITRY SMIRNOV, National High Magnetic Field Lab, LEI MA, Tianjin International Center of Nanoparticles and Nanosystems, CLAIRE BERGER, WALTER DEHEER, ZHIGANG JIANG, Georgia Inst of Tech — We report on the magneto-infrared spectroscopy study of the new generation epigraphene grown on a non-polar facet of SiC [arXiv:1910.03697]. Interband Landau level (LL) transitions are observed and fitted well with $1\times10^6$ m/s as Fermi velocity in the massless Dirac fermion model. The transitions remain visible as the magnetic field is down to 0.25 T, indicating that the carrier density is no greater than $3.6\times10^{10}$ cm$^{-2}$ as expected for charge-neutral non-polar epigraphene. When the samples are grown thicker, LL transition splittings are spotted at high magnetic fields. Failing to explain the splittings with electron-hole asymmetry, we suggest that it could arise from (twist) bilayer epigraphene components and we will discuss it with a numerical twist bilayer graphene model.  
*The work at NHMFL was supported by the NSF Cooperative Agreement No. DMR-1644779 and the State of Florida, and DoE-BES DE-FG02-07ER46451.
4:42PM U51.00012: Direct Imaging of Electronic Symmetries in Twisted Double-Bilayer Graphene  
SIMON TURKEL (Presenter), CARMEN RUBIO VERDÚ, LARRY SONG, Department of Physics, Columbia University, New York, New York 10027, USA, DANTE KENNES, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany, LEDE XIAN, Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany, HECTOR OCHOA, Department of Physics, Columbia University, New York, New York 10027, USA, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan, ANGEL RUBIO, ABHAY PASUPATHY, Department of Physics, Columbia University, New York, New York 10027, USA — When two graphene bilayers are twisted relative to one another at about one degree, the resulting system has been shown to host correlated insulating and superconducting states. Unlike in the case of simple twisted bilayer, the insulating states in the magic double bilayer are enhanced under parallel magnetic field, suggesting that electronic correlations may be mediated by ferromagnetic order. We directly image the local density of states in twisted double bilayer graphene using scanning tunneling microscopy and spectroscopy and observe the evolution of electronic wave functions within the moiré unit cell as a function of carrier density and applied electric field. In addition to corroborating theoretical band structure calculations via point spectroscopy, our observations of symmetry-broken states across a range of dopings and long-range order persisting across hundreds of nanometers offer insights into the complex charge and spin order that exists in magic angle twisted double bilayer graphene.

4:54PM U51.00013: Imaging double moiré pattern in twisted bilayer graphene grown on hBN with microwave impedance microscopy  
XIONG HUANG (Presenter), University of California, Riverside, LINGXIU CHEN, Shanghai Institute of Microsystem and Information Technology Chinese Academy of Sciences, SHUJIE TANG, Stanford University, CHENGXIN JIANG, CHEN CHEN, HUISHAN WANG, Shanghai Institute of Microsystem and Information Technology Chinese Academy of Sciences, ZHIXUN SHEN, Stanford University, HAOMIN WANG, Shanghai Institute of Microsystem and Information Technology Chinese Academy of Sciences, YONGTAO CUI, University of California, Riverside — Stacking multiple atomic layers of similar crystal structure will create moiré patterns whose periodicity and orientation are determined by the stacked layers. In this study, we image the moiré patterns in CVD grown bilayer graphene/hBN heterostructures using microwave impedance microscopy and conductive atomic force microscopy. Two sets of moiré patterns are observed: one formed between the first graphene layer with hBN and a second one between the two twisted graphene layers. The graphene/hBN moiré pattern indicates a perfect alignment between the two layers. The graphene/graphene moiré pattern has a smaller period due to a larger twist angle. This moiré pattern experiences abrupt phase change across the boundaries of the graphene/hBN moiré pattern. We present our analysis of such double moiré pattern based on lattice reconstruction occurred in the graphene layers.

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U52 DCMP: Surfaces and Thin Films of Novel Electronic Materials Mile High Ballroom 1E - Daniel Dougherty, North Carolina State University
**2:30PM U52.00001: Exploring the origin of the thickness-dependent metal-insulator transition in thin-film systems with band structures**  
SUNGSOO HAHN (Presenter), BYUNGMIN SOHN, CHANGYOUNG KIM, Department of Physics and Astronomy, Seoul National University — Metal-insulator transition (MIT) has been studied in decades and is well known to be induced by temperature, pressure, and dopants. However, the origin of MIT in thin films which occur as metallic thin films become thinner is not explained. In order to investigate the thickness-dependent MIT, transport measurements and photoemission spectroscopy have been performed, however, the conclusion is not to be determined yet. Here, we observed band structures of SrRuO$_3$ ultrathin films near the MIT-critical thickness by using *in-situ* angle-resolved photoemission spectroscopy (ARPES). We expect our experimental observation sheds light on the thickness-dependent MIT in thin-film systems.

*This work is supported by IBS-R009-G2 through the IBS Center for Correlated Electron Systems.

**2:42PM U52.00002: Scanning tunneling spectroscopy of rare earth hexaborides**  
PHILIPP BUCHSTEINER (Presenter), IV. Physikalisches Institut, Georg-August Universität Göttingen, FLORIAN SOHN, Institut für Theoretische Physik, Georg-August Universität Göttingen, LISA HARMSEN, IV. Physikalisches Institut, Georg-August Universität Göttingen, PETER E BLOECHL, Institut für theoretische Physik, Technische Universität Clausthal, MARTIN WENDEROTH, IV. Physikalisches Institut, Georg-August Universität Göttingen — The surface physics of rare earth hexaborides is of great interest for both technological applications and fundamental research. For example, LaB$_6$ is a widely used electron emitter due to its low work function and the 4f-electron system SmB$_6$ is a Kondo insulator with proposed topologically protected surface states. In order to systematically investigate the influence of 4f-electrons on the hexaboride surface physics, we performed scanning tunneling microscopy (STM) on the (001)-cleavage planes of LaB$_6$ [1] and PrB$_6$. We found that on both crystal surfaces a chain-like (2×1) reconstruction is present. Furthermore, we found uniform terminations on PrB$_6$. By performing slab calculations within the framework of density functional theory (DFT) we rationalize this reconstruction as parallel chains of rare earth ions on top of a B$_6$ framework. Using scanning tunneling spectroscopy (STS) we find a spectral feature below $E_F$, which can be described as boron dangling-bond state. For PrB$_6$, an additional contribution is visible in the spectra, which we tentatively attribute to the 4f-electrons.


*We acknowledge funding from DFG grants WE1889/10-1, BL539/10-1, PR298/19-1 and SFB 1073 projects B03, C03, C04.
2:54PM U52.00003: Synchrotron-Based Ultrafast Optical Pump/X-Ray Probe Measurements of Lattice Dynamics in Photo-Excited Pt Thin Films*  MATTHEW FORBES DECAMP (Presenter), Physics and Astronomy, Univ of Delaware, ANTHONY DICHIARA, Advanced Photon Source, Argonne National Laboratory, KARL UNRUH, Physics and Astronomy, Univ of Delaware — A synchrotron-based optical pump/x-ray probe measurement technique has been used to study the structural evolution of elemental Pt thin films following photo-excitation by ps duration optical laser pulses. High quality x-ray diffraction (XRD) patterns were obtained with a time-resolution of less than 100 ps (corresponding to the duration of a single x-ray pulse) and with time delays relative to the pump pulse ranging from 10’s of ps to ms. These measurements revealed a very rapid lattice expansion normal to the sample for several 100 ps following photo-excitation followed by a much less rapid decrease. The film response to excitation energies less than about 50 mJ/cm² was nearly reversible while greater excitation energies produced irreversible stress relaxation, and eventually film oblation. Assuming that the lattice expansion can be modelled in terms of a bulk thermal expansion coefficient, the maximum observed lattice temperature was about 1500 K.

*This material is based upon work supported by the NSF under Grant No. DMR140076. Use of the Advanced Photon Source was supported by the U.S. Department of Energy under Contract No. DE-AC02-06CH11357. Use of the BioCARS was also supported by the NIH, Grant No. R24GM111072.

3:06PM U52.00004: Ex-Situ Ozone Cleaning of SrTiO₃ Substrates for Molecular Beam Epitaxy*  CAMILLE BEAN (Presenter), TATIANA A WEBB, RUIZHE KANG, JENNIFER E. HOFFMAN, Harvard University — In molecular beam epitaxy synthesis of thin films, the quality of the substrate surface is crucial. The substrate not only provides a structural template for the deposited film, but the interaction between the film and the substrate itself determines emergent electronic properties. Therefore, it is critical to employ effective in-situ and ex-situ substrate cleaning techniques to ensure a clean substrate surface, which is necessary for high-quality film growth. Here, we report an investigation of the efficacy of cleaning with ozone as an ex-situ cleaning technique for widely used SrTiO₃ substrates. The substrates are ozone cleaned after etching and annealing. The carbon ratio on the substrate surface has been carefully examined using XPS to verify the efficacy of ozone cleaning.

*This work was funded by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4536, and by the Office of Naval Research through Grant N00014-18-1-2691
3:18PM U52.00005: Benchmarking various levels of theory for first principles modeling of iron oxide surfaces and interfaces  
SUVAĐIP DAS (Presenter), Georgia Institute of Technology, EFSTRATIOS MANOUSAKIS, Florida State University, ANDREW J MEDFORD, Georgia Institute of Technology — Surfaces of iron and its oxides are scientifically relevant due to their performance as photo-anodes for water oxidation as well as their formation during corrosion processes. Finding an accurate ab-initio approach to appropriately describe surface phenomenon of iron and its oxides is critical to enable modeling of the charge accumulation, energetics and bond formation mechanisms governing the reactivity of iron oxide surfaces. Prior work has established that incorporation of the random-phase approximation (RPA) improves the accuracy of adsorption and surface energy calculations but these techniques have not been systematically applied to iron oxides. Here, we present a benchmarking study for various levels of theory such as onsite Coulomb interaction, hybrid functionals and quasiparticle GW methodology to appropriately modulate surface phenomenon in oxides. A detailed study of GW convergence from various starting points is presented for iron monoxide establishing hybrid-level orbitals as the optimum starting point for self-consistent GW calculations. The study also establishes the hybrid functional approach as an ideal trade-off between accuracy and computational cost towards efficient convergence of electronic wavefunction and formation energy for electrochemical applications.

3:30PM U52.00006: Spin Polarized Electron Emission from Magnetite Half-metals Determined by First-principles Calculations  
LIANGLIANG XU (Presenter), NAN ZHAO, MING-CHIEH LIN, Department of Electrical and Biomedical Engineering, Hanyang University, TSAN-CHUEN LEUNG, Department of Physics, National Chung Cheng University, HUA-YI HSU, Department of Mechanical Engineering, National Taipei University of Technology — Magnetite is a mineral and one of the main iron ores. With the chemical formula Fe$_3$O$_4$, it is one of the oxides of iron. Magnetite is the earliest discovered magnet, around 1500 B.C. It crystallizes in the inverse cubic spinel structure (Fd3m) above the so-called Verwey transition temperature, which is about 120 K. In this work, we study the electronic properties of magnetite (100), (110), and (111) surfaces using first principles or ab initio calculations based on density functional theory. With a +U calculation, most of the surfaces with different terminations show half-metallic, different from those predicted by a without +U calculation. It is proposed that the magnetite as a half-metal can possibly be used as a spin-polarized electron source. The spin polarized electrons can be obtained via the field emission process as described by the Fowler–Nordheim equation. From the first principles calculations, the surfaces suitable for spin polarized emission are found.
3:42PM U52.00007: Domain Walls in the Electronic Polarization of Silver Bismuthate  FRED FLORIO (Presenter), RAVISHANKAR SUNDARARAMAN, JIAN SHI, YUWEI GUO, Rensselaer Polytechnic Institute — Ternary bismuth oxides are a new class of atypical ferroelectric materials whose polar states are primarily induced by electronic charge disproportionation rather than atomic displacement. Silver bismuthates are particularly exciting as ferroelectric semiconductors with low band gaps. Previous research has focused primarily on bulk geometry and electronic structure of the materials, identifying three structural phases of Ag$_2$BiO$_3$ as a function of temperature. Understanding domain wall structures and energetics in this material is now critical to facilitate prediction of polarization and domain switching dynamics for applications in memory and opto-electronics.

Here we present structures of candidate domain walls in Ag$_2$BiO$_3$, using ab initio methods to determine the relative energies, structural displacements and charge disproportions associated with these domain walls. We also calculate the spatial width of the domain walls, the energy landscape of the polarization order parameter, and the bulk elastic response of the material. These quantities now facilitate phase field simulations of the polarization dynamics in Ag$_2$BiO$_3$, providing insight into the domain-switching dynamics from nano to micro scales.

3:54PM U52.00008: Understanding Electrical and Thermal Transport in Single Strand Cu-Coated Carbon Fiber*  HOJOON YI (Presenter), Sungkyunkwan Univ, JI YEON KIM, Korean Institute of Carbon Convergence Technology, HAMZA ZAD GUL, SEUNGSU KANG, GIHEON KIM, EUNJI SIM, HYUNJIN JI, Sungkyunkwan Univ, JUNGWON KIM, Korea Research Institute of Chemical Technology, YOUNG CHUL CHO, WON SEOK KIM, Korean Institute of Carbon Convergence Technology, SEONGCHU LIM, Sungkyunkwan Univ — Carbon fiber is used in many parts of high-performance cars to improve its performance. Furthermore, there are many researches to improve the properties of cables that have reduced weight by coating metal on carbon fiber cores. But there is a lack of research on thermal properties, one of the important properties.

In this study, 1ω AC current was used to analyze the electrical and thermal conductivity of single-stranded metal-coated carbon fibers with different metal thicknesses. Generated 3ω voltage due to heat generation was measured and analyzed. We conclude that depositing a metal layer on CF improves the both conductivity of CF. And our results show that the thermal conductivity of CF improves as the metal thickness increases. The heat flow is also identified through the Lorenz number, which represents the ratio of thermal conductivity to electrical conductivity. The change in Lorenz number explains how heat is distributed in the MCF over temperature changes.

Our results help to understand the heat transfer of the core-shell structure and can be used to identify heat dissipation and conduction without compromising the electrical conductivity of metal-coated carbon fibers.

*This work is supported by the civil-military technology cooperation program (15-CM-MA-14).
4:06PM U52.00009: Structure and electronic states of Pt/SrTiO$_3$ (001) interface using X-ray standing wave excited photoelectron emission  
YANNA CHEN (Presenter), ANUSHEELA DAS, Northwestern University, TIEN-LIN LEE, Diamond Light Source, MICHAEL J BEDZYK, Northwestern University — In this work, we focus on Pt/SrTiO$_3$ heterostructure to discover the interfacial interaction between metal catalysts and metal oxide supports. Pt nano single crystals were grown on a SrTiO$_3$ (001) substrate using pulsed laser deposition. The Pt/SrTiO$_3$ heterostructure was characterized using X-ray standing wave (XSW) excited photoelectron emission collected in the Bragg back-reflection geometry at beamline I09 of the Diamond Light Source. Different electronic core levels of Pt 4f, 4d, 3d were collected, which showed differences in their responses to the XSW excitation. O 1s, Ti 2p, and Sr 3d core levels were also collected to understand the interfacial interaction between Pt and SrTiO$_3$. Focusing on Pt 4f, O 1s, Ti 2p, and Sr 3d, three symmetry inequivalent hkl Bragg peaks were measured to produce 3D interfacial atomic maps for each species via Fourier inversion. Among other things, these results should be beneficial for the design of oxide supported catalysts.

4:18PM U52.00010: Evolution of picosecond surface electric fields generated by photon-induced charge emission from La$_{0.67}$Sr$_{0.33}$MnO$_3$ thin films at 300 K and 77 K  
RUNZE LI (Presenter), PETER M. RENTZEPIS, Texas A&M University — The spatial-temporal distribution of picosecond surface electric fields, associated with the femtosecond-laser-induced photoemission from La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO) single crystal thin films, at 300 K and 77 K, were interrogated by sub-picosecond, 30 keV, electron pulses and reconstructed by a “three-layer” theoretical model. Around a few tens of picoseconds after femtosecond laser illumination, a surprisingly strong surface electric field on the order of hundreds kV/m was observed on the LSMO film at room temperature. This electric field strength is on the same order as the field(s) used for altering the orbital domains in lanthanum strontium manganite films. The experimental data of this study imply that the self-induced transient electric fields, generated during photoemission, may be a promising means for the control of ultrafast processes in materials that are mainly achievable through strong THz excitations.
Role of substrate vicinity on structural evolution and functional properties of lightly doped La$_{1-x}$Sr$_x$MnO$_3$ thin films

BINOD PAUDEL (Presenter), Department of Physics, New Mexico State University, AIPING CHEN, MPA-CINT, Los Alamos National Laboratory, HEINRICH NAKOTTE, Department of Physics, New Mexico State University — Epitaxial engineering has been considered an important approach to tune functional properties of oxide thin films. However, there is always a quest of other approaches that can provide more knobs to tailor and explore wide range of novel functional properties. Film substrate symmetry mismatch, thermal coefficient mismatch, substrate termination, and miscut angle and directions are also important factors to modulate growth, structure and functional properties. Here, we present the study on structural and functional properties of lightly doped La$_{0.9}$Sr$_{0.1}$MnO$_3$ (LSMO) films on SrTiO$_3$ substrates with different miscut angles (0.5°, 2°, 4° and 8°). Coherent growth was observed for films on 0.5° miscut substrate and in-plane periodic twining was observed for films grown on higher miscut angles. The out-of-plane periodic twinning was seen for films on for 0.5° miscut substrate while higher miscut substrates promote tilted domains formation. These structural distortions are attributed to monoclinic or triclinic distortion of orthorhombic LSMO films on cubic STO substrates. Curie temperature systematically reduces while magnetoresistance and temperature coefficient increase due to the reduction of domain variants and increase of out of plane tilt angles with the increase of miscut angles.

Surface structure determination of a two dimensional Au-Si-alloy formed on Au(110) by x-ray photoelectron spectroscopy (XPS) and x-ray photoelectron diffraction (XPD)*

MARIE SCHMITZ (Presenter), PETER ROESE, MALTE SCHULTE, CARSTEN WESTPHAL, TU Dortmund University — The metal-semiconductor interface has caused multiple interest in solid state physics especially in methods of metal silicides for various applications, for instance photonic and electronic devices.[1] A detailed structural as well as chemical investigation was performed by means of low energy electron diffraction (LEED), x-ray photoelectron spectroscopy (XPS), and x-ray photoelectron diffraction (XPD). High-resolution core-level-spectra of Au4f and Si2p reveal multiple chemically shifted components. Both Au4f and Si2p XPD-patterns were simulated with the EDAC[2] and MSPHD[3] packages, respectively, and compared with the measured pattern by a genetic algorithm reaching R-factors around 0.1. Therefore, we propose a surface-structure model for the Au-Si-alloy based on our measurements and simulations. The results are set in the context of an previously proposed surface-structure of the Au-Si-alloy via LEED, STM, and DFT by Enriquez et al.[4].


*The authors are grateful for financial support by the Land Nordrhein-Westfalen.
4:54PM U52.00013: Geometric models and electronic structure of Pb overlayers on Ge(111): a first-principles study* ANDRE CHILDS (Presenter), SHREE RAM ACHARYA, DUY LE, University of Central Florida, CHING YAO FONG, SHIRLEY CHIANG, University of California Davis, TALAT S. RAHMAN, University of Central Florida — Lead deposition on Ge(111) shows several low dimensional phases [1]: the (√3×√3)R30° Pb structure forms at coverages of 1/3 monolayer (ML) (α phase) and 4/3 ML (β phase), while at 1 ML the overlayer is (1 × 1). In all cases the Ge(111) surface is unreconstructed. The geometric and electronic structure of the phases are not yet fully understood. We present results from our density functional theory based calculations with and without inclusion of spin-orbit coupling (SOC) to shed light onto atomic and electronic structures of these phases and the nature of their binding to the substrate. We find that Pb atoms adsorb at the T$_4$ sites at a height of 2.94 Å, at the T$_4$ and H$_3$ sites at height of 2.84 Å, and the off-centered T$_1$ sites at height of 2.84, from the underlying Ge surface, on the α, β and 1 ML phases of the structure, respectively, and at the T$_1$ site at a height of 2.76 Å directly above the nearest Ge on the Pb(1 × 1) phase. We find that these phase are metallic. Our results reinforce the importance of SOC in reproducing geometric structures of the Pb over-layers, in good agreement with experimental observations.


*Work supported in partial by NSFDMR-1710306 (AC, SRA, DL, TSR) and NSF DMR-1701748 (SC, CF).

5:06PM U52.00014: Giant Nonlinear Tunneling Current in HfO$_2$-based Anti-Ferroelectric Tunnel Junction JINHO BYUN (Presenter), TAEWON MIN, JAEKWANG LEE, Pusan Natl Univ — Owing to the recent advances in the oxide growth technology, ferroelectricity has been stabilized even in a few nm-thick films, which makes it possible to realize the ultrathin oxides-based ferroelectric tunneling junctions (FTJs) useful for the next generation switchable diode. Among various ferroelectric oxides, HfO$_2$ is the most promising material for FTJ devices since it has the great advantage of complementary metal-oxide-semiconductor (CMOS) process compatibility. Despite their numerous advantages, low non-linearity and tunneling current have hindered their applications to electronic devices. Here, combining density functional theory (DFT) calculations and numerical tunneling current simulations of the new type of tunneling potential, we find that the antiferroelectric-like head-to-head and tail-to-tail polarizations significantly enhance the non-linearity ($>10^3$) and tunneling current at the same time, which will be an essential guideline to design high density and low power consumption electronics applications.
2:30PM U53.00001: Atomic resolution characterization of 2D materials with scanning transmission electron microscopy. [Invited] NASIM ALEM (Presenter), Department of Materials Science and Engineering, Pennsylvania State University — Selected by Focus Topic Organizer (Liuyan Zhao, Robert Hovden).

2:42PM U53.00002: Using Intercalation Chemistry to Change Interlayer Spacing and Resulting Bandgap of Two-Dimension Materials* ANDREW SMITH (Presenter), SUBASH KATTEL, ZACHARY HECHT, HENRY WLADKOWSKI, JOSEPH R MURPHY, WILLIAM RICE, ELLIOTT HULLEY, JOHN ACKERMAN, BRIAN LEONARD, Univ of Wyoming — The operating principle behind smart windows is that they can transmit, absorb or reflect different wavelengths of light at will. To achieve these properties, they must be constructed with materials that have an easily tunable bandgap, this is often done via intercalation chemistry. 2D materials have shown similar tunability in the past and often show enhanced mobility for ions. We are exploring one such material, WO$_2$Cl$_2$, and what role interlayer spacing plays in the bandgap of 2D materials. When WO$_2$Cl$_2$ is intercalated with Li, it starts as a wide bandgap material (clear) then transitions to a blue narrower bandgap material, then a coppery metallic phase. To understand these phases, we have carried out 4-point resistivity measurements, absorption and Raman spectroscopy, XRD, XPS, SEM, and TEM. These methods have shown intercalated WO$_2$Cl$_2$ to be a very tunable and versatile material. Additionally, we hypothesize a direct relationship between bandgap, interlayer spacing and ion size for WO$_2$Cl$_2$. To test this, we have examined properties of WO$_2$Cl$_2$ that has been intercalated ions of increasing size, Li<Na<K<Rb<Cs to great success.

*NSF DMR: 1229383

2:54PM U53.00003: Realization of 2D Crystalline Metal Nitrides via Selective Atomic Substitution JUN CAO (Presenter), TIANSHU LI, HONGZE GAO, XI LING, Boston Univ — Two-dimensional (2D) transition metal nitrides (TMNs) are emerging members in 2D family with promising potential for a range of applications. Their applications can be further extended to electronic and optoelectronic devices through the acquisition of high crystalline and large-area thin films. However, materials that meet such requirements have not been achieved using previous methods. Here, we report the synthesis of few-nanometer thin Mo$_5$N$_6$ crystals with satisfactory area and quality via chemical conversion of layered MoS$_2$ crystals. The lateral dimensions of Mo$_5$N$_6$ crystals are inherited from the MoS$_2$ precursors. Atomic force microscopy characterization indicates that the thicknesses of Mo$_5$N$_6$ crystal reduce to about 1/3 of the MoS$_2$ crystal, matching well with the crystal structure model. Electrical measurement shows the high conductivity of Mo$_5$N$_6$. In addition, this chemical conversion strategy is found versatile for the synthesis of various metal nitrides including W$_5$N$_6$, and TiN using corresponding metal sulfides. Our strategy offers a new direction for preparing 2D TMNs with desired characteristics, opening a door for future exploration of fundamental physics and devices applications.
3:06PM U53.00004: Step edge-mediated assembly of periodic arrays of long graphene nanoribbons on Au(111)  WENCHANG LU (Presenter), North Carolina State University, CHUANXU MA, Oak Ridge National Laboratory, ZHONGCAN XIAO, North Carolina State University, JINGSONG HUANG, KUNLUN HONG, AN-PING LI, Oak Ridge National Laboratory, JERRY BERNHOLC, North Carolina State University — Graphene nanoribbons (GNRs) can be fabricated with atomic precision via bottom-up synthesis on metal substrates, but the growth of long GNRs still remains a challenge. We have previously investigated the growth mechanism of GNRs from molecular precursors on Au substrate [1]. Recently, we have observed that the step edges of an Au (111) substrate can enhance GNR growth and yield significantly longer GNRs and periodic GNR arrays on the Au(111) surface [2]. By studying the atomic structures and electronic properties near step edges by DFT calculations, we have found that the intermediate polyanthryl structures adsorb more strongly along Au step edges due to pi-pi interactions between polyanthryls near the steps, which result in longer and more compact polymer arrays and lead to the synthesis of longer GNRs. Our findings suggest a direction for the manufacturing of longer GNRs for future applications.


3:18PM U53.00005: Preparation and growth of sulfide heterostructure thin films from designed precursors  DENNICE ROBERTS (Presenter), National Renewable Energy Laboratory, BRIAN GORMAN, Colorado School of Mines, JOHN PERKINS, ANDRIY ZAKUTAYEV, SAGE BAUERS, National Renewable Energy Laboratory — Design of chalcogenide heterostructures has enabled access to a remarkable range of material properties occurring as a result of structural flexibility at the nanoscale. A powerful approach to generating heterostructures involves the preparation of an amorphous precursor film designed to mimic the desired end product. While this has been highly successful in generating selenium-based heterostructures with novel properties, sulfur-based compounds have remained unexplored. Here we present the first crystalline sulfide heterostructure prepared using this precursor approach, forming superlattices with a tunable number of SnS layers sandwiched between monolayers of TaS$_2$. Structural measurements confirm film crystallinity and overall film smoothness, and architecture is confirmed by high resolution TEM and EDS that resolves atomically precise sequencing of SnS and TaS$_2$ layers. Formation mechanisms are assessed in terms of mobility of precursor elements upon heating. A path towards sulfide heterostructures with adjustable stacking orders allows the development of materials with precisely tuned properties that utilize phenomenon inherent in constituent compounds; such materials are promising for applications in advanced electronics.
Experimental demonstration of partial van der Waals screening by mono- and double-layer MoSe\textsubscript{2} and MoS\textsubscript{2}

STANISLAV TSOI (Presenter), United States Naval Research Laboratory, SAUJAN V SIVARAM, MATTHEW ROSENBERGER, National Research Council, US Naval Research Laboratory, Washington, DC 20375, KATHLEEN MCCREARY, United States Naval Research Laboratory, HSUN-JEN CHUANG, American Society for Engineering Education, US Naval Research Laboratory, Washington, DC 20375, BEREND THOMAS JONKER, United States Naval Research Laboratory

— Few-layer flakes of MoS\textsubscript{2} or MoSe\textsubscript{2} with lateral dimensions over 1 \(\mu\)m were grown on graphite using chemical vapor deposition, yielding layered samples MoS\textsubscript{2}/graphite or MoSe\textsubscript{2}/graphite, respectively. Next, an attractive van der Waals (vdW) force on a sharp AFM tip was measured from graphite, MoS\textsubscript{2}/graphite and MoSe\textsubscript{2}/graphite as a function of a separation between the tip and sample. The vdW force from the layered samples is significantly weaker than from graphite alone, suggesting screening of the semimetallic graphite by the semiconducting MoS\textsubscript{2} and MoSe\textsubscript{2}. Statistical analysis over 6 different measurements indicates that the single-layer MoSe\textsubscript{2} screens 59 ± 14 % and the single-layer MoS\textsubscript{2} 71 ± 12 % of the force from graphite. The double-layer samples exhibit even stronger screening, with the double-layer MoSe\textsubscript{2} screening 77 ± 24 % and the double-layer MoS\textsubscript{2} 94 ± 8 % of the vdW force from graphite. The observed results demonstrate a possibility to engineer and control the nanoscale vdW forces in a bottom-up approach, and provide a critical experimental platform for testing the quantum electrodynamic Lifshitz theory of vdW interactions.

Graphene growth on non-metallic substrates by Chemical Vapor Deposition

SANDRA RODRIGUEZ VILLANUEVA (Presenter), ALVARO INSTAN, University of Puerto Rico - Rio Piedras, FRANK MENDOZA, Physics, University of Puerto Rico at Mayaguez, BRAD R WEINER, RAM KATIYAR, GERARDO MORELL, University of Puerto Rico - Rio Piedras

— The electrical properties of graphene on dielectric substrates have many applications. Graphene is usually grown on metallic substrates then transferred onto dielectric substrates as necessary. However, to obtain graphene directly on non-metallic substrates is still challenging. In this work, we show the direct synthesis of graphene on SiO\textsubscript{2}/Si and SiC by hot-filament chemical vapor deposition. The graphene deposition was conducted at low pressures with a mixture methane in hydrogen and a substrate temperature 900°C followed by abrupt cooling to room temperature. A thin strip of copper layer was sputtered in the middle of the SiO\textsubscript{2}/Si substrates as a catalytic material. For the SiC substrate, a hydrofluoric acid treatment was used before graphene deposition. The structural properties of the graphene films were analyzed using Raman Spectroscopy, Atomic Force Microscopy (AFM), and X-ray photoelectron spectroscopy (XPS). Raman mapping and AFM measurements indicate the growth of few-layer graphene films in all cases. X-ray photoelectron spectroscopy confirmed the presence of graphene deposition on SiO\textsubscript{2}/Si and SiC substrates. The results show that the availability of copper vapors from the thin copper strip enables the growth of graphene in all surfaces of the non-metallic substrates.
3:54PM U53.00008: Direct growth of twisted bilayer graphene with controllable twist angle by plasma-enhanced chemical vapor deposition*  JIAQING WANG (Presenter), YEN-CHUN CHEN, Physics, California Institute of Technology, WEI-HSIANG LIN, Applied Physics, California Institute of Technology, WEI-SHIUAN TSENG, Physics, California Institute of Technology, CHII-DONG CHEN, Institute of physics, Academia Sinica, YU-SHU WU, physics, National Tsing-Hua University — We report a direct plasma-enhanced chemical vapor deposition (PECVD) method to grow single crystalline bilayer graphene (BLG) flakes and mm-size BLG films with the interlayer twist angle controlled by the growth parameters. The average twist angle can be controlled from 0° to approximately 20° by tuning the CH4-to-H2 pressure ratio (PCHA4/PH2). Raman spectroscopic studies on our PECVD-grown BLG together with x-ray and ultraviolet-light photoelectron spectroscopy indicate high-quality samples and reveal twist-angle dependent spectral characteristics. Atomically resolved scanning tunneling microscope (STM) is employed to identify the Moiré pattern and the value of the corresponding twist angle between two layers. Our PECVD-grown BLG provides a perfect platform to study the twist-angle dependence of its electronic properties. We performed transport measurements on our BLG samples with twist angles varying between 0° and 20°. The electronic properties of BLG of different twist angles are systematically investigated as a function of temperature and gate voltage, which provides useful information for the origin of various correlated phenomena.

*This work was jointly supported by ARO and NSF in the USA, and by the MoST in Taiwan.

4:06PM U53.00009: 2D platinum diselenides grown on 3D wide-bandgap substrates by Van der Waals epitaxy*  CHIA-HER LIN, EDWARD STOCKERT, Physics Department, Natl Sun Yat Sen Univ, CHING-WEN CHANG, Research Center for Applied Sciences, Academia Sinica, Taiwan, TING CHEN, CHIEN-CHEN KUO, YI-YING LU, LI-WEI TU, Physics Department, Natl Sun Yat Sen Univ, QUARK CHEN (Presenter), Physics and TcSUH, University of Houston, PARITOSH V WADEKAR, Physics Department, Natl Sun Yat Sen Univ — PtSe2 is a 2D material that undergoes phase transition from a semiconductor of Eg≈0.3 eV to a type-II Dirac semimetal as its thickness varies. 3D wide band gap semiconductors continue to gain wider acceptance as a substrate material and as an electrode if properly doped. To embrace for broader applications, tractable materials process design rules are essential, especially in understanding the relationships between the Van der Waals epitaxy and the resulted physical properties of the ended products. In this work, ultrathin films of Pt were first deposited by magnetron sputtering on the GaN, AlN and Al2O3 substrates followed by atmospheric pressure chemical vapor deposition (APCVD). Selenization of the Pt films forms uniform and smooth 2D/3D selenide heterostructures. The effects of deposition parameters with respect to the underlying substrates according to the physical properties are investigated. Various spectroscopic means were used to study the samples with well characterized structural properties.

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**4:18PM U53.00010: Facile Production of Macroscopic Single Crystal Monolayers and Artificial Lattices of 2D van der Waals Materials**

FANG LIU (Presenter), WENJING WU, YUSONG BAI, SANGHOON CHAE, QIUYANG LI, JUE WANG, JAMES C HONE, XIAOYANG ZHU, Columbia University — Two dimensional (2D) materials from layered van der Waals (vdW) crystals hold great promises for electronic, optoelectronic, and quantum devices, but technological implementation has been hampered by the lack of high-throughput techniques for the production of monolayers with sufficient sizes and quality. Here we report a facile method to disassemble vdW single crystals layer-by-layer into monolayers with near-unity yield and with macroscopic dimensions limited only by bulk crystal sizes. The quality of the macroscopic single crystal monolayers are comparable to those of microscopic dimensions obtained from state-of-the-art techniques. We exfoliate a range of vdW crystals and assemble the monolayers into artificial lattices, including transition metal dichalcogenides with dramatic enhancement in nonlinear optical responses. This approach takes us one step closer to commercialization of 2D materials.

*The research was supported by the Materials Science and Engineering Research Center (MRSEC) through NSF grant DMR-1420634, and National Science Foundation (NSF) grant DMR-1809680, and the Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) Postdoctoral Research Award managed by Oak Ridge Associated Universities under DOE contract number DE-SC00014664.

**4:30PM U53.00011: Automated Vacuum Stacking for Additive Assembly of 2D van der Waals Heterostructures**

ANDREW YE (Presenter), Pritzker School of Molecular Engineering, University of Chicago, ANDREW J MANNIX, James Franck Institute, University of Chicago, FAUZIA MUJID, Department of Chemistry, University of Chicago, CHIBEOM PARK, James Franck Institute, University of Chicago, JIWOONG PARK, Pritzker School of Molecular Engineering, University of Chicago — Wafer-scale synthesis of monolayer 2D materials (2DMs) address the stochastic, small-area limitations of micromechanical exfoliation. Using wafer-scale synthesized 2D semiconductors along with large-area patterning and multi-functional polymer stamps, we demonstrate a highly automated, dry-transfer, additive assembly process. Our high-vacuum system can assemble 2D heterostructures at the precision of actuator limits (few micron lateral/0.2° rotational). Identical structures have been assembled in parallel and stacks of high layer counts (25+) have been achieved, all without active user control of the system. Fabricated heterostructures include a range of 2DMs (MoS$_2$, WS$_2$, WSe$_2$, graphene) and metal electrodes (Au, Ti), and can be deposited onto a variety of substrates (SiO$_2$, Al$_2$O$_3$, 2DMs). We also demonstrate controlled twisted n-layer heterostructure assembly, where number of layers depends on area limits of single-crystal 2DMs growth.

*Work is supported by DoE EFRC NPQC & NSF PARADIM No. DMR-1539918. AY is supported by the DoD NDSEG Fellowship Program.
4:42PM U53.00012: Impact of thermal treatment on graphene films synthesized via interfacial trapping technique*  SARA CHAHID (Presenter), RAJENDRA DULAL, SERAFIM TEKNOWIJOYO, Chapman Univ, ALEXANDER RZHEVSKII, Molecular & Elemental Analysis App. Lab, Thermo Fisher Scientific, ARMEN GULIAN, Chapman Univ — Large variety of graphene applications in science and technology justify different methods to obtain pure graphene films. Among these methods, Woltornist et.al., ACS Nano 7, 7062 (2013) obtained promising results by pulverizing ultrapure graphite in water/n-heptane mixture to form continuous films on glass substrate. We report here subsequent steps of studying this method with different substrates and also of application of annealing (100°-600°, in air and in a vacuum) on the physical properties of these films. As can be deduced from Raman spectra, the quality of graphene films is enhanced in certain temperature range. We complemented Raman mapping by characterizing the morphology of films using scanning electron microscopy. Other instrumentation techniques have also been used to affect and study the physical properties of these films. Overall, the simplicity of the method and the quality of the film reveal potential areas of applications in microelectronics.

*This work was supported in part by the ONR Grants N00014-16-2269, N00014-17-1-2972, N00014-18-1-2636, and N00014-1901-2265.

4:54PM U53.00013: Fabrication and Imaging of Monolayer Phosphorene with Preferred Edge Configurations via Graphene-Assisted Layer-by-Layer Thinning  YANGJIN LEE (Presenter), SOL LEE, JUN-YEONG YOON, Department of Physics, Yonsei University, JINWOO CHEON, Center for Nanomedicine, Institute for Basic Science (IBS), HU YOUNG JEONG, UNIST Central Research Facilities (UCRF), Ulsan National Institute of Science and Technology, KWANPYO KIM, Department of Physics, Yonsei University — Phosphorene, a monolayer of black phosphorus (BP), is an elemental 2D material with interesting physical properties including high charge carrier mobility and exotic in-plane anisotropic properties. To fundamentally understand its various physical properties, the atomic-scale structural investigation, various defect and preferred edge configurations for monolayer counterpart, is of critically importance. However, it has been challenging to perform imaging of monolayer phosphorene due to technical difficulty to prepare high-quality samples and damages induced during measurements via photons or high-energy electrons. Here, we successfully fabricate monolayer phosphorene by a controlled thinning process inside a TEM and subsequently perform atomic-resolution imaging. Graphene protection suppresses the e-beam-induced damage to BP and one-side graphene lamination facilitates the layer-by-layer thinning of the samples, rendering monolayer and bilayer regions. We also observe crystalline edge predominantly aligned along zigzag and (101) terminations, which can be explained by edge kinetics under e-beam-induced sputtering process. Our study provides invaluable approach to manipulate the thickness and image beam-sensitive 2D materials.

Thursday, March 5, 2020 2:30 PM - 4:54 PM

Session U54 DCMP: Topological Crystalline Phases  Mile High Ballroom 2A
2:30PM U54.00001: Aperiodic Topological Crystalline Insulators*  HUAQING HUANG (Presenter), YONG-SHI WU, FENG LIU, University of Utah — Topological crystalline insulators (TCIs) are usually described with topological protection imposed by the crystalline symmetry. In general, however, the existence of TCI states does not necessitate the periodicity of crystals as long as an essential lattice symmetry can be identified. Here we demonstrate the compatibility of TCIs with aperiodic systems, as exemplified by an octagonal quasicrystal. In contrast to most common topological insulators and TCIs, the proposed aperiodic TCIs are attributed to a different symmetry-invoked band inversion mechanism, which inverts states with the same parities but opposite eigenvalues of a specific symmetry (such as reflection). The nontrivial topology is characterized by a nonzero integer "mirror Bott index". Moreover, we demonstrate that the topological edge states and quantized conductance of the aperiodic TCI, which are robust against disorder, can be effectively manipulated by external electric fields. Our findings not only provide a better understanding of electronic topology in relation to symmetry but also extend the experimental realization of topological states to much broader material categories beyond crystals.

*This work was supported by U.S. DOE-BES (Grant No. DE-FG02-04ER46148)

2:42PM U54.00002: Real Space Invariants: Spectral Flow of Fragile Topological State under Twisted Boundary Conditions  ZHIDA SONG (Presenter), Princeton University, LUIS ELCORO, University of the Basque Country, NICOLAS REGNAULT, ANDREI BERNEVIG, Princeton University — In this paper, we propose the twisted boundary condition as a generic approach to theoretically and experimentally detect the fragile topological state. We prove that, when the fragile phase can be written as a difference of a trivial atomic insulator and the so-called obstructed atomic insulator, the gap between the fragile phase and other bands must close under a specific twist of the boundary condition of the system. We explicitly work out all the twisted boundary conditions that can detect all the 2D fragile phases implied by symmetry eigenvalues in all wallpaper groups. We develop the concept of real space invariants, which are local good quantum numbers in real space, and which also fully characterize the eigenvalue fragile phases. We show that the number of unavoidable level crossings under the twisted boundary condition is completely determined by the real space invariants. Possible realizations of the twisted boundary condition of the fragile band in metamaterial systems are also discussed.

2:54PM U54.00003: Electron localization in fragile topological crystalline phases  RAQUEL QUEIROZ (Presenter), Weizmann Institute of Science, RONI ILAN, Tel Aviv University, ZHIDA SONG, Princeton University, ADY STERN, Weizmann Institute of Science, ANDREI BERNEVIG, Princeton University — Topological phases are known for their robustness to local perturbations. Localization of topological bands has been extensively studied, particularly those protected by local symmetries such as time-reversal or particle-hole symmetries. In the last few years, it became clear that also nonlocal, crystalline, symmetries are crucial for the protection of topology in electronic systems. Crystalline symmetry protected topology opens the way fundamentally new concepts that fall outside of the conventional knowledge in theory of localization. In this talk, I will present a numerical study of localization in fragile topological insulators, relevant for recent experimental developments.
3:06PM U54.00004: Fragile Topology Protected by Inversion Symmetry: Diagnosis, Bulk-Boundary Correspondence, and Wilson Loop*  YONSEOK HWANG (Presenter), JUNYEONG AHN, BOHM-JUNG YANG, Seoul Natl Univ — We study the bulk and boundary properties of fragile topological insulators (TIs) protected by inversion symmetry, mostly focusing on the class A insulator. First, we propose an efficient method for diagnosing fragile band topology by using the symmetry data in momentum space. Second, we study the bulk-boundary correspondence of fragile TIs protected by inversion symmetry. In particular, we show that a minimal fragile TI with the filling anomaly corresponds to the $dD$ $(d+1)$th-order TI. Although $dD$ $(d+1)$th-order TIs have no in-gap states, the boundary mass terms carry an odd winding number along the boundary, which induces localized charges on the boundary at the positions where the boundary mass terms change abruptly. Also by studying the (nested) Wilson loop spectra, we show that all the spectral windings of the (nested) Wilson loop should be unwound to resolve the Wannier obstruction of fragile TIs. By counting the minimal number of bands required to unwind the spectral winding of the Wilson loop and nested Wilson loop, we determine the minimal number of bands to resolve the Wannier obstruction, which is consistent with our diagnosis method of fragile topology.

*This work was supported by IBS (IBS-R009-D1), NRF (0426-20190008), and the U.S. Army Research Office (W911NF-18-1-0137).

3:18PM U54.00005: Crystalline topological phases without symmetry indicators  SANDER KOOI (Presenter), GUIDO VAN MIERT, CARMINE ORTIX, Univ of Utrecht — Topological insulating phases of matter are quantum phases that cannot be deformed to atomic insulators. They generically feature protected anomalous surface states, which can be used for applications in spintronics and quantum computation.

Recently, two new types of topological phases protected by crystalline symmetries have been discovered. The first are higher-order topological insulators, featuring conducting states on the hinges [1], recently observed in bismuth [2]. The other are fragile topological states, which become trivial when occupying additional bands. Twisted bilayer graphene may be a realization of a fragile phase, which may help to explain superconductivity in this system [3].

Usually, crystalline topology can be detected by computing symmetry indicators. However, there exist topological phases which cannot be detected in this way, and we present the first classification of such states [4]. We show these crystalline invariants are also well-defined in quantum spin Hall systems and use this to construct a hybrid-order weak TI [5], which is both a weak and higher-order TI.

3:30PM U54.00006: Topology of chiral insulators  MARCELO GUZMÁN (Presenter), DENIS BARTOLO, DAVID CARPENTIER, Physique, Ecole Normale Superieure de Lyon — Building on direct analogies with electronic matter, the concepts of topological insulator and topological protection have been successfully applied to a host of different physical systems as diverse as photonic metamaterials, geophysical fluids and mechanical structures. In this work, we focus on materials, or metamaterials, having a chiral symmetry, such as crystals with a sub-lattice symmetry and all mechanical systems assembled from beads and springs.

Firstly, we show that the topology of waves in chiral materials is naturally encoded in their chiral polarization, which quantifies the spatial imbalance of localized Wannier states between the two sub-lattices. Secondly, we demonstrate that the chiral polarization originates both from topological properties of the Hamiltonian and of the frame on which this Hamiltonian is defined. Our results elucidate a long-standing ambiguity on the topological characterization of the simplest, and probably oldest example of a topological state: the Su-Schrieffer-Hegger (SSH) chain. Finally, we establish a generalized bulk-boundary correspondence for chiral systems and show how to effectively use the concept of chiral polarization to predict the existence of interfacial states at the boundary of chiral insulators.

3:42PM U54.00007: Boundary obstructed topological phases  ESLAM KHALAF (Presenter), Harvard University, WLADIMIR A BENALCAZAR, The Pennsylvania State University, TAYLOR L HUGHES, University of Illinois at Urbana-Champaign, RAQUEL QUEIROZ, Weizmann Institute of Science — Symmetry protected topological (SPT) phases are gapped phases of matter that cannot be deformed to a trivial phase without breaking the symmetry or closing the bulk gap. Here, we introduce a new notion of a topological obstruction that is not captured by bulk energy gap closings in periodic boundary conditions. More specifically, we say two bulk Hamiltonians belong to distinct boundary obstructed topological ‘phases’ (BOTPs) if they can be deformed to each other on a system with periodic boundaries, but not for symmetric open boundaries without closing the gap at a high symmetry region on the surface. BOTPs are not topological phases of matter in the standard sense since they are adiabatically deformable to each other on a torus but, similar to SPTs, they are associated with surface states or fractional corner charges in the open system. We show that the double-mirror quadrupole model of [Science, 357(6346), 2018] is a prototypical example of such phases, and present a detailed analysis of boundary obstructions in this model. In addition, we introduce several three-dimensional models having boundary obstructions, which are characterized either by surface states or fractional corner charges and discuss their general formulation in terms of Wannier band representations.

3:54PM U54.00008: Topological Crystalline States with Non-trivial Relative Group Cohomology*  SYDNEY R TIMMERMAN (Presenter), YI LI, Johns Hopkins University — The method of relative homotopy group has been know useful to characterize the surface defects that are not trivial extensions of bulk defects. We develop the method of relative group cohomology to study novel topological crystalline states characterized by non-trivial relative group cohomology and their relation to fragile topological crystalline states.

*This work is supported by NSF CAREER DMR-1848349 and in part by the Alfred P. Sloan Research Fellowships.
4:06PM U54.00009: Topological Invariants of a Filling-Enforced Quantum Band Insulator

ABIJITH KRISHNAN (Presenter), Harvard University, HOI CHUN PO, Massachusetts Institute of Technology, ASHVIN VISHWANATH, Harvard University —

In the classical picture of insulators, electrons occupy localized Wannier (atomic-like) orbitals. Recently, insulators for which electron filling prohibits this atomic description have been theoretically proposed. The electronic wave functions of these insulators, termed filling-enforced Quantum Band Insulators (feQBIs), display a necessary degree of quantum entanglement due to the non-atomic filling. Currently, little is known about the relation between feQBIs and conventional topological invariants. In this work, we study such relations for a particularly interesting example of an feQBI realized with spinless fermions in space group 106.

4:18PM U54.00010: Fermions in $\mathbb{Z}_N$ Gauge Fields: From Chern Insulators to Higher-Order Topological Insulators*

VIJAY SHENOY (Presenter), SHUBHAM RANA, Indian Institute of Science —

Fermions coupled to gauge fields defined on the links of lattices have received considerable attention due to their importance in describing a variety of physical systems. Here, we show how a higher-order topological insulator emerges in a system of fermions coupled to $\mathbb{Z}_N$ gauge fields. By tuning the filling of fermions and the strength of the coupling of fermions to the gauge fields, we show that a variety of fermion phases are stabilized for different parameter regimes. We map out the phase diagram of this system and identify conditions needed to generate a higher-order topological insulating phase. This work suggests experimental routes, for example in a cold atomic system, to obtain different topological phases of fermions to study both the properties of these phases and the phase transitions between them.

*SR thanks KVPY Program, and VBS thanks SERB, DST, India for support. The authors thank visitors program at MPIPKS, Dresden, where part of this work was done.
Type-II quadrupole topological insulators

YANBIN YANG (Presenter), KAI LI, LUMING DUAN, YONG XU, Tsinghua University — Recently, the formulation of polarization based on the Berry phase has been extended to higher multipole moments, through the discovery of the so-called quadrupole topological insulator.

It has been established by a classical electromagnetic theory that in a two-dimensional material the quantized properties for the quadrupole topological insulator should satisfy a basic relation. Here we discover a new type of quadrupole topological insulator (dubbed as type-II) that violates this relation due to the breakdown of a previously established theory that a Wannier band and an edge energy spectrum are topologically equivalent in a closed quantum system. We find that, similar to the previously discovered (referred to as type-I) quadrupole topological insulator, the type-II hosts topologically protected corner states carrying fractional corner charges. However, the edge polarizations only occur at a pair of boundaries in the type-II insulating phase, leading to the violation of the classical constraint. We propose an experimental scheme to realize such a new topological phase of matter. The existence of the new topological insulating phase means that new multipole topological insulators with distinct properties can exist in broader contexts beyond classical constraints.

Layer Construction of Topological Crystalline Insulator LaSbTe

YUTING QIAN (Presenter), Institute of Physics, Chinese Academy of Science, ZHIYUN TAN, School of Physics and Electronic Science, Zunyi Normal University, TAN ZHANG, JIACHENG GAO, ZHIJUN WANG, ZHONG FANG, CHEN FANG, HONGMING WENG, Institute of Physics, Chinese Academy of Science — Topological crystalline insulator (TCI) is one of the symmetry-protected topological states. Any TCI can be looked as a simple product state of several decoupled two-dimensional (2D) topologically nontrivial layers in its lattice respecting its crystalline symmetries, so called layer construction (LC) scheme. In this work, based on first-principles calculations we have revealed that both the tetragonal LaSbTe (t-LaSbTe) and the orthorhombic LaSbTe (o-LaSbTe) can be looked as a stacking of 2D topological insulators in each lattice space. The structural phase transition from t-LaSbTe to o-LaSbTe due to soft phonon modes demonstrates how the real space change can lead to the modification of topological states. Their symmetry-based indicators and topological invariants have been analyzed based on LC. We propose that LaSbTe is an ideal paradigm perfectly demonstrating the LC scheme, which bridges the crystal structures in real space to the band topology in momentum space.
U54.00013: Filling-enforced Dirac loops and their evolutions under various perturbations
DEXI SHAO (Presenter), Chinese Academy of Sciences, Institute of Physics — Based on symmetry analysis, we find that filling-enforced Dirac loops (FEDLs) in non-magnetic systems exist in only five space groups. We further explore all possible configurations of these FEDLs in these space groups, and classify them accordingly. We study the evolutions of the FEDLs under various types of perturbations such as applied strain or field. It is interesting that the FEDL-materials can serve as both parent materials of nodal semimetals having Dirac points or nodal-loops, and topological insulators/topological crystalline insulators. Many the FEDL-materials are predicted in DFT calculations.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U55 DCMP: Topological superconductors in more than one dimension
Mile High Ballroom 2B - Tag(s): Focus

2:30PM U55.00001: Superconductivity without time-reversal or inversion symmetries
[Invited] DANIEL AGTERBERG (Presenter), University of Wisconsin - Milwaukee, PHILIP BRYDON, Physics, University of Otago, MARK H FISCHER, Physics, University of Zurich, HENRI MENKE, Physics, University of Otago, MANFRED W SIGRIST, Theoretical Physics, ETH-Zurich, CARSTEN TIMM, Theoretical Physics, Technische Universität — To ensure a superconducting instability, key symmetries are required. In three dimensions (3D), these are time-reversal (T) and inversion (I) symmetries. In two dimensions, T and I are joined by TM_z and IM_z symmetries where M_z is a mirror reflection through the basal plane. Here we discuss unusual physics that arises when one or more of these key symmetries are broken. In particular, in 3D, we show that spontaneously breaking T symmetry allows for topologically protected nodal Bogoliubov Fermi surfaces and apply this idea to URu_2Si_2 and Sr_2RuO_4. In 2D, we develop an energetic and topological superconductor classification in the unfamiliar situation that both T and I symmetries are absent. We apply this to Ising superconductors with in-plane magnetic fields and monolayer FeSe coexisting with antiferromagnetic order.
3:06PM U55.00002: Supercurrent-induced Majorana bound states in a planar geometry*
ANDRÉ MELO (Presenter), SEBASTIAN RUBBERT, ANTON AKHMEROV, Kavli Institute of Nanoscience, Delft University of Technology — We propose a new setup for creating Majorana bound states in a two-dimensional electron gas Josephson junction. Our proposal relies exclusively on a supercurrent parallel to the junction as a mechanism of breaking time-reversal symmetry. We show that combined with spin-orbit coupling, supercurrents induce a Zeeman-like spin splitting. Further, we identify a new conserved quantity—charge-momentum parity—that prevents the opening of the topological gap by the supercurrent in a straight Josephson junction. We propose breaking this conservation law by adding a third superconductor, introducing a periodic potential, or making the junction zigzag-shaped. By comparing the topological phase diagrams and practical limitations of these systems we identify the zigzag-shaped junction as the most promising option.

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3:18PM U55.00003: Dissipative chiral superconductors in 3D  MENG HUA (Presenter), LINGYU YANG, JEFFREY TEO, Univ of Virginia — Topological band theories that describe insulators, superconductors and (semi)metals are conventionally classified according to the Altland-Zirnbauer classification based on the presence or absence of local time-reversal and particle-hole symmetries. More recently, there are theoretical generalizations that incorporate non-local magnetic space group symmetries. There are more exotic combined antiunitary spatial symmetries that involve particle-hole conjugation and may be allowed in a non-Hermitian system. In this talk, we focus on the classification, model realization and topological-index characterization of dissipative topological superconductors in 3D and the corresponding dissipative chiral Majorana fermion on the boundary surface.
3:30PM U55.00004: Topological Skyrmion Phases of Matter* ASHLEY COOK (Presenter), University of California, Berkeley — We introduce two-dimensional topological phases of matter defined by non-trivial homotopy groups into the literature, characterized either by a single Skyrmion number, known as the chiral topological Skyrmion insulator, or a pair of Skyrmion numbers, known as the helical topological Skyrmion insulator, which generalize and extend the concepts of the Chern insulator and quantum spin Hall insulator, respectively. We show each topological phase of matter is protected by a combination of a mirror symmetry and a generalized particle-hole symmetry equal to the product of particle-hole symmetry and spatial inversion symmetry. Despite these phases being protected in part by crystalline point group symmetries, the phases introduced here are very different from all others known: we characterize three kinds of phase transitions by which a Skyrmion number can change. One kind of topological phase transition occurs without the closing of energy gaps, which has important consequences for study of topologically non-trivial phases of matter. We find that each phase is realized in a tight-binding model relevant to Sr2RuO4 and discuss experimental realization given that the chiral topological Skyrmion insulator phase is realized for a parameter set used to characterize Sr2RuO4.

*NSERC

3:42PM U55.00005: Triplet-Superconductivity in Triple-Band Crossings* GIBAIK SIM (Presenter), MOON JIP PARK, SUNGBIN LEE, Korea Adv Inst of Sci & Tech — In this talk, we will introduce the triplet superconductivity in the newly discovered form of the topological semimetal, where the electrons with pseudospin J=1 form triple-band crossings. The peculiar property of J=1 electrons is that Fermi statistics rules out on-site spin singlet pairing. Performing the exact decoupling of on-site electron interactions into pairing channels, we adopt the Landau theory of spin-triplet pairings and study the Landau free energy functional to plot out the global phase diagram. We find two distinct phases; (i) time-reversal symmetric (Sz) state, (ii) time-reversal broken (Sx + i Sy) state. Remarkably, both of these states have gapless Bogoliubov quasiparticles and furthermore have topological invariants for each nodal line or Bogoliubov Fermi surface.

*The authors are supported by the KAIST startup, BK21 plus program, KAIST and National Research Foundation Grant No. NRF2017R1A2B4008097.
3:54PM U55.00006: Higher-order topological superconductor in $\mathcal{P}$, $\mathcal{T}$-odd quadrupolar Dirac metal  
BITAN ROY (Presenter), Lehigh University — Presence or absence of certain symmetries in the normal state (NS) also plays important role in determining the symmetry of the Cooper pairs. We here show that two- and three-dimensional Dirac metals, realized by doping parity ($\mathcal{P}$) and time-reversal ($\mathcal{T}$) odd topologically trivial Dirac insulators, sustain a local or inter-unit cell pairing that assumes the form of a time-reversal odd and mixed parity (due to the absence of $\mathcal{T}$ and $\mathcal{P}$ in the NS, respectively) pairing around the Fermi surface. When the NS additionally breaks discrete four-fold ($C_4$) symmetry (yielding a $\mathcal{P}$, $\mathcal{T}$-odd, quadrupolar Dirac metal), the system gives birth to a higher-order $p + id$ pairing, hosting corner (in $d = 2$) or hinge (in $d = 3$) modes of codimension $d_c = 2$ of Majorana fermions. While the $p$-wave component stems from the Dirac nature of quasiparticles in the NS, appearance of the $d$-wave component is solely attributed to the lack of $C_4$ symmetry, as its restoration produces $p + i s$ pairing.

4:06PM U55.00007: Refined symmetry indicators for topological superconductors in all space groups*  
SEISHIRO ONO (Presenter), Univ of Tokyo, HOI CHUN PO, Massachusetts Institute of Technology, HARUKI WATANABE, Univ of Tokyo — Topological superconductors are exotic phases of matter featuring robust surface states that could be leveraged for topological quantum computation. A useful guiding principle for the search of topological superconductors is to relate the topological invariants with the behavior of the pairing order parameter on the normal-state Fermi surfaces. The existing formulas, however, become inadequate for the prediction of the recently proposed classes of topological crystalline superconductors. In this work, we advance the theory of symmetry indicators for topological (crystalline) superconductors to cover all space groups. Our main result is the exhaustive computation of the indicator groups for superconductors under a variety of symmetry settings.


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HCP is supported by a Pappalardo Fellowship at MIT and a Croucher Foundation Fellowship. 
HW is supported by JSPS KAKENHI Grant No. JP17K17678 and by JST PRESTO Grant No. JPMJPR18LA.
4:18PM U55.00008: Emergent spacetime and gravitational Nieh-Yan anomaly in chiral Weyl superfluids and superconductors* JAAKKO NISSINEN (Presenter), Low Temperature Laboratory, Department of Applied Physics, Aalto University — Momentum transport in topological Weyl superfluids (and superconductors) is anomalous in the presence of textures and superflow. Using the semi-classical approximation and gradient expansion, the gauge and Galilean symmetries of the system induce via the superfluid hydrodynamics an emergent "Riemann-Cartan" spacetime with torsion and curvature for the low-energy Weyl quasiparticles. Furthermore, the background exhibits local conservation laws corresponding to emergent quasi-relativistic Lorentz symmetry. We show that the momentum anomaly can be given a consistent interpretation as the chiral Nieh-Yan gravitational anomaly experienced by Weyl fermions on the emergent curved spacetime. The coefficient of this anomaly term is not universally quantized and seems to be determined by the underlying non-relativistic Fermi-liquid and Galilean symmetries. Finally, the connection and extension of the emergent spacetime to finite temperature corrections and thermal effects will be discussed.

*This work has been supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant Agreement No. 694248)

4:30PM U55.00009: Weyl-superconductor phases in the multilayer model of Weyl semimetals and superconductors RYOTA NAKAI (Presenter), KENTARO NOMURA, Tohoku University — We study the superconducting proximity effect in the bulk of Weyl semimetals by considering a multilayer structure consisting of alternating Weyl-semimetal and superconductor (WSM-SC) layers. Our model realizes Weyl-superconductor phases with 2 or 4 nodes of the Majorana fermion, and (2d) topological-superconductor phases characterized by half-odd-integer and integer Chern numbers. We found that potential barriers at the interface and/or mismatch of the Fermi velocity favor topological-superconductor phases with half-odd integer Chern numbers, while Weyl-superconductor phases with 4 nodes and topological-superconductor phases with integer Chern numbers are realized when the Fermi velocity coincides. Topological-superconductor phases are characterized by the quantization of the thermal Hall conductivity, and Weyl-superconductor phases by continuously varying thermal Hall conductivity determined by the position of nodes.

4:42PM U55.00010: Edge current and orbital angular momentum of chiral superfluids revisited WENXING NIE (Presenter), Sichuan University, WEN HUANG, Southern University of Science and Technology, HONG YAO, Institute for Advanced Study, Tsinghua University — Cooper pairs in chiral superfluids carry quantized units of orbital angular momentum (OAM). Various predictions of the total OAM of a chiral superfluid differ by several orders of magnitude. These constitute the so-called angular momentum paradox. Following several previous studies, we substantiate the semiclassical Bogoliubov-de Gennes theory of the edge current and OAM in two-dimensional chiral superfluids in the BCS limit. The analysis provides a simple intuitive understanding for the vanishing of OAM in a non-p-wave chiral superfluid (such as d+id) confined by a rigid potential. When generalized to anisotropic chiral superconductors and three-dimensional (3D) chiral superfluids, the theory similarly returns an accurate description. We will also present a numerical study of the chiral phases in the BEC limit, where the OAM density is found to vanish in the bulk and arise purely from the boundary effects.
4:54PM U55.00011: Vortices in a Monopole Superconducting Weyl Semi-metal*  SHU-PING LEE (Presenter), CANON SUN, YI LI, Johns Hopkins University — A monopole superconductor is a novel topological phase of matter with topologically protected gap nodes that result from the non-trivial Berry phase structure of Cooper pairs. In this work we study the zero-energy vortex bound states in a model of a monopole superconductor based on a time-reversal broken Weyl semi-metal with proximity-induced superconductivity. The zero modes exhibit a non-trivial phase winding in real space as a result of the non-trivial winding of the order parameter in momentum space. By mapping the Hamiltonian to the $(1 + 1)d$ Dirac Hamiltonian, it is shown that the zero modes, analogous to the Jackiw-Rebbi mode, are protected by the index theorem.

*This work is supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331 and in part by the Alfred P. Sloan Research Fellowships under grant FG-2018-10971 and the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4305.

5:06PM U55.00012: Majorana Kramers Pairs in Higher-Order Topological Insulators*  CHEN-HSUAN HSU (Presenter), PETER STANO, Center for Emergent Matter Science, RIKEN, JELENA KLINOVAJA, DANIEL LOSS, Department of Physics, University of Basel — We propose a tune-free scheme to realize Majorana bound states using higher-order topological insulators [1]. When two hinges of a higher-order topological insulator nanowire are brought into the proximity of an $s$-wave superconductor, two types of pairings arise, one being local (intra-hinge) pairing and the other nonlocal (inter-hinge) pairing. We find that, the competition between these pairings leads to a topological phase transition. The energy band is inverted in the regime where the nonlocal pairing dominates over the local one, leading to the formation of a Kramers pair of Majorana bound states at each end of the nanowire. We show that this topological condition can be fulfilled in the presence of moderate electron-electron interactions, without fine-tuning system parameters such as external magnetic fields.


*We acknowledge financial support from the JSPS Kakenhi (Grant No. 16H02204 and No.19H05610), the Swiss National Science Foundation (Switzerland), the NCCR QSIT, and the European Unions Horizon 2020 research and innovation program (ERC Starting Grant, Grant Agreement No. 757725).
5:18PM U55.00013: Topology-Bounded Superfluid Weight in Twisted Bilayer Graphene
FANG XIE (Presenter), ZHIDA SONG, BIAO LIAN, ANDREI BERNEVIG, Princeton University — We derive the superfluid weight (phase stiffness) of the TBLG superconducting flat bands with a uniform pairing, and show that it can be expressed as an integral of the Fubini-Study metric of the flat bands. This mirrors results [1] already obtained for nonzero Chern number bands even though the TBLG flat bands have zero Chern number. We further show the metric integral is lower bounded by the topological C2zT Wilson loop winding number of the TBLG flat bands, which renders the superfluid weight has a topological lower bound proportional to the pairing gap. In contrast, trivial flat bands have a zero superfluid weight. The superfluid weight is crucial in determining the BKT transition temperature of the superconductor. Based on the transition temperature measured in TBLG experiments, we estimate the topological contribution of the superfluid weight in TBLG.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U56 DCMP: SmB6 and Kondo Insulators Mile High Ballroom 2C - Xiaxin Ding, Idaho National Laboratory

2:30PM U56.00001: Kondo holes break topological protection of heavy Dirac fermions in SmB6* HARRIS PIRIE (Presenter), YU LIU, Harvard University, ERIC MASCOT, University of Illinois at Chicago, PENGCHENG CHEN, Harvard University, SHANTA SAHA, XIANGFENG WANG, JOHNPIERRE PAGLIONE, University of Maryland, College Park, MOHAMMAD H HAMIDIAN, Harvard University, CYRUS F. HIRJIBEHEDIN, University College London, UK, DIRK KLAUS MORR, University of Illinois at Chicago, JENNIFER E. HOFFMAN, Harvard University — The interplay of magnetism and strongly correlated topology is expected to generate exotic quantum phenomena. SmB6 is a leading platform, as it was recently shown to host heavy Dirac surface states that form within a screened Kondo lattice [1]. In conventional heavy fermion materials, it is well known that local magnetic structure is nucleated by Kondo holes—substitutions on the f-electron contributing lattice. If the same mechanism exists in the topological counterparts to these systems, Kondo holes would provide a local gauge of the impact of magnetism on the emergent heavy Dirac fermions. However, current experimental techniques to image the microscopic signature of a Kondo hole are challenging, and require tracking the complex heavy fermion band structure. Here, we introduce electrochemical potential imaging spectroscopy to directly visualize the impact of Kondo holes from the liberation of screening electrons around them. In SmB6, we discover that Sm-site defects create Kondo holes that locally break topological protection, allowing backscattering of heavy Dirac fermions.


*This work was supported by NSF DMR-1410480, DOE DE-FG02-05ER46225, AFOSR FA9550-14-1-0332, and Gordon and Betty Moore Foundation grant 4536 and 4419.
Electronic transport in the Kondo insulator SmB$_6$ is dominated at low temperatures by a surface state, which could arise as a consequence of a non-trivial topology of its bulk electronic structure. At ambient pressure, our thermopower measurements have suggested the surface states of SmB$_6$ to have a strongly enhanced effective mass, consistent with recent quasiparticle interference studies from STM. Pressure increases the hybridization between $f$- and conduction electrons eventually leading to a metallic state. Here we report thermopower measurements under pressure that illustrate that the Fermi energy of the surface state is unchanged as a function of pressure in the insulating regime. We discuss our results in consideration of Hall effect data that reveal a carrier density increase with increasing pressure.

*Work at Los Alamos was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering. S.S. acknowledges a Directors Postdoctoral Fellowship through the Laboratory Directed Research & Development program.
A Resonant Inelastic X-ray Scattering investigation of the 4f states in SmB$_6$*  ANDREA AMORESE (Presenter), OLIVER STOCKERT, Max Planck Institute for Chemical Physics of Solids, KURT KUMMER, NICHOLAS B BROOKES, European Synchrotron Radiation Facility, DAE-JONG KIM, ZACHARY FISK, Department of Physics and Astronomy, University of California, Irvine, MAURITS HAVERKORT, Institute for Theoretical Physics, Heidelberg University, PETER THALMEIER, LIU HAO TJENG, Max Planck Institute for Chemical Physics of Solids, ANDREA SEVERING, Institute of Physics II, University of Cologne — The crystal-field (CF) splitting of the $^6H_{5/2}$ Hund's rule ground state of Sm$^{3+}$ in the strongly correlated topological insulator SmB$_6$ [1,2] has been determined with high resolution resonant inelastic x-ray scattering (RIXS) at the Sm M$_5$ edge [3]. The valence selectivity of RIXS allows to isolate the crystal-field-split excited multiplets of the Sm$^{3+}$(4f$^5$) configuration from those of Sm$^{2+}$(4f$^6$) in intermediate valent SmB$_6$. We find that the quartet G$_8$ ground state [4] and the doublet G$_7$ excited state are split by $D_{CF}=20\pm10$meV. Considering this as an upper limit for the 4f bandwidth suggests an extremely large mass renormalization from the band structure value, which can be linked to the small coefficient of fractional parentage for the hopping of the 4f electrons [5]. The tiny band width complies with the small value of the gap and may be used to put constraints to the energies of the topological surface states.


*Financial support of the DFG under grant SE-1441/4-1 is acknowledged
3:06PM U56.00004: A Parameter-free Study of the Magnetic and Electronic Structure of the Topological Heavy-fermion Compound SmB$_6^*$  RUIQI ZHANG (Presenter), Tulane University, BAHADUR SINGH, CHRISTOPHER LANE, Northeastern University, JAMIN KIDD, YUBO ZHANG, Tulane University, BERNARDO BARBIELLINI, Lappeenranta University of Technology, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern University, JIANWEI SUN, Tulane University — We revisit the highly debated mixed-valence compound SmB$_6$, which has been widely studied in both theory and experiment. One outstanding challenge is the difficulty in obtaining accurate theoretical band structures of SmB$_6$ as the starting point for further theoretical studies. We report new first-principles electronic-structure results, finding a band structure in agreement with experiments, wherein the correct crystal field splitting of $f$ electrons is captured by considering magnetic configurations. Intermediate valency and the right ground state symmetry are also captured in our calculations. The energies for each magnetic ordering are extremely close, indicating that SmB$_6$ exhibits spin fluctuations. Moreover, our results confirm that SmB$_6$ is a robust Kondo topological insulator due to its strong $d$ and $f$ band hybridization. Our study paves the way for future mean-field theory investigations of electronic and atomic structures, phase diagrams, and band topology of $f$-electron systems and other complex materials.

*Work supported by DOE under grant DE-SC0012575

3:18PM U56.00005: Conductive dislocation lines in SmB$_6$ observed through microwave impedance microscopy* KEJUN XU (Presenter), Stanford University, JING XIA, University of California, Irvine, JAN ZAANEN, Leiden University, ZHIXUN SHEN, Stanford University — SmB$_6$ is a candidate for an important class of topological insulator arising from strong correlations. Transport studies suggest surface-dominated transport at low temperatures [1]. Photoemission also revealed 2D in-gap states [2], however the topological nature of these states are under debate [3]. Here we use scanning microwave impedance microscopy to reveal conductive dislocation lines that terminate at step edges of the SmB$_6$ surface. Temperature dependence show that these states persist up to high temperatures beyond any Kondo energy scale. These observations reveal an important conduction channel that must be taken into account for transport studies. Further studies are desired to probe the topological nature of these 1D dislocation states.


*This work is supported by the Gordon and Betty Moore foundation, the National Science Foundation, and US DOE.
3:30PM U56.00006: Electrical Transport Properties of SmB$_6$ Nanowires*  SUJOY GHOSH
(Presenter), SEAN THOMAS, YEONHOO KIM, FILIP RONNING, ERIC BAUER, JINKYOUNG YOO,
PRISCILA ROSA, Los Alamos National Laboratory — Strongly correlated electron systems based on
rare-earth elements have attracted a great deal of interest in the last few decades due to their
emergent properties, such as valence fluctuations, metal–insulator transitions and heavy-fermion
superconductivity near the quantum critical point. Among these, SmB$_6$ is a topological Kondo
insulator candidate, an ideal platform to investigate the interplay between topology and strong
interactions as well as possible exotic quasiparticles, such as Majorana fermions. In this
presentation, I will talk about our recent experimental efforts on the synthesis and
characterization of SmB$_6$ nanowires prepared via a low-temperature reaction. I will further
discuss the electrical transport properties of these nanowires under different temperatures and
magnetic fields.

*Acknowledgments: Work at Los Alamos was performed under the auspices of the U.S.
Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and
Engineering. SG and PFSR acknowledge support from the Laboratory Directed Research and
Development program under Grant No. 20190076ER.

3:42PM U56.00007: Synthesizing SmB$_6$ single crystals by various techniques  SHANTA SAHA
(Presenter), Maryland Quantum Materials Center, Department of Physics, University of Maryland College
Park, LUCAS WILLIAM, MagLab Tallahassee, WESLEY T FUHRMAN, YUN SUK EO, Maryland Quantum
Materials Center, Department of Physics, University of Maryland College Park, RYAN BAUMBACH, MagLab
Tallahassee, JOHNPIERRE PAGLIONE, Maryland Quantum Materials Center, Department of Physics,
University of Maryland College Park — Samarium Hexaboride (SmB$_6$), a mixed valence Kondo
insulator, has attracted much recent attention due to the discovery of a low temperature
conducting surface state, proposed to be a topologically protected surface state that arises due
to the formation of a Topological Kondo insulator state. To date, single crystals of SmB$_6$ have
only been synthesized by ‘aluminum flux’ and ‘floating zone’ methods, mainly due to the high
melting point of boron. Recently, quantum oscillations were observed in the both type of crystals,
but intrinsic origins of those findings are controversial due to possible extrinsic origins such as
aluminum inclusions. Therefore, growing single crystals using alternative methods is considered
important for elucidating the intrinsic electronic properties of SmB$_6$. We will discuss efforts to
produce SmB$_6$ single crystals by radiofrequency (RF) technique and by flux growth methods
using alternative fluxes, comparing the results of various techniques.
3:54PM U56.00008: Revisiting Hall coefficient measurements in samarium hexaboride*
ALEXA RAKOSKI (Presenter), Department of Physics, Univ of Michigan - Ann Arbor, YUN SUK EO, Center for Nanophysics and Advanced Materials, University of Maryland, DMITRI MIHALIOV, CAGLIYAN KURDAK, Department of Physics, Univ of Michigan - Ann Arbor, PRISCILA ROSA, Los Alamos National Laboratory, ZACHARY FISK, Department of Physics and Astronomy, University of California Irvine, BOYOUN KANG, MYUNG-SUK SONG, BEONGKI CHO, Gwangju Institute of Science and Technology, MONICA CIOMAGA HATNEAN, GEETHA BALAKRISHNAN, Department of Physics, University of Warwick — Samarium hexaboride is a correlated material in which strong f-d interactions open a small gap at the Fermi energy below ~100 K. In transport, SmB$_6$ demonstrates activated behavior down to ~4 K, terminated by a conduction mechanism attributed to the emergence of a topological surface state. We present a study of transport, especially Hall coefficient, from three perspectives. First, we discuss a method of analyzing Hall data at low temperatures, allowing for accurate extraction of mobility from the conductive surface. Next, we re-examine a well-known high-temperature feature in Hall data: the sign change from negative to positive as temperature is raised above ~65 K. This sign change has been attributed to skew scattering due to the strong f-d interactions, but it leads to an inaccurate determination of carrier density and mobility. We discuss a method to improve the accuracy of transport analysis that relies on ARPES data at high temperature to correct for the positive Hall sign. Finally, we present a method of carving a micron-sized Hall bar from SmB$_6$ to investigate the effect of sample size on transport parameters. Taken together, these results aim to provide a summary of current transport perspectives on SmB$_6$.

*Funding for this work was provided by NSF Grant No. DGE-1256260.

4:06PM U56.00009: Properties of the donor impurity band in mixed valence insulators
BRIAN SKINNER (Presenter), Ohio State Univ - Columbus — In traditional semiconductors with large effective Bohr radius, an electron donor creates a hydrogen-like bound state just below the conduction band edge. The properties of the impurity band arising from such hydrogenic impurities have been studied extensively during the last 70 years. Here I consider whether a similar bound state and a similar impurity band can exist in mixed valence insulators, such as SmB$_6$ and YbB$_{12}$. I show that the structure of the hybridized conduction band leads to an unusual bound state that can be described using the physics of the one-dimensional hydrogen atom. The properties of the resulting impurity band are consequently modified in a number of ways relative to the traditional semiconductor case; most notably, the impurity band can hold a much larger concentration without inducing an insulator-to-metal transition. I give an estimate of the DC and AC conductivities and specific heat associated with the impurity band, and show that they are consistent with experiments on SmB$_6$. 
4:18PM U56.00010: Topological surface state of Kondo insulator YbB$_{12}^*$ YUKI SATO

(Presenter), SHIGERU KASAHARA, YUICHI KASAHARA, Department of Physics, Kyoto University, ZIJI XIANG, COLIN B TINSMAN, LU CHEN, LU LI, Department of Physics, University of Michigan, TAKASADA SHIBAUCHI, Advanced Materials Science, University of Tokyo, FUMITOSHI IGA, Institute for Quantum Beam Science, Ibaraki University, JOHN SINGLETON, Los Alamos National Laboratory, NITYAN NAIR, NIKOLA MAKSIMOVIC, JAMES ANALYTIS, Department of Physics, University of California, Berkeley, YUJI MATSUDA, Department of Physics, Kyoto University — YbB$_{12}$ is a Kondo insulator which is theoretically predicted to host metallic surface states arising from the nontrivial band structure. Recent observation of quantum oscillations (QOs) in YbB$_{12}$ arouses great interest since it may indicate a Fermi surface in an insulator phase. The most important subject is to clarify whether the QOs arise from insulating bulk or metallic surface. Here we fabricated micro-devices of YbB$_{12}$ using focused ion beam technique and measured transport properties in high fields. All of the samples fabricated by FIB and mechanical polishing exhibit resistivity plateaus at low temperatures and residual resistivity decreases linearly as a function of thickness. These results provide evidence of 2D surface conduction in YbB$_{12}$. We also find the device shows positive and quasi-linear $H$-dependent magnetoresistance, which is attributed to the anti-weak localization of the surface electrons with spin-momentum locking. No discernible QOs are observed in this device, suggesting the QOs in single crystals arise from insulating 3D bulk.

*This work is supported by Overseas Challenge Program for Young Researchers, Grants-in-Aids for Science Research (KAKENHI) (Nos. 18J22138, 18H01177, 18H05227) and Innovative Areas "Topological Material Science" (No. 15H05852) from JSPS.

4:30PM U56.00011: Field-induced “exotic metal” phase in Kondo insulator YbB$_{12}$ ZIJI XIANG

(Presenter), Univ of Michigan - Ann Arbor, YUICHI KASAHARA, Department of Physics, Kyoto University, LU CHEN, TOMOYA ASABA, Univ of Michigan - Ann Arbor, YUKI SATO, Department of Physics, Kyoto University, COLIN B TINSMAN, Univ of Michigan - Ann Arbor, FUMITOSHI IGA, College of Science, Ibaraki University, JOHN SINGLETON, Los Alamos National Laboratory, YUJI MATSUDA, Department of Physics, Kyoto University, LU LI, Univ of Michigan - Ann Arbor — YbB$_{12}$, a representative Kondo insulator, has attracted attention in recent years as it exhibits Shubnikov-de Haas effect in intense magnetic fields. With the magnetic field further increasing, YbB$_{12}$ goes through an insulator-to-metal transition. We systematically studied the high field metallic phase in YbB$_{12}$ in pulsed magnetic fields. The temperature dependence of the resistivity in this phase reveals a crossover from non-Fermi-liquid behavior above 4 K to Fermi-liquid-like behavior below 2 K. The low-temperature state also shows unusually large Kadowaki-Woods ratio. Results of the proximity detector oscillator measurements provide evidences that the electronic structure of YbB$_{12}$ in the metallic phase depends on both the strength and the orientation of external magnetic fields.
4:42PM U56.00012: Magnetic Field Induced Fermi Liquid In a Candidate Topological Kondo Insulator

SATYA KUSHWAHA (Presenter), MUN K. CHAN, JOONBUM PARK, SEAN THOMAS, ERIC BAUER, JOE D THOMPSON, FILIP RONNING, PRISCILA ROSA, NEIL HARRISON, Los Alamos National Laboratory — Kondo insulators are expected to undergo an insulator-to-metal phase transition under strong magnetic fields. We show that Ce$_3$Bi$_4$Pd$_3$ is a narrow gap Kondo insulator. Our high magnetic pulse-field transport and magnetization experiments reveal the destruction of Kondo coupling and the closing of the Kondo gap at a critical magnetic field, $B_c \approx 11$ T. A Fermi liquid state emerges for fields beyond $B_c$, with a decrease in electronic correlations.


4:54PM U56.00013: First-principles study of band topology for $f$-electron materials: Ce$_3$(Pt/Pd)$_3$Bi$_4$$^*$

JAMIN KIDD (Presenter), RUIQI ZHANG, JIANWEI SUN, Tulane Univ — Recent density functional theory (DFT) calculations on the proposed topological Kondo insulator SmB$_6$ using the newly developed SCAN functional have yielded valence $f$-band splitting consistent with experiment, as well as band hybridization and $Z_2$ indices for the paramagnetic phase by following a symmetry analysis of the periodic Anderson Kondo lattice Hamiltonian.$^1$ Motivated by these promising results, we apply the SCAN functional to study the ternary Ce$_3$(Pt/Pd)$_3$Bi$_4$ systems, a new family of candidates for strongly correlated topological materials. While the Pt-based (Pd-based) compound has been predicted to be a Kondo insulator (Kondo semimetal), the topological properties of both systems are still under debate.$^{2,3}$ Here, we consider the local magnetic moment of Ce atoms and calculate the electronic structures for typical magnetic configurations. We then identify the topological phases present in both materials by calculating the appropriate invariants and comparing our results to previous experiments.

References:

1. Dzero et al., PRL 104, 106408.
2. Dzsaber et al., PRL 118, 246601.

*We acknowledge the support of the American Chemical Society Petroleum Research Fund and the Tulane University Center for Engaged Learning and Teaching.
5:06PM U56.00014: Optical Properties of Kondo Insulators*  ARI WUGALTER (Presenter), YASHAR KOMIJANI, PIERS COLEMAN, Physics & Astronomy, Rutgers, The State University of New Jersey — This talk will discuss the optical properties of Kondo insulators, including the dielectric constant and magnetic permeability. Using a large-N Abrikosov fermion representation in a treatment of a Kondo lattice model, we show that the dielectric constant is determined by the squared ratio of the plasma frequency to the direct gap, predicting dielectric constants of order 1000, diffractive indices of order 30. By treating the magnetic correlations of the f-electrons as a gapless spin-liquid, described by dispersing f-electrons coupled to a gauge field we derive an effective model for the gauge fields which includes a continuum of excitations as well as a hybridization between the external electro-magnetic gauge field and the emergent gauge field. The gradient expansion of the effective model predicts a massless `light’ mode and a massive Higgs mode. The observation of this Higgs mode would provide an interesting opportunity to establish the presence of spin fractionalization and emergent gauge fields in Kondo insulators.

*This work is supported by the NSF grant DMR-1830707.

5:18PM U56.00015: Interplay between magnetism and topology in Kondo Insulators*  DAVID RIEGLER (Presenter), MICHAEL KLETT, University of Wuerzburg, SEULGI OK, TITUS NEUPERT, University of Zurich, PETER K WOELFLE, Karlsruhe Institute of Technology, RONNY THOMALE, University of Wuerzburg — Topological Kondo insulators are a rare example of an interaction-enabled topological phase of matter, making them an intriguing but also hard case for theoretical studies. Here, we investigate the periodic Anderson model with the addition of spin orbit coupling via a fully spin-rotation invariant slave-boson treatment. Within mean-field approximation we map out the magnetic phase diagram and characterize both antiferromagnetic and paramagnetic phases by their topological properties. Moreover, we establish the stability of the mean-field solution via Gaussian fluctuations around the saddle point by the computation of the dynamical susceptibility.

*DFG-SFB 1170

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U57 DMP: Charge Density Waves, Excitonic and Correlated States in Two-Dimensional Materials and Semimetals  Frederic Joucken, University of California, Santa Cruz - Mile High Ballroom 3A - Tag(s): Focus
Mott insulating behaviors in few-layer 1T-TaSe$_2$  

SIQI WANG (Presenter), SUI YANG, University of California at Berkeley, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, KAI ROSSNAGEL, Kiel University, XIANG ZHANG, University of California at Berkeley — Material systems with strong electron correlation may exhibit exotic properties in stark contrast to conventional Fermi liquid. Among them, Mott insulators continue to attract tremendous research interest due to its close relation with unconventional superconductors and quantum spin liquids. Recent advances in layered van der Waals materials provide a novel material family which intrinsically has great in-situ tunability and therefore may act as a versatile quantum simulator for complicated systems. While the low temperature insulating phase with commensurate charge density wave (CCDW) order of the two-dimensional (2D) material 1T-TaS$_2$ has been ascribed to a Mott insulator, recent work casts doubt on this identification by considering the vertical stacking order of 2D CDWs. On the other hand, the CCDW phase in question was reported to be fragile towards mechanical exfoliation, hindering direct characterization in atomic-layer limit. Here we present electrical transport characterization of few-layer 1T-TaSe$_2$, a ‘sibling’ material with simpler phase diagram and more robust CCDW order. Our results provide evidence of Mott insulating behaviors in this long-thought trivial metal, thus hinting at an ideal platform for the investigation of strongly correlated physics in 2D systems.

Excitonic insulator in MoS$_2$ under pressure  

SAMANEH ATAEI, DANIELE VARSANO, Istituto Nanoscienze, CNR, DAVIDE SANGALLI, FLASHit, CNR-ISM, ELISA MOLINARI, FIM, University of Modena, MASSIMO RONTANI (Presenter), Istituto Nanoscienze, CNR — Among correlated insulators, a fascinating paradigm applies to narrow-gap semiconductors, whose low-energy excitations are pairs of electron ($e$) and hole ($h$) bound by Coulomb attraction, the excitons. If the binding energy overcomes the gap, then excitons spontaneously condense at thermodynamic equilibrium—similarly to Cooper pairs in a superconductor—giving rise to the ‘excitonic insulator’ (EI). Crucially, breakthrough reports [1] of the EI in transition metal dichalcogenides could not assess at which extent the condensation of $eh$ pairs was due to the formation of bound excitons or to the softening of the phonon responsible of the observed structural change. Here, by means of many-body perturbation theory from first principles, we demonstrate that MoS$_2$ at high pressure is prone to the condensation of genuine excitons of finite momentum, whereas the phonon dispersion remains regular. The self-consistent electronic charge density of the EI sustains an out-of-plane permanent electric dipole moment with an in-plane anti-ferroelectric texture. At the onset of the EI phase, those optical phonons that share the exciton momentum are folded to the zone center, providing a unique Raman fingerprint that has been observed but not explained yet.

2:54PM U57.00003: Geometric Frustration in a Monolayer TMD Alloy* MEHMET DOGAN (Presenter), AMIN AZIZI, JEFFREY D. CAIN, RAHMATOLLAH ESKANDARI, XUANZE YU, EMILY C GLAZER, ALEX ZETTL, MARVIN L COHEN, University of California, Berkeley — Geometric frustration occurs when the constituent interactions of a system cannot be simultaneously satisfied due to the underlying geometry. In an idealized frustrated system, long-range order is prevented, and degenerate ground-states with short-range order are observed, leading to extensive entropy at 0 K. In real materials, higher-order effects can lead to relieving of frustration, allowing long-range order to appear. Here, we directly observe frustrated ordering of the atomic species in a monolayer transition metal dichalcogenide (TMD) alloy, using scanning transmission electron microscopy (STEM). We find that this system is analogous to the 2D Ising model of antiferromagnetic spins in a triangular lattice, and long-range order is thoroughly suppressed. Using density functional theory, we build a lattice model that closely matches the statistical properties of the experimental atomic distribution. We also demonstrate the effects of atomic ordering on the band structure. We predict that the degree of ordering can be controlled by the growth temperature, allowing the tuning of the electronic, optical and thermal properties.

*This work was supported by the Department of Energy under Contract No. DE-AC02-05-CH11231, and the National Science Foundation under Grant #DMR1508412.

3:06PM U57.00004: van der Waals tunneling spectroscopy of WTe2 monolayer* YANYU JIA (Presenter), PENGJIE WANG, GUO YU, MICHAEL ONYSZCZAK, F. ALEXANDRE CEVALLOS, SHIMING LEI, SEBASTIAN KLEMEZ, BERTHOLD JAECK, Princeton University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, LESLIE SCHOOP, ROBERT J. CAVA, ALI YAZDANI, SANFENG WU, Princeton University — The discovery of superconducting and quantum spin Hall (QSH) states in the single layer WTe2 opens up new possibilities of engineering correlated topological quantum matter based on 2D crystals. In this talk, I will introduce a tunneling device geometry based on van der Waals heterostructures to perform spectroscopic studies of monolayer WTe2. The visualization of gate-induced changes in the monolayer's electronic structure will be discussed.

*This research was supported by NSF through the Princeton University Materials Research Science and Engineering Center DMR-1420541
3:18PM U57.00005: Anisotropic conductivity in monolayer WTe$_2$  
BOSONG SUN (Presenter), PAUL MALINOWSKI, ZAIYAO FEI, WENJIN ZHAO, University of Washington, TAUNO PALOMAKI, Sandia National Laboratory, XIONG HUANG, University of California, Reverside, ELLIOTT RUNBURG, University of Washington, YONGTAO CUI, University of California, Reverside, JIUN-HAW CHU, XIAODONG XU, DAVID COBDEN, University of Washington — The layered semimetal WTe$_2$ behaves in the monolayer limit as a topological insulator but the nature of the insulating state in the interior bulk is unclear. We study its conductivity as a function of gate doping, temperature, and current direction. Care is needed to eliminate helical edge conduction from the measurements, including along cracks, which we locate by microwave impedance microscopy. The conductivity is found to be highly anisotropic for hole doping and much less so for electron doping. Surprisingly, for hole doping the conductivity is about three times lower along the a-axis, the direction of the tungsten chains, than along the b-axis, perpendicular to the chains. We consider the implications of this observation for the possibility that the state is a kind of excitonic insulator.

3:30PM U57.00006: Probing correlated states in WTe$_2$ devices*  
PENGJIE WANG (Presenter), GUO YU, YANYU JIA, MICHAEL ONYSZCZAK, SHIMING LEI, SEBASTIAN KLEMENZ, F. ALEXANDRE CEVALLOS, Princeton University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ROBERT J. CAVA, LESLIE SCHOOP, SANFENG WU, Princeton University — Interesting behaviors, such as quantum spin Hall effect, superconductivity, non-linear Hall effect, and ferroelectricity have been observed in atomically thin tungsten ditelluride (WTe$_2$). We introduce a new device geometry to further probe the intrinsic electronic response of two-dimensional WTe$_2$. In this talk, we will report our recent transport studies on these new devices, in search of exotic correlated states.

*This research was supported by NSF through the Princeton University Materials Research Science and Engineering Center DMR-1420541.
We introduce a novel topological class of superconducting and density-wave states which exhibit monopole harmonic symmetry. This so-called “monopole harmonic order” can be realized in interacting Weyl semimetal materials. Generally, when two Fermi surfaces carry different Chern numbers, the many-body ordering between these two Fermi surfaces can exhibit a non-trivial Berry phase inherited from band structure topology. In contrast to other known many-body order, the total vorticity of the ordering gap nodes in momentum space is determined by the monopole charge of the pair Berry phase and is independent of specific ordering mechanisms. Connections to experimental realizations and signatures of monopole harmonic superconductivity and monopole harmonic charge-density-wave states are proposed.

1. Yi Li and Haldane, “Topological Nodal Cooper Pairing in Doped Weyl Metals”, Phys. Rev. Lett. 120, 067003 (2018);

*This work is supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331 and by the NSF CAREER grant DMR-1848349, and in part by the Alfred P. Sloan Research Fellowships under grant FG-2018-10971 and the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4305.
Layer-dependent charge density wave in few layer VSe$_2$ films

BYOUNG KI CHOI (Presenter), Department of Physics, University of Seoul, Republic of Korea, GANBAT DUVJIR, Department of Physics, University of Ulsan, Republic of Korea, SØREN ULSTRUP, Department of Physics and Astronomy, Aarhus University, Denmark, IN HAK LEE, HYUK JIN KIM, Department of Physics, University of Seoul, Republic of Korea, LY THI TRINH, Department of Physics, University of Ulsan, Republic of Korea, CHRIOS JOZWIAK, AARON BOSTWICK, ELI ROTENBERG, Lawrence Berkeley National Laboratory, JUNSDAE KIM, Department of Physics, University of Ulsan, Republic of Korea, YOUNG JUN CHANG, Department of Physics, University of Seoul, Republic of Korea — VSe$_2$ monolayer (ML) has recently attracted attention about charge ordering property in two-dimensional monolimit. Researches have been discussing the origin of charge ordering characteristic of VSe$_2$ ML and there is an inconsistent argument. We have reported two types of charge-ordering transitions in VSe$_2$ ML on graphene substrates. One is enhanced charge density wave (CDW) originated from bulk VSe$_2$ and one is metal-insulator transition (MIT) caused by interface effect between graphene and VSe$_2$ ML. In this presentation, we present layer dependent CDW properties in VSe$_2$ 1ML, 2ML and 3ML on graphene substrates. We will show depressed CDW effects with increasing number of layers. We will also discuss the MIT property of VSe$_2$ monolayer changing substrates and implications of interface effect between substrate and VSe$_2$ ML.

* [This work is published in Nano Letters 18, 5432 (2018). This work was supported by the Korean government (NRF-2018R1-D1A1B07050144, NRF-2019R1A6A1A11053838, NRF-2014R1-A4A1071686, and NRF-2017R1C1B2004927). The ALS is supported by the U.S. DOE under Contract No. DE-AC02-05CH11231.]

Evidence of charge density wave with anisotropic gap in monolayer VTe$_2$ film

YUAN WANG (Presenter), JUNHAI REN, JIAHENG LI, YUJIA WANG, HUINING PENG, PU YU, WENHUI DUAN, SHUYUN ZHOU, State Key Laboratory of Low Dimensional Quantum Physics and Department of Physics, Tsinghua University — We report experimental evidence of charge density wave (CDW) transition in monolayer 1T-VTe$_2$ film. Low energy electron diffraction (LEED) measurements reveal 4×4 reconstruction peaks below transition temperature. Angle-resolved photoemission spectroscopy (ARPES) measurements reveal arc-like pockets with anisotropic CDW gaps up to 50 meV. The anisotropic CDW gap is attributed to the imperfect nesting of the CDW wave vector, and first-principles calculations reveal phonon softening at the same vector. These results suggest the important roles of both Fermi surface nesting and electron-phonon interaction in the CDW mechanism of monolayer VTe$_2$ film.
4:42PM U57.00010: Ultrafast Electron Diffraction in Charge Density Wave State of TiSe$_2$*

PAUL XHORI (Presenter), ANTON ANIKIN, Physics, Drexel University, JACOB BOLDUC, Materials Science and Engineering, Drexel University, SHALIN PATEL, Physics, Drexel University, MAHER HARB, GORAN KARAPETROV, Physics and Materials Science and Engineering, Drexel University — We probe the ultrafast laser response in thin TiSe$_2$ single crystals below and above the CDW transition temperature using ultrafast electron diffraction. The electron-phonon dynamics is initiated by 150 fs pulses centered at 400 nm. While we observe a comparably fast initial diffraction intensity decay at room temperature, we do not observe any bi-exponential dynamics that was previously reported in the dynamics of <110> peaks at fluences above 1 mJ/cm$^2$ with 800 nm centered excitation. On the other hand, at temperatures below the CDW transition temperature bi-exponential dynamics is observed above the threshold fluence of 0.5 mJ/cm$^2$. This threshold fluence is more than two times larger than the threshold fluence for CDW melting with an 800 nm pump. Bi-exponential behaviour is linked to a strong electron-phonon coupling process followed by a slower electron-lattice equilibration. This shows the importance of the Jahn-Teller mechanism for charge density wave formation in TiSe$_2$. We will also present ultrafast electron diffraction results on Cu$_x$TiSe$_2$ single crystals.

*This work was supported by the National Science Foundation under Grant No. ECCS-1711015.

4:54PM U57.00011: The current-induced metastable CDW heterostructure in 2D 1T-TaS$_2$

MASARO YOSHIDA (Presenter), TAKURO SATO, RIKEN Center for Emergent Matter Science, FUMITAKA KAGAWA, YOSHIHIRO IWASA, Department of Applied Physics, The University of Tokyo — The layered 1T-TaS$_2$ is a showcase of electronic phases including complex charge density waves (CDWs), superconductivity, Mott insulator, and spin liquid. In addition to such thermodynamically stable phases, thermally inaccessible, persistent metastable metallic states can be induced by means of current [e.g.1]. We investigated the current-induced phase transition to the persistent metastable state by performing noise spectroscopy measurements [2]. We observed the emergence of a broadband noise at the transition, indicating the sliding motion of CDWs. Surprisingly, the dynamical property of the CDW was found to be preserved after the injection of current, although the electronic properties are significantly modified by the injection. It is likely that the CDW sheets slide to change their 3D structure, the stacking way, followed by the considerable change in electronic structure. We suggest that after the current injection, the CDW sheets stack in a metastable way that yields metallic electronic structure. Our discovery emphasizes the importance of the stacking degree of freedom, the concept of Van der Waals heterostructure, to create exotic electronic states in 2D material.

5:06PM U57.00012: Doping a Mott insulator at the lateral junctions of single layer 1H-1T NbSe$_2$* LIAN LI (Presenter), HUIMIN ZHANG, LIWEI LIU, Department of Physics and Astronomy, West Virginia University, ZHUOZHI GE, MICHAEL WEINERT, Department of Physics, University of Wisconsin-Milwaukee — At the single layer limit, transition metal dichalcogenides can adopt a variety of structural polymorphs with significantly different electronic properties. Here we report the selective growth of single layer 1T- and 1H-NbSe$_2$ on epitaxial graphene/SiC substrates by molecular beam epitaxy. Using a combination of scanning tunneling microscopy/spectroscopy and angle-resolved photoemission spectroscopy, we show that the 1H-NbSe$_2$ is metallic and exhibits a 3 by 3 charge density wave (CDW) at below 20K, while 1T-NbSe$_2$ is a Mott-insulator exhibiting a root 13 by root 13 CDW at room temperature. Furthermore, at the 1H-1T lateral junction, we observe a one-dimensional channel that is characterized by a V-shaped gap in tunneling spectroscopy. The spectra can be fitted by power law, similar to other substitutionally doped Mott insulators. Those finding suggests that lateral heterojunctions of different transition metal dichalcogenide polymorphs present an opportunity to engineer new quantum phases with emergent properties.

*This research is supported by NSF (DMR- DMR-1734017).

U57.00013: Infrared spectroscopy of few-layer excitonic insulator candidate Ta$_2$NiSe$_5$ CHAOYU SONG (Presenter), CHONG WANG, SHENYANG HUANG, HUGEN YAN, Fudan Univ — Ta$_2$NiSe$_5$ is proposed as an excitonic insulator, which has narrow direct bandgap and high transition temperature. In this talk, we will present our infrared spectroscopy study of few-layer Ta$_2$NiSe$_5$. In addition to the large anisotropic absorption peak at about 0.4 eV reported by many previous studies, a weak but clear excitation was newly found at lower frequency. It is possibly a signature of the electron correlation or from another electronic transition.

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U58 DCP DAMOP DLS DCMP: Ultrafast Spectroscopies and Coherent Phenomena in the X-ray Domain II Mile High Ballroom 3B - Michael Schuurman, Natl Research Council-Canada - Tag(s): Focus
2:30PM U58.00001: Ultrafast X-ray Molecular Dynamics* [Invited] STEPHEN R. LEONE
(Presenter), University of California, Berkeley — Transient absorption in the extreme ultraviolet and X-ray spectral regimes is used to probe molecular dynamics on both femtosecond and attosecond timescales. Laser-produced high-order harmonics are generated to use as the probe, while ultraviolet or visible pulses excite the molecular system by well-defined transitions. The method is used to investigate dissociating molecules, ring opening, passage through curve crossings and conical intersections, singlet-to-triplet transitions, and electronic and vibrational coherences. By extending the probe photon energies to 300 eV in the soft X-ray, carbon species are investigated to reveal atom-specific electronic orbitals during electronic transformations of organic molecules. Time domain measurements provide an assessment of multiple excited state products and key points along the reaction trajectories. Passage through curve crossings and conical intersections reveal distinct changes in electronic state character at the crossings, and shifts in core level spectroscopic features provide information on the changes in orbital energetics and occupancies, such as when bonds break. X-ray spectroscopic transitions of transient intermediate states are directly characterized. On ultrashort timescales, electronic and vibrational wave packet coherent dynamics are also observed. The results form the basis of an X-ray spectroscopic revolution in molecular dynamics, sensitive to electron state character.

*This work supported by the Department of Energy, the National Science Foundation, and the Army Research Office.

3:06PM U58.00002: Probing the ultrafast intermediate states of a divalent cobalt-manganese complex with femtosecond M-edge XANES* ELIZABETH RYLAND (Presenter), KAILI ZHANG, JOSH VURA-WEIS, Chemistry, University of Illinois at Urbana-Champaign — In this work we perform ultrafast transient M-edge XANES on divalent Cobalt-Manganese(N,N,N-tri(2-(2-pyridylamino)ethyl)amine)Cl, a heterobimetallic system with directly-interacting dual metal centers held within a non-innocent ligand scaffold. The strong metal-metal interaction facilitated by the ‘double-decker’ type ligand scaffold leads to a highly multiconfigurational electronic structure with relaxation pathways unavailable in monometallic analogues. With the ultrashort broadband probe pulse used in transient high-harmonic generation spectroscopy, we are able to perform M-edge XANES on both metal edges simultaneously with high specificity for each metal center and ligand environment. By combining transient XANES with transient UV-visible spectroscopy we can compile a full picture of the ultrafast electronic relaxation dynamics of this complex molecule. Photoinduced MM’CT is followed by distinct electronic dynamics at both metal edges and within the ligand scaffold, suggesting complex interplay of the Co, Mn, and ligand redox centers. Increased understanding of the relation of function to metal-specific photodynamics will help lay essential groundwork for the development of multimetallic catalysts with efficiencies comparable to those found in nature.

*AFOSR YIP
ACS PRF
Heme proteins are essential for respiration, neural transmission and biological signaling. The binding to and dissociation of small diatomic ligands (O₂, CO, NO, CN) from the Fe atom of the heme porphyrin represents the primary events of these processes. These can be mimicked by photodissociating them with a pulse of light and monitoring the recombination with a probe pulse. With the advent of XFELs, fs photon-in/photon-out experiments such as X-ray emission (XES), X-ray Raman scattering (XRS) and resonant-inelastic X-ray scattering (RIXS) have become possible that could never be achieved before due to their requirement for high fluxes and high temporal resolution.

We have investigated the case of Nitrosyl-Myoglobin (MbNO) in order to address crucial questions about the change from the planar low spin (LS) hexacoordinated heme configuration to the domed high spin (HS) pentacoordinated one. We excite the system into the Q-bands and probed its evolution by fs-XES using X-ray pulses from the SACLA, SwissFEL and European-XFEL free electron lasers. We found that the entire photocycle from planar to domed and back, after ligand recombination, is a series of spin cross-over (SCO) and back SCO events. We also investigated the most important electron transfer protein in our body, ferric cytochrome c, for which no ligand dissociation was ever reported, and therefore neither doming nor spin states. Here too we establish the photocycle as a SCO event, and propose that doming is crucial for the electron transfer properties of the protein, rather than heme ruffling as previously proposed.
Ultrafast X-Ray Absorption Spectroscopy as a Probe of Conical Intersection-Mediated Dynamics: Theoretical Tools and Studies [Invited]  SIMON NEVILLE (Presenter), National Research Council of Canada — Ultrafast time-resolved X-ray absorption spectroscopy (TRXAS) has emerged as a powerful tool for probing excited-state non-adiabatic molecular dynamics. Of particular interest is the sensitivity of TRXAS to the changes in valence electron density that occur as an excited-state wavepacket approaches a region of conical intersection between electronic states. In particular, the mixing of state characters in these high-coupling regions can be expected to modulate the amount of localisation of the valence electron density around the individual atomic centres, resulting in shifts in the core-orbital energies. Resultantly, shifts in the peaks in the TRXAS are expected to occur, which may be directly related to the non-adiabatic nuclear dynamics.

As the emergence of new light sources make excited-state TRXAS studies a reality, there is a need for accompanying theoretical simulations to enable a complete characterisation and understanding of the recorded spectra. In particular, rigorous, general, and tractable methods for the simulation of excited-state X-ray absorption spectra (XAS) are needed. Up until now, however, there has been a dearth of methods that can treat initial states of arbitrary character, while maintaining a low cost and black box usage. To address this issue, we have developed a new theoretical framework employing the core-valence separated combined DFT/MRCI method (CVS-DFT/MRCI). This is a method that is, perhaps, uniquely suited to the simulation of XAS for large molecules and initial states of multi-reference character, which are encountered in the vicinity of conical intersections.

In this talk, I will present recent studies using CVS-DFT/MRCI for the exploration of the sensitivity of TRXAS to conical-intersection-mediated dynamics in a range of molecules, ranging from the disentangling of competing relaxation pathways in allene to the Jahn-Teller effect-mediated dynamics in the graphene nanoflake coronene.
4:30PM U58.00005: RIXS within the coupled-cluster framework reveals the hidden transitions of transient species in ionized liquid water* KAUSHIK NANDA (Presenter), Department of Chemistry, University of Southern California, USA, LUDVIG KJELLSSON, JAN-ERIK RUBENSSON, Department of Physics and Astronomy, Uppsala University, Sweden, GILLES DOUMY, STEPHEN SOUTHWORTH, PHAY J HO, ANNE M MARCH, ANDRE AL HADDAD, YOSHIKAI KUMAGAI, MING-FENG TU, Chemical Sciences and Engineering Division, Argonne National Laboratory, USA, MUHAMMAD SHAFIQ MOHD YUSOF, TUSHAR DEBNATH, Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore, CAROLINE ARNOLD, RALPH WELSCH, LUDGER INHESTER, ROBIN SANTRA, Center for Free-Electron Laser Science, DESY, Germany, MARC SIMON, Sorbonne Université and CNRS, Laboratoire de Chimie Physique-Matière et Rayonnement, France, WILLIAM F SCHLOTTER, STEFAN MOELLER, GIACOMO COSLOVICH, JAKE KORELEK, DANIEL DEPONTE, LCLS, SLAC National Accelerator Laboratory, USA, ZHIHENG LOH, Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore, ANNA KRYLOV, Department of Chemistry, University of Southern California, USA, LINDA YOUNG, Chemical Sciences and Engineering Division, Argonne National Laboratory, USA — X-ray spectroscopies such as resonant inelastic X-ray scattering (RIXS) expand our ability to investigate the chemical structure and dynamics; in particular, when augmented with reliable theoretical tools. Computing the RIXS spectra, however, is challenging; primarily due to the difficulties in computing the underlying core-excited virtual states that are embedded inside the valence-ionization continuum in a converged fashion. We will present a novel electronic structure method within the equation-of-motion coupled cluster framework that facilitates converged calculations of the RIXS spectra for both closed- and open-shell species. We will illustrate the capabilities of our approach by measuring its performance in modeling the RIXS spectrum of the transient aqueous OH radical formed in ionized liquid water against experiments. We will provide orbital characterization of the distinct peaks in the RIXS spectrum of the OH radical for absorption below water's absorption edge. We will provide ab initio explanation of why the intermolecular charge-transfer transitions of aqueous OH radical, that are dominant in UV-visible spectrum, are suppressed in RIXS revealing the hidden localized valence transition.

*This work was supported by the U.S. National Science Foundation (No. CHE-1856342).
The emergence of X-FELs has meant that our ability to probe ultrafast structural dynamics is becoming increasingly common. Importantly, the combined structural, electronic and spin information contained within X-ray spectroscopy offers new perspectives for understanding the correlated dynamics of these degrees of freedom within the femtosecond regime. However, the complex nature and high information content of this class of techniques means that detailed theoretical studies are often essential to provide a firm link between the spectroscopic observables and the underlying molecular structure and dynamics.

Herein I will present some recent work on intersystem crossing dynamics in transition metal complexes and discuss the potential insight that could be obtained from femtosecond X-ray studies. I will also present recent work on exploiting on-the-fly quantum dynamics simulations and machine learning approaches to reduce the computational expense of simulating time-resolved X-ray signals.


Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U59 DMP: Weyl semimetals, ARPES, STM and optics Mile High Ballroom

3C - Tag(s): Focus
Probing the Ultrafast Nonlinear Response in the Transition Metal Monopnictide Family of Weyl Semimetals [Invited] NICHOLAS SIRICA (Presenter), RA’ANAN TOBEY, YAOMIN DAI, Los Alamos National Laboratory, PETER ORTH, Ames Laboratory, Ames, IA, 50011, USA, MATHIAS SCHEURER, Department of Physics, Harvard University, Cambridge, MA 02138, USA, STUART A TRUGMAN, JIAN-XIN ZHU, Los Alamos National Laboratory, NI NI, Department of Physics and Astronomy, University of California, Los Angeles, CA 90095, USA, XIANGGANG QIU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, ANTOINETTE TAYLOR, DZMITRY YAROTSKI, ROHIT P PRASANKUMAR, Los Alamos National Laboratory — Weyl semimetals have been the focus of intense experimental and theoretical investigation, due to their broad appeal in fundamental science and applied technology alike. Recently, several studies have centered on the nonlinear optical properties of these materials, where it is believed that characteristic features of Weyl physics can be observed. To date, many of these studies have been limited to static or quasi-static measurements, but new and important insight can come about through extending nonlinear optical probes into the time domain. To do so, we use terahertz (THz) emission spectroscopy and time-resolved second harmonic generation (TR-SHG) spectroscopy to provide a contact free measure of ultrafast photocurrents in the transition metal monopnictide family of type-I Weyl semimetals. On the basis of our data, we are able to clearly distinguish between helicity-dependent, transverse photocurrents generated within the $ab$-plane from polarization-independent photocurrents flowing along the noncentrosymmetric $c$-axis. By using the photocurrent response as a probe of underlying crystal symmetry, we explore the role that polarization-dependent photoexcitation has on the assignment of point group symmetry, including the possibility of transient symmetry breaking. These findings highlight the robust nonlinear response exhibited by this class of materials, making them promising candidates for next generation sources and detectors in the mid-IR and THz frequency ranges.

Giant nonlinear optical response in topological semimetals* [Invited] LIANG WU (Presenter), Physics and Astronomy, University of Pennsylvania — The second-order optical nonlinearity has been a focus of basic research and technological development for decades as it is both a probe of inversion symmetry breaking in media and the basis for generating coherent light from far-infrared to ultraviolet wavelengths. Here, we focus on experimental investigations on the relation between band geometry/topology and nonlinear optics. I would like to discuss how do the second-order responses that originates from band geometry and topology in polar and chiral topological semimetals respectively. In both cases, we observed large optical nonlinearity and the possible origins will be discussed.

*This project is supported by the Army Research Office Grant W911NF1910342.
3:42PM U59.00003: Imaging current in semimetals with cryogenic scanning NV magnetometry* URI VOOL (Presenter), ASSAF HAMO, XU ZHOU, Harvard University, JOHANNES GOOTH, CLAUDIA FELSER, MPI for chemical physics of solids, Dresden, AMIR YACOBY, Harvard University — Among their many unique features, Weyl semimetals are predicted to enable complex electron-electron and electron-phonon interactions. Such behavior has been predicted, and recently measured, to induce correlated flow of electrons through the semimetal.

We study the current profile in a tungsten ditelluride flake by imaging the local magnetic field above it using a nitrogen-vacancy (NV) center in a diamond scanning tip. Using coherent quantum sensing, we obtain magnetic field resolution of ~10nT and spatial resolution of ~100nm. The current pattern we observe differs substantially from that of a normal metal, suggesting correlated flow through the semimetal.

*This work was supported by the Army Research office (Grant W911NF-17-1-0023) and by the JHDSF program at Harvard University. Devices were fabricated at the Center for Nanoscale Systems (DMR-1541959).

3:54PM U59.00004: Observation of a Dirac nodal loop in the non-symmorphic semimetal Nb₃SiTe₆ RO-YA LIU (Presenter), Department of Physics, University of Illinois at Urbana-Champaign, ANGUS HUANG, Department of Physics, National Tsing Hua University, CHIH-CHUAN SU, RAMAN SANKAR, Institute of Physics, Academia Sinica, SHIH-CHANG WENG, National Synchrotron Radiation Research Center, MENG-KAI LIN, Department of Physics, University of Illinois at Urbana-Champaign, PENG CHEN, School of Physics and Astronomy, Shanghai Jiao Tong University, JOSEPH HLEVYACK, Department of Physics, University of Illinois at Urbana-Champaign, ALEXEI V FEDOROV, Advanced Light Source, Lawrence Berkeley National Lab, CHENG-MAW CHENG, National Synchrotron Radiation Research Center, JONATHAN DENLINGER, Advanced Light Source, Lawrence Berkeley National Lab, CHIA-SENG CHANG, Institute of Physics, Academia Sinica, HORNG-TAY JENG, Department of Physics, National Tsing Hua University, TIEN-MING CHUANG, Institute of Physics, Academia Sinica, TAI-CHANG CHIANG, Department of Physics, University of Illinois at Urbana-Champaign — In 3-dimensional non-symmorphic crystals, band crossings protected by translational symmetry can host Dirac nodal loops in a 2-dimensional cut in the momentum surface. These nodal loops, often with an hourglass shape, give rise to unusual bulk and surface properties, including anisotropic electronic transport and chiral anomaly, based on transport or optical response measurements. This talk will present a detailed study of the band structure of Nb₃SiTe₆ by angle-resolved photoemission spectroscopy. The dispersion relations along the XS direction, which is perpendicular to the sample surface, is mapped out by varying the incident photon energy. The results show that the crossing point (Dirac point) of a Dirac cone at gradually shifts to higher binding in going from X to S. The measurements provide evidence for the presence of a Dirac nodal loop in this system.
**4:06PM U59.00005: Momentum space signature of Berry curvature monopoles in a Weyl semimetal: from first principles to direct experimental observation**  
PHILIPP ECK (Presenter), MAXIMILIAN ÜNZELMANN, TIM FIGGEMEIER, FRIEDRICH REINERT, HENDRIK BENTMANN, DOMENICO DI SANTE, GIORGIO SANGIOVANNI, University of Wuerzburg (Germany) — We investigate the Fermi arcs and the Weyl points in the prototypical non-centrosymmetric time-reversal invariant Weyl semimetal family TaAs/TaP in a joint analysis of state-of-the-art Ab-initio calculations and advanced photoemission spectroscopy methods. The Weyl physics is induced by the broken inversion symmetry giving rise to a predominant orbital magnetization, which results in the interplay with the spin-orbit interaction in the emergence of Weyl points. We characterize the local orbital magnetization in the vicinity of the Weyl points and explore indeed, in agreement with the local Berry curvature, clear features of Berry monopoles at the Weyl points.


*DFG SFB 1170 “ToCoTronics”

**4:18PM U59.00006: Study of hot electrons in topological nodal-line semimetal ZrSiS using time- and angle-resolved photoemission spectroscopy**  
YANGYANG LIU (Presenter), M. MOFAZZEL HOSEN, GYANENDRA DHAKAL, CHRISTOPHER SIMS, JOHN E BEETAR, SABIN REGMI, KLAUSS DIMITRI, FIROZA KABIR, Univ of Central Florida, DARIUSZ KACZOROWSKI, Polish Academy of Sciences, MICHAEL CHINI, MADHAB NEUPANE, Univ of Central Florida — We have studied the ultrafast hot electron cooling process on topological nodal-line semimetal ZrSiS using an advanced XUV-based time- and angle-resolved photoemission spectroscopy (trARPES) with sub-30 meV energy resolution and 320 fs time resolution. The transient ARPES spectra in the vicinity of the nodal-line bulk states and surface states are individually measured using pump-probe scans employing 1.2 eV pump and 21.8 eV probe pulses. Our data reveals that the relaxation decay of the transient electronic temperature in the nodal-line bulk states (around 700 fs) is longer than the surface states (around 320 fs). Furthermore, the relaxation process of the hot electrons in the nodal-line bulk states exists not only a fast decay of ~700 fs, but also a second slow decay (> 6 ps) process, which indicates the existence of a second filling channel in the nodal-line bulk states. Our studies reveal the unique ultrafast properties of the hot electrons in the nodal-line semimetal ZrSiS.

*This project is supported by the Air Force Office of Scientific Research under Award numbers FA9550-17-1-0415 and FA9550-16-1-0149.*
4:30PM U59.00007: Symmetry-Enforced Dirac Fermions in Nonsymmorphic α-Bismuthene*
GUANG BIAN (Presenter), Univ of Missouri - Columbia — According to recent theoretical works, nonsymmorphic crystal symmetries can enforce the formation of Dirac cones, providing a new route to establishing Dirac states in 2D materials. Here we will discuss our recent work on the realization of the symmetry-enforced Dirac fermions in nonsymmorphic α-bismuthene (Bi monolayer). The bismuthene was synthesized by the method of molecular beam epitaxy (MBE). The Dirac band structure was observed by the micro-angle-resolved photoemission (μ-ARPES) experiment. The Dirac points are located at high-symmetry momentum points which are entirely determined by the lattice symmetry. This correspondence of Dirac states to the nonsymmorphic symmetry group can potentially lead to the discovery of a range wide of new 2D Dirac materials. In addition, the Dirac fermions in α-bismuthene is of spin-orbit type in contrast to the spinless Dirac states in graphene. The result will accelerate the search of 2D Dirac materials and extend “graphene” physics into new territory where strong spin-orbit coupling is present.

*This work is supported by US National Science Foundation (NSF-DMR#1809160).

4:42PM U59.00008: Molecular Beam Epitaxy, Band Structure, and Electrical Properties of the Dirac Semimetal ZrTe$_2$*
TIMOTHY PILLSBURY (Presenter), ANTHONY R. RICHARDELLA, RUN XIAO, WILSON YANEZ, MAX STANLEY, HEMIAN YI, CUI-ZU CHANG, NITIN SAMARTH, Department of Physics, The Pennsylvania State University — Topological semimetals (TSMs), a class of gapless electronic phases exhibiting topologically stable crossings of bulk energy bands, have attracted tremendous interest in the condensed matter physics community recently. Based on the origin of the band crossing, TSMs can be classified into Dirac semimetals (DSMs), Weyl semimetals (WSMs) and others. Recently, the transition metal dichalcogenide ZrTe$_2$ has been theoretically predicted and experimentally demonstrated to possess a DSM phase. We used molecular beam epitaxy to synthesize ZrTe$_2$ thin films on insulating sapphire (0001) substrates and performed systematic in vacuo angle-resolved photoemission spectroscopy (ARPES) measurements. The observation of the Dirac cone in the ARPES spectra of ZrTe$_2$ thin films confirms the DSM phase. We also measured the temperature dependence of the ex-situ magneto-transport and found that negative magnetoresistance is absent in our films. We are also exploring the quantum phase transition from DSM to WSM by transition metal doping into these ZrTe$_2$ films.

*This work is supported by 2DCC-MIP/NSF (DMR-1539916), SMART/nCORE/SRC/NIST, DOE EFRC (DE-SC0019331), and ARO (W911NF1810198).
4:54PM U59.00009: Observation of linearly dispersive edge modes in a magnetic Weyl semimetal Co$_3$Sn$_2$S$_2$* SEAN HOWARD (Presenter), LIN JIAO, ZHENYU WANG, Department of Physics, University of Illinois at Urbana-Champaign, PRAVEEN VIR, CHANDRA SHEKHAR, CLAUDIA FELSER, Max Planck Institute For Chemical and Physical Solids, TAYLOR HUGHES, Department of Physics and Institute for Condensed Matter Theory, University of Illinois Urbana Champaign, VIDYA MADHAVAN, Department of Physics, University of Illinois at Urbana-Champaign — The physical realization of Chern insulators is of fundamental and practical interest, as they are predicted to host the quantum anomalous Hall effect (QAHE) and chiral edge states which carry dissipationless current. Realization of the QAHE state has however been challenging due to the complex heterostructures and sub-Kelvin temperatures required. Magnetic Weyl semimetals, essentially stacks of Chern insulators with inter-layer coupling, may provide a new platform for the higher temperature realization of robust 2D QAHE edge states. In this work we present a combined scanning tunneling spectroscopy and theoretical investigation of a newly discovered magnetic Weyl semimetal, Co$_3$Sn$_2$S$_2$. Using numerical simulations we find that chiral edge states can be localized on partially exposed Kagome planes on the surface of a Weyl semimetal. As such, our STM dI/dV maps on narrow kagome Co$_3$Sn terraces show linearly dispersing quantum well-like states, which can be attributed to hybridized chiral edge modes. Our results suggest a new paradigm for studying chiral edge modes in time-reversal breaking Weyl semimetals. More importantly, this work leads a practical route for realizing higher temperature QAHE.

*Basic Energy Sciences DE-SC0014335, Gordon and Betty Moore Foundation Grant GBMF4860

5:06PM U59.00010: Generation of strain-induced pseudo-magnetic field in a doped type-II Weyl semimetal* SUMAN KAMBOJ (Presenter), PARSHA SARATHI RANA, Physical Sciences, IISc Bangalore, ANSHU SIROHI, AASTHA VASDEV, IISER Mohali, MANASI MANDAL, SOURAV MARIK, R P SINGH, Physical Sciences, IISER Bhopal, TANMOY DAS, Physical Sciences, IISc Bangalore, GOUTAM SHEET, IISER Mohali — As per the theory, it is in principle possible to realize a pseudo-magnetic field in strained Weyl semimetals. The basic idea is that strain alters the hopping parameter which may manifest itself as a gauge potential, which in turn may lead to a quantity analogous to the magnetic field. This pseudo-magnetic field may help the formation of quantized Landau levels and thus may become observable in Weyl semimetals. We will show the emergence of a pseudo-magnetic field in a doped and intrinsically strained type-II Weyl semimetal by Scanning Tunneling Spectroscopy (STS) down to 300 mK. In these experiments, clear Landau level oscillations are observed in the absence of an externally applied magnetic field. The system also has a known superconducting phase at very low temperature, which remains unaffected by the pseudo-magnetic field.

*DST/SJF/PSA-01/2015-16
Theoretical Study of Quasiparticle Interference in Weyl Semimetals with ab initio Band Structure Informed Tight-Binding Hamiltonian*  
ZHAO HUANG (Presenter), DZMITRY YAROTSKI, ANTOINETTE TAYLOR, JIAN-XIN ZHU, Los Alamos National Laboratory — The Weyl semimetal is a group of interesting materials where Weyl fermions emerge around singularity points of Berry curvature in the band structure (so called Weyl nodes). A direct consequence of the Weyl nodes is the anomalous surface state arising from the separation of Weyl nodes with opposite topological charges. The energy bands of the surface states cross the Fermi level and form a Fermi arc which connects the projections of Weyl nodes on the surface. Experimentally, observation of the Fermi arc is taken as a fingerprint of the Weyl semimetals. Here we theoretically study the quasiparticle interference (QPI) due to impurity scattering on surfaces in several Weyl semimetals. The scattering between Fermi arcs can lead to special patterns of QPI as indirect observation of the Fermi arcs. In particular, we adopt the accurate tight-binding multi-orbital Hamiltonian constructed from the first-principle electronic structure calculations for each material. We anticipate that our theoretical results will help interpret STM-based measurements on a more comparable footing, thus providing guidance for the identification of Weyl physics.

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This work was carried out under the auspices of the U.S. DOE NNSA (Contract No. 89233218CNA000001), and supported by the U.S. DOE BES EFRC Program.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U60 DMP: Topological Superconductivity: 3D TIs, Weyl Semimetals and TMDs Mile High Ballroom 4A - Vidya Madhavan, University of Illinois at Urbana-Champaign

2:30PM U60.00001: Valley Hall transport and superconductivity signatures in twisted transition metal dichalcogenides [Invited]  NING WANG (Presenter), Physics, The Hong Kong University of Science and Technology — Selected by Focus Topic Organizer (Peide Ye)
Most thermoelectric materials and topological insulators were made from heavy elements and have narrow band gaps and strong spin-orbit couplings. The nontrivial topological insulating states are the essential base for the topological superconductivity. It remains unclear how the thermoelectric figure of merit performs in the topological state, and whether a thermoelectric material can evolve into a topological superconductor and what is the driving force if the latter happens. By choosing an $n$-type Bi$_2$Te$_{2.7}$Se$_{0.3}$, a highly efficient thermoelectric material and topological insulator, we perform measurements of the thermoelectric and superconducting properties at high pressures. We find that the figure of merit increases with pressure and exhibits a maximum at around 1 GPa where the topological phase transition takes place. After that, superconductivity appears and the critical temperature dramatically increases with increasing pressure in the phase with the nontrivial topological state. Its upper critical field exhibits different temperature dependence compared to the other superconducting phases without topological order. The topological phase transition is proposed to serve the linkage for the high-performance thermoelectricity and topological superconductivity.

**3:18PM U60.00003: Theory of Giant In-Plane Critical Field Enhancement in Superconducting Films on a Topological Insulator Surface**

HAOYUN DENG (Presenter), PEDRO SCHLOTTMANN, PENG XIONG, NICHOLAS EVANS BONESTEEL, Florida State Univ — Majorana zero modes (MZMs) are of interest due to potential applications in topological quantum computing. Topological insulators (TIs), with spin-momentum locked surface states, may enable emergence of MZMs when coupled to an $s$-wave superconductor (SC) via the proximity effect. We recently observed a giant enhancement of the in-plane $H_c$ in thin Al, a superconductor with minimal intrinsic spin-orbit coupling (SOC), evaporated onto a 3-dimensional strong TI. $^1$ Here we present a theoretical analysis of this enhancement. Superconductivity at in-plane fields well in excess of the Chanderasekhar-Clogston (CC) limit is understood as a consequence of strong SOC induced in the thin Al films from the topological surface state through the inverse proximity effect. The CC model is combined with the Maki equation to calculate $H_c$ at different temperatures. The calculated $H_c(T)$ shows excellent quantitative agreement with the experimental result. A relatively large value of the induced spin-orbit scattering rate (in comparison to the superconducting energy gap) is derived, indicating a strong proximity coupling in this TI-SC heterostructure which may be a promising platform for observing MZMs.

$^1$Z. Lin et. al., unpublished.

*Work supported by the DARPA TEE Program and NSF grant DMR-1905843.*
3:30PM U60.00004: Characterizing the Superconducting State of Cu$_x$Bi$_2$Se$_3$ Through Muon-Spin Relaxation/Rotation  EMILY DUDEN (Presenter), Winona State University, BENJAMIN FRANDSEN, Brigham Young University, MARKUS KRIENER, RIKEN Center for Emergent Matter Science, YOICHI ANDO, University of Cologne, YASUTOMO J UEMURA, Colombia University — The discovery of topological superconductors has been a major objective in the field since they were first predicted theoretically. The doped topological insulator Cu$_x$Bi$_2$Se$_3$ is a promising candidate for topological superconductivity, but there is much conflicting evidence on the subject. Identifying the superconducting symmetry of the material is paramount in determining whether it has a topologically nontrivial ground state. Muon spin relaxation/rotation (SR) experiments provide a heretofore unexplored method of probing the superconducting state of Cu$_x$Bi$_2$Se$_3$. Here, we present SR data collected on a single-crystal sample of Cu$_{0.3}$Bi$_2$Se$_3$. Measurements conducted in zero-field conditions demonstrate that time reversal symmetry is preserved in the superconducting state, while transverse-field measurements reveal superfluid density behavior that is consistent with p-wave pairing. Such a scenario could support topological superconductivity in Cu$_x$Bi$_2$Se$_3$. However, a more conventional s-wave pairing scenario also provides a reasonable fit to the data, making an unambiguous conclusion difficult. Nevertheless, these results represent a valuable addition to the body of experimental data available for Cu$_x$Bi$_2$Se$_3$.

3:42PM U60.00005: In-plane Critical Field far beyond the Paramagnetic Limit for Thin Al Films on Topological Insulator Surface*  ZHU LIN (Presenter), Department of Physics, Florida State University, ZHILIN LI, Institute of Physics, Chinese Academy of Sciences, HAOYUN DENG, TIANHAN LIU, Department of Physics, Florida State University, GANG SHI, Institute of Physics, Chinese Academy of Sciences, PEDRO SCHLOTTMANN, NICHOLAS EVANS BONESTEEL, Department of Physics, Florida State University, YONGQING LI, Institute of Physics, Chinese Academy of Sciences, PENG XIONG, Department of Physics, Florida State University — Heterostructures of an s-wave superconductor and a strong topological insulator are regarded as a viable platform for the creation of Majorana zero mode (MZM). However, the microscopic understanding of the proximity effect between the superconductor and topological surface state has yet to be fully elucidated. Here we report measurements of the in-plane critical field (H$_{C/\parallel}$) of thin Al, a superconductor with minimal spin-orbit interaction (SOI), on the surface of (Bi$_{0.5}$Sb$_{0.5}$)$_2$TeSe$_2$ (BSTS). H$_{C/\parallel}$ of the Al films are directly compared with those of simultaneously grown control samples of Al films on SiO$_2$. Giant enhancement of H$_{C/\parallel}$ beyond the paramagnetic limit was observed for the Al on BSTS. The enhancement diminishes with increasing Al thickness. The H$_{C/\parallel}$(T) of thin Al on SiO$_2$ is consistent with the Chanderasekha-Clogston theory, while the H$_{C/\parallel}$(T) of thin Al on BSTS can be well-described by a theory based the Maki equation invoking strong induced SOI in Al. The results provide direct evidence for an electrically transparent interface and strong proximity effect between the Al and BSTS. The Al/BSTS heterostructure may be a promising system for inducing topological superconductivity and controlled generation of MZMs.

*Work supported by the DARPA TEE Program and NSF grant DMR-1905843.
3:54PM U60.00006: Uniaxial-Strain Control of Nematic Superconductivity in Sr$_x$Bi$_2$Se$_3$*

IVAN KOSTYLEV, SHINGO YONEZAWA, Kyoto Univ., ZHIWEI WANG, YOICHI ANDO, Univ. Cologne, YOSHITERU MAENO (Presenter), Kyoto Univ. — Recently, nematic superconductivity, in which the superconducting gap spontaneously lifts the rotational symmetry of the lattice, has been discovered [1]. In nematic superconductivity, multiple superconducting domains with different nematic orientations can exist. These domains can be controlled by a conjugate external stimulus, such as the strain induced by a uniaxial stress with a piezoelectric device [2]. Here, we report for the first time control of the nematic superconductivity and their domains of Sr$_x$Bi$_2$Se$_3$, through externally-applied uniaxial stress [3]. The suppression of subdomains indicates that it is the Δ$_4$ state that is most favored under compression along the basal Bi-Bi bonds. These results provide an inevitable step towards microscopic understanding and future utilization of the unique topological nematic superconductivity.


*This work was supported by JSPS KAKENHI JP15H05851, JP15H05852, JP15H05853, JP15K21717, JP17H04848, and by the JSPS Core-to-Core program. The work at Cologne was funded by the DFG-Project number 277146847-CRC 1238 (Subproject A04).

4:06PM U60.00007: Doping and pressure effects on Weyl semimetal Mo$_{1-x}$W$_x$Te$_2$* RABIN DAHAL (Presenter), LIANGZI DENG, NARAYAN POUDEL, MELISSA GOOCH, ZHENG WU, HUNG-CHENG WU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204, USA, HUNG-DUEN YANG, Department of Physics, National Sun Yat-sen University, Kaohsiung, 80424, Taiwan, CHUNG-KAI CHANG, National Synchrotron Radiation Research Center, Hsinchu, 30076, Taiwan, PAUL C. W. CHU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204, USA — Systematic pressure and doping dependent study on Mo$_{1-x}$W$_x$Te$_2$ was carried out to investigate the correlation among chemical doping, structural transition, and superconductivity. Doping dependent resistivity measurement at ambient pressure shows structural transition temperature ($T_s$) for MoTe$_2$ to be 249 K, which continuously increases as doping level ($x$) increases and reaches a maximum value of 613 K for WTe$_2$. The structural transition of WTe$_2$ at ambient pressure is also confirmed by conducting temperature dependent synchrotron X-ray diffraction from 300 K to 673 K. Three samples with different doping ($x = 0.10, 0.40, 0.75$) were selected for high pressure measurement. The superconducting transition temperature - pressure ($T_c - P$) phase diagrams have been constructed and will be discussed. Our experimental results revealed a competition between the structural transition and superconductivity in Mo$_{1-x}$W$_x$Te$_2$. Superconductivity emerges when the $T_s$ is suppressed below 175 K and $T_c$ increases as $T_s$ is suppressed.

*The work performed at Houston is supported by USAFOSR Grant FA9550-15-1-0236, TLL Temple Foundation, JJ&R Moores Endowment, and State of Texas through TCSUH.
4:18PM U60.00008: Theory on superconducting chiral crystal and its applications  ZHESHEN GAO (Presenter), WENYU HE, KAM TUEN LAW, Hong Kong University of Science and Technology — Chiral crystals are shown to have nontrivial band topology: at the time reversal invariant momenta, Kramers Weyl points and multi-fold Weyl points can emerge due to the chiral lattice symmetry. In the normal metallic state, the chiral lattice symmetry along with the band topology introduces the magnetoelectric effect and circular photogalvanic effect to modify the electromagnetic properties in the materials. However, how does the chiral lattice symmetry and the associated band topology affect the superconducting phase in chiral crystals remains unknown. In this work, we classify the possible pairing phases resulted from chiral lattice symmetry and find various topological superconducting phases. We propose the candidate topological superconducting chiral crystal and study its unique superconducting properties.

4:30PM U60.00009: Correlation-driven renormalization of Weyl nodes in the Ce-113 series
VSEVOLOD IVANOV (Presenter), SERGEY SAVRASOV, University of California, Davis — We study the electronic properties of the inversion-broken CeTX3 (T = Co, Rh, Ir, X=Si,Ge) heavy-fermion materials through a combination of LDA and LDA+Guzwiller methods. In this class of compounds the electronic mass is enhanced, causing narrowing the Ce f-electron bands. Our LDA+Guzwiller procedure captures these renormalization effects, yielding a mass enhancement that is in good agreement with experimental specific heat measurements. We also track the renormalization of Weyl points by the correlations, which move them closer to the Fermi energy. We briefly comment on the interplay of Weyl physics and pressure-induced superconductivity in these compounds.

4:42PM U60.00010: One-dimensional states residing on edges and steps in few-layer WTe$_2$
ARTEM KONONOV (Presenter), GULIBUSITAN ABULIZI, University of Basel, KEJIAN QU, JIAQIANG YAN, DAVID MANDRUS, Materials Science and Engineering, The University of Tennessee, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, CHRISTIAN SCHONENBERGER, University of Basel — WTe$_2$ is a layered material with rich topological properties. The bulk crystal is a type-II Weyl semimetal and the monolayer is a two-dimensional topological insulator. Recently, it has been predicted that higher order topological insulator state can appear in WTe$_2$. An observation of 1D, highly conductive channels, known in this case as hinge states, is hindered by the bulk conductivity of WTe$_2$. Here, we employ the Josephson effect to disentangle the contribution of the hinge states from the bulk in electronic transport. We observe 1D current carrying states on edges and steps in few-layer WTe$_2$. The width of the states is deduced to be below 100 nm. A supercurrent in them can be measured over distances up to 3 µm and in perpendicular magnetic field up to 2 T. Moreover, the dependence of the supercurrent on the magnetic field is compatible with the asymmetric Josephson effect predicted to occur in topological systems with broken inversion symmetry.

*Supported by the Georg H. Endress foundation and the European Research Council project Top-Supra (787414)
**4:54PM U60.00011: Probing Proximity Effect in Topological Insulator/Superconductor Heterostructures**  
CEQUN LI (Presenter), BRIAN BERSCH, NATALIE BRIGGS, YIFAN ZHAO, CHENGYE DONG, TIMOTHY BOWEN, HEMIAN YI, JOSHUA ROBINSON, CUI-ZU CHANG, JUN ZHU, Pennsylvania State University — Topological insulator (TI)/superconductor heterostructures are predicted to host Majorana zero modes, which are building blocks of topological qubit. In this work, we synthesize high-quality large-area TI/graphene (Gr)/gallium heterostructures combining confinement epitaxy and molecular beam epitaxy. Atomically thin Ga film superconducts at $T_c \sim 4K$ [B. Bersh, et. al, arXiv:1905.09938], and the growth of TI preserves its superconductivity. We probe the proximity effect in the TI film using four-terminal transport and tunneling spectroscopy. Hints of a proximity induced gap in the TI film are observed in transport measurements. We demonstrate the efficacy of a clean van der Waals tunnel junction in probing the superconducting gap of thin film NbSe$_2$ and present tunneling spectroscopy measurements on TI/Gr/Ga heterostructures.

**5:06PM U60.00012: Topological superconductivity in proximitized transition metal dichalcogenide Josephson junctions**  
*JOSEPH PAKIZER (Presenter), ALEX MATOS ABIAGUE, Wayne State Univ — We theoretically investigate the emergence of topological superconductivity in Josephson junctions (JJ) built of a two-dimensional transition metal dichalcogenide (TMD) layer in proximity to an s-wave superconductor and a magnetic insulator. We show that in a certain range of chemical potential and magnetic proximity strength, Majorana bound states form at the ends of the normal region of a TMD-based JJ. The evolution of the topological superconducting phase as the magnetization direction is varied is also investigated. The effect of the interplay between Ising spins, proximity exchange, and Rashba spin-orbit coupling on the system transition to the topological superconducting phase, as well as the corresponding signatures on the ground state phase and critical current, are analyzed in detail for both phase-fixed and phase-unbiased JJs.

*This work was supported by DARPA Topological Excitations in Electronics (TEE) Grant No. DP18AP900007 and US ONR Grant No. N000141712793.*
Superconductivity in Cd$_3$As$_2$ thin films

ALEXEY SUSLOV (Presenter), Natl High Magnetic Field Lab, ALEXANDER DAVYDOV, P. N. Lebedev Physical Institute, LEONID OVESHNIKOV, National Research Center “Kurchatov Institute”, LEONID MORGUN, National Research University Higher School of Economics, KLIMENT KUGEL, Institute for Theoretical and Applied Electrodynamics, VASILIY ZAKHVALINSKII, EVGENY PILYUK, Belgorod National Research University, ALEXEY KOCHURA, ALEXANDER KUZMENKO, South-West State University, ALEXEY RIL, Kurnakov Institute of General and Inorganic Chemistry, SERGEY MARENKIN, National University of Science and Technology MISIS, VLADIMIR PUDALOV, BORIS ARONZON, P. N. Lebedev Physical Institute

For the first time we observed superconductivity in Cd$_3$As$_2$ thin films without applying external pressure. We studied thin (40 nm -100 nm) films of Cd$_3$As$_2$ grown on various substrates by two various methods: thermal evaporation and magnetron sputtering from Cd$_3$As$_2$ single crystals. Both Raman spectroscopy and X-ray diffraction on the films show results typical for Cd$_3$As$_2$ with tetragonal lattice. A zero-resistance state was registered by the four-probe method on Hall bar shaped samples. Also a zero-resistance plateau was observed in dV/dI characteristics at low currents. The superconducting state was suppressed by applying a magnetic field or increasing the current above critical values $H_c$ and $I_c$, respectively. $H_c$ perpendicular to the film plane was smaller than the in-plane critical field at the same temperature. Analysis of dependences of critical magnetic field $H_c$ on critical temperature $T_c$ reveals a clearly pronounced linear behavior within the intermediate temperature range, similar to that observed for superconducting bulk Cd$_3$As$_2$ and Bi$_2$Se$_3$ under pressure.

*Russian Science Foundation grant 17-12-01345, RFBR grant 16-29-03330, NSF/DMR-1644779 and the State of Florida

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U61 DMP DCMP: Metal-Insulator transition in 4d/5d oxides
Emergent transport properties on the verge of metal-insulator transitions in pyrochlore 5d/4d oxides* [Invited] KENTARO UEDA (Presenter), Univ of Tokyo —

Magnetic Weyl semimetals have been proved to generate emergent transport properties such as giant anomalous Hall effect due to the band-crossing points acting as magnetic monopoles of Berry curvature.

A variety of 5d/4d oxides, in which the magnitude of the relativistic spin-orbit coupling is comparable to that of the electron correlation, are suggested to host such a topologically-nontrivial property. For instance, pyrochlore iridates (R$_2$Ir$_2$O$_7$) are firstly proposed as a candidate for the magnetic Weyl semimetal. Recent studies uncover that Nd$_2$Ir$_2$O$_7$ shows salient magnetotransport properties on the verge of metal-insulator transitions, attributable to the realization of multiple topological semimetals with different magnetic ordering patterns. Here, we report another examples of such states in Pr$_2$Ir$_2$O$_7$, which is known as a paramagnetic Luttinger semimetal. The resistivity is largely enhanced in the 3-in 1-out magnetic configuration of Pr-4f moments, whereas it is relatively small in the magnetically metastable state (so-called Kagome-ice state) accompanied with the plateau structure of Hall resistivity. It indicates that the quadratic-band-touching electronic structure is significantly sensitive to the localized magnetic configurations even in the weak-coupling system.

We also demonstrate that the pyrochlore 4d oxides provide a fertile playground. Particularly, Ruthenates (A$^{2+}$Ru$^{5+}$O$_7$: 4d$^3$ or R$^{3+}$Ru$^{4+}$O$_7$: 4d$^4$) exhibit wide range of magnetic/electronic phases from an antiferromagnetic insulator to a ferromagnetic-like metal as the valence of A site changes. Furthermore, the sizable anomalous Hall conductivity is observed in the intermediate A-site composition, which can be understood in the context of the topological nature of the band structures.

*This work was supported by JSPS Grant-in-Aid for Scientific Research (No. 26103006, No. 24224009, and 19K14647) from the MEXT, and by CREST (No. JPMJCR16F1 and JPMJCR1874), JST, Japan.
3:06PM U61.00002: Multiorbital effects in Sr$_2$IrO$_4$ under an external field*  LEINA ENGSTRÖM (Presenter), TAMIR PEREG-BARNEA, McGill University, WILLIAM WITCZAK-KREMPA, Université de Montréal — Many parallels have been drawn between the spin-orbit coupled Mott insulator Sr$_2$IrO$_4$ and the high-T$_c$ superconducting cuprates. In the undoped compound, a one band $J_{eff}=1/2$ model has been shown to capture the observed magnetic order. In other regimes, the applicability of this model is less clear, and the correlated phases are less understood due to potentially complex multiorbital physics. We use a multiple order parameter, self-consistent mean-field approach to explore the relevance of multiorbital effects to possible exotic phases in Sr$_2$IrO$_4$ in an external magnetic field. We study the contributions from both spin and orbital degrees of freedom to the magnetic moment. We thus unravel what role spin orbit coupling plays for emerging orders. Implications for superconductivity and thermal Hall measurements are discussed.

* - “Etablissement de nouveaux chercheurs universitaires” Grant from FRQNT
- Discovery Grant from NSERC
- Grant from Fondation Courtois

3:18PM U61.00003: Electrical resistivity relaxation under uniaxial strain in BaIrO$_3$ at room temperature  PETER SIEGFRIED (Presenter), HENGDI ZHAO, GANG CAO, MINHYEA LEE, University of Colorado, Boulder — We investigate the 5$d$ transition metal oxide BaIrO$_3$, in which the ground state is strongly dependent on the corner sharing Ir-O-Ir buckling angle between the face sharing octahedral trimers. We compare nanoindentation and resistivity under uniaxial strain, finding a strong hysteretic behavior in the resistivity that is driven by a strain dependent relaxation. This relaxation exhibits logarithmic time dependence, and also emerges in the lattice relaxation as creep. These observations highlight the strong mechanical and electrical coupling in BaIrO$_3$, and point to the relaxation mechanisms sharing the same origin. Our results promote the value of utilizing uniaxial strain testing and nanoindentation as a novel technique to probe the structural sensitivity of quantum materials.
In-situ anisotropic strain controlled metamagnetism of \( \text{Sr}_2\text{IrO}_4 \) by pseudo-Jahn-Teller distortion

HAN ZHANG (Presenter), LIN HAO, JUNYI YANG, University of Tennessee, JOSHUA MUTC, ZHAOYU LIU, University of Washington, QING HUANG, KYLE R NOORDHOEK, University of Tennessee, ANDREW MAY, Oak Ridge National Laboratory, JIUN-HAW CHU, University of Washington, JONG WOO KIM, PHILIP RYAN, APS, Argonne National Laboratory, HAIĐONG ZHOU, JIAN LIU, University of Tennessee — In recent years, iridates have been recognized as an ideal material platform where the emergent many-body phenomena mesh with Antiferromagnetic (AF) functionalities. As the prototype, \( \text{Sr}_2\text{IrO}_4 \) is a quasi-two-dimensional AF Mott insulator of pseudospin-half electrons that exhibits remarkable phenomenological analogy to the high-\( T_c \) cuprates. Meanwhile, significant magnetic responses of the AF order in both bulk and thin film samples have been demonstrated, including metamagnetism, giant magnetoresistance, and anisotropic magnetoresistance. The high controllability of the AF order is largely related to the unique electronic structure that the strong spin-orbit coupling of Ir stabilizes the pseudospin-half Kramer doublet while makes no contribution to the magnetic anisotropy. In this study, we drove the metamagnetic transition of \( \text{Sr}_2\text{IrO}_4 \) bulk crystal into distinct regimes by applying in-situ anisotropic strain. The system was studied with resonant magnetic x-ray scattering and transport measurement. We found the application of anisotropic strain is seen to modulate the pseudospin-lattice coupling, leading to highly efficient magnetoelastic control of the \( J_{\text{eff}}=1/2 \) metamagnetism as well as the associated elasto- and magnetoresistance.

Thickness Dependent Magnetic Reversal in \( \text{Sr}_4\text{Ru}_3\text{O}_{10} \) Nanosheets

YAN LIU, JIYONG YANG, High Magnetic Field Laboratory, CAS, Hefei 230026, China, ZHIQIANG MAO, Department of Physics, Pennsylvania State University, GANG CAO, Department of Physics, University of Colorado at Boulder, MINGLIANG TIAN (Presenter), High Magnetic Field Laboratory, CAS, Hefei 230026, China — While ruthenium oxide \( \text{Sr}_4\text{Ru}_3\text{O}_{10} \) has been studied extensively in the last two decades, the origin of the unusual second magnetic anomaly near \( T_M \approx 50 \) K remains elusive. Here, we investigated the thickness-dependent anisotropic magnetoresistance (AMR) of pure and 2% Fe-doped \( \text{Sr}_4\text{Ru}_3\text{O}_{10} \) nanosheets. It was clearly found that the AMR properties in pure nanosheets present thickness-dependent behavior and an unusual reversal near \( T_M \), but Fe-doping nansheet completely suppresses the second anomaly down to low temperatures. Analysis of the data demonstrates that this AMR reversal is caused by the magnetization reversal from the \( ab \) plane ferromagnetic order at \( T>T_M \) to the \( c \) direction at \( T<T_M \) due to the competition between the shape anisotropy and the inherent magnetocrystalline anisotropy. Our result suggests that the second magnetic transition in \( \text{Sr}_4\text{Ru}_3\text{O}_{10} \) nanosheets is originated from spin reorientation.
3:54PM U61.00006: Transport phenomena in ultraclean 111 oriented SrVO$_3$ thin films

JOSEPH ROTH (Presenter), TATIANA KUZNETSOVA, ROMAN ENGLER-HERBERT, Pennsylvania State University — SrVO$_3$ has proven to be an ideal testbed for studying the effects of strong electron correlation due to its simple cubic structure and single d-orbital electron. Ultraclean SrVO$_3$ films with residual ratios exceeding 200 have recently been demonstrated using self-regulated growth by hybrid MBE, allowing accurate interpretation of the intrinsic features of electron correlation [1]. In addition to allowing high quality growth, we demonstrate that SrVO$_3$ can also be grown epitaxially on (111) oriented LSAT substrates. We compare the temperature dependent electronic transport properties of (111) and (001) oriented SrVO$_3$ thin films. In addition, we discuss the formation of a low temperature Fermi liquid like phase in each case.


*This work was supported by the NSF Graduate Research Fellowship Program under Grant No. DGE1255832 and NSF-DMR 1905861.

4:06PM U61.00007: Growth and Characterization of Heterostructures of Ferromagnetic SrRuO$_3$ and Superconducting Sr$_2$RuO$_4$ by Molecular-Beam Epitaxy

NATHANIEL SCHREIBER (Presenter), HARI NAIR, JACOB RUF, LUDI MIAO, BERIT GOODGE, LENA KOURKOUTIS, KYLE M SHEN, DARRELL SCHLOM, Cornell University — Sr$_2$RuO$_4$ single crystals have been shown to exhibit unconventional superconductivity with a $T_c$ of 1.5 K. Our group recently reported a thermodynamic growth window for Sr$_{n+1}$Ru$_n$O$_{3n+1}$ thin films, including the demonstration of the reproducible growth of high-RRR Sr$_2$RuO$_4$ and SrRuO$_3$ thin films. The growth of Sr$_2$RuO$_4$ thin films and the recent $^{17}$O NMR results on single crystals offer an opportunity for the growth of Sr$_2$RuO$_4$-based heterostructures, in order to perform measurements to determine the superconducting order parameter. In this talk, we describe the growth of SrRuO$_3$/Sr$_2$RuO$_4$ heterostructures using oxide molecular-beam epitaxy. We characterize the crystallinity and structure of these heterostructures using X-ray diffraction, X-ray reflectivity, and scanning transmission electron microscopy, and finally we present magnetometry and electrical resistivity measurements on these heterostructures.

4:18PM U61.00008: Intrinsic tunable anomalous Hall effect induced by momentum-space Berry curvature in SrRuO$_3$

BYUNGMIN SOHN (Presenter), EUNWOO LEE, JI SEOP OH, WONSHIK KYUNG, HANYOUNG YOO, BOHM-JUNG YANG, CHANGYOUNG KIM, Physics and Astronomy, Seoul National University — Broken time-reversal symmetry and spin-orbit coupling (SOC) in strongly correlated ferromagnetic materials are expected to induce novel phenomena. One of these ferromagnetic materials, SrRuO$_3$ (SRO), is well-known for showing non-monotonous anomalous Hall effect (AHE), which is produced due to magnetic monopoles, or large Berry curvature in momentum space. Recently, we observed an abnormal behavior of AHE in SRO ultrathin films. To explain this, we measured angle-resolved photoemission spectroscopy (ARPES) of SRO ultrathin film. We found that non-monotonous AHE is induced by band-structure nodal lines, which open a gap due to SOC and magnetization. By changing temperature and thickness of SRO, the sign of AHE can be tunable with a variation of large Berry curvature.
4:30PM U61.00009: Spectroscopic study on band evolution and formation of relativistic Mott insulating phase in Ir doped Sr$_2$RuO$_4$  JUNYOUNG KWON (Presenter), BEOM SEO KIM, Physics, Seoul Natl Univ, JONATHAN DENLINGER, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, Lawrence Berkeley National Laboratory, YOUNG JAI CHOI, Physics and Applied Physics, Yonsei University, WONSHIK KYUNG, CHANGYOUNG KIM, Physics, Seoul Natl Univ — Recent research showed 4d, 5d transition metal oxide provides rich novel physical properties. A discovery of superconductivity in Sr$_2$RuO$_4$ is still controversial to verify the mechanism, and relativistic Mott phase of Sr$_2$IrO$_4$ expanded wide research field of spin-orbit coupling-driven physics. As one step to explore the field, doping study also become vivid that it can alter the system's key parameters and artificially create a perturbed physical system. Rh doping in Sr$_2$IrO$_4$ revealed variation of spin-orbit coupling, and doping on electrons on Sr$_2$IrO$_4$ showed charge carrier dependent collapse of Mott phase. Now we tried to study doped compound Sr$_2$(Ru,Ir)O$_4$ to show the electronic propagation of bands and evolution of relativistic Mott phase with angle-resolved photoemission spectrscopy technique. With this presentation we would clarify the role of spin-orbit coupling on the crystal-field-dominating band structure of Sr$_2$RuO$_4$, and provide a step by step evolution of relativistic Mott transition from varying spin-orbit coupling parameter.

4:42PM U61.00010: Spectroscopic evidence for electron-boson coupling in electron-doped Sr$_2$IrO$_4$  YONG HU, University of Science and Technology of China, XIANG CHEN, University of California, Santa Barbara, SHUTING PENG, University of Science and Technology of China, CHRISTOPHER LANE, MATTHEW MATZELLE, Northeastern University, ZELIANG SUN, University of Science and Technology of China, MAKOTO HASHIMOTO, DONGHUI LU, Stanford Synchrotron Radiation Lightsource, EIKE F. SCHWIER, MASASHI ARITA, Hiroshima University, TAO WU, University of Science and Technology of China, ROBERT MARKIEWICZ, Northeastern University, KENYA SHIMADA, Hiroshima University, XIANHUI CHEN, University of Science and Technology of China, ZHIXUN SHEN, Stanford University, ARUN BANSIL, Northeastern University, STEPHEN WILSON, University of California, Santa Barbara, JUNFENG HE (Presenter), University of Science and Technology of China — The pseudogap, d-wave superconductivity and electron-boson coupling are three intertwined key ingredients in the phase diagram of the cuprates. Sr$_2$IrO$_4$ is a 5d-electron counterpart of the cuprates in which both the pseudogap and a d-wave instability have been observed. Here, we report spectroscopic evidence for the presence of the third key player in electron-doped Sr$_2$IrO$_4$: electron-boson coupling. A kink in nodal dispersion is observed. The strength of the kink changes with doping, but the energy scale remains the same. These results provide the first non-cuprate platform for exploring the relationship between the pseudogap, d-wave instability and electron-boson coupling in doped Mott insulators.
4:54PM U61.00011: Relaxation Dynamics at High-symmetry Points in Sr$_2$IrO$_4$ through Time- and Angle-resolved Photoemission Spectroscopy*  DONGSUNG CHOI (Presenter), DORON AZOURY, EDOARDO BALDINI, BAIQING LYU, ALFRED ZONG, Massachusetts Institute of Technology MIT, ZACH PORTER, STEPHEN WILSON, University of California, Santa Barbara, NUH GEDIK, Massachusetts Institute of Technology MIT — The unresolved mechanism that underlies high-$T_c$ superconductivity in cuprates has stimulated the search for new material platforms that could shed light on this long-standing puzzle. A promising candidate is electron-doped Sr$_2$IrO$_4$ — an antiferromagnetic Mott insulator with strong spin-orbit coupling. Pioneering studies have shown that chemical doping modifies the electronic band structure in electron-doped Sr$_2$IrO$_4$. However, instead of chemical doping, which provides a static modification of the electronic band structure, transient photo-doping with an ultrafast laser pulse can be considered. Through time- and angle-resolved photoemission spectroscopy, we performed momentum-resolved pump-probe experiments and compared the electron relaxation behavior at high-symmetry points (Γ, M, and X) of the Brillouin zone. This time- and momentum-resolved study provides new insights into the transient charge dynamics in this Mott insulator.

*ARO MURI Grant No. W911NF-16-1-0361, U.S. Department of Energy, BES DMSE and Gordon and Betty Moore Foundations EPiQS Initiative grant GBMF4540

5:06PM U61.00012: Magnetic-field-dependent second-harmonic generation study of Sr$_2$IrO$_4$  KYLE SEYLER (Presenter), ALBERTO DE LA TORRE, Caltech, ZACH PORTER, University of California, Santa Barbara, GANG CAO, University of Colorado, Boulder, STEPHEN WILSON, University of California, Santa Barbara, DAVID HSIEH, Caltech — The quasi-two-dimensional layered oxide Sr$_2$IrO$_4$ has earned recognition for its novel spin-orbit Mott state and various analogies to cuprate physics. Neutron diffraction and x-ray scattering measurements show that it possesses a centrosymmetric magnetic ground state, consisting of a canted intralayer antiferromagnetic order with nonzero net magnetic moments in each layer stacked antiferromagnetically [1-4]. However, the onset of a second-harmonic generation (SHG) signal below the Néel temperature has suggested the presence of a distinct hidden magnetic order [5]. Using small in-plane magnetic fields, it is possible to manipulate the Néel order and help distinguish it from hidden order. In this talk, we will present magnetic-field-dependent SHG rotational anisotropy and microscopy studies that further elucidate the nature of this hidden state.

5:18PM U61.00013: Raman measurements on Sr$_2$IrO$_4$ grown in magnetic field*  NICK PELLATZ (Presenter), DMITRY REZNIK, GANG CAO, University of Colorado, Boulder — Recent experiments found a massive reduction in the low-temperature resistivity in Sr$_2$IrO$_4$ when the crystals were grown in the presence of a magnetic field. Here I will present a comparison of Raman scattering data from normal and field-grown Sr$_2$IrO$_4$. The main differences between the two appeared in scattering from magnetic excitations. Two-magnon scattering was significantly broader in the field-grown sample and exhibited unusual temperature dependence. Scattering from single magnons, clearly visible in the normal sample, was completely absent in the field-grown sample down to an energy of at most 5 cm$^{-1}$. Latest results including on doped samples will be presented.

*Work at the University of Colorado was supported by the NSF under Grant No. DMR-1410111

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U62 DCMP: Helium and Exotic Quantum Fluids  Mile High Ballroom 4C - Valeri Kotov, Univ of Vermont

2:30PM U62.00001: Chasing signs of the Kelvin-wave cascade on a single vortex using nanoscale mechanical resonators*  SAMULI AUTTI (Presenter), ANDREW GUTHRIE, RICHARD HALEY, SERGEY KAFANOV, MARK NOBLE, YURI PASHKIN, GEORGE PICKETT, VIKTOR TSEPELIN, DMITRY ZMEEV, Department of Physics, Lancaster University — It is believed that Kelvin waves propagating on a quantum vortex provide a fundamental channel of dissipation of superfluid turbulence, driven by the Kelvin-wave cascade. In spite of decades of theoretical work, no conclusive experimental evidence on the existence of such cascade has been presented. In our experiments we use nanoscale mechanical resonators operating at about 1MHz, immersed in superfluid $^4$He [1]. These probes are sensitive enough to probe single vortices. A vortex can be attached to the resonator by creating turbulence using a nearby tuning fork. This allows measuring the restoring force and the dissipation the vortex imposes on the resonator as a function of time, until the vortex is disconnected. We compare the observations with the theoretical expectation [2], and discuss possible future experiments.


*This research is supported by the U.K. EPSRC (EP/R025487/1, EP/P024203/1), the European FP7 Programme MICROKELVIN (project number 228464), and the European Union’s Horizon 2020 research and innovation programme (European Microkelvin Platform, grant agreement No. 824109). S.A. acknowledges financial support from the Jenny and Antti Wihuri Foundation via the Council of Finnish Foundations.
2:42PM U62.00002: Suppression of triplet superfluidity near magnetically-active surfaces
ANTON VORONTSOV (Presenter), Montana State University, Bozeman — Recent experiments investigating properties of the chiral A phase of superfluid $^3$He in thin slabs (P. Heikkinen et al, arXiv:1909.04210) revealed unusually large $T_C$ suppression that exceeds the fully-diffusive scattering limit. This requires re-thinking of the boundary conditions, and inclusion of magnetic degree of freedom to describe scattering of the quasiparticles on surfaces that are covered my magnetically-active solid layer of He-3 atoms. I will review existing models of magnetic scattering to prove that they cannot, in principle, give such suppression of the A phase. I will show that in order to explain the large $T_C$ suppression, the internal quantum degrees of freedom of the solid spins have to be taken into account.

2:54PM U62.00003: Emergence of a New Superfluid Phase in Quasi-2D $^3$He*
ALEXANDER SHOOK (Presenter), VAISAKH VADAKKUMBATT, PRAMODH V SENARATH YAPA ARACHCHIGE, CALLUM DOOLIN, RUFUS BOYACK, PAUL Y KIM, GREG POPOWICH, FABIEN SOURIS, HOLLY CHRISTANI, JOSEPH MACIEJKO, JOHN DAVIS, Univ of Alberta — $^3$He is a fermionic superfluid that exhibits exotic properties at ultra-low temperatures due to its unconventional $p$-wave Cooper pairing. The orbital and spin degrees of freedom of $^3$He Cooper pairs allows for a rich array of possible superfluid phases, which are determined by geometry as well as the thermodynamic properties of the fluid. Much of the current theoretical and experimental interest in $^3$He has focused on quasi-2D slabs where new phases are predicted to emerge. Our lab has created nanofluidic mechanical resonators capable of both confining $^3$He and detecting phase transitions over a wide range of pressures and temperatures. In doing so we have observed a new phase transition which is stabilized by confinement and thought to be due to the breaking of translational symmetry within the superfluid slab.

*The University of Alberta; the Natural Sciences and Engineering Research Council, Canada (Grants No. RGPIN-04523-16, No. DAS-492947-16, and No. CREATE-495446-17); Quantum Alberta; and the Canada Foundation for Innovation.
3:06PM U62.00004: Memory Effect and the Metastability of the A to B Transition in Superfluid $^3$He.*  DMYTRO LOTNYK, ANNA EYAL, NIKOLAY ZHELEV, T.S. ABHILASH, JOHN WILSON, MICHAEL TERILLI, ALDO CHAVEZ, ERIC SMITH, ERICH MUELLER, JEEVAK PARPIA (Presenter), Cornell University — We experimentally study the metastability of the A phase of superfluid $^3$He, as either temperature ($T$) or pressure ($P$) is varied. We find significant supercooling, with the A-B transition occurring well below the temperature of the thermodynamic phase boundary in bulk. The observed transition in two chambers (separated by a 1.1 $\mu$m tall channel) shadows the thermodynamic A-B line in the $T$-$P$ plane but extends below the polycritical point and terminates in the B phase (and not at $T_c$). We find significant path dependence (memory effect) in the metastability: When we sweep pressure at fixed temperature, the region of metastable A is larger than when we sweep temperature at fixed pressure. We find U-shaped depressurizing-cooling-pressurizing paths in the $T$-$P$ plane which enable the metastable A phase to exist well below the polycritical point at 21.2 bar that cannot be reached by a temperature sweep. While cooling at constant pressure, we observe A-B transitions down to 20.85 bar, whereas while depressurizing, A-B transitions are seen down to 19.5 bar. Ongoing experiments in a 50 G field show unexpected behavior. The measurements highlight the role of surfaces in nucleation and the memory effect.

*Research supported by the National Science Foundation under DMR1708341

3:18PM U62.00005: Mott Insulator to Superfluid Quantum Phase Transition for Helium on Strained Graphene*  JIANGYONG YU (Presenter), NATHAN NICHOLS, TARAS I. LAKOBA, VALERI KOTOV, ADRIAN DEL MAESTRO, Univ of Vermont — An exciting development in the field of correlated systems is the possibility of realizing two-dimensional (2D) superfluidity, particularly by adsorbing helium on novel 2D quantum materials, such as graphene. How superfluidity emerges in this system, and whether it could exist in the first, second, etc. layer, has been a topic of considerable controversy. We argue theoretically that under certain favorable external conditions where uniaxial stress is applied to graphene, 2D anisotropic superfluidity can form in the first layer. This result is based on preliminary large-scale ab initio quantum Monte Carlo simulations combined with a mapping of the problem to an effective Bose-Hubbard model. We show that a critical ratio of the onsite repulsion to hopping strength ($U/t$) can be achieved via strain, allowing for a quantum phase transition to a superfluid state below a critical value. Our analysis supports, for the first time, the existence of an unconventional first layer 2D anisotropic superfluid, possibly also exhibiting supersolid correlations reflecting the underlying graphene lattice structure.

*This work received support under NASA grant number 80NSSC19M0143.
3:30PM U62.00006: Modelling a Neutron Star in Superfluid Helium  
RENA ZIEVE (Presenter), ROBERT P PRATER, University of California, Davis — We discuss a lab experiment intended to model neutron star behavior. Superfluid helium is encased in a container that can rotate freely. The container is spun up, then monitored as it gradually slows down. Pinned vortices inside which release and repin can produce rotational glitches mimicking those of pulsars. We discuss the experimental design and the expected measurement sensitivity. The design is based on similar work from 40 years ago. We revisit the experiment now because of advances in the speed of computers and videocameras, as well as in the theoretical modelling of neutron stars.

3:42PM U62.00007: Few-body precursor of the Higgs mode in a superfluid Fermi gas - from theory to experiments.*  
JOHANNES BJERLIN (Presenter), Univ of Copenhagen — We demonstrate the presence of an undamped few-body precursor of the Higgs mode in an ultracold trapped Fermi gas.
Here, the lowest excitation mode frequency has non-monotonical dependence on the interaction strength, attaining a minimum in the crossover region.
In the many-body limit, the Higgs mode appears as a zero-energy excitation mode at the quantum phase transition point between the superfluid and the normal phase.
In the few-body limit, we observe an energy minimum that deepens with increasing particle number, reflecting the fact that we see a few-body Higgs mode analog which develops towards a zero-energy excitation.
This hallmark of the Higgs mode is persistent also for weakly anharmonic and anisotropic traps, and it can readily be observed in a new generation of microtraps where the Higgs mode is selectively excited by modulating the interaction strength via Feshbach resonances.
Using variations of the Hartree-Fock Bogoliubov method combined with exact diagonalization, we track the development of the few-body mode into the regime of N~100 particles.

*This research was supported by the Swedish Research Council, the Knut and Alice Wallenberg foundation, and NanoLund at Lund University. GMB would like to acknowledge the support of the Villum Foundation and ESF POLATOM network.
A doping-dependent switch from one- to two-component electron-hole superfluidity with high transition temperatures in coupled TMD monolayers. SARA CONTI (Presenter), Univ of Antwerp, ANDREA PERALI, University of Camerino, DAVID NEILSON, FRANCOIS M PEETERS, Univ of Antwerp — Electron-hole (e-h) superfluidity in a Transition Metal Dichalcogenide heterostructure consisting of coupled MoSe$_2$-WSe$_2$ monolayers, is investigated using mean-field approach. We include self-consistent screening of the electron-hole interaction and the multibands effects arising from the strong spin-orbit band splitting [1].

The different magnitude of the valence and conduction band splitting results in a large energy misalignment of the electron and hole bands [2]. This misalignment is completely different if the doping of the monolayers is interchanged between MoSe$_2$(e)/WSe$_2$(h) and MoSe$_2$(h)/WSe$_2$(e), and depending on the choice of doping, the superfluidity may or may not be tuneable by density from one- to two-components. We find that only MoSe$_2$(h)/WSe$_2$(e) can have both one-component and two-component superfluidity.

The electron-hole pairing is much stronger than in graphene[3] due to the large effective masses so superfluidity is predicted for densities up to $10^{13}$ cm$^{-2}$. The transition temperatures are high, up to 100 K, which is consistent with a very recent experiment on the identical system[4].


Anomalous phase fluctuations of a superfluid flowing in a random potential* TAIKI HAGA (Presenter), MASAHITO UEDA, University of Tokyo — The phase structures of driven quantum many-body systems have attracted considerable interest owing to recent experimental progress in ultracold atomic gases. A fundamental issue in this subject is to clarify how and when the long-range order of a nonequilibrium steady state is destroyed by random perturbations. In thermal equilibrium, the Mermin-Wagner theorem can be invoked to address the stability of the ordered phase against thermal fluctuations. However, in nonequilibrium situations the universal mechanisms responsible for the breakdown of the long-range order are poorly understood. In this study, we investigate the stability of the off-diagonal long-range order of a superfluid flowing in a weak random potential [1]. Within the classical field theory, we show that for an arbitrarily small flow velocity the off-diagonal long-range order is destroyed in one and two dimensions. We argue that the superfluid flowing in a random potential can be identified with the corresponding uniform system at thermal equilibrium with an effective temperature, where the long-range order is prohibited in one and two dimensions by the Mermin-Wagner theorem.


*This work was supported by JSPS KAKENHI Grant Nos. JP19J00525 and JP18H01145.
Disordered Creutz lattice: The role of flat bands in superfluid behavior

CHEN CHENG, Center for Interdisciplinary Studies, Lanzhou University, China, GEORGE BATROUNI, Universite Cote d’Azur, INPHYNI, CNRS, 0600 Nice, France, RUBEM MONDAINI (Presenter), Beijing Computational Science Research Center, China — Physical systems displaying flat or quasi-flat bands have been intensively investigated due to the enhanced effects that interactions may bring. This is for example, believed to be behind the manifestation of superconductivity in the twisted bilayer graphene, where by adjusting the twisting angles, one can induce the formation of (quasi-) flat bands close to the Fermi energy. On a typically non-interacting picture, a flat band would correspond to an infinite effective mass for the carriers, halting transport. In the case one possess attractive interactions, it has been recently shown that superfluid transport is robust and the associated superfluid weight bounded by topological invariants the bands may possess. Further, when comparing the robustness of the superfluid properties to the presence of quenched disorder, the constrast between topological and non-topological systems becomes extremely clear. In this presentation, we will show results for the disordered Hubbard model with attractive interactions in the presence of flat or dispersive bands, checking the influence topological properties may possess in stabilizing the superfluid behavior in this interacting system.

The Dynamical Structure Factor of a Fermionic Super-solid on an Optical Lattice

PATRICK KELLY (Presenter), ETTORE VITALI, ANNETTE LOPEZ, California State University, Fresno, DAVIDE GALLI, GIANLUCA BERTAINA, Physics, University of Milan — We perform a Quantum Monte Carlo simulation and study of a cold atomic Fermi gas on a 2D optical lattice. This system is modeled with a Hubbard hamiltonian with on-site attractive interaction. At half-filling, when on average one fermion occupies each lattice site, with equal numbers of fermions spin up and spin down, the system displays an interesting supersolid phase: a superfluid with a checkerboard density modulation. Combining unbiased Auxiliary-Field Monte Carlo simulations with state-of-art analytic continuation techniques, we compute the density dynamical structure factor $S(\mathbf{q},\omega)$ of the system and the density response function $\chi(\mathbf{q})$, in order to characterize this supersolid phase. These results shed light on this interesting physical regime, where s-wave pairing superfluidity coexists with a non-uniform local density.
4:42PM U62.00012: Density-wave steady-state phase of dissipative ultracold fermions with nearest-neighbor interactions

IRAKLI TITVINIDZE (Presenter), JAROMIR PANAS, MICHAEL PASEK, ITP, Goethe University Frankfurt, ARYA DHAR, ITP, Leibniz Universität Hannover, TAO QIN, Anhui University, ANDREAS GEISSLER, ISIS, University of Strasburg, MOHSEN HAFEZ-TORBATI, ITP, Goethe University Frankfurt, MAX E. SORANTIN, ITP-CP, TU Graz, WALTER HOFSTETTER, ITP, Goethe University Frankfurt — In the current work, we investigate the effect of local dissipation on the presence of density-wave ordering in spinful fermions with both local and nearest-neighbor interactions, as described by the extended Hubbard model [1]. For this purpose we use the recently developed Lindblad dynamical mean-field theory (L-DMFT) [2,3], which allows to study directly steady-state properties of strongly correlated fermionic systems. To take into account nearest-neighbor interactions we perform a mean-field decoupling. We find the density-wave order to be robust against decoherence effects up to a critical point where the system becomes homogeneous with no spatial ordering. These results will be relevant for future cold-atom experiments using fermions with nonlocal interactions arising from the dressing by highly excited Rydberg states, which have finite lifetimes due to spontaneous emission processes.


*Support by the Deutsche Forschungsgemeinschaft via DFG SPP 1929 GiRyd, SFB/TR 49, the Austrian Science Fund (FWF) within Projects P26508 and F41 (SFB ViCoM).

The high-performance computing center LOEWE-CSC is gratefully acknowledged.

4:54PM U62.00013: Squeezed Photons Reconsidered

SAMUEL BOWEN (Presenter), Chemistry and Physics, Chicago State University, JAY D. MANCINI, Physics and Chemistry, Kingsborough Community College — Using an exact one-photon thermodynamic Green's Function determined by a matrix method for the Liouville operator, the relationship between squeezed photons and the amplitude of the vector potential is determined without the use of the usual coherent states or the squeezing operator. The Hamiltonian for each photon mode is determined for all levels of uncertainty to be given by an extended simple harmonic oscillator Hamiltonian. The matrix method used and the simplest approximation for the generation of squeezed photons is presented.

5:06PM U62.00014: Anomalous hydrodynamics in condensed matter systems

ALEXANDRE ABANOV (Presenter), Department of Physics and Astronomy, Stony Brook University — Fluid dynamics is a powerful tool in studying both quantum and classical many body systems. I will review recent progress in using fluid dynamics to describe two-dimensional isotropic fluids with broken parity. The viscous stress tensor for these fluids can possess an anomalous part known as odd or Hall viscosity. This peculiar viscosity does not lead to any dissipation in the fluid. Examples of fluids with odd viscosity include rotating superfluids, plasmas in magnetic fields, quantum Hall fluids, and chiral active fluids. I will describe some manifestations of the odd viscosity. In particular, I will focus on surface waves propagating along the boundaries of such fluids.

*NSF DMR-1606591, US DOE DESC-0017662
U62.00015: Collective modes for a Fermi Liquid under Harmonic Trap  YUELIN SHAO
(Presenter), Chinese Academy of Sciences, Institute of Physics, XIDAI, Physics, Hong Kong University of Science of Technology — Based on the Boltzmann transport equation of quasi-particles, we examine the low energy excitations of a normal Fermi liquid confined in a two-dimensional harmonic trap. In the non-interacting limit, the excitation spectrum is discrete and the highly degenerate eigenfrequencies locate exactly at integer multiples of the corresponding trap frequency. When the interaction is switched on, the degeneracy will be broken and every degenerate frequency will extend to be a continuous band but with some discrete modes out of the band. The continuum and discrete modes in the spectrum can be interpreted as particle-hole excitations and collective modes ("zero sound") respectively. For a repulsive interaction, the lowest collective mode frequencies are higher than those of the corresponding particle-hole excitations and can be detected by the experiments on cold atom systems.

Thursday, March 5, 2020 2:30 PM - 5:18 PM

Session U63 DCMP: Twisted 2D Heterostructures: Computational and Theoretical Studies II  Mile High Ballroom 4D - Nicolas Leconte

2:30PM U63.00001: Geometric and conventional contribution to superfluid weight in twisted bilayer graphene*  XIANG HU (Presenter), Physics, William and Mary, TIMO HYART, International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, DMITRY I. PIKULIN, Microsoft Quantum, Microsoft Station Q, University of California, Santa Barbara, ENRICO ROSSI, Physics, William and Mary — We calculate the superfluid weight for twisted bilayer graphene (TBLG) taking into account both the conventional contribution and the contribution arising from the quantum geometry of the bands. We find that both contributions are larger than one would expect by treating the bands as well-isolated, that at the magic angle the geometric contribution is larger than the conventional one, and that for small deviations away from the magic angle the conventional contribution is larger than the geometric one. Our results show that, despite the flatness of the bands the superfluid weight in TBLG is finite and consistent with experimental observations. We also show how the superfluid weight can be tuned by varying the chemical potential and the twist angle opening the possibility to tune the nature of the superconducting transition between the standard BCS transition and the Berezinskii-Kosterlitz-Thouless transition.

*Work funded by NSF Grant No. DMR-1455233 CAREER, ARO Grant No. W911NF-18-1-0290, and BSF Grant Number 2016320
**2:42PM U63.00002: Inherited and flatband-induced ordering in twisted graphene bilayers**
LENNART KLEBL (Presenter), CARSTEN HONERKAMP, RWTH - Aachen — The nature of the insulating and superconducting states in twisted bilayer graphene systems is intensely debated. While many works seek for explanations in the few flat bands near the Fermi level, theory and a number of experiments suggest that nontwisted bilayer graphene systems do exhibit – or are at least close to – an ordered, insulating ground state related to antiferromagnetic ordering. We investigate how this magnetic ordering scenario is affected by the slight twisting. We find that at charge neutrality the ordering tendencies of twisted systems interpolate between those of untwisted AA and AB stacked bilayers at intermediate temperatures, while at lower temperatures of the order of typical flat-band dispersion energies, the ordering tendencies are even enhanced for the twisted systems. The preferred order at charge neutrality still exhibits an antiferromagnetic spin arrangement, with ordered moments alternating on the carbon-carbon bonds, with an enveloping variation on the moiré scale (inherited ordering). Even in the RPA analysis, the possible low-energy behaviors are quite versatile, and slight doping of one or more electrons per moiré cell can take the system into a, potentially flat-band induced, ferromagnetic phase.

**2:54PM U63.00003: Moiré-pattern fluctuations and electron-phason coupling in twisted bilayer graphene**
HECTOR OCHOA (Presenter), Columbia University — In twisted bilayer graphene, long-wavelength lattice fluctuations are dominated by phasons: acoustic collective modes resulting from coherent superpositions of optical phonons. At small twist angles, these modes describe the sliding motion of stacking domain walls separating regions of partial commensuration. The resulting soliton network is a soft elastic manifold, whose reduced rigidity arises from the competition between elastic and adhesion forces governing lattice relaxation. Shear deformations of the beating pattern dominate the electron-phason coupling. This coupling lifts the layer degeneracy of the Dirac cones at the corners of the moiré Brillouin zone, which could explain the observed fourfold (instead of eightfold) Landau level degeneracy. Electron-phason scattering gives rise to a linear-T resistivity that increases with decreasing twist angle due to the reduction of the stiffness of the soliton network. This contribution alone cannot explain the huge enhancement of the resistivity of the normal state close to the magic angle. I will discuss the connection between these soft collective modes and the widespread presence of twist angle disorder in the samples.

*This work has been supported by the NSF MR-SEC program Grant No. DMR-1420634.*
3:06PM U63.00004: Spin-valley density wave in moiré materials*  CONSTANTIN SCHRADE
(Presenter), LIANG FU, Massachusetts Institute of Technology MIT — We introduce and study a minimum two-orbital Hubbard model on a triangular lattice, which captures the key features of both the trilayer ABC-stacked graphene-boron nitride heterostructure and twisted transition metal dichalcogenides in a broad parameter range. Our model comprises first- and second-nearest neighbor hoppings with valley-contrasting flux that accounts for trigonal warping in the band structure. For the strong-coupling regime with one electron per site, we derive a spin-orbital exchange Hamiltonian and find the semiclassical ground state to be a spin-valley density wave. We show that a relatively small second-neighbor exchange interaction is sufficient to stabilize the ordered state against quantum fluctuations. Effects of spin- and valley Zeeman fields as well as thermal fluctuations are also examined.

*This work was supported by DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0018945. Liang Fu was supported in part by a Simons Investigator Award from the Simons Foundation.

3:18PM U63.00005: Phonon scattering induced carrier resistivity in twisted double bilayer graphene  XIAO LI (Presenter), City Univ of Hong Kong, FENGCHENG WU, University of Maryland — In this work we carry out a theoretical study of the phonon-induced resistivity in twisted double bilayer graphene (TDBG), in which two Bernal-stacked bilayer graphene devices are rotated relative to each other by a small angle $\theta$. We show that at small twist angles ($\theta \sim 1^\circ$) the effective mass of the TDBG system is greatly enhanced, leading to a drastically increased phonon-induced resistivity in the high-temperature limit where phonon scattering leads to a linearly increasing resistivity with increasing temperature. We also discuss possible implications of our theory on superconductivity in such a system, and provide an order of magnitude estimation of the superconducting transition temperature.

3:30PM U63.00006: Functional renormalization group analysis of many-body states in a large moiré unit cell systems*  LENNART KLEBL, DANTE M. KENNES, CARSTEN HONERKAMP (Presenter), RWTH Aachen University — Layers of two-dimensional materials arranged at a twist angle with respect each other lead to enlarged unit cells with potentially strongly altered band structures, offering a new arena for novel and engineered many-body ground states. For the exploration of these, renormalization group methods are an appropriate, flexible tool that takes into account the mutual influence of competing tendencies. We show how the functional renormalization group known from simpler two-dimensional systems can be employed for the large-unit cell moiré superlattices, providing a description on the atomic scale and absorbing available ab-initio information on the model parameters. For the case of twisted bilayer graphene models, we explore the leading ordering tendencies depending on the band filling and the range of interactions. The results indicate a delicate balance between distinct magnetically ordered ground states.

*DFG-RTG 1995
3:42PM U63.00007: Three-Dimensional Topological Twistorics

FENGCHENG WU (Presenter), RUIXING ZHANG, University of Maryland — We introduce a theoretical framework for the new concept of three-dimensional (3D) twistronics by developing a generalized Bloch band theory for 3D layered systems with a constant twist angle \( \theta \) between successive layers. Our theory employs a nonsymmorphic symmetry that enables a precise definition of an effective out-of-plane crystal momentum, and also captures the in-plane moire pattern formed between neighboring twisted layers. To demonstrate the novel topological physics that can be achieved through 3D twistronics, we present two examples. In the first example of chiral twisted graphite, Weyl nodes arise because of inversion-symmetry breaking, with \( \theta \)-tuned transitions between type-I and type-II Weyl fermions, as well as magic angles at which the in-plane velocity vanishes. In the second example of twisted Weyl semimetal, the twist in the lattice structure induces a chiral gauge field \( A \) that has a vortex-antivortex lattice configuration. Line modes bound to the vortex cores of the \( A \) field give rise to 3D Weyl physics in the moire scale. We also discuss possible experimental realizations of 3D twistronics.


*This work is supported by the Laboratory for Physical Sciences and Microsoft.

3:54PM U63.00008: Ferromagnetic Mott state in twisted graphene bilayers at the magic angle

KAGNJUN SEO, Univ of Oklahoma, VALERI KOTOV, Department of Physics, University of Vermont, BRUNO UCHOA (Presenter), Univ of Oklahoma — We address the effective tight-binding Hamiltonian that describes the insulating Mott state of twisted graphene bilayers at a magic angle [1]. In that configuration, twisted bilayers form a honeycomb superlattice of localized states, characterized by the appearance of flat bands with fourfold degeneracy. After calculating the maximally localized superlattice Wannier wave functions, we derive the effective spin model that describes the Mott state at quarter filling, which has an emergent SU(4) symmetry that is reminiscent of spin and valley quantum numbers. We suggest that the system is an exotic ferromagnetic Mott insulator, with well-defined experimental signatures.


*K. S. and B. U. acknowledge NSF CAREER Grant No. DMR-1352604 for support.
4:06PM U63.00009: Theory of generalized Wigner crystals in moire superlattices.  BIKASH PADHI (Presenter), University of Illinois at Urbana-Champaign, CHITRA RAMASUBRAMANIAN, Physics, ETH Zurich, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — Recent developments in moire materials (twisted layers of graphene or transition metal compounds) has opened up a new avenue to realize quasi-flat bands in condensed matter systems in which the interactions dominate. Our previous calculations suggested that the correlations in such systems could be strong enough to realize electronic solids called Wigner crystals (WC). Such states have been observed before in (continuum) 2D electron gas and recently it was also claimed to be observed in a (moire lattice of) twisted bilayer of WS/WSe2. Despite the experimental advances, a clear understanding of the physics of WC coupled to an underlying lattice is completely lacking. In this talk we present some preliminary results based on a model we construct to address this problem. In such a scenario, melting of a WC (coupled to lattice) can be understood in terms of an interplay of coulomb interaction and the tendency for forming solitons.

4:18PM U63.00010: Floquet flat-band engineering of twisted bilayer graphene*  OR KATZ (Presenter), Technion - Israel Institute of Technology, GIL REFAEL, Institute of Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, California 91125, USA, NETANEL LINDNER, Technion - Israel Institute of Technology — Twisted Bilayer Graphene at the magic twist angle features flat energy bands, which lead to superconductivity and strong correlation physics. These unique properties are typically limited to an extremely narrow range of twist angles around the magic angle. Here we demonstrate that coherent optical irradiation could lead to emergence of flat isolated Floquet-Bloch bands at a wide range of small twist angles. At small twist angles larger than 1°, these bands exhibit non-trivial topology and a non-zero chern number. We show that the effect can potentially be realized with relatively weak optical beams at the visible-infrared range, potentially allowing for realization of optically tuned flat bands.

*N.L. and O.K. acknowledge financial support from the European Research Council (ERC) under the European Union Horizon 2020 Research and Innovation Programme (Grant Agreement No. 639172). We acknowledge support from the IQIM, an NSF physics frontier center funded by Gordon and Betty Moore foundation. We are grateful for support from ARO MURI W911NF-16-61-0361 “Quantum Materials by Design with Electromagnetic Excitation” sponsored by the U.S. Army. This work was performed in part at Aspen Center for Physics, which is supported by National Science Foundation grant PHY-1607611.
4:30PM U63.00011: Mirror symmetry breaking and the stacking-shift effect in twisted trilayer graphene* CHAO LEI (Presenter), University of Texas at Austin, LUKAS LINHART, Vienna University of Technology, WEI QIN, ALLAN MACDONALD, University of Texas at Austin — A continuum model of twisted trilayer graphene devices was constructed using ab initio first principles theory to assess the dependence of electronic structure on local stacking. We have applied the model to study electronic structure and transport properties as a function of band filling. When the middle layer of Bernal stacking trilayer graphene is twisted a mirror symmetry exists which is absent in the case of twisted top layers and twisted bilayer graphene. The mirror symmetry decouples band with even and odd parity, but is lost when the top layer is shifted relative to the bottom layer or an electric field is applied. We study the consequences of mirror and C3v symmetry breaking by this top layer lateral stacking shift effect or electric field, focusing on the electronic structure and transport properties such as the longitudinal and Hall conductivities of this system. Whereas a lateral shift has no effect for either top layer twisted trilayers or bilayers, large changes in electronic structure occur for middle-layer twisted trilayers.

*Work in University of Texas at Austin was supported by DOE grant DE- FG02-02ER45958

4:42PM U63.00012: Derivation of Wannier orbitals and minimal-basis tight-binding Hamiltonians for twisted bilayer graphene: First-principles approach* STEPHEN CARR (Presenter), SHIANG FANG, Harvard University, HOI CHUN PO, Massachusetts Institute of Technology, ASHVIN VISHWANATH, EFTHIMIOS KAXIRAS, Harvard University — The complexity of the atomic-scale structures in twisted bilayer graphene (TBG) has made even the study of single-particle physics at low energies around the Fermi level challenging. We provide a convenient and physically motivated picture of single-particle physics in TBG using reduced models with the smallest possible number of localized orbitals. The reduced models exactly reproduce the low-energy bands of ab initio tight-binding models, including the effects of atomic relaxations. We obtain for the first time the corresponding Wannier orbitals that incorporate all symmetries of TBG, which are also calculated as a function of angle, a requisite first step towards incorporating electron interaction effects. We construct eight-band and five-band models for the low-energy states for twist angles between 1.3° and 0.6°.

*This work was supported by 704 the STC Center for Integrated Quantum Materials, NSF Grant 705 No. DMR-1231319 and by ARO MURI Award W911NF-706 14-0247. H.C.P. was supported by a Pappalardo Fellowship 707 at MIT and a Croucher Foundation Fellowship. A.V. was 708 supported by a Simons Investigator award and NSF-DMR 709 1411343.
We study the collective modes of the correlated insulating states in magic-angle twisted bilayer graphene (MATBG) within the framework of the generalized random phase approximation (GRPA), also known as the time-dependent Hartree-Fock approximation (TDHFA), using a continuum model and assuming insulating states that break spin/valley flavor but not translational symmetries. The calculations confirm the stability of the translationally invariant states and provide values for key energy scales associated with low-energy collective fluctuations, including spin-stiffnesses and gaps for valley-wave modes. We find that zone-boundary collective mode energies are an order of magnitude smaller than the charge gaps. By fitting to the calculated collective excitation spectra, we derive generalized spin models that fully capture the low-energy physics. Finally, we discuss how these collective mode energies vary with moiré band filling factor and the possible role of their coupling to Fermi surface quasiparticles in superconductivity and non-Fermi liquid behavior.

This work was supported by DOE grant DE- FG02-02ER45958, as well as by the National Science Foundation through the Center for Dynamics and Control of Materials: an NSF MRSEC under Cooperative Agreement No. DMR-1720595.

Lattice mismatch between graphene and a substrate produces local variations in the density of states (LDOS) as observed in STM images. These are known as moire patterns, in analogy with classical interference produced by two overlapping periodic arrays. These have been observed in twisted bilayer graphene[1], a system that can be thought of as monolayer graphene deposited on a substrate with misaligned crystalline orientations. In this regime, the resulting charge density distribution is related to superconductor and Mott insulator phases observed in experiments. It is natural to wonder if similar features could be obtained by depositing graphene on engineered substrates inducing modulated strain fields. Starting from the simplest case of two overlapping deformations, we obtain the LDOS profile for a one-dimensional array, and show the emergence of a different periodicity, a feature associated with moire patterns. We identify conditions for discrete and continuous charged regions, and extend our results to a 2D close-packed structure, demonstrating that periodic deformations can be used to generate moire patterns.

2:30PM U64.00001: Signature of Dispersing 1D Majorana Channels in an Iron-based superconductors [Invited]  ZHENYU WANG (Presenter), UIUC — Selected by Focus Topic Organizer (Seongshik Oh and Peter Armitage)

3:06PM U64.00002: Physical Properties of XTSb[(X= Eu, Sr), (T= Ag, Au)] single crystals* PARUL DEVI (Presenter), LIN-LIN WANG, CAIDEN ABEL, SERGEY L. BUD’KO, PAUL C CANFIELD, Ames Lab — Single crystals of XTSb [(X= Eu, Sr), (T= Ag, Au)] were grown by the solution growth by using self flux [1]. These single crystals were investigated by powder X-ray diffraction at room temperature and the structure was successfully refined to be the hexagonal (space group $P63/mmc$) crystal structure. Temperature dependent magnetic susceptibility measurements indicate antiferromagnetic ordering for magnetic compounds (e.g. $T_N = 6$ K for EuAgSb). Density functional theory calculations find that the band inversion giving a Dirac point is present in the non-magnetic Au compounds, but not the Ag compounds. Thermodynamic and transport data on the non-magnetic SrAgSb, SrAuSb and magnetic EuAgSb, EuAuSb will be presented and compared.

Reference:

*This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering. The research was performed at Ames laboratory. Ames laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358. PD and LLW were supported by the Center for Advancement of Topological Semimetals, an Energy Frontier Research Center funded by the U.S. DOE, Office of Basic Energy Sciences.

3:18PM U64.00003: Ab initio study of surface states in Bi$_4$Te$_3$* OMAR ASHOUR (Presenter), ZHENGLU LI, STEVEN LOUIE, Department of Physics, University of California, Berkeley, Berkeley, California 94720, USA and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, C — The crystal structure of the layered material Bi$_4$Te$_3$, a member of the adaptive series of crystals (Bi$_2$)$_n$(Bi$_2$Te$_3$)$_n$, forms a superlattice of alternating Bi$_2$ and Bi$_2$Te$_3$ layers. Given the topological properties of its individual constituents, Bi$_4$Te$_3$ is expected to be a topological insulator or semimetal. Recent experimental results indicate the presence of unusual surface states in this material. In this work, we perform ab initio density functional theory calculations of bulk and slab geometries to investigate the surface states of Bi$_4$Te$_3$.

*This work was supported by the Theory of Materials Program at the Lawrence Berkeley National Laboratory funded by the U.S. Department of Energy, Office of Basic Energy Sciences under Contract No. DE-AC02-05CH11231, and by the National Science Foundation. Computational resources were provided by NERSC and XSEDE.
3:30PM U64.00004: Bond Disproportionation in the Silver Bismuthate Ag$_2$BiO$_3$  MOHAMED OUDAH (Presenter), University of British Columbia, MINU KIM, KSENIA RABINOVICE, GRAHAM MCNALLY, BERKAY KILIC, KATHRIN KÜSTER, Max Planck Institute for Solid State Research, ROBERT GREEN, KATERYNA FOYEVTSOVA, University of British Columbia, ALEXANDER BORIS, Max Planck Institute for Solid State Research, GEORGE ALBERT SAWATZKY, University of British Columbia, ANDREAS SCHNYDER, Max Planck Institute for Solid State Research, DOUGLAS ANDREW BONN, University of British Columbia, BERNHARD KEIMER, Hidenori Takagi, Max Planck Institute for Solid State Research — The stoichiometric silver bismuthate Ag$_2$BiO$_3$ is expected to contain bismuth in the nominal Bi$^{+4}$ state, but the bismuth ions disproportionate into two distinct sites that render Ag$_2$BiO$_3$ insulating [1]. Recent theoretical predictions of metal-insulator transition and Weyl semimetal state in Ag$_2$BiO$_3$ have revived the interest in this material [2]. However, such novel properties are only expected in the absence of disproportionation of bismuth, where Ag$_2$BiO$_3$ is in the Pnma phase. Here, we examine nature of disproportionation in Ag$_2$BiO$_3$ via X-ray absorption and photoemission spectroscopies. We present an updated band structure for Ag$_2$BiO$_3$ in the Pnn2 (disproportionated) phase, where we have a band gap of 1 eV in agreement with our optical spectroscopy measurement. Furthermore, we present Raman spectroscopy results and highlight the extent of similarities to other disproportionated bismuthates despite the distinct crystal structure Ag$_2$BiO$_3$.


3:42PM U64.00005: Analytic calculation of generalized Brillouin zone in non-Hermitian bands*  ZHESEN YANG (Presenter), KAI ZHANG, CHEN FANG, JIANGPING HU, Chinese Academy of Sciences, Institute of Physics — In this talk, we introduce a systematic method to calculate the generalized Brillouin Zone (GBZ) analytically in one dimensional non-Hermitian systems. In general, a m-band non-Hermitian Hamiltonian is constituted by m distinct sub-GBZs, each of which is a piecewise analytic closed loop. All the analytic properties of the GBZ can be characterized by an algebraic equation, which is dubbed as auxiliary GBZ. As an application of our theory, we show a new kind of topological phase under open boundary condition, which is characterized by the non-zero energy winding number for each band.

*The work is supported by the Ministry of Science and Technology of China 973 program (No. 2015CB921300, No. 2017YFA0303100), National Science Foundation of China (Grant No. NSFC-11888101, 1190020, 11534014, 11334012), and the Strategic Priority Research Program of CAS (Grant No.XDB07000000).
3:54PM U64.00006: Materials database development for electromagnetic responses*  YAN SUN (Presenter), YANG ZHANG, QIUNAN BU, JONATHAN NOKY, Max Planck Institute for Chemical Physics of Solids, JAKUB ZELEZNY, Institute of Solid State Physics, Czech Academy of Sciences, KLAUS KŒPERNIK, Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany, TOMAS JUNGWIRTH, Institute of Solid State Physics, Czech Academy of Sciences, JEROEN VAN DEN BRINK, Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids — The interplay between electromagnetic response theory and symmetry is crucial to understand the transport properties in quantum materials. It is critical to fully understand these physical properties and find materials that host strong electromagnetic response, which, have an extensive impact on the development of data storage, information processing, and energy conversion, etc. Experimentally, however, such large-scale screening is very impractical, as a quantitative determination of the electromagnetic responses by electrical and optical measurements requires integrating each material separately into a complex multicomponent mesoscopic transport device. Theoretically and computationally, the situation is in principle much more straightforward. Via high throughput numerical simulations, we developed the database for intrinsic spin Hall effect in nonmagnetic compounds, shift current in inversion symmetry Weyl semimetals, anomalous Hall effect and anomalous Nernst effect in magnetic Heusler compounds based on the known materials. Our database is helpful for the full understanding of the electronic properties of materials and selecting the correcting materials for further experimental studies.

*ERC Advanced Grant No. 291472 `Idea Heusler',
ERC Advanced Grant No. 742068 `TOPMAT'.

4:06PM U64.00007: Reentrant Defect Modes in a PT-Symmetric Circuit*  ALEXANDER STEGMAIER (Presenter), TOBIAS HELBIG, TOBIAS HOFMANN, RONNY THOMALE, Theoretical physics I, University of Wuerzburg — Systems obeying PT-symmetry are a special case in non-Hermitian physics where real eigenvalue spectra can still emerge. They usually exhibit a phase diagram with different regimes of symmetry conservation or spontaneous symmetry breaking in their eigenstates. We examine a localized zero-energy defect mode within a PT-symmetric hopping model that disappears and re-emerges at different PT phase transitions and present an exhaustive explanation for this phenomenon. Our theoretical findings are confirmed by eigenstate measurements for different gain/loss profiles in an electrical circuit implementation.

Distinct multiple fermionic states in a single topological metal* [Invited]

MADHAB NEUPANE (Presenter), Univ of Central Florida — Among the quantum materials that have recently gained interest are the topological insulators, wherein symmetry-protected surface states cross in reciprocal space, and the Dirac nodal-line semimetals, where bulk bands touch along a line in momentum space. However, the existence of multiple fermion phases in a single material has not been verified yet. Using angle-resolved photoemission spectroscopy (ARPES) and first-principles electronic structure calculations, here we discuss a systematic study of the metallic ternary material discovering properties, which are unique in a single topological quantum material. We experimentally observe weak topological insulator surface states and our calculations suggest the existence of additional strong topological insulator surface states. Our first-principles calculations reveal a one-dimensional Dirac crossing—the surface Dirac-node arc —along a high-symmetry direction, which is confirmed by our ARPES and time-resolved ARPES measurements. Furthermore, we will present our recent results on the experimental observation of new topological quantum materials. These are topological superconductors and magnetic topological materials which were discovered through ARPES and time-resolved ARPES measurements with further support from first-principles calculations.

*This work is supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0415, the National Science Foundation (NSF) CAREER award DMR-1847962 and the Center for Thermal Energy Transport under Irradiation, an Energy Frontier Research Center funded by the U.S. DOE, Office of Basic Energy Sciences.

Anomalous quantum oscillations in a spin-3/2 topological semimetal: I. Experiment

HYUNSOO KIM (Presenter), JUNHYUN LEE, HALYNA HODOVANETS, KEFENG WANG, JAY SAU, JOHNPIERRE PAGLIONE, University of Maryland, College Park — Gapless spin-3/2 quasiparticles lead to an unprecedented class of high-spin topological superconductivity which hosts a Majorana fluid on the surface. The spin-3/2 Fermi surface can be realized in a crystal lattice with high symmetry. The RPtBi (R=rare earth) half-Heuslers are a family of promising candidates, in which strong spin-orbit interaction inverts the Bi p-orbital derived bands and Bi s-orbital derived bands. In this particular case, the low energy quasiparticles are adequately described by the four-band Luttinger–Kohn model. In this talk, we report compelling evidence for a spin-3/2 Fermi surface in YPtBi via studies of the angle-dependent Shubnikov-de Haas (SdH) effect uniquely explained by the anisotropic effect of Zeeman interaction on spin-3/2 quasiparticles, confirming the long-awaited high-spin nature of topological semimetal RPtBi compounds.
5:06PM U64.00010: Anomalous quantum oscillations in a spin-3/2 topological semimetal: II. Theory JUNHYUN LEE (Presenter), HYUNSOO KIM, HALYNA HODOVANETS, KEFENG WANG, JAY SAU, JOHNPIERRE PAGLIONE, University of Maryland, College Park — Gapless spin-3/2 quasiparticles lead to an unprecedented class of high-spin topological superconductivity which hosts a Majorana fluid on the surface. The spin-3/2 Fermi surface can be realized in a crystal lattice with high symmetry. The RPtBi (R=rare earth) half-Heuslers are a family of promising candidates, in which strong spin-orbit interaction inverts the Bi p-orbital derived bands and Bi s-orbital derived bands. In this particular case, the low energy quasiparticles are adequately described by the four-band Luttinger–Kohn model. In this talk, we report compelling evidence for a spin-3/2 Fermi surface in YPtBi via studies of the angle-dependent Shubnikov-de Haas (SdH) effect uniquely explained by the anisotropic effect of Zeeman interaction on spin-3/2 quasiparticles, confirming the long-awaited high-spin nature of topological semimetal RPtBi compounds.

U64.00011: Correspondence between winding numbers and skin modes in non-hermitian systems KAI ZHANG (Presenter), ZHESEN YANG, CHEN FANG, Chinese Academy of Sciences, Institute of Physics — We establish exact relations between the winding of “energy” (eigenvalue of Hamiltonian) on the complex plane as momentum traverses the Brillouin zone with periodic boundary condition, and the presence of “skin modes” with open boundary condition in non-hermitian systems. This correspondence is exactly related to our new understanding of generalized Brillouin zone, which is the curve defined on the complex plane and always surrounding the same number of zeros and poles of characteristic equation of the system. We show that the nonzero winding with respect to any complex reference energy leads to the presence of skin modes, and vice versa. We also show that both the nonzero winding and the presence of skin modes share the common physical origin that is the non-vanishing current through the system.

Thursday, March 5, 2020 2:30 PM - 5:18 PM

2:30PM U65.00001: Stable White Light-Emitting Diodes using Metal Halide Perovskites

GOPI ADHIKARI (Presenter), SAROJ THAPA, HONGYANG ZHU, PEIFEN ZHU, Department of Physics and Engineering Physics, University of Tulsa — Inorganic lead halide perovskite nanocrystals (NCs) are emerging as attractive materials for their applications in modern lighting technologies due to their excellent optoelectronic properties. However, the inclusion of toxic element (lead) and stability issues in the perovskite NCs hinder their practical applications in the devices. Here, we report on the transformation of lead halide perovskite NCs to lead depleted (by 20 %) perovskite NCs and incorporation of lead depleted perovskite NCs in the commercially available polymers. As a result, the composites retain the excellent optical properties without degrading photoluminescence quantum yield. Furthermore, we have fabricated white light-emitting diodes (WLEDs) using these composites. Bright white light is achieved with superior color quality. Thus, this work demonstrates that the halide perovskite NCs are promising alternatives to conventional phosphors for the fabrication of efficient, less-toxic, and stable WLEDs.

*The University of Tulsa Faculty Start-up Fund.

2:42PM U65.00002: Switchable Excitonic Circular Polarization in CdSe/CdMnS Nanoplatelets with Bilayer Core and Magnetically Doped Shell

ARMAN NAJAFI (Presenter), STEVEN TARASEK, Department of Physics, State University of New York at Buffalo, Buffalo, New York, SAVAS DELIKANLI, Department of Electrical and Electronics Engineering, Department of Physics, UNAM-Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey, PEIYAO ZHANG, TENZIN NORDEN, Department of Physics, State University of New York at Buffalo, Buffalo, New York, SUSHANT SHENDRE, MANOJ SHARMA, LUMINOUS! Centre of Excellence for Semiconductor Lighting and Displays, School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore, Singapore, ARINJOY BHATTACHARYYA, Department of Physics, State University of New York at Buffalo, Buffalo, New York, NIMA TAGHIPOUR, Department of Electrical and Electronics Engineering, Department of Physics, UNAM-Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey, JAMES PIENTKA, Department of Physics, St. Bonaventure University, St. Bonaventure, New York, HILMI VOLKAN DEMIR, LUMINOUS! Centre of Excellence for Semiconductor Lighting and Displays, School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore, Singapore, ATHOS PETROU, TIM THOMAY, Department of Physics, State University of New York at Buffalo, Buffalo, New York — We have utilized time-resolved photoluminescence (TRPL) to study the excitonic circular polarization from CdSe/CdMnS core/shell nanoplatelets (NPLs) with a bilayer core. This technique allows detailed study of the emission dynamics as a function of magnetic field, temperature, doping concentration, and excitation wavelength.

In the presence of an external magnetic field, pulsed excitation below the shell gap results in near-zero circular polarization at all times. In contrast, pulsed excitation with a photon energy larger than the shell gap results in a rapid (100 ps) build-up of the excitonic circular polarization which subsequently remains constant at a level of up to 40%.

We explore a model that describes these results; we also discuss possible applications.
Controlling Linear and Nonlinear Optical Properties of Boron Nitride with Moiré Superlattices

SAMUEL MOORE (Presenter), NATE FINNEY, KAIYUAN YAO, LEO MCGILLY, GUANGXIN NI, EVAN TELFORD, P. JAMES SCHUCK, CORY DEAN, JAMES C HONE, ABHAY NARAYAN, DMITRI BASOV, Columbia University — Van der Waals materials enable the creation of artificial heterostructures with exciting new emergent properties. Recently, the twist angle between adjacent layers has proved to be an important control parameter in these stacks. In this work, we use conventional dry-transfer techniques to fabricate small-twist-angle few-layer hexagonal boron nitride (hBN) heterostructures. We study the resulting moiré superlattice with a variety of linear and nonlinear atomic force microscopy probes. These techniques yield a local variation of the transverse-optical-phonon oscillator strength, near-field second harmonic generation, and the piezoelectric response. These combined demonstrations of hBN moiré physics implicate local strain as an important tuning parameter for the linear and nonlinear optical properties of Van der Waals materials.

Photoluminescence study of non-polar m-plane InGaN and near strain-balanced AlGaN/InGaN superlattices

YANG CAO (Presenter), ALEXANDER SENICHEV, BRANDON DZUBA, TRANG NGUYEN, MICHAEL MANFRA, OANA MALIS, Physics and Astronomy, Purdue Univ — We present the first detailed study of the temperature-dependence of photoluminescence (PL) from m-plane bulk In$_x$Ga$_{1-x}$N ($x<0.25$) layers and near strain-balanced AlGaN/InGaN superlattices grown by plasma-assisted molecular-beam epitaxy on free standing m-plane GaN substrates. The experimental PL peak positions were found to deviate from inter-band transition energies calculated using structural parameters obtained from high-resolution x-ray diffraction. The effect is stronger for superlattices than for bulk InGaN films. The temperature dependence of PL suggests the discrepancy is due to localization centers in InGaN. The low-temperature PL linewidths are narrower than some published results for both In$_x$Ga$_{1-x}$N ($x<0.1$) and Al$_{0.2}$Ga$_{0.8}$N/In$_{0.09}$Ga$_{0.91}$N superlattices indicating lower alloy inhomogeneity than previously reported. We also observed the PL intensity drops dramatically as temperature increases. This suggests the presence of a high-density of non-radiative defects. We will describe our efforts to optimize growth conditions to increase PL efficiency and reduce PL linewidth at room temperature.

*TN, YC, and OM acknowledge partial support from NSF grant NSF-DMR 1610893. AS and BD were supported from NSF award ECCS-1607173.
3:18PM U65.00005: Backward output-side-grooves regulated light wave resonance in a subwavelength metallic slit and an ultrahigh energy accumulator* JIAN-SHIUNG HONG (Presenter), KUAN-REN CHEN, Department of Physics, National Cheng Kung University — Featuring conceptual breakthroughs in subwavelength wave mechanics, our work studies the output-side groove effect and finds a backward coupling mechanism. The transmitted light is scattered by the grooves and then re-enters into the slit. In one case study, this causes a phase delay of the reflected wave and is considered a reduction in the resonant film thickness. The traveling wave in the slit can be more in phase to significantly enhance the transmission. For another arrangement of the grooves, we find that the wave reflection inside the slit is raised up to 100% due to backward coupling. As the same arrangement of the grooves are patterned at the entrance side of the slit, an incident wave on the slit will be trapped in roundtrips after the transmission through the entrance. At resonance, the roundtrip wave is superposed constructively. Our analysis yields that the intensity of the time-averaged energy can be five million times that of the incident wave. This finding is groundbreaking in subwavelength optics and should have many applications in nonlinear optics, particle trapping, biomedicine, etc.

*Ministry of Science and Technology, Taiwan, and National Center for High-performance Computing

3:30PM U65.00006: Nonreciprocal spatio-temporal modulated metasurfaces* DIEGO ALEJANDRO DALVIT (Presenter), ANDREW CARDIN, SINHARA SILVA, SHAI VARDENY, Los Alamos Natl Lab, WILLIE PADILLA, Duke University, AVADH SAXENA, ANTOINETTE TAYLOR, WILTON J DE MELO KORT-KAMP, HOU-TONG CHEN, ABUL AZAD, Los Alamos Natl Lab — Spatio-temporal modulated metasurfaces (STMMs) are dynamic two-dimensional arrays of sub-wavelength resonators with arbitrary reflection amplitude and phase reconfigurability, and have the potential to revolutionize fundamental and applied photonics. Just as their static counterparts, STMMs can also enable arbitrary wave-front engineering with the key advantage of on-demand reconfigurability and control of the frequency and momentum harmonic contents of scattered waves. In this talk I will report our recent theory and experimental advances in STMMs for dynamical wave-front shaping and nonreciprocal propagation of free space electromagnetic waves. Our experimental measurements reveal on-demand wave-front control of frequency conversion processes. We also demonstrate maximum violation of Lorentz reciprocity in both beam steering and focusing due to nonreciprocal excitation of surface waves. We develop an analytical generalized Bloch-Floquet theory valid for arbitrary modulations, providing excellent agreement with the experiments.

*Research presented in this paper was supported by the Laboratory Directed Research and Development program of Los Alamos National Laboratory.
3:42PM U65.00007: Bright magnetic dipole radiation from two-dimensional lead halide perovskites  
RYAN DECRESCENT (Presenter), NAVEEN VENKATESAN, CLAYTON J DAHLMAN, 
RHIANNON (RHYS) M KENNARD, XIE ZHANG, University of California, Santa Barbara, 
WENHAO LI, Brown University, XINHONG DU, MICHAEL L. CHABINYC, University of California, Santa Barbara, 
RASHID ZIA, Brown University, JON A SCHULLER, University of California, Santa Barbara — 

Two-dimensional (2D) hybrid organic-inorganic perovskites (HOIPs) comprise a versatile class of solution-processable materials with outstanding optoelectronic properties. Analogous to conventional semiconductors, light-matter interactions in 2D HOIPs have been completely described within the electric dipole (ED) approximation. Here, using energy-momentum spectroscopies, we demonstrate that the ED approximation insufficiently describes light-matter interactions in 2D HOIPs. We identify an optical transition in 2D HOIPs that exhibits striking multipolar radiation patterns at an energy 90 meV below the primary exciton emission. The transition is evidently intrinsic in origin and arises from an unconventionally fast magnetic dipole (MD) transition from a polaron-like excited state. These results suggest the presence of even-parity excited state symmetries that have not yet been established, and represent the first observation of MD optical interactions in a bulk crystal. In addition to being of fundamental interest, this demonstration may be crucial for resolving open questions regarding the previously observed bounty of complex optical signatures in 2D HOIPs, and may have implications for quantum information applications based on “dark” excitons in 2D materials.

3:54PM U65.00008: Photon circulation in photonic structures integrated with quantum dots - a consequence of multi-path geometry  
PALAK DUGAR (Presenter), MICHAEL SCHEIBNER, CHIH-CHUN CHIEN, University of California, Merced — 

The typical route to achieve circulation of photons is via artificial gauge fields. We show that even without any artificial gauge field, by using multiple path geometry such as, that of a triangle and the quantum nature of bosonic particles, the steady state photonic current can circulate in a photonic structure integrated with quantum dots. Our system is made up of three quantum dots which are connected in a triangular geometry, this geometry is embedded in photonic crystal and waveguide. The photon-exciton interaction limits the number of photons that can be transferred between the quantum dots, a phenomenon also called photon blockade. We use the Lindblad form of the quantum optical master equation to calculate the steady state currents with the maximal photon number per site set by the photon blockade. Our results show that the photon circulations have a non-trivial dependence not only on the internal system parameters such as the tunneling coefficient, or the effective photon-photon interaction but also on external parameters such as the system-reservoir coupling. This system can be tailored to function as a density independent local pump or memory device.
Temperature-dependent photoluminescence of carbon quantum dots

Temperature-dependent photoluminescence (PL) and time-resolved PL (TRPL) of carbon quantum dots (CQD) were investigated to explain the possible source of luminescence. XPS, PL, and UV-Vis absorption measurements suggest that the nitrogen-related functional groups, emission, and absorption depend on the amount of the CQD in the film. The energy loss between the absorption and emission spectra indicates the presence of vibrational relaxation in CQD films. The 0-0 transition peaks of the CQD films exhibit blueshift with faster decay time as temperature increases. This temperature-dependent blueshift and lifetimes possibly indicate the presence of thermally activated hopping sites which was also seen in another organic semiconductors. These hopping sites are related to nitrogen-based functional groups which are confirmed by the presence of additional deconvoluted peaks in the C1s high resolution XPS measurements. These measurements show that the presence of the conjugated functional groups is the primary reason for the exciton diffusion dynamics in the CQD. However, the excessive amount of CQD in the film results increases reabsorption and re-emission process. Thus, limiting the temperature-dependent PL and TRPL behaviors of films with larger amount of CQD.

Ultra-thin film nanophotonics device on various optics application

The vast majority of optical metamaterial are fabricated on rigid substrates. Ultra-thin thickness and resulting mechanical flexibility in nanophotonics is the key attribute of various optics device including flexible imaging/display arrays, wearable photonics device, spectrometer, mechanics drive holography, multi-layer stacking Photonic device. Our fabrication techniques majorly depend on stamp transfer of dielectric material or direct patterning on flexible substrate. The significant difference is that fabricated device on past researches is all on thick polymer substrate. When direct bond such kind of flexible chip to any other devices, the thick substrate will damage the optical properties because of the scattering and reflection. Our flexible substrate is 200nm - 3 um PMMA, the thickness of which can be precisely controlled. The subwavelength thickness of this PMMA film will primarily reduce scattering and reflection optical reflection, which it will also protect the device surface. Furthermore, the ultra-thin PMMA layer is easy to remove after sticking the metasurface + PMMA to devices by special removing tape. Our ultra-thin PMMA substrate flexible device enables direct integration of optical metasurface to various optical devices like another metasurafce.
Extraordinary Transmission in Coupled Nano-Bridged Nanosphere Quasi-Complimentary Arrays

TYLER DODGE (Presenter), Boston College, LINGPENG LUO, ESER METIN AKINOGLU, International Academy of Optoelectronics at Zhaoqing, South China Normal University, MICHAEL NAUGHTON, Boston College, MICHAEL GIERSIG, International Academy of Optoelectronics at Zhaoqing, South China Normal University, KRZYSZTOF KEMPA, Boston College — Ultra-sensitive structures can be based on percolation, which at the threshold radically change their response (e.g. conduction, transmission, etc.). However, due to the critical nature, such structures are very unstable at the threshold. Here, we demonstrate that the stability can be restored, with minimal loss of sensitivity, by engineering weak links between the units of a percolation system. Our system consists of a pair of strongly coupled complementary arrays made of metallic films, obtained by depositing plasmonic metal on a periodic array of spheres with submicron dimensions through a modified standard nanosphere lithography (NSL). In an earlier work we demonstrated, that the modification of NSL leads to the formation inter-sphere nano-bridges, which after metallic deposition work as the weak links. We simulate plasmonics of these arrays, demonstrating ultrahigh sensitivity and stability of the extraordinary optical transmission (EOT) of this structure near the percolation threshold.

Exciton–phonon coupling in resonant Raman scattering: intrinsic attributes and extrinsic tunability in ZnTe of different dimensionalities

YINGYAN YI, JASON K MARMON, Univ of North Carolina - Charlotte, YUANPING CHEN, US Army Research Laboratory, FAN ZHANG, TAO SHENG, Univ of North Carolina - Charlotte, PRIYALAL S. WIJEWARNASURIYA, US Army Research Laboratory, HAOTAO ZHANG, YONG ZHANG (Presenter), Univ of North Carolina - Charlotte — The dependence of electron-phonon coupling (EPC) on nanostructure size has been controversial over three decades. Often, the EPC was probed by resonant Raman scattering (RRS) using the 2LO to 1LO intensity ratio R21 to extract the Huang-Rhys factor (S) by applying Albrecht’s theory, where the bulk reference S was calculated using a theoretical model developed for a bound exciton with Fröhlich interaction. We show that in ZnTe, in contrast to the previous reports, R21 exhibits a much larger intrinsic value and minimal change from bulk to 30 nm nanowire [1], indicating previously reported size dependences were likely affected by extrinsic mechanisms. Indeed, the ratio can be tuned extrinsically over one order in magnitude controllably either during or post growth, allowing for programing EPC in nanoscale devices. We point out that R21 is not directly related to Huang-Rhys factor, lattice relaxation is minimal for bulk and moderately small nanostructures, and Albrecht’s theory is not applicable to RRS [2]. This work provides unambiguous experimental results for validating EPC theories with reduced dimensionality.


*Supported by ARO/Electronics (W911NF-16-1-0263)
4:54PM U65.00013: Analysis of $\chi^{(2)}$ of III-V quantum-well structures using transfer matrix techniques
NATALIE FOSTER (Presenter), Physics, University of Texas at Austin, ANN KATHRYN ROCKWELL, SETH BANK, Electrical Engineering, University of Texas at Austin, MICHAEL C DOWNER, Physics, University of Texas at Austin — Nano-layered quantum wells (QWs) composed of III-V semiconductors provide unexplored opportunities to engineer $\chi^{(2)}$ (e.g. for electro-optic and quantum information applications) by optimizing thickness, separation, and shape of individual QW layers as well as the number N of repeated layers. A digital alloys growth technique was used, which avoids phase segregation that often plagues III-V alloy growth, and also lends itself readily to nano-structuring to enhance $\chi^{(2)}$. Second harmonic generation (SHG) was used to probe the total nonlinear $\chi^{(2)}$ response of a series of N multiple-QW (MQW) layers made up of InAs QWs and AlSb barriers, sandwiched in between a GaSb oxidation cap and GaSb buffer layer, grown on GaSb substrate. The measured SHG signal is composed of a contribution from each of the layers that interfere with each other. To isolate the N-dependent SHG polarization of the MQW layer of interest, we implemented a SHG transfer matrix formalism to model the SHG signal as a coherent superposition of a variable-N MQW layer with fixed substrate and cap layer SH polarizations. Experimental results show up to 25x stronger SHG from MQW structures than from GaSb substrate. The model attributes this enhancement partly to geometrical effects and to enhanced $\chi^{(2)}$ of the MQW structures.

5:06PM U65.00014: Optically-induced dressed states in $\alpha$ materials: electronic and transport properties
ANDRII IUROV (Presenter), Medgar Evers College, LIUBOV ZHEMCHUZHNA, DIPENDRA DAHAL, GODFREY GUMBS, Hunter college, CUNY, DANHONG HUANG, Air Force Research Lab — We have obtained the energy dispersion relations and their wave functions for the so-called interacting Floquet states in pseudospin-1 $\alpha$-T$_3$ materials for various value of the parameter $\alpha$ in the presence of an external off-resonant dressing field. The obtained dressed states and their basic electronic properties significantly depend on the polarization of the applied radiation, while our derived results now depend on both the parameter and the light intensity. The energy subbands become directly dependent on the valley index $\tau$ once elliptically polarized irradiation is applied. We have calculated optical and transport conductivities for an irradiated dice lattice, which represents a limiting case of an $\alpha$-T$_3$ structure for $\alpha$ equal to 1.
2:30PM U66.00001: Electronic nematic softening in cuprate superconductors probed by resonant ultrasound spectroscopy [Invited]  PAULA GIRALDO-GALLO (Presenter), University of the Andes — Electronic-nematic order has been shown to be the driver of the structural and magnetic transitions in the Ba-pnictide superconductors. For cuprate superconductors, the determination of the existence of long-range electronic-nematic order and fluctuations is not as clearly established as for the pnictides. In this talk I will present Resonant Ultrasound Spectroscopy (RUS) measurements in single crystals of La$_{2-x}$Sr$_x$CuO$_4$ of different Sr compositions, through which we have determined the temperature dependence of all elastic moduli in the tetragonal phase of this compound. A strong softening of the C66 elastic shear moduli, associated with the B2g symmetry channel, is observed as temperature is decreased, even for the compositions for which the tetragonal to orthorhombic structural transition is not seen. The temperature dependence of this softening is consistent with a Curie-like temperature dependence, $1/(T-T_0)$. The B2g softening is truncated by the opening of the superconducting gap at $T_c$=$T_0$, evidenced by the stiffening of C66 below $T_c$. These observations suggest an electronic nematic origin for this softening.

3:06PM U66.00002: Strange Metal Transport in Electron-doped La$_{2-x}$Ce$_x$CuO$_4$* [Invited]  RICHARD GREENE (Presenter), University of Maryland, College Park — I present new measurements of resistivity, Hall Effect, magnetoresistance (MR) and thermopower in the electron-doped cuprate La$_{2-x}$Ce$_x$CuO$_4$ for 0.19$\geq$ x $\geq$0.08 as a function of temperature and magnetic field. The surprising results are:
1) The normal state MR has an anomalous linear-in-H behavior [1] at the same doping (0.14 to 0.175) where a linear-in-T resistivity was previously observed for $H>H_{c2}$ [2]. Beyond the SC dome (x $>$ 0.175) conventional metallic behavior is found.
2) The normal state Seebeck coefficient, S/T, exhibits a low temperature $-$lnT dependence at the same dopings [3]. Conventional S/T = constant metallic behavior is found for x $>$0.175.
3) Itinerant ferromagnetism is found below 4K for doping beyond the SC dome [4].
I conclude that conventional Fermi liquid theory cannot explain (1) and (2). Moreover, the magnitude of the anomalous magnetoresistance and thermopower scales with $T_c$, suggesting that the origin of the superconductivity is correlated with the anomalous normal state properties.

*Research supported by the NSF DMR. Work done in collaboration with T. Sarkar, P. Mandal, and N. Poniatowski
**What determines the Hall and Thermal Hall coefficients of metals, magnets and superconductors?**

**ASSA AUERBACH (Presenter), Technion - Israel Institute of Technology —**

The Hall coefficient has long been used to characterize the number and sign of charge carriers in metals and semiconductors. This assignment has only been justified in the weak disorder and interactions regimes. Unexpected Hall coefficient sign reversals (a.k.a. “Hall anomalies”) have been observed in strongly interacting metals, thermal Hall effect in antiferromagnets, and in the flux flow regime of cuprate superconductors.

I review recent theoretical advances [1,2] which shed light on Hall anomalies. New computable formulas [1] for Hall, Nernst and Thermal Hall coefficients in gapless (metallic) phases are applied to strongly correlated Hubbard and Heisenberg models, where traditional Chern number calculations and Drude-Boltzmann theory are inapplicable. We show that Hall sign reversal is a consequence of proximity to a Mott insulator, and that a negative thermal Hall coefficient is produced in the square lattice antiferromagnet with three-spin exchanges. A revised theory of magnetotransport in the flux flow regime of superconductors [3] explains Hall anomalies caused by moving vortex charge.

3. A. Auerbach and D.P. Arovas, to be published.

*US-Israel Binational Science Foundation, Grant 2016168, Israel Science Foundation, Grant 2021367, Aspen Center for Physics, Grant NSF-PHY-1066293.*
4:18PM U66.00004: Sign reversal of the flux flow Hall effect* [Invited] VALERII VINOKOUR (Presenter), Argonne Natl Lab — We present a phenomenological theory of the Hall effect sign reversal in type II superconductors taking into account the normal carriers scattering and the topological contribution to Hall conductivity and show that the latter contribution leads to a double sign change of the Hall conductivity. We report an experimental observation of the double sign reversal in atomically thin BSCCO and find a quantitative agreement between the experimentally observed Hall resistance and our theoretical predictions.

In collaboration with: Frank Zhao, Margaret G. Panetta, Cyndia Yu, Jedediah Johnson, Hyobin Yoo, Philip Kim, Harvard University; Nicola Poccia, Institute of Metallic Materials at IFW; Ruidan Zhong, Genda Gu, Brookhaven National Laboratory; Kenji Watanabe, Takashi Taniguchi, National Institute for Materials Science, Tsukuba; Svetlana Postolova, Institute for Physics of Microstructures RAS, Nizhny Novgorod; Mikhail Feigelman, Landau Institute; Vadim B. Geshkenbein, ETH-Zuerich; Anatoly Larkin, University of Minnesota

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4:54PM U66.00005: Scale-invariant magnetoresistance in a cuprate superconductor* [Invited]

PAULA GIRALDO-GALLO, University of the Andes, JOSE A GALVIS, Universidad Central, Colombia, ZACHARY A STEGEN, National High Magnetic Field Laboratory, KIMBERLY MODIC, Max Planck Institute for Chemical Physics of Solids, FEDOR BALAKIREV, JONATHAN B BETTS, Los Alamos National Laboratory, XIUJUN LIAN, National High Magnetic Field Laboratory, CAMILLA MOIR, CRIEPI, JIE WU, ANTHONY TRAVIS BOLLINGER, XI HE, IVAN BOZOVIC, Brookhaven National Laboratory, BRAD J RAMSHAW, Cornell University, ROSS MCDONALD, Los Alamos National Laboratory, GREGORY SCOTT BOEBINGER (Presenter), ARKADY SHEKHTER, National High Magnetic Field Laboratory — The anomalous metallic state in the high-temperature superconducting cuprates is masked by superconductivity near a quantum critical point. Applying high magnetic fields to suppress superconductivity has enabled detailed studies of the normal state, yet the direct effect of strong magnetic fields on the metallic state is poorly understood. In this talk, we report the high-field magnetoresistance of thin-film La$_{2-x}$Sr$_x$CuO$_4$ cuprate in the vicinity of the critical doping, 0.161 ≤ p ≤ 0.190. We find that the metallic state exposed by suppressing superconductivity is characterized by magnetoresistance that is linear in magnetic fields up to 80 tesla. The magnitude of the linear-in-field resistivity mirrors the magnitude and doping evolution of the well-known linear-in-temperature resistivity that has been associated with quantum criticality in high-temperature superconductors.

*The high-field resistivity measurements were performed in the 60 T long-pulse and 100 T magnet systems at the NHMFL Pulsed Field Facility, which is supported by NSF grant DMR-1157490 and the U.S. Department of Energy, Basic Energy Sciences (DOE/BES) "Science at 100 T" grant. Molecular beam epitaxy synthesis, lithography, and characterization of the samples were done at Brookhaven National Laboratory, which is supported by DOE/BES, Materials Sciences and Engineering Division.

Thursday, March 5, 2020 2:30 PM - 5:30 PM

Session U67 DCMP: Nano-Plasmonics in Van Der Waals Materials and Beyond Four Seasons 2-3 - Alexander McLeod - Tag(s): Invited
Moiré patterns are well-known phenomena in art, textiles and mathematics, which originate from the overlay of two periodic patterns. Intriguingly, atomically thin materials can be stacked on top of each other such that a new periodic pattern can emerge: the moiré superlattice. This can result in a dramatic modification of the electronic and optical properties of twisted 2D materials, compared to those of a single layer. The moiré superlattice can give rise to a plethora of interesting phenomena such as topological bands [1] and many-body phases like superconductivity and magnetism [2].

In this talk, we give an overview of the nano-optical properties of 2D material superlattices, obtained by twisting or nanostructuring. Nanoscale optical techniques such as near-field optical microscopy reveal unique observations of topological domain wall boundaries, hyperbolic phononic lattices, and interband collective modes in charge neutral TBG near the magic angle [3]. The freedom to engineer these so-called optical and electronic quantum metamaterials [4] is expected to expose a myriad of unexpected phenomena.

References

*This work was supported by the ERC consolidator grant Toponanop.

3:06PM U67.00002: Michael M Fogler Invited Talk [Invited] —
MAIKEN MIKKELSEN (Presenter), Duke University — Tailoring light–matter interactions in monolayer MoS$_2$ is critical for its use in optoelectronic and nanophotonic devices. Optical cavities with multiple tunable resonances have the potential to provide unique electromagnetic environments at two or more distinct wavelengths—critical for control of optical processes such as nonlinear generation, entangled photon generation, or photoluminescence (PL) enhancement. Here, we show a plasmonic nanocavity based on a nanopatch antenna design that has two tunable resonant modes in the visible spectrum. The importance of utilizing two resonances simultaneously is demonstrated by integrating monolayer MoS$_2$, a two-dimensional semiconductor, into the colloidal synthesized nanocavities. We observe a 2000-fold enhancement in the PL intensity of MoS$_2$—which has intrinsically low absorption and small quantum yield—at room temperature, enabled by the combination of tailored absorption enhancement at the first harmonic and PL quantum-yield enhancement at the fundamental resonance [1]. Next, we explore how the emission spectrum can be tailored, including complex excitonic states. We demonstrate that the peak emission wavelengths of the A and B excitons can be tuned up to 40 and 25 nm, respectively, by integrating monolayer MoS$_2$ into a plasmonic nanocavity with tunable plasmon resonances [2]. Contrary to the intrinsic photoluminescence spectrum of monolayer MoS$_2$, we are also able to create a dominant B exciton peak when the nanocavity is resonant with its emission. Additionally, we observe a 1200-fold enhancement of the A exciton emission and a 6100-fold enhancement of the B exciton emission when normalized to the area under a single nanocavity and compared to a control sample on thermal oxide.

4:18PM U67.00004: Collective mode spontaneous symmetry breaking: out-of-equilibrium plasmonic magnetism* [Invited] JUSTIN SONG (Presenter), Nanyang Tech Univ — Spontaneous symmetry breaking lies at the heart of the description of interacting phases of matter. We will argue that a driven interacting system subject to a linearly polarized (achiral) driving field can spontaneously magnetize (acquire chirality). In particular, we find when a metal is driven close to its plasmon resonance, it hosts strong internal ac fields that enable Berryogenesis: the spontaneous generation of a self-induced Bloch band Berry flux, which supports and is sustained by a circulating plasmonic motion, even for a linear polarized driving field. This non-equilibrium phase transition occurs above a critical driving amplitude, and depending on system parameters, can enter the spontaneously magnetized state in either a discontinuous or continuous fashion. Berryogenesis relies on nontrivial interband coherences for electronic states near the Fermi energy generated by ac fields readily found in a wide variety of multiband systems. We anticipate that graphene devices, in particular, which can host high quality plasmons, provide a natural and easily available platform to achieve Berryogenesis and spontaneous non-equilibrium (plasmon-mediated) magnetization in present-day devices, e.g., those based on graphene plasmonics.

*J.C.W.S. gratefully acknowledges the support of the Singapore National Research Foundation (NRF) under NRF fellowship award NRF- NRFF2016-05, a Nanyang Technological University start-up grant (NTU-SUG), and Singapore MOE Academic Research Fund Tier 3 Grant MOE2018-T3-1-002.

4:54PM U67.00005: Nano-polaritonics in twisted van der Waals heterostructures [Invited] GUANGXIN NI (Presenter), Columbia Univ — Interlayer coupling in atomic van der Waals heterostructures plays a rather unique role in controlling their optical and electronic properties. The character of the interlayer coupling can be manipulated by a particular stacking arrangement of the proximal layers and by adjusting the orientation of the neighboring planes. The latter method is known to trigger the long-range periodic modulations referred to as twisted moiré superlattices. The presence of periodic moiré patterns enables further fine tuning of the electronic band structure and yielding rich insights into the electronic phenomenon. This has been manifested in graphene/hexagonal boron nitride (G/hBN) moiré patterns, twisted bilayer graphene structures as well as twisted hBN crystals. Using nano-infrared optical microscopy we have experimentally studied the collective excitations in these twisted moiré structures. We analyzed these soliton networks and obtained the local electrodynamical characters based on the infrared active polaritonics at the nanoscale.

Reference:

Thursday, March 5, 2020 2:30 PM - 5:30 PM
Using Information Geometry to find simple models of complex processes*

MARK TRANSTRUM (Presenter), Physics & Astronomy, Brigham Young University —

Effective theories play a fundamental role in how we organize our knowledge about the world. Although reality is much more complicated than our models, we justify parsimonious representations by judiciously ignoring degrees of freedom that are irrelevant for the predictions of interest. Often, these models are related through a hierarchy of simplifying approximations that formally justify their respective domains of validity. I demonstrate how information geometry can be used to construct such effective theories for many complex systems, including systems beyond the reach of traditional methods. Embedded in the mathematical form of many model classes is a hierarchy of natural approximations. These approximations are manifest as boundaries of high-dimensional manifolds. These approximations are not black-boxes. They remain expressed in terms of the relevant combinations of mechanistic parameters and reflect the physical principles from which the complicated model was built. Furthermore, these approximations can be identified in a data-driven way for models with thousands of parameters.

*This work was supported by the US National Science Foundation under Award NSF-1753357.

Finding and explaining structural hierarchies in models of complex systems

KATHERINE QUINN (Presenter), The Graduate Center, City University of New York —

Sloppy models form a universality class of complex, nonlinear models in which outcomes are significantly affected by only a small subset of parameter combinations, arising in disparate fields from systems biology to accelerator physics. By unifying information geometric interpretations of sloppiness with Chebyshev approximation theory, I will derive a formal and systematic explanation of why sloppiness occurs. I will then extend this framework to general probabilistic models and data, to derive a widely-applicable manifold-learning method called InPCA that ameliorates a canonical problem in machine learning: the "curse of dimensionality".
4:18PM U68.00004: Identifiability, uncertainty, and parameter reduction in mathematical biology* [Invited] MARISA EISENBERG (Presenter), Univ of Michigan - Ann Arbor — The interactions between parameters, model structure, and outputs can determine what inferences, predictions, and control strategies are possible for a given system. Identifiability, estimability, and parameter space reduction methods are thus essential for many questions in mathematical modeling and uncertainty quantification. These approaches can help to determine what inferences and predictions are possible from a given model and data set, and help guide control strategies and new data collection. In this talk, I will discuss some of the ideas and methods from identifiability, how they link to ideas of model reduction and model selection, and present public health applications to recent epidemics of polio and cholera. We will illustrate how reparameterization and alternative data collection may help resolve various types of unidentifiability and allow for successful intervention predictions.

*This project was funded through the Models of Infectious Disease Agent Study program within the National Institute of General Medical Sciences of the National Institutes of Health (Grant U01GM110712), and the National Science Foundation (Grant OCE-1115881).

4:54PM U68.00005: Manifold Learning for Parameter Reduction [Invited] YANNIS KEVREKIDIS (Presenter), Johns Hopkins University — Large scale dynamical systems (e.g. many nonlinear coupled differential equations) can often be summarized in terms of only a few state variables (a few equations), a trait that reduces complexity and facilitates exploration of behavioral aspects of otherwise intractable models. High model dimensionality and complexity makes symbolic, pen-and-paper model reduction tedious and impractical, a difficulty addressed by recently developed frameworks that computerize reduction. As the interest in mapping out and optimizing complex input--output relations keeps growing, it becomes clear that combating the curse of dimensionality also requires efficient schemes for input space exploration and reduction. Here, we explore systematic, data-driven parameter reduction by means of effective parameter identification, starting from current nonlinear manifold-learning techniques enabling state space reduction. Our approach aspires to extend the data-driven determination of effective state variables with the data-driven discovery of effective model parameters, and thus to accelerate the exploration of high-dimensional parameter spaces associated with complex models. We also discuss the data-driven exploration of conjugacies between different models/observations.

In collaboration with: M. Khooshkbaghi, A. Zagaris, A. Holiday, and J. Bello-Rivas

Thursday, March 5, 2020 2:30 PM - 4:54 PM

Session U70 DCMP DCOMP: Frontiers in Interdisciplinary Theory and Phenomena 208
2:30PM U70.00001: No-Go Experiment Confirms Superdeterminism Loophole*  MANUEL MORALES (Presenter), Rowan University — Nonlocal hidden variables of motion served to obtain absolute internal validity in a twelve-year no-go experiment (2000-2012) that confirmed it is impossible for a test taker to conduct experiments or observations without the mechanical functions of direct or indirect selection. In other words, the natural world prohibits the will of the test taker from conducting any and all experiments prior to the predetermined first-order functions of selection. Therefore, the mechanisms of selection, commonly known as choice or free will, are mandatory functions not a freedom. In physical terms, external validity of the findings means that effects of existence such as energy and mass are not conserved because they are predetermined effects of how they are determined, i.e., superdeterminism as predicted by John S Bell. The unambiguous empirical evidence obtained from the no-go experiment confirmed that Albert Einstein was indeed correct to suspect that quantum mechanics is not a fundamental theory due to hidden variables at play. However, he was incorrect as to the domain of their origin.

*Funded by Manuel S Morales

2:42PM U70.00002: A Covariant Field Reformulation of Classical Electrodynamics*  WILLIAM BRYAN MAIER (Presenter), Physics, Naval Postgraduate School — Classical electrodynamics is here reformulated as a field theory rather than a particle and field theory. Electromagnetic fields are taken to be continuous and differentiable everywhere. Maxwell's equations are assumed to be valid at all scale lengths, and second order variations on the vector potentials $A_k$ are used to obtain fundamental equations from a covariant action in which the usual term involving particle mass $m$ has been replaced by the covariant mass density $\mu$ associated with the fields. Point, line, and surface charges are not allowed. Stable charge distributions having finite extent and charge of only one sign are found. These bodies are stabilized by the charge motion in the distribution's self-field. Their mass is finite and equivalent to the energy of the electromagnetic field integrated over all space. Spin, magnetic moment, and electric dipole and quadrupole moments of these bodies can be calculated. The Lorentz force law plus radiation reaction is shown to govern the motion of these charged objects in an imposed electromagnetic field. Ordinary classical electromagnetism is thus reproduced, and the classical structures of fundamental charged bodies are obtained. Structures of the electron and proton in this theory are briefly discussed.

*Naval Postgraduate School
2:54PM U70.00003: A New, Unified, Non-Relativistic Quantum Quaternal Physics  CLAUDE MASSOT (Presenter), Theoretical Physics, Independant Scientist — Despite its impressive results, the relativistic Standard Model, remains unrealistic because of quantum incompatibilities. String and GUT theories are exciting, but far from being validated. To confront these theoretical contradictions and to develop a mathematical model for de Broglie's wave-particle, I did propose the new Hypothesis of the Complex Nature of Matter. It was presented in 1994 at the french Academy of Sciences, by Andre Lichnerowicz. I do extend it, now, by quaternion algebra, to link, without any relativistic postulate, mass and time dilation with Planck's and de Broglie's laws, and to take into account spin and helicity. I start with a new interpretation of Michelson's experiment, assuming that its photons are carried by the gravitational field of the earth. This discards the need for the hypothesis of space contraction and gravitation as a curvature of space. Instead, I consider gravitation as a very tiny residual attractive Coulomb's force between the electric fields of protons and electrons. This allows a unification of atomic forces and gravitation and leads to a solar system quantified by an extended Bohr's model with a link between the orbital and daily spin of the Earth.

3:06PM U70.00004: Mikowski Space may be interpreted as a Theory of Orbitals  RICHARD KRISKE (Presenter), Physics, MIT — When one compares the work of Kepler, with Mikowski Space, they are both Cones joined at a nexus. In Kepler Space, one is viewing the Cones from the outside, and there are three types of Conic Sections, the Ellipse, the Parabola, and the Hyperbola. In Aeronautical Engineering, they are the Elliptical Orbit, the Parabolic Orbit, and the Hyperbolic Obital. The Minkowski Diagram is somewhat in error, in that the observer views one cone as the future and one cone as the past. We know from Quantum Mechanics that an observation is a measurement. So the nexus is not a point, but is planck's constant / two, as a minimum overlap. This over lap is an elliptical orbital, so the Conservation of Angular Momentum comes about due to Special Relativity, and the overlap of the Minkowski Space Cones. The Parabolic Orbital is the Speed of Light in a Vacuum. The Hyperbolic Orbital is the a Quantum Leap. An Electron Changing Orbitals needs only the Speed of Light as the escape velocity. Where does on see the Hyperbolic Orbital? That occurs when an Electron or other Elementary particle is measured from its wavefunction and collapses into a particle, far from its origin. This new view of Mikowski Space may solve the problem of Unitary Entities comprising Space Time, they are in orbit like planets.
Anomaly of the Electromagnetic Duality of Maxwell Theory

Every physicist knows that classical electromagnetism is described by Maxwell's equations, and that it is invariant under the electromagnetic duality $S: (E, B) \rightarrow (B, -E)$. The properties of the electromagnetic duality in the quantum theory, represented by an SL(2, Z) group acting on the lattice $\mathbb{Z}^2$ of the electric and magnetic charges, might not be as well known to physicists in general. This is particularly true when going around a nontrivial path in the spacetime results in a duality transformation. In this work, we uncover a feature of the Maxwell theory and its duality symmetry in such a situation, namely that it has a quantum anomaly. We find that the anomaly of this system in a particular formulation is 56 times that of a Weyl fermion. The interpretation of this result is twofold: one is by using the bulk symmetry-protected topological phase in 4+1 dimensions characterizing the anomaly, and the other is by considering the properties of some (5+1)-dimensional superconformal field theory. Our result reproduces, as a special case, the known anomaly of the all-fermion electrodynamics—a version of the Maxwell theory where all particles of odd charge are fermions—discovered in the last few years.

C.-T. H. is supported in part by JSPS KAKENHI Grant-in-Aid No. 19K14608.

A Number of Early 20th Century Important Physics Formulas, Some Nobel Prize Winning, Must Be Slightly Corrected Because They Lack Rotational and Vibrational Factors Not Known To Be Necessary When The Formulas Were Discovered

In 1905 Einstein derived the total energy of a mass at slow speeds to be $E = mc^2 + \frac{1}{2}mv^2$. Later, in the 20th century it was discovered that all masses can also be rotating and vibrating. Thus, the total energy of a mass at slow speeds must be $E = mc^2 + \frac{1}{2}mv^2 + \frac{1}{2}I\omega^2 + \frac{1}{2}kx_0^2 + \frac{1}{2}I(x_0)^2 + \frac{1}{2}Gm_1m_2/r^2 + \frac{1}{2}kq_1q_2/r^2$ also including gravitational, electrostatic potential energies and all kinetic energies. Einstein stated the relativistic kinetic energy at low speeds to be $T = (E - E_0)$. Thus, the relativistic kinetic energy is $T = (\frac{1}{2}mv^2 + \frac{1}{2}I(\omega)^2 + \frac{1}{2}k(x_0)^2 + (Gm_1m_2)/r^2 + (kq_1q_2)/r^2$. The Photoelectric Effect Equation must include rotational and vibrational factors: Maximum energy of the ejected electron must be: $hf = (\frac{1}{2}mv^2 + \frac{1}{2}I(\omega)^2 + \frac{1}{2}k(x_0)^2)_{\text{max}} + \Phi$. The Virial Theorem astrophysics equation and Compton Effect energy equation must both be updated including rotational and vibrational factors: $\frac{1}{2}mv^2 + \frac{1}{2}I(\omega)^2 + \frac{1}{2}k(x_0)^2 + U = 0$, where $U$ is the gravitational energy for Virial. The Compton should be: $h\nu/(\lambda)^2 + (m_0)c^2 + \frac{1}{2}m(v_1)^2 + \frac{1}{2}I(\omega)^2 + \frac{1}{2}k(x_0)^2 = h\nu/(\lambda)^2 + m_0c^2 + \frac{1}{2}(m_2)v^2 + \frac{1}{2}I(\omega)^2 + \frac{1}{2}k(x_0)^2$.

Many other early 20th century physics equations, then assumed correct, some of possibly Nobel Prize quality as those above, may need to be updated by adding rotational and vibrational factors not then even considered essential.
3:42PM U70.00007: A quantum interpretation of the physical basis of mass-energy equivalence* DONALD CHANG (Presenter), Hong Kong University of Science and Technology — We know energy and mass of a particle can be connected by $E = mc^2$. What is the physical basis behind this relation? Historically, it was thought that it is based on the principle of relativity (PR). However, a careful examination of the literature indicated that this relation was not directly derived from PR. Instead, Einstein came to this conclusion mainly based on his intuitive thinking that radiation and matters behave similarly. Following this hint, we suspect that the mass-energy equivalence could be based on the quantum principle of wave-particle duality. It is well known that both photon and electron can behave as a particle as well as a wave. Using a wave model which treats particles as excitations of the vacuum, we show that the relations $E = mc^2$ can be directly derived from Planck's relation. This wave hypothesis has several advantages; not only can it explain naturally why particles can be created in the vacuum; it also predicts that a particle cannot travel faster than the speed of light. This hypothesis can also be tested in experiment.

*This work was supported by the Macro-science project of HKUST.

3:54PM U70.00008: Adding a Dynamic to Gravitation Reveals How Extra Gravity Halos are Projected from Galactic Cores* JOHN HUENEFELD (Presenter), APS — It is unfortunate that the term dark matter was used to describe the extra gravity observed in galaxy clusters. The name presupposes a material answer, but the only thing actually observed is an Extra Gravity Halo (EGH). The mysterious source of this extra gravity remains unresolved. Or does it?

A new theory, sets GR in motion, predicting an ongoing space-time contraction within a gravitational field. Unlike Hubble expansion, this contraction field is non linear with distance from the source and projects more strongly with the increasing amount of concentrated matter generating the field. No assumed additional mass is needed to boost the orbital velocity of stars around a galactic core. The contraction field augments the acceleration of gravity to achieve galaxy rotation curves consistent with observation.

Dark matter is not a particle. EGHs are the result of relativity, and are an integral part of gravitation. The contraction field acts to scale up gravity. The scale factor, which falls easily from the math, has exactly the right mathematical shape to replicate assumed dark matter distributions. Not only do these contraction fields explain galaxy rotation curves, they also explain the Bullet Cluster, and Ultra Diffuse galaxies which have either a very strong EGH or none at all.

*N/A
Each Force has a function. Each function has a Particle Force Carrier.

Existence is a function of Time. Without Time, nothing exists.

It is my hypothesis that an unrecognized Fifth Force exists along with the currently known Four Forces, which are: The Electro-Magnetic Force whose Particle Force Carrier is the Photon, The Strong Force whose Particle Force Carrier is the Gluon, The Weak Force whose Particle Force Carriers are the W-, W+ and Z Bosons, and the last and currently the weakest of the Four known Forces, Gravity whose Particle Force Carrier is the yet to be seen Graviton (I have a separate hypothesis on Gravity and the Graviton, but that’s an altogether separate Abstract).

This Fifth Force is so pervasive throughout the Universe, is it any wonder it’s been overlooked?

This Fifth Force also has its own Particle Force Carrier, and it is the first Particle Force Carrier to have been discovered before its Force was even recognized.

To me this might be called “Aquilina’s Assumption, but the only choice for the Particle Force Carrier for Time is the Higgs Boson.

The identification of Time as a Force would also tie the Four other Forces together since they all fall under the umbrella of “Existence”.

Rich Aquilina 04/17/2018 @11:56pm

Quantum electrodynamics (QED) is the fundamental theory of electromagnetic interactions. Thus, the Schrödinger equation, which yields the electron wavefunction in low energy electromagnetic interactions, must be a condition that can be derived from the fundamental QED theory. Due to the small value of the electromagnetic coupling constant, we can adequately describe low-energy interactions by classical potentials. Furthermore, the dominant (lowest order) term of the electron wavefunction is a superposition of plane waves. As a result, we show that to fulfill the total energy relations, the electron wavefunction must satisfy at each space-time point the Schrödinger, Pauli, and Dirac equations.
4:30PM U70.00011: Mathematical proof of electromagnetic wave nature of photons in hydrogen emission spectrum and theoretical derivation of Planck’s constant*  JUNHO JEONG (Presenter), Dong-A University — The photons emitted from electron transitions are electromagnetic waves, but there is no mathematical demonstration as to why this is so. According to the electromagnetic theory, electromagnetic radiation is emitted as magnetic dipole radiation when a charge revolving in an orbit of radius \( r_0 \) flows as an alternating current. This paper presents a mathematical proof for the emission of infrared-to-ultraviolet electromagnetic waves of the hydrogen emission spectrum when an alternating current is generated by the oscillation and revolution of an electron around a hydrogen-atom proton at a radius \( r_{nor} \) due to external energy. The mathematical results have demonstrated that the photon is not wave–particle duality of light but an electromagnetic wave of energy form, and the empirical Planck’s constant, \( h \), is mathematically derived for the first time. Therefore, the electromagnetic spectrum above the infrared region can be explained with oscillating and revolving particles with a constant electric charge.

*I wish to thank SBN Science LTd. for supporting funding.

4:42PM U70.00012: Wavefunction; Guided Energy of Wave*  DESMOND AGBOLADE ADEMOLA (Presenter), Olabisi Onabanjo Univ — This paper expound on true nature of wavefunction and answered questions that arise from quantum foundation. The fundamental analysis presented in this work show that mathematical formalism of wavefunction was wrongly formulated. On this basis, we therefore mathematically formalized new wavefunction equation which applicable to any forms of particles. We further introduced diffraction concept which mathematically establishes space-time quantization. We further show that wavefunction does not collapse, only converges and diverges gradually. The gradual process of divergence of wavefunction display how particle-like behavior return to wave-like behavior, and the gradual process of convergence of wavefunction also display how wave-like behavior return to particle-like behavior. The fundamental equations and analysis presented in this work hereby provides single description for both wave properties of smallest tiny particles (e.g. electrons) and matter properties of large particles (celestial bodies). The fundamental analysis presented here confirms that quantum mechanics needs to be profoundly modified to absorbs ideas of fundamentals analysis presented in this paper so that it might become a unique theory that accounts for dynamics behaviors of all particles regardless of sizes.

*NIL
We propose a double inflection point inflationary model. In which one of the inflection point predicts the power spectra consistent with CMB observations at large scales and the other generates a large peak in the power spectrum of scalar perturbations at small scales. Such a peak allows for the generation of primordial black holes at small scales, which can account for a significant fraction of dark matter. We also calculate the energy spectrum of induce gravitational waves from primordial scalar perturbations and find that the gravitational-wave signal can be detected by future space-based laser interferometers.

*This work was supported by “the National Natural Science Foundation of China” (NNSFC) with Grant No. 11705133
8:00AM W01.00001: Anisotropic Wave Breaking in Highly Nonlinear Thermal Media  GIULIA MARCUCCI (Presenter), Physics Department, Sapienza University of Rome, PHILLIP CALA, WEINING MAN, Department of Physics and Astronomy, San Francisco State University, DAVIDE PIERANGELI, CLAUDIO CONTI, Physics Department, Sapienza University of Rome, ZHIGANG CHEN, Department of Physics and Astronomy, San Francisco State University — In optics, many phenomena are ruled by the nonlinear Schrödinger equation (NLSE), as solitons and dispersive shock waves (DSWs). We report experiments on 2D-optical DSWs with anisotropic singularity in m-cresol/nylon, and provide theoretical description by time asymmetric quantum mechanics (TAQM) [1].

M-cresol/nylon is a chemical solution with an isotropic giant self-defocusing nonlinearity. When it is enlightened by a CW laser beam, the material experiences a thermo-optical effect, governed by the nonlocal version of the defocusing NLSE.

By choosing an initial beam shape (propagating along z) that has null intensity along x = 0, a new kind of wave breaking emerges: the shock develops undular bores on the beam external borders, but around the singularity it presents an abrupt intensity discontinuity.

We analyze this shock and find that it is caused by the interplay of a trapping/focusing potential along x and an antitrapping/defocusing potential along y. While the trapping potential is the standard harmonic oscillator (HO), the antitrapping potential is the reversed HO, a paradigmatic model in TAQM. Indeed, light propagation is described by a superposition of exponential decays with quantized decay rates, a fundamental TAQM signature.


8:12AM W01.00002: Strong-Field Ionization in Bicircular Laser Fields  JAN CHALOUPKA (Presenter), Dept of Physics & Astronomy, Univ of Northern Colorado — We ordinarily take Einstein's description of the photoelectric effect to mean that atoms can absorb only one photon at a time, thereby prohibiting ionization by weak, low-frequency light. But shortly after the invention of the laser, it was found that under intense illumination, atoms could simultaneously absorb many photons, leading to so-called multiphoton ionization. It was also discovered that a second electron could be liberated with surprising efficiency through a process known as rescattering, where the first electron is driven back to the ion leading to impact double ionization. Since this process relies on trajectories that bring the first electron back to the parent ion, it is most effective with linear polarization and absent with circular polarization. But there has recently been great interest in ionization dynamics driven by intense bicircular light, generated by combining two colors of circularly polarized light. Here we present new results using a classical ensemble approach and utilizing a high-performance computational cluster. We uncover novel patterns in recollision timing, identify classes of complex trajectories that contribute to double ionization, and map various ionization processes onto the resulting transverse electron momentum distributions.
HONGXIA ZHENG (Presenter), Fudan Univ, YIKUN JIANG, Department of Physics, Cornell University, HUAJIN CHEN, Guangxi University of Science and Technology, XIAO LI, The Hong Kong University of Science and Technology, XINNING YU, Fudan Univ, WANLI LU, China University of Mining and Technology, JACK NG, Southern University of Science and Technology, ZHIFANG LIN, Fudan Univ — Based on either mathematics or physics, it is natural to split the optical forces acting on small particles into the conservative gradient force and the nonconservative scattering force. While the former can trap small particles at a potential energy minimum, the latter can push or even pull small particles, thus transporting them. Nevertheless, although its importance in understanding optical micromanipulation is recognized, these forces are only calculated for particles small or large compared to the light wavelength. Their true profiles for Mie sized particles, which are the most commonly encountered particles in real experiment, were not available. The difficulty lies in the complicated mathematics. Here, we report several algorithms we developed to calculate the decomposed force for spherical particle with arbitrary size and composition and present some interesting results calculated by these algorithms [1-4].

[4] Y. Jiang et. al., accepted by ACS Photonics, 10.1021/acsphotonics.9b00746

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ASMA AL-QASIMI (Presenter), DANIEL FV JAMES, University of Toronto — Coherence properties of light are known to change upon propagation in linear optical systems [1-4]. Here, we study coherence properties of classical light using convenient techniques from Matrix Algebra. We apply those techniques, first, to a set up of a Young's Interference Experiment, finding maximal coherence properties, such as those pertaining to polarization and which-path distinguishibility. Second, we find the maximal polarization obtainable of a partially coherent beam propagating in space [5].


*This work is supported in part by the M. Hildred Blewett Fellowship of the American Physical Society, www.aps.org and by the Natural Sciences and Engineering Research Council of Canada (NSERC).
8:48AM W01.00005: Generating photon-added states without adding a photon*  SAURABH SHRINGARPURE (Presenter), JAMES D FRANSON, Univ of Maryland-Baltimore County — Optical Parametric Amplifiers convert pump photons to pairs of signal and idler photons. In this work, we demonstrate that a continuous range of non-classical states, including a displaced number state and photon-added state, can be prepared in the signal when the input idler mode contains a pure single-photon state and the output idler mode is post-selected to be unchanged by the OPA, depending on the gain of the OPA. The ability to continuously tune the gain and hence the non-classical states provide an advantage over a similar approach for conventional beam splitter with fixed reflectivity.

Reference

*This work was supported in part by the National Science Foundation under grant number PHY-1802472.

9:00AM W01.00006: Limits to Single Photon Detection: Amplification*  TZULA PROPP (Presenter), STEVEN J VAN ENK, Univ of Oregon — We have constructed a model of photo detection that is both idealized and realistic enough to calculate the limits and tradeoffs inherent to single photon detector (SPD) figures of merit. This model consists of three parts: transmission [1], amplification [2], and measurement. In this talk, we discuss the effects of signal amplification post-filtering; by first writing correct commutator-preserving transformations for non-linear photon-number amplification (e.g. avalanche photodiode, electron-hole pair creation, electron shelving), we derive alternative noise limits that out-perform the well-known Caves limits for linear amplification of bosonic mode amplitudes and possess no zero-temperature noise contribution to boson number SNR. We then discuss the optimistic implications for single photon detection. Lastly, we briefly discuss the pre-amplification filtering process (transmission) along with the construction of POVMs completely describing photo detectors (measurement), from which we can calculate all standard SPD figures of merit.


*This work was supported by funding from DARPA under Contract No. W911NF-17-1-0267.
9:12AM W01.00007: Optical attenuation without absorption*  IAN NODURFT (Presenter), RICHARD A BREWSTER, TODD BUTLER PITTMAN, JAMES D FRANSON, Univ of Maryland-Baltimore County — We simulate a coherent state of light passing through an atomic medium. Upon transmission, the atoms’ states are observed and all cases in which any are excited are rejected, and the final output is calculated. Depending on initial amplitude and coupling strength, the output can be attenuated to a greater degree or even amplified when compared to the output where the atoms’ states are ignored.


*This work was supported in part by the National ScienceFoundation under Grant No. PHY-1802472.

9:24AM W01.00008: A computational design of cylindrically symmetric 2D dielectric grating meta-lens with optical limiting effect based on saturable absorption by FDTD simulation  YUQI ZHAO (Presenter), HAMIDREZA CHALABI, EDO WAKS, University of Maryland, College Park — Meta-surface materials can shape the amplitude and phase with high spatial resolution and exhibit properties not occurring in natural materials, receiving considerable attention nowadays. Many exotic phenomena have been successfully demonstrated in linear optics. However, to meet the growing demand for the integration of more functionalities into a single optoelectronic circuit, the tailorable nonlinear optical properties of meta-surfaces will also need to be exploited. Here, by carefully tailoring meta-atoms' dimensions using FDTD simulation, we manage to design an optical limiting cylindrically symmetric 2D grating meta-lens with GaAs meta-atoms on SiO2 substrate. The nonlinearity based on saturable absorption is obtained by embedding quantum dots inside meta-atoms. Each quantum dot is treated as a two-level quantum system and optical Bloch equations are used for refractive index calculations and meta-lens simulations. Good focusing and optical limiting effect is observed and analyzed.
9:36AM W01.00009: Optical pulse propagation in transverse Anderson localization optical fibers*  ARASH MAFI (Presenter), CODY BASSETT, University of New Mexico, MATTHEW TUGGLE, Clemson University, MOSTAFA PEYSOKHAN, ESMAEIL MOBINI, University of New Mexico, JOHN M BALLATO, Clemson University — We study the optical pulse propagation in transverse Anderson localization optical fibers (TALOFs). TALOFs are a novel class of optical fibers that guide light, not in a conventional core-cladding setting, but by means of Anderson localization, where any location across the transverse profile of the fiber can be used to guide light. In particular, we investigate the group velocity distribution of guided modes in TALOFs. We observe that the narrowest distribution of group velocities is obtained in the presence of a small amount of disorder; therefore, the modal dispersion of an optical pulse is minimized when there is only a slight disorder in TALOF. Our investigation is primarily aimed at the nonlinear optical properties of TALOFs, but the results can apply to the usage of TALOFs in optical communications as well. We will also discuss other nonlinear behavior of TALOFs, e.g., four-wave-mixing and heralded single-photon generation for quantum information processing.


*NSF: 1807857; 1808232

9:48AM W01.00010: Characterization and design of radiation-balanced Yb-doped ZBLAN fiber laser*  MOSTAFA PEYSOKHAN (Presenter), ESMAEIL MOBINI, ARASH MAFI, University of New Mexico — Thermal instability degrades laser beam quality and is a substantial hurdle in the power-scaling of fiber lasers. Radiation balancing is suggested as a viable method for heat mitigation and is based on balancing the anti-stokes fluorescence cooling against conventional sources of heating in a laser. In designing a radiation-balanced fiber laser, characterization plays a vital role. Moreover, for the laser cavity design, one needs to present a viable geometry and select the appropriate pump and signal wavelengths to achieve optimum efficiency while maintaining the radiation-balanced condition. In this study, we introduce a non-constructive and non-contact method for fully characterizing the Yb-doped ZBLAN fiber. We extract such parameters as the parasitic absorption, background absorption, quantum external efficiency, and cooling efficiency for the different pump wavelengths. We also find the optimal pump wavelength for maximum cooling efficiency.


*AFOSR MURI: FA9550-16-1-0362
**10:00AM W01.00011: A synthetic Hall effect creates strong photonic nonreciprocity**

CHRISTOPHER PETERSON (Presenter), University of Illinois at Urbana-Champaign, WLADIMIR A BENALCAZAR, The Pennsylvania State University, MAO LIN, TAYLOR L HUGHES, GAURAV BAHL, University of Illinois at Urbana-Champaign — The ordinary Hall effect is a historically well-known physical phenomenon where a transverse electric field is produced when a magnetic field is applied perpendicular to a current. The inverse of this effect, where orthogonal electric and magnetic fields induce an electric current in the E x B direction, is a less well-known but an equally valid application of the same principle. Here, we experimentally realize this combination of effective electric and magnetic fields in a photonic resonator chain through use of synthetic dimensions. We then demonstrate the photonic equivalent of the Hall effect, where the combination of fields creates a “photon current” such that transmission of photons is unidirectionally suppressed. We show that this synthetic Hall effect can induce strongly nonreciprocal transmission, with greater than 58 dB of contrast, when both synthetic fields are tuned to maximize their respective symmetry breaking. This mechanism is general can be applied to break reciprocity in a wide variety of domains, including optical, microwave, and mechanical systems.

*We acknowledge support from the US National Science Foundation and U.S. Office of Naval Research

**10:12AM W01.00012: High Harmonic Generation In Single-Walled Carbon Nanotubes Driven By A Circularly Polarized Incident Field**

WALTER FURMAN (Presenter), LINDA E REICHL, University of Texas at Austin — High-order harmonic generation occurs in single-walled carbon nanotubes when a time-periodic field is applied at a large enough intensity to induce significant nonlinearities in the electron current. Regularized delta-function potentials were used to approximate the energy band structure of graphene and nanotubes. Then 10-10 armchair nanotubes were modeled using Floquet-Bloch theory driven by a circularly polarized field propagating parallel to the tube axis. Quasienergy, average energy, and electron current are computed, and the nature of the high harmonic emission spectrum will be discussed.

*Welsh Goverment Learning Grant*
10:24AM W01.00013: Electromagnetically induced transparency without control field in giant atoms* ANDREAS ASK (Presenter), Chalmers Univ of Tech, YAO-LUNG L. FANG, Brookhaven National Lab, Computational Science Initiative, ANTON FRISK KOCKUM, Chalmers Univ of Tech — Quantum interference between different excitation pathways in a three-level system can make an otherwise opaque medium transparent. The transparency window is achieved by turning on a control field, and is therefore named electromagnetically induced transparency (EIT). Since EIT is accompanied by a drastic change in refractive index, it gives rise to highly non-linear effects, such as slow light. We have investigated the creation of EIT in systems without the need for an explicit control field: two two-level atoms coupled to a waveguide. In particular, these atoms can be giant, i.e., couple to the waveguide at two spatially separated points. By tuning the distance between the two coupling points, a giant atom can decouple from the waveguide, thus forming a dark state, a key component in EIT physics. Since our proposed system does not involve neither an explicit three-level system, nor a control field, the complexity of achieving EIT is drastically reduced. Our proposal can be realized in several experimental setups, e.g., superconducting qubits coupled to microwave photons or surface-acoustic-wave phonons.

*Y.-L. L. Fang acknowledges support from grant LDRD 19-002.

10:36AM W01.00014: Topological Spaser in a Non-uniform Field* RUPESH GHIMIRE (Presenter), JHIH-SHENG WU, VADYM APALKOV, MARK I STOCKMAN, Department of Physics and Center of Nano Optics, Georgia State University — We propose a nanospaser made of an achiral plasmonic-metal nanodisc and a two-dimensional chiral gain medium, e.g., a monolayer transition-metal dichalcogenide (TMDC). Such a gain medium can pumped by circularly-polarized radiation into a valley-polarized (topologically-charged) state where the population-inversion of the K and K' valleys may be different. Each valley's population inversion independently feeds a chiral spasing mode of the nanodisk. There are two such modes that carry opposite topological charges; they do not compete with or cross-talk to each other, and are highly independent. The local fields of these modes rotate in time in opposite directions and are highly nonuniform in space.

*1. Office of Naval Research (DOD); N000-14-17-1-2588
2. Emory University, subcontracted by the National Science Foundation (NSF); T883032 is the subaward number; the Federal Award no. is EFMA-1741691
3. Department of Energy (DOE); DE-FG02-01ER15213
4. Department of Energy (DOE); DE-SC0007043
5. University of Central Florida, subcontracted by the Air Force Office of Scientific Research (AFOSR); 24086151 is the subaward number; the Federal Award no. is FA9550-15-1-0037
10:48AM W01.00015: Arbitrary optical wave evolution with Fourier transforms and phase masks  VICTOR JOSE LOPEZ PASTOR (Presenter), Max Planck Inst for Sci Light, JEFF LUNDEEN, Department of Physics, University of Ottawa, FLORIAN MARQUARDT, Max Planck Inst for Sci Light — A large number of applications in classical and quantum photonics require the capability of implementing arbitrary linear unitary transformations on a set of optical modes. In a seminal work by Reck et al. [1] it was shown how to build such multiport universal interferometers with a mesh of beam splitters and phase shifters, and this design became the basis for most experimental implementations in the last decades. However, the design of Reck et al. is difficult to scale up to a large number of modes, which would be required for many applications. Here we present a constructive proof that it is possible to realize a multiport universal interferometer on N modes with a succession of 6N Fourier transforms and 6N+1 phase masks, for any even integer N. Since Fourier transforms and phase masks are routinely implemented in several optical setups and they do not suffer from the scalability issues associated with building extensive meshes of beam splitters, we believe that our design can be useful for many applications in photonics.


Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W02 GSCCM: Materials in Extremes: Simulations of Materials at Extreme Conditions

8:00AM W02.00001: Force-based interatomic potential for strength and toughness in brittle solids  MD HOSSAIN (Presenter), Univ of Delaware — Most of the available potentials (such as Tersoff, Stillinger-Weber, ReaxFF, EDIP, Vashishta, etc.) produce reliable properties (such as bulk modulus) of a solid under symmetry-preserving deformation or symmetry-breaking deformation around the linear regime of mechanical deformation. However, despite the incorporation of long-range interactions, they have sizable accuracies in producing extreme mechanical properties such as strength and toughness (which are two critical extreme mechanical properties of a solid). To address the limitations, we developed a force-based scheme that gives first-principles accurate strength and toughness. We validated the approach for a number of brittle solids including diamond, SiC, hBN, and graphene. In addition to fitting the equilibrium material properties, the approach allows fitting the potential to the forcing behavior as well as the mechanical strength of the solid, without requiring any ad hoc modifications of the nearest-neighbor interactions to avoid artificial stiffening at larger deformation. The talk will discuss the development of the force-based scheme and its application for a number of brittle solids. It will highlight a number of failure mechanisms that emerge from an accurate description of the interatomic interactions.
8:12AM W02.00002: Automated generation of machine learning-based atomistic potentials for extreme conditions*  
BEN NEBGEN (Presenter), JUSTIN SMITH, NITHIN MATHEW, JIE CHEN, LEONID BURAKOVSKY, SARYU FENSIN, KIPTON BARROS, Los Alamos Natl Lab — Neural Network (NN) interatomic potentials are a powerful tool for atomistic scale simulations, combining the generality and accuracy of ab-initio methods with costs approaching those of classical potentials. A robust training dataset covering many atomic configurations must be computed with ab-initio methods to train an accurate NN potential. Recently, active learning (AL) algorithms have demonstrated the ability to generate training datasets quickly and efficiently by selecting atomic configurations for which a NN potential has high uncertainty. This facilitates the generation of training datasets through a minimum number of ab-initio calculations with little or no human intervention. A LAMMPS interface for our NN potential, named ANI, has facilitated large-scale GPU-accelerated MD simulations using domain decomposition. Utilizing this interface, we validate an autonomously generated ANI aluminum potential using both static and dynamic simulated properties, including a partial phase diagram. Additionally, we present million-atom shock simulations of aluminum to illustrate robustness and demonstrate extensibility to the prediction of high-pressure phases.

*We acknowledge resources provided by the NNSA ASC program, the LANL LDRD program, and LANL Institutional Computing.

8:24AM W02.00003: Quantum-accurate SNAP Potential For Large-Scale Molecular Dynamics Simulations of Carbon at Extreme Conditions  
JONATHAN T WILLMAN (Presenter), ASHLEY WILLIAMS, KIEN NGUYEN-CONG, University of South Florida, ANATOLY BELONOSHKO, Royal Institute of Technology, MITCHELL WOOD, AIDAN THOMPSON, Sandia National Laboratories, IVAN OLEYNIK, University of South Florida — Highly accurate interatomic potentials are of critical importance for trustworthy MD simulations of materials at extreme conditions of high pressures, temperatures, and high strain-rates. A new quantum accurate Spectral Neighbor Analysis Potential (SNAP) for carbon has been developed to describe the behavior of carbon at multi-megabar pressures and up to 10,000 K. SNAP is formulated in terms of the bispectrum components, which play a role of descriptors that characterize the local neighborhood of each atom. Machine learning is used to train the quadratic SNAP on a large set of first-principles training data. The SNAP development involves (1) the generation of the training database comprising a consistent and meaningful set of first-principles DFT data; (2) the robust and physically guided fit of SNAP parameters; and (3) the validation of the SNAP potential in simulations of carbon at extreme conditions. In this presentation, several applications of SNAP to study carbon at extreme conditions are described.
8:36AM W02.00004: Time dependent boundary conditions for large scale atomistic simulations of shocked surface instabilities* JAMES HAMMERBERG (Presenter), Los Alamos Natl Lab, RAMON JOSE RAVELO, University of Texas El Paso, TIMOTHY GERMANN, Los Alamos Natl Lab — Shock induced surface instabilities such as Richtmyer-Meshkov instabilities at perturbed metal vacuum/gas interfaces result in metal material ejecta. For strong shock waves the material ejected is initially in the form of fluid sheets when the surface perturbation is two-dimensional. These sheets ultimately break up to form a distribution of droplets. Large-scale non-equilibrium molecular dynamics simulations of such instabilities allow the investigation of the dynamics of the breakup process but are limited in length and time scales by rarefaction wave reflections at the boundaries ultimately leading to spall that may affect the instability growth. A time-dependent boundary condition based on the self-similar character of the release wave is presented that mitigates boundary reflections and reduces unwanted tensile waves behind the perturbed interface zone. This boundary condition can be used to increase the wavelength and time scale for breakup simulations. We discuss the details of this method and results of NEMD simulations of a shocked Cu interface with a single mode perturbation characterized by a wavelength of $\lambda = 13$ nm and a wavenumber amplitude product $kh_0 = 1/2$.

*This work was funded by the LANL LDRD ER program, grant 20180721ER, whose support is gratefully acknowledged.

8:48AM W02.00005: Molecular dynamics simulation of shock compressed cis-polybutadiene : from in situ synthesis to mechanical analyses of long-term relaxation processes GAUTIER LECOUTRE, CLAIRE LEMARCHAND, LAURENT SOULARD, NICOLAS PINEAU (Presenter), CEA/DAM/DIF — We used a recently devised procedure based on molecular dynamics to generate cis-polybutadiene melts with various chain lengths [1] and study their mechanical behaviour under shock compression with the non-reactive OPLS all-atom force-field. The resulting samples show properties in excellent agreement with previous works [2] with negligible influence of the chain length. Comparison of direct shock with shock equilibrium (hugoniotstat) simulations shows a discrepancy in the shear stresses. Based on a careful mechanical analysis of the time-dependance of this difference behind the shock front, we show that their timescale is compatible with the typical equilibrium relaxation times at play in these complexe materials.

References
9:00AM W02.00006: Structure and dynamics of liquid Fe at high pressure and temperature. **A first principles study**  
DAVID J GONZALEZ (Presenter), MIRIAM MARQUES, LUIS GONZALEZ, Dpt. Fisica Teorica, Atomica y Optica, Univ. de Valladolid — The static and dynamic properties of bulk liquid Fe at high pressure and temperature conditions have been studied by using first principles molecular dynamics simulations based on the density functional theory. Results are reported for some thermodynamic states resembling those found in the Earth's outer core. We have evaluated some structural magnitudes such as static structure factors, pair distribution functions and coordination numbers. The static structure factors show an asymmetric second peak which suggests local icosahedral order in the liquid. Several dynamical properties have been calculated, such as velocity autocorrelation function, dynamic structure factors, longitudinal and transverse current spectral functions. The dispersion relations of longitudinal and transverse excitations reveal two branches of transverse collective modes. Results are also reported for some transport coefficients, namely, self-diffusion and shear viscosity.

*Funding provided by the spanish MEC and EU FEDER funds (PGC2018-093745-B-I00) and by JCyL (VA124G18)

9:12AM W02.00007: Extreme Dynamic Tension Theory: Preliminary Research**  
SEOKBIN LIM (Presenter), New Mexico Tech, PHILIPP BALDOVI, NSWC Indian Head — The dynamic tension fracture has brought much interests in various engineering applications ranging from the pressure vessel/pipe failure to the explosively driven fragmentations in the commercial/space or military applications. There has been great improvement in this area of study by many researchers, but the question regarding the fundamental mechanism of extreme tension remains unanswered. In this report, an extreme dynamic tension theory based on the conservation equations is proposed, and it is evaluated by a series of MD (molecular dynamic) and hydrocode simulations. In-depth descriptions of tension wave speed, wave profile, tension pressure/profile, particle velocity of the plastic tension wave, etc. are present, hoping to provide a clue to understand the extreme dynamic tension physics prior to the crack formation.

*This work is mainly supported by FAA-COE-CST Task 377. Authors would like to show their gratitude to NASA EPSCoR CAN (grant #: 80NSSC17M0050) and NASA's Space Grant College and Fellowship Program for the partial support of this research.
**9:24AM W02.00008: Electron-Phonon Interactions in Condensed Phases under Compression**

ANGUANG HU (Presenter), Suffield Research Centre, Defence Research and Development Canada — Electron-phonon interactions in condensed phases are central to all important temperature-dependent properties of materials such as electrical resistance in metals, carrier mobility in semiconductors, and phase transitions in conventional superconductors. Based on all-electron quantum solid-state chemistry using density functional theory, non-perturbative calculations of electron-phonon interactions have been recently developed in condensed phases under compression. Such calculations can provide a clear understanding on the thermal dependence of electron energy bands and thermomechanically induced distortion of band structures to raise or lower the Fermi level, leading to the generation of charge and spin density waves mainly determined by amplitudes of vibrational motion under mechanical compression. More importantly, calculations also show how vibrational mode energies in the measure by vibrational amplitudes distribute to reach an equilibrium state and even to create a superconducting state with the temperature-dependent energy gap. High-pressure superconductors $\text{H}_3\text{S}$ and $\text{LaH}_{10}$ are taken as examples to show calculation results in comparison with experiments.

**9:36AM W02.00009: Molecular simulations of ultrafast radiation induced melting at metal-semiconductor interfaces**

ASHWIN RAVICHANDRAN (Presenter), NASA Ames Research Center - SGT Inc, JOHN LAWSON, Intelligent Systems Division, NASA Ames Research Center — Understanding radiation induced ultrafast melting at material interfaces is essential in designing robust electronic devices for aviation/space applications and in laser machining. While it is difficult to achieve the spatial and temporal resolution required to quantify the phenomenon experimentally, simulations can provide the detailed mechanisms of the structural changes that happen during phase transition. In this work, we use molecular simulations to study the effect of radiation damage on silicon carbide (SiC) - tungsten (W) interfaces which is of interest in high power electronics. A multi-scale approach is involved wherein the reactions at the interfaces are quantified using \textit{ab-initio} molecular dynamics (MD) simulations and classical MD simulations are employed to understand the structural and diffusional changes across the material interface. Finally, coarse-grained Lennard-Jones type models are used to study the larger scale mechanisms and structures obtained due to the induced damages. We show that the response of the material to radiation damage depends on factors such as energy of the incident radiation, thermal properties, and molecular structure of the material.
9:48AM W02.00010: Accelerated Molecular Dynamics Simulations of Dislocation-Obstacle Interactions in Tungsten: Enabling Micro-Second Simulations  NITHIN MATHEW (Presenter), ENRIQUE MARTINEZ SAEZ, DANNY PEREZ, Los Alamos National Laboratory — Plasma Facing Materials (PFMs) in fusion reactors have to withstand extreme temperatures and high particle flux of Hydrogen (H) isotopes and Helium (He). Tungsten (W) is the main candidate for PFM in the International Thermonuclear Experimental Reactor but He irradiation of W results in modification of surface microstructure due to creation of Helium-Vacancy (HeₙVm) complexes. This leads to increased retention of H isotopes and degradation of thermomechanical stability. In this work, we study the interaction of these HeₙVm complexes with edge dislocations using accelerated molecular dynamics. We use a novel Parallel Replica Dynamics method where states and transitions are identified on-the-fly using a diffusion distance metric calculated from an approximation of the Koopman operator of the dynamics. Using up to 600 replicas, we are able to investigate the interactions between edge dislocations and HeₙVm complexes at temperatures ranging from 300-1200 K and applied stresses well below the critical resolved shear stress. The calculated rates for the dislocation to overcome the obstacle span ≈3 orders of magnitude, reaching micro-second timescales at low temperatures/stresses, and show a strong dependence on the applied stress.

10:00AM W02.00011: Periodic Boundary Condition for Large Material Deformation*  DUAN ZHANG (Presenter), MIN WANG, PAUL BARCLAY, Los Alamos Natl Lab — The use of periodic boundary conditions has been a common practice in numerical simulations for the study of constitutive response of materials. To consider material deformation, the common method of enforcing the periodic boundaries is to deform the computational domain with the material, which limits the strain of the material to order one. The method fails when strains are large or the deformation gradients are complicated, such as those containing large rotation or twist. For instance, it is quite difficulty to perform a simulation under a large pure shear deformation because of the distorted and elongated computational domain.

To avoid this difficulty, a different method has been developed by decomposing the velocity gradient matrix into the upper triangle part and the antisymmetric part representing a pure rotation. The antisymmetric part is then canceled by performing the simulation in a rotating reference frame and considering the associated inertial forces. Advantages of this method will be shown using examples.

*Work sponsored by Exascale Computing Program of LANL under auspice of US DOE.
10:12AM W02.00012: Phase transitions and new states under extreme conditions from first-principles* [Invited] JIAN SUN (Presenter), Nanjing University — High pressure is an important method to modify the free energy surface of materials and overcome the barriers for synthesizing new functional materials. On the other hand, crystal structure search based on ab initio calculations has been successfully used to prediction new materials. In this talk, I will introduce some of our recent work on theoretical prediction on high pressure phase transitions, functional materials with interesting properties, and new states of matter under extreme conditions, such as superionic states.

REFERENCE

*MOST of China, NSFC

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W07 DQI: Quantum Amplifiers, Bolometers, and Detectors 102 -
Guilhem Ribeill, BBN Technology - Massachusetts
8:00AM W07.00001: Sensitive and fast bolometer integrable with superconducting qubit readout* MIKKO MOTTONEN (Presenter), ROOPLE KOKKONIEMI, JEAN-PHILIPPE GIRARD, QCD Labs, QTF Centre of Excellence, Department of Applied Physics, Aalto University, DIBYENDU HAZRA, Micro & Nanoelectronics, VTT Technical Research Centre of Finland, ANTTI LAITINEN, NANO group, QTF Centre of Excellence, Department of Applied Physics, Aalto University, JOONAS GOVENIUS, Micro & Nanoelectronics, VTT Technical Research Centre of Finland, RUSSELL LAKE, IIRO SALLINEN, QCD Labs, QTF Centre of Excellence, Department of Applied Physics, Aalto University, VISA VESTERINEN, Micro & Nanoelectronics, VTT Technical Research Centre of Finland, EEMIL VISAKORPI, QCD Labs, QTF Centre of Excellence, Department of Applied Physics, Aalto University, SANNA ARPIAINEN, MIKA PRUNNILA, Micro & Nanoelectronics, VTT Technical Research Centre of Finland, PERTTI JUHANI HAKONEN, NANO group, QTF Centre of Excellence, Department of Applied Physics, Aalto University — Traditionally, bolometers have been too slow and inaccurate to operate in quantum sensing applications in the microwave regime. Thus their benefits such as simple setup, broad input band, absence of quantum noise, and energy-resolving calorimetry has not been harnessed in microwave quantum sensing. We report on a new type of a bolometer that simultaneously reaches the lowest noise reported for any bolometer, 20 zW/Hz$^{0.5}$ [1], and is roughly three orders of magnitude faster than the previous ultralow-noise bolometers. The thermal time constant, measured at the 100-ns range, corresponds to the typical speed of state-of-the-art high-fidelity qubit readout schemes [2]. The extracted energy resolution of this bolometer being in the 10-GHz range it manifests as a potentially important future tool in reading out superconducting qubits [3] or in quantum sensing applications in the microwave regime [4].


*We acknowledge EU Quantum Flagship project QMiCS and Academy of Finland (312300, 314449) for funding.
Towards a Microwave Single Photon Detector Using Inelastic Cooper Pair Tunneling

JOËL GRIESMAR (Presenter), Université de Sherbrooke, ROMAIN ALBERT, CEA Grenoble, JUHA LEPPÄKANGAS, Karlsruher Institut für Technologie, MAX HOFHEINZ, Université de Sherbrooke — The detection of single photons is a fundamental quantum measurement, complementary to linear amplification. However, in the microwave domain this is a difficult task due to the low energy of the photons. We present here a photo-multiplier using the energy of a Cooper pair tunneling across a voltage-biased Josephson junction to convert one microwave photon into several photons at a different frequency. This process relies on the strong non-linearity provided by the interaction between a Josephson junction and its high-impedance electromagnetic environment. We have fabricated and measured a device composed of a low critical current SQUID galvanically coupled to two high-impedance resonators. It showed conversion from one to two photons with an efficiency of 80% and also exhibited conversion from one to three photons. By cascading two of these multiplication stages and adding a quantum limited amplifier, it should be possible to discriminate itinerant single photon states from vacuum without dead time.

*This research was supported by Canada First Research Excellence Fund, Natural Sciences and Engineering Research Council of Canada, Agence Nationale de la Recherche and Grenoble Nanosciences Foundation.

Josephson single infrared photon detector

EVAN D. WALSH, Massachusetts Institute of Technology, GIL-HO LEE, WOOCHAN JUNG, Pohang University of Science and Technology, K.-F. HUANG, Harvard University, BAE-IAN WU, Air Force Research Laboratory, DMITRI EFETOV, ICFO - The Institute of Photonic Sciences, THOMAS A OHKI, BBN Technology - Massachusetts, PHILIP KIM, Harvard University, DIRK R. ENGLUND, Massachusetts Institute of Technology, KIN CHUNG FONG (Presenter), BBN Technology - Massachusetts — Josephson junction (JJ) enables many high sensitivity detectors such as SQUID amplifier, magnetometer, microwave mixer, bolometer, and parametric amplifier. In the earliest realization of Josephson detectors during the 70’s, photodetection was one of the target applications before it fell out of competition due to the lack of good detection and coupling mechanism. However, new opportunities are now opening up for photodetection by exploiting the electrical and thermal properties of graphene in the superconducting-graphene-superconducting junctions. In this talk, we report the experimental detection of near-infrared (NIR) single photons by a graphene-based JJ via non-resonant Cooper-pair breaking and the resulting quasiparticle diffusion. Our method demonstrates an efficient mechanism for the electromagnetic wave to interact directly with the JJ. Such single photon detector is an enabling technology for quantum communication, quantum computing, and could be used as cryogenic optical interconnects.
**8:36AM W07.00004: Frequency tunable single microwave photodetector based on irreversible qubit-photon coupling**  
EMANUELE ALBERTINALE (Presenter), CEA-Saclay, RAPHAËL LESCANNE, École Normale Superieure, SAMUEL DÉLEGLISE, LKB Sorbonne, ZAKI LEGHTAS, École Normale Superieure, DANIEL ESTEVE, PATRICE BERTET, EMMANUEL FLURIN, CEA-Saclay — Single photon detection is a key resource for sensing at the quantum limit and is the enabling technology for measurement-based quantum computing, however microwave photons have energies 5 orders of magnitude lower than optical ones and are therefore ineffective at triggering measurable phenomena at macroscopic scales.
We report the observation of a new type of interaction between a two level system and a microwave resonator. These two quantum systems do not interact coherently but share a common dissipative mechanism to a cold bath: the qubit irreversibly switches to its excited state if and only if a photon enters the resonator. This highly correlated dissipation mechanism is used to detect itinerant photons impinging on a frequency tunable resonator. The scheme does not require any prior knowledge of photon waveform or arrival time, and dominant decoherence mechanisms do not trigger spurious events. We demonstrate a detection efficiency of 65%, a record low dark count rate of 1/ms over a frequency tuning range of 200 MHz and the capability to operate the detector in cyclic mode with a 50% duty cycle on a 10 µs detection sequence, making it a practical tool for quantum sensing and measurement-based computing in microwave domain.

*EU Horizon 2020 Marie Curie grant agreement 765267*

**8:48AM W07.00005: A Superconducting Detector That Counts Microwave Photons up to Two**  
ANDRII SOKOLOV (Presenter), Universität des Saarlandes, Institute of Physics of the National Academy of Sciences of Ukraine, FRANK WILHELM, Universität des Saarlandes — We propose a detector of microwave photons which can distinguish the vacuum state, one-photon state, and the states with two or more photons. Its operation is based on the two-photon transition. The detection occurs when a Josephson junction switches from a superconducting to a normal state, which provides a macroscopic voltage. We model the detector theoretically and evaluate its performance.

*Work of A.S. was partly supported by a DAAD scholarship (2016).*
9:00AM W07.00006: Primary thermometry of propagating microwaves in the quantum regime  MARCO SCIGLIUZZO, ANDREAS BENGTSSON, Chalmers Univ of Tech, JEAN-CLAUDE BESSE, ANDREAS WALLRAFF, ETH Zurich, PER DELSING, SIMONE GASPARINETTI (Presenter), Chalmers Univ of Tech — The ability to control and measure the photonic occupation of propagating microwave modes down to very low temperatures is indispensable for quantum information processing with superconducting circuits, and may open opportunities for studies of thermodynamics at the nanoscale. Yet, the methods used so far are indirect, require sophisticated time-resolved measurements, and have poor temporal resolution. Here we propose and experimentally demonstrate primary thermometry of propagating microwave modes, using a transmon-type superconducting circuit. We illustrate our method by measuring the radiation temperature of a highly attenuated coaxial cable connecting room-temperature electronics to the base plate of a dilution cryostat, in the range of 200 mK down to 35 mK and with resolution well below one per mil in thermal occupation. To increase the radiation temperature in a controlled fashion, we either inject calibrated, wideband digital noise, or heat the device and its environment. In the latter case, we observe the thermalization dynamics of the microwave modes in real time. Our technique can be used to benchmark filtering and attenuation schemes for superconducting quantum information processors; at the same time, it provides a novel tool for experiments in quantum thermodynamics.

9:12AM W07.00007: Using Superconducting Qubits for Axion Dark Matter Detection  AKASH DIXIT (Presenter), SRIVATSAN CHAKRAM, ANKUR AGRAWAL, University of Chicago, RAVI KAUSHIK NAIK, University of California, Berkeley, DAVID I SCHUSTER, University of Chicago, AARON CHOU, Fermilab — The axion is a potential solution to the strong CP problem in QCD and could account for the abundance of dark matter observed in the universe. In the presence of an applied magnetic field, the axion field will source a current used to drive a resonant cavity to single photon occupation. A transmon qubit operating as a microwave photon sensor is a viable readout system at frequencies where the added noise of quantum limited amplifiers overwhelms the signal rate. The use of a direct dispersive quantum non-demolition measurement of the photon number decouples the measurement back action from the experimental uncertainties. In this regime dark counts are the dominant sources of detector error. For a transmon qubit operating as a photon counter, dark counts occur due to qubit errors which occur with probability 1-10%. In order to mitigate the effect of individual qubit flip errors of the detector, repeated measurements of the same photon are performed. The error rate of the joint N measurements could be significantly suppressed. The detector errors are then no longer the dominant source of false positives when attempting to measure weak signals sourced by the dark matter.
9:24AM W07.00008: High-Q Photonic Bandgap Microwave Cavity for Dark Matter Axion Searches*  ANKUR AGRAWAL (Presenter), AKASH DIXIT, University of Chicago, WENJIE YAO, STEVEN G. JOHNSON, Massachusetts Institute of Technology, MOHAMED AWIDA, Fermilab, DAVID I SCHUSTER, University of Chicago, AARON CHOU, Fermilab — A 3D photonic bandgap (PBG) crystal forbids the propagation of electromagnetic waves with energy within a certain range in all directions. We create an electromagnetic cavity by designing a defect inside the crystal such that its frequency lies within the forbidden gap. With enough number of periods in the crystal, the Q-factor is only limited by the dielectric loss in the material. One of the potential applications is in the Axion Dark Matter search, which is currently limited by the usage of low Q-factor copper cavities due to the presence of a strong magnetic field. We present various designs and experimental results of dielectric materials which can significantly increase the sensitivity and scanning rate of axion search. We predict the Q-factor of a PBG cavity to increase in the presence of a large magnetic field due to the shift in the two-level system energies to a higher level.

*Supported by the Heising-Simons Foundation

9:36AM W07.00009: Her Dark Materials: Comparison of Semiconducting Targets for Multi-Channel Direct Detection of Light Dark Matter  KATHERINE INZANI (Presenter), Lawrence Berkeley National Laboratory, TANNER TRICKLE, ZHENGKANG ZHANG, Department of Physics, University of California, Berkeley, KATHRYN ZUREK, Walter Burke Institute for Theoretical Physics, California Institute of Technology, SINÉAD GRIFFIN, Lawrence Berkeley National Laboratory — The nature of dark matter (DM) remains one of the greatest mysteries of physics. Experiments searching for DM on the mass scale of WIMPs have not established a DM signal, whilst the lighter mass range of keV to GeV is well-motivated yet unexplored. Expanding the reach of direct detection experiments down to light DM masses requires new ideas for the types of excitation that are possible and efficient pathways for their detection. Correspondingly, materials with a strong response must be identified for use as targets.

We have designed a methodology for evaluating the sensitivity of semiconducting materials to DM excitations based on density functional theory calculations.\(^1\) The model takes into account three complementary interactions: nuclear recoils, electron transitions across band gaps and single phonon excitations. We include a novel multi-channel response.

Using this framework, we have calculated the performance of 25 materials for a comparison of target sensitivities.\(^2\) We identify the materials parameters that must be optimized in order to maximize experimental reach. Furthermore, we evaluate a two-dimensional material which can exhibit the “smoking gun” DM signature of daily and annual modulation.

\(^{1}\)arXiv:1910.08092
\(^{2}\)arXiv:1910.10716
9:48AM W07.00010: Interfacial effects on phonon propagation through quantum sensors used for dark matter detection  THOMAS HARRELSON (Presenter), SINEAD GRIFFIN, Lawrence Berkeley National Laboratory — Several proposals for the direct detection of dark matter (DM) of keV-MeV masses involve the scattering and absorption of DM with quasiparticles in the meV-eV energy transfer range. At these energy scales, phonons are the dominant energy carrier in most materials. Therefore, the task of detecting DM particles reduces to the detection of athermal distributions of phonons in a target material, which is accomplished using a transition edge sensor (TES). The phonons generated by DM scattering events in the target material propagate to the interface of the TES, and are either reflected or transmitted into the TES. We use density functional theory simulations to describe the probability at which phonon distributions are transmitted through the target/TES interface, and the coherence losses in quasiparticle transmission to the sensor. Specifically we calculate currently used targets Si and GaAs, with an Al TES. We consider the commercially available crystal faces for the target materials, and use these simulations to find the best target/TES interfaces for optimizing the phonon transmission coefficients. We use this information to create more accurate models of DM detection, which allows the optimization of the target material and interfaces in the quantum sensor.

10:00AM W07.00011: Gain calibration of a cryogenic amplification chain using normal-metal–insulator–superconductor junctions  MÁTÉ JENEI (Presenter), ERIC HYYPPÄ, SHUMPEI MASUDA, KUAN YEN TAN, VASILII SEVRIUK, QCD Labs, QTF Center of Excellence, Department of Applied Physics, Aalto University, MATTI SILVERI, Research Unit of Nano and Molecular Systems, University of Oulu, JAN GOETZ, MATTI PARTANEN, RUSSELL LAKE, QCD Labs, QTF Center of Excellence, Department of Applied Physics, Aalto University, LEIF GRÖNBERG, QTF Center of Excellence, VTT Technical Research Centre of Finland, MIKKO MOTTONEN, QCD Labs, QTF Center of Excellence, Department of Applied Physics, Aalto University — To achieve a high-efficiency readout in a low-temperature microwave circuit using both cryogenic and room temperature electronics, the signal has to go through one or more amplifiers to obtain a reasonable signal-to-noise ratio. In practice, the readout line has additional losses and reflections due to different microwave components which hinder the gain estimation. We present a gain calibration scheme [1] that utilizes a normal-metal–insulator–superconductor junction, which is capacitively coupled to a superconducting microwave resonator [2]. Depending on the bias voltage applied to the junction, the nanostructure can be employed as a quantum-circuit refrigerator [3] or as an incoherent photon source [4]. For the latter case, we derive an analytic expression for the total gain that is based on only a single fitting parameter. We present our experimental results where we reach 0.1 dB relative uncertainty of the total gain in a three-stage amplification chain.

10:12AM W07.00012: Josephson Parametric Amplifiers Fabricated in Wafer-scale with Side-wall Passivated Spacer Junction Technology* VISA VESTERINEN (Presenter), SLAWOMIR SIMBIEROWICZ, LEIF GRÖNBERG, JANNE LEHTINEN, ROBAB NAJAFI JABDARAGHI, MIKA PRUNNILA, JOONAS GOVENIUS, VTT Technical Research Centre of Finland Ltd — We present our latest experimental results on Josephson parametric amplifiers (JPAs) fabricated with our Nb/Al-AlOx/Nb junction process. The fabrication relies on UV photolithography and semi-automated 150-mm wafer processing steps, while minimizing the amount of deposited lossy dielectric materials [1]. The first JPA category is a flux-driven reflection amplifier for sub-GHz frequencies. It has found applications in the rf reflectometry of quantum dots, as well as in the rf readout of microwave nanobolometers [2] and charge detectors. Secondly, we report on the development of a 4-8 GHz traveling wave parametric amplifier tailored for the readout of superconducting quantum bits.


*This research was funded by EU Quantum Flagship (OpenSuperQ, QMiCS), and Academy of Finland (312059, 312294, 321700).

10:24AM W07.00013: Noise performance of a three-wave mixing kinetic inductance traveling-wave parametric amplifier MAXIME MALNOU (Presenter), JIANSONG GAO, MICHAEL R. VISSERS, JOEL N ULLOM, National Institute of Standards and Technology — Kinetic inductance traveling wave parametric amplifiers (KITs) have the potential to read out large numbers of qubits and cryogenic sensors due to their wide bandwidth, high saturation power, and potentially quantum-limited noise performance. However, noise in KITs has so far not been carefully studied, including its dependencies on device design and operating conditions. Here, we present a KIT based on a sub-micron resolution structure that is biased with a dc current and pumped in a three-wave mixing fashion. We experimentally evaluate its noise properties, which approach the quantum limit, and discuss its suitability for readout applications.
Overlap junction-based Josephson parametric amplifiers (O-JPA)

MUSTAFA BAL (Presenter), JUNLING LONG, RUICHEN ZHAO, HAOZHI WANG, COREY RAE MCRAE, RUSSELL LAKE, SUNGOH PARK, XIAN WU, HSIANG-SHENG KU, National Institute of Standards and Technology Boulder, DANIEL FROLOV, ROMAN PILIPENKO, SILVIA ZORZETTI, ERIC T HOLLAND, ALEXANDER ROMANENKO, Fermi National Accelerator Laboratory, DAVID PAPPAS, National Institute of Standards and Technology Boulder — We have recently developed submicron scale overlap Josephson junction fabrication process suitable for superconducting qubits with long coherence times [1]. Here, we extend the fab process to micron scale overlap junctions to enable other superconducting quantum devices such as overlap junction-based Josephson parametric amplifiers (O-JPA). We realize frequency tunable O-JPAs with negligible insertion loss. Compared to other competing processes, overlap junction process for micron scale junctions allows the fabrication of O-JPAs with high yield and good device performance at a much lower infrastructure requirements. We present the fabrication details as well as the characterization of O-JPAs.


Fabrication tolerances for traveling wave parametric amplifiers

DENNIS FENG (Presenter), MEHRNOOSH VAHIDPOUR, YUVRAJ MOHAN, SAM STANWYCK, TYLER WHYLAND, NICHOLAS SHARAC, GANESH RAMACHANDRAN, MICHAEL SELVANAYAGAM, Rigetti Quantum Computing — Resonantly phase matched traveling wave parametric amplifiers (TWPAs) [1] are sensitive to device fabrication errors. We develop a method to analyze the performance of the TWPA with emulated fabrication variations and different process parameters. We begin with an ideal analytic model and use circuit analysis and full-wave modeling to perturbatively calculate the full-circuit dispersion relation. We use this to find fabrication tolerances to different circuit parameters as well as ways to mitigate that sensitivity. We demonstrate that these robust designs with fabricated amplifiers achieve reasonable parametric gain and instantaneous bandwidth, suitable for multi-qubit multiplexed readout.


Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W08 DQI: Superconducting Qubits: Materials, Fabrication and Coherence III 104 - Anna Stockklauser, Rigetti Quantum Computing
8:00AM W08.00001: Superconducting qubit devices: fabrication suite*  KOK WAI CHAN  
(Presenter), TIANYI LI, WEI LIU, JOHANNES HEINSOO, VASILII SEVRIUK, CASPAR OCKELOEN-KORPPI,  
JANI TUORILA, JUHA HASSEL, JUHA VARTIAINEN, KUAN YEN TAN, JAN GOETZ, MIKKO MOTTONEN,  
IQM Finland Oy — Scalable quantum computing architecture and fabrication processes have been  
a hot research topic in the past decade. We focus on the realization of a quantum computer  
based on superconducting qubits with a fast qubit reset and initialization techniques, utilizing a  
quantum-circuit refrigerator [1]. We present the fabricated devices and results achieved to date,  
which includes resonators with high quality factors, > 1e6, long qubit lifetime > 0.02 ms and 3D  
integration techniques such as airbridges.  

*We acknowledge the provision of facilities and technical support by Aalto University at OtaNano - Micronova Nanofabrication Centre. We thank Quantum Technologies Flagship members for scientific discussions.

8:12AM W08.00002: NbN-based superconducting qubit on Si substrate*  SUNMI KIM  
(Presenter), TOMOKO FUSE, FUMIKI YOSHIHARA, WEI QIU, Advanced ICT research institute, NICT, TARO  
YAMASHITA, Department of Engineering, Nagoya University, ZIQIAO AO, KOUICHI SEMBA, HIROTAKA  
TERAI, Advanced ICT research institute, NICT — In the superconducting qubit composed of  
aluminum-based Josephson junctions (JJs), the decoherence from microscopic two-level systems  
in amorphous aluminum oxide is concerned. As alternative materials for qubits, fully epitaxial  
NbN/AlN/NbN JJs are an attractive candidate with the potential to solve the above problems  
because of its high crystal quality, its chemical stability against oxidization, and relatively high  
transition temperature (~ 16 K) of NbN. Here we note that AlN is grown in cubic phase to avoid  
piezoelectricity. Early studies of superconducting qubits using epitaxially grown nitride JJs showed  
significant potential, but the qubit energy relaxation time was limited due to dielectric loss from  
the MgO substrate. [Y. Nakamura et al., APL, 99, 212502 (2011)]. In order to solve this problem,  
we have employed a Si substrate with TiN buffer layer for the epitaxial growth of this nitride JJs  
a λ/2 coplanar waveguide resonator. We observed clear Rabi oscillations and Ramsey  
interference patterns. We will discuss the detailed coherence characteristics.  

*Part of this work has been supported by JST-CREST (Grant No. JPMJCR1775) and KAKENHI  
(JP19H05615).
8:24AM W08.00003: Flux qubits fabricated using a high-coherence transmon process*
TREVOR CHISTOLINI (Presenter), WILLIAM LIVINGSTON, BRADLEY MITCHELL, IRFAN SIDDIQI, University of California, Berkeley — Over the past years, superconducting circuit qubit lifetimes have been continuing to increase, largely due to design enhancements in addition to processing and fabrication evolution. While the earliest designs of Cooper pair boxes exhibited $T_1$ coherence times on the order of 1 ns, there are recent reports of transmon lifetimes exceeding 100 μs. We now apply these advances in processing to look back upon flux qubits, and we present an 8-qubit ring of alternating flux qubits and tunable transmons, with coupling between nearest neighbors. Preliminary work focuses on optimizing flux qubit design and increasing experimentally observed coherence times, with motivation from theoretical studies and numerical simulations targeting energy structure and noise coupling. Meanwhile, further theoretical investigations into novel two qubit gate designs between flux qubits and transmons, which leverage their opposing anharmonicities, are underway.

*This work was funded by the Army Research Office. This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE 1752814.

8:36AM W08.00004: Fabrication and characterization of compact vacuum gap transmon qubits* MARTIN ZEMLICKA (Presenter), MATILDA PERUZZO, FARID HASSANI, SHABIR BARZANJEH, ELENA REDCHENKO, ANDREA TRIONI, JOHANNES FINK, Institute of Science and Technology Austria — The large shunt capacitance of the transmon qubit decreases its sensitivity to charge fluctuations but requires sizeable qubit dimensions. Very large capacitor designs furthermore lower the coupling to parasitic losses localized in material interfaces, an approach that improves coherence times consistently, but lowers the achievable integration density and increases parasitic cross coupling and leakage in superconducting processors. Our goal is the development of a compact low-loss transmon qubit by minimizing the electric field participation ratio of metal-dielectric and dielectric-air interfaces. Several attempts to realize vacuum gap capacitors were already implemented [1, 2], usually relying on an out-of-plane geometry that involved a sacrificial layer before releasing the structure. We utilize silicon membranes to fabricate micro-machined resonators and transmon qubits based on suspended in-plane vacuum capacitors [3] with qubits sizes as low as 20 x 20 μm^2.


*Supported by the Austrian Science Fund (FWF) through BeyondC (F71)
8:48AM W08.00005: Characterization of Al-based Airbridges for Superconducting Microwave Devices. ROBAB NAJAFI JABDARAGHI (Presenter), LEIF GRÖNBERG, VISA VESTERINEN, MIKA PRUNNILA, VTT Technical Research Centre of Finland Ltd — The realization of a co-planar waveguide (CPW) for quantum circuits requires only a single wiring layer. However, the usability of the structure is limited by parasitic slotline modes which can modify couplings and act as a loss channel in complex superconducting integrated circuits. Free-standing metallic crossovers known as airbridges [1,2] commonly provide electrical connectivity between ground planes to suppress the parasitic modes. Here, we demonstrate our latest development of Al airbridges in conjunction with Nb CPWs. Our fabrication method relies on three separate optical lithography steps with Al deposition combined with the CPW structures using re-flowed photoresist as a scaffold. We are striving for low-loss airbridges that are robust against sonication and etches during further processing. At present, more than 90% of our airbridges survive the sonication. [1] Z. Chen et al., Applied Physics Letters 104, 052602 (2014). [2] Y. Kwon et al., IEEE microwave and wireless components letters 11, 59 (2001).

*This research was funded by Academy of Finland (312059, 312294), the Technology Industries of Finland Centennial Foundation, and the Jane and Aatos Erkko Foundation.

9:00AM W08.00006: Epitaxial GaAs Loss Measurements and the Merged Element Transmon* COREY RAE MCRAE (Presenter), NIST Boulder / CU Boulder, ANTHONY P MCFADDEN, UCSB, RUICHEN ZHAO, HAOZHI WANG, SUNGOH PARK, JUNLING LONG, NIST Boulder / CU Boulder, CHRIS J PALMSTROM, UCSB, DAVID PAPPAS, National Institute of Standards and Technology Boulder — Transmon qubits are traditionally composed of two components: a Josephson junction, which is commonly made up of a pair of superconducting aluminum films separated by a thin layer of amorphous aluminum oxide, and a large paddle capacitor. The presence of lossy materials in this design, as well as the significant size of the capacitor paddles, limits the transmon’s performance and scalability. In contrast, the merged element transmon design combines the qubit’s nonlinear inductance and capacitance into a single trilayer junction with extremely low dielectric loss. GaAs is a good candidate test material for these trilayer junctions as its epitaxial growth and interface with Al is well-characterized, and single crystal growth and lattice matching is possible. In this work, we use dielectric loss extraction methods to accurately measure the TLS loss for Al/GaAs/Al trilayers.

*Army Research Office
9:12AM W08.00007: Frequency Fluctuations in Tunable Superconducting Microwave Cavities

BENJAMIN BROCK (Presenter), MILES BLENCOWE, ALEXANDER J RIMBERG, Dartmouth Coll — We present a model for measurements of the scattering matrix elements of tunable microwave cavities in the presence of resonant frequency fluctuations induced by fluctuations in the tuning parameter. We apply this model to the specific case of a two-sided cavity and find an analytic expression for the average scattering matrix elements. A key signature of this `fluctuating model' is a subtle deformation of the trajectories swept out by scattering matrix elements in the complex plane. We apply this model to experimental data and report a direct observation of this deformation in the data. Despite this signature, we show that the fluctuating and non-fluctuating models are qualitatively similar enough to be mistaken for one another, especially in the presence of measurement noise. However, if one applies the non-fluctuating model to data for which frequency fluctuations are significant then one will find damping rates that appear to depend on the tuning parameter, which is a common observation in tunable superconducting microwave cavities. We propose this model as both a potential explanation of and remedy to this apparent phenomenon.

*Supported by NSF grants DMR-1807785 and DMR-1507383

9:24AM W08.00008: Investigation of surface induced loss mechanisms in high-quality superconducting Nb resonators

JEROEN VERJAUW (Presenter), MASSIMO MONGILLO, ANTON POTOCNIK, ROHITH ACHARYA, ANTOINE PACCO, TSVETAN IVANOV, DANNY WAN, LAURENT SOURIAU, JULIEN JUSSOT, ARAME THIAM, JOHAN SWERTS, XIAOYU PIAO, SEBASTIEN COUET, BOGDAN GOVOREANU, IULIANA RADU, MARC HEYNS, IMEC — Performance of superconducting qubit devices is limited by two-level system (TLS) defects, predominately found in amorphous interface layers. Reducing microwave loss contributions from these interfaces by proper surface treatments is key to push the device performance forward. We study niobium resonators where the native oxides at the metal-air & substrate-air interface are selectively etched with Hydrofluoric (HF) acid. Although HF treatment right before the low temperature characterization is known to yield an order of magnitude improvement in the resonator's quality factor, the precise loss contribution from various residual oxides and other defects at the interfaces is still unknown. By combining resonator quality factor measurements with X-ray photoelectron spectroscopy (XPS), electron energy loss spectroscopy (EELS) and other surface characterization techniques, we investigate the reappearance of loss mechanisms introduced by exposure to ambient conditions. This is of particular interest for fabricating air resilient, high-quality superconducting qubit devices as they share the same loss mechanisms with resonators.
9:36AM W08.00009: Flux Noise and Spin Dynamics of Multiple Interacting Adsorbates on Superconducting Qubits* KEITH RAY (Presenter), YANIV J ROSEN, JONATHAN L DUBOIS, VINCENZO LORDI, Lawrence Livermore Natl Lab — Molecular oxygen, OH group, and atomic hydrogen surface adsorbates have been identified as possible sources of magnetic flux noise in superconducting qubits. This noise causes decoherence and frequency jitter that can hinder tunable multi-qubit devices. To better understand the spin dynamics of these fluctuating adsorbates we have extended our model for interacting adsorbed paramagnetic $O_2$ molecules to include other species adsorbed from the device operation atmosphere, including water at different coverages. We calculate the effects of applied fields on the phases of the spin system, its dynamics, and the charge and flux noise generated. To do this we utilize a thermodynamic ensemble generated with Monte Carlo simulations along with Landau-Lifshitz-Gilbert equation simulations for the dynamics, both parametrized with vdW-corrected density functional theory calculations.

*Prepared by LLNL under Contract DE-AC52-07NA27344.

9:48AM W08.00010: Positive- and negative-frequency noise from an ensemble of two-level fluctuators* XINYUAN YOU (Presenter), Northwestern University, AASHISH CLERK, University of Chicago, JENS KOCH, Northwestern University — Depolarization of superconducting qubits with intrinsic protection, such as heavy fluxonium or the 0-π qubit, is dominated by excitation rather than relaxation processes. To extract the corresponding excitation rates, it is thus crucial to carefully consider the negative-frequency components of the noise spectral density. We are particularly interested in noise sources with the ubiquitous 1/f spectrum at positive frequencies. Existing models based on an ensemble of two-level fluctuators predict a symmetric noise spectral density valid in the high-temperature limit. We extend the analysis beyond this limit, and derive results explicitly obeying the fluctuation–dissipation theorem. We discuss deviations from pure 1/f behavior and compare with recent experimental observations.

*This research was supported by the U.S. Army Research Office under contract number W911NF-17-C-0024 and the Northwestern–Fermilab Center for Applied Physics and Superconducting Technologies.

10:00AM W08.00011: Random two-level defects in polycrystalline and amorphous alumina CHIH-CHIAO HUNG (Presenter), KEVIN OSBORN, NEDA FOROUZANI, BAHMAN SARABI, University of Maryland, College Park — Atomic two-level system (TLSs) are ubiquitous defects in superconducting qubits, however the TLS host material is generally amorphous alumina. We extend a characterization technique to, for the first time, study TLSs in two states of the same material: amorphous and polycrystalline alumina. A large distribution of approximately 400 individual TLS dipole moments are obtained in polycrystalline AlOx along a common axis. The averaged dipole moment in material is approximately 3.1 Debye. On the other hand, the average dipole moment is much larger in amorphous alumina, which is contradicted by expectations. We observe strong TLS frequency drifting phenomenon in the amorphous sample which relates to its TLS-TLS interactions. For the first time, a material characterization technique shows that one can collect a large amount of individual TLS data for material optimization, such as TLS dipole moments and TLS frequency stability.
10:12AM W08.00012: Coplanar silicon/aluminum resonators with internal quality factor above 2M: fabrication*  AIDAR GABIDULLIN (Presenter), FMN Laboratory, Bauman Moscow State Technical University, ALINA ALEKSANDROVNA DOBRONOSOVA, Dukhov Automatics Research Institute, (VNIIA), ANTON IVANOV, FMN Laboratory, Bauman Moscow State Technical University, LUCIA ALMIROVNA GANIEVA, Dukhov Automatics Research Institute, (VNIIA), DMITRIY MOSKALEV, ANDRONIC MICHAEL, NIKITA SERGEEVICH SMIRNOV, DMITRIY BAKLYKOV, FMN Laboratory, Bauman Moscow State Technical University, OLGA SOROKINA, Dukhov Automatics Research Institute, (VNIIA), GLEB PETROVICH FEDOROV, Moscow Institute of Physics and Technology, ILYA RODIONOV, FMN Laboratory, Bauman Moscow State Technical University — Extremely low intrinsic loss coplanar resonators are critical elements in superconducting quantum computing devices, photon detectors, parametric amplifiers and quantum memories. Here we describe the fabrication and measurement of superconducting coplanar waveguide microwave resonators on silicon substrates with internal quality factors over 2 millions at low powers, corresponding to single-photon regime. These quality factors are achieved by careful optimization of resonators geometry, measurement setup and key TLS-containing interfaces: metal-air, metal-substrate, and substrate-air. We provide a detailed analysis of the design and technological factors impact on resonators quality, including multi-step substrates cleaning, aluminum films crystalline structure, low-damage dry etching, design features and air-bridges application. Finally, using the same process flow we fabricate and characterize superconducting tunable X-mon qubits with the coherence over 100 us, confirming well-known correlations between resonators and qubits quality.

*Devices were fabricated at the BMSTU Nanofabrication Facility (Functional Micro/Nanosystems, FMNS REC, ID 74300).

10:24AM W08.00013: Long Relaxation Times of a C-shunt Flux Qubit Coupled to a 3D Cavity*  LEONID ABDURAKHIMOV (Presenter), IMRAN MAHBOOB, HIRAKU TOIDA, KOUSUKE KAKUYANAGI, SHIRO SAITO, NTT Basic Research Laboratories, NTT Corporation — We present measurements of relaxation times of a capacitively shunted flux qubit embedded in a 3D microwave cavity. Qubit energy-relaxation times T_{1} were found to be in the range of 60-90 μs, and Hahn-echo coherence time T_{2E} was about 80 μs. Using the CPMG dynamical decoupling sequence, the T_{1}-limited coherence time T_{2CPMG} of 160 μs was reached. Qubit energy relaxation could be attributed to quasiparticle tunneling, while dephasing times were limited by charge and critical-current noises at the optimal flux bias point and by 1/f flux noise elsewhere. With their relaxation times being comparable or exceeding previously reported values for other types of flux qubits, 3D c-shunt flux qubits can be utilized for quantum annealing, quantum magnetometry and spin sensing.

*This work was partially supported by JST CREST (JPMJCR1774).
10:36AM W08.00014: Coplanar silicon/aluminum resonators with internal quality factor above 2M: measurements*

ANTON IVANOV (Presenter), FMN Laboratory, Bauman Moscow State Technical University, VIKTOR IVANOVICH POLOZOVA, ELIZAVETA IL'INICHNA MALEVANNAYA, Dukhov

10:36AM W08.00014: Coplanar silicon/aluminum resonators with internal quality factor above 2M: measurements*

ANTON IVANOV (Presenter), FMN Laboratory, Bauman Moscow State Technical University, VIKTOR IVANOVICH POLOZOVA, ELIZAVETA IL'INICHNA MALEVANNAYA, Dukhov

10:36AM W08.00014: Coplanar silicon/aluminum resonators with internal quality factor above 2M: measurements*

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10:36AM W08.00014: Coplanar silicon/aluminum resonators with internal quality factor above 2M: measurements*

ANTON IVANOV (Presenter), FMN Laboratory, Bauman Moscow State Technical University, VIKTOR IVANOVICH POLOZOVA, ELIZAVETA IL'INICHNA MALEVANNAYA, Dukhov

10:36AM W08.00014: Coplanar silicon/aluminum resonators with internal quality factor above 2M: measurements*

ANTON IVANOV (Presenter), FMN Laboratory, Bauman Moscow State Technical University, VIKTOR IVANOVICH POLOZOVA, ELIZAVETA IL'INICHNA MALEVANNAYA, Dukhov

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W16 DQI: Superconducting Qubits: QEC and Ultrastrong Coupling

201 - Christian Kraglund Andersen, ETH Zurich
**8:00AM W16.00001: Ground state of a circuit QED system in the deep-strong-coupling regime coupled to an environment**

TOMOHIRO SHITARA (Presenter), Tokyo Medical and Dental University, MOTOAKI BAMBA, Japan Science and Technology Agency, FUMIKI YOSHIHARA, TOMOKO FUSE, KOUICHI SEMBA, National Institute of Information and Communications Technology, KAZUKI KOSHINO, Tokyo Medical and Dental University — We investigate theoretically how the ground state of a qubit-resonator system in the deep-strong coupling regime is modified by the coupling to an environment. We employ the qubit-dependent coherent/squeezed-coherent state as the variational state for the ground state of the enlarged qubit-resonator-environment system and observe the following points. (i) The number of virtual photons increases by the coupling to an environment, proportionally to the square root of the loss rate \( \kappa \) of photons in the resonator. (ii) The ground state of the qubit-resonator system becomes mixed even at the zero temperature. The decrease in purity is proportional to the loss rate \( \kappa \). (iii) There exists an optimal value of the qubit-resonator coupling to maximize the nonclassicality of the qubit-resonator system, which is quantified by the metrological power.

*This work was supported by JST CREST Grant Number JPMJCR1775 and JST PRESTO Grant Number JPMJPR1767, Japan.

**8:12AM W16.00002: Time-domain measurements of an ultra-strongly coupled qubit-resonator circuit**

TOMOKO FUSE (Presenter), FUMIKI YOSHIHARA, National Institute of Information and Communications Technology, SAHEL ASHHAB, Qatar Environment and Energy Research Institute, KOUSUKE KAKUYANAGI, SHIRO SAITO, NTT, KOUICHI SEMBA, National Institute of Information and Communications Technology — In cavity- and circuit QED, when the coupling energy becomes \( \sim 10 \% \) or more of a photon and qubit energies (ultra- to deep-strong coupling regime), interesting physics are predicted [1]. So far, ultra- and deep-strong coupling [2-5] were achieved and the transition energy spectra of their circuits were studied. In this work, we have measured the coherence properties of an ultra-strongly coupled flux qubit-resonator circuit by driving the qubit while probing the resonator transition, which is also flux-bias dependent due to its very strong coupling to the qubit. The coherence times of \( \sim 1 \) \( \mu \)s were obtained for the qubit at the optimal point. In the presentation, a possible origin of the decoherence will also be discussed.


*This work was supported by Japan Society for the Promotion of Science Grant-in-Aid for Scientific Research (Grant No. JP19K03693), and Japan Science and Technology Agency Core Research For Evolutionary Science and Technology (Grant No. JPMJCR1775).
8:24AM W16.00003: Rabi model in the dispersive regime  CLEMENS MUELLER (Presenter), IBM Research - Zurich — The dispersive regime of circuit QED is the main workhorse for today's quantum computing prototypes based on superconducting qubits. Analytic descriptions of this model typically rely on the rotating wave approximation of the interaction between qubits and resonator fields, using the Jaynes-Cummings model as starting point for the dispersive transformation.

Here we present our results on the dispersive regime of the Rabi model, without taking the rotating wave approximation of the underlying Hamiltonian. Using a recently developed hybrid perturbation theory based on the expansion of the time evolution on the Keldysh contour [1], we derived simple analytic expressions for all experimentally relevant parameters like dispersive shift and resonator induced Purcell decay rate, both for idealized two-level systems as well as for realistic multi-level and weakly anharmonic qubits.

The analytical equations are easily tractable and reduce to the known Jaynes-Cummings results in the relevant limit, but show qualitative differences at large detuning, allowing for more accurate modelling of the interaction between superconducting qubits and resonators.


8:36AM W16.00004: Conical intersections and Berry phase in deep-strongly coupled superconducting qubit-resonator system* KOUICHI SEMBA (Presenter), National Institute of Information and Communications Technology, Japan., SAHEL ASHHAB, Qatar Environment and Energy Research Institute, Qatar Foundation, Qatar. — Conical intersections, or Dirac cones, have been observed in various modern physical systems. Measuring Berry phases and curvatures are interesting themes [1-2]. Flux-qubit resonator circuits can be well described by a simple model, the quantum Rabi-model, even in the deep strong coupling regime [3]. Numerical analysis reveals that conical intersections occur not only in the symmetric quantum Rabi-model which has clear parity symmetry, but also in the asymmetric quantum Rabi-model which has no obvious symmetry [4]. The occurrence of conical intersections in the asymmetric Rabi-model provides indirect evidence that there should be a hidden symmetry. Here, we propose an experimental scheme to observe conical intersections in the energy landscape and the Berry phase in ultra- or deep-strongly coupled qubit-resonator systems. This will also provide a clue to understand the hidden symmetry in the system.


*This work was supported by Japan Science and Technology Agency Core Research for Evolutionary Science and Technology (Grant No. JPMJCR1775).
Quantum impurity physics meets circuit QED: observation of finite lifetime photons

ROMAN KUZMIN (Presenter), NICHOLAS GRABON, NITISH JITENDRAKUMAR MEHTA, University of Maryland, College Park, MOSHE GOLDSTEIN, Tel Aviv University, VLADIMIR MANUCHARYAN, University of Maryland, College Park

We report a new regime of quantum electrodynamics (QED) where a single photon acquires a finite lifetime due to spontaneous decay to many lower-frequency photons. This phenomenon is a hallmark of ultra-strong coupling between a sufficiently non-linear quantum system (the quantum impurity) and a continuum of 1D bosonic modes. While this situation is impossible in atomic physics, it is ubiquitously in the bosonic description of strongly-correlated 1D electronic systems. We implemented bosonic versions of two key quantum impurity models: the boundary sine-Gordon model and the Kondo model. Physically our system is a long section of a high-impedance transmission line (the bosons) connected to a single small capacitance Josephson junction (the BSG impurity) or to a fluxonium qubit (the Kondo impurity). The many-body correlation functions of these two quantum impurity problems can be extracted from the measured inelastic spectrum of microwave photons, which implements a quantum simulation of a classically difficult computational problem.

Cavity-free circuit quantum electrodynamics: interfacing a high-coherence qubit with propagating photons

YEN-HSIANG LIN (Presenter), HAONAN XIONG, Physics, Univ of Maryland-College Park, NATHANAEL PIERRE COTTET, Physics, Univ Lyon, ENS de Lyon, LONG NGUYEN, RAY MENCIA, AARON SOMOROFF, VLADIMIR MANUCHARYAN, Physics, Univ of Maryland-College Park

We report experiments with a fluxonium artificial atom directly connected to a 1D transmission line. Unlike conventional circuit quantum electrodynamics (cQED), here there is no extra cavity mode degree of freedom buffering the qubit from the readout environment. Thanks to the highly anharmonic fluxonium spectrum, we simultaneously achieved a strong coupling of a high-frequency “cycling” readout transition (0→3 or 1→2) to the traveling waves and a nearly complete suppression of the spontaneous emission of the low-frequency “clocking” qubit transition (0→1). Notably, the cycling dynamics during the readout is confined to a small Hilbert space of a single quantum degree of freedom, and it can be understood within a minimal optical pumping model. Our system realizes the simplest possible interface between a highly-coherent qubit and propagating photons for constructing quantum communication networks.
Experimental Demonstration of Quantum Error Detection with a Small Surface Code

CHRISTIAN KRAGLUND ANDERSEN (Presenter), ANTS REMM, STEFANIA LAZAR, NATHAN LACROIX, SEBASTIAN KRINNER, GRAHAM J. NORRIS, MIHAI GABUREAC, CHRISTOPHER EICHLER, ANDREAS WALLRAFF, ETH Zurich — One of the most promising approaches for quantum error correction is the surface code, which consists of a $d \times d$ grid of data qubits combined with a set of ancilla qubits. The surface code implements a distance-$d$ quantum error correction code that allows for the detection of $d-1$ errors per stabilizer-measurement cycle. The smallest non-trivial surface code that allows for complete quantum error detection of a logical qubit subspace is the $d=2$ surface code, consisting of 4 data qubits and 3 ancilla qubits for the stabilizer measurements. Here we present experimental results obtained on a small seven-qubit surface code device implemented in superconducting circuits. We present measurements of all three stabilizers with high fidelity and repeated detection of errors on the data qubits using the stabilizer readout.

We acknowledge support by the ODNI, IARPA, via grant W911NF-16-1-0071, by NCCR QSIT, the EU Flagship H2020-FETFLAG-2018-03 project 820363 OpenSuperQ and by ETH Zurich.

Evaluation of the Performance of a 7-Qubit Surface Code

ANTS REMM (Presenter), CHRISTIAN KRAGLUND ANDERSEN, STEFANIA LAZAR, NATHAN LACROIX, SEBASTIAN KRINNER, GRAHAM J. NORRIS, MIHAI GABUREAC, CHRISTOPHER EICHLER, ANDREAS WALLRAFF, ETH Zurich — One of the promising approaches to fault tolerant quantum computation is based on the surface code. The existence of an error rate threshold, below which increasing the code size exponentially suppresses logical errors, has been shown for many common error mechanisms [R. Raussendorf and J. Harrington, Phys. Rev. Lett. 98, 190504 (2007)]. In this talk we analyse the physical error mechanisms of a seven-qubit superconducting quantum device on which we implement the elementary operations required for a surface code. By repeated stabilizer measurements we implement a distance $d=2$ surface code enabling the detection of any single-qubit error. We identify the error mechanisms which have the most significant effect on the logical error rate. We further discuss how to extend our scheme to larger distance surface codes given the current performance of our device.

We acknowledge support by the ODNI, IARPA, via grant W911NF-16-1-0071, by NCCR QSIT, the EU Flagship H2020-FETFLAG-2018-03 project 820363 OpenSuperQ and by ETH Zurich.
9:36AM W16.00009: Real-time decoding of repeated stabilizer measurements in a bit-flip code

* DIEGO RISTÈ (Presenter), LUKE GOVIA, Raytheon BBN Technologies, BRIAN DONOVAN, Systems & Technology Research, SPENCER FALLEK, WILLIAM KALFUS, Raytheon BBN Technologies, MAIKA TAKITA, ANTONIO D CORCOLES, MARKUS BRINK, NICHOLAS T BRONN, JERRY M. CHOW, IBM Thomas J. Watson Research Center — Although qubit coherences and gate fidelities are continuously improving, logical encoding is essential to achieve fault tolerance in quantum computing. In most encoding schemes, correcting or tracking errors throughout the computation is necessary to implement a universal gate set without delaying the processor. Here we present a classical control architecture for the fast extraction of errors based on multiple rounds of stabilizer measurements, and subsequent optional correction. We demonstrate its application on a minimal bitflip code with five transmon qubits, showing that error tracking based on multiple stabilizer rounds is superior to round-by-round correction, while introducing minimal latency. This co-processing of classical and quantum information will be crucial in running a logical circuit at its full speed to outpace error accumulation.

*This document does not contain technology or technical data controlled under either the U.S. ITAR or the U.S. EAR. The project depicted was sponsored by the Department of Army, US Army Research Office. The content of the information does not necessarily reflect the position or policy of the federal government, and no official endorsement should be inferred.

9:48AM W16.00010: Real-time Quantum Error Correction for a Surface-Code Logical Qubit

*MIGUEL MOREIRA (Presenter), BRIAN M TARASINSKI, JORDY GLOUDEMANS, VIACHESLAV P. OSTROUKH, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, WOUTER VLOTHUIZEN, QuTech, Netherlands Organization for Applied Scientific Research, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Achieving fault-tolerant universal quantum computation hinges on performing multi-round quantum error correction in real time. Several technical challenges, from instruction bandwidth to timing considerations, make it challenging to engineer a control system capable of real-time error correction. We present a control architecture for surface code with a tightly-coupled real-time quantum error decoder. We demonstrate real-time decoding of error syndromes for a Surface-17 logical qubit satisfying experimental timing constraints. We present the realization of multiple error decoding strategies and compare the hardware resources required for each implementation.

*This research is funded by IARPA (U.S. Army Research Office Grant No. W911NF-16-1-0071), Intel Corporation, and QuTech.
10:00AM W16.00011: Continuous Parity Measurement and Error Correction*  WILLIAM LIVINGSTON (Presenter), MACHIEL S BLOK, JUAN ATALAYA, University of California, Berkeley, RAZIEH MOHSENINIA, Univ of Southern California, JING YANG, ANDREW N JORDAN, University of Rochester, JUSTIN DRESSEL, Chapman University, IRFAN SIDDIQI, University of California, Berkeley — In a multi-qubit system, performing continuous measurements of joint properties such as parity allows us to study the collapse dynamics of multipartite states. Simultaneous parity measurements in a three-qubit system also act as continuous stabilizer detection for a quantum error correction code, allowing us to observe a single qubit flip in real time. The parity of two superconducting transmons may be directly measured without qubit ancilla by coupling them to a single readout resonator, using identical dispersive coupling chis much larger than the resonator bandwidth kappa. Using a chip with three qubits and connecting each of two pairs to a parity readout resonator, we implement the two parity measurements needed to perform the conventional three-qubit bit-flip code. We control the qubits from a field programmable gate array board which also continuously monitors the parity, allowing for low latency correction pulses to be applied when a qubit flip occurs.

*This work was funded by the Army Research Office.

10:12AM W16.00012: Topological and subsystem codes on low-degree graphs with flag qubits  GUANYU ZHU (Presenter), CHRISTOPHER CHAMBERLAND, THEODORE YODER, JARED HERTZBERG, ANDREW CROSS, IBM Tj Watson Research Center — In this work we introduce two code families, the heavy hexagon code and heavy square code. Both code families are implemented by assigning physical data and ancilla qubits to both vertices and edges of low degree graphs. Such a layout is particularly suitable for superconducting qubit architectures to minimize frequency collision and crosstalk. In some cases, frequency collisions can be reduced by several orders of magnitude. The heavy hexagon code is a hybrid surface/Bacon-Shor code mapped onto a (heavy) hexagonal lattice whereas the heavy square code is the surface code mapped onto a (heavy) square lattice. In both cases, the lattice includes all the ancilla qubits required for fault-tolerant error-correction. Naively, the limited qubit connectivity might be thought to limit the error-correcting capability of the code to less than its full distance. Therefore, essential to our construction is the use of flag qubits. We modify minimum weight perfect matching decoding to efficiently and scalably incorporate information from measurements of the flag qubits and correct up to the full code distance while respecting the limited connectivity. Simulations show that high threshold values for both codes can be obtained using our decoding protocol.
Qubit leakage is present in leading quantum computing platforms, including superconducting transmon qubits. These errors fall outside the stabilizer formalism of quantum error correction (QEC), thus constituting a threatening error source for fault tolerance. While the performance of QEC codes, such as the surface code, has been investigated for simplistic leakage error models, an analysis with respect to a physically-motivated leakage error model for transmons has not been undertaken so far. In this work, we employ realistic full-trajectory simulations of the CZ gate in a transmon system (the dominant source of leakage in this system). We find novel effects within the leakage subspace of two transmons, including leakage mobility and leakage conditional phases. We use this in density-matrix simulations of the distance-3 surface code Surface-17 and study the leakage build-up, its lifetime, and how leaked qubits spread errors onto neighboring qubits.

*F.B., B.V. and B.M.Te. are supported by ERC grant EQEC No. 682726; B.M.Ta., V.P.O. and L.D.C. by ODNI and IARPA, via the U.S. Army Research Office grant W911NF-16-1-0071; T.E.O. by NWO/OCW under the NanoFront and StartImpuls programs, and by Shell Global Solutions BV.
Detection and mitigation of leakage in simulations of a transmon implementation of the surface code, Part 2: Scalable Hidden Markov models for the identification of leakage

BORIS VARBANOV (Presenter), FRANCESCO BATTISTEL, QuTech, Delft University of Technology - Netherlands, BRIAN M TARASINSKI, VIACHESLAV P. OSTROUKH, QuTech and Kavli Institute of Nanoscience, Delft University of Technology - Netherlands, THOMAS O'BRIEN, Instituut-Lorentz for Theoretical Physics, Leiden University - Netherlands, BARBARA MARIA TERHAL, QuTech; JARA Institute for Quantum Information, Delft University of Technology - Netherlands; Forschungszentrum Jülich - Germany, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology - Netherlands — The detection and mitigation of leakage, a threatening error source for stabilizer quantum error correction (QEC) on leading physical hardware, is an important step towards demonstrations of fault tolerance. We explore the effects of leakage on the performance of the distance-3 surface code Surface-17 by performing density-matrix simulations, employing realistic error models for transmon qubits in a circuit QED processor. We demonstrate the indirect detection of leakage via a network of local, independent and scalable Hidden Markov models. We show that post-selecting on detection of leakage restores the logical fidelity of the encoded information. We explore the integration of leakage detection into a minimum-weight perfect-matching decoder.

*F.B., B.V. and B.M.Te. are supported by ERC grant EQEC No. 682726; B.M.Ta., V.P.O. and L.D.C. by ODNI and IARPA, via the U.S. Army Research Office grant W911NF-16-1-0071; T.E.O. by NWO/OCW under the NanoFront and StartImpuls programs, and by Shell Global Solutions BV.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W17 DQI: Quantum Machine Learning II

8:00AM W17.00001: Advances in Quantum Reinforcement Learning [Invited] VEDRAN DUNJKO (Presenter), Leiden — Vedran Dunjko has made key advances in understanding how reinforcement learning can assist in quantum computing and quantum error correction.
**8:36AM W17.00002: Artificial Spiking Quantum Neural Networks**  
LASSE KRISTENSEN  
(Presenter), Department of Physics and Astronomy, Aarhus University, MATTHIAS DEGROOTE, Department of Chemistry, University of Toronto, PETER WITTEK, Rotman School of Management, University of Toronto, ALAN ASPURU-GUZIK, Department of Chemistry, University of Toronto, NIKOLAJ T. ZINNER, Department of Physics and Astronomy, Aarhus University — Within the realm of classical computing, the paradigm of artificial spiking neural networks has found a wide range of applications in settings where the temporal aspects of such networks are advantageous, such as in time-series prediction and signal analysis. In this talk, we will present a class of simple quantum spin-network models inspired by this classical paradigm, combining both an explicit neural network structure and explicit temporality through quantum evolution, and with the inherent ability to operate on quantum data as input. A set of neuron-like building blocks for such networks will be presented, and a network combining these objects into a structure capable of comparing pairs of Bell states will be proposed, a task with applications in quantum certification. Finally, a few comments on inherent properties related to the generation of entanglement and measurement back-action through these networks will be given.

The content of this talk is based on the arXiv-preprint 1907.06269

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**8:48AM W17.00003: A Path Towards Obtaining Quantum Advantage in Training Classical Deep Generative Models with Quantum Priors**  
WALTER VINCI (Presenter), NASA Ames Research Center, LORENZO BUFFONI, University of Florence, HOSSEIN SADEGHI, D-Wave Systems Inc., DANIEL O’CONNOR, University College London, EVGENY ANDRIYASH, MOHAMMAD AMIN, D-Wave Systems Inc. — A class of quantum-classical hybrid machine-learning algorithms can be obtained by integrating classical deep generative models with quantum probability distributions as 'priors' over their latent variables. We introduce a hybrid implementation of variational autoencoders (QVAE) and also present a technique to hybridize flow-based invertible generative models. We demonstrate the use of D-Wave quantum annealers as physical simulators of quantum Boltzmann machines (QBM) to perform quantum-assisted training of QVAE. Latent-space QBM develop slowly mixing modes, opening a path to obtain quantum advantage in generative modeling with available quantum devices.

*We are grateful for support from NASA Ames Research Center. We also appreciate support from the AFRL Information Directorate under grant F4HBKC4162G001 and the Intelligence Advanced Research Projects Activity (IARPA), via IAA 145483. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of IARPA, AFRL, or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Governmental purpose notwithstanding any copyright annotation thereon.
9:00AM W17.00004: Experimental demonstration of quantum-enhanced machine learning in NV center system  
WENGANG ZHANG (Presenter), XIAOLONG OUYANG, XIANZHI HUANG, DONGLING DENG, LUMING DUAN, Tsinghua University — We demonstrate the quantum-enhanced supervised classification of vectors in an NV center system using the algorithm of Lloyd, Mohseni and Rebentrost [arXiv:1307.0411 (2013)]. A $^{13}$C nuclear spin is employed to encode the vectors with the spin-triplet state of the NV center as an ancilla. We design efficient methods to prepare the initial electron-nuclear entangled state within the coherence time $T_2^*$ of the electron spin, and then compute the distance between the test vector and the center of each class by measuring the level population through maximum likelihood estimation. Our experiment allows more than one reference vectors in each class, thus forms an important enabling step toward quantum-enhanced machine learning.

9:12AM W17.00005: Cost function embedding and dataset encoding for machine learning with parameterized quantum circuits* 
SHUXIANG CAO (Presenter), University of Oxford, LEONARD P WOSSNIG, Computer Science, University College London, BRIAN VLASTAKIS, PETER J LEEK, University of Oxford, EDWARD GRANT, Computer Science, University College London — Machine learning is seen as a promising application of quantum computation. For near-term noisy intermediate-scale quantum (NISQ) devices, parametrized quantum circuits (PQCs) have been proposed as machine learning models due to their robustness and ease of implementation. However, the cost function is normally calculated classically from repeated measurement outcomes, such that it is no longer encoded in a quantum state. This prevents the value from being directly manipulated by a quantum computer for algorithms such as gradient estimation using the Hadamard Test. In this talk, we introduce a routine to embed a cost function for machine learning into a quantum circuit, which accepts a training dataset encoded in superposition or an easily preparable mixed state. We characterize the utility of such a routine using numerical simulations and introduce proof-of-principle experiments in an optimized superconducting qubit device.

*E.G. is supported by the UK Engineering and Physical Sciences Research Council (EPSRC) [EP/P510270/1]. L.W. acknowledges support through the Google PhD Fellowship in Quantum Computing. B.V. acknowledges support from an EU Marie Curie fellowship. P.L. acknowledges support from the EPSRC [EP/M013243/1] and Oxford Quantum Circuits Limited.
9:24AM W17.00006: Physical-Layer Supervised Learning Assisted by an Entangled Sensor Network* QUNTAO ZHUANG (Presenter), Electrical & Computer Engineering, University of Arizona, ZHESHEN ZHANG, Materials Science & Engineering, University of Arizona — Many existing quantum supervised learning (SL) schemes consider data given in a classical description. There, however, also exist a multitude of SL tasks whose data are acquired by sensors, e.g., pattern classification based on data produced by imaging sensors. Solving such SL tasks naturally requires an integrated approach harnessing tools from both quantum sensing and quantum computing. We introduce supervised learning assisted by an entangled sensor network (SLAEN) as a means to carry out SL tasks at the physical layer. The entanglement shared by the sensors in SLAEN boosts the performance of extracting global features of the object under investigation. We leverage SLAEN to construct an entanglement-assisted support-vector machine for data classification and entanglement-assisted principal component analyzer for data compression. In both schemes, variational circuits are employed to seek the optimum entangled probe states and measurement settings to maximize the entanglement-enabled enhancement. We observe that SLAEN enjoys an appreciable entanglement-enabled performance gain, even in the presence of loss, over conventional strategies in which classical data are acquired by separable sensors and subsequently processed by classical SL algorithms.

*ONR, GeoFlow

9:36AM W17.00007: Quantum-inspired nonlocal parallel tempering with approximate tensor network contractions MASOUD MOHSENI, DANIEL EPPENS (Presenter), Google Inc., MAREK M RAMS, Marian Smoluchowski Institute of Physics,, Jagiellonian University, SERGIO BOIXO, HARTMUT NEVEN, Google Inc. — We use tensor networks to represent probability distribution of spin-glass models that are encoding combinatorial optimization problems. We then develop greedy approximation tensor contraction for efficient Gibbs sampling of the low energy states for structured quasi-2D spin-glass models. Our deterministic approach can reveal certain geometrical properties of such hard optimization problems known as “droplet excitations”. The knowledge of such droplets can be used to enhance traditional probabilistic Monte Carlo techniques. Specifically we provide two new cluster Monte Carlo techniques in which we combine tensor network contractions with “parallel tempering” (PT). In the first method the tensor networks provide certain high-quality initial states for PT instead of traditional random restarts. In the second method, the tensor network contraction provide droplet information that can be used for dynamical cluster updates unfreezing low-temperature replicas near a computational phase transition. We demonstrate several orders of magnitude improvement in time-to-solutions in comparison to local Monte Carlo techniques such as PT. We also observe significant improvement over commercial solvers, such as Gurobi, or other heuristic cluster PT approaches powered by iso-energetic moves.
Generative models are able to produce new data according to an underlying probability distribution that they learn from a given data set. Inspired by the probabilistic nature of quantum mechanics, we employ a generative model, known as the "Born machine", which uses quantum state representation and learns the joint probabilities over such quantum degrees of freedom. To represent the quantum states we train tensor network architectures that could provide efficient expressivity, training, and sampling when the quantum probability distribution has some local structure. Specifically, we train two types of tensor networks known as matrix product states (MPS) and tree tensor network (TTN) over both classical and quantum data. We first show that our TTN model can generate the MNIST handwritten digits efficiently. In the next step, we variationally train tensor network models to generate desired quantum entanglement produced by shallow quantum circuits given iterative input-output information from actual quantum hardware with typically unknown systematic and random errors.

The variational quantum eigensolver (VQE) is a leading near-term hybrid classical/quantum algorithm for calculating spectra of molecular Hamiltonians. As with any variational approach, its performance depends sensitively on the selection of an appropriate variational form. Recent work has detailed the effectiveness of ADAPT-VQE, an adaptive approach to VQE in which the variational form is grown iteratively, resulting in ansatze which yield high performance with minimal numbers of variational parameters. This approach, however, is quantum resource intensive, requiring many quantum circuit executions and state measurements to grow the ansatze. Here we present RNN-VQE, a machine learning model which uses recurrent neural networks to learn and quickly generate effective variational ansatze for VQE.
10:12AM W17.00010: Measuring Correlation Scaling in Images via Logistic Regression*  IAN CONVY (Presenter), WILLIAM HUGGINS, BIRGITTA K WHALEY, Chemistry, University of California, Berkeley — It is well known in quantum many-body physics that local Hamiltonians often have ground states whose entanglement entropies scale with the boundary of the bipartition (known as an "area law"), allowing them to be characterized efficiently using tensor networks. Given recent interest in using tensor network models for machine learning, we explore whether correlations in classical image data may possess analogous scaling behavior in the mutual information (MI) between bipartitions of the pixels. Building on techniques developed in the context of generative machine learning, we recast the MI estimation problem as logistic regression on samples drawn from the joint and marginal distributions of the image partitions. We test the accuracy of our model using Gaussian Markov random fields designed to have analytic boundary law and volume law scaling patterns, and perform regression on the well-known MNIST and CIFAR image datasets to evaluate the MI scaling in real-world images. We find that our model can capture the scaling behavior of the Markov random fields even with hundreds of pixels, while the large MI values found in CIFAR and MNIST remain challenging to reproduce.

*This work was supported by a grant from Siemens Corporation.

10:24AM W17.00011: Quantum neural network for generating quantum states*  RONGXIN XIA (Presenter), SABRE KAIS, Department of Chemistry, Department of Physics and Astronomy, and Birck Nanotechnology Center, Purdue University — Quantum machine learning has become a research focus in quantum computation nowadays. One direction of quantum machine learning is developing quantum neural network based on parametrized quantum circuits. However, previous works of quantum neural network based on parameterized quantum circuits provide few systemic and general ways to introduce non-linear activation function. In the meantime, non-linear activation function is one of the most important parts in classical neural network as it makes the multi-layer neural network not work as a single layer. In this work, we give a new construction of quantum neural network to introduce non-linear activation functions. To demonstrate the new approach, we present results of using the quantum neural network to generate ground states as well as excited states for different quantum chemistry systems. The generated states approximate exact states closely, which not only show the potential of the new construction of quantum neural network, but also may be a new approach to solve quantum chemistry problems.

*We acknowledge the funding from the U.S. Department of Energy, Office of Basic Energy Sciences under award number DE-SC0019215.
10:36AM W17.00012: Gauge Enhanced Quantum Criticality and Time Reversal Domain Wall: SU(2) Yang-Mills Dynamics with Topological Terms  
YUNQIN ZHENG (Presenter), Princeton University, YIZHUANG YOU, Department of Physics, University of California, San Diego, JUVEN C WANG, Center of Mathematical Sciences and Applications, Harvard University — We study the low energy dynamics of the four siblings of Lorentz symmetry enriched SU(2) Yang-Mills theory with a theta term at $\theta = \pi$. Since there exists a mixed anomaly between time reversal symmetry and the center symmetry, the low energy dynamics must be nontrivial. We focus on two possible scenarios: 1) time reversal symmetry is spontaneously broken by the two confining vacua, and 2) the low energy theory describes a U(1) spin liquid which is deconfined and gapless while preserving time reversal symmetry. In the first scenario, we first identify the global symmetry on the time reversal domain wall, where time reversal symmetry in the bulk induces a Z2 unitary symmetry on the domain wall. We explore how the Lorentz symmetry and the unitary Z2 symmetry enriches the domain wall theory. In the second scenario, we relate the symmetry enrichments of the SU(2) Yang-Mills to that of the U(1) spin liquids. This further opens up the possibility that SU(2) QCD with large and odd flavors of fermions could be a second order phase transition between two phases of U(1) spin liquids as well as between a U(1) spin liquid and the a trivial paramagnet, where the gauge symmetry is enhanced to be non-Abelian at and only at the transition. We name them as Gauge Enhanced Quantum Critical Points.

10:48AM W17.00013: Robust Decomposition of Quantum States  
JONATHAN MOUSSA (Presenter), Molecular Sciences Software Institute — We show that quantum states over multiple subsystems can be recursively decomposed into states on one fewer subsystem and quantum operations that extend the state onto the omitted subsystem. This decomposition is robust in the sense that dephasing errors on subsystems between operations do not alter the marginal state on error-free subsystems. By restricting the form of these operations to a truncated cluster expansion, their classical simulation cost is reduced to the cost of simulating the maximal clusters. Such simulations provide direct access to independent statistical samples of observables and systematically improvable lower bounds on the von Neumann entropy, which together enable variational free energy minimization.

*The Molecular Sciences Software Institute is supported by grant ACI-1450169 from the National Science Foundation.

Friday, March 6, 2020 8:00 AM - 10:24 AM

Session W18 DSOFT: Bio-Mineralization, Hydration & Hardening in Colloidal Gels: Building Solid Materials Out of Soft Gels 205 - Tag(s): Invited
8:00AM W18.00001: Compositional and structural gradients in dental enamel: from nanoto microscale* [Invited]  KAREN DEROCHER, PAUL JM SMEETS, Northwestern University, BERIT GOODGE, MICHAEL J ZACHMANN, Cornell University, PRASANNA VENKATARAMAN BALACHANDRAN, University of Virginia, LINUS STEGBAUER, MICHAEL COHEN, LYLE M GORDON, JAMES RONDINELLI, Northwestern University, LENA FITTING KOURKOUTIS, Cornell University, DERK JOESTER (Presenter), Northwestern University — Dental enamel has evolved to bear large masticatory forces, resist mechanical fatigue, and withstand wear over decades of use. Functional impairment or loss, as a consequence of developmental defects or tooth decay, has a dramatic impact on health and quality of life. While the last decade has seen great progress in our understanding of enamel formation and the functional properties of mature enamel, attempts to repair enamel lesions or synthesize enamel in vitro have had limited success. This is partly due to the highly hierarchical structure of enamel and the additional complexities arising from chemical gradients that we are only beginning to understand. Herein we show, using atomic-scale quantitative imaging and correlative spectroscopies, that human enamel is comprised of crystalline apatite and a Mg-rich amorphous intergranular phase. Individual crystallites have core-shell structure. The core is comprised of two thin layers enriched in Mg flanking a region that is poor in Mg and enriched in Na. Fluoride is often also present in layers. The sandwich core is surrounded by a shell largely free of substitutional defects. A mechanical model of coherent crystallites based on DFT calculations predicts that significant residual stresses, with important implications for enamel dissolution, crystallite and tissue mechanical properties, and crystal growth processes during amelogenesis. In addition to these gradients at length scales from single digit to 10s of nanometers, we will report on systematic changes in average lattice parameters and coherence length across single enamel rods, i.e. length scales on the order of 1-10 µm.

*NIH-NIDCR R03 DE025303-01, R01 DE025702-01; NSF DMR-1508399; NSF PARADIM DMR-1539918; University of Virginia
ROSA ESPINOSA-MARZAL (Presenter), BINXIN FU, JOSUE LOPEZ-BERGANZA, CHING-WEI LEE, SIMON A ROGERS, University of Illinois at Urbana-Champaign — Marine organisms exploit varied physical and chemical interactions between calcium carbonate and organic additives to yield mineral-organic complexes that are not only visually stunning but also highly functional. Despite recent leaps in the understanding of these systems, knowledge of the relation between kinetics of mineral growth, microstructure of the composite and mechanical response is still lacking. Our aim is to mechanistically elucidate potential pathways that afford control of the mineralization pathway of hydrogels and of their microstructure, and yield composites with tunable mechanical response. Our previous studies demonstrated that the formation of amorphous calcium carbonate precursors (ACC) throughout agarose hydrogels is a diffusion-limited process, and therefore, it is strongly affected by the solution composition and by the hydrogel composition. In contrast, amorphous precursors in the hydrogel control tightly the inclusion of the polymer into calcite, and crystal morphology, as well as the rate of crystal growth, affording a uniform crystal growth throughout the hydrogels, in the absence of concentration gradients, over a wide range of solution conditions and hydrogel compositions. Based on these findings, we have extended these studies to phosphates, and show that amorphous precursors also modulate the mineralization kinetics quite tightly. Furthermore, the phosphate-mineralized hydrogels exhibit key advantages with regard to microstructure -as provided by hydroxyapatite nanosheets- and mechanical response, compared to the mineralized hydrogels in the absence of phosphates. The results of this work not only reveal an important mechanism underlying (bio)mineralization but it can also inspire new avenues to craft biomimetic materials.

*National Science Foundation, No. CMMI-1435920

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W19 GMAG: Spin Ice - From Freezing to Cerenkov Radiation

Kate Ross, Colorado State University - Tag(s): Invited
Tuning dipolar interactions in artificial spin ices - From Ising to Potts spins

FRANCOIS MONTAIGNE (Presenter), DAMIEN LOUIS, MARYAM MASSOURAS, MICHEL HEHN, THOMAS HAUET, DANIEL LACOUR, Universite de Lorraine — Since the proposal in 2006 [1] to use nanomagnets patterned by top-down techniques to mimic "artificial spins", the studies of artificial spin systems has attracted wide interest [2]. As a matter of facts, the possibility to design "upon request" arbitrary network thanks to lithography and the possibility to determine completely the "spin" configuration with magnetic imaging offer a wide playground for statistical physics. Up to now only Ising spin systems have been studied. However, beyond Ising spins, statistical physics and condensed matter physics have shown the interest of other spin models like q-state Potts models (q different spin orientation) or even XY model (isotropic in plane orientation).

In this talk, we introduce the dipolar 4-state Potts model. It is shown that on a square lattice, depending on the angle between spins and lattice, the system present very different properties like antiferromagnetic order, spin ice state (2 in-2 out ice rule) and even dipolar ferromagnetism.

This model has been realized experimentally. At room temperature, the magnets present a uniform state with 4 equivalent directions. Upon heating at 350 °C the magnets switch from one direction to another. It is therefore possible to simply drive the system toward its ground state. The magnetic configurations determined by magnetic force microscopy reveals the importance of the dipolar coupling as the different expected ground states (antiferromagnetic, spin ice and ferromagnetic) are indeed observed [3]. It is noticeable that these very different properties are obtained with the same "spins" (magnetic elements) and same lattice. The exact process of magnetization evolution, differences with "Ising" systems and future prospects will be discussed.


Slow dynamics in classical and quantum spin ice systems

CLAUDIO CASTELNOVO (Presenter), Univ of Cambridge — The low temperature properties of magnetic systems with fractionalised point-like excitations are determined by the interplay between a small density of quasiparticles and the underlying spin degrees of freedom out of which they are borne. Spin ice materials are a case in point. Even in their simplest classical modelling, a dramatic slowing down is expected due to the excitations becoming exponentially sparse. Once more realistic details are taken into account, and in particular quantum fluctuations are included, the situation becomes far more complex and interesting. The phenomenology uncovered thus far includes the formation of long-lived metastable states, structural as well as correlation-driven disorder that alters the local quantum mechanical spin fluctuations, and a prominent freezing of the dynamics whose origin continues to elude our understanding. This talk presents a selection of results and observations that highlight the uniquely rich, tunable and experimentally accessible playground to study slow dynamics in frustrated magnetism offered by spin ice systems.
9:12AM W19.00003: Machine learning assisted analysis of neutron scattering: new insights into spin ice* [Invited]  DAVID TENNANT (Presenter), ANJANA SAMARAKOON, Oak Ridge National Lab, SANTIAGO GRIGERA, CONICET La Plata Argentina, ALEXANDER KIRSTE, PTB Berlin, BASTIAN KLEMKE, Helmholtz Center Berlin, LUDOVIC DC JAUBERT, CNRS-Bordeaux, CLAUDIO CASTELNOVO, Univ of Cambridge, RODERICH MOESSNER, MPIPKS Dresden — The macroscopic manifolds of ground states in highly frustrated magnets are responsible for their rich physical behavior. Thermal and quantum fluctuations within these manifolds gives rise to liquid states with remarkable properties which are receiving intense interest. An open question is, what is the fate of these liquid states as the system cools? To gain insight into this we have undertaken a comprehensive study of Dy$_2$Ti$_2$O$_7$. Dy$_2$Ti$_2$O$_7$ is well known as a prototypical spin ice material that shows a U(1) gauge liquid behavior with magnetic monopole quasiparticles. From a combination of neutron scattering, magnetic noise, and thermodynamic measurements we have developed a model for the material using machine learning. The analysis involves use of autoencoders to identify phases and by optimizing in the network’s latent space highly accurate interaction parameters are extracted. A key part of this analysis is the ability to discriminate artifacts from physical signals in the neutron scattering data and to perform analysis on three-dimensional diffuse data sets. The extracted model is shown to reproduce glass formation in the material and provides microscopic understanding of a range of observations including the arresting of order as freezing occurs and $1/f^\alpha$ magnetic noise. High performance computer modeling has also been used to map the development of short-range order and changes in dimensionality and topology in monopole pathways. Our results suggest ways in which spin glass formation could occur from simple interactions even without intrinsic disorder.

*The research was sponsored by the DOE Office of Science, Laboratory Directed Research and Development program (LDRD) of Oak Ridge National Laboratory, managed by UT-Battelle, LLC for the U.S. Department of Energy. (Project ID 9566). A portion of this research used resources at Spallation Neutron Source, ORNL.
MASAFUMI UDAGAWA (Presenter), Department of Physics, Gakushuin University — Fractionalization is one of the most remarkable phenomena in the systems of nontrivial topological character. Magnetic monopoles in quantum spin ice (QSI) give a typical example of fractional excitations, and a keen interest is focused on their role in dynamical and transport properties of QSI candidate materials. However, due to the fractional nature of excitations, magnetic monopoles behave quite differently from conventional excitations such as magnons, and their character still remains quite elusive. In this contribution, in order to understand the nature of magnetic monopoles, we address the anisotropic limit ($J^\pm \ll J^z$) of spin-1/2 quantum XXZ model defined on a pyrochlore lattice. In particular, we focus on the temperature region, $J^\pm^3/J^z^2 << T << J^\pm$, where the ground state spin ice manifold is still incoherent, while the monopole excitations already show coherent quantum motion. In this region, we obtained the local dynamical structure factor by the exact diagonalization of 32 site cluster [1]. The obtained spectrum shows a steep edge discontinuity at low energy attributed to the van Hove singularity of monopole spectrum, which results from the dimensional transmutation due to the coupling to background gauge field. We clarify the origin of this dimensional transmutation in terms of the state graph description, by mapping the monopole motion to a free particle Hamiltonian on a virtual Husimi cactus graph.


*This work was supported by JSPS KAKENHI (Nos. JP15H05852 and JP16H04026), MEXT, Japan

SIDDHARDH MORAMPUDI, Boston Univ, FRANK WILCZEK, Center for Theoretical Physics, MIT, CHRISTOPHER LAUMANN (Presenter), Boston Univ — Quantum spin liquids are low temperature phases of magnetic materials in which quantum fluctuations prevent the establishment of long-range magnetic order. These phases support exotic fractionalized spin excitations (spinons) and emergent gauge fields. In this talk, I will briefly review the basic theoretical picture of how a quantum Coulomb phase emerges in spin ice and then turn to recent results regarding the observable consequences in neutron scattering. The emergent Coulomb interaction modifies the threshold cross-section for spinon production dramatically, changing the weak turn-on expected from a mean-field treatment to an abrupt onset reflecting the basic coupling parameters. The slow photon typical in existing lattice models and materials suppresses the intensity at finite momentum and allows profuse Cerenkov radiation beyond a critical momentum. These features are broadly consistent with recent numerical and experimental results.

*FW's work is supported by the U.S. Department of Energy under grant Contract Number DE-SC0012567, by the European Research Council under grant 742104, and by the Swedish Research Council under Contract No. 335-2014-7424. CRL acknowledges support from the NSF through grant PHY-1752727.
8:00AM W20.00001: Harmonic oscillation frequencies of cellular contractility support a wave shape model* [Invited]  MICHAEL E WERNER, DYLAN D RAY, COLEMAN BREEN, ADAM SATTLER, Univ of NC - Chapel Hill, FLORIAN JUG, Molecular Cell Biology and Genetics, Max Planck Institute, AMY SHAUB MADOX (Presenter), Univ of NC - Chapel Hill — Animal cell shape changes such as cytokinesis are driven by poorly understood rearrangements of the actomyosin cortical cytoskeleton. To gain novel insights into cell-autonomous cytokinetic contractility, we used the C. elegans zygote as a model cell and imaged cytokinesis with unprecedented temporal resolution. Cytokinetic ring closure underwent cycles of acceleration and deceleration. We quantified contractile oscillations via continuous wavelet transform and mode decomposition. Ring inward displacement dynamics were the composite of co-existing amplitude- and frequency-modulated wave modes with ~ 18, 36 and 72-second periodicity. The periodicities of speed oscillations were only subtly changed by depletion of a panel of conserved actomyosin regulators and structural components, but oscillation amplitudes were suppressed by reduction of force generation, and enhanced by reduction of network crosslinking. As suggested by the relationship of the modes’ periodicities as a fundamental frequency, a harmonic and a subharmonic, the range of speed oscillations was well described by a wave-shape model with a single time-varying amplitude, a single time-varying frequency, and a shape factor. Finally, to retain the spatial relationships among contracting segments of the cytokinetic ring, we performed mode decomposition in three dimensions on a space-time-frequency kymocube of our wavelet transform output. We found three major classes of frequency surfaces varying little over space and time. Principal component analysis of these two-dimensional modes confirmed that the frequencies of contractile oscillations are related as a harmonic and sub-harmonic around a fundamental frequency. We propose that the latter reflects the Rho pacemaker driving contractility, and that the harmonic is emergent due to non-linearities in the system. Dissipation of contractility within the network may explain the slower, sub-harmonic contractile oscillations.

*Supported by GM102390 to ASM.
8:36AM W20.00002: Actomyosin-driven mechanics of starfish oocytes*  
(Presenter), NIKA FAKHRI, Massachusetts Institute of Technology MIT — Actomyosin networks underlie most force generation by eukaryotic cells. These networks are driven out of equilibrium in part by myosin which crosslinks and exerts forces on actin filaments. While myosin’s role in force generation is well studied, how actin structure and dynamics influence the active mechanics of the networks during force generation is not understood. Here, we address this issue using oocytes from the starfish Patiria miniate. During maturation, the oocytes undergo surface contraction waves driven by the actomyosin cortex. Using pharmacological inhibitions, which target actin polymerization dynamics, we find that cellular deformation during the contraction wave is not a monotonic function of cortical actin density and is peaked near the wild type. This is reminiscent of in vitro actomyosin networks, which have been shown to have maximal contractility at intermediate levels of network connectivity. To test if this is also the case in starfish oocytes, we probe the oocyte’s mechanical properties and how these change under targeted molecular perturbations.

*PJF acknowledges the Gordon and Betty Moore Foundation for support as a Physics of Living Systems Fellow through grant no. GBMF4513

8:48AM W20.00003: Spatiotemporal dynamics of the neuronal cytoskeleton across scales during development*  
(KATE M O’NEILL (Presenter), EMILY K ROBINSON, WOLFGANG LOSERT, University of Maryland, College Park) — Neuronal structure is intrinsically tied to neuronal function because the spatial arrangement of the output (axon) and inputs (dendrites) of a neuron determines how it integrates into the neuronal network. A critical component of the cytoskeleton that drives neuronal morphology is actin, which is necessary for establishing connections (synapses) early in development to refining connections as networks mature. Using live confocal imaging, we study how the dynamics of actin change as cultures of in vitro primary rat cortical neurons develop. We employ two-dimensional Laplacian of Gaussian (LoG) filtering to identify neuronal processes and a pixel-based optical flow algorithm to track actin dynamics in developing neurons. We observe micron-scale actin dynamics in younger neurons (1-5 days in vitro) that clearly drive the pathfinding of growth cones, whereas older neurons display actin dynamics on a much smaller scale, confined to small regions of dendrites and to synaptic spines. Future work will further characterize these dynamics at key developmental timepoints.

*KMO was funded by MURI grant #FA9550-16-1-0052 to WL.
9:00AM W20.00004: Computational model of mitotic spindle positioning in polarized cells
JEFFREY M MOORE (Presenter), ADAM R LAMSON, MATTHEW A. GLASER, MEREDITH BETTERTON, University of Colorado, Boulder — The microtubule cytoskeleton plays important roles during the cell life cycle, in events including mitotic spindle assembly, chromosome segregation, nuclear elongation, and spindle positioning. During cell division in budding yeast, interactions between astral microtubules and proteins at the cell cortex position the spindle and nucleus at the bud neck before cytokinesis. The spindle moves due to pulling forces on the microtubules generated by the minus-end-directed motor dynein, which are activated by binding to protein domains localized at the cell cortex. Both the asymmetric distribution of cortical dynein binding domains and microtubule buckling and stabilization are thought to be important for regulating spindle positioning, but how the interplay between microtubule dynamics and motor-driven pulling forces lead to proper positioning at the site of cytokinesis is not well understood. We present results from simulations of a minimal spindle positioning model in a polarized cell driven by interactions between astral filaments, motorized tethers, and cortical binding domains. Our results show how binding domain localization and filament dynamics affect spindle positioning in polarized cells.

9:12AM W20.00005: Flagellar length control in biflagellate eukaryotes: Cooperative phenomena of generating and regenerating the flagellum
SWAYAMSHREE PATRA (Presenter), IIT Kanpur, FRANK JULICHER, Max-Planck-Institute for the Physics of Complex Systems, DEBASHISH CHOWDHURY, IIT Kanpur — Chlamydomonas Reinhardtii is a biflagellate eukaryote which generates its own flagella of correct length (in a controlled manner) after cell division (ciliogenesis), regenerates both of them after deflagellation and regenerates the amputated flagellum. A pool of proteins needed to form, maintain and regenerate the flagella is synthesized in the cell body. These proteins are transported from the pool to the distal tips for flagellar assembly and those released from the flagellar tip due to ongoing turnover are shuttled back to the pool by intraflagellar transport trains. Combining the dynamics of trafficking intraflagellar transport trains, the pool and the kinetics of flagellar assembly and disassembly, we have developed a stochastic model for understanding the collective phenomena of flagellar length control. Our model accounts for all key features of experimentally known phenomena which include ciliogenesis, resorption, deflagellation as well as regeneration after selective amputation of one of the two flagella. Moreover, we show how the communication among both the flagella through the common pool influences the nature, duration and extent of regeneration under different circumstances and governs the correlations between the fluctuating lengths of the two flagella.
9:24AM W20.00006: Bridging microtubules promote centering of kinetochores by length-dependent pulling forces  AGNEZA BOSILJ, Department of Physics, Faculty of Science, University of Zagreb, Zagreb, IVA TOLIĆ, Ruder Bošković Institute, Zagreb, NENAD PAVIN (Presenter), Department of Physics, Faculty of Science, University of Zagreb, Zagreb — The mitotic spindle, by exerting forces, segregates chromosomes into two daughter cells during cell division. During metaphase, chromosome are positioned in the equatorial plane of the mitotic spindle, which is necessary to prevent lagging chromosomes and abnormal nuclear envelope reformation. It has been proposed that two centering mechanisms play a key role here, microtubule catastrophe promoted by kinesin-8 motors and pushing forces exerted by chromokinesins. Here we show, by combining a theoretical model and quantitative experiments, that kinetochore microtubules cross-linked by bridging microtubules exert length-dependent centering pulling forces. Our model also shows that length-dependent catastrophe and rescue regulated by motor proteins and passive cross-linkers are necessary for well defined length of microtubules and their antiparallel overlap, respectively. We predict that stable antiparallel overlaps exert length-dependent forces on kinetochores to navigate their positioning in the center of the metaphase plate.

9:36AM W20.00007: Effects of rapid impact loading on neural progenitor cells*  DELANY RODRIGUEZ, LUKE H. C. PATTERSON, JENNIFER L. WALKER, University of California, Santa Barbara, EVELYN RODRIGUEZ-MESA, KEVIN SHIELDS, JOHN S. FOSTER, Owl Biomedical, ADELE M. DOYLE, University of California, Santa Barbara, KIMBERLY L. FOSTER, Tulane University, MEGAN VALENTINE (Presenter), University of California, Santa Barbara — We recently developed a high throughput microfluidic MEMS device, the μHammer, to subject individual cells to rapid impact loading, at strains of up to 40% over typical impact durations of ~10 μs. With the μHammer, we can subject >100,000 cells to controlled impacts per experiment, allowing measurement of both single cell properties and statistically-relevant population averages. Cells are collected post-impact and cultured, allowing the time course of damage and recovery to be determined through subsequent analysis. Here, we report the range of cytoskeletal structures and dynamics observed in neural progenitor cells (NPC) before and after sub-lethal impacts, as assessed by high-resolution confocal microscopy. These studies establish important baseline properties of the NPC cytoskeleton, while providing insight into the effects of traumatic injuries on cells and tissues.

*National Science Foundation through grants CBET-1631656, CMMI-1254893, and DBI-1625770.
**9:48AM W20.00008: Assemblies of Calcium/Calmodulin Dependent Kinase II with Actin and Their Dynamic Regulation by Calmodulin in Dendritic Spines**

QIAN WANG, MINGCHEN CHEN, NICHOLAS SCHAFFER, CARLOS BUENO, Rice University, SARAH SONG, University of Texas, Health Science Center, ANDY HUDMON, Purdue University, PETER G WOLYNES, Rice University, NEAL WAXHAM, University of Texas, Health Science Center, MARGARET CHEUNG (Presenter), Univ of Houston — Calcium-calmodulin dependent kinase II (CaMKII) plays a key role in the plasticity of dendritic spines. Calcium signals cause calcium-calmodulin to activate CaMKII, which leads to remodeling of the actin filament (F-actin) network in the spine. We elucidate the mechanism of the remodeling by combining computer simulations with protein array experiments and electron microscopic imaging, to arrive at a structural model for the dodecameric complex of CaMKII with F-actin. The binding interface involves multiple domains of CaMKII. This structure explains the architecture of the micron-scale CaMKII/F-actin bundles arising from the multivalence of CaMKII. We also show that the regulatory domain of CaMKII may either bind calmodulin or F-actin, but not both. This frustration along with the multipartite nature of the binding interface allows calmodulin transiently to strip CaMKII from actin assemblies so that they can reorganize. This observation therefore provides a simple mechanism by which the structural dynamics of CaMKII establishes the link between calcium signaling and the morphological plasticity of dendritic spines.

*This work was supported by the NSF Grant PHY-1427654, CHE-1614101 and CHE- 1743392.

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**10:00AM W20.00009: A generalized clutch model to explain cell adhesion mechanics**

CHIARA VENTURINI, PABLO SAEZ (Presenter), Univ Politecnica de Catalunya — Integrin-based cell adhesion is a key mechanism in a large number of physiological processes and diseases. The composition and nanoscale organization of adhesion complexes have shown that the integrin-talin-actin chain plays a central role in the formation of small nascent adhesion and further maturation into focal adhesions. The role of ligand spacing and substrate rigidity has been also clearly demonstrated. Clutch models have been widely used to describe how cell adhesion works. However, they have not been capable of rationalizing many of the aspects described above; probably, because current clutch models are built under a number of simplifications of the adhesion mechanisms. Here, we extend the classical clutch model with a detail description of the talin rod as well as a space-dependent ligand distribution. We will show the minimal building block and adhesion length of focal adhesion. Following the same computational model, we will also show that focal adhesion forms for stiff substrates for low spacing while they form in soft substrates for large spacing. In summary, we proposed a model that unifies our current understanding of cell adhesion architecture and turnover while replicating previous experimental results.

*The European Commission, H2020-FETPROACT-01-2016-731957.

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**Friday, March 6, 2020 8:00 AM - 10:12 AM**

**Session W21 DCP: Dynamics and Spectroscopy** 302 - Scott Sayres, Arizona State Univ
**8:00AM W21.00001: Broadband Microwave Spectroscopy of Lignin, Biofuels, and Their Pyrolysis Intermediates**

ALICIA HERNANDEZ-CASTILLO (Presenter), Molecular Physics, Fritz-Haber Institute, TIMOTHY SCOTT ZWIER, Chemistry, Purdue University, JOHN F STANTON, Chemistry, University of Florida — The chemical complexity of the fast-expanding list of potential plant derived biofuels pose a challenge to the scientific community seeking to provide a molecular understanding of their combustion. The direct relationship between molecular structure and rotational frequencies makes rotational spectroscopy highly structure specific; therefore, it is an ideal tool to characterize resonance-stabilized radicals. A high-temperature flash pyrolysis micro-reactor coupled with a supersonic expansion were used to generate the radicals, and a protocol called “strong-field coherence breaking (SFCB)” was used to analyze and speed up the line assignments. The 2-furanyloxy radical, a primary, resonance-stabilized radical formed by loss of a methyl group in the pyrolysis of 2-methoxy furan, was detected and its molecular parameters were determined. Furthermore, the phenoxy radical was investigated and structurally characterized by doing mass-correlated microwave studies. The new structural insights derived from analysis of the observed radicals and the new broadband rotational techniques will be discussed.

*Donors of the American Chemical Society Petroleum Research, Grant No. PRF#55152-ND6. Department of Energy Basic Energy Sciences, Chemical Sciences Division, Grant No.DEFG02-96ER145

**8:12AM W21.00002: Making a pure beam of cold, state-selected particles with tuneable velocity**

JUTTA TOSCANO (Presenter), JILA, University of Colorado, Boulder, CHRISTOPHER J. RENNICK, National Physical Laboratory, UK, MICHAL HEJDUK, Physical and Theoretical Chemistry, University of Oxford, UK, TIMOTHY P. SOFTLEY, University of Birmingham, UK, BRIANNA R. HEAZLEWOOD, Physical and Theoretical Chemistry, University of Oxford, UK — Generating a controllable and pure source of molecular free-radicals or open-shell atoms has been one of the primary barriers hindering the detailed study of radical processes in the laboratory. Radicals are intrinsically highly reactive species that are challenging to isolate as a pure sample. As a result of this, detailed information on the kinetics and dynamics of elementary reactions involving radicals is extremely scarce.

In order to obtain a source of cold state-selected radicals, we combine a Zeeman decelerator, which slows down a subset of the radicals in a supersonic beam using pulsed magnetic fields, with a newly designed magnetic guide. The latter serves to purify the output of the decelerator, yielding a pure beam of cold, state- and velocity-selected radicals which is ideal for collision studies. The magnetic guide can be used after a Zeeman decelerator — or after any supersonic or effusive beam — to select only radical species with a specific desired velocity within a narrow velocity distribution, affording exceptional control over the properties of the particles.

8:24AM W21.00003: Production of O\textsubscript{2} from Ultrafast Pump-Probe CO\textsubscript{2} Photodissociation

JACOB GARCIA, RYAN SHAFFER, SCOTT SAYRES (Presenter), School of Molecular Sciences, Arizona State Univ — Carbon dioxide (CO\textsubscript{2}) is ubiquitous in our atmosphere and plays important roles in the life cycle, the greenhouse effect, and has potential applications in industrial processes as a chemical feedstock. Concern over the ever-increasing concentration of CO\textsubscript{2} in our environment has sparked a renewed interest in its photoabsorption dynamics. Photodissociation of CO\textsubscript{2} proceeds via multiple pathways depending on available energy, but commonly into CO and O. Here, ultrafast pump-probe spectroscopy is applied to study the excited state dynamics of CO\textsubscript{2}. Multiphoton excitation from a 35 fs pump laser impulsively transfers CO\textsubscript{2} from the X \rightarrow A state, preparing a bending vibrational wavepacket that influences its dissociation. Using mass spectrometry, we report changes in the fragmentation pattern as a function of time delay between the pump and probe laser pulses that reflect the vibrational motion. At well-defined time delays the dissociation oscillates between observable CO\textsuperscript{+} and O\textsubscript{2}\textsuperscript{+} fragments. The state relaxes to the ground state through a conical intersection.

8:36AM W21.00004: Non-adiabatic dynamics of the highly excited uracil cation

PATRICIA VINDEL ZANDBERGEN (Presenter), Rutgers University, Newark, SPIRIDOULA C MATSIKA, Department of Chemistry, Temple University, Philadelphia, NEEPA MAITRA, Rutgers University, Newark — Conical intersections facilitating non-adiabatic transitions have been found to play a key role in many photo-physical pathways. Radical cations of nuclear acid bases involved in charge transfer processes in DNA exhibit ultrafast dynamics governed by the existence of non-adiabatic couplings between excited states, where electron-nuclei coupled dynamics become important. We investigate the dynamics of the uracil cation, using highly-accurate coupled electron-ion dynamics methods and compare the results with more commonly used and less computationally intensive methods. In particular, trajectory-based surface hopping dynamics has proven to be a powerful tool to study coupled nuclear-electronic dynamics, but it does not properly account for quantum decoherence. Instead, a new coupled-trajectory approach has been proposed based on the exact electron-nuclear correlation from the exact factorization of a full molecular wave function. Numerical simulations with model systems have shown that the electron–nuclear coupling beyond the non adiabatic coupling terms can describe the quantum coherence properly. Within this method the quantum (de)-coherence in large molecules can be treated correctly at the same computational cost as the original surface hopping dynamics.

*DOE DE-SC0019394
8:48AM W21.00005: Feshbach-Dyson method for calculations of Auger decay rates
WOJCIECH SKOMOROWSKI (Presenter), ANNA KRYLOV, Univ of Southern California — Photon absorption in the X-ray domain generally leads to creation of highly excited species with core-electron vacancies. One of the major relaxation channels for such states is Auger decay - a process accompanied by spontaneous emission of free electron(s). While Auger decay in atoms and molecules has been known for long now, its predictive modeling still poses a significant challenge for theorists, as it intrinsically involves electronic continuum and many-body electronic states which are formally unbound (metastable).

Here we present a novel approach to calculate Auger decay rates and spectra based on Fano-Feshbach resonance theory and equation-of-motion coupled-cluster method (EOM-CCSD). We apply core-valence separation (CVS) technique and appropriate EOM models to obtain the correct (both initial and final) electronic states that occur in the Auger decay. Then, all Auger partial rates and energy corrections are computed via contraction of two-body Dyson functions (an equivalent of two-particle transition density matrix) with proper two-electron integrals involving a free electron orbital. Results of our benchmark calculations for atomic and molecular systems demonstrate that the presented method yields highly robust and accurate Auger parameters.

9:00AM W21.00006: Sub-20-fs broadband transient transmission spectroscopy in the UV range used to track primary photoinduced processes in thiobases* DANIELLE CRISTINA FERREIRA (Presenter), Física, UFMG, IRENE CONTI, Chimica Industriale, Università degli Studi di Bologna, ROCIO BORREGO-VARILLAS, Dipartimento di Fisica, Politecnico di Milano, ARTUR NENOV, Chimica Industriale, Università degli Studi di Bologna, LUCIA GANZER, CRISTIAN MANZONI, Dipartimento di Fisica, Politecnico di Milano, MARCO GARAVELLI, Chimica Industriale, Università degli Studi di Bologna, GIULIO CERULLO, Dipartimento di Fisica, Politecnico di Milano, ANA MARIA DE PAULA, Física, UFMG — Thiation induces a red-shift in the absorption spectrum and causes also a dramatic change in the photophysics with respect to the canonical nucleobases: while in nucleobases internal conversion from the photoexcited singlet state to the ground state mediated by a conical intersection is the main deactivation channel, the major relaxation pathway in thiobases is via the population of triplet states through an ultrafast intersystem crossing.

We employ ultrafast transient transmission spectroscopy in the near-UV range together with CASPT2/MM decay path calculations to unravel the excited-state lifetimes and decay pathways of thiouracils solvated systems. Their linear absorption spectra show overlapping bright states bands leading to different/parallel bright states decay pathways which we systematically track. This comprehensive evaluation together shows with different processes lead to the triplet population, both directly from the bright absorbing state and via the dark intermediate state.

*This work was supported by CAPES, CNPq and Fapemig.
Effect of polar molecules in spin crossover transition of Fe(H$_2$B(pz)$_2$)$_2$(bipy)  

THILINI EKANAYAKA (Presenter), PAULO S COSTA, GUANHUA HAO, University of Nebraska - Lincoln, ALPHA T. N’DIAYE, Lawrence Berkeley National Laboratory, LUCIE ROUTABOUL, Université Paul Sabatier, PIERRE BRAUNSTEIN, Université de Strasbourg, XIN ZHANG, JIAN ZHANG, QIN-YIN SHI, VICKI SCHLEGEL, University of Nebraska - Lincoln, BERNARD DOUDIN, Université de Strasbourg, AXEL ENDERS, Universität Bayreuth, PETER A DOWBEN, University of Nebraska - Lincoln — The spin crossover phenomenon is a temperature-induced transition of diamagnetic low spin (LS) state to paramagnetic high spin (HS) state. This transition can also be triggered by pressure, light or magnetic field. The Fe(II) spin crossover molecules are known to exhibit spin-crossover transition and we have shown that [Fe{H$_2$B(pz)$_2$}$_2$(bipy)] exhibits a temperature dependent spin-crossover transition from its LS state to the HS state, if the temperature is increased above approximately 160 K. The temperature dependence of the spin state occupancy Fe(II) complex can be affected by addition of polar molecules. The highly polar p-benzoquinonemonoimine zwitterion mixed with [Fe{H$_2$B(pz)$_2$}$_2$(bipy)] resulted in locking [Fe{H$_2$B(pz)$_2$}$_2$(bipy)] largely into a low spin state while addition of the di-ethyl derivative of p-benzoquinonemonoimine zwitterion mixed with [Fe{H$_2$B(pz)$_2$}$_2$(bipy)] did not appear to perturb the spin crossover transition. Addition of different polar molecule, benzimidazole with small dipole moment results in a re-entrant spin crossover transition.

Chemical reaction pathways estimated by a transformation between manifolds*  

MARK PALENIK (Presenter), United States Naval Research Laboratory — Chemical reaction pathways are often estimated by linearly interpolating a set of internal coordinates, such as bond lengths, between reactant and product structures. However, these internal coordinates are not generally isomorphic to atomic positions. For example, the number of bond lengths between N atoms is N(N−1)/2, which is usually greater than the 3N -6 coordinates that specify unique molecular geometries. If arbitrarily chosen, the bond lengths may not be physically realizable because they violate the triangle inequality. The solution used in the method known as linear synchronous transit is to employ a least squares minimization to approximate the desired set of generalized coordinates. However, this method is prone to generating discontinuous reaction pathways and outright failure at generating transition states. As an alternative, we treat the spaces of generalized coordinates and Cartesian coordinates as separate manifolds and locally transform a velocity vector from the former into the latter. This results in a first-order differential equation for the reaction path which is numerically integrable even when linear synchronous transit fails.

*This work was supported by the Office of Naval Research, directly and through the Naval Research Laboratory.
9:36AM W21.00009: Harvesting force and energy from the thermal motion of gas molecules
   TOM ZHU (Presenter), Tom Zhu — This presentation will describe a few methods for producing force and energy from the thermal motion of gas molecules. The force that exerts to a surface by the gas molecules in collision with the surface is due to the change of the momentum of the gas molecules. For an elastic collision, there is no lost in the kinetic energy of the gas molecule. The rebound speed is the same as the initial speed. However, for a real system, there is always lost or gain in the kinetic energy in the collision. The force exerted to the surface by the gas molecule in collision with the surface will be smaller if there is kinetic energy lost in the collision because lower rebound speed. We may design a high-lost surface and a low-lost surface to produce a net force, to do work with this force, and at the same time to lower the gas temperature which could be maintained by absorbing the heat from external source. The net result is transfer the heat to work which can be used to, for example, generate electricity, without producing the waste heat. The force can also be used as propulsion means, or to lift weight against the gravity, for example elevating the vehicle of the hyper-loop, without consuming any energy.

9:48AM W21.00010: Theory of Diffusion-Limited Reactions between Proteins in a Confined Environment*  CHEN LIN (Presenter), JOSEPH RUDNICK, ROBIJN F BRUINSMA, University of California, Los Angeles — Smoluchowski theory is extensively used to compute diffusion-limited reaction rates. It is based on the assumption that the reactants diffuse in from infinity. However, in many cases, this assumption fails for association reactions between biological macromolecules because they initially are confined inside a certain volume. Examples are association reactions between the linked subdomains of polyproteins, such as the Gag protein of HIV-1 and the assembly reactions of the molecular components of a virus in a "virus factories". Confinement greatly increases reaction rates. The talk will discuss how Smoluchowski’s theory is generalized to include a confined environment by introducing particles at the finite range.

* We would like to thank the NSF for support under DMR Grant No.1836404.

10:00AM W21.00011: Chemical Cloaking*  FRANCESCO AVANZINI (Presenter), GIANMARIO FALASCO, MASSIMILIANO ESPOSITO, University of Luxembourg Limpertsberg — Any object embedded in a chemical gradient will typically distort it. We propose a strategy to hide an object in a gradient by coating it with a chemical reaction-diffusion network which can act as an active cloaking device. By controlling the concentration of some species in its immediate surroundings, the chemical reactions redirect the gradient as if the object was not there. We also show that the energy required to cloak can be extracted from the chemical gradient itself.

*European Research Council project NanoThermo (ERC-2015-CoG Agreement No. 681456)

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W22 DBIO: Robophysics III  303 - Nick Gravish, University of California, San Diego - Tag(s): Focus
8:00AM W22.00001: Collective Robot Sex on Dynamic Resource Landscapes* [Invited] GAO WANG, Physics, Chongqing University, TRUNG PHAN, ROBERT AUSTIN (Presenter), Princeton University, JUNLE QU, Physics, Shenzen University, LIYU LIU, Physics, Chongqing University — We present a community of robots (``Jeeps''), which move over a resource landscape consisting of a large light-emitting diode (LED) light board whose local RGB intensity represents fitness, the local intensity can change due to robot local presence, making the landscape dynamic. Each Jeep has a basic digital genotype that carries the response (phenotype) to a given local fitness value, down-ward firing RGB sensors to measure local intensity and RGB color, and side-firing sensors and LEDs to communicate with neighboring Jeeps and engage in gene exchange (robot sex) with neighboring Jeeps. The Jeeps move in response to the current local fitness gradient given by the gradient in color intensity of their position on the light board. The jeeps ``genes’’ mutate at a rate inversely proportional to the color intensity at their position, breed genomes, and consume resources. This robot community has great generality which spans the space of many-body soft-matter physics, evolutionary biology and multi-cell disease states. We show robots on the dynamic landscape exhibit the self-organization of a collective, distributed intelligent complexity
*This work was supported by NSF PHY-1659940 and the BBSRC(grant number BB/R012415/1

8:36AM W22.00002: Delay Induced Swarm Pattern Bifurcations in Mixed Reality Experiments* VICTORIA EDWARDS, IRA SCHWARTZ, United States Naval Research Laboratory, KLEMENTYNA SZWAYKOWSKA, Georgia Tech Research Institute, JASON HINDES, United States Naval Research Laboratory, M. ANI HSIEH, University of Pennsylvania, IOANA TRIANDAF (Presenter), United States Naval Research Laboratory — Swarms of coupled mobile agents with communication-time delay are known to exhibit multiple dynamic patterns in space, which depend on interaction strength and delay. We demonstrate experimentally delay-induced bifurcations between spatio-temporal patterns with two separate robotic platforms using a mixed-reality framework, and isolate parameter regions where transitions occur. We show that multiple rotation patterns persist in the presence of collision-avoidance and uncertainties in the real robot dynamics. Moreover, we show the existence of multi-stability of rotational patterns not predicted by usual mean field dynamics. Our experimental results increase understanding of swarm-pattern robustness in the physical world, and may form the basis for improved reproducible models of swarms with physical robots.
*We thank the NRL base funding program, N0001414WX00023, and the Office of Naval Research, N0001419WX01166 for their support.
8:48AM W22.00003: Robotic control of live jellyfish swimming to enhance propulsion*

NICOLE XU (Presenter), Stanford Univ, JOHN O DABIRI, California Institute of Technology — Animal locomotion and bioinspiration have the potential to expand the performance capabilities of robots, but current implementations are limited. Mechanical soft robots leverage engineered materials and are highly controllable, but these biomimetic robots consume more power than corresponding animal counterparts. Biological soft robots from a bottom-up approach offer advantages such as speed and controllability, but are limited to survival in cell media. Instead, biohybrid robots that comprise live animals and self-contained microelectronic systems leverage the animals’ own metabolism to reduce power constraints and body as a natural scaffold with damage tolerance. We demonstrate that by integrating onboard microelectronics into live jellyfish, we can enhance propulsion up to threefold, using only 10 mW of external power input to the microelectronics and at only a twofold increase in cost of transport to the animal. This robotic system uses 10 to 1000 times less external power per mass than existing swimming robots in literature, and can be used in future applications for ocean monitoring.

*NSF GRFP awarded to NWX

9:00AM W22.00004: Neuromuscular actuation of biohybrid motile bots*

MATTIA GAZZOLA (Presenter), ONUR ADYIN, XIAOTIAN ZHANG, TAHER SAIF, University of Illinois at Urbana-Champaign — The integration of muscle cells with soft robotics in recent years has led to the development of biohybrid machines capable of untethered locomotion. A major frontier that currently remains unexplored is neuronal actuation and control of such muscle-powered biohybrid machines. As a step toward this goal, we computationally designed, optimized, and implemented light-sensitive flagellar swimmers driven by on-board neuromuscular units. The body of the swimmer consists of a free-standing soft scaffold, skeletal muscle tissue, and optogenetic stem cell-derived neural cluster containing motor neurons. Neural stimulation triggers cyclic muscle contractions, driving time-irreversible flagellar dynamics, thereby providing thrust for untethered forward locomotion of the swimmer. Overall, this work demonstrates an example of a biohybrid robot implementing neuromuscular actuation and illustrates a path toward the forward design and control of neuron-enabled biohybrid machines.

*NSF Science and Technology Center for Emergent Behaviors of Integrated Cellular Systems Grant 0939511
NSF Emerging Frontiers in Research and Innovation (EFRI): Continuum, Compliant, and Configurable Soft Robotics Engineering (C3 SoRo) Grant 1830881
NSF Career Award 1846742
Gait coordination and hydrodynamic performance of a quadriflagellate robophysical model  
TOMMIE ROBINSON (Presenter), KELIMAR DIAZ, YASEMIN OZKAN-AYDIN, Georgia Inst of Tech, KIRSTY WAN, Physics, University of Exeter, DANIEL I GOLDMAN, Georgia Inst of Tech — Multi-legged animals coordinate their limbs in distinctive patterns known as gaits. At the microscopic scale, quadriflagellate algae have been found to exhibit similar capabilities, coordinating their flagella to numerous rhythmic patterns to generate propulsion (Wan & Goldstein, 2016). To study quadriflagellate gait coordination, we developed a robophysical model which replicates quadriflagellate swimming at low-Reynolds number. We focus on two distinct gaits, the pronk and the trot, and explored the effects of flagellar orientation. When the flagella were oriented parallel to the cell body, forward motion was measured at 0.30±0.09 body lengths per gait cycle (BL/cyc) for the trot and at 0.19±0.03 BL/cyc for the pronk. Results are comparable to microorganisms' performance, where using the trot enables a higher speed (0.39±0.18 BL/cyc) than the pronk (0.18±0.05 BL/cyc). Surprisingly, when the flagella beat planes were perpendicular to the cell body, hydrodynamic performance improved significantly. Forward motion was measured at 0.66±0.13 BL/cyc for the trot and at 0.38±0.10 BL/cyc for the pronk. The results show that hydrodynamic performance is highly sensitive to swimming gait and flagellar orientation.

Locomotion of Soft Robots with Flexible Uni-flagellum in low Reynolds Number Fluid  
YAYUN DU (Presenter), University of California, Los Angeles — In nature, more than 90% of the bacteria propel using a single flagellum. The uniflagellar bacterium is comprised of a basal body and a flagellum, with a flexible hook connecting the two. Experimental and numerical observations indicate that the flexibility of the flagellum and its buckling are essential to change the swimming direction of the bacterium. We simulate the locomotion and deformation of the flagellated system in low Reynolds number conditions using a combination of the Discrete Elastic Rods and the Lighthill Slender Body Theory. The simulator shows that the robot is able to follow a prescribed three-dimensional trajectory by simply controlling the angular velocity of the flagellum. Inspired by natural bacterial structure, we fabricate a self-contained robot with a rigid and a motor-actuated elastomeric helical rod - our analog for the flagellum. With a motor, sensors, and a flexible control circuit embedded inside the head, the robot is able to follow a prescribed nonlinear trajectory by flagellum buckling. This robotic system demonstrates how structural instability can be harnessed for control of soft robots. It can also serve as an analog model for the natural bacterium to help us understand the fluid dynamics and biophysics underlying the propulsion of bacteria.
Simply controlled 1DOF adaptive soft robotic fish with multiple swimming behaviors

BANGYUAN LIU (Presenter), DANIEL I GOLDMAN, FRANK L. HAMMOND III, Mechanical Engineering, Georgia Inst of Tech —

Research in robotic grasping and soft machines has demonstrated that the use of “smart” mechanical structures in robotic systems can enable complex behaviors in dynamically changing, uncertain environments without the need for complicated, low-level control strategies. Upon that premise, we designed an 1DOF simply controlled robotic fish to explore the ability to achieve different locomotion patterns and passively generate adaptive swimming behaviors, simply by changing the servo’s output parameters. This 1-DOF, cable-driven robotic fish mimics the cascaded skeletal structure of soft spine tissue and hard spine bone seen in many fish species using a series of rigid segments and elastic joints. By changing the frequency of actuator motion, the robotic fish can not only change its lateral swimming pattern from oscillatory (2.3cm/s) to undulatory (11.0cm/s), but also change swimming direction from forward to backward and steering by biasing servo sweeping offset. Preliminary tests also show that the robot can swim downward to 7m successfully. In addition, the soft body helps the fish passively navigate through gaps and around obstacles without any feedback control, greatly enhancing the locomotion robustness in complex, cluttered environments.

Magnetic Actuation and Biological Sensing for Soft Micro Bio Robots*

ELIZABETH HUNTER (Presenter), EDWARD STEAGER, VIJAY KUMAR, University of Pennsylvania —

Small-scale robotic systems have the potential to drive technological development in biological research and medicine. Similar in size to insects or as small as a single cell, robots at these scales have manipulated cells and tissues, delivered therapeutics, and monitored biological environments. In order to perform these tasks, small-scale robots must be able to precisely locomote, take measurements, and use those measurements to make decisions. In this talk, we will discuss our distinct approach to actuation and sensing through the design and fabrication of soft micro bio robots composed of an organic hydrogel embedded with iron oxide nanoparticles. Due to its biocompatible, soft, and porous scaffold, this robot can transport and deliver chemical, cellular, and bimolecular payloads. We drive these robots using uniform, rotating magnetic fields across a range of rotational frequencies and within various fluids spanning three orders of magnitude in viscosity. Inspired by developments in synthetic biology, we genetically engineer sensors and processing units harbored within bacteria which are grown and function on-board the robot. These results showcase a hybrid strategy to actuate and integrate sensors on-board biologically relevant small-scale robots.

*NSF Grant CNS-1446592
10:00AM W22.00009: Surface electrochemical actuators for micron-scale fluid pumping and autonomous swimming*  
MICHAEL REYNOLDS (Presenter), ALEJANDRO CORTESE, QINGKUN LIU, WEI WANG, MICHAEL CAO, DAVID ANTHONY MULLER, Cornell University, MARC MISKIN, University of Pennsylvania, ITAI COHEN, PAUL L MCEUEN, Cornell University — Recently, our group demonstrated a new class of electronic actuators called surface electrochemical actuators (SEAs). They use surface adsorption on a nanometer-thick cantilever to produce micron-scale radii of curvature with only fractions of a volt for actuation. Here we use SEAs to mechanically pump fluid at the micron-scale in several different geometries, both in the rigid panel (Purcell) and flexible (flagella) limits. We further discuss ongoing work to integrate SEAs with photovoltaics to create optically powered swimmers. Our ultimate goal is to create fully autonomous swimming microrobots with onboard electronics that can sense and respond to their environment in complex ways, yet are too small to be resolved by the naked eye.

*This work was supported by the Cornell Center for Materials Research (DMR-1719875), the Air Force Office of Scientific Research (MURI: FA9550-16-1-0031), the Army Research Office (ARO W911NF-18-1-0032) and the Kavli Institute at Cornell for Nanoscale Science. This work was performed in part at Cornell NanoScale Facility, an NNCI member supported by NSF Grant NNCI-1542018.

10:12AM W22.00010: Material remodeling on granular terrain yields robustness benefits for a robophysical rover  
SIDDHARTH SHRIVASTAVA (Presenter), ANDRAS KARSAI, YASEMIN OZKAN-AYDIN, Georgia Inst of Tech, ROSS PETTINGER, Jacobs Engineering Group, WILLIAM BLUETHMANN, ROBERT O AMBROSE, Software Robotics and Simulation Division, NASA Johnson Space Center, DANIEL I GOLDMAN, Georgia Inst of Tech — Planetary rovers face the risk of entrapment during extraterrestrial exploration; these risks led NASA JSC to develop RP-15, a 300 kg rover capable of lifting and sweeping each wheel to execute a crawling behavior to escape entrapment. We created a miniature rover (2.1 kg) as a robophysical model of RP-15 and conducted systematic and automated experiments in a tilting bed containing a model granular medium (poppy seeds) to discover gaits which allow progress in various conditions. A combination of stepping, paddling, and wheeling (“RS gait”) allows climbing of loose granular slopes. The RS gait produces up to 4x greater tractive (drawbar) forces than wheel rotation alone on dry granular media. Drawbar results were validated through experiments on RP-15 at JSC. On slopes near the maximum angle of stability, a different gait used the front wheels as agitators while paddling the rear wheels to climb granular slopes successfully via controlled avalanching. While substrate disturbance typically hinders granular locomotion, using appropriate active granular reconfiguration can create localized granular structures that facilitate effective locomotion.
10:24AM W22.00011: Investigating Growth and Granular Fluidization in a Minimally Invasive Burrowing Robot

NICHOLAS NACLERIO (Presenter), Mechanical Engineering, University of California, Santa Barbara, MASON MURRAY-COOPER, ANDRAS KARS AI, YASEMIN OZKAN-AYDIN, DANIEL I GOLDMAN, Physics, Georgia Institute of Technology, ELLIOT W. HAWKES, Mechanical Engineering, University of California, Santa Barbara — Subterranean navigation is simply hard to do. The forces resisting underground motion are orders of magnitude higher than in air or water. Here we present a paradigm for minimally invasive robotic burrowing that results in movement an order of magnitude faster and deeper than previous low-impact approaches. Three principles enable this behavior: tip-extension to eliminate skin drag; granular fluidization to reduce form drag; and granular fluidization to control lift forces, a heretofore unstudied phenomenon. We present experimental results from controlled intrusion tests, studying the effects of fluidization direction, depth, and flow rate on both drag and lift. We show that lift is highly dependent on fluidization angle (i.e., the direction of air flow at the tip), decreasing as the fluidization is changed from horizontal to vertically downward, but drag reduction is insensitive to fluidization angle. With the use of pneumatic artificial muscles for steering, we demonstrate a functional burrowing robot, capable of navigating through sand and subterranean obstacles. Our results advance the understanding and capabilities of robotic subterranean locomotion, and the forces at play.

*This work is funded by a NASA Space Technology Research Fellowship, and the NSF (grant no. 1637446).

10:36AM W22.00012: Force response of running up a sand dune

BRIAN CHANG (Presenter), ALEXANDER GREENWOOD, WALEE D NOWAYTI, TONIA HSIEH, Temple Univ — Running up a sand dune is challenging because: (1) sand fluidizes when an external force exceeding the material yield stress is applied; and (2) at inclines approaching the angle of repose, the sand pile is increasingly unstable. In this study, we experimentally examined the impact force normal to a flat plate against a bed of poppy seeds, to determine how intrusion kinematics affect force generation. We tested a range of impact speeds (0.01-1.2 m/s), substrate angles, and impact angles. We identified two regimes with distinct force production patterns: 1) the gravity regime (<0.6 m/s) and 2) the inertial regime (>=0.6 m/s). In the gravity regime, the force-depth relation tends to diverge when comparing, for example, \((\theta_{\text{Intrusion}}, \theta_{\text{substrate}})=(40,0)\) and \((0,40)\). This difference is likely due to the propensity of the angled substrate to avalanche and reduce the material force response. On the other hand, the same set would converge at higher impact speeds, indicating that inertia dominates the system with particle movement instigated by the intruder exceeding that due to avalanching. This insight will help inform how animals and robots may navigate up sand dunes efficiently.
10:48 AM W22.00013: Generation GrowBots: learning from plants how to design self-morphing, growing robots  BARBARA MAZZOLAI (Presenter), EMANUELA DEL DOTTORE, LAURA MARGHERI, ALESSIO MONDINI, FRANCESCA TRAMACERE, Center for Micro-BioRobotics, Istituto Italiano di Tecnologia — Plants show unique capabilities of endurance and the ability to adapt their morphology to different environmental conditions. This plasticity is materialized through a variety of strategies, including moving-by-growing to search for nutrients, lights, or for external supports; rapid movements to capture prays; or passive movements for spreading seeds and fruits. Together with plant biologists and materials scientists, we are deeply investigating the biomechanics, materials, energy efficiency mechanisms, and behavior of a variety of plant species. For the first time, we have proposed a growing robot inspired by the movements and the behaviors of plant roots, able to create its own structure exploiting a 3D printer-like system integrated into its tip and depositing a thermoplastic material. With a focus on climbing plants, we are now taking inspiration from their material properties, biomechanics, and searching&anchoring capabilities for the design of new multi-functional, self-morphing, adaptable, growing robots. This new generation of plant-inspired “growbots”, able to self-create their structure, will find potential applications in a variety of sectors, including the exploration and monitoring of archaeological sites, future urban architecture, or extra-terrestrial areas.

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W23 DBIO DPOLY DSOFT GSNP: Macromolecular Phase Separation in Biology III 304 - Patrick McCall, Max Planck Institute for the Physics of Complex Systems - Tag(s): Focus
8:00AM W23.00001: Valence and Patterning of Aromatic Residues Determine the Phase Behavior of Disordered Prion-Like Domains* [Invited] ALEX S HOLEHOUSE (Presenter), Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, ERIK W MARTIN, IVAN PERAN, Department of Structural Biology, St. Jude Children's Research Hospital, ROHIT V PAPPU, Department of Biomedical Engineering, Washington University in St. Louis, TANJA MITTAG, Department of Structural Biology, St. Jude Children's Research Hospital — Prion-like domains (PLDs) are intrinsically disordered protein regions that can drive functional liquid-liquid phase separation (LLPS) in vitro and in cells. Curiously, in many neurodegenerative diseases these regions contain mutations, leading to the formation of aggregates which are strongly correlated with disease pathology. An open question reflects the underlying molecular details that explain why some sequences form dynamic reversible assemblies, while others form solid-like aggregates. Here, we use multipronged biophysical approaches that integrates across simulation, experiment, and theory to address this question and uncover the physical principles underlying how an archetypal PLD derived from hnRNPA1 avoids aggregation in favor of LLPS. The extent of compaction of individual PLDs in dilute solutions mirrors the driving forces for temperature-dependent LLPS. This compaction is directly determined by the valence of aromatic residues in PLDs. As a result, the sequence-dependent phase behaviour for PLDs can be predicted using a stickers-and-spacers model. We uncover an evolutionary preference for aromatic residues to be uniformly distributed, as opposed to being clustered, along PLD sequences. We demonstrate that this non-random patterning drives reversible LLPS whereas its disruption leads to aggregation. We conclude that the valence and patterning of aromatic residues are key determinants of LLPS in PLDs. More generally, the valence and patterning of stickers in a stickers-and-spacers model offers a quantitative approach to relate sequence features to full binodal curves.

*Funding was provided by St. Jude Children's Research Hospital Research Collaborative (to RVP and TM), NSF grant MCB1614766 to RVP), and HFSP grant (RGP0034/2017 to RVP).

8:36AM W23.00002: A Random Heteropolymer Model of Protein Aggregation* MARTIN FALK (Presenter), Physics, University of Chicago, CATHERINE TRIANDAFILLOU, Biophysics, University of Chicago, ARVIND MURUGAN, Physics, University of Chicago — There have been dramatic developments in our ability to functionalize submicron scale objects with molecules enabling specific interactions between building blocks. To guide exploration in this design space, it is natural to look towards biology. In this context, the phenomenon of protein aggregation is a particularly appealing subject of study. Proteins navigate a complex and rugged energy landscape, and the design rules underlying their ability to avoid or take advantage of aggregated states in this landscape can be instructive for synthetic systems as well. We study a simple system consisting of a solution of random heteropolymers, and identify parameters that determine the structure of the aggregated phase.

*We acknowledge NSF-MRSEC 1420709 for funding.
8:48AM W23.00003: Actin(g) on phase separation* TINA WIEGAND (Presenter), Max Planck Institute for the Physics of Complex Systems, ANTHONY HYMAN, STEPHAN GRILL, Max Planck Institute of Molecular Cell Biology and Genetics — F-actin networks play a crucial role for cellular integrity and induction of shape changes during development and homeostasis. Actin polymerization is highly regulated by multiple pathways involving nucleating and sequestering factors, or mechanisms that regulate local monomer concentration. Recently, actin partitioning into biomolecular condensates has been reported as an additional mechanism to enhance polymerization kinetics. We reconstitute phase separated droplets of the components wsp-1 and the arp2/3 complex in vitro and study their interaction with actin. We find that actin partitions inside phase separated drops, where it polymerizes into fibers which extrude. We use this assay to study the effect of locally enhanced concentration on branched actin polymerization, the dynamics of active condensates and the mechanical interplay between established actin networks and biomolecular condensates. Our aim is to recapitulate the complex spectrum of kinetic behaviors observed for actomyosin in vivo.

*ELBE postdoctoral fellow program

9:00AM W23.00004: Elasticity dominated small molecule migration in polymer mixtures and gels* BUDDHAPRIYA CHAKRABARTI (Presenter), BISWAROOP MUKHERJEE, Univ of Sheffield — Surface segregation of the low-molecular weight component in a polymeric mixture leads to degradation of industrial formulations. We report a simultaneous phase separation and surface migration phenomena in oligomer-polymer and oligomer-gel systems following a temperature quench. We compute equilibrium and time varying migrant density profiles and wetting layer thickness using coarse grained molecular dynamics and mesoscale hydrodynamics simulations to demonstrate that surface migration in oligomer-gel systems is significantly reduced due to network elasticity. Further, phase separation processes are significantly slowed in gels, modifying the Lifshitz-Slyozov-Wagner (LSW) law. Our work allows for rational design of polymer/gel-oligomer mixtures with predictable surface segregation characteristics.

*EP/P07864/1
9:12AM W23.00005: Looped liquid-liquid coexistence in protein crystallization  JENS GLASER (Presenter), SHARON C GLOTZER, Univ of Michigan - Ann Arbor — The potential of proteins to realize enzyme crystals or act as nanomachines in dense assemblies makes them excellent candidates for the de-novo design of biological materials. In view of the notorious complexity of protein-protein interactions, simplified models of proteins treated as patchy particles offer a promising strategy to obtain insight into the mechanism of crystallization. Here we report liquid-liquid phase separation (LLPS) with a highly asymmetric coexistence region in a computational model of rubredoxin with real molecular shape. The coexistence region terminates in both an upper (UCST) and a lower (LCST) critical solution temperature, and the complex molecular shape explains the closed-loop behavior of the LLPS. A popular conceptual framework of protein crystallization predicts that nucleation is a two-step process controlled by a metastable liquid-liquid critical point. Here, LLPS occurs via the formation of ring-like nucleation precursors if and only if the proteins are capable of crystallizing. Our findings dispute the notion that the nucleation rate may be enhanced by indirectly controlling nucleation through an independent, metastable critical point. Conversely, we show that metastable LLPS is an essential feature of crystallization.

9:24AM W23.00006: Intermolecular association of the variable domain of dynamin related protein 1 in crowding conditions suggests a role in dynamin assembly  JAMES HARDEN (Presenter), AMMON POSEY, Biomedical Engineering, Washington University, MEHRAN BAGHERI, Univ of Ottawa, MEGAN HARWIG, NOLAN W. KENNEDY, Biochemistry, Medical College of Wisconsin, VINCENT HILSER, Program in Molecular Biophysics, Johns Hopkins University, R. BLAKE HILL, Biochemistry, Medical College of Wisconsin — Dynamins are an essential superfamily of mechanoenzymes that remodel membranes and often contain a “variable domain” (VD) important for regulation. For the mitochondrial fission dynamin, Drp1, a regulatory role for the VD is demonstrated by mutations that can elongate, or fragment, mitochondria. How the VD encodes inhibitory, and stimulatory, activity is an unresolved issue. This talk focuses on the behaviour of isolated VD from Drp1 isoform 1. Using spectroscopy methods (NMR and circular dichroism) and molecular dynamics (MD) simulations, this VD is shown to be intrinsically disordered (ID). Somewhat surprisingly, microscopy and light scattering studies also indicate that this VD in solution undergoes a liquid-liquid phase separation under the influence of an osmolyte that normally induces ID proteins to fold. Interestingly, these crowding conditions also enhance binding to cardiolipin, a mitochondrial lipid. MD simulations suggest this liquid-liquid phase separation arises from weak, multivalent interactions similar to other systems involving intrinsically disordered regions. These new findings support a model where the variable domain mediates phase separation that enables rapid tuning of Drp1 assembly necessary for fission.
9:36AM W23.00007: Model for intrinsically disordered proteins with a strong dependence of liquid-liquid phase separation on sequence  
ANTONIA STATT (Presenter), Materials Science and Engineering, University of Illinois, HELENA CASADEMUNT, Department of Physics, Harvard University, CLIFF BRANGWYNNE, ATHANASSIOS PANAGIOTOPoulos, Princeton University — Phase separation of intrinsically disordered proteins is important for the formation of membraneless organelles, or biomolecular condensates, which play key roles in the regulation of biochemical processes within the cells. In this talk, we present the phase separation behavior of different sequences of a coarse-grained model for intrinsically disordered proteins and show that they exhibit a surprisingly rich phase behavior. Both the fraction of total hydrophobic parts and the distribution hydrophobic parts are investigated. We observed not only conventional liquid-liquid phase separation, but also reentrant phase behavior, in which the liquid phase density decreases at lower temperatures. For some sequences, we also observe formation of open phases consisting of aggregates, rather than a normal liquid. These aggregates had overall lower densities than the conventional liquid phases and complex geometries with large interconnected fibril-like or membrane-like clusters. Minor alterations in the ordering of a given set of amino acids may lead to large changes in the overall phase behavior, a fact of significant potential relevance for biology.

9:48AM W23.00008: Quantitative droplet FRAP based on physical principles  
LARS HUBATSCH (Presenter), LOUISE JAWERTH, Max Planck Institute for the Physics of Complex Systems, ANTHONY HYMAN, Max Planck Institute for Cell Biology and Genetics, CHRISTOPH WEBER, Max Planck Institute for the Physics of Complex Systems — Fluorescence recovery after photobleaching (FRAP) is used to characterize a range of dynamic processes, for example binding kinetics and mobility of intracellular proteins, and recently liquid-liquid phase separation (LLPS) in vitro and in vivo. To gain an understanding of the relevant molecular mechanisms, data analysis must be based on the underlying physics. Strikingly, for FRAP of phase-separated droplets, no physical model from first principles has been derived, which severely restricts data interpretation. Here, we first derive a FRAP model from the physical principles underlying LLPS. Second, we use the full spatio-temporal imaging data within the droplet for fitting. This results in the following improvements: we can (i) distinguish the time scales of exchange through the droplet interface (set by bulk diffusion and boundary kinetics) from diffusion inside the droplet, (ii) quantify the impact of the interface (iii) provide improved measurements for several biologically important proteins, and (iv) use our analysis framework to explore several multi-component scenarios. Finally, we provide experimental guidelines for highly quantitative in vitro FRAP, e.g. the necessity to perform a full bleach to allow robust analysis and routines to allow spatio-temporal fitting.
**10:00AM W23.00009: Probing ATPase Dependent Physical Properties of Biological Condensates**
SEBASTIAN COUPE (Presenter), YOON JUNG, NIKTA FAKHRI, Massachusetts Institute of Technology MIT — Biological condensates are membraneless organelles, formed through nonspecific or multivalent ribonucleoprotein interactions, which are thought to be involved in the biochemical organization of the cell. There is increasing evidence for the regulation of these biological condensates by DEAD-box RNA helicases, which canonically remodel RNA-protein and RNA-RNA interactions in an ATP-dependent manner. The specific relationship between helicase activity and condensate properties such as viscosity, elasticity, and network architecture has not been investigated to date. DEAD-box helicase LAF-1, a critical component of the P granule condensate of *C. elegans*, phase separates in vitro. The ability for LAF-1 to interact with RNA and the effect of RNA on its droplet fluidity have been previously studied, however the interplay between its enzymatic function and droplet properties has not been established. We analyze the diffusion of single-walled carbon nanotubes, which are infrared-fluorescent, photostable, passive probes, to analyze the physical properties of LAF-1 droplets. In studying how this model condensate system responds to base-pairing RNAs, ATP, and accessory proteins we will shed light on principles underlying energetic regulation of condensate fluidity.

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**10:12AM W23.00010: The robust bioinformatic analysis of the protein sequences with phase behavior**
ALEKSANDRA ELZBIETA BADACZEWSKA-DAWID (Presenter), DAVIT POTOYAN, Iowa State University — Liquid-liquid phase separation (LLPS) of many proteins is critical in the biological function of membrane-less organelles. Reversible nature of biomolecular PS in cells suggests that phases of proteins and nucleic acids are like to be tightly regulated. Post-translational modifications and single-residue mutations have been shown to lead to the dissolution of biomolecular droplets or phase transition into aggregated forms. Based on the wealth of experimental data, it reasonable to expect that the PS of proteins is highly sequence-specific.

To reveal common motifs of protein sequences that promote PS, we have carried out large-scale statistical analysis of phase separating protein deposited in the LLPSDB database. For each motif, the most significant interactions have been identified (e.g. charge, hydropathy, polarity, pi-stacking). The bioinformatic analysis provides us with crucial knowledge about sequence conservation, secondary structure preferences, aggregation tendency, post-translational modification prediction, and binding affinity.

The long-term goal of our research is the creation of a publically accessible database that would be used by both experimentalists for designing controlled mutations and for computationally-oriented scientists for developing new modeling tools.
10:24 AM W23.00011: Effects of protein charge and charge patterning on complex coacervation for enzymatic microreactors  
NICHOLAS ZERVOUNDIS (Presenter), ALLIE OBERMEYER, Columbia University — Complex coacervation is a liquid-liquid phase separation phenomenon that has shown promise encapsulating proteins and improving protein stability to a variety of perturbations. Cells utilize the process of complex coacervation to create microcompartments, termed membraneless organelles, for increased spatiotemporal control in cellular functions. Here, polypeptide-tagged green fluorescent protein (GFP) mutants and poly(4-vinyl N-methylpyridinium) were used to investigate the effects of protein charge patterning on coacervate phase behavior. Tagged mutants achieved coacervate concentrations higher than previously reported while retaining their secondary structure, suggesting that complex coacervation is a potentially attractive avenue for encapsulating enzymes for biocatalytic applications. Preliminary data has indicated the ability to form liquid-liquid phase separated microcompartments containing multiple enzymes. Using a model colorimetric cascade reaction, these multi-enzyme-polyelectrolyte coacervates have been used to evaluate the catalytic efficiency in biomimetic microcompartments and have the potential to inform the design of novel microcompartments for the production of industrially-relevant chemicals.

10:36 AM W23.00012: The role of a hidden ordered domain in controlling the material properties of RNA-protein condensates  
IAN SEIM (Presenter), DAPHNE KLOTSA, AMY S GLADFELTER, Univ of NC - Chapel Hill — Biomolecular condensates are a diverse class of membraneless, intracellular bodies that organize biochemistry. The constituent molecules, often RNA and protein, phase separate from a soluble pool into condensates which are crucial for normal physiological function but are also implicated in the development of several neurological diseases. Condensates can range from liquid-like droplets to solid-like aggregates. However, the distribution of condensate material properties along the viscoelastic continuum has not been well characterized, the molecular basis is poorly understood, and the corresponding functional consequences for cells are largely unknown. We have identified a coiled-coil (CC) motif within the disordered polyQ tract of a phase separating protein that strongly influences the material states of resulting RNA-protein condensates. By mutating specific residues in the CC, we demonstrate a range of material states in vitro, characterized by kinetic mean-field modeling of condensate formation. The CC domain structure is predicted by atomistic monte carlo simulations which are complemented by circular dichroism. Finally, integration of CC mutants into cells provides an in vivo system that demonstrates a link between the material state of condensates and cell function.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W24 GSNP: The Statistical Physics of Real-world Networks I  
Guido Caldarelli, IMT Alti Studi Lucca - Tag(s): Undergrad Friendly
Scale-free networks revealed from finite-size scaling

MATTEO SERAFINO, IMT Alti Studi Lucca, GIULIO CIMINI (Presenter), CNR-ISC Inst for Complex Systems, AMOS MARITAN, SAMIR SUWEIS, University of Padova, JAYANTH R BANavar, University of Oregon, GUIDO CALDARELLI, IMT Alti Studi Lucca — Network theory is a powerful tool to develop predictive models of physical, biological and social collective phenomena. A remarkable feature of many networks observed in nature is that they are approximately scale free: the fraction of nodes with $k$ incident links (the degree) follows a power law for sufficiently large $k$. The value of the power law exponent as well as deviations from such scaling behavior provide invaluable information on the mechanisms underlying the formation of the network. Importantly, real networks are not infinitely large and the largest degree cannot be larger than the number of nodes. Finite size scaling is a useful tool for analyzing deviations from power law behavior in the vicinity of a critical point in a physical system arising due to a finite correlation length. Here we show that despite the essential differences between networks and critical phenomena, finite size scaling provides a powerful framework for analyzing self-similarity and the scale free nature of real networks. We analyze about two hundred naturally occurring networks with distinct dynamical origins, and find that a large number of these follow the finite size scaling hypothesis without any self-tuning.

Statistical Physics and Twitter analysis*

GUIDO CALDARELLI (Presenter), CAROLINA BECATTI, ROCCO DE NICOLA, IMT Alti Studi Lucca, FABIO DEL VIGNA, ISC, Consiglio Nazionale delle Ricerche, RENAUD LAMBIOTTE, Mathematics, University of Oxford, MARINELLA PETROCCHI, IIT, Consiglio Nazionale delle Ricerche, FABIO SARACCO, IMT Alti Studi Lucca — In this work we analyse approximately $10^6$ tweets exchanged during the last Italian elections held on March 4, 2018. Using an entropy-based null model discounting the activity of the users, we first identify potential political alliances within the group of verified accounts: if two verified users are retweeted more than expected by the non-verified ones, they are likely to be related. Then, we derive the users’ affiliation to a coalition measuring the polarisation of unverified accounts. Finally, we study the bipartite directed representation of the tweets and retweets network, in which tweets and users are collected on the two layers. Unexpectedly for most of the users, automated accounts, also known as social bots, contribute more and more to this process of news spreading. Results show that social bots play a central role in the exchange of significant content. Indeed, not only the strongest hubs have a number of bots among their followers higher than expected, but furthermore a group of them, that can be assigned to the same political tendency, share a common set of bots as followers.

*EU Tender Smart (Grant No. 2017/0090 LC-00704693), IMT PAI Project TOFFEE
8:24AM W24.00003: Using Correlated Stochastic Differential Equations to Model Cryptocurrency Rates and Social Media Activities* STEPHEN DIPPLE, ABHISHEK CHAUDHARY, JAMES FLAMINO, BOLESLAW SZYMANSKI, GYORGY KORNISS (Presenter), Rensselaer Polytechnic Institute — Increasingly interconnected financial systems and online social networks present both critical challenges and opportunities. Volatility in the former (e.g., cryptocurrency rates) can give rise to increased volume of activities in online social networks on relevant topics, while sentiments and rumors in online social networks can also have a significant impact on the corresponding financial time series. Here, we analyze and exploit correlations between the price fluctuations of selected cryptocurrencies and social media activities, and develop a predictive framework using noise-correlated stochastic differential equations. We employ the standard Geometric Brownian Motion to model cryptocurrency rates, while for social media activities and trading volume of cryptocurrencies we use the Geometric Ornstein-Uhlenbeck process. In our model, correlations between the different stochastic variables are introduced through the noise in the respective stochastic differential equation. Using a Maximum Likelihood Estimation on historical data of the corresponding cryptocurrencies and social media activities, we estimate parameters, and using the observed correlations, forecast selected time series.

*This work was supported in part by DARPA/ARO, ARL NS-CTA, and ONR.

8:36AM W24.00004: Optimizing Network Structure in a Network Model of Human Aging GARRETT STUBBINGS (Presenter), ANDREW RUTENBERG, Dalhousie Univ — Our network model of aging represents aspects of human health as nodes in a complex network, these nodes damage stochastically over time based on the health of their neighbours. This represents the accumulation of damage leading to poor health and eventual mortality. Previous work has shown that by using a scale free network this model captures the phenomenology of health and mortality in human populations. Why do scale free networks best capture this phenomenology? Do these scale free networks represent an organism's robustness to damage in a meaningful way? We address this question from the bottom up using a network optimization approach. Beginning at a random network structure, we optimize the network structure with respect to various health outcomes, such as longevity and health-related quality of life. We investigate which network motifs emerge depending on the optimization health outcome, and how these aspects of the network structure affect damage propagation. Knowledge of how damage propagates between different types of nodes will aid our understanding of how different aspects of human health interact, and how humans accumulate health deficits over time.
8:48AM W24.00005: Cascading dynamic slowdowns around hacked vehicles  SKANDA VIVEK (Presenter), Georgia Gwinnett College, DAVID B YANNI, Georgia Institute of Technology, JESSE L SILVERBERG, Multiscale Systems, Inc., PETER YUNKER, Georgia Institute of Technology — Almost 40% of vehicles in the US can connect to the internet. While there are significant benefits of increased connectivity, hackers have illustrated that internet connected vehicles can be compromised remotely. Further, large-scale hacks have the potential to cause disastrous city-wide disruptions. Recently, it was shown using percolation theory that randomly stalling 20% of cars in Manhattan would cause a total freeze of city traffic. While this upper-bound estimate served as the first quantification of city-scale disruptions when vehicles are hacked, dynamic effects potentially cause significant slowdowns at lower fractions of hacked vehicles. Here, we perform simulations of traffic dynamics around hacked vehicles on grids of one-lane roads, using the SUMO traffic simulation platform. We consider slowdowns, when vehicles encounter road blocks from hacked vehicles and find that shortly post-hack, blocked roads cascade to neighboring regions, leading to significant slowdowns across the grid. We find that slowdowns are a function of hacked vehicle density, time since hack, and grid size. At large enough wait times, even low fractions of hacked vehicles cause significant gridlocks. Our results provide insights for recovery and rerouting to mitigate impacts of a large-scale hack.

9:00AM W24.00006: Inference of Network Communities using Random Walks  ADITYA BALLAL (Presenter), WILLOW KION-CROSBY, ALEXANDRE MOROZOV, Rutgers University, New Brunswick — Community structures are very common in real-world networks. For example, social networks such as Facebook, Instagram and Twitter, biological networks such as gene co-expression networks, protein-protein interaction networks or link based networks such as Wikipedia all exhibit pronounced community structure. We propose a novel stochastic method, based on random walks, for community detection on undirected networks with weighted or unweighted edges. The method employs first-passage properties of random walks on networks, providing key statistics of network community structure such as the number of communities and the size of each community after only a small fraction of nodes have been explored. This method provides robust results on large-scale networks in which the complete transition matrix is unavailable due to network size.
Resolution limit revisited: community detection using generalized modularity density

Various attempts have been made in recent years to solve the Resolution Limit (RL) problem in community detection by considering variants of the modularity metric in the detection algorithms. These metrics purportedly largely mitigate the RL problem and are preferable to modularity in many realistic scenarios. However, they are not generally suitable for analyzing weighted networks or for detecting hierarchical community structure. Resolution limit problems can be complicated, though, and in particular it can be unclear when it should be considered as problem. In this paper, we introduce a metric that we call generalized modularity density $Q_g$ that eliminates the RL problem at any desired resolution scale and is easily extendable to study weighted, directed, and hierarchical networks. We also propose a benchmark test to quantify the resolution limit problem, examine various modularity-like metrics to show that the new metric $Q_g$ performs best, and show that $Q_g$ can identify modular structures in real-world and artificial networks that are otherwise hidden.

This work was supported by the NSF through grants DMR-1507371 and IOS-1546858. Some of the computations were done on the uHPC cluster at the University of Houston, acquired through NSF grant 1531814.

A novel community detection method improves detection of functional gene modules in big gene expression data.

We identify communities of functionally related genes in the network inferred from the gene expression data of eukaryotic model organisms Arabidopsis thaliana & Saccharomyces cerevisiae by finding the network partition that maximizes the recently introduced generalized modularity density metric $Q_g$. This new metric does not suffer from the resolution limit problem and, with its tunable control parameter, can be used to study the hierarchical structure of communities. We use the Reduced Network Extremal Ensemble Learning (RenEEL) scheme [Sci. Rep. 9, 14234 (2019)] to optimize the metric. Statistical significance comparisons with the gene ontology indicate that the $Q_g$ method outperforms other clustering methods. Orphan genes have been found in all sequenced species. These are genes unique to particular species. They are thought to play a key role in speciation, but their regulatory interactions remain largely unknown. Focusing on highly significant functional modules that contain orphan genes, regulatory interaction patterns involving these genes are discovered and testable predictions are made about their specific biological functions.

Supported by the NSF grants DMR-1507371 and IOS-1546858.
9:36AM W24.00009: The broken symmetry of music: applying statistical physics to understand the structure of musical harmony  JESSE BEREZOVSKY (Presenter), Case Western Reserve University — Despite myriad musical systems and styles, certain characteristics are nearly universal across cultures and throughout history, including a restriction to a discrete set of sound frequencies (pitches). In this talk, I will present a bottom-up approach to a theory of musical harmony, starting from two basic (and conflicting) principles: a system of music is most effective when it 1. minimizes dissonant sounds, and 2. permits sufficient complexity to allow the desired artistic expression. By quantifying these principles and assuming a parameter (temperature) that specifies the balance between them, the problem directly maps onto standard statistical mechanics [1]. A mean field treatment reveals phase transitions from disordered sound to ordered phases with distributions of pitches that closely match musical tuning systems used throughout the history of both western and non-western music. A numerical model with nearest-neighbor interactions displays the behavior of an XY system, including the appearance of topological defects following a quench. These defects, arising from the Kibble-Zurek mechanism, are interpreted as chords, with their arrangement reflecting a system of harmony.


9:48AM W24.00010: Evolution of coauthorship networks in view of simplicial complex  BYUNGNAM KAHNG, YONGSUN LEE (Presenter), DEOKJAE LEE, Seoul Natl Univ — Graph, composed of nodes and links, is a simple representation for constituents and pairwise interactions, respectively. This simple method was successful for explaining diverse properties of complex systems to some extent. Hypergraph including simplicial complex is a generalization of graph, which takes into account of more than pairwise interactions between multiple nodes. Here, using this simplicial complex representation based on algebraic topology, we consider the evolution of coauthorship networks, a prototypical example of large-scale social relationships, based on empirical datasets on specific subfields in science. We found that the facet degree distribution exhibits power-law decaying behavior more elaborately than the graph degree distribution, and the first Betti number is useful for representing the emergence of a large-scale cooperative phenomenon. Moreover, we construct a model to reproduce such results, which would be useful for understanding further structural properties of such simplex complexes.
10:00AM W24.00011: Impact Factor volatility to a single paper: A comprehensive analysis of 11639 journals  MANOLIS ANTONOYIANNAKIS (Presenter), Department of Applied Physics & Applied Mathematics, Columbia University — We study how a single paper affects the Impact Factor (IF) by analyzing data from 3,088,511 papers published in 11639 journals in the 2017 Journal Citation Reports of Clarivate Analytics. We find that IFs are highly volatile. For example, the top-cited paper of 381 journals caused their IF to increase by more than 0.5 points, while for 818 journals the relative increase exceeded 25%. And one in 10 journals had their IF boosted by more than 50% by their top three cited papers. Because the single-paper effect on the IF is inversely proportional to journal size, small journals are rewarded much more strongly than large journals for a highly-cited paper, while they are penalized more for a low-cited paper, especially if their IF is high. This skewed reward mechanism incentivizes high-IF journals to stay small, to remain competitive in rankings. We discuss the implications for breakthrough papers to appear in prestigious journals. We also question the reliability of IF rankings given the high IF sensitivity to a handful of papers for thousands of journals.

10:12AM W24.00012: A mathematical analysis of Stock price oscillations within financial markets.  LEONARD MUSHUNJE (Presenter), Applied Mathematics and Statistics, Midlands State University — The application of econophysics in modeling investment assets' market behavior is considerably increasing and is highly becoming an area of interest for econophysicists. This study investigated stock price oscillatory behavior in stock markets. We applied mathematical methods to derive the stock market price oscillatory model from the physics field. We considered two distinct price level cases that is, high and low price cases and presented/ derived a corresponding model for each case. We managed also to derive an explicit time function which measures and calculate the time taken by stock prices to oscillate between two values. Also, from the low-price oscillation model we managed to investigate stock price motion at different times with all other external forces held constant. Results obtained showed that, although stock price movement (volatility) is time dependent, it is propelled and fueled by market forces such as stock volume, market size and classical forces of demand and supply. Above all we evaluated our model using means difference test of hypothesis using actual and estimated stock price data. We failed to reject our null hypothesis and concluded that, there is no statistical significant difference in the means which highly support the precision of our model.
10:24AM W24.00013: When money beats time: the effect of length-dependent costs on transport driven by long-range connections  

JAYSON PAULOSE (Presenter), Physics, University of Oregon, TOM SUTER, École polytechnique fédérale de Lausanne, OSKAR HALLATSCHEK, Physics and Integrative Biology, University of California, Berkeley — Finding the optimal route between pairs of spatially-separated points is a prevalent problem in technology (transport and communication networks) and nature (foraging and migration). In many situations, each segment of a route is associated with a stochastic waiting time determined by the frequency of making connections over a given distance (the jump rate), and a deterministic travel cost which is a growing function of the connection length (the cost function). The optimal route minimizes a weighted combination of time and cost. When deterministic costs are ignored, broad jump-rate distributions which fall off slowly with distance can dramatically speed up optimal routes: nearly all the distance between origin and destination is covered in a single segment which can be found in a short time. However, introducing a deterministic cost makes these long connections prohibitively expensive, and less useful for optimal routing. We study the trade-off between broad jump rate distributions and growing cost functions in a model that generates ensembles of optimal routes for specified jump rates and cost functions. We find that even gently-growing cost functions (which grow slower than linearly with distance) can strongly suppress the acceleration due to broad jump-rate distributions.

10:36AM W24.00014: Quantum mechanism of price stabilization in financial markets*  

JACK SARKISSIAN (Presenter), Algostox Trading — We study the mechanism of price stabilization in financial instruments using the quantum coupled-wave model and show that security mispricing results in persistent execution imbalance, which drives the price towards its fair value. In the course of stabilization the bid-ask spread widens, which is in agreement with observed market data. If initial mispricing is large, price may exhibit oscillatory behavior as the normally present random phase jumps are suppressed. This also is a widely observed empirical pattern. When the fair price is achieved, imbalance stabilizes at zero value and fluctuates around it. These fluctuations are smaller for highly liquid securities, and larger for less liquid securities, which shows that liquid securities are less tolerable to mispricing. This behaviour is again in agreement with market data. These results show that price stabilization can be viewed as a quantum-chaotic process resulting from balance between buyers and sellers quoting prices on different bid and ask levels, rather than agreeing on a single price, as is widely believed in the economic supply-demand balance paradigm.

*None
10:48AM W24.00015: Hybrid phase transitions driven by tug-of-war mechanism in complex
dynamic systems  BYUNGNAM KAHNG (Presenter), JINHA PARK, Seoul Natl Univ, SUDO YI, school of
physics, korea institute for advanced studies, KWANGJONG CHOI, Seoul Natl Univ — Hybrid phase
transitions, exhibiting a jump of the order parameter and criticality at a transition point, are
observed in diverse complex systems. Examples include k-core percolation, cascading breakdown
in interdependent networks, contagion dynamics, restricted cluster coagulations,
synchronization, etc. For such dynamical systems, it is a challenging task to uncover underlying
mechanisms, and according to which the hybrid phase transitions are classified into universality
classes. Here, we perform such tasks. Particularly, we focus on the case that the so-called tug-of-
war mechanism between two temporal subgroups of the system induces hybrid phase
transitions in dynamical systems such as percolation and synchronization. We show that in such
dynamics, inter-event times between two successive crossings in the tug-of-war process have an
inter-event time distribution that exhibits power-law decay behavior. The associated exponent
determines the criticality of the hybrid percolation transition through cluster merging dynamics.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W25 GSNP: Pattern Formation, Chaos, Nonlinear Dynamics II
402 - Tankut Can, The Graduate Center, City University of New York

8:00AM W25.00001: Concentration-measure theory of waves: new perspectives of the
fundamentals of nonequilibrium statistical physics and mesoscopic physics  PING FANG
(Presenter), Beijing University of Posts and Telecommunications —
The foundations of statistical physics are currently under renovations. A number of scenarios for
the arising of statistical physics in an individual system has been proposed. However, most
studies have focused on equilibrium statistical physics. In this talk, I shall report our recent
progress on the fundamentals of nonequilibrium statistical physics. I will show a theory for
structures and fluctuations of waves in individual disordered media, using the mathematical tool
of the concentration of measure. Applying this theory, we can see how the elementary
nonequilibrium process of diffusion can arise from a single scattering state of wave equation,
without the canonical hypothesis of ensembles. Furthermore, fluctuations associated with the
change in incoming waves exhibit a new kind of universalities, which does not exist in
conventional mesoscopic fluctuations associated with the change in disorder realizations, and
originate from the coherence between the natural channels of waves – the transmission
eigenchannels.
Coherent Perfect Absorption in Chaotic Microwave Graphs* LEI CHEN
(Presenter), Department of Electrical and Computer Engineering, University of Maryland, College Park, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, STEVEN ANLAGE, Department of Physics and Department of Electrical and Computer Engineering, University of Maryland, College Park — Coherent perfect absorption (CPA) has been of great interest to the physics community, in part because it represents the time-reversed version of a laser. The CPA process works by taking waves of particular amplitude and phase (coherent illumination) from multiple input channels and causing them to interfere and to be completely absorbed by losses in the system. Its implementation promises the realization of a novel family of extremely efficient absorbers, tunable and highly-selective notch filters, and high-efficiency energy conversion systems. We experimentally demonstrate the concept of coherent perfect absorption in a microwave graph constructed from coaxial cables connected by Tee-junctions. By adding a simple variable lossy attenuator into the system, we can effectively identify the CPA frequencies as the complex zeros of the scattering matrix which crosses the real axis and achieve perfect absorption in this chaotic setup. Most importantly, our experimental set-up allows us to demonstrate that the concept of CPA can be extended beyond the case where time-reversal (TR) symmetry holds, by introducing a circulator into the microwave graph.

*We acknowledge support under contract AFOSR COE Grant FA9550-15-10171 and the ONR Grants N000141912481 and N00014-19-1-2480.

Tailored Noise Correlations and Generalized Levy Wave Dynamics in Multimode Systems* YAXIN LI (Presenter), Wesleyan Univ, DORON COHEN, Department of Physics, Ben-Gurion University, TSAMPIKOS KOTTOS, Wesleyan Univ — Multi-mode systems, like cavities, fibers etc, often suffer from the presence of environmental noise which causes mode mixing and subsequent interferences between various modes. In many occasions the study of the exact wave dynamic is a formidable task due to the many degrees of freedom that have to be taken into account in the equations of motion that describe such systems. Instead, a statistical theory of wave propagation might be a best way to describe the transport in such framework. We have utilized a Random Matrix Theory modeling which allow us to study the spreading of an initial mode excitation in the mode-space due to the environmental noise. Using this method we have developed a systematic approach that enforces a generalized Levy-type wave dynamics with a power law that it is imposed from the noise correlations. Our theoretical predictions have been tested in realistic circumstances like in paraxial light propagation in multimode fibers with tailored quenched disorder or in quantum dots with time-modulated boundaries.

*Partial support by an AFOSR Grant No. FA9550-14-1-0037, and by an NSF Grant No. EFMA-1641109.
Efficient Hybrid Model of Field and Energy Flow in Interconnected Wave Chaotic Systems*

STEVEN ANLAGE (Presenter), SHUKAI MA, University of Maryland, College Park, SENDY PHANG, George Green Institute for Electromagnetics Research, University of Nottingham, ZACHARY DRIKAS, BISRAT ADDISIE, RONALD HONG, US Naval Research Laboratory, Washington, DC, VALON BLAKAJ, GABRIELE GRADONI, GREGOR TANNER, School of Mathematical Sciences, University of Nottingham, THOMAS M ANTONSEN, EDWARD OTT, University of Maryland, College Park — Predicting energy flow through interconnected complex billiards is of keen interest to many fields. The Random Coupling Model (RCM) has been successfully applied to predicting the electromagnetic (EM) field statistical properties of various wave chaotic systems. Recent studies extend RCM to networks of coupled systems with multiple connecting channels [arXiv:1909.03827]. However the model becomes computationally costly as more billiards are added to the network. The Power Balance Model (PWB) can produce fast predictions for the averaged power density of waves in electrically-large systems. However the fluctuations of the wave field are lost in PWB, and many other mean-field approaches. Here we combine the best aspects of each model to create a hybrid treatment and study the EM fields in arrays of coupled complex systems. The proposed hybrid approach provides both mean and fluctuation information of the EM fields without the full computational demand of RCM. We compare the hybrid model predictions with experiments on linear cascades of overmoded cavities of various degrees of loss and find good agreement. The range of validity and applicability of the hybrid method is also discussed.

*ONR Grants N000141512134, and N000141912481, and AFOSR COE Grant FA9550-15-10171.

Breakdown of the Metastable State in the β Fermi-Pasta-Ulam-Tsingou Lattice*

KEVIN REISS (Presenter), SALVATORE PACE, DAVID K CAMPBELL, Physics, Boston University — We investigate numerically the formation and disappearance of Fermi-Pasta-Ulam-Tsingou (FPUT) recurrences in the β FPUT lattice, with special consideration to the lifespan of the metastable state. First, we consider different initial energies (E) and system sizes (N), to determine which initial parameters cause FPUT recurrences to form. We find that for large N, recurrences cease to form above a critical $E\beta$, a product of the energy and nonlinear parameter $\beta$. We explore the relationship between their disappearance and the breakdown of the metastable state to explain this critical $E\beta$, and also to estimate the time scale to the metastable state breakdown. In so doing, we define and measure a quantity called “shareable energy” and use this to show that systems with a negative $\beta$ have a much lower level of energy sharing than those with positive $\beta$.

*We thank Boston University's Undergraduate Research Opportunities Program and Boston University's Research Computing Services.
9:00AM W25.00006: The $\beta$ Fermi-Pasta-Ulam-Tsingou Recurrence Problem*  
SALVATORE PACE (Presenter), KEVIN REISS, DAVID K CAMPBELL, Physics, Boston University — One of the most remarkable and longest-studied problems in nonlinear dynamics is Fermi-Pasta-Ulam-Tsingou (FPUT) recurrences. We perform a thorough investigation of the first FPUT recurrence in the $\beta$-FPUT chain for both $\beta > 0$ and $\beta < 0$. We show numerically that the rescaled FPUT recurrence time $T_r = t_r(N + 1)^{-3}$ depends, for large $N$, only on the parameter $S = E\beta(N + 1)$. Our numerics also reveal that for large $|S|$, $T_r$ is proportional to $|S|^{-1/2}$ for both $\beta > 0$ and $\beta < 0$ but with different multiplicative constants. We numerically study the continuum limit and find the recurrence time closely follows the $|S|^{-1/2}$ scaling and can be interpreted in terms of mKdV solitons, and the difference in the multiplicative factors between positive and negative $\beta$ arises from soliton-kink interactions. We complement our numerical results with analytical considerations in the nearly linear regime (small $|S|$) and the highly nonlinear regime (large $|S|$). For the former, we extend previous results using a shifted-frequency perturbation theory and find a closed form for $T_r$, which depends only on $S$. In the latter regime, we show that the soliton theory correctly predicts $T_r \sim |S|^{-1/2}$ in the continuum limit.

*We thank Boston University's Undergraduate Research Opportunities Program.

9:12AM W25.00007: Statistical model and universality class for interacting puffs in transitional turbulence  
GRÉGOIRE LEMOULT, Normandie Université and Institute of Science and Technology Austria, MUKUND VASUDEVAN, JOSE M LOPEZ, Institute of Science and Technology Austria, HONG-YAN SHIH (Presenter), Institute of Physics, Academia Sinica and Department of Physics, University of Illinois at Urbana-Champaign, GAUTE LINGA, The Njord Center, University of Oslo and Niels Bohr Institute, University of Copenhagen, BJOERN HOF, Institute of Science and Technology Austria, JOACHIM MATHIESEN, Niels Bohr Institute, University of Copenhagen, NIGEL GOLDENFELD, Department of Physics, University of Illinois at Urbana-Champaign, BJOERN HOF, Institute of Science and Technology Austria — To understand the universality class of the laminar-turbulent transition in pipe flow, we measure how turbulent regions known as puffs proliferate and interact. Because of the huge length and time scales required to reach the critical regime, we model the dynamics from the effective forces we measure in experiments. Away from the transition, we find a crystal-like pattern with spatio-temporal intermittency. Renormalization group analysis and numerical simulations of both discrete and continuous models of puff interactions show that interactions are irrelevant at the 1+1-dimensional directed percolation fixed point but several finite-size artifacts mask the critical scaling regime in practice.
9:24AM W25.00008: A reduced model for a single cardiac cell  SHANGJUNG WU (Presenter), KUO-AN WU, Natl Tsing Hua Univ — The leading cause of sudden cardiac death is due to ventricular fibrillation (VF). VF is a heart rhythm disease that occurs from irregular dynamics behavior-discordant alternas. Therefore, it is vital to investigate the dynamics of a cardiac cell. In the past, typical mathematical models for dynamics of a cardiac cell involve intricate interplay between the membrane potential, ion channels, calcium cycling, etc, which would reproduce realistic responses such as cardiac alternas. Although above-mentioned models can reproduce genuine dynamics of a cardiac cell, they are generally complicated to analyze due to their high dimensional phase space. Hence, we propose a reduced model derived from an existing cardiac ionic model, and show that this three-variable dynamical system exhibits similar bifurcation diagram as that of the ionic model. The dynamical response and bifurcation behavior of a cardiac cell are investigated with the proposed reduced model.

9:36AM W25.00009: Diffusive behavior in walking droplets  AMINUR RAHMAN (Presenter), Texas Tech University, GIUSEPPE PUCCI, Université de Rennes, DANIEL M HARRIS, Brown University — Fluid droplets walking on a vibrating fluid bath have been observed to display deterministic diffusion. We present an experimental and theoretical investigation of such droplets. In our experiments a droplet is placed into an annular region on a vibrating fluid bath. The droplet motion becomes increasingly diffusive as the bath vibration is intensified above the Faraday wave threshold. This is also captured in our hydrodynamic – kinematic models, which shows close agreement between theory and experiments. Since the model can be studied at a much higher spatio-temporal resolutions than experiments, we use the model to numerically investigate bifurcations and chaotic dynamics suggested by experiments. Finally, we briefly discuss the possibility of model reduction to mitigate computational costs.

9:48AM W25.00010: Sloppy model analysis of dynamical systems near bifurcations*  CHRISTIAN ANDERSON (Presenter), MARK TRANSTRUM, Brigham Young Univ - Provo — In dynamical systems, bifurcations refer to topological changes in phase space trajectories in response to relatively small changes in parameter values. They are useful for identifying tipping points between qualitatively different types of behaviors such a phase transitions or from regulated to cancerous cellular pathways. Bifurcations are classified by the nature of the topological change in phase space with classes being typified by a "normal form", indicating that only a few parameters are responsible for driving a system through a bifurcation. Sloppy models provide a framework for identifying relevant parameters in a data-driven way. We apply sloppy model analysis to several dynamical systems near their bifurcations. We show that after an appropriate coarse-graining procedure, sloppy model analysis is able to correctly identify the bifurcation parameters. This suggests that sloppy model analysis can be used to identify the relevant control knobs in multi-parameter models of complex dynamical systems in a data-driven way.

*This work was supported by the US National Science Foundation under Award NSF-1753357.
10:00AM W25.00011: A mathematical approach to the effects of gender bias and cross gender interactions on careers in STEM. JENNIFER PEARCE (Presenter), JESSICA JENSEN, DARRELL VALENTI, JULIETTE M CAFFREY, Roger Williams University — Creating a mathematical model to predict participation in STEM fields would allow communities such as the APS understand better how to influence participation in physics. We propose a model that simulates the progression of women in male-dominated fields starting from the equations for a model predator-prey type system. We include interactions between the dominant and non-dominant populations and investigate how they effect the percent of the non-dominant population. We believe that such a model effectively captures some of the dynamics reported by researchers directly collecting data about the experiences of women in these fields.

10:12AM W25.00012: Hysteresis Experiments in Coupled Oscillators near Daido's Aging Transition OLAFUR HAUKSSON (Presenter), DAVID MERTENS, Physics, Eckerd College — One way to experimentally characterize collective oscillations is to measure the magnitude of the steady-state response. In order to examine more dynamic aspects of the behavior, we have measured the hysteresis of the collective response as we vary the collective bifurcation value. Specifically, in our collection of electronic oscillators, we produce a hysteresis by sequentially lowering then raising the bifurcation setting of each oscillator such that the collective bifurcation parameter goes below and above is critical value. The shape of the hysteresis loop exhibits a strong dependence on the rate at which we drive the system through the transition. We find that the area of the hysteresis loop exhibits a square-root dependence on the driving frequency. This is in contrast to ferromagnetic and ferroelectric systems, which exhibit power-law frequency dependence with much weaker exponents.

10:24AM W25.00013: Conformal field theory and the web of quantum chaos diagnostics* JONAH KUDLER-FLAM, LAIMEI NIE (Presenter), SHINSEI RYU, University of Chicago — We study three prominent diagnostics of chaos and scrambling in the context of two-dimensional conformal field theory: the spectral form factor, out-of-time-ordered correlators, and unitary operator entanglement. With the observation that all three quantities may be obtained by different analytic continuations of the torus partition function, we address the connections and distinctions between the information that each quantity provides us. In this process, we study the emergence of irrationality from “large-N” limits of rational conformal field theories (RCFTs) as well as the explicit breakdown of rationality for theories with central charges greater than the number of their conserved currents. Our analysis begins to elucidate the intermediate dynamical behavior of theories that bridge the gap between integrable RCFTs and maximally chaotic holographic CFTs.

*Simons Investigator Grant from the Simons Foundation; Kadanoff Fellowship from the University of Chicago.
10:36AM W25.00014: Cryptographic analysis of chaotic systems*  WILLIAM GILPIN (Presenter), Quantitative Biology Initiative, Harvard University — In computer science, hash functions are elementary operators that convert arbitrary-length inputs into finite-length outputs. We describe a direct analogy between these functions and the trajectories of particles advected by fluid flows, and we show that, when the governing flow is chaotic, hydrodynamic hash functions exhibit statistical properties typically associated with hash functions used for digital cryptography. These include non-invertibility, sensitivity to initial input, and avoidance of collisions—a phenomenon in which two similar inputs produce identical outputs. We show that this analogy originates from the tendency of certain chaotic flows to braid together particle trajectories across space in time in an irreducible manner, and we describe how techniques used to probe the properties of digital hash functions can be used to characterize the properties of flows when only limited observational data is available. Our findings have potential applications in microfluidic proof-of-work systems, as well as for characterizing large-scale transport in ocean flows and living systems.

*National Science Foundation, Simons Foundation

10:48AM W25.00015: Universality in Kinetic Models of Circadian Rhythms in Arabidopsis thaliana  YIAN XU (Presenter), Department of Physics and Astronomy, Trinity University, MASOUD ASADI-ZEYDABADI, RANDALL TAGG, Department of Physics, University of Colorado Denver, ORRIN SHINDELL, Department of Physics and Astronomy, Trinity University — Adapting to the 24-hour periodic environment on the Earth, plants have evolved sets of chemical reactions that regulate their circadian rhythms. Over the past fifteen years, researchers studying these circadian reactions in the common laboratory plant Arabidopsis thaliana have developed eleven, increasingly elaborate, chemical kinetic models based on genetic feedback loops. Each model consists of a system of coupled nonlinear ordinary differential equations. We find these models are all situated near a Hopf bifurcation in parameter space. This suggests that there may be some biological significance corresponding to this mathematical property.

To illustrate the special nature of these systems, we numerically compute the solutions to the kinetic models for Arabidopsis thaliana. Separately, we perform a weakly nonlinear analysis on each model near bifurcation to predict the amplitude and frequency of the oscillating concentration of chemical species from the Stuart-Landau amplitude equation. By scaling the numerical frequencies and amplitudes by our theoretical predictions, we show that the solutions to all these models collapse into a universal parameter-free form. We further comment on some implications of our results for improving future modeling efforts.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W26 DBIO DSOFT DCP DFD: Interrogating Biomolecules with Synthetic Nanostructures 403 - Binquan Luan, IBM TJ Watson Research Center - Tag(s): Focus
8:00AM W26.00001: Optimal Signal Transduction with Silicon Transistors Enable Therapeutic Enzyme Regulation  ARVIND BALIJEPALLI (Presenter), SON LE, MICHELLE A MORRIS, National Institute of Standards and Technology, HARISH C PANT, NINDS, National Institutes of Health, CURT RICHTER, National Institute of Standards and Technology — We used commercially sourced n-channel silicon field-effect transistors (nFETs) operating under PID control to demonstrate pH measurements with a resolution of $(7.2\pm0.3)\times10^{-3}$ at 10 Hz. The results represent a 3-fold improvement over open loop operation of the nFETs and over ion sensitive field-effective transistors (ISFETs). The improved performance was realized when the pH sensing membrane was separated from the nFETs and connected electrically to the transistor gate. The technique leverages key operating procedures from our previous work with dual-gate 2D field-effect transistors (dg2DFET) fabricated with 2D semi-conducting MoS$_2$ channels [1]. The devices were used to measure the function of the enzyme Cdk5, which facilitates signaling within cells by modifying proteins via the hydrolysis of adenosine triphosphate (ATP), and thereby changing the pH of the surrounding solution by a very small amount. By measuring this subtle change in pH, we quantified the activity of Cdk5, which has been previously implicated in Alzheimer's disease, under physiological conditions. Finally, we demonstrated the effectiveness of a custom polypeptide, p5, as a therapeutic agent in restoring the function of the pathological form of Cdk5.


8:12AM W26.00002: Protein-Corona-by-Design in 2D: A Molecular Dynamics study to Decode Bio-Nano Interactions for Quality-by-Design Nanomedicines* MOHAMED ALI AL-BADRI (Presenter), Physics, King's College London, KHULOUD AL-JAMAL, Institute of Pharmaceutical Science, King's College London, CHRISTIAN LORENZ, Physics, King's College London — Nanoparticles and nanomaterials are increasingly studied for use in biomedical applications including drug delivery, imaging and hyperthermic therapies. However, upon their introduction to a biological medium, the nanomaterial's size, shape, surface charge, surface functional groups, and hydrophilicity/hydrophobicity all play a role in the formation of a hard protein corona. The components of which affect the biological fate of nanomedicine carried by the material, these have consequences on the cellular uptake and toxicity of the corona-nanomaterial complex.

Understanding and controlling the interaction of graphene-based materials with proteins is key to the development of graphene-enabled biomedical technologies and to the successful delivery of chemotherapy drugs. Little is known about the fundamental atomistic behaviour of the interactions of proteins exposed to functional groups on 2D synthetic materials. Here we investigate the interaction of graphitic materials with an array of proteins with all-atom molecular dynamics simulations and perform analytical modelling ito identify safe and toxic protein corona profiles in 2D that could pave the way for future quality by design 2D/3D nanomedicines & better clinical translation.

*This work was supported by BBSRC (grant BB/M009513/1)
8:24AM W26.00003: Single-Molecule Characterization of Nanoparticle Bioconjugates using Microwell Array Analysis*  

MOHAMMAD ABDUL-MOQUEET (Presenter), LEEANA TOVIAS, KATHRYN MAYER, University of Texas at San Antonio — Nanoparticles functionalized with biomolecules have been studied extensively for their applications in nanomedicine. A need for characterizing these nanoparticle bioconjugates at the single-particle level using optical methods is needed. Microwell array analysis is a useful tool for single-molecule studies in which enzyme molecules are isolated in femtoliter wells; the enzymes convert non-fluorescent substrates into fluorescent products which can be measured using optical microscopy. Gold bipyramids were synthesized and functionalized with a self-assembled-monolayer (SAM). These particles were then bioconjugated using carbodiimide crosslinking with mouse anti-human epidermal growth factor receptor (EGFR)[KM1] antibodies, followed by human EGFR labeled with horseradish peroxidase (HRP). Microwell arrays were loaded with the nanoparticle bioconjugates such only that a small number of wells were occupied according to Poisson statistics. The fluorescence intensity of the microwells was then used to determine the number of antibodies that were conjugated to the gold bipyramids.

*National Institute of General Medical Sciences of the National Institutes of Health (SC2GM118273). Institute on Minority Health and Health Disparities (G12MD007591) from the National Institutes of Health.

8:36AM W26.00004: Single-Molecule Kinetics of Taq Polymerase up to 94 °C*  

MACKENZIE WALKER TURVEY (Presenter), WONBAE LEE, JEFFREY J TAULBEE, CALVIN J LAU, KRISTIN GABRIEL, REBECCA VARGAS, GREGORY WEISS, PHILIP G COLLINS, University of California, Irvine — Single-molecule enzymology is a useful tool for understanding protein kinetics, function, and inhibition, but common techniques work in a limited temperature range. Here, we extend single-molecule science up to 94 °C with MHz resolution using solid-state, carbon nanotube biosensors. Their operation, which is essentially independent of temperature, provides unprecedented access to commercially important enzymes such as Taq, the DNA polymerase I from Thermus aquaticus. Taq is the linchpin protein for the polymerase chain reaction (PCR) amplification of DNA [1]. Our electronic biosensor approach provides direct access to single-nucleotide incorporation activity [2] from room temperature up to 94 °C. For example, the incorporation rate of a single Taq molecule was monitored from 1 bp/s at 22 °C to greater than 100 bp/s at 72 °C, the typical PCR operating temperature. In addition, the biosensor transduces the distinct motions of Taq subdomains, such as brief, 20-µsec flutters as the fingers domain tests nucleotides for complementarity.


*NIH NHGRI (1R01HG009188)
8:48AM W26.00005: Monitoring Antipsychotic Drug Effects on Stimulated Dopamine Release Using Carbon Nanotube Transistors with Nafion-Radical Hybrid Films  INKYOUNG PARK (Presenter), VIET ANH PHAM BA, DONG-GUK CHO, Department of Physics and Astronomy, and Institute of Applied Physics, Seoul Natl Univ, SEUNGHUN HONG, Department of Physics and Astronomy, and Institute of Applied Physics, and Department of Biophysics and Chemical Biology, Seoul National University — We developed floating electrode-based carbon nanotube biosensors for the monitoring of antipsychotic drug effects on the dopamine release from nerve cells (PC12) under potassium stimulation. In this work, carbon nanotube field-effect transistors with floating electrodes were functionalized with nafion films containing 2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS●) radicals to build selective biosensors for the dopamine detection. The selective interaction between ABTS● radicals and dopamine allowed us to discriminate dopamine from the simultaneous presence of other neurotransmitters such as glutamate and acetylcholine with a detection limit down to 10 nM. Furthermore, we demonstrated the real-time monitoring of dopamine release from PC12 cells under the stimulation of potassium solutions at various concentrations. Significantly, we could also evaluate the effects of antipsychotic drug (pimozide) on the dopamine release from potassium-stimulated PC12 cells. Since our method enables the quantitative and real-time evaluation of drug effects on living cells, it should be a versatile tool for both biomedical researches and applications.

9:00AM W26.00006: Synthesis and toxicity of bio-templated fluorescent metal nanoclusters in human Neuro-2a cells  SHASHI P KARNA, KARIMA JENEH PERRY (Presenter), Weapons and Materials Research Directorate, APG, MD 21005, CCDC Army Research Laboratory, RAJ KUMAR, Radiation Biotechnology Lab, INMAS Delhi, India 110052, RAJ K. GUPTA, DoD Blast Injury Research Program Coordinating Office, Ft Detrick, MD 21702, USAMRDC — Bio-templated fluorescent metal nanoclusters (fMNC) have attracted a great deal of attention recently for their potential applications in sensing, cellular imaging, and as photonic probes. More recently, there have been reports of in situ synthesis of fluorescent MNC by tumorigenic (cancerous) as well as healthy animal cell cultures. Here we present the synthesis of Au and Fe nanoclusters synthesized in vitro using human neuro-2a cells. Additionally, protein (BSA and Chicken Egg-White) synthesized fMNCs were also incubated in neuro-2a cells. The cells exhibit significant uptake of protein-templated fMNCs. In both cases the cells exhibited significant viability at relatively elevated metal concentration, up to tens of micrograms.

*Author to whom correspondence should be addressed: Electronic mail: karima.j.perry.ctr@mail.mil
Protein Aggregation Characterization by Nanopore technology

JIALI LI (Presenter), Univ of Arkansas-Fayetteville — Protein aggregation is one of the leading causes of many neurodegenerative diseases such as Alzheimer’s and Parkinson’s. In this talk, we report our study on characterizing protein aggregation with a solid-state nanopore device, together with AFM and DLS techniques. Our model proteins used in these studies are β-lactoglobulin variant A (bLGa) and neuronal Tau and tubulin proteins. The main component of a nanopore device is a nanometer size pore fabricated in free-standing silicon nitride membrane supported by a silicon substrate which separates two PDMA chambers containing salt solution. A stable ionic current is established by applying a biased voltage on a pair of silver chloride (AgCl) electrodes across the nanopore membrane. When charged protein molecules are added to the grounded chamber, applying a correct bias potential to the other chamber drives a protein molecule into the nanopore which partially blocks ionic flow that can be measured as a transient current drop signal. A protein aggregate which has larger volume than a single protein molecule would block larger amount of current or generate a greater current drop amplitude, therefore a nanopore device can be used to characterize protein aggregation at single molecule level. The volume of translocating protein aggregates are estimated using a calibrated nanopore by a standard that has known geometry such as a dsDNA molecule. We show that solid state nanopore method is capable of measuring protein aggregation number and the aggregation number distribution in the conditions close to their native aqueous environment. The nanopore experiments were performed under applied voltages from 60-210 mV at different pH, temperature, and salt concentrations. We present data of bLga, and Tau and tubulin aggregations measured by nanopore method, and compare them with the results from AFM and DLS.

Active and stable palladium nano-thin-film structure development for rapid and direct biomolecules conjugation and sensing

CHIA-CHING CHANG (Presenter), CHIA-YU CHANG, YUN-TZU HUANG, WEI CHEN, Natl Chiao Tung Univ — Metal atoms on surface edges or with specific coordinates possess high surface potentials and serve as core atoms for organic molecule bonding. Unlike self-organized or surface modified nanoparticles, these active metal nanostructures may lose their activity by surface self-diffusion process. It is challenging to create a metal surface structure which possesses both active and stable properties. However, a surface template with native nano-roughness may solve this dilemma. In this study, a PET substrate has been selected for metal atoms absorption and a stable and active Pd nano-thin-film (NTF) surface has been developed. Further studies indicated that the surface contains an (1,1,1) like structure and Pd-NTF growth followed a Stranski-Krastanov-like growth model. This nanostructure thin-film (Pd NTF-PET) electrode has been developed for electrochemical impedance spectroscopy (EIS) usage. Both DNA and protein can be immobilized on the Pd NTF-PET electrodes directly, within 15 min and its biosensing sensitivity was as low as 0.1 ng per-test in 1 µl. In summary, we have developed an active and stable Pd NTF-PET electrode for biosensing applications.

This study was supported by MOST 107-2112-M-009-016-MY3 and Ministry of Education through the SPROUT Project-IDS²B of NCTU, Taiwan.
10:00AM W26.00009: Spontaneous ssDNA Stretching on Graphene and Hexagonal Boron Nitride In-plane Heterostructures  BINQUAN LUAN (Presenter), IBM TJ Watson Research Center — Because single-stranded DNA (ssDNA) molecules in solution typically form coiled structures, stretching ssDNA is extremely crucial when applying any nanotechnology for ssDNA analysis. Recent advances in material fabrication enable the deployment of nanochannels to manipulate, stretch, sort and map double-stranded DNA (dsDNA) molecules, however nanochannels fail to stretch ssDNA molecules due to the ultra-short persistence length and the potential nonspecific-interaction-induced clogging. Given the significance of ssDNA stretching in genome analysis, here a novel ssDNA stretching platform is proposed: two dimensional in-plane heterostructure comprising graphene and hexagonal boron nitride (h-BN), and I show that ssDNA can be stretched on a h-BN nanostripe sandwiched between two adjacent graphene domains ("nanochannel"). Additionally, with a biasing voltage the stretched ssDNA can be electrophoretically transported along the "nanochannel", allowing easy controls/manipulations. When being conveniently integrated with existing atomic resolution sensors, the heterostructure platform paves the way for sequencing DNA on a planar surface [see Nat. Commun. 10, 4610 (2019)].

10:12AM W26.00010: Block Optical DNA Sequencing with Plasmonic Substrates for Rapid Biomarker Diagnostics  LEE KORSHOJ, AMEYA GAJANAN PRABHUNE (Presenter), PRASHANT NAGPAL, University of Colorado, Boulder — Precision medicine requires high-throughput point-of-care diagnostics with multiomics capability for sensing biomolecules and their molecular variants. In a push for improved precision diagnostics, we describe an optical sequencing platform that uses surface-enhanced Raman spectroscopy (SERS) measurements from plasmonic nanostructured surfaces and nanoparticles for label-free determination of nucleobase content in DNA k-mer blocks. With SERS on cationic silver nanoparticles, we achieved >93% accuracy for predicting A-G-C-T content in 10-mer DNA blocks. The high-accuracy measurements were used with a content-scoring bioinformatics algorithm to correctly identify a β-lactamase antibiotic resistance gene and confirm the Pseudomonas aeruginosa pathogen from merely <12 measurements (<15% coverage of the gene) [1,2]. We further proved applicability on RNA and chemically modified nucleobases for extensions to transcriptomics and epigenomics. With the versatility of plasmonic substrates for simple data acquisition, resolution to single-molecules, and multiplexing, optical sequencing can provide rapid biomarker diagnostics in the clinical setting [3].

10:24AM W26.00011: Dynamics of DNA in periodic temperature gradient field created by plasmonic heating*  RYOKO SHIMADA (Presenter), Japan Women's University, HIROSHI WATANABE, Kyoto University — Different molecules in a solution can be separated from each other along a temperature gradient. This phenomenon, so-called Soret effect, offers an interesting method of molecular manipulation in various research fields. Plasmonic heating from periodic metal domains is one of the effective ways to create a periodic temperature gradient. In this work, we utilized the plasmonic heating from periodic silver (Ag) domains under emission of blue light (400 – 440 nm) to create the periodic temperature gradient (with a large amplitude of ~ 0.5 K/um), thereby attempting to observe the Soret effect on DNA molecules mixed in polyethylene glycol (PEG) solutions. The DNA molecules, labeled with fluorescent dyes, were concentrated in high temperature zones, confirming the positive Soret effect. In addition, for large DNA molecules (~ 166 Kbp), stretched conformations bridging two hot zones were occasionally observed and their diffusion appeared to deviate from the simple Fickian behavior, possibly because of the microscopic Soret effect within the molecule. Details of this observation will be discussed on site.

*This work was supported by JSPS KAKENHI grant number 18K03570.

10:36AM W26.00012: Tunneling Spectroscopy on Engineered Surfaces for RNA Nucleotide and Structural Label Identification  LEE KORSHOJ (Presenter), GARY R ABEL JR., ANUSHREE CHATTERJEE, PRASHANT NAGPAL, University of Colorado, Boulder — Although several advances have been made in RNA sequencing and structural characterization, the lack of a method for directly determining the sequence and structure of single RNA molecules has limited our ability to probe heterogeneity in gene expression at the level of single cells. We present a method for identification of RNA nucleotides and structural labels for mapping of single RNA molecules. With non-perturbative tunneling spectroscopy, we probed the molecular orbitals of distinct nucleobases within RNA macromolecules immobilized with restricted conformational freedom on a chemically modified surface. From the measurements, models for tunneling were combined to obtain twelve biophysical parameters unique to the ribonucleotides within the electronic junction [1]. The twelve parameters serve as a comprehensive molecular fingerprint, enabling ribonucleotide discrimination and identification of structure-dependent chemical labels with machine learning. We show high accuracy for both ribonucleotide discrimination (>99%) and chemical label identification (>98%) with a modest 35 repeat measurements [2]. This technique facilitates probing the transcriptome with a previously unattainable level of detail.

Conformational heterogeneity in human interphase chromosome organization reconciles the FISH and Hi-C paradox*

GUANG SHI (Presenter), DAVE THIRUMALAI, University of Texas at Austin — Hi-C experiments are used to infer the contact probabilities between loci separated by varying genome lengths. Contact probability should decrease as the spatial distance between two loci increases. However, studies comparing Hi-C and FISH data show that in some cases the distance between one pair of loci, with larger Hi-C readout, is paradoxically larger compared to another pair with a smaller value of the contact probability. Here, we show that the FISH-Hi-C paradox can be resolved using a theory based on a Generalized Rouse Model for Chromosomes (GRMC). The FISH-Hi-C paradox arises because the cell population is highly heterogeneous, which means that a given contact is present in only a fraction of cells. Insights from the GRMC is used to construct a theory, without any adjustable parameters, to extract the distribution of subpopulations from the FISH data, which quantitatively reproduces the Hi-C data. Our results show that heterogeneity is pervasive in genome organization at all length scales, reflecting large cell-to-cell variations.

*This work is supported by National Science Foundation (CHE 19-00093) and CollieWelch Regents Chair (F-0019)

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W27 DBIO: Microbiological Physics 404 - Seth Coleman, Rice Univ

Temperature-dependent Motility in *H. pylori*

JYOT ANTANI (Presenter), PUSHKAR LELE, Texas A&M Univ — *Helicobacter pylori* employ a run-reversal strategy in contrast to the run-tumble strategy employed by *E. coli* during navigation. As a result, their migration patterns are anticipated to be different from those in *E. coli*. We have quantitatively determined the effect of medium temperatures on the two modes of *H. pylori* motility – a pusher mode in which the flagella lag behind the body and a puller mode in which the flagella precede the body. Our data show that the cells swam faster in one mode relative to another as a function of temperature. The mean durations of the runs in either mode also depended on the temperature, as did the fraction of the time that the flagellar filaments rotated counterclockwise. We analyzed the mean squared displacements of the cell populations and determined that the bacterial spread was the highest at temperatures close to physiological temperatures. We will present a quantitative model that accounts for the anisotropic random walk to predict the temperature dependence of the bacterial diffusion. The fundamental insights from this work are likely to provide a handle for determining the motile responses of *H. pylori* to various types of environmental stressors.

*High Impact/High Risk Award RP170805, Cancer Prevention and Research Institute of Texas
8:12AM W27.00002: Developing Methods for Two-Way Communication to Explore the Dynamic Sense of Touch in Bacteria*  ZHOU XU (Presenter), WUQI NIU, SYLVIA RIVERA, SLOAN SIEGRIST, MARK THOMAS TUOMINEN, MARIA SANTORE, Univ of Mass - Amherst — Living organisms usually utilize chemical or biomolecular signals that travel relatively slowly. However, bacterial cells can respond very quickly, yielding interesting opportunities for interfacing with bacteria. In this work, we study the bacterial sense of touch to establish the new research area of sensory-based bacterial communication. The focus is on fast two-way transmission of mechanical and electrical signals between bacteria and man-made devices. Bacterial touch acts through mechanical and electrical stimuli at timescales much less than chemical- and nutrient-based bacterial interactions. Employing high resolution microscopy with a flow cell system, we investigate the adsorption rate and growth of E. coli on different surfaces such as poly-l-lysine coated surface and hydrophobic. We use indium tin oxide coated glass as electrodes to apply electric stimulus on bacterial and measure the response. Using biomolecular engineering, we investigate the response to stimuli based on their gene expression.

*This research is supported by NSF grant # CBET 1848065

8:24AM W27.00003: Comparative study of bacterial growth on different surfaces and the effect of weak magnetic field on the growth rates  SAMINA MASOOD (Presenter), University of Houston, Clear Lake — We investigate the growth of bacteria on different surfaces. The presence of nanoripple structure on glass is known to affect the growth rate. The growth of bacteria in the weak field is also affected by the type of the applied field, if all other conditions remains unchanged. Affect of weak magnetic field sustains for more than one generation. Moreover, the growth rate of bacteria and the structure of bacteria is also affected if it is grown over different materials including gold and silver surfaces.

8:36AM W27.00004: Rigid Body Dynamics of Motile Bacteria Near Surfaces*  ORRIN SHINDELL (Presenter), KEATON HOLT, Department of Physics & Astronomy, Trinity University, QUAN HOANG, NAM DUNG HOANG, Department of Mathematics, Vietnam National University, FRANK HEALY, Department of Biology, Trinity University, HOA NGUYEN, Department of Mathematics, Trinity University — Motile bacteria in their natural environment commonly interact with surfaces. Using total internal reflection fluorescence microscopy, we record the trajectories of Escherichia coli cells swimming near surfaces. By fitting ellipsoids to the fluorescent intensity profiles of the bacteria via a novel method, we extract their translational and rotational dynamics. We present results from our analysis for experiments with both wild-type and smooth-swimming E. coli strains.

*National Science Foundation grant DMS-1720323 and Trinity University.
8:48AM W27.00005: Fast Modulation of Phenotypic Diversity in Bacterial Chemotaxis*
KEITA KAMINO (Presenter), AMOLF Institute, Yale University, JOHANNES M KEEGSTRA, AMOLF Institute, JUNJIAJIA LONG, THIERRY EMONET, Yale University, THOMAS S SHIMIZU, AMOLF Institute — A central question in cell biology is how cell populations deal with ever-changing environments. It has been shown that gene regulatory networks can modulate in an environment-dependent manner not only the average phenotype, but also its diversity within isogenic populations. Here, we demonstrate that cells can also tune the level of phenotypic diversity much more rapidly than is possible by gene expression, using covalent modification of signaling proteins. In the E.coli chemotaxis pathway, we find that the diversity of a key sensory parameter, the response sensitivity, is modulated depending on the presence or absence of ambient chemoattractant molecules. We show how this diversity tuning originates from an environment-dependent mapping between the sensitivity phenotype and the standing cell-to-cell variation in the number of allosterically-coupled receptors. This diversity tuning enhances the population's readiness for uncertain future signals in the absence of any signal, but allows the population to rapidly switch to tracking the signal once it is perceived.

*KK and TE* were funded by NIH award R01GM106189. KK, JL, TE*, and TSS* were funded by Paul G. Allen Family Foundation award 11562. KK, JMK, and TSS* were funded by NWO VIDI award 680-47-515. *Corresponding.

9:00AM W27.00006: Flow-induced symmetry breaking in growing bacterial biofilms
PHILIP PEARCE, Department of Systems Biology, Harvard Medical School, BOYA SONG (Presenter), DOMINIC SKINNER, RACHEL V MOK, Department of Mathematics, Massachusetts Institute of Technology, RAIMO HARTMANN, PRAVEEN SINGH, HANNAH JECKEL, Max Planck Institute for Terrestrial Microbiology, JEFFREY S OISHI, Department of Physics, Bates College, KNUT DRESCHER, Max Planck Institute for Terrestrial Microbiology, JÖRN DUNKEL, Department of Mathematics, Massachusetts Institute of Technology — Bacterial biofilms represent a major form of microbial life on Earth and serve as a model active nematic system, in which activity results from growth of the rod-shaped bacterial cells. In their natural environments, ranging from human organs to industrial pipelines, biofilms have evolved to grow robustly under significant fluid shear. Despite intense practical and theoretical interest, it is unclear how strong fluid flow alters the local and global architectures of biofilms. Here, we combine highly time-resolved single-cell live imaging with 3D multi-scale modeling to investigate the mechanisms by which flow affects the dynamics of all individual cells in growing biofilms. Our experiments and cell-based simulations reveal three quantitatively different growth phases in strong external flow, and the transitions between them. In the initial stages of biofilm development, flow induces a downstream gradient in cell orientation, causing asymmetrical droplet-like biofilm shapes. In the later developmental stages, when the majority of cells are sheltered from the flow by the surrounding extracellular matrix, buckling-induced cell verticalization in the biofilm core restores radially symmetric biofilm growth, in agreement with predictions of a 3D continuum model.
9:12AM W27.00007: Resource allocation model for bacterial shape control under growth perturbations*  DIANA SERBANESCU (Presenter), NIKOLA OJKIC, SHILADITYA BANERJEE, Univ Coll London — Single bacterial cells adapt their growth rates and morphologies to changes in environmental conditions in order to optimize their fitness for proliferation. Control of cell size demands making tradeoffs between cellular resources allocated towards growth and division. Understanding the nature of these tradeoffs remains an outstanding challenge. Here we propose a coarse-grained theory for how bacteria allocate their molecular resources to regulate their cell shapes and growth rates in varying nutrient environments and antibiotic induced perturbations. We propose that a balanced tradeoff between ribosomal resources allocated towards growth and division determines the control of bacterial cell volume and surface area. The results from our model are in excellent quantitative agreement with available experimental data on single-cell growth and shape under nutrient and translational perturbations. By calibrating our model with experimental data, we further predict that a combination of antibiotics that induce cell filamentation and inhibit translation may be more efficient in bacterial killing.

*University College London
Institute for the Physics of Living Systems
The Royal Society
Engineering and Physical Sciences Research Council

9:24AM W27.00008: Multi-scale dynamical description Gram-negative bacterial responses to antibiotics towards drug resistance PEDRO MANRIQUE (Presenter), Theoretical Biology and Biophysics, Los Alamos National Laboratory, KUMKUM GANGULY, Bioscience Division, Los Alamos National Laboratory, S GNANAKARAN, Theoretical Biology and Biophysics, Los Alamos National Laboratory — Contemporary medicine struggles with bacterial infections on a daily basis. The ongoing challenge is to describe how these organisms adapt and protect at different levels when attacked by drugs. In the presence of these agents, colonies of bacteria carry out myriad processes at the molecular, genetic, and cellular scales that grant resistant against intruders threatening its survival. Even though mechanisms of specific processes in different scales have been characterized, a framework that integrates the processes at different scales remains absent. Here we propose a dynamical model that integrates these scales in the context of bacterial survival and efficacy of drugs. Using experimental inputs, our approach produces testable outputs that are in agreement with empirical data. In general, this framework provides a mathematical tool to test stress response strategies in organisms that can potentially guide experiments in natural and synthetic cellular systems.
9:36AM W27.00009: A Facile Accelerated Specific Therapeutic (FAST) Platform that Reverses Carbapenem Resistance in Multi-Drug Resistant *E. coli*  THOMAS AUNINS (Presenter), KEESHA ERICKSON, ANUSHREE CHATTERJEE, University of Colorado, Boulder — Carabapenems are a powerful class of antibiotics, often used as a last-resort treatment to eradicate multidrug-resistant (MDR) infections. However, as carbapenem-resistant pathogens have become more common, the need for new strategies to combat resistance has emerged as a critical public health priority. Here, we show that the Facile Accelerated Specific Therapeutic (FAST) platform can use transcriptomic data for the rapid (<1 week) design, synthesis, and testing of antisense inhibitors that are able to re-sensitize a strain of MDR *E. coli* to carbapenem treatment. We used total and small RNA-seq data to determine genes that may be important to the meropenem (to which the strain is sensitive) and ertapenem (resistant) responses. These observations, combined with genome sequencing of the MDR *E. coli*, allowed us to use FAST to create peptide nucleic acids (PNA) to knock down the translation of specific genes. Using PNA in combination with both antibiotics, we demonstrated the ability to inhibit bacterial growth at antibiotic concentrations to which MDR *E. coli* strain was initially resistant. This work confirmed FAST’s ability to use transcriptomics to design novel antibiotic strategies, and identified gene expression-based resistance mechanisms that warrant further exploration.

9:48AM W27.00010: A Comparative Analysis of Various Cas Proteins in CRISPRi Gene Circuits  LIOR KREINDLER (Presenter), GUILLAUME LAMBERT, Applied and Engineering Physics, Cornell University — Cas proteins with deactivated cutting domains can be used as programmable components in genetic circuits in E. Coli. While dSpCas9 and dFnCas12a have proven functional in gene circuits, there exist Cas proteins from other species of bacteria that have yet to be explored and fully understood. A particularly new and mysterious Cas protein is CasX, which is completely distinct from both Cas9 and Cas12a. CasX is much smaller than both Cas9 and Cas12a; it could potentially be preferable for use in gene circuits. Cas9 and Cas12a proteins from varying species of bacteria recognize unique PAM sequences, and thus function slightly differently. To explore these differences, six versions of a CRISPRi inverter circuit that previously worked with FnCas12a in E. Coli were developed, each using the deactivated version of a different Cas protein (SaCas9, St1Cas9, TdCas9, NmCas9, AsCas12a, and CasX) programmed to target a cassette of tetA (tetracycline resistance) and sacB (sucrose sensitivity). The circuits are transformed into E. Coli, which are then selected for growth in tetracycline and sucrose. Additionally, another version of each circuit targeting GFP is tested, to confirm the results of the multiplexed tetA-sacB selection serially and to compare the effects of targeting different genes.
10:00AM W27.00011: Tuning programmable CRISPR-based toggle switches with buffer sites in Escherichia coli  
YASU XU (Presenter), GUILLAUME LAMBERT, Cornell University — Recent developments and advances in CRISPR-Cas systems have ushered a new generation of powerful genetic engineering tools in synthetic biology. In particular, a catalytically ‘dead’ version of Cas proteins that lack nuclease activity can essentially function as a logic NOT gate by selectively binding to a promoter and preventing transcription initiation. In this work, we first create programmable genetic toggle switches (TSs) using pairs of mutually repressible orthogonal CRISPR-based NOT gates and measure the strength of these TSs using massive parallel CRISPRi assay called “Xseq”. Specifically, hundred pairs of CRISPR nodes with different barcoded targets are simultaneously cloned into a plasmid that contains a TetA-SacB cassette as a reporter, then transformed into E. coli. Each cell has a single TS construct. By selecting cell survival under sucrose and tetracycline conditions, we are able to sort out matched CRISPR TSs among numerous randomized promoter-target pairs and quantify relative strength of each NOT gate in all possible combination at the same time. Later, adding a second plasmid that shares the same target as the TS and competes with TS for dCas pool, we can tune the efficiency of each NOT gate via manipulating the number of buffers, and thus the performance of TS.

10:12AM W27.00012: Development of non-linear gradient microfluidic devices*  
DRAGOS AMARIE (Presenter), ILEENE HARDEN, ARTURO DIAZ, ELIJAH WATERS, Physics and Astronomy, Georgia Southern University, DWAYNE G. STUPACK, Obstetrics Gynecology and Reproductive Sciences, University of California, San Diego — Mechanical stress introduced by the flow in microfluidic chambers induces shear stress thus impacting the live cells migration patterns. Our last-year work showed that constructing a flowless linear gradient requires two mirrored gradient chambers. In this work we present microfluidic devices that generates non-linear chemical gradients. By splitting and recombining the input flows through a combination of bifurcated (mixers and splitters) and trifurcated (splitters) channels one can generate a chemical gradient across a microfluidics chamber. As the input chemicals flowing downstream mix, a linear gradient can only achieve relative lateral gradients either from 0% to 50% or from 50% to 100%. However, we demonstrate that these mirrored gradient can be non-linear in order to accommodate a steeper flowless gradient. By introducing bias when recombining the flows in the mixers one can generate non-linear gradients. Different bias between mixers input channels can accommodate steeper lateral gradients from 100% to: (a) 37% for a 2:1 bias, (b) 30% for a 3:1 bias, (c) 27% for a 4:1 bias and (d) 24% for a 5:1 bias. This type of separated, flowless gradient offers new opportunities to study the migration of live cells free of physical flow.

*Office of Research, Georgia Southern University
10:24AM W27.00013: Acoustic Micromotors for Cellular Manipulation*  
JEFFREY MCNEILL, University of Pennsylvania, AUSTIN MAADDI, SAMBEETA DAS (Presenter), Univ of Delaware — Cell manipulation is an important aspect of many studies such as single cell analysis, tissue engineering, and mechanobiology. Despite the recent surge of activity in this area, there still does not exist a system that contains most of the practical components for carrying out high-throughput cellular manipulation. The small size of cells and lack of bio-compatibility are critical challenges in cell manipulation, especially for mammalian cells. Here, we demonstrate the use of acoustically powered micromotors steered by an applied magnetic field for mammalian cell rotation and manipulation. The acoustic propulsion mechanism provides a variety of highly desirable features, such as high speed, precision, short-range attractive forces utilized as an end effector, and orthogonality in any aqueous medium. The potential power of this approach is also highlighted by cargo pickup and delivery to individual cells.

*We gratefully acknowledge the support of the National Science Foundation DMR-1420620, the Singh Center for Nanotechnology under grant NNCI-1542153 and the Department of Mechanical Engineering at the University of Delaware.

10:36AM W27.00014: The biophysics of cellular counting — uncovering how viral copy number drives cell-fate decision  
SETH COLEMAN (Presenter), Bioengineering, Rice University, TIANYOU YAO, THU VU PHUC NGUYEN, Verna and Marrs McLean Department of Biochemistry and Molecular Biology, Baylor College of Medicine, OLEG A IGOSHIN, Bioengineering, Rice University, IDO GOLDING, Physics, University of Illinois Urbana-Champaign — After infecting an E. coli cell, the virus lambda either kills the host cell (lysis) or enters a stable, dormant state (lysogeny). Such cell-fate decisions are ubiquitous in biology, but few are well understood mechanistically. The lambda decision is an attractive model system, as it is comparatively simple, well-studied, and shares multiple features with more complex systems. A key factor affecting the decision is the multiplicity of infection (MOI), i.e. the number of co-infecting viruses. Increasing MOI raises the likelihood of a lysogenic outcome, but the mechanisms by which viral copy number drives the decision are unclear. To determine these mechanisms, we combine single-cell resolution experiments with coarse-grained modeling of infection over a range of MOI. We find that the expression of essential genes in the decision network exhibits power-law scaling with MOI. Notably, the expression of cro, a key lytic gene, scales sublinearly, whereas the expression of cI, the gene responsible for establishing the lysogenic state, scales superlinearly. This nonlinear, gene-specific response to MOI is a consequence of negative and positive feedback loops in the regulatory network. This feedback causes increasing MOI to drive expression of cI, pushing the decision towards lysogeny.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W28 DCMP: New Physics and Quantum Technology at Ultra-Low Temperatures 405-407 - William Halperin, Northwestern University - Tag(s): Invited
8:00AM W28.00001: Precision experiments at ultralow temperatures enabled by quantum technology and superconducting electronics [Invited] CHRISTIAN ENSS (Presenter), Kirchhoff Institute for Physics, Heidelberg University — Ultralow temperatures are favorable conditions for the realization of quantum technology in general and for quantum sensors in particular. One type of such quantum sensors are cryogenic detectors for particles and radiation, which have begun to revolutionize experiments in many areas of physics. Here we will discuss a specific kind of cryogenic detector, namely a metallic magnetic calorimeter (MMC) consisting of an absorber suitable for the particles to be detected, in close thermal contact with a paramagnetic temperature sensor. Together the two are connected by a weak thermal link to a thermal bath. Their universal applicability for the detection of different particles and radiation as well as their high resolution, wide bandwidth, fast and linear response make them a popular choice in many different applications today. Here we will discuss their principle of operation and their impact on precision gamma spectroscopy and neutrino mass determination.

8:36AM W28.00002: Topological Superfluid $^3$He under mesoscopic confinement* [Invited] JOHN SAUNDERS (Presenter), Department of Physics, Royal Holloway University of London — Confinement of superfluid $^3$He in a nanofabricated cavity of height comparable to the superfluid coherence length is a powerful tool to modify the p-wave superfluid order parameter [1]. This enables the creation of superfluid $^3$He hybrid nanostructures, with interfaces between two $^3$He material phases stabilized by a step in cavity height [2]. Measurements on the chiral A-phase, stabilized at low pressure in a 200 nm tall cavity, show that the order parameter suppression and the spectrum of surface bound states are fragile with respect to details of quasiparticle scattering [3]. We show that magnetic surface scattering leads to an unexpectedly large suppression of the transition temperature, corresponding to an increased density of low energy bound states. On the other hand specular surface scattering eliminates gap suppression and surface states. In taller cavities an AB transition is observed; the 0.7 and 1.1 micron cavities show a universal phase boundary, with minute super-cooling, which is potential evidence for an intrinsic nucleation mechanism under confinement [4]. Near to the AB transition the confined B-phase is predicted to be unstable to spontaneous formation of domains, with a predicted stripe phase [5]. However our NMR measurements find a two-dimensional spatially modulated superfluid (pair density wave) [6]. The future quest is to identify and manipulate Majorana zero modes in the only firmly establish topological “superconductor”.


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9:12AM W28.00003: Superconducting Quantum Circuits for Quantum Computing and Quantum Simulation [Invited] JENS KOCH (Presenter), Northwestern University — Quantum research has undergone a remarkable transition from probing quantum phenomena intrinsic to nature, to developing engineered and fully controllable quantum systems with new functionality. Experimental capabilities to reach milli-Kelvin temperatures have played an important role in enabling new quantum technology. An exciting example of such low-temperature quantum devices are superconducting circuits which have facilitated impressive progress towards quantum computation and quantum simulation. I will review the journey from the early superconducting qubits to presently employed circuits with coherence times in the micro- to millisecond range, and discuss the ongoing development of even more robust superconducting qubits with intrinsic error protection. These next-generation circuits, including the heavy-fluxonium and 0-π qubits, have the potential to outperform and ultimately replace the widely used transmon qubit.

9:48AM W28.00004: Innovation at the cold frontier for current and future quantum devices and sensors* [Invited] RICHARD HALEY (Presenter), SAMULI AUTTI, DAVID IAN BRADLEY, ANTHONY GUÉNAULT, ALEXANDER JONES, SERGEY KAFANOV, YURI PASHKIN, GEORGE PICKETT, MALCOLM POOLE, JONATHAN PRANCE, MICHAEL THOMPSON, VIKTOR TSEPELIN, DMITRY ZMEEV, Physics, Lancaster University — The Low Temperature Physics Laboratory at Lancaster University, a founder member of the European Microkelvin Platform, designs and constructs record-breaking millikelvin dilution refrigerators and sub-millikelvin adiabatic demagnetisation stages, building on the expertise, infrastructure and technical capabilities that have been developed and refined over many years. Research runs from blue-skies work in superfluid helium-3 and helium-4 at temperatures close to absolute zero, through to innovation and technology transfer of refrigeration, instrumentation and ultra-sensitive measurement techniques to academic and commercial collaborators. This talk will describe some of our recent research highlights including: the discovery of super-critical superfluid condensate flow; exploiting high quality factor nanomechanical resonators as force sensors over many orders of magnitude; and developing new techniques for delivering microkelvin electron temperatures in nano-fabricated on-chip devices.

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U.K. EPSRC (EP/M508354/1, M028305/1, EP/L000016/1, EP/I028285/1, EP/N019199/1, EP/P024203/1).
Research in quantum fluids, where are we?*  

YOONSEOK LEE  
(Presenter)  
University of Florida — In this paper, we present a review of the recent progresses in the field of quantum fluids with a forward-looking perspective. The main research in this field is on superfluid phases of two helium isotopes and can be classified in two realms. One is to use helium as a platform for other related physics. For example, efforts in realizing ultra-high sensitive detection and qubits using superfluid helium-4 have attracted interests of researchers in related fields with potential impact for technology. In parallel a group of researchers continue their effort in unveiling the nature of these unique quantum systems with novel experimental techniques and fresh perspectives. Active investigation of the topological nature and the capability of engineering novel superfluid phases in helium-3 widened the scope of the research in this field. The recent progress in quantitative investigation of quantum turbulence are expected to produce exciting results in the near future. This discussion is based on the works presented at the conferences in the field and the record of publications in recent years [1].


*This work is supported by NSF DMR-1708818.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W29 DSOFT DPOLY DBIO DFD: Electrostatic Manipulation of Fluids and Soft Matter II: Self-Assembly  
Jonathan Singer, Rutgers University, New Brunswick - Tag(s): Focus

8:00AM W29.00001: Precision measurement of tribocharging in acoustically levitated sub-millimeter grains  
ADAM KLINE (Presenter), MELODY LIM, HEINRICH M. JAEGGER, University of Chicago — Contact electrification of dielectric grains forms the basis for a myriad of physical phenomena. However, even the basic aspects of collisional charging between grains are still unclear. In this talk, we present a new experimental method [1], extending a prior approach [2] based on acoustic levitation, which allows us to controllably and repeatedly collide two sub-millimeter grains head-on and measure the evolution of their electric charges. This is the first collisional tribocharging experiment to provide complete electric isolation of the grain-grain system from its surroundings. We use this method to measure collisional charging rates between pairs of grains for three different material combinations: polyethylene-polyethylene, polystyrene-polystyrene, and polystyrene-sulfonated polystyrene. The ability to directly and noninvasively collide particles of different constituent materials, chemical functionality, size, and shape opens the door to detailed studies of collisional charging in granular materials.

8:12AM W29.00002: Tuning friction and slip at solid-nanoparticle suspension interfaces by electric fields.* CAITLIN M SEED (Presenter), BIPLAV ACHARYA, DONALD W BRENNER, ALEX I SMIRNOV, JACQUELINE KRIM, North Carolina State University — Pathways to achieve climate stabilization consistently require a diverse mix of technologies, with energy efficiency being the largest contributor, ranging from 35-40% in virtually all proposed scenarios. Reductions in frictional energy losses and improved lubrication methodologies are key to such energy savings. Nanoparticles in aqueous suspensions hold particular promise for such purposes. We report an experimental Quartz Crystal Microbalance (QCM) study of tuning interfacial friction and slip lengths for aqueous suspensions of ceramic (Al₂O₃, TiO₂ and SiO₂) nanoparticles on planar platinum surfaces by external electric fields. Attraction and retraction of particles perpendicular to the surface by means of an externally applied fields resulted in increased and decreased interfacial friction levels and slip lengths. The variation was observed to be non-monotonic, with a profile attributed to the physical properties of interstitial water layers present between the nanoparticles and the platinum substrate. The results are compared and contrasted with macroscale friction measurements performed on the same materials.

*NSF#DMR1535082

8:24AM W29.00003: Particle assembly using confined electro-hydrodynamics: Driven versus active assembly* [Invited] JON OTTO FOSSUM (Presenter), PAUL DOMMERSNES, Norwegian Univ Tech (NTNU) — We give examples of driven colloidal shell assembly on drop interfaces by application of DC-electrohydrodynamics and dielectrophoresis, using standard leaky dielectric carrier fluids for non-polarisable and/or polarizable colloids. We summarize how this can be used to fabricate static or dynamic colloidal shells with patchy structure and functionality. Secondly, we give examples of active granular bead assembly in suspension by exploiting the electrohydrodynamic Quincke-rotation effect (i.e. electric field induced rotational motion of non-electrically-conducting particles suspended in a leaky-dielectric fluid). We study a system in quasi-2D microfluidic confinement with an applied DC-electric field perpendicular to the 2D-plane, where a monolayer of Quincke rotors are forced to “live” near a flat solid surface, and thus become a monolayer of self-propelled Quincke rollers. A Quincke roller’s direction of motion in the 2D plane is individual and normal to the applied electric field, with any direction possible, i.e. the electric field supplies energy (“food”), but not direction. Unlike animals, the “metabolism” of Quincke-rollers is instantaneous, and their “food” is translated into motion immediately. We have demonstrated several types of assemblies that emerge from populations of such confined granular Quincke-rollers confined, such as crystallites, dynamic clusters, clusters of clusters, vortices, swirls, and polar liquids with uniform direction of motion.

*Research Council of Norway - RCN - Petromask2 program, project number 280643
Research Council of Norway - RCN - Nano2021 program, project number 250619
M-Era.Net/RCN-Nano2021 program, project number 272919
9:00AM W29.00004: Electrostatic patterns from peeling tape*  MARY REITER (Presenter), MATTHEW VANDUSEN-GROSS, TROY SHINBROT, Rutgers University, New Brunswick — It has been known since the 17th century that as mercury rolls from glass, “barometric light” is emitted[1]. Similarly, as tape is pulled from surfaces, light is emitted that can even extend to produce enough x-rays to image bones within a finger[2]. It has been proposed that the light is generated by discharges that follow triboelectric charging by the tape. In this talk, we discuss new and surprising aspects of triboelectric charging associated with tape peeling including entirely different charge patterns on formerly adjoining surfaces. We describe these unique patterns as well as implications for the charging and adhesion of surfaces and particles in nature and industry.


*This research was funded by the National Science Foundation via the award NSF/CBET-1804286.

9:12AM W29.00005: Sublattice Melting in Binary Superionic Colloidal Crystals*  YANGE LIN (Presenter), MONICA OLVERA DE LA CRUZ, Northwestern University — In superionic compounds one component pre-melts providing high ionic conductivity to solid state electrolytes. Here, we find sublattice melting in colloidal crystals of oppositely charged particles that are highly asymmetric in size and charge in salt solutions. The small particles in ionic compounds melt when the temperature increases forming a superionic phase. These delocalized small particles in a crystal of large oppositely charged particles, in contrast to superionic phases in atomic systems, form crystals with non-electroneutral stoichiometric ratios. This generates structures with multiple domains of ionic crystals in percolated superionic phases with adjustable stoichiometries.

*This work has been funded by NSF DMR Award No. 1611076.

9:24AM W29.00006: Band-collision gel electrophoresis (BCGE) for visualizing molecular and colloidal interactions  DIMITRI BIKOS (Presenter), Center for Biofilm Engineering, Montana State University, THOMAS MASON, Physics & Astronomy and Chemistry & Biochemistry, UCLA — Electrophoretic mobility shift assays (EMSAs) are widely used to study binding interactions between different molecular species loaded into a single well within an electrophoresis gel. However, shift assays can explore only a subset of reaction possibilities that would otherwise be accessible if separate bands of reagent species were instead collisionally reacted. We fabricate a gel with two or more wells within a single lane and load these wells with different reagent species. By applying an electric field, we produce collisional reactions between propagating pulse-like bands of these species and record the images optically. We observe cases where bands pass through one another undisturbed, while in other cases, we observe complexing and precipitation, indicating strong attractive interactions. This band-collision gel electrophoresis (BCGE) approach is generalizable to a variety of reaction types, such as acid-base, ligand exchange, and redox, as well as to colloidal species in passivated large-pore gels.
9:36AM W29.00007: Controlling surfactant self-assembly in dodecane via applied potential*

MAISA VUORTE (Presenter), AAPO LOKKA, MARIA SAMMALKORPI, Aalto University, Finland — The response of colloidal assemblies in apolar solvents to applied electrostatic potential plays a key role in both electrostatic stabilization and manipulation of the resulting nanoemulsion, drug delivery, and synthesis platforms. Here, we present a molecular modelling study of the aggregation of dioctyl sodium sulfosuccinate (AOT) surfactant in apolar dodecane solvent under applied potential. We probe the sensitivity of the self-assembling, reverse micellar surfactant structures and their dynamics to the magnitude of the applied potential and presence of moisture in the system. While the anionic AOT surfactant readily forms reverse micellar aggregates even in the absence of trace water, presence of moisture greatly increases the size of the formed aggregates and their dynamics. The applied potential controls the AOT sodium counterion mobility but the charge transfer via the counterions is also influenced strongly by the degree of hydration of the AOT head groups. We discuss the significance of the findings against literature and experimental data.

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9:48AM W29.00008: Dumbbell model for the simulation of polyelectrolytes in combination of flow and electric fields*

ANGELO SETARO (Presenter), PATRICK UNDERHILL, Rensselaer Polytechnic Institute — The combination of Poiseuille flow and electric fields has been used to drive the transverse migration of charged polyelectrolytes in channels, resulting in non-uniform concentration profiles. Manipulation of these profiles can be used to drive separations of charged polyelectrolytes such as double stranded DNA. Interestingly, the amount of migration is not monotonic in electric field strength. Rather the migration peaks at intermediate electric fields before decreasing. To date, the mechanism for this non-monotonic trend has been poorly understood as prior models have been unable to reproduce this behavior. To gain insight to the underlying phenomena, we used a combination of theoretical calculations and Brownian Dynamics simulations in order to understand the mechanism of migration and why it results in a non-monotonic trend. It was found that at high electric field strengths, the migratory flux of polymers was able to impact the conformational distribution, altering the electrophoretic mobility and, in turn, limiting the migration. Further, when comparing to experimental migration data, our model captures the position of the maximal migration with near quantitative accuracy.

*We acknowledge support from NSF Grant CBET-1826788.
10:00AM W29.00009: Electrostatically Stabilized Microphase Separation in Polyelectrolyte Blends: Analogy to Nuclear "Pasta" Phases  ARTEM RUMYANTSEV (Presenter), JUAN DE PABLO, University of Chicago — We develop the weak segregation theory of microphase separation in stoichiometric blends of oppositely and weakly charged polyelectrolytes, which would be immiscible in the absence of charged units. Short-range repulsions between polycation and polyanion monomers induce the formation of oppositely charged domains, whose size is controlled by their excess Coulomb energy. The diagram of blend morphologies is constructed in the framework of a Leibler's mean-field approach and, to account for fluctuations, within a Brazovskii-Fredrickson-Helfand approximation. Phase behavior of the polyelectrolyte blends is fully analogous to that of neutral diblock copolymers. In asymmetric blends, increasing incompatibility between polyelectrolytes triggers the usual cascade of first order phase transitions, disordered blend $\rightarrow$ bcc $\rightarrow$ hex $\rightarrow$ lam. We also discuss that microphase separation in polyelectrolyte blends (and hence neutral diblock copolymers) and the formation of nuclear “pasta” phases arising within neutron stars are governed by similar physical principles, despite the six orders of magnitude difference in the periods of these structures (nanometers vs femtometers, respectively).

10:12AM W29.00010: Determination of diffusion constant of antimicrobial peptide nisin interacting with Langmuir monolayers of DPPC and DPPG molecules*  IMRAN PASHA, BHARAT KUMAR (Presenter), Central University of Karnataka — We present a method of determining the diffusion constant of peptides interacting with lipid films. The method involves studying the interactions of diffusing peptides with the lipid Langmuir monolayer at the air-water interface. Due to the interaction between peptides and lipid molecules in the monolayer at the air-water interface, the surface pressure of the monolayer changes as a function of time which can be measured from the surface manometry technique. A model based on the diffusion of particles under the influence of a constant force is developed to obtain an analytical expression for change in the surface pressure of Langmuir monolayer as a function of time. The expression was found to fit well with the experimental data. The average hydrodynamic radius and the translational diffusion constant of the nisin molecules are calculated from the fit parameters for the different subphase pH solutions. The diffusion constant was found to vary with the pH of the media.

*Dr. Bharat Kumar acknowledges the support from DST-INSPIRE faculty award and SERB, Govt. of India. Mr. Imranpasha acknowledges the fellowship from Directorate of Minorities, Govt. of Karnataka, India.
Capture and Translocation of a Rod-like dsDNA by a Nanopore: A Lattice Boltzmann Simulation Study

LE QIAO (Presenter), Physics, University of Ottawa, CHRISTIAN L. HOLM, KAI SZUTTOR, Physics, University of Stuttgart, GARY W. SLATER, Physics, University of Ottawa — Short dsDNA, viruses like the tobacco mosaic virus and filamentous bacteriophages can be considered as a rigid rods. We previously argued that the field-driven orientation of a rod-like object will impact its capture by a nanopore because both its translational diffusion coefficient $D$ and electrophoretic mobility $\mu$ vary with orientation. We also introduced a critical orientational capture radius to describe this effect. In this talk, we investigate this problem further using a coarse-grained (CG) model of a charged double-stranded DNA where the hydrodynamic interactions are added by coupling the CG DNA with a lattice-Boltzmann fluid via a raspberry approach. The electrostatic interactions with the salt ions are modeled with the P3M algorithm. We also discuss the capture of modified DNAs, including partially charged and branched DNAs. In all cases, we examine how molecular orientation affect capture and entry into the pore.

The authors acknowledge the support of the University of Ottawa, NSERC, Mitacs Globalink research award and CSC.

Nontrivial effects of dielectric mismatch on the conformational behavior of confined polyelectrolytes

TRUNG NGUYEN (Presenter), MONICA OLVERA DE LA CRUZ, Northwestern University — We investigate the conformational behavior of a highly charged polyelectrolyte confined in a spherical cavity where the media inside and outside the cavity have different dielectric constants. Depending on the charge density of the cavity surface and dielectric mismatch, the polyelectrolyte either collapses into amorphous conformations, or folds into a four-fold symmetry conformation. On the contrary to the common wisdom that polarization effects would be negligible for charged surfaces, we find that such effects influence the polyelectrolyte conformational behavior in a nontrivial manner. Our study provides insight into the effects of dielectric mismatch in packaging and delivery of polyelectrolytes across media with different relative permittivities. Moreover, the reversible transformation of the polyelectrolyte conformations in response to environmental permittivity suggests potential applications in biosensing and medical monitoring.
10:48AM W29.00013: Interaction of highly charged rigid polymer in monovalent salt*
YAOHUA LI (Presenter), FELIPE JIMENEZ-ANGELES, MONICA OLVERA DE LA CRUZ, Northwestern University — Charged polymers such as DNA bear important biological functions and have useful applications as a nanomaterial. Experiments of these polyelectrolytes are often performed in aqueous salt solutions. Using an empirical ion potential that reproduces pair correlations from all atom molecular dynamics (MD) simulations, we study ion distributions and DNA-DNA interactions by coarse-grained MD simulations with explicit salt ions. We focus on high concentration regimes, and found that at concentrations greater than 2M, both the ion distribution profile and the potential of mean force between DNAs becomes non-monotonic and has attractive wells. These results are in good agreement with our liquid state theory predictions. Furthermore, the importance of detailed DNA structure will be discussed using all atom MD simulation of DNAs. Our study can help interpret experimental results and help control the phase behavior of charged polymer using salts.

*We thank the support of the grant DE-FG02-08ER46539 from the Department of Energy Basic Energy Science Office, and the Sherman Fairchild Foundation.

Friday, March 6, 2020 8:00 AM - 10:48 AM


8:00AM W31.00001: Hydrodynamic coupling to the electrical response of fluid suspensions of non-Brownian conducting particles MATTHEW SNELL (Presenter), JEFFREY RICHARDS, Northwestern University — We report on the electrical response of conducting non-Brownian suspensions to applied steady shear. We show using dc-conductivity measurements in a rheo-dielectric device that a shear-rate dependent conductivity increases both with the shear intensity and the particle volume fraction. The conductivity increases instantaneously upon flow start-up and returns instantaneously and reversibly to the quiescent value upon flow cessation. For volume fractions exceeding 30 vol% microspheres, the ratio of the conductivity under flow to that in the quiescent state can exceed a factor of $10^5$. We rationalize these results based on a simplistic scaling law that confirms the hydrodynamic forces couple to the interparticle electron transfer rate. These observations help to reconcile emerging experimental evidence for the role of particle mobility in determining electrical transport in colloidal fluids and suspensions and could prove a basis for new mechano-electric sensing modalities as well as improved electrochemical storage technologies.
8:12AM W31.00002: Rheological analysis of hydrocolloidal Basil seed mucilage in the context of seed physiology  BHUVSMITA BHARGAVA (Presenter), JACOB JOHN, SUSY VARUGHESE, Indian Inst of Tech-Madras — Hydration of the seeds of the *Ocimum basilicum* develops a translucent mucilage around the seed that plays a vital role in its germination, adhesion and dispersal. This functionality stems from the structure of the mucilage, which comprises of adherent and non-adherent layers, that have varying concentrations of complex polysaccharides such as pectin, cellulose, and hemicellulose. Pectin crosslinks in the presence of Ca$^{+2}$ ions to form hydrocolloidal gels. The interplay between the pectin and calcium concentrations and degree of esterification determines the nature and extent of crosslinking. However, the extent to which it contributes to the gel structure, its rheology and the resulting seed physiology is not completely understood. This work uses Large Amplitude Oscillatory Shear (LAOS) rheology as a tool to estimate the factors that affect crosslinking in the Basil seed mucilage. We observe that the mucilage behavior is gel-like, with a constant modulus plateau at low strains and shear thinning at higher strains. The non-linear signatures such as the loss modulus overshoot and strain stiffening observed for mucilage gels are compared with those of the pectin-Ca gels to estimate the extent of Ca$^{+2}$ crosslinking and the degree of esterification of the pectin present in the mucilage.

8:24AM W31.00003: Rheology of glassy and jammed emulsions*  CONG CAO (Presenter), Emory University, JIANSAN LIAO, VICTOR BREEDVELD, School of chemical & Biomolecular Engineering, Georgia Institute of Technology, ERIC WEEKS, Emory University — We study the rheology of monodisperse and polydisperse emulsions with various mean droplet sizes. Above a critical volume fraction $\varphi$, these systems exhibit solid-like behavior and possess a yield stress. Previous simulation work suggests that for small thermal particles, rheology will see a glass transition at $\varphi\approx0.58$; for large athermal systems, rheology will see a jamming transition at $\varphi\approx0.63$. However, for intermediate sized droplets at the crossover of thermal and athermal regimes, the glass and jamming transitions may both be observable in the same sample. We use a rheometer to shear different sizes of TPM emulsion droplets. By varying the shear rate and particle size, our experiments cover a wide range of Péclet number (the ratio of shear and thermal motions), including the crossover regime. We successfully measure rheological properties near the critical volume fraction(s). We then further measure how their yield stress change with volume fraction.

*This work is supported by National Science Foundation (DMR-1609763).
8:36AM W31.00004: Athermal Shear-Driven Flow of Mixtures of Frictionless Rods and Disks in Two Dimensions*  STEPHEN TEITEL (Presenter), THEODORE A MARSCHALL, University of Rochester — We numerically simulate the athermal steady-state shearing of a mixture of frictionless circular disks and elongated spherocylinders (rods) in two dimensions, suspended in a host medium. We study behavior as the total packing fraction and the fraction of rods are varied, at slow shear strain rates. We find that the average angular velocity of the shear-driven rod rotations decreases, and the extent of the nematic ordering of the rods increases, as the fraction of the rods decreases. In the limit of a single rod in a sea of disks, the rod appears to cease rotating, except at very low packing fractions. We find that, as one shears from an initial random configuration, the system tends to form clusters of parallel contacting rods. We believe that such clusters form so as to reduce the pressure in the system, and that these clusters play an important role in the shear-driven rotation of the rods.

*Supported in part by NSF Grants CBET-1435861 and DMR-1809318. Computations were carried out at the Center for Integrated Research Computing at the University of Rochester.

8:48AM W31.00005: Brownian motion in near-surface pressure driven flows with 3D-nanometric spatial resolution*  ALEXANDRE VILQUIN (Presenter), PIERRE SOULARD, VINCENT BERTIN, ESPCI Paris, GABRIEL GUYARD, Université Paris Sud, DAVID LACOSTE, ELIE RAPHAEL, ESPCI Paris, FREDERIC RESTAGNO, Université Paris Sud, THOMAS SALEZ, Université de Bordeaux, JOSHUA MCGRAW, ESPCI Paris — In near-surface flows, interfaces play a major role by imposing (typically) no-slip boundary conditions, greatly reducing the fluid velocity compared to the central part of a channel. With total internal reflection fluorescence (TIRF), a flow is illuminated with an evanescent field decaying over a few hundred nanometers into the channel; this decay allowing a determination of nanoparticle altitudes. Combined with particle tracking, experimental determination of the velocity profile and local velocity distributions in three dimensions are possible. Here we present a detailed look at the statistics of near-surface particle motions in pressure-driven water for which diffusion is important compared to advection. The distribution of displacements in the invariant flow direction is Gaussian as for normal diffusion. Significant anomalies are however observed for both of the other spatial dimensions. Combining experiments and simulations, we disentangle contributions from so-called Taylor-Aris dispersion, nanoparticle polydispersity and the optical measurement system. This description of TIRF allows for the study of many Brownian motion problems, such as near-surface polymer solution dynamics or particle motion near soft boundaries.

*ANR ENCORE, ANR CoPinS
9:00AM W31.00006: Effect of Roughness and Elasticity on Interactions between Charged Colloidal Spheres* JOSEPH MONTI (Presenter), PATRICIA M MCGUIGGAN, MARK ROBBINS, Johns Hopkins University — The effects of realistic roughness and elasticity on the interactions between charged silica spheres are studied as a function of surface potential, screening length, interfacial energy, and roughness. The repulsive force $F_{re}$ that must be overcome to bring charged spheres into contact is relatively insensitive to elasticity unless spheres are hundreds of times softer than silica. $F_{re}$ is also insensitive to roughness and interfacial energy. In contrast, roughness has a large effect on the binding energy of spheres and the force $F_{sep}$ to separate them. Both are lowered by 1 to 2 orders of magnitude by the measured surface roughness of less than 1 nm on 1 μm silica spheres. The reason is that interactions between rigid spheres are dominated by the highest surface peaks rather than the entire spherical surface. Elasticity can increase the pull-off force of rough spheres by a factor of 2 or more because additional surface area can be brought into contact. The implications of these results for shear-thickening transitions are discussed.

*Support provided by NSF Grant No. DMR-1411144.

9:12AM W31.00007: Near-surface dynamics of semidilute polymer solutions: diffusion, nonlinear rheology, and the hydrodynamic boundary condition* GABRIEL GUYARD, JOSHUA MCGRAW (Presenter), ALEXANDRE VILQUIN, ESPCI Paris, FREDERIC RESTAGNO, Université de Paris Sud — Near-surface dynamics of polymer solutions challenge both experimental and theoretical efforts — especially in the case of semi-dilute solutions for which the chains overlap — yet evanescent wave microscopy allows for a three-dimensional characterization of such interfacial flows. Here we report nanoscale-resolved particle motions in microfluidic channels for pressure-driven flows of semidilute polymer solutions. The results using polymer-free water are in good agreement with Stokes-flow hydrodynamic and diffusive theory. Experiments using hydrogenated polyacrylamide at different volume fractions close to and above the overlap concentration are done in the same chips as for the water experiments. In contrast to Newtonian fluid behaviour, the shear-rate/pressure drop relation is non-linear for the polymer solution flows, suggesting nanometrically-resolved, shear-thinning effects, accompanied with a non-trivial hydrodynamic boundary condition. The diffusive motion of the tracer particles is also distinguished from that of the water experiments, and such motions are detailed here. These results set the basis for a study of near-wall hydrodynamic flow and diffusion in complex fluids, notably including semidilute polymer solutions.

*ANR ENCORE, ANR CoPinS, Total
9:24AM W31.00008: Emergence of surface roughness from plastic deformation of amorphous materials

RICHARD LEUTE (Presenter), Department of Microsystem Engineering, University of Freiburg, TILL JUNGE, Department of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, LARS PASTEWKA, Department of Microsystem Engineering, University of Freiburg — Many man made and natural surfaces show intrinsic surface roughness which controls material properties such as adhesion or friction. Over several length scales and in different materials, ranging from rocks to gold crystals, roughness shows a self-affine scaling behaviour. We investigate the emergence of self-affine surface roughness in amorphous solids through plastic deformation. Our simulations are performed using a fast Fourier transform (FFT)-based continuum mechanics solver. The typical plastic deformation avalanche dynamics of an amorphous material is simulated by a fully tensorial stochastic plasticity model. The crucial role of avalanches for self-affine surface roughness is shown by comparing the stochastic plasticity model with a finite strain $J^2$-plasticity formulation with linear isotropic hardening. We present avalanche statistics and analyse the spatiotemporal distribution of the plastic events. The non-affine deformations in the bulk of the material is related to the self-affine surface roughness of the free surface.

9:36AM W31.00009: Determining the Structural Characteristics of Deforming Objects from Their Scattering Signature

GUAN-RONG HUANG (Presenter), YANGYANG WANG, YUYA SHINOHARA, CHANGWOO DO, TAKESHI EGAMI, WEI-REN CHEN, Oak Ridge National Lab — There has been much interest in understanding the structural characteristics of deforming materials on different length scales. In the context of scattering, the domain of interest can be splitted into a microscopic region within which the local configurational translation and rotation can be treated in detail, and a larger regime where the description of global shape is appropriate. From a perspective of geometric interpretation at the micro/macroscopic level, a central issue is how to quantitatively determine the structural characteristics from the anisotropic scattering intensity in a model-free manner.

We present a general approach to deal with this problem. In the mean-field limit, we first show that the radius of gyration is the source term of intra-particle structure factor. Using the real spherical harmonic expansion (RSHE), we derive the exact expression of gyration tensor in terms of the anisotropic spatial correlation functions. Meanwhile, we derive the orientational distribution functions to describe the local configurational alignment. Theoretical benchmarks verify that our approach not only facilitates quantitative scattering studies of flowing materials, but also provides insightful information regarding the deformation behavior of materials at the molecular level.
9:48AM W31.00010: Maximum strain energy density drives path selection in dynamic
cracks*  LITAL ROZEN-LEVY, The Racah Institute of Physics, The Hebrew University of Jerusalem, Israel,
JOHN KOLINSKI (Presenter), Ecole Polytechnique Federale de Lausanne, GIL COHEN, JAY FINEBERG, The
Racah Institute of Physics, The Hebrew University of Jerusalem, Israel — Our fundamental
understanding of dynamic ‘simple’ cracks in brittle solids is excellent, yet the criteria for path
selection of moving cracks remain unknown. We evaluate the criteria for path selection in
dynamic fracture in two ways: first, we deflect dynamic cracks using sparsely implanted defects,
and second, we drive them to undergo an intrinsic oscillatory instability in defect-free media. Our
experiments cover a wide range of crack velocities, from 10-95% of their limiting velocity within
the brittle material. Our high-speed imaging data are used to obtain measurements of the strain
fields very near the crack tip - and these measurements reveal that path selection for such rapid
and strongly perturbed cracks is determined by the direction of maximal strain energy density
rather than by the principle of local symmetry. These results suggest a novel mechanism for
material toughening in brittle solids, whereby a crack is steered, deflected and even stopped by
embedded inclusions.

*US-Israel Binational Science Foundation (grant 2016950); Israel Science Foundation (grant
1523/15)

10:00AM W31.00011: A scaling law to determine cracking lengths in shrinkable granular
packings*  HAN-JAE JEREMY CHO (Presenter), Mechanical Engineering, University of Nevada, Las Vegas,
SUJIT DATTA, Chemical and Biological Engineering, Princeton University — Hydrated granular packings
can shrink and crack into discrete clusters of grains when dried. Cracking in paint and mud are
familiar examples of this phenomenon. Despite its ubiquity, however, an accurate prediction of
cracking length scales remains elusive. Here, we uncover the previously overlooked role of
individual grain shrinkage in determining crack patterning. We perform experiments with
shrinkable hydrogel particles and discrete-element simulations. By incorporating grain shrinkage
into classical Griffith crack theory, we obtain a scaling law that quantifies how cluster size
depends on the interplay between grain shrinkage, stiffness, and size—in agreement with
experiments and simulations. The cracking predictions are applicable to a diverse array of
shrinkable granular materials.

*This work was partially supported by the Alfred Rheinstein Faculty Award, the Grand Challenges
Initiative of the Princeton Environmental Institute, and the Princeton Center for Complex
Materials, a Materials Research Science and Engineering Center supported by National Science
Foundation Grant No. DMR-1420541.
10:12AM W31.00012: The Prince's Dilemma: How Local Heterogeneities Affect the Onset of Frictional Slip  MARY AGAJANIAN (Presenter), SAM DILLAVOU, Harvard University, VINCENT STIN, ESPCI Paris, AMIR SAGY, Geological Survey of Israel, EMILY BRODSKY, University of California, Santa Cruz, SHMUEL RUBINSTEIN, Harvard University — Peas in eider-down beds and asperities at frictional interfaces trouble fairy-tale princesses and nucleate slip events, respectively. We study the onset of such slip events at a two-dimensional frictional interface using soft, transparent elastomer slabs separated by a layer of sand. This system slows rupture propagation to time scales easy to capture experimentally and allows us to directly visualize the full displacement field at the interface. As the top plate is sheared across the interface, stress aggregation forces contact points at the frictional interface to slide and initiates slip events. We systematically introduce localized pockets of stress (peas) to the interface geometry and characterize the effects of these peas on the dynamics of slip nucleation and growth. By tracking the displacement field near the interface, we observe a plethora of these nucleation behaviors, including partial ruptures and local and traveling nucleation.

10:24AM W31.00013: Role of Mesoscopic Friction and Morphology in Large Deformation of Carbon Nanotube Network: a Distinct Element Method Study  YUEZHOUS WANG (Presenter), Integrated Engineering, Minnesota State University, Mankato, GRIGORII DROZDOV, Scientific Computing Program, University of Minnesota, Twin Cities, TRAIAN DUMITRICA, Mechanical Engineering, University of Minnesota, Twin Cities — Carbon nanotubes (CNTs) are game-changing materials in various disciplines, but the limited capability for simulating CNT in bulk represents a significant obstacle for realizing their promising applications. We address this challenge by developing a new simulation methodology titled the mesoscopic Distinct Element Method (mDEM). With parameters input from atomistic simulations, mDEM bridges across the atomistic and mesoscopic length scales, providing an efficient tool to predict the large deformation mechanism of CNT network. Validated through experiments, mDEM is utilized in hypothesis-driven research to demonstrate the internal structural evolution of CNT network stretched until fracture. At small and moderate deformations, zipping relaxations along the applied strain direction dictates the microstructural evolution. At larger deformations, the occurrence of energetic elasticity promotes yarn densification, by relaxing CNT waviness and eliminating squashed pores. Besides the strain-induced alignment process, phononic and polymeric friction promote CNT alignment by enabling load transfer. Our parametric studies not only offer guidance in manufacturing industry to achieve high quality yarn, but also potentially offer an effective way to model fibrous materials in general.
10:36AM W31.00014: Tracking Tabletop Earthquake Nucleation  SAM DILLAVOU (Presenter), Harvard University, VINCENT STIN, ESPCI, MARY AGAJANIAN, Harvard University, AMIR SAGY, Geological Survey of Israel, EMILY BRODSKY, UC Santa Cruz, SHMUEL RUBINSTEIN, Harvard University — Where, when, and how does an earthquake start? Stress concentrations are thought to play an important role in nucleating earthquakes, but their roles are far from trivial. How stressed areas (known as asperities) interact to control the location and timing of quake nucleation is an inherently two-dimensional elasto-dynamic crack problem where the effects of heterogeneity are far from obvious. We experimentally probe the dynamics of nucleation using a tabletop model fault. We reduce the speed of the dynamic ruptures by using soft transparent elastomers and filling the interface with a thin layer of sand. Heterogeneous stress concentrations are imposed by compressing the interface with a rigid plate and adjustable beads to form localized asperities. The clear material allows us to directly image the propagating slip, which would not be possible in natural rock. We find that nucleation location and style is controlled by the stress concentrations. Weaker concentrations result in more migratory nucleation and more global slip events. Furthermore the location of these regions dictates their interactions; widely spaced concentrations are less likely to slip simultaneously, resulting in fewer global events and slower stress release in the case of a global event.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W32 DPOLY DSOFT: Polymers with Special Architectures: From Molecular Design to Physical Properties II 504 - Reika Katsumata, Univ of Mass - Amherst - Tag(s): Focus

8:00AM W32.00001: Molecular conformation of rigid cyclic and branched polymers in solution* [Invited] KEN TERAO (Presenter), Macromolecular Science, Osaka University — Local conformational properties of rigid cyclic and branched polymers are not always the same as those for the corresponding linear chain unlike flexible polymers. We recently investigated rigid cyclic amylose derivatives and 3-arm star poly(quinoxaline-2,3-diyl) to determine their molecular conformation and intermolecular interactions in dilute solution. We found that local helical structure for the cyclic polymers are appreciably extended and therefore the main chain is more flexible than that for the corresponding linear chain. Regarding with this, the chiral separation columns made of the cyclic amylose derivative are substantially different separation behavior from those for the linear chain, indicating that the local conformation plays an important role for the molecular recognition ability. Both the linear and star chains have lyotropic liquid crystallinity. The phase diagram of isotropic and nematic phases are explained by a modified scaled particle theory when we assume some specific conformation in the nematic phase.

*JSPS KAKENHI Grant Numbers JP17K05884, JP25410130, 23750128

Friday, March 6, 2020 8:00 AM - 11:00 AM
8:36AM W32.00002: Scattering from Melts of Combs and Bottlebrushes: Molecular Dynamics Simulations and Theoretical Study*  HEYI LIANG, ZILU WANG (Presenter), ANDREY DOBRYNIN, Univ of Akron — We use coarse-grained molecular dynamics simulations to establish correlations between peak position in the static structure factor $S(q)$ of combs and bottlebrushes in a melt and their architectural parameters such as degree of polymerization of the side chains $n_{sc}$ and number of backbone bonds $n_g$ between side chain grafting points. Analysis of the scattering function derived in the framework of the Random Phase Approximation and one obtained in simulations shows that in the comb regime with dilute side chains, $n_g > n_{sc}$, the wave number $q^*$ corresponding to the peak position in function $S(q)$ scales with macromolecular parameters as $q^* \propto (n_{sc} n_g)^{-1/4}$. A new scaling law $q^* \propto n_{sc}^{-3/8}$ emerges in the bottlebrush regime, where interactions between side chains stiffen the backbone at short length scales causing the effective backbone Kuhn length to increase with the degree of polymerization of the side chains as $b_K \propto n_{sc}^{1/2}$. The established correlation between the peak position $q^*$ and bottlebrush Kuhn length provides foundation for a new method of obtaining the Kuhn length from scattering data. This approach does not require labeling of bottlebrush backbone and relays on natural contrast between side chains and backbones in the bottlebrush melts.

*NSF DMR-1535412

8:48AM W32.00003: Impact of Architectural Asymmetry on Frank-Kasper Phase Formation in Block Polymer Melts  ALICE CHANG (Presenter), FRANK S BATES, University of Minnesota — Block polymer self-assembly reflects a multiscale competition between enthalpic and entropic factors, producing periodic nanostructures with rich potential to tune the composition, geometry, and length scales. Until recently, the body-centered cubic lattice was believed to be the universal equilibrium state in the sphere-forming region. However, the recent discoveries of equilibrium Frank-Kasper $\sigma$ and A15 phases in diblock polymer melts have revealed remarkable new complexity in these ostensibly simple materials. These complex low-symmetry phases have been experimentally identified in two types of neat block polymers: (1) linear AB diblocks and (2) linear ABA'C tetrablocks. To the best of our knowledge, non-linear architectures remain unexplored. In this talk, we will discuss the connections between molecular architecture and symmetry selection in block polymers. We have systematically tuned the architectural asymmetry in block polymers via living polymerization, from the linear-$b$-linear to linear-$b$-bottlebrush limits. Analysis by small-angle X-ray scattering provides insight into the impact of architectural asymmetry on block polymer self-assembly. Increasing the asymmetry between blocks skews the phase diagram and introduces new potential for block polymer design.
9:00AM W32.00004: Molecular architecture directs linear-bottlebrush-linear triblock copolymers self-assemble to soft, reprocessable elastomers  SHIFENG NIAN (Presenter), Department of Materials Science and Engineering, University of Virginia, HUADA LIAN, Department of Chemical Engineering, Stanford University, ZIHAO GONG, Department of Materials Science and Engineering, University of Virginia, MIKHAIL ZHERNENKOV, National Synchrotron Light Source-II, Brookhaven National Laboratory, JIAN QIN, Department of Chemical Engineering, Stanford University, LIHENG CAI, Department of Materials Science and Engineering, University of Virginia — Linear-bottlebrush-linear (LBBL) triblock copolymers represent an emerging system for creating multifunctional nanostructures. Their self-assembly depends on molecular architecture but remains poorly explored. We synthesize polystyrene-block-bottlebrush polydimethylsiloxane-block-polystyrene triblock copolymers with controlled molecular architecture, and use them as a model system to study the self-assembly of LBBL polymers. Unlike the classical stiff rod-flexible linear block copolymers that are prone to form highly ordered nanostructures such as lamellae, at small weight fractions of the linear blocks, LBBL polymers self-assemble to a disordered sphere phase regardless of the bottlebrush stiffness. Microscopically, the characteristic lengths of the self-assembled nanostructures increase with the stiffness of bottlebrush block by a power law, which is captured by a scaling analysis. Macroscopically, the formed nanostructures are ultrasoft, reprocessable elastomers with shear moduli of about 1 kPa, two orders of magnitude lower than that of conventional polydimethylsiloxane elastomers. Our results provide insights on exploiting the self-assembly of LBBL polymers to create soft functional nanostructures.

9:12AM W32.00005: Structure of bottlebrush polymers end-grafted to a planar surface* JAROSLAW PATUREJ (Presenter), Institute of Physics, University of Silesia, Katowice, Poland, PAUL JUNGMANN, JENZ-UWE SOMMER, IPF Dresden, Germany, TORSTEN KREER, Johannes Gutenberg-Universität, Mainz, Germany — Polymer brush is a hybrid material composed of a solid substrate coated with end-grafted polymers. We conducted coarse-grained molecular dynamics simulations and scaling theory of the equilibrium structure of planar brushes formed by bottlebrush polymers. Bottlebrushes are branched macromolecules consisting of densely spaced linear side chains grafted along a central (linear) backbone. We elucidate the relationship between bottlebrush architecture, surface coverage \( \sigma \) and polymer brush thickness \( H \). We study the impact of three length scales on the brush height \( H: D_0 \), the cross-section radius of bottlebrushes determined by the degree of polymerization of side chains \( N_{sc}, R_0 \) the (overall) size of bottlebrushes controlled by the degree of polymerization of backbone \( N_{bb} \) and \( d \) the distance between nearest-neighbor tethering sites. The latter quantity provides a measure of molecular coverage \( \sigma \) of a substrate defined as the number of bottlebrush polymers per unit surface area \( \sigma \propto 1/d^2 \). Our theoretical analysis identifies three conformational regimes for the height \( H \), which gradually establish upon increasing substrate coverage and stem from interplay between relevant length scales: \( d, D_0 \) and \( R_0 \).

*Polish National Science Center (Grant No. 2018/30/E/ST3/00428)
9:24AM W32.00006: Self-assembly of Bottlebrush Amphiphilic Polymers Near/On Surfaces: Coarse-grained Molecular Dynamics Simulation Study  MICHIEL WESSELS (Presenter), ARTHI JAYARAMAN, Department of Chemical and Biomolecular Engineering, University of Delaware — Nanostructured materials for a wide range of applications such as electronics, optics, and sensing are engineered by the self-assembly of block polymers on surfaces. Significant number of past experimental, theoretical, and computational studies have tackled the self-assembly of linear block polymers, both in bulk and on/near surfaces. Relatively fewer studies have been focused on self-assembly of non-linear architectures (e.g., bottlebrush, star, comb) near/on surfaces. In this talk, we will present our recent work using coarse-grained molecular dynamics simulations to elucidate how branched polymer architecture affects the assembly in solutions of amphiphilic block copolymers near/on surfaces. We establish the role of side chain length versus backbone length, side chain grafting density on the backbone of amphiphilic block polymers as well as surface attraction strength on the chain conformations and the shapes, sizes and patterns of domains assembled on attractive surfaces.

9:36AM W32.00007: Effects of Ionic Groups on Dynamics of Linear-Star Polymer Blends: A Molecular Dynamics Simulation Study* MANJULA SENANAYAKE (Presenter), Department of Chemistry, Clemson University, Clemson, SC, United States,29634, GARY GREST, Sandia National Laboratories, Albuquerque, NM, United States,87123, DVORA PERAHIA, Department of Chemistry/Department of Physics, Clemson University, Clemson, SC, United States, 29634 — Tethering ionic groups to polymers influence their phase behavior and dynamics, and in turn affect their blending with other macromolecules. Here, using MD simulations we probe the effects of ionic groups on the dynamics of linear-star polymer blends, where both the ionic groups and the topology affect the behavior. The polymer chains are modeled by the beads-spring model and the ionic groups are incorporated in the form of stickers (0-5%) on either the linear or star polymers or on both. The fraction $f_{\text{star}}$ of star polymer is varied from 0 to 1. We find that for non-charged blends the short linear and star polymer chains are miscible. Introducing ionic groups on either the linear or the star polymers results in ionic clustering and phase separation. We find that the mobility of the linear ionizable melt is slower than the non-ionic polymers. In contrast, stickers increase the mobility of star polymer melts. In the presence of small amounts of stickers, the mobility of the chains is not affected by chain architecture.

*Supported in part by DOE Grant No. DE-SC007908
9:48AM W32.00008: Complete photonic band gaps with nonfrustrated ABC bottlebrush copolymers  JOSHUA LEQUIEU (Presenter), KRIS T DELANEY, GLENN H FREDRICKSON, University of California, Santa Barbara — Block polymers are a promising platform for photonic materials, yet progress has been limited due to the scarcity of suitable morphologies with complete photonic band gaps and the large domain sizes necessary to manipulate visible light. Here we show that nonfrustrated ABC bottlebrush copolymers can surmount both of these limitations and can be used to form materials with complete photonic band gaps. To achieve this, we have developed a computational tool that couples self-consistent field theory (SCFT) simulations to Maxwell's equations, thereby permitting a direct link between molecular design, self-assembly and the resulting photonic band structure. Using this approach, we calculate the phase diagram of ABC bottlebrush copolymers, and show that complete photonic band gaps can open in the alternating gyroid and alternating diamond phases for modest dielectric contrast between the A, B, and C components. We show that the gap width increases with segregation strength, and depends strongly of the volume fractions of the A and C networks. Notably, the maximum band gap for the alternating gyroid corresponds to a region of the bottlebrush phase diagram where SCFT predicts this phase to be stable, suggesting that these photonic materials could be realized experimentally.

10:00AM W32.00009: Polydispersity Stabilized Complex Morphologies in Poly(styrene-b-methyl methacrylate) Diblock Copolymers  INHO KIM (Presenter), SHENG LI, KAIST — Block copolymers have the unique property to self-assemble into ordered microstructures with well-defined periodicity. Among the various attainable microdomain morphologies, complex bicontinuous morphologies are highly desirable due to their inherent structural connectivity. While such complex structures are difficult to obtain in monodisperse block copolymers, they may be stabilized by increasing block dispersity. In this study, we synthesized a series of poly(styrene-b-methyl methacrylate) (PS-PMMA) diblocks where dispersity of both blocks were systematically varied. The domain morphologies of the resulting diblocks were examined by combination of small-angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). At fixed volume fraction of the PS block, dispersity dictated phase transition was observed. In particular, in the case where dispersity of both blocks were high, the polymers were found to exhibit perforated lamellae (PL) and disordered bicontinuous (BIC) morphologies. These results showed that dispersity control can be used to widen the accessibility window for complex morphologies in block copolymers.
10:12AM W32.00010: Molecular Design of Post-functionalizing Block Copolymers for Versatile Morphologies* TERUAKI HAYAKAWA (Presenter), SEINA YAMAZAKI, YASUNARI YOSHIMURA, YUTA NABAE, Tokyo Inst of Tech - Tokyo — One of the challenges in block copolymer study is to produce bicontinuous structures with various types of polymers with high reproducibility. Conventionally, two methods are known: a method of synthesizing a polymer having a target composition ratio by precise polymerization, and a polymer blend in which fine adjustment of the composition ratio is performed while accurately blending one polymer. However, there are some problems such as lack of reproducibility, limited polymers that can be used, and macrophase separation.
In this study, we demonstrated a new approach for creating bicontinuous microphase-separated structures using the post-functionalization of side-chain type block copolymers. The molecular design of the block copolymers having a vinyl group or glycidyl group in the side chain group was carried out, and the composition ratio was precisely controlled based on the high-yield reactions in the post-functionalization. It was found that the bicontinuous gyroid structure can be obtained with good reproducibility by precisely controlling the amount of side chains introduced.

*This work was supported by JSPS KAKENHI (17H03113) and the Cooperative Research Program of "Network Joint Research Center for Materials and Devices".

10:24AM W32.00011: Poly(Styrene-block-Glycidyl Methacrylate-block-Methyl Methacrylate) as a Versatile Platform for Exploring the Phase Diagram of Linear Triblock Copolymers* KEVIN WYLIE (Presenter), LEI DONG, YUTA NABAE, TERUAKI HAYAKAWA, Tokyo Inst of Tech - Tokyo — Block copolymers have been of great interest because of their intrinsic ability to self-assemble into myriad ordered structures with characteristic dimensions on the order of nanometers. In particular, diblock copolymers have been the primary focus of most research because of their simple architecture leading to a comprehensive understanding of their phase diagram. In contrast, adding a third block greatly increases the number of parameters affecting the self-assembly behavior which in turn greatly increases the number of phases accessible.
We have designed a new linear triblock consisting of poly(styrene-b-glycidyl methacrylate-b-methyl methacrylate) as a new platform for exploring the phase diagram of linear triblock copolymers. The reactive glycidyl methacrylate block can be functionalized with small molecules to modify the Flory-Huggins χ parameter between the middle block and the outer blocks. Thus, we can observe the effect of the changing χ values directly since they are all derived from the same batch.

*This work was supported by KAKENHI (Grant #17H03113), NEDO, the Ogasawara Foundation, and the Cooperative Research Program of Network Joint Research Center for Materials and Devices: Dynamic Alliance for Open Innovation Bridging Human, Environment and Materials.
10:36AM W32.00012: Helical sense of wrapped belts in star terpolymers via slice and view scanning electron microscopy  \( \text{WENPENG SHAN (Presenter), XUEYAN FENG, Rice Univ, GEORGE POLYMEROPoulos, NIKOS HADJICHRISTIDIS, King Abdullah University of Science and Technology, EDWIN THOMAS, Rice Univ} \) — We study the self-assembly behavior of well-defined 3-miktoarm star terpolymers consisting of polyisoprene (PI), polystyrene (PS), and poly(2-vinylpyridine) (P2VP), (PI)\(_2\)-b-PS-b-P2VP. By adjusting the volume fractions of each block (40 vol % for PI, 27 vol % for PS and 33 vol % for P2VP), a unique structure was formed, in which hexagonally packed P2VP cylinders are wrapped by helically twisting PS belts in a matrix of PI. This structure was initially characterized by small angle X-ray scattering of bulk samples and bright field transmission electron microscopy (BF-TEM) of thin microtomed sections. By using I\(_2\) to selectively stain P2VP and OsO\(_4\) for PI, we can distinguish all 3 types of microdomains. In order to study the helical sense and coherent packing between adjacent cylinders, slice and view scanning electron microscopy (SVSEM) tomography is employed. The 3D tomograms of large regions provide information on the detailed nature and packing of the helical PS belts.

10:48AM W32.00013: Molecular dynamics simulations and neutron scattering provide an atomistic level understanding of the self-assembly of poloxamines* \( \text{ROBERT ZIOLEK (Presenter), Department of Physics, King's College London, GUSTAVO GONZALEZ-GAITANO, Department of Chemistry, University of Navarra, CECILE A. DREISS, Institute of Pharmaceutical Science, King's College London, CHRISTIAN D. LORENZ, Department of Physics, King's College London} \) — By integrating molecular dynamics simulations and neutron scattering, we have studied different poloxamines (Tetronics), a family of star-shaped block copolymers that show promise as controlled release drug delivery agents. Their amphiphilicity and the basicity of their central diamine unit control their pH-sensitive self-assembly into supramolecular complexes.

We have studied Tetronic 904 (T904), a medium-sized poloxamine, and Tetronic 304 (T304), a smaller analogue, by all-atom molecular dynamics simulations and neutron scattering. While it is well-known that T904 readily forms micelles over a range of temperatures and concentrations, T304 has previously been found to have a more limited ability to self-assemble. Together, our simulations and experiments provide a detailed microscopic picture of the structure, dynamics and hydration of the self-assembled structures formed by both T904 and T304, and for the first time have uncovered the mechanisms that typically hinder T304 self-assembly.


Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W33 DPOLY DSOFT DMP: Polymer Crystals and Crystallization

I 505 - Christopher Li, Drexel Univ - Tag(s): Focus
8:00AM W33.00001: Polymer epitaxy under heterogeneous confinement
JASON LIU (Presenter), YANG XIA, GEOFFREY ZHENG, MIKKO HAATAJA, CRAIG ARNOLD, RODNEY PRIESTLEY, Princeton University — It is challenging to grow polymer crystals which are aligned over long length scales due to the inherent tendency of polymer lamellae to undergo spherulitic branching and splaying during growth. One approach to the creation of ordered and aligned polymer structures is by epitaxial crystallization. Typically, crystallization proceeds in a film of uniform thickness, in which polymer crystals nucleate and grow along rotationally symmetric, epitaxially matched crystallographic directions. In this work, we heterogeneously confine the film into spatially disparate regions of varying thickness to separate the nucleation and growth processes, allowing oriented arrays of epitaxial crystals to grow unimpeded over long distances. We uncover the hierarchical structure of polymers crystallized under heterogeneous confinement and elucidate the undercooling and molecular weight dependencies of pattern formation with experiments and phase-field simulations.

8:12AM W33.00002: Understanding polymer crystallization undergoing zone annealing*
ALEJANDRO KRAUSKOPF (Presenter), ANDREW JIMENEZ, SANAT KUMAR, Department of Chemical Engineering, Columbia University, ELIZABETH LEWIS, BRYAN VOGT, Department of Polymer Engineering, The University of Akron, JULIA PRIBYL, BRIAN C BENICEWICZ, Department of Chemistry and Biochemistry, University of South Carolina — Zone annealing is a process through which a temperature gradient is translated at a set velocity across a polymer sample of interest, differentiating it from other crystallization processes by its inherent directionality. Through the application of the Hermans orientation function to our small-angle X-ray scattering detector patterns, we explore the extent of anisotropy that the process imparts on both the pure polymer and the polymer nanocomposite systems, with a focus on the lamellar orientation for the former and the nanoparticle arrangement for the latter. We also utilize differential scanning calorimetry to quantify the effects that the process has on the crystalline content and the melting temperature of the materials.

*United States Department of Energy, Office of Science
Gates Millennium Scholars Program
Columbia University Soft Matter Grant
SEONG HYUK CHO (Presenter), RICHARD REGISTER, Princeton University — The Huang-Brown (HB) model predicts that tie molecules (TM), polymer chains that connect different crystalline lamellae across the amorphous layer, form when the end-to-end distance of the coil in the melt (R) exceeds the intercrystalline spacing (d) in the solid state, i.e., the TM probability should scale with R/d. To test the HB model, we synthesize narrowly-distributed (dispersity < 1.2) linear PEs of varying molecular weight (M) using ring-opening metathesis polymerization of cyclopentene followed by hydrogenation. Each PE is either quenched or slowly-cooled from the melt to vary the thermal history, giving two different d values. Uniaxial tensile tests of these PEs show a rather abrupt brittle-to-ductile transition (BDT) with increasing M, but the transition occurs at different R/d for the different crystallization conditions, in the contrast to the HB prediction. Quenched blends with variable contents of high-M PE in a low-M PE matrix show a BDT at the same HB tie chain probability as the quenched PEs. The differences among the values of R/d at the BDT for PEs with different thermal histories and hydrogenated polybutadiene (literature data) suggest that the degree of crystallinity has a significant influence on the value of R/d at the BDT.

*NSF Polymers Program (DMR-1402180)

DAVID NICHOLSON, PENG YI, GREGORY RUTLEDGE (Presenter), Massachusetts Institute of Technology MIT — Crystallization is an essential step in the processing of most polymers. It takes place under conditions of rapid cooling and high strain rate, and is strongly accelerated relative to quiescent conditions. The initial step in this process is flow-enhanced nucleation (FEN), which occurs on time and length scales that are hard to capture experimentally. To resolve this problem, we use nonequilibrium molecular dynamics simulations to characterize FEN from a melt of linear polyethylene-like chains. Both short and long (entangled) chains are simulated. First, methods are described for identifying the critical nucleation event using mean first-passage times (MPFT). Fitting of the data to a master equation is used to extract important thermodynamic and kinetic quantities. Results for nucleation kinetics accelerated under different modes of deformation, e.g. simple shear or uniaxial extension, and rates of strain are used to assess several of the existing models in the literature for flow-enhanced nucleation, based on their abilities to describe the data accurately, and new models based on the orientational ordering of Kuhn segments induced by flow are proposed. Evidence is presented for a breakdown of classical nucleation theory for entangled polymer melts at high strain rates, which in turn is traced to the flow-induced formation of nematic domains in the melt. The appearance of such domains suggests a different perspective on the underlying physics of flow-enhanced nucleation of long chain molecules.

*The authors gratefully acknowledge the support of ExxonMobil Chemicals Co.
9:12AM W33.00005: Stereoregularity, Molecular Dynamics, and Unusual Crystallinity of Hydrogenated Polynorbornenes: Configurational Disorder*  TOSHIKAZU MIYOSHI (Presenter), NAVIN KAFLE, YUTA MAKITA, Univ of Akron — Solid-state NMR spectroscopy can be used to study both the structure and dynamics of macromolecular systems that exhibit different degrees of order to understand the fundamental properties of materials. One such point of interest is to determine the difference of a polymer's structure, local dynamics and phase transition between various isomers of semicrystalline polymers. Recently, a thorough study on stereospecific ring-opening metathesis polymerization has been conducted on norbornenes making the synthesis and the study of hydrogenated polynorbornene (hPNB) stereoisomers possible. The unique local dynamics, phase structure, and phase transition of atactic-syndiotactic- and isotactic-hPNBs will be shown and their relationships will be discussed.

*NSF DMR Polymers 1708999

9:24AM W33.00006: Crystallization of Asymmetric PEO-b-PCL from Different Solvents*  RYAN VAN HORN (Presenter), Lafayette Coll — Poly(ethylene oxide)-b-poly(caprolactone) (PEO-b-PCL) copolymers have received a lot of attention due to their biocompatibility and amphiphilicity. One unique characteristic is that PEO and PCL have similar crystallization behavior, thus making them a robust model for phase behavior studies. Our previous work showed that the crystallization order could be switched in symmetric copolymers (nearly equal mass fraction) through selective solvent interactions. Further work has been done to identify similar behavior in asymmetric systems. Relative crystallinity and morphology are varied in as-cast films based on solvent characteristics.

*This work was supported by the National Science Foundation.

9:36AM W33.00007: Symmetry breaking via polymer chain overcrowding in molecular bottlebrush crystallization*  CHRISTOPHER LI (Presenter), HAO QI, MARK STAUB, Drexel Univ, DANIEL HENN, BIN ZHAO, University of Tennessee — One of the fundamental laws in crystallization is translational symmetry, which accounts for the profound shapes observed in natural mineral crystals and snowflakes. Spherical polymer crystalsomes have been grown and investigated in the context of spherical crystallography, where translational symmetry is broken by confining crystal growth in a curved liquid/liquid interface. In this talk, we present the spontaneous formation of spherical hollow crystals with broken translational symmetry in crystalline molecular bottlebrush (mBB) polymers. The unique structure was named as mBB crystalsome (mBBC), highlighting its similarity to the classical molecular vesicles. Fluorescence resonance energy transfer (FRET) experiments showed that the mBBC formation was driven by local chain overcrowding-induced asymmetrical lamella bending.

*This work was supported by the National Science Foundation Grant DMR 1709136 and DMR 1607076
Improving Crystallite Size and Orientation in Organic Semiconductor Thin Films using PDMS-Assisted Crystallization

VESTA ZHELYASKOVA (Presenter), PRACHI SHARMA, Department of Electrical, Computer, and Energy Engineering, University of Colorado Boulder, DANIEL DESSAU, Department of Physics, University of Colorado Boulder, SEAN SHAHEEN, Department of Electrical, Computer, and Energy Engineering, University of Colorado Boulder — We aim to develop a scalable, solution-based method for growing crystalline organic semiconductor thin films, which can be used in a variety of electronic charge transport, metal doping, and device integration studies. Using a polydimethylsiloxane (PDMS)-assisted deposition method for fullerenes, we grew polycrystalline C₆₀ thin films on plain glass, between gold electrodes on glass, and on silicon substrates under a range of growth conditions. AFM characterization revealed that the films (1) were typically 200-300 nm thick, (2) were made up of crystallites extending up to 200 μm, and (3) had crystalline microstructures that vary with choice of solvent, temperature, and substrate pre-treatment. Films grown from carbon disulfide solutions covered larger areas than those grown out of o-dichlorobenzene—an interplay between the C₆₀’s low solubility and the PDMS’s absorption of nonpolar solvents. Growth at lower temperatures resulted in uniformly aligned crystallites, which formed farther from the PDMS-substrate boundary. Growth along and between gold contacts resulted in nucleation of similarly aligned crystallites at the gold’s edge. Here we discuss the growth kinetics of these films along with their electronic, structural, and spectroscopic characterizations.

W. M. Keck Foundation

Wang-Landau Simulation of the Free Energy Surface of Crystallization in a Polymer Melt

PIERRE KAWAK (Presenter), ANDREW SCOTT GIBSON, LOGAN STEWART BROWN, BEVERLY DELGADO, DOUGLAS TREE, Chemical Engineering Department, Brigham Young Univ-Provo — Semicrystalline polymers comprise as much as 70% of the hundreds of million of tons of polymers produced worldwide. However, the polymer crystallization process remains imperfectly understood. Recently, there has been a lively debate in the literature concerning the applicability of classical nucleation theory to the primary nucleation process in a polymer melt. Recent experimental observations have lead several authors to propose mesomorphic phases that mediate the melt-crystal transition. To investigate these claims, we have constructed a GPU-accelerated Wang-Landau Monte Carlo algorithm that employs both configurational bias and bond breaking moves. Our algorithm has the ability to directly sample the density of states, which can be used to construct a free energy surface as a function of relevant order parameters for crystallization. Our initial results show that we are able to capture both melt and crystalline phases with speed increases of about two orders of magnitude greater than with a comparable serial algorithm.

We acknowledge financial support from the American Chemical Society Petroleum Research Fund (PRF# 59244-DN16) and BYU Board of Trustees as well as computational resources from the BYU Office of Research Computing and Fulton Supercomputing Lab.
10:12AM W33.00010: Crystallization and self-nucleation of conjugated polymers*  LUCIA FERNANDEZ-BALLESTER (Presenter), RAMIN HOSSEINABAD, JESSE KUEBLER, University of Nebraska - Lincoln — It is well known that the specific conditions under which polymer crystallization occurs dictate the resulting semicrystalline morphology and, therefore, the final mechanical, optical, and diffusive properties of the solidified material. For conjugated polymers, even seemingly small differences in crystallinity, orientation, or tie chains can result in significant changes in charge transport properties; however, the interplay between chain structure, crystallization conditions, and structure development remains elusive because they are typically processed in solution (for example, by spin-coating) where ill-defined conditions are prevalent. Here, we explore the role of molecular attributes on the crystallization behavior of poly-3-hexylthiophene under well-defined conditions. The results indicate that molecular characteristics play an important role in the way crystallization proceeds, and that self-nucleation strategies can be used effectively to manipulate crystallization conditions.

*Funding provided by National Science Foundation under award DMR-1809888.

10:24AM W33.00011: Paradigm on the Growth Kinetics of Lamellar Polymer Crystals*  WENBING HU (Presenter), Nanjing University — Growth kinetics of lamellar polymer crystals is the holy grail topic in the crystallization mechanism of polymers. There exist so far many controversial arguments, but only three of them have derived the kinetic equations of the linear crystal growth rate at the lateral front of lamellar crystals: Lauritzen-Hoffman model, Sadler-Gilmer Model and the intramolecular crystal nucleation model. Three equations hold however similar forms. This fact reveals the long-existing paradigm during the development of these three models. The latest intramolecular nucleation model provides interpretations to those unique kinetic phenomena of polymer crystallization, such as the origin of chain-folding, the determination of fold-length, molecular-length segregation, sequence-length segregation, three-regime transitions, linear concentration dependence, and self-poisoning growth with integer-folding of short chains.

*National Natural Science Foundation of China (Grant No. 21734005).
10:36AM W33.00012: Tuning Nanoparticle Dispersion to Control Confined Polymer Crystallization for Induced Ordering* ANDREW JIMENEZ (Presenter), ABDULLAH AL TORBAQ, Columbia Univ, ALEJANDRO J MÜLLER, University of the Basque Country, SANAT KUMAR, Columbia Univ — Extremely slow isothermal processing presents the ability to control nanoparticle dispersion in semicrystalline polymers, hierarchically ordering them in the amorphous regions of the crystal structure and providing mechanical reinforcement to the composite. The necessity for “extremely slow processing” is, of course, not ideal despite its favorable outcome. Recent work began to understand the tradeoff of crystallization rate and the subsequent particle alignment, both of which depend strongly on nanoparticle grafting and concentration. Building from these insights, we have worked to tune nanoparticle parameters (size and grafting) to manipulate their influence on nucleation and crystal growth rate by effectively controlling polymer confinement and polymer-particle interactions. Designing relative differences in nanoparticle dispersion and mobility allows for increased control over the crystallization rate of the polymer matrix and the subsequent nanoparticle structure of the composite.

*DE-SC0018111
DE-SC0018135
DE-SC0018182

10:48AM W33.00013: Kinetics of Shape-fixing in Semicrystalline Shape-memory Networks* JEH-CHANG YANG (Presenter), MITCHELL ANTHAMATTEN, Chemical Engineering, University of Rochester — Crystallization of elastic polymer networks can enable shape-fixing of elastically deformed shapes which can subsequently be melted to regenerate stress or revert to the original shape. The initial step of a shape-memory cycle is shape-programming and involves the formation of connected crystal domains that can prevent the release of stored elastic strain energy. Crystallization kinetics play a critical role in determining the conditions required for sufficient shape-fixing. Here, we assess how imposed strain and undercooling affect crystallization kinetics and concomitant stress loss of crosslinked poly(caprolactone)s. Isothermal crystallization experiments were performed that involve in situ x-ray scattering combined with stress decay measurements. The main finding is that only a small amount of crystallization is needed to significantly reduce tensile stress. This result is valid for low levels of strain and undercooling, and it has broad implications for engineering new shape memory materials.

*Funding was provided by NSF under Grant ECCS-1530540 and Cornell High Energy Synchrotron Source (CHESS) through NSF under DMR-1332208. J.-C.Y. was supported by a Horton Fellowship from the Laboratory of Laser Energetics.

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W34 DPOLY GSCCM DCP: Polymers Under Extreme Environmental Conditions 506 - Nir Goldman, Lawrence Livermore Natl Lab - Tag(s): Focus
Anisotropic hydrolysis susceptibility in deformed polydimethylsiloxanes*  
MATTHEW KROONBLAWD (Presenter), NIR GOLDMAN, JAMES LEWICKI, Lawrence Livermore Natl Lab — Environmental factors such as humidity have potential to drive chemical degradation of polymer networks in ways that compound with mechanical stressors. Using two levels of quantum chemical theory, we identify a possible electronic driver for strain-induced chemical susceptibility in deformed polydimethylsiloxane (PDMS) chains. High throughput sampling with a validated semiempirical density functional tight binding (DFTB) model is used to explore the complicated interplay between hydrolytic chain scissioning reactions, mechanical deformations of the backbone, water attack vector, and chain mobility. We show that sustaining tension through concerted strains of the backbone over at least a few monomer units is necessary to significantly increase hydrolysis susceptibility. A reactive order parameter is developed that describes chain scission probabilities as a complicated function of the backbone degrees of freedom. The trends identified suggest simple physical descriptions for the synergistic coupling of local mechanical deformation and chemistry in silicones.


Relating Electrical Properties of Highly Disordered Insulating Materials via the Dispersion Parameter*  
ZACHARY GIBSON (Presenter), JOHN R DENNISON, Utah State University — Relations between electrical properties, critical transitions (CT), and the dispersion parameter $\alpha$ for highly disordered insulating materials (HDIM) are presented. The dispersion parameter is often defined as the thermal energy (low field regime) or field energy (high field regime) scaled by a material-dependent characteristic energy (energetic width of DOS within mobility gap). For dispersive transport, $0<\alpha<1$; $\alpha=1$ defines a CT in both temperature (T) and electric field. A kink is observed in double logarithmic current-time plots measured at constant voltage, similar to Scher-Montroll curves for pulsed photoconductivity. Dark conductivity measurements transition from $T^{-1}$ to $T^{-1/4}$ dependence on a double logarithmic current-T plot at the temperature CT, indicative of a transition from multiple trapping to variable range hopping dominated transport. A field CT is apparent in pulsed electroacoustic measurements of charge distributions where normal transport is observed at high fields, corresponding to the onset of normal transport and electrostatic breakdown. As an example of a prototypical HDIM, various measurements are presented for low-density polyethylene.

*Supported by AFRL STTR FA 9453-13-C-0067 and a USU Presidential Doctoral Research Fellowship.
8:24AM W34.00003: Atomistic analysis of PBO carbonization process with ReaxFF Reactive Force Field* MALGORZATA KOWALIK (Presenter), CHOWDHURY M. ASHRAF, Department of Mechanical Engineering, Penn State University, SIAVASH RAJABPOUR, Department of Chemical Engineering, Penn State University, BEHZAD DAMIRCHI, DOOMAN AKBARIAN, QIAN MAO, ADRI C.T. VAN DUIN, Department of Mechanical Engineering, Penn State University — There is a constant need for an alternative precursor polymer for the carbon fibers (CFs) production with lowering the costs without compromising CFs mechanical properties. We report an atomistic simulation of a direct carbonization of poly(p-phenylene-2,6-benzobisoxazole) (PBO) that can be transformed into high strength carbon fiber. The possibility of using various heating rates is considered and observed gaseous molecules as well as 6-membered all-carbon ring production analyzed. Based on our ReaxFF atomistic-scale reactive molecular dynamics simulations of the direct carbonization of the PBO we proposed a mechanism that might be responsible for an improvement of the mechanical characteristics of the PBO-based CFs with ultrafast heating rate treatment observed in experiment.

*This project is funded by the Department of Energy Grant No. DE-EE0008195.

8:36AM W34.00004: Characterization of the shock response of heterogenous polymer foams using multi-point PDV measurements JOHN LANG (Presenter), RACHEL HUBER, KATHY MAERZKE, DANA DATTELBAUM, Los Alamos Natl Lab — SX358 is a cross-linked polydimethylsiloxane (PDMS) that can be synthesized in a range of densities (0-65% porous). When porous, it is a stochastic, open cell heterogenous foam with varying pore sizes (10-1000s µm). To model SX358, experimental data is needed to inform equation of state (EOS) models over the range of initial densities. Gas gun planar impact was used to measure high pressure, high temperature material response and shock compression with traditional configurations and diagnostics. The results vary widely, which we attribute to the heterogenous structure of the foam. The diagnostics may interrogate areas where the local density is less than (e.g., a large pore) or greater than the average density. To explore pore variability, we interrogated a large sample area with many velocimetry probes, and then combined the data to obtain an ‘average’ material response. As with past experiments the individual probes showed a varied response. When the data are combined, the ‘average’ response provides a better measure of the continuum response of the stochastic foam with a reduced uncertainty. Phase contrast imaging of the propagating shock front and velocimetry diagnostics with interrogation areas larger than the pore sizes are under investigation to better constrain the EOS.
**8:48AM W34.00005: Investigating the Shock Properties of Polycarbonate**  
JAMES HAWRELIAK (Presenter), Washington State Univ — Polycarbonate is an impact resistant optically transparent thermal plastic used in many engineering applications. The optical transparency and low-Z composition of the polymer chains which make up polycarbonate have made it a candidate window material for dynamic compression experiments. Specifically, experiments which uses x-rays to probe the lattice structure. The low-Z allows for high x-ray transmission and low x-ray scattering for performing x-ray diffraction experiments to measure the atomistic properties, and the optical transparency is suited for using optical probes to measure the bulk material response. We present measurements of the optical properties of polycarbonate at 1550nm and 532nm, the two wavelengths used for velocity interferometry in shock wave experiments.

*The work was supported by the grant DE-SC0016360 funded by the U.S. Department of Energy, Office of Science. The author acknowledges the support of the DOE/NNSA for the Institute for Shock Physics' research activities.*

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**9:00AM W34.00006: Polyimide Two-Wave Structure Produced by Shock Compression**  
RACHEL HUBER (Presenter), BRIAN BARTRAM, Dana DATTELBAUM, LLOYD L GIBSON, JOHN LANG, Los Alamos National Laboratory — Polymeric materials undergo densification when dynamically compressed, transitioning the polymer from reactants to products. During gas gun-driven planar impact, we can observe this decomposition with velocimetry probes capturing the particle velocity (movement of the material) history that results from the impinging shock wave. This transition produces a shock wave for both the reactants and the products. If the volume change is large enough, the reactants wave will separate from products wave, generating a two-wave structure in the velocimetry profiles. If the polymer is shocked above or below this transition region, a single wave will be observed. Polyimide (PI) is composed of imide monomer units (-OC=NC-C=O-); it is used as a thermoplastic for high pressure, high temperature applications. Understanding how this polymer reacts within its transition region (17.8-30 GPa) provides vital information for equation of state (EOS) modeling. PI has a large volume change, 20.3%, when shocked into its transition region. Through gas gun-driven planar impact we have observed a two-wave structure in PI with velocimetry probes. The two-wave structure measurement provides kinetic parameters for the reactants-to-products transition that informs the kinetics for EOS models.

*Science Campaign 2*
9:12AM W34.00007: 3D-printed polymeric foam under constant compressive strain: constitutive and multiscale models of long-term property changes [Invited] AMITESH MAITI (Presenter), Lawrence Livermore Natl Lab — Cellular solids or foams constitute an important class of materials with diverse applications. Traditional processes to create such materials lead to significant dispersion in pore size, shape, thickness, and topology. However, recent LLNL advances in 3D printing of polymeric foams by direct-ink-write has enabled the creation of cellular materials of programmable microstructure, customizable shapes, and tunable mechanical response. Success of these 3D printed parts as viable replacement for traditional stochastic foams depends critically on their performance and stability under long-term mechanical strain. To study such effects, we carried out accelerated aging experiments on foams, both stochastic and 3D printed, under a state of constant compression. We monitored the time-evolution of permanent structural change (compression set), altered load-bearing capacity, and changed modulus. This talk will highlight several recent results based on the above measurements, including: (1) the prediction of long-term property changes through time-temperature superposition, with uncertainty margins created using statistical bootstrap; (2) the development of an “age aware” constitutive materials model using the Ogden hyperfoam formalism in a Tobolsky two-network scheme; and (3) finite-element stress analysis within X-ray-CT-imaged foam microstructures that illustrates the superior stability of certain 3D printed close-packed frameworks. The basic steps to a reptation-tube-encompassing coarse-grained strategy to model macroscale aging effects in rubber will also be discussed.

Acknowledgement: This work is a result of close collaboration with LLNL colleagues W. Small, J. Lewicki, A. Saab, T. Weisgraber, S. Chinn, J. Lenhardt, T. Wilson, E. Duoss, C. Spadaccini, and R. Maxwell, and academic collaborator Prof. Y. Li at U. Connecticut. The work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
9:48AM W34.00008: Features of shock Hugoniot measurements of underdense materials*
DANA DATTELBAUM (Presenter), JOSHUA COE, Los Alamos Natl Lab, BRITTANY BRANCH, Sandia National Laboratories — An important challenge pertaining to equation of state model improvements for underdense materials is the quality of experimental measurements. A recent analysis of errors associated with historical explosively-driven experiments yielded large values (>10%) – due, in part, to the near-equivalencies of the shock and mass velocities, which give rise to large errors in density, and spatiotemporal limitations on diagnostics. Other challenges include material heterogeneity and high shock temperatures, both of which contribute to difficulties in experimental measurements. Shock heating, for example, can dominate the compressive response resulting in “anomalous compression.” In the anomalous regime, the Hugoniot curves often bend back, with increases in shock pressure resulting in no volume change, even at modest porosities. We present a summary of features of shock Hugoniots of porous polymers over a range of initial densities, and show the interplays between initial density, shock stress, and normal vs. anomalous regimes. We also describe how penetrating x-ray-based imaging can be used to drive down errors. Recommendations will be made for future improvements and their impacts on theoretical model development.

*Triad LLC operates Los Alamos National Laboratory for the U.S. DOE

10:00AM W34.00009: Efficient Shockwave Energy Dissipation in Dynamic PDMS Networks
CHRISTOPHER EVANS (Presenter), NANCY SOTTOS, JAEJUN LEE, LAURA PORATH, BRIAN JING, University of Illinois at Urbana-Champaign — Polymer networks containing dynamic bonds have received increasing attention over the past decade. Depending on the specific bond, a certain amount of energy is required for the bonds to undergo an exchange process. We hypothesize and demonstrate that dynamic bonds in polydimethylsiloxane (PDMS) networks can be used as an effective mechanism for dissipating energy, in particular from a shockwave. The density of dynamic bonds can be controlled which controls the modulus while the network Tg is unchanged. Using a classical laser induced shockwave technique, superior energy dissipation is observed in a PDMS dynamic rubber compared to the benchmark polyurea. The dynamic PDMS also outperforms covalently crosslinked PDMS and shows a monotonic improvement in dissipation performance with increasing density of dynamic boronic ester bonds. In all cases, the Tg is invariant in the different networks (-125 °C) implying a minimal role of segmental dynamics on dissipation in these specific networks. The dynamic networks can be shocked multiple times with invariant performance suggesting the mechanism is non-destructive and related to bond exchange rather than breakage.
10:12AM W34.00010: Synthesis and Self-Assembly of Multi-Patch Functional Colloids* [Invited]

ALEXANDER BÖKER (Presenter), Fraunhofer-Institute for Applied Polymer Research IAP — This talk will discuss the creation of artificial materials systems which can be programmed to self-assemble and may even allow self-replication of structures. To achieve this, an indispensable prerequisite is the multi-directional control of interactions between the building blocks of materials. Thus, we describe a new class of multi-patch colloidal particles via an advanced micro-contact printing technique yielding patches of different chemical or physical functionalities. The new production process allows precise control over the patch location and chemistry even with low molecular weight inks and thus also yields particles that go well beyond known ABA- or ABC-type Janus particles. In addition chemical approaches for selective interaction and their influence on the self-assembly behavior will be discussed[1-5].

"Characteristics of Microcontact Printing with Polyelectrolyte Ink for the Precise Preparation of Patches on Silica Particles" RSC Advances 2018, 8, 39241.


*This work has been funded in the framework of the European Research Council (ERC) project REPLICOLL (grant number 648365).
W34.00011: Surface hardness enhancement of ion bombarded polycarbonate*  SUNMOG YEO (Presenter), CHANG YOUNG LEE, WON-JE CHO, YONG-SEOK HWANG, CHORONG KIM, DONG-SEOK KIM, KOMAC, Korea Atomic Energy Research Institute — The surface hardness of polycarbonate (PC) can be enhanced by ion bombardment with energy of a few hundred KeV. Nano indentation measurement on ion bombardment PC shows that the hardness of PC increases with increasing the ion dose. In addition, the surface properties examined by FT-IR show that the lighter ion mass causes the increase of C=O (1680-1750 cm\(^{-1}\)) and C=C (1500-1700 cm\(^{-1}\)) stretching vibration and the relative ratio of C-O-C peak near the wave number of 1200 cm\(^{-1}\) decreases with increasing dose and energy of H\(^{+}\) ion. We discuss the surface hardness enhancement of PC based on these results.

*This work has been supported through KOMAC (Korea Multi-purpose Accelerator Complex) operation fund and the Creative Research Program of KAERI by MSIP (Ministry of Science, ICT and Future Planning)

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W35 DPOLY: Dynamics in Polyelectrolyte Complexes and Associative Polymer Networks 507 - Jelena Dinic, Argonne Natl Lab - Tag(s): Focus

8:00AM W35.00001: Engineering hydrogel viscoelastic mechanics via bio-inspired supramolecular metal-coordinate dynamics  NIELS HOLTEN-ANDERSEN (Presenter), Massachusetts Institute of Technology MIT — Growing evidence supports a critical role of metal-coordinate supramolecular crosslinking in governing stimuli-responsive properties of soft biological materials. As such, bio-inspired metal-coordinate crosslinking provides unique opportunities to further our understanding of how to directly correlate macroscopic hydrogel mechanics with microscopic crosslink dynamics. Recent insights generated from such fundamental studies of metal-coordinate supramolecular chemo-mechanical couplings in hydrogels will be presented.
8:12AM W35.00002: Experimental evidence of universal behavior in ion-induced volume phase transition in polyelectrolyte gels* MATAN MUSSEL (Presenter), PETER BASSER, FERENC HORKAY, National Institutes of Health - NIH — Introduction of high valence counterions into polyelectrolyte solutions and gels results in a reversible volume phase transition. The volume change can be induced by a small change in the concentration of the equilibrium salt solution. In the present work new results are reported for the volume transition induced by calcium-sodium ion exchange in sodium polyacrylate gels made by osmotic swelling pressure and small angle neutron scattering measurements. We show that the threshold Ca\(^{2+}\) ion concentration at which the transition occurs increases with increasing NaCl concentration in the surrounding bath, decreases with increasing the concentration of the ionized groups on the polymer backbone and the temperature, and is practically unaffected by changing the crosslink density of the network. It is demonstrated that the normalized swelling data fall on a master curve, indicating that the volume transition exhibits universal behavior. These findings imply that gel volume transition is primarily governed by changes in the electrostatic interactions as a consequence of the divalent-monovalent ion exchange.

*No funding.

8:24AM W35.00003: pH modulated nanoparticle diffusion in silica-polyacrylamide hydrogels* KATIE ROSE (Presenter), DAEYEON LEE, Chemical and Biomolecular Engineering, University of Pennsylvania, RUSSELL COMPOSTO, Materials Science and Engineering, University of Pennsylvania — Using single particle tracking (SPT), we investigate nanoparticle (NP) diffusion in polyacrylamide hydrogels containing immobile silica particles (0% - 10% volume). For low concentrations of silica particles, two distinct populations of diffusing NPs are observed, localized and diffusive, whereas only diffusive NPs are found in the neat hydrogel. Primarily diffusive behavior is recovered for high concentrations of silica, attributed to an incomplete formation of the mesh as indicated by rheology. A proposed mechanism for the localized behavior of the NP probes is the pH mediated attraction via hydrogen bonding interaction between the PEG brush grafted to the surface of the NP and the silanol groups on the silica surface. The extent of the PEG-silica interaction and its subsequent impact on NP dynamics is examined at different pH values using quartz crystal microbalance with dissipation (QCM-D). This study provides valuable insight into controlling the diffusion of NPs in hydrogels based on pH mediated interactions with an incorporated tertiary component, with implications in drug delivery and filtration.

*This work is supported by NSF-PIRE #1545884 and NSF-GRFP.
Length-scale dependent anomalous diffusion regimes in associative protein hydrogels*

AMEYA RAO (Presenter), HELEN YAO, BRADLEY OLSEN, Massachusetts Institute of Technology MIT — Associative polymer gels are of interest as tunable, responsive materials for biomedical and soft robotics applications. Although theories can describe the effect of crosslink reversibility on network viscoelasticity, diffusion of chains through the network is poorly understood due to the complex interplay between sticker association and strand relaxation. Here, we use forced Rayleigh scattering and neutron spin echo to study self-diffusion in model coiled-coil protein hydrogels over a range of 8 decades of length-squared. We show the first experimental evidence for multiple diffusion regimes spanning from the submolecular to the Fickian, including anomalous caging and superdiffusive regimes, which depend on the concentration and length scale probed. Interpreting these results in the context of Brownian dynamics simulations allows characterization of various diffusive modes and molecular parameters (e.g., sticker dissociation and strand relaxation time) governing transitions between these regimes. Finally, tracer diffusion of single coiled-coils is measured in a matrix of proteins containing 4 such domains to link quantitatively single-sticker dynamics to overall chain diffusion rates at various length scales.

*NSF DMR-1709315; DOE DE-SC0007106. AR acknowledges an NDSEG fellowship.

Anomalous diffusion in a model associative network with high sticker density.*

IRINA MAHMAD RASID (Presenter), NIELS HOLTEN-ANDERSEN, BRADLEY OLSEN, Massachusetts Institute of Technology MIT — The dynamic nature of the bonds in associative polymer networks has led to their use in the design of tough and self-healing hydrogels. The ability to self-heal in these networks relies on the reformation of the original network and is strongly affected by the timescale for self-diffusion. This work measured the self-diffusion of a model associative network, consisting of a linear polymer functionalized with histidine side-groups, using forced Rayleigh scattering. The effect of sticker density was investigated by synthesizing random copolymers through RAFT polymerization, with up to 15 histidine groups per chain. The polymers showed anomalous diffusion that persisted even for the highest sticker density. Earlier work has shown that anomalous diffusion as observed from FRS measurements in other associative networks, with up to four stickers per chain, primarily result from molecular hopping. These results indicate that molecular hopping could still be an important mode of self-diffusion in these networks, even at high sticker densities.

*Institute for Soldier Nanotechnologies (ISN)
-Office of Naval Research (ONR)
-Center for Materials Science and Engineering (CMSE)
-National Science Foundation (NSF)
9:00AM W35.00006: Scattering Investigations of Structure and Dynamics of Triblock Polyelectrolyte Complex Hydrogels  DEFU LI (Presenter), SAMANVAYA SRIVASTAVA, Chemical and Biomolecular Engineering, University of California, Los Angeles — Polyelectrolyte complex (PEC) hydrogels are physically crosslinked 3-D networks that form upon complexation between oppositely charged polyelectrolytes. The development and use of PEC hydrogels for diverse biomedical applications require an in-depth understanding of the thermodynamics and kinetics of hydrogel assembly as well as their mesoscale structures and bulk properties. In this talk, we introduce the intimate correlations between PEC domain morphologies and material relaxation timescales in hydrogels comprising oppositely charged ABA triblock polyelectrolytes. Polymer size and concentration as well as solution ionic strength were all found to dictate the PEC domain morphologies, size and arrangements. X-ray photon correlation spectroscopy (XPCS) investigations revealed two distinct relaxation modes of the nanoscale PEC domains. The polymer concentration-independent faster relaxation was expected to capture the dynamic processes inside the PEC domains, while the slower polymer concentration-dependent domain relaxation timescales were found to be inherently linked with the equilibrium hydrogel structure. Upon addition of salt, both relaxation modes became faster, indicating speeding of the intra-domain relaxations and smaller, faster-relaxing PEC domains.

9:12AM W35.00007: Stimuli-responsive polyelectrolyte gels and the role of ion and polymer solvation*  ALEXANDROS CHREMOS (Presenter), MATAN MUSSEL, PETER BASSER, Section on Quantitative Imaging and Tissue Sciences, National Institutes of Health, JACK DOUGLAS, National Institute of Standards and Technology, FERENC HORKAY, Section on Quantitative Imaging and Tissue Sciences, National Institutes of Health — Polyelectrolyte gels are essential components of living systems, since biological tissues are largely composed of polyelectrolyte gels providing a medium for the transport of ions and molecules more easily and effectively while at the same time providing structural integrity. The challenge of modeling the influence of solvation and ion partition on the swelling of gels is due to the coupling between the polyelectrolyte chain configurations and the spatial distribution of the ionic species in solution. We perform molecular dynamics simulations of a minimal model of a polyelectrolyte nanogel particle in solution with an explicit solvent and ions, where the relative strength of dispersion interactions between the solvent and the charged species defines the solvent quality and the position of the ion along the Hofmeister series. Our findings demonstrate that the solvent plays a crucial role in gel swelling and the sensitivity of swelling to the addition of salt and the ion partitioning between the gel and the surrounding solution. Overall, our findings provide a guideline for the development of a more predictive theory of the thermodynamic and transport properties of these complex systems.

*National Institutes of Health
9:24AM W35.00008: Influence of temperature, salt and molecular weight on the dynamics of polyelectrolyte complexes. MO YANG (Presenter), Department of Chemistry and Biochemistry, Florida State University, JIANBING SHI, School of Materials Science and Engineering, Beijing Institute of Technology, JOSEPH SCHLENOFF, Department of Chemistry and Biochemistry, Florida State University — Oppositely-charged polyelectrolytes can spontaneously associate into either solid-like complexes or liquid-like coacervates based on the external salt concentration. The linear viscoelasticity of polyelectrolyte complexes/coacervates (PEC) can be influenced by a variety of factors, such as temperature, salt and pH. Due to the insufficient chain length of polyelectrolyte, few works have reported the entanglement behavior of PEC and only reptation time ($\tau_{\text{rep}}$) has been found. Here, we prepared five pairs of PEC with different molecular weight and matched polycation/polyanion chain length. Rheology experiments were carried out for all PEC pairs at different temperatures and salt concentrations. Time-temperature (TTS) and time-temperature-salt (TTSS) superpositions were achieved with good fit to sticky association theory. Relaxation times for polymer partnering ($\tau_b$), entanglement ($\tau_e$) and reptation ($\tau_{\text{rep}}$) were revealed directly from the TTS data. All these characteristic lifetimes were slowed by the sticky dynamics of Pol$^+$Pol$^-$ pairs. We found that the relaxation kinetics of temperature showed Arrhenius dependence, whereas changing the salt concentration impacted the lifetime of Pol$^+$Pol$^-$ pairs, the number of stickers per chain and the volume fraction of polymer.

9:36AM W35.00009: Water binding and mobility in polyelectrolyte complexes* PIOTR BATYS, Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Poland, SOUSA JAVAN NIKKHAH, Aalto University, Finland, YANPU ZHANG, SUVESHW LALWANI, JODIE LUTKENHAUS, Texas A&M University, TX, United States, MARIA SAMMALKORPI (Presenter), Aalto University, Finland — Water is central in the assembly and the dynamics of charged macromolecular systems including polyelectrolyte assemblies. Nevertheless, it remains a challenge to resolve how water influences assembly characteristics and materials properties of these systems. We have examined via molecular modelling and interconnected experiments the role of water at molecular level on polyelectrolyte complexes and multilayers. We compare different polyelectrolyte systems under varying hydration and salt content and report that the hydration and water binding at especially intrinsic ion pairs connects with the thermal and mechanical response of hydrated polyelectrolyte assemblies. The findings rise attention to water and water partitioning as a control parameter of polyelectrolyte materials properties.


*This work was supported by the Academy of Finland (Grant. No. 309324) (M.S.) and National Science Foundation (Grant No. 1609696) (J.L.L.).
9:48AM W35.00010: Water's effect on the glass transition and dynamic mechanical properties of polyelectrolyte complexes* [Invited] JODIE LUTKENHAUS (Presenter), Texas A&M Univ, MARIA SAMMALKORPI, Aalto University, PIOTR BATYS, Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences — Charged assemblies bearing opposite or complementary charges span natural (proteins, enzymes, DNA) to synthetic materials (surfactants, synthetic polyelectrolytes). Assembly is facilitated by electrostatic attraction and entropic release of counterions, and most often occurs in aqueous media. Notably decades ago, Michaels described synthetic polyelectrolyte complexes as brittle when dry but “leathery or rubberlike” when wet, which points to the strong effect of water on the mobility of a charged assembly. Here, the molecular origin of the glass transition is quantified for several charged macromolecular systems is investigated using calorimetry and molecular modeling as a function of water content. A general relationship is revealed as it holds for two completely different types of charged systems (pH- and salt-sensitive) and for both polyelectrolyte complexes and polyelectrolyte multilayers, which are made by different paths. This suggests that water facilitates the relaxation of charged assemblies by reducing attractions between oppositely charged intrinsic ion pairs. We further demonstrate the dual role of water and temperature in the dynamics of polyelectrolyte complexes by showing time-temperature and time-water superpositioning in a single polyelectrolyte complex system. This is accomplished by changing the relative humidity to adjust the water content in the complex during testing. Results indicate the existence of a water-based shift factor ($a_w$) that bears a log-linear relationship.

*This work was supported by the National Science Foundation (Grant Nos. 1609696) (J.L.L.) and Academy of Finland (Grant. No. 309324) (M.S.). This work was also supported by CSC – IT Center for Science, Finland, and RAMI – RawMatTERS Finland Infrastructure by computational resources.

10:24AM W35.00011: Electric field-dependent metastable phenomena in polyelectrolyte solutions* KATCHER MARGOSSIAN (Presenter), MURUGAPPAN MUTHUKUMAR, Department of Polymer Science and Engineering, University of Massachusetts Amherst — We have recorded the response of various polyelectrolyte systems to applied voltages. Here, we explore the effects of chain length, architecture, and concentration on the charge transport properties of our solutions in order to determine the origin of nonlinear behavior demonstrated by these materials. Our findings suggest the existence of several mechanisms by which ions can flow through charged polymers, each of which can be observed within distinct voltage regimes and solution conditions. With these findings, we can understand similar characteristics seen in other charged networks.

*NSF DMR-1504265
NSF Soft Materials in the Life Sciences National Research Traineeship-1545399
10:36AM W35.00012: Electrospinning Coacervates – No Chain Entanglements Required
Xiangxi Meng, Department of Chemical Engineering, University of Massachusetts Amherst, Yifeng Du, Department of Polymer Science & Engineering, University of Massachusetts Amherst, Yalin Liu, Department of Chemical Engineering, University of Massachusetts Amherst, Bryan Coughlin, Department of Polymer Science & Engineering, University of Massachusetts Amherst, Jessica Schiffman, Sarah Perry (Presenter), Department of Chemical Engineering, University of Massachusetts Amherst — Electrospun fibers have utility across a range of fields. However, electrospinning traditionally requires long-chain, entangled polymer solutions. This combination of factors is necessary to create physical entanglements that relax slower than the timescale for electrospinning to prevent capillary breakup of the polymer jet. This requirement has also meant that spinning polyelectrolytes is particularly challenging as electrostatic repulsions along the polymer backbone dramatically increase the solution viscosity. We have reported a strategy for electrospinning charged polymers via complex coacervation. The coacervate liquid resulting from the complexation of oppositely-charged polymers can be used for electrospinning, resulting in solid fibers that are stable against dissolution in water and organic solvents. Here, we explore the potential for using the cooperative electrostatic interactions between polymer chains in place of physical entanglements. We investigated the electrospinnability of coacervates as a function of chain length. We demonstrated successful spinning of fibers using coacervates of oligomers of length <10. These results suggest the potential for using coacervates as a new class of electrospun materials where fiber formation is decoupled from chain length.

10:48AM W35.00013: Phase Separation and Gelation in Solutions of A–B Associative Polymers
Scott Danielsen (Presenter), Michael Rubinstein, Mechanical Engineering and Materials Science, Duke University — An equilibrium theory for reversible network formation in two-component solutions of associative polymers is presented to account for the phase behavior due to hydrogen bonding, metal–ligand, electrostatic, or other pairwise associative interactions. We consider polymers of types A and B with many associating groups per chain and consider only A–B association between the groups. A simple analytical expression for the free energy is derived and is shown to be consistent with the classical Flory-Stockmayer gelation theory. It is shown that association and formation of a reversible network is always accompanied by a tendency for phase separation, even at good solvent conditions, a significant difference from self-associative polymers. Homogeneous networks are most easily stabilized near stoichiometric conditions between A and B associative groups, resulting in a sol–gel–sol transition as the overall composition is altered. Chemical incompatibility between the A and B polymers drives a competition between attractively and repulsively-driven phase separation, leading to microphase formation and eutectic behavior.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W36 DCOMP: Twenty years of the Quantum Cluster Theory: recent progress 601/603 - Juana Moreno, Louisiana State University, Baton Rouge - Tag(s): Invited
8:00AM W36.00001: Impurity models and the development of quantum cluster approaches to lattice models of quantum condensed matter [Invited]  HULIKAL KRISHNAMURTHY (Presenter), Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science — My aim in this talk will be to provide a historical perspective of the evolution of computational quantum many-body ideas and methods connected with the first numerical solutions of quantum impurity problems leading on to the development of modern quantum cluster theories of strongly correlated and disordered condensed matter systems, the subject of this symposium. I will review the advances that took place, both in understanding and in the techniques of solution, of quantum impurity models in the 70s and 80s, the development of the dynamical mean-field theory in the late 80s and early 90s, and of its cluster extensions in the late 90s and early 2000s.

8:36AM W36.00002: Quantum Cluster Theory of Unconventional Superconductivity* [Invited] THOMAS MAIER (Presenter), Oak Ridge National Laboratory — Quantum cluster theories provide an important framework to give insight into the complex behavior and different quantum states observed in correlated electron materials. In particular, they can provide an understanding of the mechanisms that give rise to superconductivity in unconventional superconductors, in which pairing is driven by electron-electron interactions. Here we discuss how dynamic cluster approximation quantum Monte Carlo calculations of Hubbard models have progressed in addressing this problem, and how this progress is linked to advances in algorithms and high-end computing hardware.

*This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

9:12AM W36.00003: Multiscale approaches to strongly correlated systems in and out of equilibrium [Invited] HERBERT FOTSO (Presenter), University at Albany — The degrees of freedom that confer to strongly correlated systems their many intriguing properties also render them fairly intractable through typical perturbative treatments. For this reason, many of the mechanisms responsible for these technologically promising properties remain rather elusive. Computational approaches have played a major role in helping to fill this void. In particular, dynamical mean field theory (DMFT) and its cluster extension, the dynamical cluster approximation (DCA) have allowed significant progress. However, despite all the insightful results of the dynamical cluster approximation, computational constraints (sign problem, exponential growth of the Hilbert space) still limit the length scale within which correlations can be treated exactly in the formalism. A natural next step is the development of multiscale many body approaches whereby this challenge is addressed by introducing, between the short length scale where correlations are treated exactly using a cluster solver such Quantum Monte Carlo (QMC) or exact diagonalization, and the long length scale where correlations are treated in a mean field, an intermediate length scale within which correlations can be treated perturbatively. We will discuss implementations of this multiscale many body approach and the results they have yielded. In addition, we will discuss the framework for extension of quantum cluster approximations to the nonequilibrium problem.
9:48AM W36.00004: Quantum cluster typical medium methods for the study of localization in strongly disordered electronic systems.* [Invited] HANNA TERLETSKA (Presenter), Middle Tennessee State Univ — Disorder is a common feature of many materials and often plays a key role in changing and controlling their mechanical, electronic and other functional properties. Anderson localization is one of the fascinating effects of disorder in materials, which is often hard to capture numerically. There has been great progress made in the last several years towards understanding the properties of disordered electronic systems and electron localization, in particular, based on the effective medium methods. We have recently developed the Typical Medium Dynamical Cluster Approximation (TMDCA) for disordered electronic systems [1, 2]. The TMDCA enables quantitative analysis of electron localized states in disordered electron systems. The method is an effective medium approach that maps a given disorder lattice problem onto a quantum cluster embedded in an effective typical medium, which is determined self-consistently. Following the ideas of Dobrosavljevic et al. [3], the TMDCA employs the cluster typical (geometrically averaged) density of states as an order parameter to detect the localized electrons states. It has been shown that TMDCA not only correctly captures non-local effects but also recovers exact analytical results in simple disorder models [1]. In this talk, I will provide an overview of various recent applications of the TMDCA to a variety of models and systems, including application of the method to interacting disordered electrons as well as realistic systems in the framework of the ab-initio methods.


*This work is supported by NSF OAC grant 1931367 and US DOE de-sc0017861.

10:24AM W36.00005: Cluster dynamical mean field studies of two-particle response functions in the Hubbard model* [Invited] EMANUEL GULL (Presenter), XINYANG DONG, Univ of Michigan - Ann Arbor, XI CHEN, Simons Foundation — Over the last twenty years, the cluster dynamical mean field theory has generated useful insight into the Hubbard model and its relation to the pseudogap and superconductivity in the two-dimensional Hubbard model. While the behavior of single-particle properties of the model is well understood, this was so far not the case for higher order correlation functions. This talk will introduce susceptibility calculations and show comparisons to a range of experimental two-particle probes in the cuprates, including NMR, neutron spectroscopy, and M-EELS. We will also show how two-particle quantities can be used to identify the leading fluctuations.

*This work was funded by NSF DMR 1606348
8:00 AM W37.00001: The Making of Modern Physics in Colonial India [Invited] SOMADITYA BANERJEE (Presenter), Austin Peay State University — How did modern physics establish itself in India—a British colony—in the early 20th century? Who were the key actors and why did they develop physics in a colonized country far away from a European metropole? By using the case studies of Jagadish Chandra Bose, Satyendranath Bose and Chandrasekhara Venkata Raman, this talk will explore their physics, nationalism and social identity as "well-mannered intelligentsia" who played a key role in the making of modern physics in a country still under colonial domination. Finally, it will be argued how the local and the global were entangled in the worldview of these colonial intellectuals and the correlations between the discontinuous 'light quantum' and Indian history that played a key role in the ushering in of modern Indian physics.

8:36 AM W37.00002: Women and Physical Sciences in India: Bimla Buti and efforts to flourish a physical plasma community in her home country [Invited] INDIANARA SILVA (Presenter), Graduate Program in History, Philosophy and Science Teaching, Federal University of Bahia — Bimla Buti is the first Indian woman Physicist Fellow of Indian National Science Academy (INSA) and The Academy of Sciences of the Developing World (TWAS). Her contributions to physical sciences have been celebrated with awards, such as INSA-Vainu Bappu Award, Vikram Sarabhai Award, and Jawaharlal Nehru Birth Centenary Lectureship Award. Buti received her scientific recognitions with surprise as, using her own words, “it was almost impossible for me, a woman scientist in a man-dominated field, to get nominated for prestigious awards like the Bhatnagar award” (Buti, 2008, p. 38). The man-dominated field was plasma physics. To Indian physical sciences, besides writing papers and books, she contributed to developing a research program on plasma physics at the Physical Research Laboratory (PRL) and founded The Plasma Science Society in India. “We managed to establish a very strong group in plasma physics, both theoretical and experimental, at PRL” (Buti, 2008, p. 39). This talk will trace her contributions to physical sciences, struggles to become a female physicist, and efforts to build a career and community in plasma physics, contributing, thus, to the History of Science in India.
9:12AM W37.00003: “The free side of the meter”: Trustworthiness, theft and class identity in reading the domestic electric meter in early twentieth-century Calcutta [Invited]
ANIMESH CHATTERJEE (Presenter), Leeds Trinity University — Of all the devices used in early electric supply projects in early twentieth century Calcutta, the domestic meter was perhaps the most controversial. Introduced as a reliable billing method to measure consumption by customers connected to the newly introduced electric supply system, the electric meter was also at the centre of cases of “improper use” of electricity supply. The term “improper use” is used broadly here to refer to a variety of consumer practices that the Calcutta Electric Supply Corporation believed to be interferences to their property and operations. These included theft of electricity by bypassing or breaking seals on electric meters, or using electricity for purposes other than that for which it was supplied to the customer. This paper examines some of the disputes between customers, and engineers and inspectors of Calcutta Electric Supply Corporation on the deployment and use of electric supply and meters in early twentieth century Calcutta. Following recent works on users and non-users of technologies, and trust and the morality of measurements, this paper examines how electric meters became central to concerns over issues of quantities measures by meters, the class identity of customers, and trust between the supplier, consumers and the electric meter. In doing so, this paper will focus on both the design of measurements instruments, and the agency and discretion of the electrical consumer, thereby providing new perspectives on how consumers, suppliers and electrical measurement technologies interacted during the early days of electricity supply in colonial Calcutta.

9:48AM W37.00004: Scientific Creativity in Peripheral Locations: The Madras Triple Helix Model of G.N. Ramachandran [Invited] DEEPANWITA DASGUPTA (Presenter), The University of Texas at El Paso — The name of the Indian scientist G. N. Ramachandran is associated forever with the discovery of the structure of Collagen. Present in almost all connective tissues, such as skins, bones or muscles, collagen was the third great discovery in biophysics right after the discovery of alpha helix by Linus Pauling and the DNA double helix by Crick and Watson. Unlike the first two however, this third discovery came from a young peripheral scientist who worked from an obscure newly-founded Department at the University of Madras. The discovery of the triple helix structure in collagen, and the subsequent creation of the Ramachandran Plot, was thus truly a case when a peripheral scientist won the race for discovery against numerous Goliaths in the field. In this presentation, my goal will be to trace the outlines of the reasoning that led Ramachandran from his early X-ray diffraction diagrams to the final triple helix structure and the controversy that created the Ramachandran Plot.

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W38 DQI: Control and Characterization Tools for Quantum Error Mitigation 607 - Timothy Proctor, Sandia National Laboratories - Tag(s): Focus
8:00AM W38.00001: Demonstrating error rate homogenization using dynamically corrected gates in a trapped ion system  CLAIRE EDMUNDS (Presenter), CORNELIUS HEMPEL, ALISTAIR MILNE, MICHAEL BIERCUK, Univ of Sydney — High quality, error-robust gates are a fundamental element of scalable quantum computing architectures; however, their performance is often limited by their high sensitivity to external perturbations and imperfections in the control field. We experimentally demonstrate that replacing “primitive” physical gates with error-suppressing, dynamically corrected gates (DCGs) can homogenize error rates across a qubit register in both space and time, in addition to reducing net error rates.

We perform parallel single-qubit operations on a multi-qubit register of $^{171}$Yb$^+$ ions using a microwave field. We achieve a best case single-qubit average error rate of 1.9e-5 using primitive gates, although inhomogeneous fields lead to an order of magnitude variation across the 10 qubit register. By using DCGs, we observe an 8.5x reduction in the spread of error rates across the register, and a 2.4x improvement of the average value. Furthermore, DCGs provide an added robustness to slow drifts in the control, reducing the overhead required for regular calibrations. Finally, we discuss a microwave synthesis chain using a cryogenic sapphire oscillator and an arbitrary waveform generator, aimed at improving the control-field phase noise and reducing the calibration requirements compared to traditional I/Q.

8:12AM W38.00002: Error Mitigation Via Simulated Measurement of Stabilizers*  AMY GREENE (Presenter), MORTEN KJAERGAARD, Massachusetts Institute of Technology MIT, MOLLIE SCHWARTZ, MIT Lincoln Laboratory, GABRIEL SAMACH, Massachusetts Institute of Technology MIT, ANDREAS BENTSSON, Chalmers University of Technology, MICHAEL O'KEEFFE, MIT Lincoln Laboratory, MILAD MARVIAN, RONI WINIK, Massachusetts Institute of Technology MIT, DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, JONILYN YODER, DANNA ROSENBERG, KEVIN OBENLAND, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, Massachusetts Institute of Technology MIT, IMAN MARVIAN, Duke, WILLIAM OLIVER, Massachusetts Institute of Technology MIT — While closed-loop control is the ideal for quantum error correction, open-loop techniques are more accessible given current technologies. Dynamical decoupling is the go-to error mitigation technique, but many of the noise mechanisms encountered in experimental implementations, such as microwave cross-talk or coherent gate errors, are not amenable to simple dynamical decoupling schemes. An alternative technique for these errors is to simulate measurement of stabilizer operators via the stochastic application of gates from the set of stabilizers. We demonstrate the error-mitigating effects of this simulated quantum measurement protocol on a small superconducting qubit processor.

*This research was funded in part by the ARO grant No. W911NF-18-1-0411; and was funded in part by the Assistant Secretary of Defense for Research & Engineering via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002; and was funded in part by a Google Fellowship in Quantum Computing. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.
8:24AM W38.00003: SPAM Error Correction: Transition Matrix versus Quasiprobabilities
MINGYU SUN (Presenter), MICHAEL RAY GELLER, University of Georgia — State preparation and measurement (SPAM) errors limit the performance of noisy intermediate-scale quantum computers and their potential for practical application. Two techniques have been used to partially mitigate these SPAM errors. Both approaches build approximate models of the errors via tomography and then attempt to invert it. The first technique is to measure the transition matrix between all initial and final classical states, and to use this information to classically correct subsequently measured data. The second technique recently proposed by Temme, Bravyi, and Gambetta decomposes an ideal circuit into a quasiprobabilistic mixture of noisy measured ones. While neither approach is scalable, it would be useful to know their effectiveness when applied to real SPAM errors. Here apply both methods to online IBM qubits, and find very similar predictions for one- and two-qubit corrected Pauli expectation values, with some indication that the simpler transition matrix method performs slightly better than the quasiprobability representation, at least for the SPAM errors encountered in superconducting qubits.

8:36AM W38.00004: Experimental Realization of Randomized Compiling for in-situ Error Reduction
AKEL HASHIM (Presenter), University of California, Berkeley, KASRA NOWROUZI, ALEXIS MORVAN, Lawrence Berkeley National Laboratory, RAVI KAUSHIK NAIK, JOHN MARK KREIKEBAUM, IRFAN SIDDIQI, University of California, Berkeley — We present work on reducing the average error during the operation of an algorithm through randomized compiling (RC) [1], which tailors arbitrary Markovian noise into stochastic Pauli errors. By compiling random single-qubit twirling gates into the bare sequence of an algorithm and averaging over many initializations of an RC circuit, the total error of an algorithm is reduced because the error per single qubit gate has been averaged into a stochastic noise channel that is independent of the gate itself. Here, we demonstrate experimental work towards implementing RC in both random circuits and quantum protocols for optimization problems. We show that RC suppresses coherent errors in a circuit and that it increases the probability of measuring the correct solution of an algorithm.


*This work was supported by the testbed program of the Advanced Scientific Computing Research for Basic Energy Sciences program, Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and the National Defense Science & Engineering Graduate (NDSEG) Fellowship.
8:48AM W38.00005: Optimizing stability and performance of cloud-based quantum systems

NEEREJA SUNDARESAN (Presenter), ISAAC LAUER, SRIKANTH SRINIVASAN, CINDY WANG, WILLIAM LANDERS, MICHAEL STUART GORDON, DOUGLAS T. MCCLURE, IBM Thomas J. Watson Research Center — Since the launch of the first five-qubit device on the IBM Q Experience platform in 2016, we have made steady increases in the number of devices available for cloud access, as well as their fidelity, stability, speed and uptime. Here we will discuss some of the challenges encountered, lessons learned, and best practices adopted in the bring-up, operation, and maintenance of these devices.

9:00AM W38.00006: Fidelity of sequences of SWAP operations in chains of multiple coupled qubits

ROBERT THROCKMORTON (Presenter), University of Maryland, College Park — We investigate the swapping of qubit states between neighboring qubits in a chain of multiple qubits with quasi-static noise both in the (nearest-neighbor) couplings between them and in fields applied to the individual qubits. We will assume no intentionally applied fields, so that all such fields that appear are due entirely to noise. We consider chains of several different lengths and different sequences of SWAP operations (i.e., different pairs of neighboring qubits to perform the operation on and different lengths). We determine the fidelity of these sequences as a function of sequence and qubit chain length for different noise strengths.

*This work was funded by the Laboratory for Physical Sciences.

9:12AM W38.00007: Noise-resistant Landau-Zener sweeps from geometrical curves

FEI ZHUANG (Presenter), JUNKAI ZENG, EDWIN BARNES, SOPHIA E. ECONOMOU, Virginia Tech — The decoherence of a qubit due to environmental noise is a long-standing problem in quantum information science. Recent work provided a new recipe for designing dynamically corrected gates analytically using a simple geometric formalism. By adapting that formalism, we demonstrate how to design noise-resistant Landau-Zener sweeps through an avoided crossing. In the case where the avoided crossing is created purely from noise, we demonstrate identity gates and phase gates that are robust against error up to second order. In the more general case where the avoided crossing exists in the absence of noise, we show that robust sweeping protocols are in one-to-one correspondence with curves lying on a sphere that obey certain constraints. We show how to exploit this correspondence to systematically construct noise-resistant Landau-Zener sweeps for generic avoided crossings.

*This work is supported by DOE grant no. de-sc0018326.
High-performance nonlinear optimization module for quantum control

HARRY SLATYER (Presenter), PER LIEBERMANN, MICHAEL HUSH, ANDRÉ CARVALHO, HARRISON BALL, STEPHEN GORE, MICHAEL BIERCUK, Q-CTRL — Precise manipulation of quantum systems via shaped control pulses has emerged as a key area of development for quantum physics and chemistry. In near-term quantum computers, for example, substitution of primitive operations with optimized noise-robust controls can yield improved fidelities for single- and multi-qubit gates without hardware modifications. However, for all but the most basic of systems, identifying ideal control pulses via analytic approaches is intractable, motivating an approach based on numerical optimization. In this talk we introduce a custom GPU-compatible optimization toolkit purpose-built for rapidly creating high-fidelity, noise-robust quantum controls in high-dimensional Hilbert spaces. We describe the design of the toolkit, provide examples of standard and custom workflows, and present benchmarking results that demonstrate the speedup enabled by the GPU-compatible graph architecture.

Implementation of a canonical phase measurement with quantum feedback

IRFAN SIDDIQI (Presenter), University of California, Berkeley — In many sectors of modern metrology and communication technology, information is encoded in electromagnetic waves, typically as an amplitude or phase. While current hardware can perform near-ideal measurements of photon number or field amplitude, a device that can perform an ideal phase measurement is elusive. In this work, we implement a single-shot canonical phase measurement on a one-photon wave packet which surpasses the current standard of heterodyne detection and is optimal for single-shot phase estimation. By applying quantum feedback to a Josephson parametric amplifier, our system adaptively changes its measurement basis during photon arrival and allows us to validate the detector’s performance by tracking the quantum state of the photon source. These results demonstrate that quantum feedback can both enhance the precision of a detector and enable it to measure new classes of physical observables.

*This work was supported by the ARO/LPS.
10:12AM W38.00010: Two-qubit Pauli-frame randomization in a superconducting system
MATTHEW WARE (Presenter), GUILHEM RIBEILL, LUKE GOVIA, Quantum Engineering and Computation, Raytheon BBN Technologies — Coherent noise and non-Markovianity are projected to be significant sources of non-ideal behavior in large scale quantum computers. One approach to dealing with such noise sources is called Randomized Compiling where quantum circuits are permuted by the insertion of random gates whose effect is tracked and inverted at the end of the circuit on a shot-by-shot basis. While this technique effectively removes coherent error and significantly reduces non-Markovianity, it can be quite challenging to implement experimentally due to the large number of random circuits that need to be generated and data that needs to be post processed. To remove some of the experimental overhead, we have implemented control system firmware that randomizes quantum circuits on-the-fly using custom control electronics. Here we build on previous work accomplishing this in a single qubit system extending it to circuits with two qubit gates.

“This document does not contain technology or technical data controlled under either the ITAR or the EAR.”

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10:24AM W38.00011: Deep Reinforcement Learning for Quantum Control: Learning to Optimally Navigate in Complex Noisy Environments
GREGORY QUIROZ (Presenter), PARAJ TITUM, KEVIN SCHULTZ, Johns Hopkins University Applied Physics Lab — Quantum control seeks to establish control over a quantum system in such a way so that logical operations are implemented while simultaneously mitigating unwanted interactions between the system and its environment. From the point of view of quantum computation, quantum control can potentially provide significant improvements in computational accuracy when quantum logic operations are tailored for the particular noise plaguing the hardware. Specifically tailoring each controlled operation can be quite demanding if one wishes to perform this task for every instantiation of a quantum algorithm. Here, we examine how one can leverage reinforcement learning to learn and predict quantum gates in the presence of temporally correlated noise. We discuss how this information provides knowledge about optimal gate construction for noise-tailored quantum algorithms, as well as how this approach potentially informs noise characterization.

*Army Research Office, DOE Office of Science
Assigning Hamiltonians to Open Quantum Systems

EUGEN DUMITRESCU (Presenter), PAVEL LOUGOVSKI, Oak Ridge National Lab — Building on recent efforts illustrating that one may characterize a closed system of k-local interacting particles, we study the task of identifying a local-Hamiltonian in the presence of additional environmental interactions. Beginning with a candidate system consisting of an XX-interacting spin chain subject to thermal relaxation noise, we show how both the Hamiltonian and the underlying Lindbladian can models can be inferred. Moreover, we study open-systems learning in the settings where one is given i) access to steady states, ii) dynamical information, as well as iii) in the presence of stochastic noise on the measurement output.

*The authors acknowledge DOE ASCR funding under the Quantum Computing Application Teams program, FWP number ERKJ347.

Friday, March 6, 2020 8:00 AM - 10:12 AM

Session W39 DCOMP GDS DMP: Machine Learning for Quantum Matter

8:00AM W39.00001: Differentiable programming tensor networks and quantum circuits

JINGUO LIU (Presenter), LEI WANG, Institute of Physics — Computation is playing an increasingly important role in the studies of complex quantum systems. Efficient and exact gradients from automatic differentiation (AD) changes the way we program. This talk covers a brief survey of the state of the art differential programming frameworks, and their applications to condensed matter physics and quantum computing. These application range from optimizing infinite tensor network states to simulating variational quantum algorithms. Lastly, I will introduce reversible computing as the host of next generation differential programming framework, which may unleash the full power of AD for differentiable scientific computing.

*This project supported by the National Key Research and Development Project of China Grant No. 2017YFA0302901 and No. 2016YFA0302400, the National Natural Science Foundation of China Grant No. 11888101 and No. 11774398, the Strategic Priority Research Program of Chinese Academy of Sciences Grant No. XDB28000000.
8:36AM W39.00002: Machine learning effective models from a Boltzmann perspective*
JONAS RIGO (Presenter), ANDREW MITCHELL, Univ Coll Dublin — We investigate the derivation of effective models for quantum impurity type problems using machine learning methods. Parameters of the effective model are optimized with respect to the parent Hamiltonian by using a classical probability distribution extracted from a diagrammatic expansion of the partition function. The classical probability distributions are naturally in the form of an energy-based model within this framework, making clear the connection to Boltzmann machines. In this case, the energy-based model is the effective model and has a physical meaning. The information geometry inspired derivation of the cost function predicts that the best fitting effective model has the same thermal expectation value of effective interactions as in the parent model. However, we show that this does not necessarily yield an effective model with the same low-energy physics as the parent model due to information monotonicity along RG flow [1].


8:48AM W39.00003: Automatic design of Hamiltonians*
KIRYL PAKROUSKI (Presenter), Princeton University — We formulate an optimization problem of Hamiltonian design. Given a variational ansatz for a Hamiltonian we construct a loss function to be minimised as a weighted sum of relevant Hamiltonian properties specifying thereby the search query. Using fractional quantum Hall effect as a test system we illustrate how the framework can be used to determine a generating Hamiltonian of a finite-size model wavefunction (Moore-Read Pfaffian and Read-Rezayi states) or to find optimal conditions for an experiment. We also discuss how the search for approximate generating Hamiltonians may be used to find simpler and more realistic models implementing the given exotic phase of matter by experimentally accessible interaction terms. Based on arXiv:1907.05898.

*Swiss National Supercomputing Centre (CSCS), Project IDs s395 and s551. Princeton's Institute for Computational Science & Engineering and OIT Research Computing. Swiss National Science Foundation, Early Postdoc.Mobility grant P2EZP2 172168. DOE grant No. DE-SC0002140.
9:00AM W39.00004: Direct and Reverse Structure-Electronic Property Relationship Prediction with Deep Learning and Bayesian Optimization*  ARTEM PIMACHEV (Presenter), SANGHAMITRA NEOGI, Aerospace Engineering, University of Colorado at Boulder — Ab-initio computational approaches fail to predict electronic properties of systems with increasing size and complexity. It is highly desirable to formulate methods that can translate the information from ab-initio techniques across length scales, and predict electronic properties of technological applications at relevant length scales. We use a deep learning model to find the complex relationship between the geometrical attributes of heterostructures (HS) and the electronic structure properties predicted by ab-initio calculations. We test the usefulness of the model by predicting electronic transport properties of unknown Si/Ge HS based on the relationship, and comparing with experimental data. We consider the local atomic environment features and the global HS features as the descriptors of the model. The advantage of deep learning models becomes evident since the configuration space is vast due to the variability of HS fabrication. We propose a reverse approach based on Bayesian optimization to predict the structure from measured system's properties of interest. This method is generically applicable to predict electronic properties of dynamically varying heterostructures and the discovery of new structures.

*The project is funded by DARPA (DSO) [Agreement No.: HR0011-16-2-0043].

9:12AM W39.00005: Machine Learning of Single-Atom Defects in 2D Transition Metal Dichalcogenides with Sub-Picometer Precision*  ABID KHAN (Presenter), BRYAN CLARK, CHIAHAO LEE, DI LUO, CHUQIAO SHI, SANGMIN KANG, WENJUAN ZHU, PINSHANE HUANG, University of Illinois at Urbana-Champaign — Deep learning techniques based on fully convolutional networks (FCNs) have revolutionized image recognition in fields ranging from medical diagnosis to facial recognition. The ability of FCNs to identify objects in images opens new opportunities for accessing the underlying information in atomic-resolution images obtained using scanning transmission electron microscopy (STEM). The properties of two-dimensional transition metal dichalcogenides (2D TMDCs) are strongly influenced by atomic defects such as vacancies and substitutional dopants, but high-precision characterization of single-atom defects remains challenging because 2D materials are irradiation sensitive, produce low scattering signals, and require low-voltage imaging modes. While identifying defects by hand is possible, it severely limits our ability to process large quantities of atoms and obtain large-scale statistics. By employing deep learning techniques, we quickly identify and classify various defect species, including metal substitutions, chalcogen vacancies, and chalcogen substitutions. This approach lets us observe changes in atomic separations induced by these defects with sub-picometer precision.

*DOE DE-SC0020190
9:24AM W39.00006: Dictionary Learning in Fourier Transform Scanning Tunneling Spectroscopy*  JEDRZEJ WIETESKA, YENSON LAU (Presenter), Columbia Univ, TETSUO HANAGURI, Center for Emergent Matter Science, RIKEN, JOHN WRIGHT, Columbia Univ, ILYA EREMIN, Institute for Theoretical Physics, Ruhr-Universität Bochum, ABHAY PASUPATHY, Columbia Univ — Modern high-resolution microscopes, such as the scanning tunneling microscope, are commonly used to study specimens that have dense and aperiodic spatial structure. Extracting meaningful information from images obtained from such microscopes remains a formidable challenge. Fourier analysis is commonly used to analyze the underlying structure of fundamental motifs present in an image. However, the Fourier transform fundamentally suffers from severe phase noise when applied to aperiodic images. We have developed a new algorithm based on nonconvex optimization, applicable to any microscopy modality, that directly uncovers the fundamental motifs present in a real-space image. Apart from being quantitatively superior to traditional Fourier analysis, this novel algorithm also uncovers phase sensitive information about the underlying motif structure. We apply this algorithm to scanning tunneling microscopy images of an S-doped iron selenide superconductor to recover phase-sensitive quasiparticle interference in this material as function of sulfur doping. Implications of our results on the evolution of the superconducting gap structure across the putative nematic quantum critical point will be discussed.

*NSF

9:36AM W39.00007: Machine Learning Tool for Crystal Structure Predictions  VALENTIN STANEV (Presenter), HAOTONG LIANG, University of Maryland, College Park, AARON KUSNE, National Institute of Standards and Technology, Gaithersburg, MD, ICHIRO TAKEUCHI, University of Maryland, College Park — Structure is the most basic and important property of crystalline solids; it determines directly or indirectly most other materials characteristics. However, predicting the crystal structure of solids remains a formidable and not fully solved problem; standard theoretical tools for the task are computationally expensive and not always reliable. In this talk I will present an alternative approach that utilizes machine learning for crystal structure predictions. We developed a tool that can predict the Bravais lattice, space group and lattice parameters of a material based only on its chemical composition. It consists of a series of neural network models with predictors based on aggregate properties of the elements constituting the compound. The tool was trained and validated on more than 100,000 entries from the Inorganic Crystal Structure Database (ICSD). It demonstrates good predictive power and significantly outperforms alternative strategies. This machine learning tool is easy to use, and can be utilized both as an independent prediction engine or as a data-informed method to generate candidate structures for further exploration.
Transferable and interpretable machine learning model for four-dimensional scanning transmission electron microscopy data

Michael Matty (Presenter), Physics, Cornell University, Michael Cao, Zhen Chen, Applied and Engineering Physics, Cornell University, Li Li, Google Research, David Muller, Applied and Engineering Physics, Cornell University — The challenge brought to scientific discovery by the data revolution may be overcome by data scientific approaches. Here we focus on 4D scanning transmission electron microscopy (STEM) data. With advances in detector technology, STEM records the full scattering distribution at each scan position in real space, producing a 4D phase-space distribution. An efficient approach is needed to turn these data into a real space image with subatomic resolution. Existing approaches are limited: annular dark field (ADF) imaging by low dose efficiency and resolution, and ptychography to a few atomic layers and by high computational cost. Here, we develop an efficient, interpretable machine learning model to map the entire STEM dataset to real space images. Our model has higher contrast than ADF, still distinguishes atomic species, and transfers well between samples of different lattice symmetry. We benchmark against conventional approaches using quantitative metrics for resolution and contrast.

*We acknowledge support from DOE DE-SC0018946, the Cornell Center for Materials Research with funding from the NSF MRSEC programme (DMR-1719875), and NSF (Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)) under Cooperative Agreement No. DMR-1539918.

Tight-binding deep learning approach to band structures calculations

Florian Sapper (Presenter), Vittorio Peano, Florian Marquardt, Max Planck Inst for Sci Light — Band structures are ubiquitous in physics as they describe natural as well as engineered materials. Even for systems for which the numerical calculation of the band structure for a single configuration is in itself not prohibitively expensive, efficient numerical methods are highly valuable as they allow the systematic investigation of large sets of configurations. This is often required because configuration spaces are typically huge.

In this talk we present a numerical method for band structure calculations that is based on deep neural networks (NNs). In our approach, the NN does not predict the band structure directly but rather makes it easily accessible via the parameters of a tight-binding model. This is, thus, an example of so-called known-operator learning.

Our tight-binding learning NN goes beyond other existing NN based approaches to band structure calculations in that: (i) It does not focus on a few selected model parameters but rather provides a full mapping from arbitrary unit cell geometry to bands. (ii) It allows to better interpret the network's predictions. (iii) It gives access to the space-group symmetries of the underlying normal modes (especially important for topological systems).
Using structural disorder to design terahertz optical response of ferromagnetic metal alloys

MING LEI (Presenter), SINISA COH, University of California, Riverside

We study the intrinsic anomalous Hall conductivity of Fe-Co-Al alloys in the terahertz (THz) region by first-principles calculations. We find that alloying is a feasible way to tune the THz optical feature of ferromagnetic metals. The optical conductivity (sigma_xy) response of these alloys generically shows a lot of features in the range between 2 THz and 20 THz as it is driven by the spin-orbit interaction. In addition to sharp features in the spectrum, we also find that in some alloys sigma_xy can even change the sign in the THz regime.

This work was supported by grant NSF DMR-1848074.

Evolution of physical properties of RE$_3$Ni$_5$Al$_{19}$ family (RE = Y, Nd, Sm, Gd, Tb, Dy, Ho, Er)

ZUZANNA RYZYNSKA (Presenter), MICHAL J. WINIARSKI, Applied Physics and Mathematics, Gdansk University of Technology, WEIWEI XIE, Chemistry, Louisiana State University, TOMASZ KLIMCZUK, Applied Physics and Mathematics, Gdansk University of Technology

Single crystals of RE$_3$Ni$_5$Al$_{19}$ series (RE = Y, Nd, Sm, Gd, Tb, Dy, Ho, Er) were grown using a self-flux method. The crystal structure was examined with x-ray powder diffraction measurements and single crystal refinement. Physical properties were studied for the first time for RE$_3$Ni$_5$Al$_{19}$ (RE = Y, Nd, Gd, Tb, Dy, Ho and Er) by means of magnetic susceptibility, electrical resistivity and heat capacity measurements. Complex magnetic behavior for all of the studied compounds will be briefly discussed.

The research was supported by the National Science Centre (Poland) grant (UMO-2018/29/N/ST5/01286).

Morphology of the glassy phase of a disordered ferromagnet

JUAN CARLOS ANDRESEN (Presenter), MOSHE SCHECHTER, Ben-Gurion University of the Negev

Previous work established the existence of a novel ferromagnetic disordering mechanism in ferromagnetic disordered systems with random fields [Phys. Rev. Lett. 111, 177202 (2013)]. This mechanism lies in between the standard random field ferromagnetic disordering mechanism and the Imry-Ma disordering mechanism. The interplay of the quenched disorder and the small but finite random fields favors domains with a spin-glass like spin alignment destroying the ferromagnetic phase. Making use of large-scale Monte Carlo simulations of disordered spin models in a random field at different dimensionalities we study the morphology of the spin-glass like domains at different points of the phase diagram and unveil the microscopic structure of the quasi-spin glass phase.
High Curie temperature in Eu-doped GaN caused by Ga-vacancies*  

AKIRA MASAGO (Presenter), Graduate School of Engineering Science, Osaka University, HIKARI SHINYA, Research Institute of Electrical Communication, Tohoku University, TETSUYA FUKUSHIMA, The Institute of Solid State Physics, The University of Tokyo, KAZUNORI SATO, Graduate School of Engineering, Osaka University, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering, The University of Tokyo — The present study computationally demonstrates that room-temperature ferromagnetism, which has been experimentally observed in Eu-doped GaN, is induced by holes in N 2p states (i.e., Zener's double exchange interaction) that arise on the assumption that Ga vacancies appear as a result of the introduction of Eu ions (i.e., volume compensation). The calculated Curie temperature ($T_C$) suddenly increases over a certain range of Ga vacancy concentrations and gradually increases with increasing concentration of Eu ions. High $T_C$ above room temperature is dominated by Zener's double exchange mechanism in partially occupied N 2p hole-states which itinerate throughout the whole crystals, and low $T_C$ is dominated by Zener’s p-f exchange mechanism in Eu 4f and N 2p hybridization. We can explain reasonably a surprising experimental data of 4000 μB per Gd atom in Gd-doped GaN reported by Dhar et al. [S. Dhar et al., Phys. Rev. Lett. 94, 037205 (2005)]

*This work is supported by JST-CREST (JPMJCR1777), JSPS-KAKENHI (18K04926 and 18H05212), and SpiN-RNJ.

Defect-related Optical and Electronic Properties of Ion-bombarded Hexagonal Boron Nitride*  

GABRIEL LÓPEZ-MORALES (Presenter), Chemistry PhD Program, The Graduate Center, City University of New York, MINGXING LI, HARISHANKAR JAYAKUMAR, NICHOLAS PROSCIA, DANIELA PAGLIERO, Physics, The City College of New York, GUSTAVO E LOPEZ, Chemistry, Lehman College of New York, VINOD M MENON, CARLOS MERILES, Physics, The City College of New York — Hexagonal boron nitride (hBN), a well-known 2-dimensional (2D) Van der Waals material, is emerging as an attractive platform for spin-based nanoscale applications, owing to its defect-related single-photon emitters (SPE) and their recently shown magneto-optical response. Unfortunately, only a small fraction of emitters displays possible spin-selective transitions, while their atomic structures remain elusive. We report on work towards circumventing some of these limitations by implanting rare-earth impurities. Cerium (Ce3+) bombarded hBN flakes show a distribution of isolated defects with broadened spectral features (centered at ~ 575 nm), good optical stability and strong magneto-optical response when excited via circularly polarized light. These results help pave the way towards defect engineering in low-dimensional materials for applications in opto-electronics, nanoscale sensing and quantum information processing.


*G.I.L.M and N.V.P acknowledge funding from CREST IDEALS, NSF-1547830. V.M.M. and C.A.M acknowledge support from the National Science foundation (USA) through grant NSF-1906096
9:00AM W40.00006: Slowing down of spin glass correlation length growth: simulations meet experiments* RAYMOND ORBACH (Presenter), QIANG Zhai, University of Texas at Austin, VICTOR MARTIN-MAYOR, Fisica Teiruca, Universidad Complutense, DEBORAH SCHLAGEL, Division of Materials Science and Engineering, Ames Laboratory — The aging rate, \( \frac{d \ln t_w}{d \ln \xi} = \left( \frac{T_c}{T} \right)^z_c(T, \xi) \), of the spin glass correlation length \( \xi \) has been measured in a single crystal of CuMn (6 at.\%) as a function of the waiting time, \( t_w \), where \( T_c \) is the critical temperature. Dynamic slowing down is observed with \( \xi \) reaching a value of \( \xi = 152 \text{ nm} \). The measurements were performed at \( T/T_c = 0.89 \) and for times \( 2 \times 10^3 \leq t_w \leq 8 \times 10^4 \text{ s} \). The value of the crossover variable, \( x(t_w, T) = l(J)/\xi(t_w, T) \), where \( l(J) \) is the Josephson length, is sufficiently small (0.091 \( \leq x \leq 0.12 \)) that the experimental results are free from critical effects. The measured aging rate (\( z_c = 12.37 \pm 0.07 \)) was compared with simulation results from the Janus Collaboration. An extrapolation of the Janus results yields \( z_c(115 \text{ nm}) = 11.94 \pm 0.08 \) and \( z_c(152 \text{ nm}) = 12.76 \pm 0.08 \). This relationship between simulations and experiments allows exploration of phenomena, especially in complex systems, with the particular insights of each partner fueling the interpretation and development of the other. [Phys. Rev. B 100, 094202 (2019)]

*This work was supported by the U.S. Department of Energy, Award No. DE-SC0013599, and Contract No. DE-AC02-07CH11358; and MINECO; Spain, Grants No. FIS2015-65078-C2 and No. PGC2018-094684-B-C21, partially funded by FEDER.

9:12AM W40.00007: Response Time Reveals Temperature Chaos in Spin Glasses* QIANG ZHAI (Presenter), RAYMOND ORBACH, University of Texas at Austin, DAVID HARRISON, University of Minnesota — We have measured the zero field cooled magnetization \( M_{ZFC}(t) \) for Cu\textsubscript{86.5}Mn\textsubscript{13.5} multilayer thin films of different thickness using a one-step quench protocol and two-step temperature drop protocol. The response time, \( t_w^{\text{eff}} \), was extracted from the relaxation rate \( S(t) = \frac{dM_{ZFC}(t)}{d\ln t} \). We found that in the one-step temperature quench to \( T_2 \) experiments, \( t_w^{\text{eff}} \) was a monotonic function of waiting time \( t_w \) until the system reached a quasi-equilibrium state. In the two-step temperature drop experiments, the sample was aged at an intermediate temperature \( T_1 \) until the quasi-equilibrium state established. The temperature was then lowered to \( T_2 \), the same final temperature in one-step quench experiment. After the system regained its quasi-equilibrium state, the response time \( t_w^{\text{eff}} \) was compared with the maximum response time \( t_w^{\text{ref}} \) in one-step quench protocol. The results are rather counterintuitive: there exists a temperature range \( \Delta T \) in which the two-step effective waiting times \( t_w^{\text{eff}} \) are either smaller or larger than \( t_w^{\text{ref}} \). Above the range \( \Delta T \), \( t_w^{\text{eff}} \) recovers to \( t_w^{\text{ref}} \). The existence of a \( \Delta T \) and the recovery to reference response time may be indicative of temperature chaos in spin glasses.

*This work was supported by the U.S. Department of Energy, Award No. DE-SC0013599.
9:24AM W40.00008: Probing spin glass energy landscapes with 1/f noise

DAVID HARRISON (Presenter), E. DAN DAHLBERG, University of Minnesota, RAYMOND ORBACH, University of Texas at Austin — We have measured the 1/f noise in the electrical resistance of thin (<10nm) CuMn wires in order to explore the spin glass state. Consistent with previous measurements, the magnitude of the 1/f noise rises rather abruptly when the system is cooled through its freezing temperature. In thin spin glass films, at temperatures near the freezing temperature, the time-dependent correlation length can grow to reach the thickness of the film on experimental timescales. This fixes the maximum barrier height, which determines the subsequent dynamics. We compare our 1/f noise data, as well as our data on the second spectrum (the noise in the 1/f noise), with previously published results on thicker CuMn films. We attribute differences to accessible time scales (frequencies) associated with the barrier heights of the thinner films.

*This work was supported by the U.S. Department of Energy, Award No. DE-SC0013599.

9:36AM W40.00009: Experimental Determination of the Critical Spin Glass Correlation Length

GREGORY KENNING (Presenter), Indiana Univ of Pennsylvania — We have made detailed measurements of the waiting time effect of the thermoremanent magnetization (TRM) near the spin glass transition temperature $T_g$. In previous measurements we found that the timescale $t_{weff}$ associated with the decay, rapidly decreases near $T_g$ (where $T_g$ is defined by the onset of remanence). This effect has been systematically mapped out for waiting times ranging from 300 s to 100,000 s. Using $t_{weff}$ to determine the length scale of the glassy correlations, $\xi_{glassy}$ (observed in both numerical studies and experiment) we see both growth of this correlation length as $T_g$ is approached (from lower temperatures), and then a rapid reduction of this correlation length very close to $T_g$. We interpret this reduction in $\xi_{glassy}$ for all waiting times, as being governed by the critical correlation length $\xi_{crit}$. The data from all waiting times collapse on a master curve that can be fit to $(T-T_c)^{-zn}$.

*This work was supported by the U.S. Department of Energy, Award No. DE-SC0013599.
Demonstration and quantitative characterization of effective random exchange fields in ferromagnet/antiferromagnet bilayers

Dylan James Collette (Presenter), Guanxiong Chen, Sergei Urazhdin, Department of Physics, Emory University

It was conjectured over 30 years ago that some of the unusual magnetic properties of ferromagnet/antiferromagnet bilayers are associated with the effective random field arising due to the frustration of exchange interaction at their interface [1]. This conjecture was supported by recent measurements demonstrating a correlated spin glass state in these systems [2], but has not yet been directly confirmed.

We utilize magnetoelectronic measurements of anisotropic magnetoresistance in Permalloy(Py)/CoO bilayers to confirm the predicted random-field effects and quantify the random field. In particular, we show that the component of magnetization of F perpendicular to the external field scales as a power-law with the exponent dependent on the thickness of Py. Scaling analysis and micromagnetic simulations confirm that these dependences are consistent with the expected effects of random field, and allow us to determine its magnitude. Our results open a route for analyzing and controlling magnetic frustration in heterostructures.


This work was supported by the grant # DE-SC2218976 funded by the U.S. DOE Office of Science.

Demagnetizing field dependent dynamic spin freezing model with random easy axes orientation in nanoparticles ensembles

Korobi Konwar (Presenter), Tezpur University, Som Datta Kaushik, UGC DAE CSR, Mumbai, Debasis Sen, Bhabha Atomic Research Centre, Pritam Deb, Tezpur University

We investigate the dynamic freezing of magnetic ensembles with varied self-arrangement of constituent Zinc Ferrite nanoparticles in their hierarchical ensembles. The small angle X-ray scattering and small angle neutron scattering experiments provide the overall information of the arrangement of primary nanoparticles in their secondary hierarchical ensembles. The extensive study of dc magnetization reveals the prevalence of strength of dipolar interaction among the nanoparticles on the magnetic memory effect [arXiv: 1907.11116]. The enhancement in magnetic memory effect in both the Field-Cooling and Zero Field-Cooling conditions is observed in an ensemble having higher demagnetizing field resulting higher degree of randomness in easy axes orientation with spin-glassy state at low temperature range.

The authors would like to acknowledge UGC-DAE-CSR, Mumbai Centre for providing financial support (vide grant no. UDCSR/MUM/AO/CSR-M-249/2017)
10:12AM W40.00012: Tuning the Properties of Colloidal Magnetic Particles for Thermometry on the Nanoscale  
ADAM BIACCHI (Presenter), THINH BUI, EDUARDO DE LIMA CORREA, THOMAS MOFFAT, WESTON L TEW, MICHAEL DONAHUE, SOLOMON ISAAC WOODS, CINDI DENNIS, ANGELA HIGHT WALKER, National Institute of Standards and Technology — Accurate, local, remote, and real-time temperature measurements are essential for many technological applications. While conventional thermometry can accurately measure the temperature of a microscale spot on a surface, magnetic nanothermometry is being developed to measure temperature at comparable spatial resolution throughout a volume. However, commercially available nanomaterials display only modest magnetic thermosensitivity; this response must be strengthened to improve the signal-to-noise ratio as a prerequisite to practical volumetric nanothermometry. Here, we engineer solution-synthesized nanoparticles and measure their magnetization dependence on the temperature of their local environment. Modulation of composition, size, and structure allows for different magnetic transition temperature regimes and sensitivities to improve these nanothermometers’ performance. Over the range 100 K to 350 K, under an applied magnetic field of 0.01 T, these structurally complex samples show considerable temperature-dependent change to their magnetization. Results collected from X-ray scattering and diffraction, Raman spectroscopy, and high-resolution electron microscopies provide correlations between the nanoscale structure of these particles with their magnetic thermosensititivy.

10:24AM W40.00013: Classical and Tunneling Percolation Transitions in Nanoparticle Composites  
SHIVA P POKHREL (Presenter), BRENDON WATERS, ZHI FENG HUANG, BORIS NADGORYNY, Wayne State Univ — Electrical conductivity in nanoparticle composites, which consist of insulating and conducting nanoparticles, is determined by two competing mechanisms, percolation in a continuous conducting network (governed by classical percolation with universal critical exponents) and tunneling between isolated conducting particles (described by tunneling percolation with non-universal critical exponents). In this work, we investigate a flexible model system based on half-metallic spherocylindrical CrO$_2$ nanoparticles, which can be gradually converted by annealing from metallic (CrO$_2$) to insulating (Cr$_2$O$_3$) state. Hence we can study a transition from classical to tunneling percolation with the variation of insulating Cr$_2$O$_3$ shell barrier (which can be controlled with sub-nanometer precision), through both experimental measurements and computer simulations - by utilizing a combination of hard-particle Monte Carlo and mechanical contraction methods. Our experimental and theoretical results for the percolation thresholds and critical exponents for classical percolation are in good agreement. We will also report the results of tunneling percolation, as well as magnetoencestivity measurements for different tunnel barrier thicknesses.
10:36AM W40.00014: Spin excitation spectrum in strong disorder spin system using spectrum bifurcation renormalization group  HONG-YE HU (Presenter), University of California, San Diego, HUI-KE JIN, Department of Physics, Zhejiang University, YIZHUANG YOU, University of California, San Diego — Recently the interplay between frustration and disorder has attracted much attention. In the experiment, there is hint that YbMgGaO4 is related to a quantum spin liquid state with a spinon Fermi surface. However, it is still under debate that whether the observed spin-excitation spectrum of YbMgGaO4 is due to effect of spin liquid or disorder. We developed a numerical tool called spectrum bifurcation renormalization group(SBRG) to study strong disordered quantum magnet. Using SBRG, we calculated the spin excitation spectrum of a strong disorder spin model on triangle lattice. We found the spin excitation spectrum agrees well with the experiment, and the result is robust with respect to model parameters.

10:48AM W40.00015: Enhanced non-collinear magnetic phase in mixed anisotropy antiferromagnet*  SOPHIE MORLEY (Presenter), SUJOY ROY, Lawrence Berkeley National Laboratory, DAVID LEDERMAN, Physics, University of California Santa Cruz — Antiferromagnetic (AFM) materials and non-collinear spin textures have recently become popular for their possible technological advantages, such as THz dynamics and topological protection. We have grown AFM epitaxial thin films of (110) Fe_xNi_{1-x}F_2 on MgF_2 substrates using molecular beam epitaxy (MBE). FeF_2 has a strong uniaxial anisotropy along its tetragonal c-axis, whereas NiF_2 has an anisotropy in the a-b plane. Orthogonal anisotropies such as these can be described by the Dzyaloshinskii-Moriya interaction (DMI) and are responsible for interesting spin textures, such as helices and skyrmions. DMI is enhanced via coupling to a high spin-orbit material. We observe an enhancement of a secondary phase close to the AFM Néel ordering temperature in our Pt capped films. We also measured temperature-dependent X-ray resonant magnetic scattering that scales well with the magnetisation. We argue that an AFM skyrmionic-like phase is stabilised in this mixed anisotropy system which is further enhanced upon proximity to a high spin orbit heavy metal.

*Funding provided by the University of California Multicampus Research Programs and Initiatives (grant MRP-17- 454963). Support in the initial stages of the project provided by the National Science Foundation (grant 1434897).

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W41 GMAG DMP: Transport Phenomena of Spin Textures 707 -

Nikolai S. Kiselev
8:00AM W41.00001: Evidence of Topological Hall Effect in Pt/Antiferromagnetic-Insulator Bilayers* YANG CHENG (Presenter), SISHENG YU, MENGLIN ZHU, JINWOO HWANG, FENGYUAN YANG, Ohio State Univ - Columbus — Topological Hall effect has been a primary indicator of spin textures in magnetic materials. We observe unambiguous the evidence of topological Hall effect in Pt/Cr$_2$O$_3$ bilayers grown on Al$_2$O$_3$(0001) and Al$_2$O$_3$(11-20), where Cr$_2$O$_3$ epitaxial film is an antiferromagnetic insulator. The Pt/Cr$_2$O$_3$ bilayers exhibit clear topological Hall resistivity for Cr$_2$O$_3$ thicknesses below 6 nm near and above room temperature, which is above the Néel temperature of Cr$_2$O$_3$, revealing the key role of thermal fluctuations in the formation of spin textures. The similarity of topological Hall signals in (0001) and (11-20)-oriented Cr$_2$O$_3$ films indicates that the emergence of spin textures is insensitive to crystalline orientation. This first observational evidence of topological Hall effect in HM/AFI bilayers significantly expands our materials base to include the large family of AF insulators for the exploration of AF-based skyrmion technology.

*This work was supported primarily by the US Department of Energy (DOE) under Grant No. DE-SC0001304. Partial support is provided by DARPA under Grant No. D18AP00008

8:12AM W41.00002: Control of ferromagnetic Curie temperature and topological Hall effect in chromium telluride thin films IN HAK LEE (Presenter), BYOUNG KI CHOI, HYUK JIN KIM, MIN JAE KIM, Department of Physics, University of Seoul, Seoul 02504, Republic of Korea, KYEONG JUN LEE, TAE YANG CHOI, SEO HYOUNG CHANG, Department of Physics, Chung-Ang University, Seoul 06974, Republic of Korea, HU YOUNG JEONG, UNIST Central Research Facilities (UCRF) and School of Materials Science and Engineering, UNIST, Ulsan, Republic of Korea, YOUNGHAK KIM, Pohang Accelerator Laboratory, POSTECH, Pohang, 37673, Republic of Korea, SUYOUN LEE, Center for Electronic Materials, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea, YOUNG JUN CHANG, Department of Physics, University of Seoul, Seoul 02504, Republic of Korea — Chromium telluride (Cr$_{1.8}$Te) has been known as a p-type ferromagnetic metal with varied Curie temperatures ($T_C = 170$ K – 340 K). Recently report of topological Hall effect (THE) suggested the skyrmion phase formation (Nano Research, 11, 3116 (2017)). However, the origin of THE as well as the various $T_C$ among the Cr$_{1.8}$Te phases was not clearly understood yet. Here, we investigate two different types of Cr$_{1.8}$Te thin films with different $T_C$ via different growth conditions to understand the origin of the various $T_C$. We also discuss the THE-like signal in our Hall measurements, with complementary microscopic and spectroscopic evidences, to address the origin of observed THE-like signal in this peculiar magnetic thin film system.
8:24AM W41.00003: Large topological Hall effect in a non-coplanar ferromagnet Cr$_{0.9}$TeB$_{0.1}$

YANGKUN HE (Presenter), GERHARD FECHER, JOHANNES KRODER, CHENGUANG FU, YU PAN, WALTER SCHNELLE, HORST BORRMANN, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids — The Berry phase understanding of electronic properties has attracted special interest in condensed matter physics, leading to phenomena such as anomalous Hall effect (AHE) and topological Hall effect (THE). A non-zero Berry phase, induced by band structure in momentum space or non-coplanar spin structure is the origin of both effects. Here, we report a sign change in AHE and the origin of THE in Cr$_{0.9}$TeB$_{0.1}$ single crystal, due to a non-coplanar canted magnetic structure and the momentum space Berry curvature. At high temperatures, the moments are aligning ferromagnetically along the $c$ axis, while non-coplanar canted magnetic structure is found below 140 K. The cone angle subtended by the spins depends on the temperature. This spin-reorientation leads to the change of Berry curvature, which influences both AHE and THE in the presence of an applied magnetic field and current. Our study provides a deep understanding of the relation between spin structure and Hall signal.

8:36AM W41.00004: Topological Hall effect in Shastry-Sutherland lattice*

MUNIR SHAHZAD (Presenter), Department of Physics & Physical Oceanography, Memorial University of Newfoundland, Canada, NYAYABANTA SWAIN, PINAKI SENGUPTA, School of Physical & Mathematical Sciences, Nanyang Technological University, Singapore — We study the classical Heisenberg model on the geometrically frustrated Shastry-Sutherland lattice with additional Dzyaloshinskii-Moriya (DM) interaction. We show that several noncollinear and noncoplanar magnetic states such as flux, all-out, 3in-1out, canted-flux are stabilized over wide range of parametric space in the presence of DM interaction. We discuss the role of different DM vectors in the stabilization of these complex configurations of localized moments. These ordered states not only drive exotic magnetic properties but also anomalous magneto-transport. The spin of itinerant electron moving on the background of these localized spins acquires a Berry phase which manifests itself by contributing an extra term in Hall conductivity known as geometrical or topological Hall effect. We demonstrate this effect by calculating the energy bands and transverse conductivity for conduction electrons hopping on these localized moments. It is shown that transverse conductivity is non-zero for several of these noncoplanar ordered states even in the absence of magnetic field coupling to the conduction electrons.

*The work is partially supported by Grant No. MOE2014-T2-2-112 of the Ministry of Education, Singapore.
**8:48AM W41.00005: Recent Developments in Spin Superfluid Transport**

(DANIEL HILL, Presenter), Institute for Quantum Matter, Johns Hopkins University, YAROSLAV TSERKOVNYAK, Physics and Astronomy, University of California, Los Angeles — Spin Superfluidity, also called Dissipative Exchange Flow to emphasize its distinguishing features from traditional superfluids, is coherent spin transport mediated by topological winding in the texture of a magnetic order parameter. Experimental signatures for Spin Superfluids have been observed in recent years, most notably in antiferromagnets and amorphous magnets; however, in some respects experimental progress has been surprisingly elusive, especially for ferromagnets. Experimental observation of ferromagnetic spin superfluids may require overcoming various problems, such as pinning due to the effective anisotropy induced by strong demagnetizing fields of thin films, as well as spin current screening due to soliton formation at the boundary. We discuss how some of these problems are actually features which lead to a rich and potentially useful non-equilibrium phase diagram. In addition, we show how spin superfluid signals could propagate through a 3D amorphous magnet, despite the spin superfluid being unstable due to a lack of barriers to phase slips.

*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331

**9:00AM W41.00006: Magnetic and electrical transport properties of MnBi$_2$Te$_4$**

(DONGLIANG GONG, Presenter), RONGYING JIN, Louisiana State University, Baton Rouge — MnBi$_2$Te$_4$ is considered as an intrinsic antiferromagnetic topological insulator. We have successfully synthesized MnBi$_2$Te$_4$ single crystals. The magnetic susceptibility measurements indicate that the Neel temperature T$_N$ = 25 K with the easy axis along the c direction. Below T$_N$, the system undergoes a spin flop transition at H$_{sf}$ when the magnetic field (H) is applied along the c axis with H > H$_{sf}$. The critical field H$_{sf}$ increases with decreasing temperature, reaching 3.5 Tesla at 2 K. Correspondingly, both the magnetoresistance and Hall resistivity show anomaly at H$_{sf}$. Detailed data analysis and implication will be presented.

*Louisiana Consortium for Neutron Scattering (LaCNS)

**9:12AM W41.00007: Magnetization and transport measurement of Cr$_{11}$Ge$_{19}$ single crystal**

(YU LI, Presenter), DAVID P YOUNG, JOHN DITUSA, Louisiana State University, Baton Rouge — We have successfully synthesized single crystal of Cr$_{11}$Ge$_{19}$ which has been proved as a candidate hosting magnetic bi-skyrmion. We carried out a series of measurements on its magnetic susceptibility and transport properties. Our results demonstrate the complex magnetism in Cr$_{11}$Ge$_{19}$ and confirmed the existence of nontrivial spin texture in this material.

*Our research is supported by US Department of Energy under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents.*
Giant anomalous Hall effect related to scalar spin chirality induced by spin-cluster scattering

HIROAKI ISHIZUKA (Presenter), Univ of Tokyo, NAOTO NAGAOSA, CEMS, RIKEN — Anomalous Hall effect (AHE) related to spin chirality, so-called topological Hall effect (THE), has been an important topic that involves a wide range of fields such as transport phenomena, topological materials, and magnetism. Since its proposal, most of the studies on THE focuses on the intrinsic mechanism. On the other hand, a recent theory proposed that an extrinsic mechanism for the chirality-related Hall effect also exists, in which the skew scattering of electrons by three-spin clusters produces a Hall effect proportional to the spin chirality. This mechanism is qualitatively different from the other AHEs because the spin-orbit interaction is unnecessary, potentially showing a distinct behavior from the conventional notion of AHE.

In this work, we discuss that the skew scattering by spin clusters shows a large skew angle in the order of 10 deg when the coupling between the electrons and the localized moments is strong. This large skew angle results in a large Hall angle up to 10 deg. Consequently, the scaling relation of AHE breaks down; the scaling relation between longitudinal and transverse conductivity shows skew-scattering-like relation even in the intrinsic regime, where the intrinsic Hall effect is usually dominant.

Giant anomalous Hall effect from spin-chirality scattering in a chiral magnet

YUKAKO FUJISHIRO (Presenter), NAOYA KANAZAWA, RYOSUKE KURIHARA, Univ of Tokyo, ATSUSHI TSUKAZAKI, Tohoku Univ., MASAKAZU ICHIKAWA, MASASHI KAWASAKI, MASASHI TOKUNAGA, Univ of Tokyo, YOSHINORI TOKURA, CEMS, RIKEN — Topological spin textures give rise to various emergent phenomena, which originate from the interplay between scalar-spin chirality and conduction electrons. In that sense, a spin hedgehog lattice in MnGe provides one distinct example, where the dense emergent magnetic field (~ 40 T) and its fluctuations lead to novel electrodynamics.

We report the observation of giant anomalous Hall effect (AHE) in MnGe thin films. The Hall conductivity and the Hall angle simultaneously reach $\Omega^{-1} \text{cm}^{-1}$ and , respectively, which are an order of magnitude larger than the typical ferromagnets. The exceptionally large value of $\sigma_{xy}$ as well as its transport life-time dependence ($\sigma_{xy} \sim \sigma_{xx}$) suggest that the AHE is induced by some electron scattering mechanism which is beyond the conventional paradigm. We demonstrate the whole picture of this unusual AHE by showing its temperature, magnetic field, mobility, and film-thickness dependences. The possible origins will also be discussed, especially in terms of a novel skew scattering mechanism arising from the fluctuation-induced scalar-spin chirality.
9:48AM W41.00010: Thermal Response Functions of Insulating Magnets Near and Beyond Critical Temperature* CAITLIN CARNAHAN (Presenter), YINHAN ZHANG, DI XIAO, Carnegie Mellon Univ — Thermal response coefficients of magnetic materials are of significant interest in the field of spintronics; understanding spin dynamics in response to a thermal gradient paves the way for energy-efficient spin manipulation via thermal fluctuations. We investigate thermal response in magnetic systems, particularly near and above the critical temperature, by simulating the dynamics of these systems and calculating the spin and energy currents that appear. Applying linear response theory, we predict the thermal conductivities of both spin and energy, which provide insight into how thermally-induced fluctuations impact transport in magnetic systems and deepen the understanding of the general effect of fluctuations on non-trivial magnetic topology.

*This work is supported by the Defense Advanced Research Project Agency (DARPA) program on Topological Excitations in Electronics (TEE) under Grant No. D18AP00011.

10:00AM W41.00011: Anomalous Hall Effect sensor based on CoFeB with ultrahigh magnetic field detectability* YIOU ZHANG (Presenter), KANG WANG, GANG XIAO, Brown University — The anomalous Hall Effect (AHE) in ferromagnetic metals and alloys have been widely studied as a potential candidate for magnetic sensing applications, due to the relative easiness of fabrication, broad frequency response and lower intrinsic noise. Nevertheless, AHE sensor suffers from relatively low sensitivity in comparison with semiconductor Hall sensor. In this work, we have demonstrated that sensitivity of AHE sensor based on Ta/CoFeB/MgO/Ta multi-layer structure can be greatly enhanced, through engineering of magnetic anisotropy. By tuning thickness of CoFeB layer as well as the annealing temperature, ultra-high sensitivity (1000 V/A/T, comparable to that of semiconductor Hall sensor) and zero hysteresis can be achieved. We have also performed noise measurement over a broad frequency range. The low-frequency 1/f noise is found to strongly depend on input current and bias magnetic field, while the high-frequency white noise shows much weaker dependence. The best magnetic field detectability of our AHE sensor reaches 70 nT/rtHz at 1 Hz and 10 nT/rtHz at 1 kHz. Our work shows that AHE sensors are suitable for ultra-small magnetic field sensing applications.

*The work was supported by King Abdullah University of Science and Technology (KAUST) through the Sensor Initiative.
10:12AM W41.00012: Atomic antiferromagnetic domain wall propagation beyond the relativistic limit  
HUANHUAN YANG (Presenter), University of Electronic Science and Technology of China, 
HUAIYANG YUAN, Southern University of Science and Technology, MING YAN, Shanghai University, 
H. W. ZHANG, PENG YAN, University of Electronic Science and Technology of China — We theoretically investigate the dynamics of atomic domain walls (DWs) in antiferromagnets driven by a spin-orbit field. For a DW with a width of a few lattice constants, we identify a Peierls-like pinning effect, with the depinning field exponentially decaying with the DW width, so that a spin-orbit field moderately larger than the threshold can drive the propagation of an atomic DW in a stepwise manner. For a broad DW, the Peierls pinning is negligibly small. However, the external spin-orbit field can induce a fast DW propagation, accompanied by a significant shrinking of its width down to atomic scales. Before stepping into the pinning region, noticeable spin waves are emitted at the tail of the DW. The spin-wave emission event not only broadens the effective width of the DW but also pushes the DW velocity over the magnonic barrier, which is generally believed to be the relativistic limit of the DW speed. While the existing dynamic theory based on the continuum approximation fails in the atomic scale, we develop an energy conversion theory to interpret the DW dynamics beyond the relativistic limit.

10:24AM W41.00013: Transport signature of the BKT transition in 2D easy-plane magnets  
SU K BUM CHUNG (Presenter), Univ of Seoul, SE KWON KIM, Univ of Missouri — The theory of the Berezinskii-Kosterlitz-Thouless (BKT) phase transition was formulated to describe the 2D phase transition of easy-plane magnets as well as 2D superconductors and superfluids. The BKT transition being topological in nature, i.e. not characterized by a local order parameter, its detection has been challenging. The BKT transitions in the latter cases have been observed in experiments, much of which involves transport signatures, such as the current-voltage relation being non-linear below the BKT temperature and linear above the BTK temperature. By contrast, the experimental study of the solid-state 2D magnetic material emerged only in the last few years. The accompanied recent development of spin-transport measurements offers a tantalizing opportunity to discover novel transport phenomena of spin, which should be expected as the spin, unlike the particle number, is not conserved. In this Letter, we show here that this non-conservation of spin in the 2D easy-plane magnets leads to a distinct spin transport signature at the BKT transition, the crossover between the infinitely long-range spin transport and the exponentially decaying spin transport. We also present how this can be detected in the van der Waals easy-plane magnetic materials such as the monolayer NiPS$_3$. 
10:36AM W41.00014: Frequency Dependence of Magnetic and Magnetoelastic Properties of Magnetostrictive Materials for Multiferroic Antennae  PETER FINKEL (Presenter), United States Naval Research Laboratory, NICHOLAS JONES, NSWC, MARGO STARUCH, United States Naval Research Laboratory — Magnetoelectric (ME) resonators are of significant interest for pure mechanically driven antennae targeting the ULF/VLF radio frequency range. Direct coupling of magnetostrictive and piezoelectric phases in the ME composites enables time variable magnetic field generation with exceptionally low operational power requirements. A dynamic stress loading of the magnetoelastic/magnetostrictive material by piezoelectric element results in a fluctuating magnetic field. In this work we fully characterize magnetostrictive materials Fe_{81.6}Ga_{18.4} and Terfenol-D at high frequencies up to several kHz and studied the effect of eddy current losses that potentially curtail the magnetic response of the material. We evaluated the dynamic response of Galfenol rod up to 1000 Hz comparing both its sensing response (changing dynamic stresses) to its actuation response (changing dynamic magnetic fields) in both solid and laminated rods.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W42 GMAG: Spin Hall Effect 709/711 - Eric Montoya, University of California, Irvine -
Tag(s): Focus
8:00AM W42.00001: Strong voltage-induced tunability of threshold current and frequency in spin Hall nano-oscillators [Invited] HIMANSHU FULARA (Presenter), MOHAMMAD ZAHEDINEJAD, ROMAN KHYMYN, MYKOLA DVORNIK, Physics, University of Gothenburg, 412 96 Gothenburg, Sweden, SHUNSUKE FUKAMI, SHUN KANAI, HIDEO OHNO, Laboratory for Nanoelectronics and Spintronics, Research Institute of Electrical Communication, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan, JOHAN AKERMAN, Physics, University of Gothenburg, 412 96 Gothenburg, Sweden — Spin Hall nano-oscillators (SHNOs) utilize pure spin currents to excite auto-oscillations at microwave frequencies in nanoscopic regions of magnetic thin films\(^1\)-\(^3\). Thanks to their wide frequency tunability\(^1,2\), their robust mutual synchronization in chains as well as in 2D arrays\(^1,3\), and their CMOS compatibility\(^2\), SHNOs have recently emerged as a promising spintronic device for neuromorphic computing\(^3\). While the SHNO frequency can be tuned with both current and external field, the lack of fine individual SHNO control in synchronized networks limits cognitive tasks in oscillator-based computing. It would be highly advantageous if an energy efficient route such as electrostatic gating can independently tune the SHNO characteristics in a synchronized network to perform more complex neuromorphic tasks\(^3,4\).

Here we demonstrate how electrostatic gating in nano-constriction based W(5nm)/CoFeB(1.7nm)/MgO(2nm) SHNOs can lead to substantial voltage-controlled tunability of threshold current and auto-oscillation frequency. High frequency microwave measurements show a large overall modulation of about 22% in threshold current with \(\Delta V_G = 4\, \text{V}\) and a moderate frequency tunability of 12 MHz/V. Our detailed analysis based on ST-FMR measurements combined with micromagnetic simulations unveil that the observed tunabilities are caused by minor voltage-induced changes in the perpendicular magnetic anisotropy, which, in our case, not only tunes the frequency but also significantly modifies the localization of the auto-oscillating mode resulting in a large change of the effective damping. Our demonstration introduces a new insight to critically control the effective damping and represents a significant step towards the realization of complex neuromorphic tasks\(^3,4\).

References

Large spin Hall effect in room-temperature sputtered W₃Ta thin films grown on SiO₂ and Al₂O₃

MOHSIN ZAMIR MINHAS (Presenter), BHARAT GROVER, ILYA KOSTANOVSKIY, STUART PARKIN, MAZHAR NAWAZ ALI, Max Planck Institute for Microstructure Physics — The spin Hall effect (SHE), in non-magnetic (NM) metals with strong spin-orbit coupling (SOC) has received much attention due to potential technological applications like magnetic random-access memory (MRAM) and spin-logic devices. Large spin Hall angles (SHA, the ratio of Jₛ/Jₖ) have been observed in materials like Pt and the metastable phase, β-W (a.k.a. W₃W in the A15-structure). Recently, W₃Ta (and other A15 compounds) was theoretically predicted to host an even larger intrinsic SHE than β-W, originating from the large spin Berry curvature of its electronic band structure. Here we report the SHE of W₄₋ₓTaₓ films including W₃Ta, deposited by DC magnetron co-sputtering on SiO₂ and Al₂O₃ substrates. Spin-torque ferromagnetic resonance (ST-FMR) and optically detected ferromagnetic resonance (ODFMR) techniques were used to measure the SHA of various W₄₋ₓTaₓ compositions and thicknesses with CoFeB as the magnetic layer. We find that W₃Ta in the A15 structure could be stabilized on both types of substrates at room temperature and hosts a large SHA in W₃Ta similar to theoretical predictions opening the door to facile device fabrication of Pt-free spintronic devices.

*Alexander von Humbolt Foundation Sofia Kovalevskaja Award Max Planck Society

Critical spin fluctuation mechanism for the spin Hall effect

SATOSHI OKAMOTO (Presenter), Oak Ridge National Lab, TAKESHI EGAMI, Department of Materials Science and Engineering, University of Tennessee, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo — We propose mechanisms for the spin Hall effect in metallic systems arising from the coupling between conduction electrons and local magnetic moments that are dynamically fluctuating. We consider a microscopic model proposed by Kondo [1] for the coupling between electrons and local moments and describe the fluctuation of local moments using the self-consistent renormalization method by Moriya [2]. Both a side-jump-type mechanism and a skew-scattering-type mechanism naturally arise and give rise to a nontrivial temperature dependence in the spin Hall conductivity. This leads to the enhancement in the spin Hall conductivity at non-zero temperatures near the ferromagnetic instability [3]. The proposed mechanisms could be observed in 4d or 5d metallic compounds.


*The research by S.O. and T.E. is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. N.N. was supported by JST CREST Grant Number JPMJCR1874 and JPMJCR16F1, Japan, and JSPS KAKENHI Grant numbers 18H03676 and 26103006.
9:00AM W42.00004: Quantitative X-ray Imaging of Spin Accumulation due to the Spin Hall Effect in Ni<sub>x</sub>Cu<sub>1-x</sub> Nanowires  MARK KELLER (Presenter), MONIKA ARORA, JUSTIN SHAW, THOMAS SILVA, BASTIEN DASSONNEVILLE, National Institute of Standards and Technology Boulder, JOACHIM GRAEFE, Max Planck Institute for Intelligent Systems, MARKUS WEIGAND, Helmholtz-Zentrum Berlin für Materialien und Energie — We recently reported a spin Hall ratio \( \theta_{\text{SH}} = 1.05 \pm 0.18 \) in Ni<sub>60</sub>Cu<sub>40</sub>, an alloy that is nonmagnetic at room temperature, based on FMR measurements of unpatterned Ni<sub>80</sub>Fe<sub>20</sub> films deposited in a bilayer with the alloy [1]. Like previous studies of spin Hall effect (SHE) in heavy metals such as Pt and W, this work inferred spin accumulation indirectly, in this case from its effect on the FMR resonance. An alloy containing Ni enables scanning transmission x-ray microscopy (STXM) to directly image spin accumulation using circularly polarized x-rays tuned to the Ni L3 absorption edge. Importantly, this technique can quantify the spin accumulation without resorting to a theoretical model of spin transport. In wires of Ni<sub>60</sub>Cu<sub>35</sub>Al<sub>5</sub> with a cross section \( \approx 80 \text{ nm} \times 30 \text{ nm} \) and driven at a current density \( \approx 5 \times 10^{11} \text{ A/m}^2 \), fabricated on Si<sub>3</sub>N<sub>4</sub> membranes, we observed spin polarization along each wire edge in normal-incidence STXM images. The amount of spin accumulation is consistent with \( \theta_{\text{SH}} \approx 1 \) and it obeys three symmetries expected for SHE measured via STXM: 1) opposite sign on opposite edges of the wire, 2) opposite sign with reversal of the driving current, and 3) opposite sign with opposite x-ray helicity.


9:12AM W42.00005: Mutually synchronized 2D spin Hall nano-oscillator arrays with quality factors up to 170,000  JOHAN AKERMAN (Presenter), MOHAMMAD ZAHEDINEJAD, AHMAD AWAD, SHREYAS MURALIDHAR, ROMAN KHYMYN, HIMANSHU FULARA, HAMID MAZRAATI, MYKOLA DVORNIK, Goteborg Univ — Nano-constriction based Spin Hall nano-oscillators (SHNOs) have emerged as an attractive alternative to spin torque nano-oscillators [1,2], as their auto-oscillating mode exhibits substantial spatial expansion in out-of-plane fields [3], propagating spin waves can be generated [4], and long chains of nano-constrictions can be mutually synchronized [5]. Here we demonstrate that it is also possible to synchronize nano-constriction SHNOs in two dimensions. We fabricate 2D square SHNO arrays ranging from 2 x 2 to 10 x 10 constrictions and study their microwave signal properties in out-of-plane fields using both electrical measurements and Brillouin Light Scattering microscopy. We observe robust mutual synchronization in up to 8 x 8 arrays and find that their quality factor, \( Q = f/\Delta f \), increases in direct proportion to the number of mutually synchronized constrictions, with the largest arrays showing \( Q = 170,000 \).

9:24AM W42.00006: Magnetization-Independent Spin Hall Effect in Ferromagnetic Metals
JOSEPH MITTELSTAEDT (Presenter), ROBERT BUHRMAN, DANIEL RALPH, Physics, Cornell University —
The anomalous spin Hall effect, which creates charge-to-spin conversion in metallic ferromagnets, offers an exciting opportunity to generate spin currents for which the spin direction is controllable. Here we report spin-torque ferromagnetic resonance measurements of current-induced torques in ferromagnet-spacer-ferromagnet trilayers with NiFe, Co and CoFeB as our magnetic layers, allowing us to clearly separate signals from the different ferromagnetic layers. We observe signals with the symmetry of a magnetization-independent spin Hall effect with spin-to-charge efficiencies as large as 10% in NiFe, which is comparable to heavy metal-ferromagnet bilayers investigated previously. This research illustrates some of the competing effects which must be considered when investigating spin-to-charge conversion in ferromagnets, and also confirms that the spin current polarization and local magnetic moment in a ferromagnet do not need to be aligned.

9:36AM W42.00007: Maximizing the spin Hall ratio of Pt: Trade-off between intrinsic spin Hall conductivity and carrier lifetime
LIJUN ZHU (Presenter), Cornell University, LUJUN ZHU, Shaanxi Normal University, SHENGJIE SHI, Cornell University, MANLING SUI, Beijing University of Technology, DANIEL RALPH, ROBERT BUHRMAN, Cornell University — Spin Hall metals with high spin-torque efficiencies and relatively low resistivities are key for developing practical spin-orbit torque technologies (e.g. memories, oscillators, and logic). Pt-based spin Hall metals are the most attractive for such applications due to their relatively low resistivity, giant intrinsic spin Hall conductivity, easy growth, and ability to be readily integrated into experimental and/or manufacturing processes. This talk will report on an unambiguous determination of the intrinsic nature of spin Hall effect in Pt [1] and how the intrinsic spin Hall conductivity and spin Hall ratio of Pt varies with carrier lifetime, strain, and interruption of crystal order [2,3]. Based on this physical understanding, we have developed several low-resistivity spin Hall metals for spin-orbit torque technologies whose power consumption is estimated to be only 1% of that of the topological insulator Bi\textsubscript{x}Se\textsubscript{1-x} [4] based devices.

9:48 AM W42.00008: Spin pumping and non-uniform magnetic excitation in spin-torque FMR studies of the spin Hall effect  
RYAN TAPPING (Presenter), YONGXI OU, LUIS HENRIQUE VILELA-LEÃO, LIJUN ZHU, DANIEL C. RALPH, ROBERT BUHRMAN, Cornell University — Early on, spin-torque ferromagnetic resonance (ST-FMR) was used to establish an initially surprisingly strong spin Hall effect (SHE) in certain heavy metals (HM), and has since been widely deployed in the study of spin-orbit torques in HM/FM bilayers. However, there are questions as to whether ST-FMR always provides accurate, quantitative measures of the dampinglike spin-torque efficiency $\xi_{DL}$, principally because of the unsettled role of spin-pumping and the inverse SHE in ST-FMR, but also because of the assumption that only the uniform mode is excited. Here we report on an extensive ST-FMR study of Pt/FM and β-W/FM bilayers and HM/spacer/FM trilayers chosen such that the spin pumping effect is both strong and variable. We show that spin pumping, when significant, substracts from the antidamping torque signal, resulting in $\xi_{FMR} < \xi_{DL}$. In conjunction with the spin pumping model, the FMR studies also clearly indicate that there can be significant coupling of the incident spin current to non-uniform modes in the FM layer, which also contributes to a lower apparent $\xi_{DL}$. These results explain why ST-FMR often underestimates $\xi_{DL}$ in comparison to quasi-static second harmonic results, the latter of which are generally confirmed by ST switching of MTJs.

10:00 AM W42.00009: Electrical Measurement of Thermally Driven Spin Hall Voltage in Platinum with Permalloy contacts*  
SEONDO PARK (Presenter), YUN DANIEL PARK, Dept. of Physics and Astronomy, Seoul National University — A group of effects coupling spin current with heat has drawn considerable attention due to their large potential for applications in spin-caloritronics[1]. Recently, a new member of the family which converts thermal gradient into pure spin current in nonmagnetic conductors, named the spin Nernst effect, was observed. Here, we report a surprisingly large magnetic-field dependent voltage (<800 nV) across two permalloy contacts on a platinum channel patterned into a cross shape, while in the orthogonal channel, electrical current is utilized to create local thermal gradient by Joule heating. From finite element analysis as well as local electrical transport thermometry measurements, we estimate thermal gradients to be 1.5 K/micron near the permalloy contacts at electrical current of 10 mA. We will further discuss the origins of the large observed voltage by presenting several experimental results which we strongly feel rules out any unintended electrical effects such as spin Hall effect. [1] G. E. W. Bauer et al., Nat. Mat., 11, 391 (2012).

*This work was supported by National Research Foundation of Korea (2017R1E1A1A01074650).
Ferromagnetic materials can generate spin currents with controllable spin polarization via the anomalous spin Hall effect, a property potentially useful for driving spin torque oscillators (STOs), which have recently found applications for performing neurotrophic tasks. Iron rhodium (FeRh) exhibits a transition between a low-temperature antiferromagnetic (AFM) state and a high-temperature ferromagnetic (FM) state. For appropriate growth parameters, this transition can be found close to 300K, such that both the FM and AFM states are stable at room temperature, making it an ideal material to compare the effectiveness of FM and AFM spin sources for STOs. The transition also provides a high level of versatility for device design. We present measurements of the spin torque efficiency in iron rhodium as the temperature is varied to drive the FeRh through its magnetic transition. We compare FeRh's efficiency for driving STOs in the stable AFM and FM states at the same temperature, and compare the effectiveness of FeRh as a spin source with ordinary spin Hall materials.

*The work was supported as part of the Q-MEEN-C, an Energy Frontier Research Center funded by the U.S. Department of Energy.
**10:24AM W42.00011: Very high spin Hall conductivities and spin Hall ratios in epitaxial Iridium di-oxide films**  
ARNAB BOSE (Presenter), School of Applied and Engineering Physics, Cornell University, JOCIENNE NELSON, Department of Physics, Cornell University, Cornell University, XIYUE ZHANG, RAKSIT JAIN, SHENGJIE SHI, School of Applied and Engineering Physics, Cornell University, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University, DANIEL C. RALPH, Department of Physics, Cornell University, Cornell University, DAVID MULLER, School of Applied and Engineering Physics, Cornell University, KYLE M SHEN, Department of Physics, Cornell University, Cornell University, ROBERT BUHRMAN, School of Applied and Engineering Physics, Cornell University — New metallic materials with exceptionally high spin Hall conductivities and accompanying high spin Hall ratios are desirable both to produce more efficient systems for spin-orbit torque applications and to further test the fundamental understanding of intrinsic spin-orbit interactions. A particularly interesting candidate for such research is the metallic rutile oxide Iridium di-oxide which angle resolved photoemission spectroscopy studies have shown exhibits Dirac nodal lines in the band structure, a feature that could enable a very high . Here we report spin-torque ferromagnetic resonance studies of the damping-like and field-like torques exerted on an adjacent ferromagnetic layer as the result of current flowing in epitaxial (110) and (001) IrO$_2$ films. The (110) films exhibit a damping-like torque efficiency $\approx 0.18$ at 293 K, which sets a lower bound for the spin Hall conductivity . The higher resistivity (~ 300 $\mu\Omega$-cm) (001) films exhibit even stronger spin-orbit torques, with ranging from ~0.45 at 293K to 0.8 at 30 K as decreases, behavior indicative of the dirty metal regime. The very high value for (001) IrO$_2$, ≥ , is both a challenge for current theoretical understanding and an exciting prospect for more efficient SOT applications.

**10:36AM W42.00012: Extrinsic Spin Hall Effect in Inhomogeneous Systems**  
TAKUMI FUNATO (Presenter), HIROSHI KOHNO, Science, Nagoya University — Interconversion between spin and charge signals is one of the most important processes in spintronics. This is done most commonly by the direct and inverse spin Hall effects (SHE). Recently, An et al. observed an enhanced charge-to-spin conversion, comparable to heavy metals, in naturally oxidized Cu (nox-Cu) [1]. Okano et al. reported a non-reciprocal charge-spin interconversion in nox-Cu [2]. The so-called spin-vorticity coupling (SVC) was suggested as the origin of these results.

In this work, we take a different approach and study the problem in terms of the extrinsic SHE in an inhomogeneous system. We model the nox-Cu system by nearly free electrons subject to impurities with spin-orbit interaction and with spatially modulated distribution. We calculate spin accumulation and spin current induced by an electric field using Kubo formula and discuss the relation between them. The results are summarized by a generalized spin diffusion equation with a spin source term given by the divergence of the spin Hall current. This source term can be put in a form of SVC only if the spin Hall angle is independent of impurity concentration, as in the case of skew scattering.

Large Spin Hall and Edelstein effects in Weyl semimetal WTe2 up to Room Temperature

BING ZHAO, DMITRII KHOKHRIAKOV, BOGDAN KARPIAK, MD ANAMUL HOQUE, SAROJ DASH (Presenter), Chalmers University of Technology, Sweden — The discovery of topological semimetals has revealed the opportunities to realize several extraordinary physical phenomena in condensed matter physics. Here, we report current-induced spin polarization, i.e. the spin Hall effect [1] and the Edelstein effect [2] and its inverse phenomenon in type-II Weyl semimetal WTe2 up to room temperature. In addition, to spin Hall and Rashba-Edelstein effects, our measurements also show an out-of-plane electrical field-induced spin polarization in WTe2 due to spin momentum locking of the spin-polarized bulk Fermi states [2]. These findings open opportunities for spin-orbit based spintronic technologies and possibilities for the realization of new states of topological matter with novel spin textures.


*Graphene Flagship, Swedish Research Council, FlagEra

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W43 DCOMP DMP: Computational Design and Discovery of Novel Materials VI: Machine Learning and High Throughput Computing 702 - Yuanxi Wang, Pennsylvania State University - Tag(s): Focus
**8:00AM W43.00001: New tools for detecting strong correlation in automated transition metal complex screening** [Invited]  
FANG LIU (Presenter), CHENRU DUAN, HEATHER J KULIK, Massachusetts Institute of Technology MIT — There are several prominent challenges in conducting quantum chemistry studies of transition metal complexes: generation of molecule structure, selection of electronic structure method, workflow control, and post-processing of simulation results. molSimplify is a user-friendly open-source toolkit that enables the seamless generation of candidate inorganic molecule structures, preparation, and execution of Density Functional Theory (DFT) calculations, and post-processing DFT results. Here we focus on extending the capability of molSimplify, enabling automated selection of electronic structure methods including both DFT and wavefunction based methods and automated control of simulations. For automatic method selection, we develop a python module, MultirefPredict, which is a high-level cross-platform workflow that calculates widely used multi-reference diagnostics for a given molecular system, without users handling the input and output of quantum chemistry packages. The backend of MultirefPredict supports several quantum chemistry packages based on both DFT and wavefunction theory methods, with calculation performed on both CPU and GPU. MultirefPredict guides a user to choose between single-reference and multi-reference based methods, which is essential for obtaining accurate results for transition metal-containing systems. For in-situ simulation control, we developed an automated workflow that checks the current status of geometry optimization using a “dynamic classifier” that predicts the probability of failure based on geometric and electronic structure information collected on the fly. This workflow terminates the simulation when it is predicted to fail, saving numerous computational resources. These open-source tools, which are accessible to the whole transition metal chemistry community, are anticipated to make transition metal chemistry simulation more automated and transparent.

*DOE Grant DE-SC0018096

**8:36AM W43.00002: High-throughput Design of Lead-free Organic-inorganic Lead Halide Semiconductors Beyond Perovskites**  
KESONG YANG (Presenter), YUHENG LI, University of California, San Diego — Organic-inorganic lead halide perovskites (including 2D hybrid perovskites) show great promise in optoelectronic applications such as light-emitting diodes and solar energy conversion. However, the poor stability and toxicity of lead halide perovskites severely limit their large-scale applications. In this talk, I am going to present our high-throughput design strategy of lead-free hybrid halide semiconductors with robust materials stability and desired material properties beyond perovskites. On the basis of 24 prototype structures that include perovskite and non-perovskite structures and several typical organic cations, a comprehensive quantum materials repository that contains 4507 hypothetical hybrid compounds was built using large-scale first-principles calculations. After a high-throughput screening of this repository, we have rapidly identified 23 candidates for light-emitting diodes and 13 candidates for solar energy conversion.

*National Science Foundation under award number ACI-1550404 and Global Research Outreach (GRO) Program of Samsung Advanced Institute of Technology under the award number 20164974.
8:48AM W43.00003: Perovskite Genomics: Optimizing the performance of large sets of perovskite materials with atomistic simulations  GIANAURELIO CUNIBERTI (Presenter), HAGEN ECKERT, FLORIAN PUMP, Chair Materials Science and Nanotechnology, TU Dresden, JOSUA VIETEN, MARTIN ROEB, CHRISTIAN SATTLER, Institute of Solar Research, German Aerospace Center (DLR) — Perovskites are ideal candidates to be applied in two-step redox cycles to convert, store and utilize energy from concentrated solar radiation by heating the perovskite materials to high temperatures (up to 1,500 °C) and thus transferring them to an energy-rich state. In a second step at lower temperatures, this energy can be used for a variety of chemical processes. As the overall performance of such redox materials is dominated by the diffusion rate of oxide ions through the constituting lattice, tuning the redox thermodynamics of such materials through composition adjustment allows the design of ideal perovskite materials. For an enhanced insight into the diffusion properties of a large set of perovskite materials, Molecular Dynamics simulations are applied for an efficient funneling of up to 58,000 candidate oxides to a few hundred for subsequent intensive studies. A major challenge lies in the generalization of the force field generation for datasets including large numbers of different oxides involving the characteristic electrostatic properties to be known for each material. To this end, we use data obtained by DFT stored in the database of the Materials Project. In this way, we are able to suggest materials with optimized and tailored dynamic properties.

9:00AM W43.00004: Computational discovery of semiconducting high-entropy chalcogenide alloys*  ZIHAO DENG (Presenter), LOGAN WILLIAMS, GUANGSHA SHI, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — High-entropy materials are formed by mixing typically five or more principal components into a single crystal structure. While significant progress has been made to synthesize entropy-stabilized metals and ceramics for structural applications, little attention has been paid to the discovery of new entropy-stabilized semiconductors. Here, we present a new class of entropy-stabilized semiconducting alloys based on the IV-VI binary chalcogenides, namely Ge_xSn_yPb_{1-x-y}S_zS_e_{1-t} high-entropy chalcogenides (HECs). By utilizing high-throughput first-principles calculations, we investigate the thermodynamic stability of HECs over their entire composition space, and show that more than 50% of the investigated compositions are stable with respect to phase segregation. We further studied the enthalpic effect of the individual elements via machine learning on the high-throughput data. Our work demonstrates the potential of entropy stabilization in the discovery of novel multicomponent semiconductor alloys.

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High-throughput discovery of metal-organic frameworks for cooperative CO2 adsorption

ERIC TAW (Presenter), Chemical Engineering, University of California, Berkeley, JEFFREY R LONG, Chemistry, University of California, Berkeley, JEFFREY B NEATON, Chemical Engineering, University of California, Berkeley, MACIEJ HARANCZYK, IMDEA Institute — Recently, a new class of post-synthetically modified metal-organic frameworks (MOFs) with non-Langmiur stepped isotherms have been discovered and tuned to reversibly and selectively adsorb CO2 under common flue gas conditions. However, very few MOFs are known to exhibit step-like isotherms, a result of a cooperative adsorption phenomenon. Here, we present a computational screening procedure to discover new CO2 adsorbent MOFs with the potential for step-like isotherms and cooperative adsorption. Our workflow is based on the hypothesis that the distance between accessible, undercoordinated metal sites is a key indicator for whether a MOF modified with ethylenediamine will exhibit cooperative adsorption. We screen the Computational-Ready Experimental MOF (CoRE-MOF) database using the fast marching algorithm to assess metal site distances given arbitrary pore geometries, and discuss candidate materials for experimental validation.

*This work is supported by the Department of Energy; computational resources provided by NETL.

Machine Learning Accelerated Discovery of Mixed Anion Materials

JIAHONG SHEN (Presenter), CHEOL WOO PARK, JIANGANG HE, CHRISTOPHER MARK WOLVERTON, Northwestern University — Mixed-anion materials are interesting counterparts to their more widely studied single-anion compounds due to the increased flexibility and tunability of properties afforded by the presence of multiple anions. Here, we demonstrate how computational approaches, based on DFT datasets can be combined with materials informatics and machine learning (ML) models to accelerate materials discovery. We utilize and compare a variety of materials representations, including a recently proposed improved crystal graph convolutional neural network (iCGCNN) model, and the Voronoi tessellation approach incorporated in the Materials-Agnostic Platform for Informatics and Exploration (MAGPIE). ML models are trained on a set of 450,000 DFT data prior calculated in the Open Quantum Materials Database (OQMD) and evaluated on a separate test set of 3,000 mixed-anion compounds where iCGCNN outperforms random forest models in predictive accuracy by ~300%. By introducing more mixed-anion compounds into the training set, the performance of the iCGCNN model is further improved, and it allows us to make predictions of a large number of stable (and hence, likely synthesizeable) new ternary oxychalcogenides, which are subsequently validated by DFT calculations.

*NSF MRSEC Grant No. DMR-1720139
9:36AM W43.00007: High-throughput Computational Study of Double Perovskite Oxides*
JIANGANG HE (Presenter), CHRISTOPHER MARK WOLVERTON, Northwestern University — Perovskite oxides have been intensively studied for decades due to the extraordinary variability of compositions and structures and their attractive applications in superconductivity, magnetoresistance, multiferroicity, catalysis, solid oxide fuel cells, and etc. Extending from single perovskite $\text{ABO}_3$ to double perovskite $\text{A}_2\text{BB'}\text{O}_6$ significantly increases the tunability towards the targeted physical and chemical properties. However, the number of possible compositions of double perovskite is prohibitively large to explore entirely experimentally. In this talk, we will present how to use a multi-step high-throughput computational method to screen $\sim 5000$ compositions of double perovskite $\text{A}_2\text{BB'}\text{O}_6$ ($\text{A}=$Ca, Sr, Ba, and La; $\text{B}$ and $\text{B'}$ are metal elements). With the $\sim 2000$ stable/metastable (and so likely synthesizable) compounds predicted by our calculations, we will show how statistical learning of the large dataset can capture the correlation among composition, stability, and crystal structure (i.e., cubic perovskite, distorted perovskite, and non-perovskite). The results will accelerate new double perovskite oxides prediction and discovery.

*U.S. Department of Energy, under Award Number DE-EE0008089

9:48AM W43.00008: Automated phase mapping of high throughput X-ray diffraction data
YIZHOU ZHU (Presenter), CHRISTOPHER MARK WOLVERTON, Northwestern University — Combinatorial synthesis and high-throughput characterization have become powerful tools to accelerate the discovery and design of novel materials. However, one key question in the high-throughput workflow is the phase mapping problem. Correct, automatic identification of the number, identity, and fraction of phases in XRD data is a crucial step to perform autonomous high-throughput characterization and establish further understanding on the composition-structure-property relationships. Traditional analysis performed manually could take days for a single material system, while an automatic solver, if lacks the domain-specific knowledge, is likely to give unphysical results. In this work, we demonstrate how we use phase diagrams generated based on DFT calculations databases, such as the Open Quantum Materials Database (OQMD), to provide domain-specific knowledge and enforce reasonable constraints. We show how DFT provides a good initial guess to phase mapping algorithms, we can address the “peak-shifting” caused by alloying behavior using machine learning techniques, and the method is capable of uncovering minor phases present in the XRD data. By combining first-principles calculations and machine learning techniques, our approach enables rapid phase identification and mapping.
A class of materials that has gained community attention recently is electrides. These rare materials stabilize “free” electrons, loosely bound to a low-dimensional cavity space, which act as anions to chemically stabilize the structure. This characteristic feature makes them highly desirable for applications such as battery anodes, superconductors, and topological electronics. However, very few electrides have been synthesized due to their chemical instability; they often undergo degradation in ambient conditions. Thus, a challenge in this field is to discover electrides with higher stability. In this work ternary electrides of the chemical species A-B-C were targeted; the choice of species and the stoichiometry between them allows a vast space within which to engineer compounds with enhanced stabilities and desirable properties. Properties of interest include magnetic, electronic carrier density, and band topology. A global structure search was performed with first-principles calculations to identify stable and metastable structures for a given composition. Highly parallelized GPU-accelerated DFT codes were used to explore the vast parameter space. Our database will guide experimental synthesis efforts of new ternary electrides with multidimensional functional properties.

Through employing the layered-crystal determination program based on the topology-scaling algorithm, 450 M_mN_nX_x (M, N = metal elements, X = S, Se) layered di-metal chalcogenides (LDCs) are identified from the 1602011 crystalline materials known in two Material Genome databases (Materials Project and OQMD). Their structures are classified into three types, standard structures, hetero-layered structures and large-cation intercalated layered structures. 312 cation-intercalated LDCs are hard to be exfoliated into few-layer 2D structures. In contrast, the other two types of structures may be exfoliated into stable few-layer 2D structures due to the weak inter-layer van der Waals interaction. The band structure screening identifies 24 semiconductors with small in-plane effective masses and thus high mobility of carriers. Furthermore, 83 found LDCs composed of the magnetic metal elements provide a new platform for search of 2D magnetic crystals. This work extends the search of layered materials from metal dichalcogenides to ternary chalcogenides and can serve as a map for the future discovery of novel 2D semiconductors and magnetic materials.
**10:24AM W43.00011: Effect of a Parameter in a Descriptor on the Efficiency of a Crystal Structure Search Using Bayesian Optimization**  
NOBUYA SATO (Presenter), National Institute of Advanced Industrial Science and Technology, TOMOKI YAMASHITA, National Institute for Materials Science, TAMIO OGUCHI, Osaka University, KOJI HUKUSHIMA, The University of Tokyo, TAKASHI MIYAKE, National Institute of Advanced Industrial Science and Technology — A crystal structure search method using Bayesian optimization (BO) has been developed recently. BO is a machine learning technique for the global optimization. It has been reported that the method can search a stable structure efficiently. In this method, a crystal structure is represented by a numerical vector referred to as a descriptor. Descriptors often have a parameter which should be predetermined. We reveal by case studies for crystalline silicon, silicon oxide, and yttrium–cobalt alloy that the efficiency of a crystal structure search depends heavily on a parameter value. Our analysis indicates that the efficiency is related to the distribution of the descriptor. Therefore, we introduce an information measure based on the descriptor distribution, which is evaluated only from a set of crystal structures. The measure succeeds in estimating a parameter value where the crystal structure search works efficiently, and thus, can be used to predetermine the value of a parameter.

**10:36AM W43.00012: An active-learning framework for the discovery of new crystalline materials**  
KIRSTEN WINTHER (Presenter), RAUL FLORES, Chemical Engineering, Stanford University, CHRISTOPHER PAOLUCCI, Chemical Engineering, University of Virginia, ANKIT JAIN, Mechanical Engineering, IIT Bombay, MICHAL BAJDICH, SUNCAT, SLAC National Accelerator Laboratory, THOMAS BLIGAARD, Department of Energy, Technical University of Denmark — A challenging problem in materials science is that the space of possible crystal structures is so vast that it is impossible to sample with brute-force screening approaches. However, electronic structure methods combined with machine-learning (ML) techniques have a huge potential to speed up the search [1][2], which hold a great promise for the discovery of novel materials and/or catalysts for energy applications. Here, we present a ML based active-learning framework to search for stable and meta-stable inorganic materials. It has already been applied to the discovery of new stable polymorphs of IrO, using a search space of experimentally observed crystal prototypes with element substitutions. We extend this search to hypothetical crystal structures that are generated with a crystal prototype enumeration scheme combined with a ML aided search for appropriate lattice parameters. Using a graph-theory based distinction, we identify a finite number of geometries to span a highly diverse material sub-space, which is used for the active-learning exploration.


*This work was supported by, and done in collaboration with, the Toyota Research Institute.*
10:48AM W43.00013: Unraveling nanoscale features controlling the diffusion of multi-component alloys through machine learning methods*  
S. MOHADESEH TAHERI-MOUSAVI (Presenter), S. SINA MOEINI-ARDAKANI, RYAN W. PENNY, JU LI, JOHN HART, Massachusetts Institute of Technology MIT — The immense compositional breadth of non-dilute multi-component alloys has made their well-targeted design extremely challenging. Yet, with the emergence of additive manufacturing which allows pointwise specification of the alloying components, new methods to predict alloy compositions and properties are needed. Here, we present a newly-developed numerical framework whereby a machine-learning algorithm supervised by atomistic-scale simulations is used to explore the nanoscale features controlling the diffusivity of atomic components in these heavily alloyed compounds. Analysis of all possible atomic configurations within a model medium-entropy alloy reveals how the size and cohesive energy of alloying elements alter the tendency of alloying elements to exchange their sites. Our developed theoretical model provides a pathway to calculate a macroscopic diffusivity rate from the information obtained from the nanoscale mechanisms. In the future, this approach can guide the selection of composition and processing parameters for conventional as well as additive manufacturing methods, and it could enable design of metals with tailored gradient diffusivity.

*ArcelorMittal, MIT-Portugal Program

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W44 DCOMP DMP: Electrons, Phonons, Electron Phophon Scattering, and Phononics VII 704 - Mu Wang, Nanjing University

8:00AM W44.00001: Nonperturbative Estimates of Electrical Current in 2D Dirac Systems - A MoS2 Example*  
DAVID N. CARVALHO (Presenter), NORDITA — The term “Dirac materials” refers to a large set of seemingly-disparate materials which share many universal properties and may be described by the Dirac equation. The effect of external time-dependent fields on their carrier dynamics is of great importance. However, due to the non-commutativity of the Dirac Hamiltonian in time domain, non-perturbative estimates of the propagator of a Dirac spinor are challenging to obtain.

Here, we propose an approach to construct observables, through the use of a suitable Magnus expansion and, with it, study the effect of shining light and deforming the sample on the produced current of arbitrary chemical potential and temperature. These two processes are captured by the coupling of electromagnetic and valley-dependent pseudo-electromagnetic fields. For appropriate excitation regimes, we show how (a) both fields create currents and (b) how these two fields can undergo interference and create both electrical and valley current and charge densities.

*DNC and AVB acknowledge support from VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744), the European Research Council under the European Unions Seventh Framework ERS-2018-SYG 810451 HERO, and the Knut and Alice Wallenberg Foundation.
8:12AM W44.00002: Driven Imposters: Controlling Expectations in Solid State Systems

GERARD MCCAUL (Presenter), Physics, Tulane Univ, CHRISTOPHER ORTHODOXOU, Physics, King's College London, KURT JACOBS, Physics, University of Massachusetts, GEORGE BOOTH, Physics, King's College London, DENYS BONDAR, Physics, Tulane Univ — We present a model to control the observables of a general many-body electron system driven by an incident laser field. The main result is a non-linear, field free equation of motion for tracking observables, together with a constraint on the functional form of expectations which may be reproduced via tracking. As a first test, the strategy is used in the Fermi-Hubbard model to make the current expectation conform to an arbitrary function under a range of model parameters. Additionally, using two reference spectra for materials in the conducting and insulating regimes respectively, we demonstrate that using the developed tracking strategy allows one to make the dipole acceleration spectrum of each material mimic the reference spectra of the other, creating a 'driven imposter'.

*We are supported by the Air Force Office of Scientific Research (AFOSR), Young Investigator Research Program (grant FA9550-16-1-0254) and the Army Research Office (ARO) (grant W911NF-19-1-0377).

8:24AM W44.00003: Noise mediated mixing in a tunnel junction

SAMUEL HOULE (Presenter), EDOUARD PINOSOLLE, JOFFREY RIVARD, CHRISTIAN LUPIN, BERTRAND M REULET, Université de Sherbrooke — The microwave mixer is a key element in the detection of all sort of signals. It is based on a nonlinear element such as a semiconducting diode or a Josephson junction, and allows for example the downconversion of microwave signals to low frequency for digitization. In the quantum regime, the mixing of vacuum fluctuations with an ac excitation leads to the generation of squeezed microwaves.

A normal metal tunnel junction with a linear current-voltage cannot be used to mix signals. It has however been shown to generate squeezed vacuum thanks to another type of nonlinearity, that of noise vs. bias voltage. We demonstrate the use of a tunnel junction as a noise mediated mixer: the junction excited at two frequencies (around 20GHz) generates a noise which amplitude is modulated at the difference frequency. We compare our data with theoretical predictions of photon-assisted noise and observe small deviations that seem to indicate an extra frequency cutoff possibly related to the thermalization time of electrons in the electrodes.
Modeling Spontaneous Charge Transfer at Metal / Organic Hybrid Heterostructures

ONGUN OZCELIK (Presenter), YINGMIN LI, WEI XIONG, FRANCESCO PAESANI, University of California, San Diego — Hybrid heterostructures are crucial in photovoltaics where the overall efficiency of the materials are closely related to the level of charge transfer at their interfaces. Here, using a combined computational and experimental approach, we show that heterodyne vibrational sum frequency generation (HD-VSFG) measurements provide an effective way of monitoring the interfacial charge transfer in these heterostructures [1]. Using ab-initio quantum chemical calculations, we show that inducing regio-randomness into the organic polymer modifies the interfacial electronic states, level of hybridization and the electronic wave function of these materials. We present the HD-VSFG responses of the metal/P3HT heterojunctions containing both regio-regular and regio-random P3HT structures and show that the intensity of non-resonant signal is directly correlated with the computed electronic structure and the level of spontaneous charge transfer at these interfaces.


This research was supported by the National Science Foundation (NSF) through grant CHE-1808111.

Enhancement of superconductivity in organic-inorganic hybrid topological materials

HAOXIONG ZHANG (Presenter), AWABAIKEI ROUSULI, SHENGCHUN SHEN, KENAN ZHANG, CHONG WANG, LAIPENG LUO, JIZHANG WANG, YANG WU, YONG XU, DUAN WENHUI, HONG YAO, PU YU, SHUYUN ZHOU, Tsinghua University — Inducing or enhancing superconductivity in topological materials has attracted extensive research interests partly due to its fundamental importance toward topological superconductivity. Reducing the thickness of transition metal dichalcogenides has provided an important pathway to engineer superconductivity in topological matters, emergent superconductivity with $T_c \sim 0.82$ K in monolayer WTe$_2$ which also hosts intriguing high-temperature quantum spin Hall effect. However, such monolayer samples are often difficult to obtain and extremely sensitive in air. Here we report a generic, experimentally convenient approach to manipulate the interlayer coupling in bulk MoTe$_2$ and WTe$_2$ single crystals through organic cation intercalation. The as-formed organic-inorganic hybrid crystals exhibit dramatically enhanced superconductivity with $T_c$ of 7.0 K for intercalated MoTe$_2$ (as compared with 0.25 K for bulk crystal) and 2.3 K for intercalated WTe$_2$ (record high compared to monolayer WTe$_2$ and with greatly improved sample stability). This organic-cation-intercalation method can be readily applied to many other layered crystals, forming a promising research platform to manipulate their corresponding electronic states, including possible topological superconductivity with significantly enhanced $T_c$. 
9:00AM W44.00006: Pressure Control of Crystal Symmetry, Fermi Surface Reconstruction and Superconductivity in Weyl semimetal MoTe$_2$  TANER YILDIRIM (Presenter), National Institute of Standards and Technology, I-LIN LIU, Physics Department, University of Maryland, COLIN HEIKES, National Institute of Standards and Technology, CHRIS ECKBERG, TRISTIN METZ, SHENG RAN, Physics Department, University of Maryland, WILLIAM RATCLIFF, National Institute of Standards and Technology, JOHNPIERRE PAGLIONE, Physics Department, University of Maryland, NICHOLAS BUTCH, National Institute of Standards and Technology — Layered transition metal chalcogenides are promising hosts of electronic Weyl nodes and topological superconductivity. MoTe$_2$ is a striking example that harbors both non-centrosymmetric T$_d$ and centrosymmetric T' phases. In this talk we present neutron scattering and transport measurements along with Density functional theory (DFT) calculations to suggest a path towards the realization and control of these topological states of the type-II Weyl semimetal and superconductor MoTe$_2$ through the application of pressure [1]. DFT calculations reveal that the strength of the electron-phonon coupling is similar for both crystal structures. Finally, we show that there is a critical pressure characterized by unique coherent quantum oscillations, indicating that the change in topology between two phases give rise to a new topological interface state[2]. We present periodic and finite slab calculations of this new interface state which is in excellent agreement with the observed quantum oscillation frequencies.


9:12AM W44.00007: Discovering topological surface states of Dirac points in an acoustic crystal  HENGBIN CHENG (Presenter), Institute of Physics, Chinese Academy of Sciences/Beijing National Laboratory for Condensed Matter Physics, Beijing, China, YIXIN SHA, School of Electronics Engineering and Computer Science, Peking University, Beijing, China, RONGJUAN LIU, CHEN FANG, LING LU, Institute of Physics, Chinese Academy of Sciences/Beijing National Laboratory for Condensed Matter Physics, Beijing, China — Dirac materials, unlike the Weyl materials, have not been found in experiments to support intrinsic topological surface states, as the surface arcs in existing systems are unstable against symmetry-preserving perturbations. Utilizing the proposed glide and time-reversal symmetries, we theoretically design and experimentally verify an acoustic crystal of two frequency-isolated three-dimensional Dirac points with Z$_2$ monopole charges and four gapless helicoid surface sheets. Under symmetry breakings, the 3D ideal Dirac point breaks into Z$_2$ Weyl dipoles, Z$_2$ nodal rings or a full bandgap.
9:24AM W44.00008: Time-resolved x-ray diffraction study of acoustic phonons in TaAs
MIN-CHEOL LEE (Presenter), NICHOLAS SIRICA, Los Alamos National Laboratory, SAMUEL W. TEITELBAUM, MARIANO TRIGO, GILBERTO ANTONIO DE LA PEAN MUNOZ, Stanford PULSE Institute, SLAC National Accelerator Laboratory, VIKTOR KRAPIVIN, YIJING HUANG, DAVID A REIS, Department of Applied Physics, Stanford University, ALEXEI MAZNEV, JIAOJIAN SHI, KEITH ADAM NELSON, Department of Chemistry, Massachusetts Institute of Technology, ROXANNE TUTCHTON, JIAN-XIN ZHU, Los Alamos National Laboratory, XIANGGANG QIU, Institute of Physics, Chinese Academy of Sciences, DZMITRY YAROTSKI, ROHIT P PRASANKUMAR, Los Alamos National Laboratory — We utilized femtosecond x-ray pulses to investigate acoustic phonon oscillations in TaAs. We observed that time-resolved x-ray diffraction reveals coherent phonon oscillations of binary acoustic modes in truncation rod scattering. The phonon oscillations correspond to the transverse and longitudinal acoustic modes propagating along the surface normal vector. We suggest that the off-axis orientation of the surface normal makes it possible to observe the transverse phonon oscillation, in contrast to conventional laser-induced acoustic phonon oscillations due to a single longitudinal mode. We also found an asymmetric Fano-like feature in the longitudinal phonon oscillations, suggestive of strong electron-phonon coupling in TaAs.

9:36AM W44.00009: Spectral signatures of exciton-polarons in two-dimensional hybrid lead-halide perovskites
FELIX THOUIN (Presenter), CARLOS SILVA, Georgia Inst of Tech — Two-dimensional hybrid organic inorganic perovskites (2D-HOIPs) feature a previously unexplained excitonic fine-structure in their absorption and emission spectra. We here show using advanced optical probes that features within this fine-structure correspond to exciton-polarons of distinct polaronic nature. We first successfully reproduce their absorption spectrum by supposing distinct excitonic states with contrasting couplings to the lattice. This hypothesis is then unambiguously confirmed by high-resolution resonant impulsive Raman spectroscopy which reveals the polaronic nature of each excitons within this fine structure. We then show that their distinct polaronic nature drives the relaxation dynamics down this excitonic manifold. We also show that these effects protect the excitons from many-body interactions hinting at their importance in polaritonic microcavities based on these materials. Finally, we also observe stable biexcitons in these materials up to room temperature. Our conclusions are of broad fundamental importance to this class of materials which, due to the high degree of tunability of their crystalline structure, offer an ideal system on which to test models of exciton-polaronic effects.

* I acknowledge support from NSERC Canada and Quebec's FRQ:NT
9:48AM W44.00010: Density functional perturbation theory with subspace iteration  SAEED BOHLOUL (Presenter), VINCENT MICHAUD, NanoAcademic technologies, HONG GUO, McGill Univ — Density functional perturbation theory (DFPT) is a useful framework for calculating material responses that can be casted as total energy derivatives with respect to perturbation fields. These responses give access to important properties including the dynamical matrix, dielectric functions, optical properties, electron-phonon coupling, etc. A major advantage of DFPT is circumventing the computational burden of direct methods by replacing DFT supercell calculations, one for each possible perturbation, by a system of coupled linear equations for primitive cells which are solved self-consistently. Nevertheless, for unit cells containing a large number of atoms, solving this linear system becomes a major bottleneck. In this work, we report a new approach to overcome this bottleneck of DFPT, the perturbed Chebyshev-filtered subspace iteration (PCFSI) method, implemented in real space. It allows us to calculate responses of materials in much larger systems than was possible before. Dielectric functions and phonon spectra will be used as examples to demonstrate the impressive power of the PCFSI method.

10:00AM W44.00011: Theories, designs, and applications of thermal metamaterials* LIUJUN XU (Presenter), SHUAI YANG, JIPING HUANG, Fudan Univ — With the growing concerns about energy issues, many researchers have paid their attention to thermal management. This trend was mainly driven by the emerging field of thermal metamaterials in the last decade. This report mainly introduces the new progress of thermal metamaterials in three aspects: new functions, multi-particle systems, and intelligentization. The new functions include the thermal "golden touch" and the thermal Janus structures. The former is a method to extend the core property to the shell with an extremely small core fraction. The latter is essentially a core-shell structure whose core has two distinct thermal conductivities, and the mechanical rotation of the core can realize different functions. Multi-particle systems extend the core-shell design, and the multi-particle interaction helps us achieve thermal invisibility. Intelligentization means that the effective thermal conductivity of a shell is always the same as that of the environment.

*We acknowledge the financial support by the National Natural Science Foundation of China under Grant No. 11725521.
10:12AM W44.00012: Optical Properties of Complex Oxides RbFe(MoO$_4$)$_2$, RbFe(SO$_4$)$_2$, and RbFe(SeO$_4$)$_2$*

RACHEL OWEN (Presenter), ELIZABETH DRUEKE, CHARLOTTE ALBUNIO, Department of Physics, University of Michigan, ALEMAYEHU S ADMASU, Rutgers Center for Emergent Materials, Rutgers University, JUNJIE YANG, Department of Physics, New Jersey Institute of Technology, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials, Rutgers University, STEVEN THOMAS CUNDIFF, LIUYAN ZHAO, Department of Physics, University of Michigan — The structural and magnetic properties of the archetype type-II multiferroic RbFe(MoO$_4$)$_2$ have been well studied due to interest in the low temperature antiferromagnetic order and its coupling to the induced ferroelectric order. However, little is known about the optical properties of this complex oxide. There have been low energy spectroscopic characterizations, but no reported linear characterization up into the band edge. Here we explore a group of similar such complex oxides: RbFe(MoO$_4$)$_2$, RbFe(SO$_4$)$_2$, and RbFe(SeO$_4$)$_2$. Substitution of the A-site in RbFe(AO$_4$)$_2$ can result in comparable, spectrally tunable absorption features that appear below the optical transition band edges. Their absorption spectra show strikingly similar thickness and temperature dependence, despite their different growth conditions and electronic/magnetic properties. We further discuss the potential origin and impact of these tunable optical transition states in the RbFe(AO$_4$)$_2$ complex oxide family.

*NSF CAREER Grant No. DMR-1749774

10:24AM W44.00013: Nonlinear optics with ionizing radiation and ultrafast lasers: progress toward measuring the complete electric field of XFEL pulses

WILLIAM PETERS (Presenter), TRAVIS JONES, RICHARD L SANDBERG, PAMELA BOWLAN, Los Alamos National Laboratory — Newly developed X-ray free electron lasers (XFELs) promise to transform nearly all areas of modern science. However, there is a significant need for more sophisticated tools to measure the X-ray pulses themselves. Complete measurements of the pulse's electric field are needed to improve the light source technology and to enable new spectroscopy and scattering experiments. Here we describe measurement approaches in which an optical laser interacts with an interference pattern from the unknown XFEL pulse, referred to as a transient grating or as four wave mixing. This geometry largely isolates the instantaneous wave-mixing response necessary for the FROG algorithm and removes the long-lived response seen in other X-ray-pump optical-probe measurements. The measurement also transfers the phase information of the X-ray electric field onto a readily-detectable optical laser field, allowing us to fully characterize the unknown pulses with visible spectrometers and cameras. Crucially, our strategy promises to be broadly applicable across the entire energy range accessible by existing and planned XFEL facilities. Lab-scale UV demonstration experiments will be presented as well as results from an upcoming beam time at the FERMI soft X-ray FEL.
Critical Behaviors of Anderson Transitions in Three Dimensional Orthogonal Classes with Particle-hole Symmetries

XUNLONG LUO (Presenter), BAOLONG XU, Peking Univ., TOMI OHTSUKI, Sophia Univ., RYUICHI SHINDOU, Peking Univ. — From transfer-matrix calculation of localization lengths and their finite-size scaling analyses, we evaluate critical exponent of the Anderson transition in three dimensional (3D) orthogonal class with particle-hole symmetry, class CI, as $\nu = 1.16 \pm 0.14, 0.18$. We further study disorder-driven quantum phase transitions in the 3D nodal line Dirac semimetal model, which belongs to class BDI, and estimate critical exponent as $\nu = 0.80 \pm 0.02, 0.04$. From a comparison of the critical exponents, we conclude that a disorder-driven re-entrant insulator-metal transition from the topological insulator phase in the class BDI to the diffusive metal phase belongs to the same universality class as the Anderson transition in the 3D class BDI. We also discover a topological quantum critical point (TQCP) between one-dimensional (1D) class BDI topological insulator and Anderson insulator and showed that the re-entrant transition in the 3D model is connected to the TQCP in its 1D limit. We argue that an infinitesimally small disorder drives the nodal line Dirac semimetal in the clean limit to the diffusive metal.


Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W45 DCOMP: Quantum Manybody Systems and Computational Physics

8:00 AM W45.00001: Isometric Tensor Network Representation of String-Net Liquids

TOMOHIRO SOEJIMA (Presenter), KARTHIK SIVA, NICK BULTINCK, SHUBHAYU CHATTERJEE, University of California, Berkeley, FRANK POLLMANN, Physics, Technische Universitat Munchen, MICHAEL ZALETEL, University of California, Berkeley — Recently, a class of tensor networks called isometric tensor network states (isoTNS) was proposed which generalizes the canonical form of matrix product states to tensor networks in higher dimensions. While this ansatz allows for efficient numerical computations, it remained unclear which phases admit an isoTNS representation. In this work, we show that two-dimensional string-net liquids, which represent a wide variety of topological phases including discrete gauge theories, admit an exact isoTNS representation. We further show that the isometric form can be preserved after applying a finite depth local quantum circuit. Taken together, these results show that long-range entanglement by itself is not an obstruction to isoTNS representation and suggest that all two-dimensional gapped phases with gappable edges admit an isoTNS representation.

*KS acknowledges support from the NSF GRFP. SC acknowledges support from the ERC synergy grant UQUAM. MZ and NB were supported by the DOE, office of Basic Energy Sciences under contract no. DE-AC02-05-CH11231. FP acknowledges the support of the Deutsche Forschungsgemeinschaft (DFG) Research Unit.
**8:12AM W45.00002: Dynamical phases of interacting Andre-Aubry-Harper model**  
YONG-CHAN YOO (Presenter), Condensed Matter Theory Center and Department of Physics, University of Maryland, College Park, JUNHYUN LEE, Condensed Matter Theory Center, Joint Quantum Institute and Department of Physics, University of Maryland, College Park, BRIAN SWINGLE, Condensed Matter Theory Center, Maryland Center for Fundamental Physics, Joint Center for Quantum Information and Computer Science, and Department of Physics, University of Maryland — The dynamics of non-integrable quantum many-body systems have received extensive attention for both theoretical and practical purposes. One important issue we address in this talk is the phase transition between thermal and many-body-localized states and the dynamical properties of their possible intermediate states. We calculate the non-equilibrium steady states (NESS) of the boundary-driven strongly interacting Andre-Aubry-Harper model by employing the time-evolving block decimation on matrix product density operators. The spin and energy transport properties of the system are obtained from the NESS, which reveals a rich phase diagram while tuning the quasiperiodic potential strength. We uncover an exotic dynamical phase following the thermal phase where the spin transport becomes sub-diffusive while the butterfly velocity remains non-zero, and also investigate the entanglement properties of each phase.

**8:24AM W45.00003: Topological signatures of Multipartite Entanglement**  
FABIO LINGUA (Presenter), Clark University, WEI WANG, Division of Condensed Matter, Max Planck Institute for the Physics of Complex Systems, LIANA SHPANI, BARBARA CAPOGROSSO-SANSONE, Clark University — We present a proposal to relate topological structure of worldline configurations to multipartite entanglement. Configurations result from the path-integral formulation of the density matrix in the limit of zero temperature. We consider hard-core bosons for which configurations, i.e. collections of particle paths, can be seen as geometric braids with a certain topological structure. We propose that properties of worldline configurations may realize a more comprehensive deciphering of multipartite entanglement. By means of Monte Carlo calculations, we study checkerboard, stripe, valence-bond solids, $Z_2$ topologically ordered spin liquid, and superfluid phase. We find that each ground-state is characterized by a certain `topological spectrum` which can be used to differentiate among different ground-states.

**8:36AM W45.00004: Dynamical properties of correlated many-body systems from Quantum Monte Carlo simulations**  
ETTORE VITALI (Presenter), PATRICK KELLY, ANNETTE LOPEZ, KAELYN DAUER, California State University, Fresno — I will discuss recent advances in the ab-initio study of correlated many-body quantum systems, and in particular the possibility to compute dynamical correlation functions from first principles using Quantum Monte Carlo techniques. Using the Hubbard model as an example, I will address the calculation of the spectral function, that can be experimentally measured in spectroscopy experiments, and the density structure factors, that can be measured in scattering experiments. The purpose is to allow us to directly compare the predictions of Quantum Monte Carlo techniques with experiments. I will present results for cold atomic Fermi systems in the BEC-BCS crossover in two and three dimensions and for cold atoms on optical lattices. I will also discuss results and perspectives for repulsive models, in connection with high-temperature superconductivity.
8:48AM W45.00005: Padé resummation of the linked cluster expansion of the many-particle path-integral.* ANISH BHARDWAJ (Presenter), Florida State University Tallahassee FL USA; National High Magnetic Field Laboratory FL USA, EFSTRATIOS MANOUSAKIS, Florida State University, Tallahassee, FL, USA; National High Magnetic Field Laboratory FL USA; University of Athens, Panepistimioupolis, Zografos, Athens, Greece — We have developed a quantum cluster expansion, analogous to the well-known Mayer cluster expansion for the classical partition function and the pair distribution function, and a quantum version of the virial expansion by starting from the many-body path-integral. We first derive the diagrammatic series expansion for the pair distribution function and show that the expansion is linked. This expansion can also be thought of as a power series expansion in the particle density. To resum the series, we use a Padé approximation scheme in momentum space, which is constrained to yield the calculated order by order expansion terms and the classical limit correctly. We have tested the approach on a Lennard-Jones and a hard-sphere system and our results agree very well with those obtained from the path-integral Monte Carlo. Our method has immediate application to the case of short-range hard-core potential where the established analytical and semi-analytical tools of many-body perturbation theory and quantum statistical mechanics cannot be applied in a straightforward manner.

*This work was supported in part by the U.S. National High Magnetic Field Laboratory, which is funded by NSF DMR-1157490 and the State of Florida

9:00AM W45.00006: An approach to discovering the low-energy space for effective quantum models of realistic systems.* BRIAN BUSEMEYER (Presenter), Center for Computational Quantum Physics, Flatiron Institute, JOAO N. B. RODRIGUES, Center for Natural Sciences and Humanities, Federal University of ABC - UFABC, SHIVESH PATHAK, LUCAS K. WAGNER, University of Illinois at Urbana-Champaign — Low-energy effective models can be powerful tools for understanding realistic systems, but in many cases it is difficult to quantify the accuracy of those models for a specific system. Density matrix downfolding (DMD) [1] is one approach to determining accurate effective models from first-principles many-body calculations, but requires a sample of low-energy wave functions with varying properties. We present a new method, constrained variational Monte Carlo, which targets low-energy wave functions while varying other properties, such as the average double-occupation of orbitals. We tested the approach on the hydrogen molecule at stretched and compressed bond lengths, and use it to explore how the low-energy space changes with bond length. For example, when the bond is stretched the low-energy space shifts such that interactions become necessary to accurately describe it. Models fitted to the generated states were solved and reproduced the exact low-energy spectrum of the first-principles Hamiltonian. The method provides a systematic many-body approach to exploring the low-energy space of realistic systems. [1] Changlani et al., J. Chem. Phys., 143, 10, 102814, (2015).

*We gratefully acknowledge the Simons Foundation for funding.
9:12AM W45.00007: Variational-Correlations Approach to Quantum Many-body Problems
ARBEL HAIM (Presenter), GIL REFAEL, Caltech — We investigate an approach for studying the ground state of a quantum many-body Hamiltonian that is based on treating the correlation functions as variational parameters. In this approach, the challenge set by the exponentially-large Hilbert space is circumvented by approximating the positivity of the density matrix, order-by-order, in a way that keeps track of a limited set of correlation functions. In particular, the density-matrix description is replaced by a correlation matrix whose dimension is kept linear in system size, to all orders of the approximation. Unlike the conventional variational principle which provides an upper bound on the ground-state energy, in this approach one obtains a lower bound instead. By treating several one-dimensional spin 1/2 Hamiltonians, we demonstrate the ability of this approach to produce long-range correlations, and a ground-state energy that converges to the exact result. Possible extensions, including to higher-excited states are discussed.

9:24AM W45.00008: Emergence of diffusive dynamics in an efficiently-solvable quantum lattice model  
JIE ZOU (Presenter), XIAOPENG LI, Department of Physics, Fudan University — Thermalization is a common phenomenon in nature, having a characteristic feature of irreversibility due to entropy increase. However, quantum mechanics, the principle for the microscopic world, is reversible. In past few decades, much effort has been devoted to this field in order to reconcile this conflict, and the eigenstate thermalization hypothesis has been proposed as one way to formulate quantum thermalization. In this talk, I will present our recent work on a one-dimension spinless hardcore fermion model with a variable range of interactions. We solve this problem by mapping it into a free fermion case, and we calculate its time evolution with an efficient Monte Carlo sampling algorithm. We observe that although our model is integrable in energy level spacing, the physical observables show certain thermalization behaviors. Furthermore, with increasing temperature, our system shows a crossover from ballistic to diffusive. It is worth mentioning that in our study we can reach a number of lattice sites of hundreds to thousands, much larger than typical numerical studies on quantum dynamics, which allows us to exclude finite-size artifacts.
Off-shell effective energy theory: a unified treatment of the Hubbard model from d=1 to d=∞
ZHENGQIAN CHENG (Presenter), CHRIS MARIANETTI, Columbia Univ — Here we propose an exact formalism, off-shell effective energy theory (OET), which provides a thermodynamic description of a generic quantum Hamiltonian. The OET is based on a partitioning of the Hamiltonian and a corresponding density matrix ansatz constructed from an off-shell extension of the equilibrium density matrix. To approximate OET, we introduce the central point expansion (CPE), which is an expansion of the density matrix ansatz, and we renormalize the CPE using a standard expansion of the ground state energy. We present dual realizations of OET based on a partitioning of the kinetic and potential energy, denoted as K and X, respectively. We showcase the OET for the one band Hubbard model in d=1, 2, and ∞ , showing favorable agreement with exact or state-of-the-art results over all parameter space; and a negligible computational cost. Physically, K describes the Fermi liquid, while X gives an analogous description of both the Luttinger liquid and the Mott insulator. Our approach should find broad applicability in lattice model Hamiltonians, in addition to real materials systems.

*This work was supported by the grant DE-SC0016507 funded by the U.S. Department of Energy, Office of Science.

The Superfluid Pairing Gap for an Ultracold Atomic Unitary Fermi Gas
ANNETTE LOPEZ (Presenter), ETTORE VITALI, PATRICK KELLY, California State University, Fresno — We address the problem of computing the superfluid pairing gap of a fermionic cold gas from first principles. Cold atomic Fermi systems are unique laboratories to explore many-body systems, due to the unprecedented experimental control that can be currently achieved. The ability to provide robust theoretical predictions for cold atoms can have a significant impact in condensed matter physics, nuclear physics, and nuclear astrophysics. In particular, cold gases can shed light into some of the most mysterious physical systems in the universe, like the interiors of neutron stars. In this work we use unbiased Quantum Monte Carlo techniques interfaced with state of art analytic continuation technique to compute the spectral function of a unitary Fermi gas and the superfluid gap.
10:00AM W45.00011: Normalizing Cluster Wavefunctions in the Interstitial Region Within the Muffin-tin Approximation*  DANIEL GEBREMEDHIN (Presenter), CHARLES ALBERT WEATHERFORD, Florida A&M University, BRIAN WILSON, Lawrence Livermore Natnl Lab — In multi-scattering methods, overlap integrals of cluster wavefunctions for an interstitial region, which lies inside the Watson sphere and outside all the enclosed ionspheres, are discussed. When the potential inside this interstitial region is taken to be constant, and hence, obeys the Helmholtz equation, the resulting solutions are known to involve Bessel functions. Normalizing the cluster wavefunctions inside this intricate region naturally leads to two-center integrals of various Bessel-type functions. In this article, all of the numerous types of integrals that might arise are exhaustively presented. Analytical expressions that are suitable for efficient computation of the overlap integrals are worked out by employing known addition theorems for the Bessel functions. These integrals require careful attention as they otherwise lead to an artificial singularity that may not cancel. Results for sample implementations will be discussed.

*DHG and CAW were partially supported by the Department of Energy, National Nuclear Security Administration, under Award Number (s) DE-NA0003866. DHG was also supported in part by Minority Serving Institutions Partnership Program and by the HED center at the Lawrence Livermore National Laboratory.

10:12AM W45.00012: Temperature scaling in Monte Carlo nonequilibrium relaxation  YOSHIHIKO NONOMURA (Presenter), MANA, National Institute for Materials Science, YUSUKE TOMITA, College of Engineering, Shibaura Institute of Technology — The nonequilibrium relaxation (NER) method is an alternative approach to overcome the critical slowing down in Monte Carlo simulations. In local-update algorithms, NER is based on the power-law critical relaxation derived from the dynamical finite-size scaling (DFSS) theory, and off-critical scaling behaviors are also derived from the same formalism. In cluster-update algorithms, critical nonequilibrium relaxation is described by the stretched-exponential formula [1-4], which can be derived phenomenologically [5]. In the present talk, we show that off-critical scaling behaviors in cluster-update algorithms can be formulated by generalizing the nonequilibrium-to-equilibrium scaling [1,3-5]. By taking the magnetic susceptibility as an example, from the early-time critical relaxation, $\chi(t) \sim \exp(\alpha t^\beta)$, and the equilibrium behavior near the critical point $T_c$, $\chi(T) \sim (T-T_c)^\gamma$, we have $\chi(t,T) \sim (T-T_c)^\gamma f_{sc}(ct^\beta + \log(T-T_c)^\gamma)$ with a scaling function $f_{sc}(x)$. This scaling is confirmed numerically, and the one derived similarly in local-update algorithms holds better than that from DFSS.

10:24AM W45.00013: A statistical mechanics definition of the hydration shell of a membrane in an open system Molecular Dynamics Simulation. JOHN WHITTAKER (Presenter), LUIGI DELLE SITE, Freie Univ Berlin — Defining and quantifying the solvation shell of a biological macromolecule poses a major challenge, and even with state of the art equipment and methods, the question of the extent of hydration can vary depending on the quantity of interest, emphasizing the need for an unambiguous definition. The adaptive resolution simulation (AdResS) technique offers the unique ability to estimate the extent of the hydration shell around a biomolecule through the use of an open boundary atomistic system embedded within a thermodynamic reservoir of non-interacting, structureless particles. Here, we apply the latest AdResS scheme to the study of a pure DPPC membrane solvated in liquid water and determine that the mandatory solvation shell of a DPPC membrane extends to ~1.5 nm away from the DPPC phosphate headgroups, well beyond distances predicted from radial distribution functions.

10:36AM W45.00014: Topologically induced pre-scrambling and dynamical detection of topological phase transitions at infinite temperature* CEREN DAG (Presenter), Univ of Michigan - Ann Arbor, LUMING DUAN, Center for Quantum Information, IIIS, Tsinghua University, KAI SUN, Univ of Michigan - Ann Arbor — Out-of-time-order correlators (OTOCs) measured at infinite temperature are well-established tools to study quantum chaos in quantum many-body systems as well as information properties of black holes. Here we report that infinite-temperature OTOCs could also directly probe quantum phase transitions at zero temperature in contrast to common intuition. We reveal the mechanism that allows OTOC to prioritize the low energy effects over strong thermal fluctuations at infinite temperature and find that the mechanism is driven by topological degeneracy and hence is highly universal and robust, as long as the underlying system can be formulated in 1D Majorana basis. Using the Majorana representation, we analytically and numerically show that the infinite-temperature OTOCs detect the presence of Majorana zero modes at the ends of the chain that is associated with 1D Z2 topological order. Such sensitivity to zero modes introduces a new time-scale to the dynamics of non-integrable systems where the information scrambling temporarily freezes, suggesting a restricted scrambling for the topologically-protected quantum information. We dub the phenomenon as topologically induced pre-scrambling.

*This work was supported by National Science Foundation under Grant No. EFRI1741618.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W46 GMAG: Low-Dimensional Magnetism and Single Molecule Magnets 708 - Selvan Demir, Michigan State Univ - Tag(s): Focus
Remarkable magnetic field effects in quasi-one dimensional Ising-like antiferromagnet BaCo$_2$V$_2$O$_8$ studied by neutron scattering [Invited] BEATRICE GRENIER (Presenter), Univ. Grenoble Alpes & CEA-Grenoble — BaCo$_2$V$_2$O$_8$ is a realization of a spin-1/2 Ising-like quasi-one dimensional antiferromagnet (AF) with fascinating static and dynamical behaviors. In zero-field, the weak interchain interactions stabilize below 5.6 K a peculiar Néel ordering, characterized by magnetic moments aligned along the chain c-axis and dressed with confined two spinon excitations [1,2]. We have explored the influence of an external magnetic field both on the AF ordering and on the spin dynamics by single-crystal neutron scattering. Different behaviors are observed for a transverse and a longitudinal magnetic field (i.e. perpendicular and parallel to the direction of the moments, respectively), nicely reproduced by TEBD numerical calculations.

In a transverse magnetic field $H$ // $b$, a staggered field is induced along the $a$ direction, due to the non-diagonal anisotropic $g$-tensor of BaCo$_2$V$_2$O$_8$. As a result, a high field novel phase settles above a critical field of 10 T, when the staggered field overcomes both the Ising anisotropy and the interchain coupling. The nature of the excitations is also strongly modified. As I will show, our results reveal the occurrence of a topological quantum phase transition between two types of solitonic topological objects [3].

In a longitudinal magnetic field $H$ // $c$, the Néel ordering turns at a critical field of 3.8 T into a longitudinal incommensurate (IC) one, with magnetic IC excitations, due to the Ising character of the system [1]. This phase has raised a strong interest as it is a unique example of the Tomonaga-Luttinger liquid (TLL) physics experimentally accessible under moderate magnetic field. I will present our results on the dispersion spectrum in this exotic phase together with its magnetic field dependence, in the light of the TLL theory [4].

8:36AM W46.00002: Comparison of magnetic disorder at low temperature in Ca$_3$Co$_2$O$_6$ and Ca$_3$Co$_{1.9}$Zn$_{0.1}$O$_6$*  
BENJAMIN WHITE (Presenter), ALEXANDER B. C. MANTILLA, JANI JESENOVEC, Central Washington University — The compound Ca$_3$Co$_2$O$_6$ undergoes a transition into a spin-density wave (SDW) state near 24 K. Below ~10 K, this unstable SDW state coexists with a nearly-degenerate commensurate antiferromagnetic state as well as short-range magnetic order. Clear signatures of this strong magnetic disorder have been observed in the response of entropy to changing magnetic field and temperature. We performed a calorimetry study of Ca$_3$Co$_2$O$_6$ and Ca$_3$Co$_{1.9}$Zn$_{0.1}$O$_6$ in order to compare their entropic responses at low temperature. Our results for Ca$_3$Co$_2$O$_6$ reveal that $\Delta S(T, H) = S(T, H) - S(T, H = 0)$ increases as either temperature or magnetic field increase. In contrast, $\Delta S$ data for Ca$_3$Co$_{1.9}$Zn$_{0.1}$O$_6$ were relatively unresponsive to changes in temperature or field, suggesting that Zn substitution may reduce the low-temperature magnetic disorder observed in Ca$_3$Co$_2$O$_6$. These results will be discussed within the context of two cases (Ca$_3$Co$_2$O$_6$ under applied pressure and Ca$_{2.75}$R$_{0.25}$Co$_2$O$_6$ ($R$ = Dy, Lu)) in which a single magnetic ground state is stabilized.

*Research supported by Central Washington University (CWU) Science Phase II Project, the CWU Office of Undergraduate Research, and start-up funds from CWU.

8:48AM W46.00003: Electronic and magnetic properties of the cluster magnet Ba$_3$LaRu$_2$O$_9$
QIANG CHEN (Presenter), Department of Physics and Astronomy, University of Tennessee, Knoxville, AMANDA CLUNE, Department of Chemistry, University of Tennessee, Knoxville, JIE MA, Department of Physics and Astronomy, Shanghai Jiaotong University, JINGUANG CHENG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, KEITH TADDEI, CLARINA RELOJ DELA CRUZ, MATTHEW STONE, ALEXANDER KOLESNIKOV, Neutron Scattering Division, Oak Ridge National Laboratory, JANICE LYNN MUSFELDT, Department of Chemistry, University of Tennessee, Knoxville, HAIDONG ZHOU, Department of Physics and Astronomy, University of Tennessee, Knoxville, ADAM ACZEL, Neutron Scattering Division, Oak Ridge National Laboratory — Magnetic materials with electrons delocalized over small molecular clusters, so-called cluster Mott insulators, have recently attracted significant interest in the quest for novel magnetic properties. The extremely short metal-metal distances within the molecular clusters promote significant electron hopping, thus leading to the formation of unusual electronic ground state configurations based on quasi-molecular orbitals. In this talk, we discuss the electronic and magnetic properties of the cluster magnet Ba$_3$LaRu$_2$O$_9$. We present magnetic susceptibility and inelastic neutron scattering data supporting an unusual spin-3/2 per dimer electronic ground state that cannot be understood in a local moment picture. We also present bulk characterization, muon spin relaxation, neutron diffraction, and inelastic neutron scattering data that are indicative of an ordered state arising from a quasi-2D frustrated lattice of Ru dimer building blocks. Finally, we present preliminary results of Raman spectroscopy and neutron diffraction under pressure that reveal a coincident structural/spin state transition at ~1 GPa.
Large positive zero field splitting in the cluster magnet $\text{Ba}_3\text{CeRu}_2\text{O}_9$

ADAM ACZEL (Presenter), Oak Ridge National Lab, QIANG CHEN, SHIYU FAN, University of Tennessee, KEITH TADDEI, MATTHEW STONE, ALEXANDER KOLESNIKOV, Oak Ridge National Lab, JINGUANG CHENG, Chinese Academy of Sciences, JANICE LYNN MUSFELDT, HAIDONG ZHOU, University of Tennessee — We present the synthesis and magnetic characterization of a polycrystalline sample of the 6H-perovskite $\text{Ba}_3\text{CeRu}_2\text{O}_9$, which consists of Ru dimers based on face-sharing RuO$_6$ octahedra. Our low-temperature magnetic susceptibility, magnetization and neutron powder diffraction results reveal a non-magnetic singlet ground state for the dimers. Inelastic neutron scattering, infrared spectroscopy, and the magnetic susceptibility over a wide temperature range are best explained by a molecular orbital model with a zero-field splitting parameter $D \approx 85\text{meV}$ for the $S_{\text{tot}} \approx 1$ electronic ground state multiplet. This large value is likely due to strong mixing between this ground state multiplet and low-lying excited multiplets, arising from a sizable spin molecular orbital coupling combined with an axial distortion of the Ru$_2$O$_9$ units. Although the positive sign for the splitting ensures that $\text{Ba}_3\text{CeRu}_2\text{O}_9$ is not a single molecule magnet, our work suggests that the search for these interesting materials should be extended beyond $\text{Ba}_3\text{CeRu}_2\text{O}_9$ to other molecular magnets based on metal-metal bonding.

Lanthanide-based single molecule magnets through the prism of ab-initio calculations*

BORIS LEGUENNIC (Presenter), Institut des Sciences Chimiques de Rennes, University of Rennes 1 — In the beginning of the century, the emergence of lanthanide-based systems exhibiting slow relaxation of their magnetization opened a new chapter in the field of molecular magnetism. These so called Single-Molecule Magnets (SMMs) may find in a near future many important applications such as high-density data storage, molecular spintronic or quantum computing. Over the recent years, quantum chemical approaches, going from multiconfigurational wavefunction-based methodologies to (periodic) density functional theory have shown to be powerful tools to gain deep insight into electronic and magnetic features of such lanthanide-based SMMs. This presentation will focus on recent applications of such state-of-the-art computational protocols in the understanding of Ln-based SMMs behaviors.

*Project that has received funding from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation program (ERC-CoG MULTIPROSMM grant agreement N725184). French Research National Agency (ANR) is also acknowledged (grant ANR-19-CE29-0012-02).
Nature of hyperfine interactions in TbPc$_2$ single-molecule magnets: *Multireference ab-initio study*  
ALEKSANDER WYSOCKI (Presenter), KYUNGWHA PARK,  
Department of Physics, Virginia Tech — Lanthanide-based single-ion magnetic molecules can have large magnetic hyperfine interactions as well as large magnetic anisotropy. Recent experimental studies reported the tunability of these properties by changes of chemical environments or by application of external stimuli for device applications. In order to provide insight into the origin and mechanism of such tunability, here we investigate the magnetic hyperfine and nuclear quadrupole interactions of TbPc$_2$ single-molecule magnets using first-principles multireference methods including spin-orbit interaction. The microscopic Hamiltonian is mapped onto an effective Hamiltonian with an electronic pseudo-spin $S=1/2$. We discuss the physical origin of *ab-initio*-calculated hyperfine interaction parameters and their dependence on the experimental molecular geometry and structure distortions. We show the *ab-initio*-calculated electronic-nuclear spectrum and compare it with experimental data. We further analyze the role of the non-axial quadrupole interactions in the formation of avoided level crossings and magnetization dynamics.

* Funded by the Department of Energy Basic Energy Sciences grant No DE-SC0018326.  
Computational support by Virginia Tech ARC.

A first-principles study of the phase stability and electronic properties of monolayer Vanadium-based Janus dichalcogenides  
DIBYENDU DEY (Presenter), ANTIA S. BOTANA, Arizona State Univ — We investigate the vibrational and electronic properties of 2D van der Waals Vanadium-based Janus dichalcogenides (VSSe, VSeTe, VSTe) at the monolayer level in both 2H and 1T phases by using first-principles calculations. We have found the 2H phase is energetically favorable in VSSe and VSeTe, whereas the 1T phase is lower in energy in VSTe. Within density functional theory, ferromagnetism (FM) allows splitting of the d-bands in the 2H phase with a trigonal prismatic environment, leading to a low-bandgap $S=1/2$ ferromagnetic insulator. On the other hand, no such splitting is observed in the distorted octahedral environment of the 1T phase, and the system remains metallic. In the presence of electronic correlations, we have found the magnetic ground state is FM for VSSe and VSeTe. On the contrary, a 120$^\circ$ canted AFM state is the magnetic ground state for VSTe. The semiconducting nature of FM two-dimensional Janus VSSe and VSeTe makes them potential materials for spintronics.
10:12AM W46.00008: Strong anisotropic spin-dipole coupling in electron-withdrawing Br-based system Cu$_2$(OH)$_3$Br*  
TATHAMAY BASU (Presenter), HEDA ZHANG, Michigan State Univ, ZHIYING ZHAO, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, XIANGLIN KE, Michigan State Univ — The compound Cu$_2$(OH)$_3$Br, belonging to an interesting hydroxyl salts of potential interests, crystallizes in monoclinic structure. This system consists of quasi-1D Cu-chains and undergoes complex antiferromagnetic ordering below around 10 K, with a magnetic field ($H$) induced spin-flop transitions below ordering. Here, we have investigated the detailed dielectric behavior of single crystalline compound in different orientations. We show that the temperature dependent dielectric constant clearly traces the magnetic ordering in presence of magnetic field, indicating the presence of magnetodielectric (MD) coupling. The MD coupling is further confirmed by isothermal $H$-dependent dielectric constant which captures the spin-flop transitions. These features are ascribable to electron withdrawing Br-atom to break the spatial inversion symmetry of the Cu-system, which creates local dipole moment and thereby governs strong MD coupling. This will create a path to design new magnetoelectric materials.

*Work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Award No. DE-SC0019259.

10:24AM W46.00009: Tailoring Non-Innocence in a Family of 2D Coordination Solids [Invited]  
KASPER PEDERSEN (Presenter), Department of Chemistry, Technical University of Denmark — Metal-organic frameworks (MOFs) and their non-porous analogues, coordination solids, constitute a new class of materials with highly multifaceted physical and chemical properties and virtually unlimited possibilities for synthetic modification and tuning. The realization of magnetic MOFs has been hampered by the large spatial separation between spin-carriers leading to magnetic order setting in at only low temperatures. A particularly attractive approach to magnetic MOFs is rooted in the use of radical ligands as spacers between paramagnetic metal ions, which alleviates the inter-metallic distance issue and have resulted in materials featuring extremely strong super-exchange interactions. Unfortunately, relatively few isolatable radical ligands possess the stability to allow their incorporation into MOF structures. An interesting approach to realize otherwise elusive radical ligands consists in the use of highly reducible metal ions, that will reduce even ligands considered wholly redox-inactive. We recently reported a quadratic, 2D coordination solid, CrCl$_2$(pyrazine)$_2$, that features Cr(III) and a partially reduced ligand scaffold, ensuing strong magnetic Cr(III)-radical exchange interactions [1].

In this talk, recent progress in the development of metal-organic solids with extremely strong magnetic exchange interactions will be presented. Focussing on a family of isostructural, quadratic 2D coordination solids, MX$_2$(pyrazine)$_2$, we show (1) how the occurrence of redox events between the metal ion, M, and the pyrazine ligand may be controlled by chemical tuning and external stimuli, and (2) how the macroscopic materials properties (magnetic, conductive, optical) relate to the redox state of the coordination solid.

8:00AM W47.00001: Coexistence of Magnetic Orders in Two-Dimensional Magnet CrI$_3$  

Ben Niu (Presenter), Tang Su, Brian A Francisco, Subhajit Ghosh, Fariborz Kargar, Xiong Huang, Mark I Lohmann, Junxue Li, Yadong Xu, University of California, Riverside, Di Wu, Department of Materials Science and Engineering, Nanjing University, Alexander Balandin, Jing Shi, Yongtao Cui, University of California, Riverside — The magnetic properties in two-dimensional van der Waals materials depend sensitively on structure. CrI$_3$, as an example, has been recently demonstrated to exhibit distinct magnetic properties depending on the layer thickness and stacking order. Bulk CrI$_3$ is ferromagnetic (FM) with a Curie temperature of 61 K and a rhombohedral layer stacking, while few-layer CrI$_3$ has a layered antiferromagnetic (AFM) phase with a lower ordering temperature of 45 K and a monoclinic stacking. In this work, we use cryogenic magnetic force microscopy to investigate CrI$_3$ flakes in the intermediate thickness range (25 – 200 nm) and find that the two types of magnetic orders can coexist in the same flake, with a layer of ~13 nm at each surface being in the layered AFM phase similar to few-layer CrI$_3$ and the rest in the bulk FM phase. The switching of the bulk moment proceeds through a remnant state with nearly compensated magnetic moment along the c-axis, indicating formation of c-axis domains allowed by a weak interlayer coupling strength in the rhombohedral phase.
8:12AM W47.00002: The honeycomb quantum Heisenberg ferromagnet model with anisotropic exchange interactions*  JOREN VANHERCK (Presenter), Physics Department, University of Antwerp, BART SOREE, Department of Electrical Engineering (ESAT), KU Leuven, WIM MAGNUS, Physics Department, University of Antwerp — Since the discovery of magnetism in single-layered CrI$_3$ about two years ago [1], research into the magnetic properties of this type of monolayer materials has ever been growing. However, a fundamental theory describing the origin of two-dimensional ferromagnetism, which is key in understanding its properties, is still missing.

We modelled these two-dimensional materials using a honeycomb quantum Heisenberg ferromagnet, accounting not only for the exchange interactions up to third nearest neighbours, but also allowing an overal exchange anisotropy. The latter turns out to be key for the ferromagnetic ordering. Here, we present analytical results that were obtained using double-time temperature-dependent Green's functions [2]. We furthermore discuss the influence of temperature, anisotropies and exchange constants on the resulting magnetization.


*We acknowledge funding from IMEC.

8:24AM W47.00003: Two-dimensional Ferromagnetic van der Waals CrX$_3$ (X=Cl, Br, I) Monolayers with Enhanced Anisotropy and Curie Temperature*  FENG XUE (Presenter), Fudan Univ, RUQIAN WU, UCI — Among the recently widely studied van der Waals layered magnets CrX$_3$ (X=Cl, Br, I), CrCl$_3$ monolayer (ML) is particularly puzzling as it is solely shown by experiments to have an in-plane magnetic easy axis and, furthermore, all of previous first-principles calculation results contradict this. Through systematical first-principles calculations, we unveil that its in-plane shape anisotropy that dominates over its weak perpendicular magnetocrystalline anisotropy is responsible for the in-plane magnetic easy axis of CrCl$_3$ ML. To tune the in-plane ferromagnetism of CrCl$_3$ ML into the desirable perpendicular one, we propose substituting Cr with isovalent tungsten (W). We find that CrWCl$_6$ has a strong perpendicular magnetic anisotropy and a high Curie temperature up to 76 K. Our work not only gives insight into understanding the two-dimensional ferromagnetism of van der Waals MLs but also sheds new light on engineering their performances for nanodevices.

*Work was supported by DOE-BES (Grant No. DE-FG02-05ER46237). Computer simulations were partially performed at the U.S. Department of Energy Supercomputer Facility (NERSC). F.X and Z.W. acknowledge support by the Basic Research Program of China under Grant No. 2015CB921400.
Spin wave excitations in van der Waals honeycomb ferromagnets

[Invited] JAE-HO CHUNG (Presenter), Korea Univ — Recent discoveries of robust two-dimensional magnetism brought about a great research interest in van der Waals ferromagnets [1]. Experimental observations of their spin wave excitations are important because the underlying spin Hamiltonian can provide crucial information regarding thermal stability of their long-range order. In this talk, we focus on honeycomb ferromagnets where linear Dirac crossings in their magnon bands similarly to the electronic band of graphene [2]. We used inelastic neutron scattering to observe spin wave excitations in CrI$_3$ and Cr$_2$Ge$_2$Te$_6$ single crystals, where robust ferromagnetism was observed in monolayers [1]. The spin wave band of CrI$_3$ at $T = 5$ K consisted of two distinctive bands of ferromagnetic excitations separated by a ~ 2 meV gap at the Dirac points [3]. These results can only be understood by considering a Heisenberg Hamiltonian with Dzyaloshinskii-Moriya interaction, thus providing experimental evidence that spin waves in CrI$_3$ can have robust topological properties. As the temperature was increased to and beyond $T_C = 61$ K, the anisotropy gap at the zone center vanished following the power law behavior whereas the stiffness of the spin waves remained finite. These results strongly indicate that the magnetic anisotropy plays a decisive role in determining the Curie temperature in CrI$_3$, which is in contrast with typical three-dimensional Heisenberg ferromagnets where exchange interactions controlling the Curie temperature. In comparison, Cr$_2$Ge$_2$Te$_6$ showed no evidence of Dirac gap but revealed the significant next nearest neighbor exchanges due to Ge ions. Finally, we will report the quantitative estimates of exchange parameters in their spin Hamiltonian, and compared their values with those of CrBr$_3$ and Cr$_2$Si$_2$Te$_6$.


Observation of 2D magnons in atomically thin CrI$_3$

JOHN CENKER (Presenter), BEVIN HUANG, Physics, University of Washington, NISHCHAY SURI, Physics, Carnegie Mellon University, PEARL THIJSSEN, AARON MILLER, Physics, University of Washington, MICHAEL MCGUIRE, Materials Science and Technology Division, Oak Ridge National Laboratory, DI XIAO, Physics, Carnegie Mellon University, XIAODONG XU, Physics, University of Washington — The collective excitations in magnetic materials, i.e. spin waves or magnons, may couple to inelastically scattered light. Despite the recent interest in two-dimensional (2D) van der Waals magnets, a direct observation of magnons in the monolayer limit is lacking. Here, we report the observation of 2D magnons in atomically thin CrI$_3$ by magneto-optical Raman measurements. In monolayer and bilayer CrI$_3$, we observe a sharp one-magnon feature at a zero-field energy of ~0.3 meV which blue-shifts with a g factor of 2. However, at the metamagnetic transition from the layered antiferromagnetic to spin-polarized state in bilayer, the magnon exhibits a discontinuous red-shift. This confirms that the magnetic anisotropy is much larger than the interlayer exchange in CrI$_3$. In addition, we observe a magnon feature at ~19 meV (~4.6 THz) for bilayer and thicker samples, significantly higher than $\Gamma$ point magnons in standard ferromagnetic systems, i.e. YIG. Our results establish CrI$_3$ as a potential candidate in miniaturized terahertz magnonic devices.
9:24AM W47.00006: Tuning Inelastic Light Scattering via Symmetry Control in 2D Magnet CrI$_3$

BEVIN HUANG (Presenter), JOHN CENKER, University of Washington, XIAOOU ZHANG, Physics, Carnegie Mellon University, ESSANCE RAY, TIANCHENG SONG, University of Washington, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, MICHAEL MCGUIRE, Materials Science and Technology Division, Oak Ridge National Laboratory, DI XIAO, Physics, Carnegie Mellon University, XIAODONG XU, University of Washington — The coupling between spin and charge degrees of freedom in a crystal imparts strong optical signatures on scattered electromagnetic waves. This has led to magneto-optical effects with a host of applications, from the sensitive detection of local magnetic order to data storage technologies. Here, we demonstrate a new magneto-optical effect: the tuning of inelastically scattered light through symmetry control in atomically thin chromium triiodide (CrI$_3$). In monolayers, we found an extraordinarily large magneto-optical Raman effect from an A$_{1g}$ phonon mode due to ferromagnetic order. The linearly polarized, inelastically scattered light rotates by ~40°, more than two orders of magnitude larger than the rotation from MOKE under the same experimental conditions. In CrI$_3$ bilayers, we show that the same A$_{1g}$ phonon mode becomes Davydov-split into two modes of opposite parity, exhibiting selection rules that depend on inversion symmetry and magnetic order. Applied magnetic and electric fields allow for magnetoelectrical control over these selection rules. Our work highlights the unique opportunities provided by 2D magnets for controlling underlying symmetries to manipulate Raman optical selection rules and for exploring emergent magneto-optical effects and spin-phonon coupled physics.

9:36AM W47.00007: Phonon-mediated magnetic order control of bilayer antiferromagnets*

MARTIN RODRIGUERZ-VEGA (Presenter), ZEXUN LIN, University of Texas at Austin, GAURAV CHAUDHARY, Physics, University of Chicago, ARITZ LEONARDO, University of the Basque Country, MAIA VERGNIORY, Donostia International Physics Center, GREG FIETE, Northeastern University — We study theoretically the effects of non-linear phonon processes after the ultra-fast photo-excitation of an infrared-active mode in the magnetic order of bilayer antiferromagnets. As a prototypical example, we consider bilayer CrI$_3$, a van der Waals crystal composed of ferromagnetic (FM) layers with out-of-plane magnetization. Between the layers, the exchange coupling is antiferromagnetic (AFM) in the ground state, as determined experimentally, and such coupling is connected with the relative stacking between the layers. We employ group theory methods to determine the nature of the phonons modes and their allowed non-linear coupling terms in the AFM groundstate. Then, we use first-principles calculations to determine their frequencies and coupling strengths. We then use those results as inputs for the phonon equations of motion after photo-excitation and find that the Raman modes involving relative movement between the layers have the potential to influence the interlayer exchange interaction. Finally, we comment on the feasibility of the experimental detection of the changes in the magnetic order.

*This work was supported by the NSF Materials Research Science and Engineering Center Grant No. DMR-1720595 and NSF Grant No. DMR-1949701.
9:48AM W47.00008: Strain effect on magnetism of atomically thin CrI₃  QIAN SONG (Presenter), CONNOR A OCCHIALINI, DIFEI ZHANG, JIARUI LI, ABRAHAM L LEVITAN, RICCARDO COMIN, Massachusetts Institute of Technology MIT — The structural stacking order plays an important role for the magnetic ground state of atomically thin CrI₃. While bulk crystals undergo a transition from Monoclinic structure at room temperature to Rhombohedral structure at low temperature, bilayer CrI₃ maintains a monoclinic structure for all temperatures. Despite several studies, the absence of a structural transition in bilayer CrI₃ remains to be understood. Here we report on the study of bilayer CrI₃ on different substrates, using Raman and magneto-optical Kerr effect measurements to reveal the interplay between epitaxial strain, lattice structure, and spin ordering. We find that the lattice mismatch and resulting strain between the substrate and the CrI₃ flakes has a dramatic impact on the structure of the atomically thin CrI₃.

10:00AM W47.00009: Intrinsic Ferromagnetism in 2D CrₓSe₁₋ₓ Crystals*  MENGYING BIAN (Presenter), KEKE HE, FAN SUN, PEIJIAN WANG, ALIREZA JALOULI, JONATHAN P BIRD, State Univ of NY - Buffalo, YANGLONG HOU, Peking University, HAO ZENG, State Univ of NY - Buffalo — In the last two years, several two-dimensional (2D) materials of magnetic order, including CrI₃ and Cr₂Ge₂Te₆, have been observed, which represents a breakthrough in the field of 2D magnetism and opens up opportunities for device applications integrating these magnets with other van der Waals (vdW) crystals. However, most of these materials are vdW structures which rely on the mechanical exfoliation technique to obtain ultra-thin flakes. Furthermore, most 2D magnets have poor stability and low magnetic transition temperature, which limit their practical application. To search for 2D materials with improved magnetic properties, one needs to look beyond vdW crystals. In this work, a 2D non-vdW magnetic material, CrₓSe₁₋ₓ, has been synthesized using an ambient pressure chemical vapor deposition method. The magnetic characterization demonstrated that the thin flakes exhibit ferromagnetic properties with ordering temperature above 250 K. These results may pave the way for practical applications of 2D magnets.

*NSF DMR-1104994 and CBET-1510121
Temperature dependent study of magnetization dynamics in CrCl$_3$ – a layered antiferromagnet*  

SUPRIYA MANDAL (Presenter), LUCKY N. KAPOOR, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research (TIFR), SOHAM MANNI, Department of Physics, Indian Institute of Technology (IIT) Palakkad, MEGHAN P. PATANKAR, A. THAMIZHAVEL, MANDAR M DESHMUKH, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research (TIFR) — Chromium trichloride (CrCl$_3$) is a layered antiferromagnet. Recently it has found renewed interest due to its antiferromagnetic resonance in GHz frequencies, two-dimensional (2D) layered structure with low cleavage energy and complex magnetization dynamics [1]. We report a detailed study of magnetization dynamics of bulk CrCl$_3$ placed on a coplanar waveguide (CPW) as a function of temperature. We observe prominent ferromagnetic, antiferromagnetic and paramagnetic resonances depending on temperature and in-plane magnetic field. We also observe magnon-magnon coupling and presence of multiple spin-wave modes by introducing an additional out-of-plane magnetic field by tilting the sample with respect to magnetic field direction. We extract useful system parameters and study their dependence on temperature and angle of tilting by fitting to experimental data. Ability to easily exfoliate 2D layers of CrCl$_3$ opens up possibility of coupling it to CPW resonators and application in antiferromagnetic spintronics and hybrid quantum systems.

Reference:

*We acknowledge funding support from Department of Atomic Energy and Department of Science and Technology of India.
Two-dimensional (2D) magnetic materials are of great current interest for their promising applications in spintronics. Here we propose the van der Waals (vdW) material $\text{VI}_3$ to be a 2D Ising ferromagnet (FM), using density functional calculations, crystal field level diagrams, superexchange model analyses, and Monte Carlo simulations. The $a_{1g}^1e_{-1}^1$ state in the trigonal crystal field turns out to be the ground state, and it gives rise to the 2D Ising FM due to a significant single ion anisotropy (SIA) associated with the $S_z=1$ and $L_z=-1$ state of $V^{3+}$ ions. Moreover, a tensile strain on the $\text{VI}_3$ monolayer further stabilizes the $a_{1g}^1e_{-1}^1$ ground state, and the enhanced FM superexchange and the strong SIA would raise the Curie temperature of the $\text{VI}_3$ monolayer from 70 K to 90-110 K under a 2.5-5% tensile strain. This prediction is worth a prompt experimental verification.

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Two-dimensional magnetism in a van der Waals semiconductor

Since the recent discovery of ferromagnetism in exfoliated flakes of $\text{CrI}_3$ and $\text{Cr}_2\text{Ge}_2\text{Te}_6$, interest in two-dimensional (2D) ferromagnetic systems has increased. Previously predicted to be prohibited by thermal fluctuations, the existence of 2D magnetically ordered systems offers an ideal platform for examining novel quantum phenomena and opens up opportunities for emerging applications, including magneto-optic and magneto-electronic devices, spintronics, and quantum computing. For use in applications, there is a crucial need to develop 2D materials that simultaneously exhibit ferromagnetism and semiconducting behaviors. Towards this end, we recently synthesized an air stable van der Waals magnetic semiconductor. 2D sheets can be prepared through mechanical exfoliation for measurement and incorporation into more complex heterostructures. Using electrical transport, second harmonic generation spectroscopy, photoluminescence spectroscopy, and scanning tunneling spectroscopy, we investigate the electrical and magnetic properties of this material in the 2D limit. We present clear evidence of layered antiferromagnetic ordering at ~130K, below which the spins in each sheet are aligned ferromagnetically parallel to the plane while the interlayer coupling is antiferromagnetic.
W47.00013: Giant and nonreciprocal second harmonic generation from layered antiferromagnetism in bilayer CrI$_3$  
ZEYUAN SUN (Presenter), YANGFAN YI, Fudan University, TIANCHENG SONG, GENEVIEVE CLARK, BEVIN HUANG, University of Washington, YUWEI SHAN, SHUANG WU, DI HUANG, CHUNLEI GAO, ZHANGHAI CHEN, Fudan University, MICHAEL MCGUIRE, Oak Ridge National Laboratory, TING CAO, University of Washington, DI XIAO, Carnegie Mellon University, WEI-TAO LIU, Fudan University, WANG YAO, University of Hong Kong, XIAODONG XU, University of Washington, SHIWEI WU, Fudan University — Layered antiferromagnetism is the spatial arrangement of ferromagnetic layers with antiferromagnetic interlayer coupling. Recently, the van der Waals magnet, chromium triiodide (CrI$_3$), emerged as the first layered antiferromagnetic insulator in its few-layer form. In this talk, we present an emergent nonreciprocal second-order nonlinear optical effect in bilayer CrI$_3$. The observed second-harmonic generation (SHG) is giant: several orders of magnitude larger than known magnetization induced SHG and comparable to SHG in the best 2D nonlinear optical materials studied so far. We show that while the parent lattice of bilayer CrI$_3$ is centrosymmetric and thus does not contribute to the SHG signal, the observed nonreciprocal SHG originates purely from the layered antiferromagnetic order, which breaks both spatial inversion and time reversal symmetries. Furthermore, polarization-resolved measurements reveal the underlying C$_{2h}$ symmetry, and thus monoclinic stacking order in CrI$_3$ bilayers, providing key structural information for the microscopic origin of layered antiferromagnetism. Our results indicate that SHG is a highly sensitive probe of subtle magnetic orders and open up possibilities for the use of two-dimensional magnets in nonlinear and nonreciprocal optical devices.

Friday, March 6, 2020 8:00 AM - 10:24 AM

Session W48 DCMP: Superconductivity: Theories and Models III  
Mile High Ballroom 1A - Volodymyr Turkowski, Univ of Central Florida

8:00AM W48.00001: On the equivalence of Peierls and Holstein models in perovskite structures  
YAU CHUEN YAM (Presenter), MONA BERCIU, GEORGE ALBERT SAWATZKY, University of British Columbia — We consider the effects of electron-phonon coupling in a perovskite ABO$_3$, modelled in terms of uncorrelated s-orbitals on the B sites that hybridize with ligand p-orbitals at the O sites. Both the s-p and the p-p hopping matrices are modulated by vibrations of the O, described as Einstein optical phonons. For a single B0$_6$ cluster, we show that the effects of this Peierls electron-phonon coupling are described well in terms of an effective Holstein model, which couples the carrier to the single "molecular" phonon with A1g symmetry. For a single polaron in an infinite crystal, however, we demonstrate that the Peierls model has sharp transitions as the coupling is varied, where the ground-state momentum jumps between different high-symmetry points of the Brillouin zone. Such transitions are impossible for a Holstein model, showing that there are regions of the parameter-space where the two types of models are not equivalent.
8:12AM W48.00002: Mottness induced phase fluctuation in overdoped superconducting cuprates  WEI KU (Presenter), ZIJIAN LANG, Tsung-Dao Lee Institute & Shanghai JiaoTong University, FAN YANG, School of Physics, Beijing Institute of Technology — Recent observations of diminishing supefluid phase stiffness in overdoped cuprate high-temperature superconductors challenges the conventional picture of superconductivity. Here, through analytic estimation and verified via variational Monte Carlo calculation of an emergent Bose liquid, we point out that Mottness of the underlying doped holes dictates a strong phase fluctuation of the supefluid at moderate carrier density. This effect turns the expected doping-increased phase stiffness into a dome shape, in good agreement with the recent observation. Specifically, the effective mass divergence due to "jamming" of the low-energy bosons reproduces the observed nonlinear relation between phase stiffness and transition temperature. Our results suggest a new paradigm, in which the high-temperature superconductivity in the cuprates is dominated by physics of Bose-Einstein condensation, as opposed to pairing-strength limited Cooper pairing.

8:24AM W48.00003: Ground state properties of the Emery model in the underdoped regime*  ADAM CHICIAK (Presenter), William & Mary College, ETTORE VITALI, California State University, Fresno, SHIWEI ZHANG, Flatiron Institute — We perform extensive Auxiliary-Field Quantum Monte Carlo (AFQMC) calculations for the three-band Hubbard (Emery) model in the underdoped regime, in order to study the ground-state properties of Copper-Oxygen planes in the cuprates. Interfacing generalized Hartree-Fock calculations with cutting-edge AFQMC techniques in a self-consistent scheme, we are able to resolve small energy scales, which is crucial for determining the complex candidate orders in such a system. We explore the charge order, spin order, and localization properties as a function of charge-transfer energy.

*Supported by NSF and Simons Foundation
A dynamical cluster approximation study of \( T_c \) in a composite superconducting-metallic two-component model.  

PHILIP DEE (Presenter), Department of Physics and Astronomy, The University of Tennessee, Knoxville, THOMAS MAIER, Computational Sciences and Engineering Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Can we realize enhanced \( T_c \) in a low superfluid density superconductor by coupling it to a metal? This idea, which was postulated in [1] and shown perturbatively in [2], suggests that coupling a layer with a large pairing scale \( \Delta_0 \) but small phase stiffness to a non-interacting metallic layer can raise \( T_c \) to its mean-field value \( T_{MF} = \Delta_0 / 2 \). We studied this system nonperturbatively using the dynamical cluster approximation for a 2D attractive Hubbard model coupled to a noninteracting metallic layer via interlayer hopping. In contrast to prior work, our results for \( T_c \) appear only to decrease with increasing interlayer coupling.


Effect of non-phonon modes on the isotope effect and Hall resistivity in cuprates  
DA WANG (Presenter), Nanjing Univ — Non-phonon boson modes are widely observed in cuprates. Their existence may cause many interesting phenomena. In this work, we investigate their effects on the \( T_c \) isotope coefficient and Hall resistivity. (1) The coexistence of phonon and non-phonon modes leads to anomalous isotope effect. In special, if one of the boson modes (either phonon or non-phonon) is pair-breaking, large isotope coefficient \( \alpha > 0.5 \) can be obtained and a scaling of \( \alpha \sim \ln^2(T_c) \) as \( T_c \to 0 \) is predicted. This study indicates that \( \alpha > 0.5 \) may be caused by pair-breaking phonon. (2) If the non-phonon boson mode is stabilized by the magnetic field, the Hall coefficient shows a strong field dependence, in special near a van Hove filling. This may challenge the current understanding of the \( \text{``Hall number''}: p \to 1+p \) or \( p \to \infty \)?

This work is supported by NSFC under grant Nos. 11874205 and 11574134.
9:00AM W48.00006: Magnetic impurities as hosts of odd-frequency superconductivity*
DUSHKO KUZMANOVSKI (Presenter), ALEXANDER BALATSKY, NORDITA, Stockholm University — Odd-frequency (odd-$\omega$) superconductivity is an example of unconventional dynamical order, where the Cooper pair correlations are both non-local and odd in relative time. Historically, the most important role regarding proximity-induced odd-$\omega$ pairing was played by superconductor-ferromagnet heterostructures. Shrinking the magnetic domain of this setup to the extreme, we demonstrate that all the necessary ingredients for generating odd-$\omega$ pairing are present in the vicinity of a paramagnetic impurity embedded in a conventional single-band bulk spin-singlet s-wave superconductor. We investigate the appearance of all possible pair amplitudes in accordance with the Berezinskii SPOT = -1 rule, which in our single-orbital case, trivially has O = +1. We study the spatial and frequency dependence of components classified by spatial parity, their evolution with impurity strength, and identify a reciprocity between different symmetries related through impurity scattering. We present calculations of physically measurable observables, such as spin-polarized local density of states, local spin susceptibility that carry signatures of odd-$\omega$ in some of their features.

*DK and AVB acknowledge support from the European Research Council under the European Union's Seventh Framework ERS-2018-SYG 810451HERO

9:12AM W48.00007: Harmonic Fingerprint of Unconventional Superconductivity*
MICHAEL KLETT (Presenter), XIANXIN WU, TILMAN SCHWEMMER, MARIO FINK, WERNER R HANKE, RONNY THOMALE, Institute for Theoretical Physics, University of Wuerzburg — The structure of superconducting pairing is determined by microscopic details such as the interaction profile and Fermiology beyond the spatial symmetry classification along irreducible point group representations of the underlying lattice. The pairing wave function unfolds in its orbital-resolved Fourier profile which we call the harmonic fingerprint (HFP), allowing us to formulate a concise connection between microscopic parameter changes and their impact on superconductivity. We present an analysis - based on random phase approximation calculations - of twisted bilayer graphene (TBG) involving d+id, s±, and f-wave order. Including nonlocal interactions - which unavoidably enter the low-energy electronic description of TBG - increases the weight of higher lattice harmonics and furthermore has a significant effect on the orbital structure of the paring states.

*The work in Wuerzburg is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through Project-ID 258499086 - SFB 1170 and through the Wuerzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter –ct.qmat Project-ID 39085490 - EXC 2147.
In heavy fermion system, multipole degree of freedom induce interesting phenomena, such as unconventional superconductivity (SC) and Anomalous Hall Effect (AHE). Recent experiments have revealed that unconventional s-wave SC state without any sigh-reversal emerges near the AFM phase in heavy fermion compound CeCu$_2$Si$_2$. However, this fact cannot be explained by conventional Migdal-Eliashberg (ME) theory. To overcome this difficulty, we study the microscopic SC paring mechanism in the presence of strong spin-orbit interaction (SOI) and higher-order many body effects ignored in ME theory. As a result, we find that unconventional s-wave state is realized near the AFM phase against the strong magnetic fluctuations. Moreover, obtained s-wave SC originates from interference between electric and magnetic multipole fluctuations due to the mode coupling effects given by many body effects. In addition, we propose large AHE will be induced due to the multi-orbital nature and strong SOI in the present system. [1] R. Tazai and H. kontani, J. Phys, Soc. Jpn. 88, 063701 (2019).

We study the effect of spin-orbit coupling (SOC) on the Hund's coupling induced orbital-singlet spin-triplet superconductivity in the three-orbital Hubbard model with rotationally-invariant slave-boson (RISB) mean-field theory. In the absence of SOC, RISB reproduces the phase diagram similar to the one obtained from dynamical mean-field theory, where the superconducting state emerges from the Hund's metal crossover regime. In the presence of SOC, the intrinsic particle-hole asymmetry in atomic levels, introduced by SOC, leads to different superconducting behaviors for above and below half-filling; the SOC suppresses the superconductivity in these two regimes with distinct manners. We analyze how these behaviors are connected to the spin and charge fluctuations and the atomic multiplets statistics. Our results provide insight into the pairing mechanism in Sr$_2$RuO$_4$ and iron-based superconductors.
9:48AM W48.00010: Influence of the Rutgers Relation on underdoped cuprate properties*

PATRICIA SALAS CASALES (Presenter), M. A. SOLÍS, Instituto de Física, UNAM — Within the extended Layered Boson-Fermion Model of Superconductivity [1,2] the Rutgers Relation, which relates the difference between the normal and the superconducting isobaric specific heats with the thermodynamic critical field, is combined with the first-principles relation of the critical field derivative as well as with the penetration and coherence lengths to get a novel expression for the penetration length $\lambda(T)$, which is more suitable for high temperature superconductors, as we have seen after applying it to underdoped cuprate superconductors $YBa_2Cu_3O_{6+x}$.

We compare our current results for the penetration length and the normalized superfluid density as functions of temperature as well as of doping $x$, with experiments and our previously reported results, obtaining a substantial improvement.


*We thank partial support form grants CONACyT 221030, DGAPA-PAPIIT IN107616 and DGAPA-PAPIIT IN110319.

10:00AM W48.00011: DMRG and weak coupling studies of the two-leg Hubbard ladder*

YUVAL GANNOT (Presenter), YI-FAN JIANG, STEVEN KIVELSON, Stanford Univ — The Hubbard model is of paradigmatic significance in the study of highly correlated electron systems. Hubbard ladders are particularly interesting as they exhibit a subtle interplay between multiple phases even at weak coupling. Here, we reexamine the ground state phase diagram of the two-leg ladder in the limit of asymptotically weak coupling, an approach pioneered by Balents and Fisher (BF).

Among other things we find that the presence of a dangerously irrelevant operator leads to an instability of a previously predicted partially gapped phase. The result is a Luther-Emery (LE) liquid - the 1D analogue of a superconductor - characterized by a hierarchy of energy scales: the principle gap depends exponentially on $1/U$ in the asymptotic $U \to 0^+$ limit, as found by BA, while the additional gaps are smaller still by factors of $U^{1/2}$ compared to the dominant gap. Using DMRG to study the same ladder for intermediate values of $U$ (as small as $U = 4t$), we find qualitative behavior (LE phase and the existence of two distinct gap scales) similar to that predicted by the weak coupling theory.

*This work was supported in part by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515.
10:12AM W48.00012: Beyond s- and d-waves: $d + d$ intra- and inter-band pairing in multiband superconductors* QIMIAO SI (Presenter), Department of Physics and Astronomy, Rice University, EMILIAN NICA, Department of Physics, Arizona State Univ — Recent experiments in multiband Fe-based and heavy-fermion superconductors have challenged the long-standing dichotomy between standard s- and d-waves. We discuss an alternative in the form of a gapped $d + d$ intra- and inter-band pairing which provides a natural interpolation between standard s and d-waves. We illustrate that this is equivalent to an $s\tau_3$ pairing initially proposed in the context of Fe-based superconductors [1]. We demonstrate that similar candidates are possible outside of the Fe-based family by constructing an analog for the heavy-fermion superconductor CeCu$_2$Si$_2$. We compare and contrast $d + d$ with similar pairings which occur in $^3$He.


*Supported by the DOE BES Award # DE-SC0018197 and the Robert A.Welch Foundation Grant No. C-1411 (Q.S.)

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W49 DCMP: Superconductivity and Competing phases Mile High Ballroom 1B - David Tanner, University of Florida

8:00AM W49.00001: Signatures of a pair density wave in striped cuprates at high magnetic fields ($H$)* PAUL BAITY (Presenter), ZHENZHONG SHI, JASMINKA TERZIC, DRAGANA POPOVIC, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ., TAKAO SASAGAWA, Tokyo Inst. of Tech. — In underdoped cuprates, a putative pair density wave (PDW) state has been suggested to be responsible for the pseudogap regime, but the evidence for a PDW remains inconclusive. To test the interlayer frustration, the crucial component of the PDW picture, we performed transport measurements on La$_{1.7}$Eu$_{0.2}$Sr$_{0.1}$CuO$_4$ and La$_{1.48}$Nd$_{0.4}$Sr$_{0.12}$CuO$_4$ with “striped” spin and charge orders in perpendicular magnetic fields $H_{\text{perp}}$, and we also applied an additional field parallel to CuO$_2$ layers ($H_{\text{para}}$). We detected several phenomena predicted to arise from the existence of a PDW, including an enhancement of interlayer superconducting (SC) phase coherence with increasing $H_{\text{para}}$. Our results are consistent with the presence of local, PDW pairing correlations that compete with the uniform SC order at temperatures $T^0_c < T < (2-6)T^0_c$, where $T^0_c$ is the zero-field SC transition temperature, and become dominant at high enough $H_{\text{perp}}$ as $T \rightarrow 0$.

8:12AM W49.00002: Re-investigating the pseudogap phase of cuprates.  PAOLO ABRAMI (Presenter), SVEN BADOUX, ANTONY CARRINGTON, Physics, University of Bristol — The nature of the pseudogap state and the role it plays in the rich phase diagram of cuprate superconductors is yet to be fully understood. It is still an open question whether the transition to this state is a true phase transition or a slow crossover. A further question is whether the phase transition terminates at a zero temperature quantum critical point and what influence this has on the superconductivity. Recently, measurements of in-plane magnetic torque have suggested an abrupt transition close to the estimated edge of the pseudogap phase; suggesting a thermodynamic transition to an electronically nematic state. Here we further investigate these effects in different high Tc cuprates and how extrinsic effects can influence the signals seen.

8:24AM W49.00003: Diffuse Scattering Studies of Local Correlations in ErBa$_2$Cu$_3$O$_{6+x}$* BISHAM POUDEL (Presenter), BOGDAN M DABROWSKI, Physics, Northern Illinois University, DANIEL PHELAN, MATTHEW KROGSTAD, RAYMOND OSBORN, STEPHAN ROSENKRANZ, OMAR CHMAISSEM, Materials Science Division, Argonne National Lab — The origin of unconventional superconductivity in cuprate superconductors remains a great challenge. Early observations of stripe correlations in La$_{2-x-y}$Nd$_x$Sr$_y$CuO$_4$ confirmed the existence of spin and charge density wave orders near a “magical” p = 1/8 hole-doping where superconductivity disappears. At about the same time, ARPES measurements observed a pseudogap at temperatures much higher than T$_C$. The observation of CDW and pseudogap states appearing together and vanishing near optimal doping led to the speculation that these parameters are correlated and have a common origin. However, with the detection of weak charge density waves in YBCO near optimal doping (away from p = 1/8), these claims need to be re-evaluated. In that regard, rare-earth crystal field spectroscopy, used as a probe of the local structural and electronic environment in ErBa$_2$Cu$_3$O$_{6+x}$, provided evidence for charge-transfer between the copper chains and planes and the formation of clusters with three distinct states. In this talk, I will discuss recent single crystal diffuse scattering work to elucidate the nature of local short-range order and its correlation with CDW and the pseudogap states.

*Work at Argonne (data collection and analysis) was supported by the U.S. DOE, Office of Science, BES, DMSE
Spatially Inhomogeneous Competition between Superconductivity and the Charge Density Wave in YBa$_2$Cu$_3$O$_{6.67}$

JAEWON CHOI (Presenter), Physik-Institut, University of Zurich, OLEH IVASHKO, Deutsches Elektronen-Synchrotron DESY, ELIZABETH BLACKBURN, Department of Physics, Lund University, RUIXING LIANG, DOUGLAS ANDREW BONN, WALTER N HARDY, Department of Physics & Astronomy, University of British Columbia, ALEXANDER HOLMES, European Spallation Source, NIELS BECH CHRISTENSEN, Department of Physics, Technical University of Denmark, MARKUS HUECKER, Department of Condensed Matter Physics, Weizmann Institute of Science, SIMON GERBER, Laboratory for Micro and Nanotechnology, Paul Scherrer Institut, OLOF GUTOWSKI, UTARUETT, MARTIN VON ZIMMERMANN, Deutsches Elektronen-Synchrotron DESY, EDWARD M. FORGAN, Department of Physics & Astronomy, University of Birmingham, STEPHEN HAYDEN, H. H. Wills Physics Laboratory, University of Bristol, JOHAN CHANG, Physik-Institut, University of Zurich — Application of magnetic field induces new charge density wave (CDW) order in the high-temperature superconductor YBa$_2$Cu$_3$O$_{7-x}$ (YBCO), which is defined here as ferro-coupled CDW (F-CDW). It can be differentiated from the conventional antiferro-coupled CDW (or AF-CDW) by their c-axis correlations. This discovery has provoked a number of questions such as how does superconductivity compete with two CDW orders? and are either of these orders responsible for the electronic reconstruction? High-energy x-ray diffraction experiments were carried out to find a clue to those questions. The intensity of F-CDW order in YBa$_2$Cu$_3$O$_{6.67}$ was investigated as a function of magnetic field and temperature. We found that F-CDW order exists from low-field range B ~ 5 T, and regions of the sample with F-CDW order suppress superconductivity stronger than those with AF-CDW order. It implies that the superconducting state in some regions is more fragile than that in the other regions. In addition, F-CDW order has sufficiently long correlation length to explain the reconstruction of the electronic state. Our study sheds a light on the role of F-CDW order in superconducting and normal state properties of underdoped YBCO.
8:48AM W49.00005: No pseudogap magnetism detected in optimally to heavily overdoped

**Bi$_{2+x}$Sr$_2-x$CaCu$_2$O$_{8+d}$** single crystals by $\mu$SR*  

SHAYAN GHEIDI (Presenter), ANDRE M CÔTÉ, Simon Fraser Univ, SARAH DUNSIGER, CMMS, TRIUMF, KOLAWOLE ABAYOMI AKINTOLA, ALEX FANG, SHYAM SUNDAR, Simon Fraser Univ, GENDA GU, Brookhaven National Laboratory, JEFF SONIER, Simon Fraser Univ — Weak, temperature-dependent, quasi-static magnetism has been detected within the pseudogap (PG) phase of optimally-doped ($T_c = 91$ K) and overdoped ($T_c = 80$ K) Bi$_{2+x}$Sr$_2-x$CaCu$_2$O$_{8+d}$ (Bi2212) single crystals by zero-field (ZF) muon spin relaxation (mSR) [A. Pal et al., Phys. Rev. B 97, 060502(R) (2018)]. However, in this study it was not possible to determine whether the magnetism onsets at the PG temperature ($T^*$) due to the occurrence of muon diffusion above $T \sim 150$ K. To address this issue, we performed a similar ZF-mSR investigation of overdoped single crystals ($T_c = 70$ K and 55 K) in which $T^*$ lies below the muon diffusion temperature. The results are similar to that obtained for the lower doped samples, indicating that the anomalous magnetism is independent of hole-doping concentration and thus apparently not associated with the PG. We have carried out additional ZF-mSR measurements on these samples using an ultra-low background spectrometer. The new measurements verify the source of the magnetism comes from the Bi2212 samples. Potential origins of the anomalous magnetism will be discussed.

*Acknowledged support from Natural Sciences and Engineering Research Council of Canada (NSERC).

9:00AM W49.00006: Nematic Cooper-pair mass renormalization in copper oxide superconductors  

JONATHAN WARDH (Presenter), MATS GRANATH, Goteborg Univ, JIE WU, IVAN BOZOVIĆ, Brookhaven National Laboratory — We show that the observation of rotational symmetry breaking from transverse resistivity measurements in the normal state of LaSrCuO by Wu et al.$^1$ can be accounted for by the thermal fluctuations of a 2D superconductor with significant in-plane phase stiffness anisotropy. The conductivity tensor is modeled by distinct normal state and paraconducting components, with different effective mass tensors corresponding in general to non-aligned nematic directors and different mass anisotropies. The model is supported by new experimental data showing the rotation of the measured nematic director in the presence of a magnetic field that suppresses superconductivity. The pair mass/phase stiffness anisotropy grows dramatically with underdoping, pointing to an exotic pseudogap state with quasi-one-dimensional pair fluctuations, despite a relatively weak single-particle anisotropy.

9:12AM W49.00007: Magnetic-field-tuned superconducting quantum phase transition in underdoped Bi$_{2}$Sr$_{2-x}$La$_x$CuO$_{6+\delta}$* 

JASMINKA TERZIC (Presenter), BAL POKHAREL, PAUL BAITY, LILY STANLEY, DRAGANA POPOVIC, Department of Physics and National High Magnetic Field Lab, Florida State University, SHIMPEI ONO, Central Research Institute of Electric Power, Japan — In underdoped cuprates, the value of the upper critical magnetic field ($B_{c2}$) has been under debate. However, recent studies on the La-214 family have firmly established vortex phase diagrams that include an intermediate, viscous vortex liquid regime, regardless of the presence of charge order. We perform similar studies in underdoped Bi$_{2}$Sr$_{2-x}$La$_x$CuO$_{6+\delta}$ (La-Bi2201), which exhibits short-range charge order, by measuring linear transport, voltage-current characteristics and Hall effect in $B$ up to 45 T and temperatures ($T$) down to 0.017 K. Our data reveal an insulatinglike high-field normal state and a qualitatively the same vortex phase diagram as in underdoped La-214 cuprates, thus supporting the universality of the vortex phase diagram with an intermediate phase, i.e. the importance of quantum phase fluctuations as $T \rightarrow 0$, in underdoped cuprates. The properties of the apparent two-stage superconductor-insulator transition are discussed and compared to that in highly underdoped La$_{2-x}$Sr$_x$CuO$_4$.


9:24AM W49.00008: Incommensurability of the dynamic spin modulations in La$_{2-x}$Sr$_x$CuO$_4$ ($x=0.12$)*

WEI HE (Presenter), Department of Materials Science and Engineering, Stanford University, JIAJIA WEN, Department of Applied Physics, Stanford University, K. M. SUZUKI, SHUN ASANO, Institute for Materials Research, Tohoku University, WEI TIAN, Neutron Scattering Division, Oak Ridge National Laboratory, MASAKI FUJITA, Institute for Materials Research, Tohoku University, YOUNG SANG LEE, Department of Applied Physics, Stanford University — The high-temperature superconducting cuprates display intriguing physical phenomena due to the presence of competing or intertwined phases. One of the remarkable observations in both Sr-doped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) system and O-doped La$_2$CuO$_{4+y}$ is the so-called Y-shift, which refers to a small shift of both spin density wave (SDW) and charge density wave (CDW) peak positions from the high-symmetry Cu-Cu bond direction. However, the ordering temperatures for the SDW and CDW are different. Above the superconducting transition temperature ($T_c$), there is only incipient spin fluctuation coexisting with the CDW order. In this talk, I will present our recent high-resolution inelastic neutron scattering experiment which characterized the Y-shift in the spin fluctuation regime in LSCO ($x=0.12$). The implication of the result will be discussed. Our study provides important information on the nature of the spin fluctuation in this system.

*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under contract No. DE-AC02-76SF00515. Research conducted at ORNL’s High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.
Emergence of superconductivity in two transition metal chalcogenides

NIKOLAOS BINISKOS, SAJNA HAMEED, DAMJAN PELC (Presenter), School of Physics and Astronomy, University of Minnesota, YUAN LI, International Center for Quantum Materials, School of Physics, Peking University, XIANGDE ZHU, CEDOMIR PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, MARTIN GREVEN, School of Physics and Astronomy, University of Minnesota — Superconducting (SC) and charge-density-wave (CDW) states are pair condensates of electrons and of electrons and holes, respectively. In many quantum materials, these two states are found to coexist or compete. Transition-metal chalcogenides such as TaSe$_{2-x}$S$_x$[1] and ZrTe$_{3-x}$Se$_x$[2] exhibit both SC and CDW phases and may be viewed as model systems to study the interplay between these two types of order. In both systems, substitutional disorder enhances SC order and suppresses CDW order [1,2]. We use AC nonlinear magnetic response, a probe that was recently shown to be highly sensitive to SC fluctuations [3], to correlate the diamagnetic response above the superconducting transition temperature with the substitutional disorder. Our results indicate rather narrow SC fluctuation regimes, yet with unconventional temperature dependences of the diamagnetic signal. We discuss these findings in the context of recent work on oxide superconductors [3].


Direct observation of an incommensurate charge density wave in the superconductor Ta$_4$Pd$_3$Te$_{16}$

ZHENZHONG SHI (Presenter), STEPHEN J KUHN, Department of Physics, Duke University, FELIX FLICKER, Rudolph Peierls Centre for Theoretical Physics, Department of Physics, Clarendon Laboratory, University of Oxford, WILLIAM STEINHARDT, SACHITH DISSANAYAKE, Department of Physics, Duke University, TONI HELM, Max Planck Institute for Chemical Physics of Solids, JOOSEOP LEE, JACOB RUFF, Cornell High Energy Synchrotron Source, Cornell University, GILBERTO F L FABBRI, Advanced Photon Source, Argonne National Laboratory, DAVID E GRAF, National High Magnetic Field Laboratory, Florida State University, JOERG STREMPFER, DANIEL HASKEL, Advanced Photon Source, Argonne National Laboratory, SARA HARAVIFARD, Department of Physics, Department of Mechanical Engineering & Materials Science, Duke University — The various electronic instabilities such as superconductivity (SC) and charge density wave (CDW) in low dimensions often conspire to determine some novel ground states in strongly correlated systems. In this talk we present our experimental and theoretical results. We report the observation of a highly unusual incommensurate charge density wave (CDW) in the superconductor Ta$_4$Pd$_3$Te$_{16}$, using synchrotron X-ray diffraction. Additionally, our de Haas-van Alphen (dHvA) quantum oscillation measurements detect no evidence of Fermi surface reconstruction across the CDW transition. The temperature-pressure phase diagram was also determined, and the SC dome is found to be centered at the pressure where the CDW vanishes.
10:00AM W49.00011: Nematic order and Charge order in $\text{Ba}_{0.6}\text{Sr}_{0.4}\text{Ni}_{2}\text{As}_{2}$  PRARTHUM SARAF
(Presenter), CHRIS ECKBERG, University of Maryland, College Park, SANGJUN LEE, Department of Physics, Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, JOHN COLLINI, University of Maryland, College Park, STELLA SUN, Department of Physics, Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, DANIEL J CAMPBELL, University of Maryland, College Park, JEFFREY LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology, PETER MICHAEL ABBAMONTE, Department of Physics, Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, JOHNPIERRE PAGLIONE, University of Maryland, College Park — Studies in the Cuprates and the Fe-based superconductors have hinted at a relationship between charge order order and superconductivity. The recent study on $\text{Ba}_{1-x}\text{Sr}_{x}\text{Ni}_{2}\text{As}_{2}$ shows strong nematic susceptibility for the B1G symmetry with increasing Sr doping corresponding to an enhancement in $T_c$. $\text{Ba}_{0.6}\text{Sr}_{0.4}\text{Ni}_{2}\text{As}_{2}$ is at the border of lattice driven nematic order and electronically driven nematic order. We report on X-ray and Neutron measurements on $\text{Ba}_{0.6}\text{Sr}_{0.40}\text{Ni}_{2}\text{As}_{2}$ that show the existence of three charge density waves. An incommensurate CDW in the tetragonal phase with $q=(0.27,0,0)$ and two commensurate CDWs in the triclinic phase with $q=(0.33,0,0)$ and $(0.5,0,0)$ are observed. The commensurate CDWs in the triclinic phase exist down to base temperature. We will discuss these results as well as elastoresistance measurements in $\text{Ba}_{0.6}\text{Sr}_{0.4}\text{Ni}_{2}\text{As}_{2}$.

10:12AM W49.00012: Charge Order in Tunable Electronic Nematic Superconductor $\text{Ba}_{1-x}\text{Sr}_x\text{Ni}_2\text{As}_2$  JOHN COLLINI (Presenter), University of Maryland, College Park, SANGJUN LEE, STELLA SUN, University of Illinois, Urbana Champaign, CHRIS ECKBERG, University of Maryland, College Park, JEFFREY LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology, PETER ABBAMONTE, University of Illinois, Urbana Champaign, JOHNPIERRE PAGLIONE, University of Maryland, College Park — Recent discoveries of charge order in the cuprates and electron nematic order in the iron-based superconductors has pointed towards the possibilities of both orderings being tied to mechanisms of high $T_c$ superconductivity. The $\text{Ba}(1-x)\text{Sr}(x)\text{Ni}_2\text{As}_2$ system, closely related to the $\text{BaFe}_2\text{As}_2$ system, has recently been shown to exhibit both types of ordering without the presence of any magnetic order. We report single crystal X-ray diffraction observations that show a unidirectional charge order with wavevector $(0.27,0,0)$ in $\text{BaNi}_2\text{As}_2$ decays and vanishes by $x=0.65$. We also show that the $(0.33,0,0)$ CDW in the triclinic phase evolves into a $(0.5,0,0)$ CDW by $x=0.65$. The evolution of the charge order in this system correlates well with the reported evolution of nematicity and superconductivity, suggesting a strong link between the three phases.
**10:24AM W49.00013: Interstitial Oxygen Dopant Dynamics in La$_2$CuO$_{4+y}$ Probed by Coherent X-rays**  
MINGDE JIANG (Presenter), WEI HE, JIAJIA WEN, Stanford Univ, ANDREI FLUERASU, YUGANG ZHANG, LUTZ WIEGART, NSLS-II, Brookhaven National Lab, YOUNG SANG LEE, Stanford Univ — Oxygen doping La$_2$CuO$_4$ (LCO) yields the superconductor La$_2$CuO$_{4+y}$ with the highest $T_c$ in the LCO family. The interstitial oxygen dopants are mobile and can be annealed to form an ordered lattice, manifested as a satellite Bragg peak in x-ray diffraction. We present x-ray photon correlation spectroscopy (XPCS) data, measuring the dynamic timescale of the corresponding oxygen ordering diffraction peaks in order to infer the interstitial oxygen dopant mobility and its temperature dependence.

*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under contract No. DE-AC02-76SF00515. This research used beamline 11-ID of the National Synchrotron Light Source II, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Brookhaven National Laboratory under Contract No. DE-SC0012704.*

**10:36AM W49.00014: An evidence of the three-dimensional superconductivity evolution through apical oxygen in YBCO**  
HAI HUANG (Presenter), SANG JUN LEE, SLAC - Natl Accelerator Lab, MASAKI FUJITA, Institute for Materials Research, Tohoku University, TERUKAZU NISHIZAKI, Department of Electrical Engineering, Kyushu Sangyo University, CHI-CHANG KAO, JUN-SIK LEE, SLAC - Natl Accelerator Lab — Superconductivity in the high-$T_c$ cuprates originates from transport phenomena in their universal structural CuO$_2$ plane. Meanwhile, the role of the apical oxygen which locates between CuO$_2$ planes has brought significant attention. This is because the superconducting temperature ($T_c$) varies based on cuprates, even though they have the same CuO$_2$ structure and doping. Here, we investigated the oxygen order at the Cu-O chain layer in YBa$_2$Cu$_3$O$_{6.73}$ (YBCO), which is connected with CuO$_2$ plane through the apical oxygen. For this purpose, we performed resonant soft x-ray scattering measurement around the Cu $L_3$-edge. We found that the evolution of the three-dimensional (3D) superconductivity in YBCO is strongly correlated with the oxygen order. More details will be introduced in the presentation.

*All soft x-ray experiments were carried out at the SSRL (beamline 13-3), SLAC National Accelerator Laboratory, supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515.*
10:48AM W49.00015: Fast moving superconducting vortices and determination of the critical current in high pulsed magnetic fields* BORIS MAIOROV (Presenter), MAXIME LEROUX, IVAN NEKRASHEVICH, Los Alamos National Laboratory, MASASHI MIURA, Seikei University, FEDOR BALAKIREV, LEONARDO CIVALE, Los Alamos National Laboratory — Expanding non-linear transport (I-V) studies to magnetic fields above those accessible by DC magnets can bring valuable information about systems such as superconductors, charge-density waves and topological semi-metals. All-superconducting very-high field magnets also make it technologically relevant to study vortex matter in this regime. However, pulsed magnetic fields reaching 100T in milliseconds impose technical and fundamental challenges that have prevented the realization of these studies. Here, we present a fast I-V DC technique that enables determination of the superconducting critical current in pulsed magnetic fields, beyond the reach of DC magnets. We demonstrate this technique on Cu- and Fe-based superconductors on single-crystalline and metallic substrates with excellent agreement with DC field measurements. The I-V characteristics change with the magnetic field rate (dH/dt). We capture this unexplored vortex physics through a model based on the broken symmetry of the vortex velocity profile produced by the applied current

*Work funded by the US DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division. Work performed at NHMFL pulsed field facility at Los Alamos National Laboratory was funded by NSF by Grant number 1157490/1644779.

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W50 DCMP: Correlated Chains and 1D Models Mile High Ballroom 1C -

Daniel Agterberg, University of Wisconsin - Milwaukee

8:00AM W50.00001: Spin chains with long range RKKY interaction* LUHANG YANG (Presenter), ADRIAN FEIGUIN, Physics, Northeastern University — Spin-chains are not well ordered antiferromagnets: their correlations decay algebraically and they do not develop true long-range order. Higher dimensional magnets may develop long-range order and, in such a case, the excitations are gapless magnons with well-defined Goldstone modes. To reconcile these two pictures we interpret magnons as bound states of spinons. The introduction of antiferromagnetic long-range RKKY interactions effectively increases the dimensionality of the chains and allow them to develop long range AFM order without violating Mermin-Wagner's theorem. We study the transition from gapless disordered to gapless ordered phases through the spin dynamical structure factor with the DMRG method. We identify signatures of bound states leaking out from the spinon continuum and the formation of coherent Goldstone modes. We also consider the effects of easy-axis anisotropy and we compare to predictions from spin-wave theory.

*We thank the NSF for support through Grant No. DMR-1807814
8:12AM W50.00002: Dynamics of a tunable spin chain with three-body interactions
KHAGENDRA ADHIKARI (Presenter), KEVIN STUART DAVID BEACH, Univ of Mississippi — We formulate a projective Monte Carlo scheme for a spin-half chain with tunable 3-body interactions that encompass the Fredkin model and its t-deformed extension. Dynamical correlation functions are measured directly in various regions of the phase diagram. We report a high-quality numerical estimate of the large dynamical exponent at the Fredkin point.

8:24AM W50.00003: Universality and Quantum Criticality in Quasiperiodic Spin Chains*
UTKARSH AGRAWAL (Presenter), ROMAIN VASSEUR, Univ of Mass - Amherst, SARANG GOPALAKRISHNAN, CUNY College of Staten Island, Staten Island — Quasiperiodic systems are aperiodic but deterministic, so their critical behavior differs from that of clean systems as well as disordered ones. Quasiperiodic criticality was previously understood only in the special limit where the couplings follow discrete quasiperiodic sequences. Here we consider generic quasiperiodic modulations; we find, remarkably, that for a wide class of spin chains, generic quasiperiodic modulations flow to discrete sequences under a real-space renormalization group transformation. These discrete sequences are therefore fixed points of a functional renormalization group. This observation allows for an asymptotically exact treatment of the critical points. We use this approach to analyze the quasiperiodic Heisenberg, Ising, and Potts spin chains, as well as a phenomenological model for the quasiperiodic many-body localization transition.

*This work was supported by the US Department of Energy, Office of Science, Basic Energy Sciences, under Early Career Award No. de-sc0019168 (Utkarsh Agrawal and Romain Vasseur), the Sloan Foundation through a Sloan Research Fellowship (Romain Vasseur), and by NSF Grant No. DMR-1653271 (Sarang Gopalakrishnan).

8:36AM W50.00004: Universal Spin Dynamics in Infinite-Temperature One-Dimensional Quantum Magnets*
MAXIME DUPONT, JOEL MOORE (Presenter), University of California, Berkeley — We address the nature of spin dynamics in various integrable and non-integrable, isotropic and anisotropic quantum spin-S chains, beyond the paradigmatic S=1/2 Heisenberg model. In particular, we investigate the algebraic long-time decay \( \sim t^{-1/z} \) of the spin-spin correlation function at infinite temperature, using state-of-the-art simulations based on tensor network methods. We identify three universal regimes for the spin transport, independent of the exact microscopic model: (i) superdiffusive with \( z=3/2 \), as in the Kardar-Parisi-Zhang universality class, when the model is integrable with extra symmetries such as spin isotropy that drive the Drude weight to zero, (ii) ballistic with \( z=1 \) when the model is integrable with a finite Drude weight, and (iii) diffusive with \( z=2 \) with easy-axis anisotropy or without integrability, at variance with previous observations.

*This work was funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05-CH11231 through the Scientific Discovery through Advanced Computing (SciDAC) program (KC23DAC Topological and Correlated Matter via Tensor Networks and Quantum Monte Carlo).
8:48AM W50.00005: Excitations of critical quantum spin chains from non-equilibrium classical dynamics  
STÉPHANE VINET (Presenter), GABRIEL LONGPRÉ, WILLIAM WITCZAK-KREMPA, Université de Montreal — We study critical quantum spin chains with spin 1/2 that are dual to the non-equilibrium dynamics of a classical spin chain coupled to a bath. One example is the Kawasaki dynamics of an Ising chain. We give the exact groundstates, and single magnon excitations. Solutions for the two-magnon spectra are derived via the Bethe Ansatz. We discuss the corresponding dynamical critical exponents, which suggest that these chains host multiple dynamics at low energy. We also discuss a generalization to higher dimensions.

9:00AM W50.00006: Critical quantum spin chains from non-equilibrium classical dynamics: level statistics and entanglement entropy*  
GABRIEL LONGPRÉ (Presenter), STÉPHANE VINET, WILLIAM WITCZAK-KREMPA, Université de Montreal — A critical quantum spin 1/2 chain dual to the non-equilibrium Kawasaki dynamics of an Ising chain coupled to a bath is presented. Its level spacing distributions are analysed in the context of random matrix theory. The implications on the integrability of the system are discussed. Scaling of the entanglement entropy of exact states is studied against the eigenstate thermalization hypothesis.

*This research was partly funded by the Alexander Graham Bell Canada Graduate Scholarship from the Natural Sciences and Engineering Research Council of Canada.

9:12AM W50.00007: 1D spin chain with topologically constrained dynamics  
ZHEHAO DAI (Presenter), Massachusetts Institute of Technology MIT, ADAM NAHUM, Physics, Oxford University — We discuss a new type of quantum critical point in 1+1D realizing topologically constrained dynamics different from blastic or diffusive transport. We discuss the scaling structure and intuitive understandings of the operator contents.
9:24AM W50.00008: Dynamical properties of a driven dissipative dimerized $S = 1/2$ chain

BRUCE NORMAND (Presenter), Neutrons and Muons Research Division, Paul Scherrer Institute, MOHSEN YARMOHammadi, Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, CONSTANTIN MEYER, Institut für Theoretische Physik, Georg-August-Universität Göttingen, BENEDIKT FAUSEWEH, Los Alamos National Laboratory, GOETZ S UHRIG, Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund — We consider the dynamical properties of a gapped quantum spin system coupled to the electric field of a laser, which drives the resonant excitation of specific phonon modes that modulate the magnetic interactions. We deduce the quantum master equations governing the time-evolution of both the lattice and spin sectors, by developing a Lindblad formalism with bath operators providing an explicit description of their respective phonon-mediated damping terms. We investigate the non-equilibrium steady states (NESS) of the spin system established by a continuous driving, delineating parameter regimes in driving frequency, damping, and spin-phonon coupling for the establishment of non-trivial properties. We characterize these NESS by their frequency and wave-vector content, explore the timescales for transient and relaxation behavior, and discuss the critical role of the type of bath adopted. Our study lays a foundation for the quantitative modelling of experiments currently being designed to control coherent many-body spin states in quantum magnetic materials.

*We thank the Swiss National Science Foundation (SNF) and the German Research Foundation (DFG).

9:36AM W50.00009: Generalization of the Haldane conjecture to SU(n) chains

KYLE WAMER (Presenter), Physics and Astronomy, University of British Columbia, MIKLÓS LAJKÓ, FREDERIC MILA, Institute of Physics, Ecole Polytechnique Federale de Lausanne, IAN AFFLECK, Physics and Astronomy, University of British Columbia — Recently, SU(3) chains in the symmetric and self-conjugate representations have been studied using field theory techniques. For certain representations, namely rank-p symmetric ones with p not a multiple of 3, it was argued that the the ground state exhibits gapless excitations. For the remaining representations considered, a finite energy gap exists above the ground state. In this paper, we extend these results to SU(n) chains in the symmetric representation. For a rank-p symmetric representation with n and p coprime, we predict gapless excitations above the ground state. If p is a multiple of n, we predict a unique ground state with a finite energy gap. Finally, if p and n have a greatest common divisor 1<q<n, we predict a ground state degeneracy of n/q, with a finite energy gap. To arrive at these results, we derive a non-Lorentz invariant flag manifold sigma model description of the SU(n) chains, and use the renormalization group to show that Lorentz invariance is restored at low energies. We then make use of recently developed anomaly matching conditions for these Lorentz-invariant models. We also review the Lieb-Shultz-Mattis-Affleck theorem, and extend it to SU(n) models with longer range interactions.
9:48AM W50.00010: Constructing Low-Energy Effective Models for the Hydrogen Chain using sb-DMRG* RANDY SAWAYA (Presenter), STEVEN ROBERT WHITE, University of California, Irvine — Sliced-basis DMRG(sb-DMRG) is used to simulate a chain of hydrogen atoms which is then transformed to an effective low-energy model. The downfolding procedure involves a change of basis from the real-space grid of the hydrogen chain to a set of atom-centered Wannier functions. Instead of conventional Wannier functions constructed from mean-field bands, we construct them directly from the exact DMRG one particle density matrix. We consider two versions of this. In the first, we use only the ground state to construct the density matrix. This more conventional approach produces a model which poorly reproduces spin and charge gaps. We obtain much better models using Wannier functions constructed from an average density matrix over a small set of low lying DMRG eigenstates.

*We are thankful for support from the Simons Foundation.

10:00AM W50.00011: Fractons from confinement in one dimension* SHRIYA PAI, MICHAEL PRETKO (Presenter), University of Colorado, Boulder — Recent work has shown that two seemingly different physical mechanisms, namely fracton behavior and confinement, can give rise to non-ergodicity in one-dimensional quantum many-body systems. We demonstrate an intrinsic link between these two mechanisms by studying the dynamics of 1d confining theories, such as lattice gauge theories. We show that, within certain parameter regimes, these models exhibit effective fracton dynamics, characterized by immobility of stable single-particle excitations and free motion of dipolar bound states. By perturbatively integrating out the linearly confining field, we obtain an effective fracton Hamiltonian for the confined charges which exhibits conservation of dipole moment. We discuss an intuitive understanding of these results in terms of the motion of the confining strings, leading to potential extensions to higher dimensions. We thereby interpret recent observations of nonthermal eigenstates and glassy dynamics in confining theories in terms of corresponding results in the fracton literature.

*The work of MP is supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0183. The work of SP is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences (BES) under Award number de-sc0014415.

10:12AM W50.00012: Emptiness Formation Probability in 1D Bose Liquids. HSIU-CHUNG YEH (Presenter), ALEX KAMENEV, University of Minnesota — We study emptiness formation probability (EFP) in interacting 1D Bose liquids. That is the probability that a snapshot of its ground state reveals exactly zero number of particles within the interval $|x| < R$. For a weakly interacting liquid there is parametrically wide regime $1/n < R < \xi$ (here $n$ is the average density and $\xi$ is the healing length), where EFP exhibits a non-trivial crossover from the Poisson to the Gaussian behavior. We employ the instanton technique [A. Abanov, 2004] to study quantitative details of these regime and compare it with previously reported limited cases.

This work was supported by NSF grant DMR-1608238.
10:24AM W50.00013: One-dimensional repulsive Hubbard model with mass imbalance
YUCHI HE (Presenter), Carnegie Mellon University, DAVID PEKKER, ROGER MONG, University of Pittsburgh — We investigate the phase diagram of the one-dimensional repulsive Hubbard model with mass imbalance away from half-filling. Using DMRG we show that this model has a triplet paired phase at generic fillings, consistent with previous theoretical analyses. We argue that this phase is a topological critical phase, based on our observation of a long-range string order and the absence of an odd-even effect. We also find, using DMRG, that at $1/3$ filling, commensurate effects lead to two additional phases: a crystal phase and a trion phase. Finally, we demonstrate how all of these phases descend from Tomonaga-Luttinger liquid theory.

10:36AM W50.00014: Dielectric breakdown of strongly correlated insulators in one dimension: Universal formula from non-Hermitian sine-Gordon theory
KAZUAKI TAKASAN (Presenter), University of California, Berkeley, MASAYA NAKAGAWA, Department of Physics, University of Tokyo, NORIO KAWAKAMI, Department of Physics, Kyoto University — Application of sufficiently strong electric fields to insulators induces finite currents and then the insulators become metallic. This phenomenon is called dielectric breakdown. In this talk, we present our recent study about the dielectric breakdown of generic strongly correlated insulators in one dimension [1]. Combining bosonization techniques with a theory of quantum tunneling, we develop an effective field-theoretical description of dielectric breakdown with a non-Hermitian sine-Gordon theory. Then, we derive an analytic formula of the threshold field which is a many-body generalization of the Landau-Zener formula. Importantly, we point out that the threshold field contains a previously overlooked factor originating from charges of elementary excitations, which should be significant when a system has fractionalized excitations. We apply our results to integrable lattice models and confirm that our formula is valid in a broad range including the weak coupling regime, indicating its wide and potential applicability. Our results unveil universal aspects in nonlinear and nonequilibrium transport phenomena for various strongly correlated insulators.

**W50.00015: Deconfined quantum criticality in a spin chain with long-range interactions**

SIBIN YANG (Presenter), Boston Univ, DAO-XIN YAO, Physics, Sun Yat-Sen University, ANDERS W SANDVIK, Boston Univ — We study a 1D spin-1/2 model with long-range power-law decaying unfrustrated (bipartite) Heisenberg exchange interactions \( J_r \propto r^{-\alpha} \) (for odd distances \( r \)) and a competing multi-spin interaction \( Q \) favoring a dimerized (valence-bond solid, VBS) ground state. Employing quantum Monte Carlo techniques and Lanczos exact diagonalization, we analyze order parameters and excited-state level crossings to characterize quantum phase transitions between the different ground states hosted by the model in the \((\alpha, Q)\) plane. For \( 1 < \alpha < 1.3 \), we find a direct continuous quantum phase transition between a long-range ordered antiferromagnetic state and a VBS state, providing an analogy to the two-dimensional deconfined quantum-critical point. Unlike previous 1D analogies of deconfined quantum criticality, where the two ordered phases both have fractional excitations, in our model the excitations fractionalize at the critical point, changing from anomalous, sublinearly dispersing spin waves in the antiferromagnetic phase to deconfined spinons in the VBS phase. We extract critical exponents and also use order-parameter histograms to study possible emergent symmetries.


**Friday, March 6, 2020 8:00 AM - 10:24 AM**

**Session W51 DCMP: Graphene: Valleytronics, Plasmonics, and Excitonics** Mile High Ballroom 1D - Aubrey Hanbicki

**8:00AM W51.00001: Strain-induced valley polarization in monolayer graphene**

DUXING HAO (Presenter), CHEN-CHIH HSU, MARCUS L TEAGUE, JIAQING WANG, NAI-CHANG YEH, Caltech — We use nearly strain-free PECVD-grown graphene [1] to induce controllable strain and pseudo-magnetic fields by nanoscale strain engineering [2]. By placing strain-free monolayer graphene and monolayer h-BN on architected silicon nanostructures fabricated by electron-beam lithography, we demonstrate broken global inversion symmetry and provide experimental evidences for strain-induced giant pseudo-magnetic fields and valley polarization by scanning tunneling spectroscopic studies at room temperature. Here we report transport properties of monolayer graphene devices using both DC and low-frequency lock-in techniques. Non-local resistance and non-local magnetoresistance are measured on both strained and unstrained graphene devices to confirm the strain-induced valley Hall effect. We further use different circularly-polarized light to enhance or suppress the valley Hall effect via selectively exciting electrons in the corresponding valley. Our approach thus paves a new way to realize scalable graphene-based valleytronics.


*This work is jointly supported by ARO under the MURI program (Award #W911NF-16-1-0472) and NSF under the Physics Frontier Centers program at Caltech (Award #1733907).
Plasmonic Doppler Effect in Graphene

YINAN DONG (Presenter), LIN XIONG, Columbia University, ISABELLE PHINNEY, Massachusetts Institute of Technology, RAN JING, ZHIYUAN SUN, ALEXANDER MCLEOD, SHUAI ZHANG, Columbia University, MICHAEL M FOGLER, University of California San Diego, PABLO JARILLO-HERRERO, LEONID LEVITOV, DENIS BANDURIN, Massachusetts Institute of Technology, DMITRI BASOV, Columbia University — High mobility two-dimensional electron gases reveal an intriguing phenomenon of the plasmonic Doppler shift. The plasmonic response is altered when direct current (DC) is applied provided the drift velocity of electrons reaches a substantial fraction of the Fermi velocity. When plasmons are coupled with light, surface plasmon polaritons (SPP) are predicted to acquire a quasi-relativistic Doppler effect [D.S. Borgnia and L.Levitov, arXiv: 1512.09044]. Here we utilize cryogenic nano-imaging technique to search for the current-induced Doppler effect in the SPP dynamics in graphene. Directional carrier flow breaks time-reversal symmetry and causes non-reciprocal plasmonic responses in infrared frequencies. Changes of SPP wavelength in real space are attributable to the Doppler effect. SPP imaging data inform us of the behavior of hybrid quasiparticles under current flow.

Plasmonic Nonreciprocity and Doppler Effect: The Role of Electron-Electron Interactions

HAOYANG GAO, ZHIYU DONG (Presenter), EGOR KISELEV, LEONID LEVITOV, Physics, Massachusetts Institute of Technology — Plasmonic modes propagating in the presence of an electrical DC current offer an appealing tool for achieving optical nonreciprocity at the nanoscale. This talk will discuss an approach relying on the DC-current-induced plasmonic Doppler effect, wherein downstream (upstream) propagation results in a blue (red) frequency shift of plasmon resonance, respectively. The carrier drift velocity in modern high-mobility two-dimensional electron systems can reach a substantial fraction of the Fermi velocity, leading to a strong Doppler effect. Since time reversal symmetry is broken in the presence of a flow, neither nonlinear coupling nor pumping, conventionally used to achieve nonreciprocity, are required in this case. We find that electron-electron interactions impact the magnitude of the effect, enhancing the Doppler shift substantially relative to the free-particle base value. Estimates of this effect based on Landau Fermi-liquid theory will be discussed and compared with the results of a microscopic approach.
8:36AM W51.00004: Valley polarization braiding in strained graphene*  
DAIARA FARIA  
(Presenter), Instituto Politécnico, Universidade do Estado do Rio de Janeiro, CARLOS LEÓN, Instituto de Física, Universidade Federal Fluminense, LEANDRO R. F. LIMA, Departamento de Física, Universidade Federal Rural do Rio de Janeiro, ANDREA LATGÉ, Instituto de Física, Universidade Federal Fluminense, NANCY SANDLER, Department of Physics and Astronomy, Ohio University — Previous works on deformed graphene predict the existence of valley-polarized states, however, optimal conditions for their detection remain challenging. We show that in the quantum Hall regime, edge-like states in strained regions can be isolated in energy within Landau gaps. We identify precise conditions for new conducting edges-like states to be valley polarized, with the flexibility of positioning them at chosen locations in the system. A map of local density of states as a function of energy and position reveals a unique braid pattern that serves as a fingerprint to identify valley polarization[1].


*IRTA-APS (DF, NS), CAPES (PrInt), CNPq (AL, CL), FAPERJ E-26/202.953/2016 (AL) and E-26/202.768/2016 (LRFL), INCT Carbon Nanomaterials (AL, DF), NSF-DMR 1508325 (DF, NS), Aspen Center for Physics NSF PHY-1607611 (NS), Ohio Supercomputer Center PHS0265. DF is the Glidden Visiting Professor at OU.

8:48AM W51.00005: Interacting Valley Chern Insulator in Moiré Systems*  
XIAOCHUAN WU  
(Presenter), YICHEN XU, University of California, Santa Barbara, CHAO-MING JIAN, Kavli Institute of Theoretical Physics, Santa Barbara, CENKE XU, University of California, Santa Barbara — One salient feature of systems with Moiré superlattice is that the Chern number of “minibands” originating from each valley of the original graphene Brillouin zone becomes a well-defined quantized number because the miniband from each valley can be isolated from the rest of the spectrum due to the Moiré potential. Then a Moiré system with a well-defined valley Chern number can become a nonchiral topological insulator with U(1) × Z_3 symmetry and a Z classification at the free fermion level. Here we demonstrate that the strongly interacting nature of the Moiré system reduces the classification of the valley Chern insulator from Z to Z_3, which is very different from the previously known examples of interaction reduced classification of topological insulators. We also show that an interacting valley Chern insulator is topologically equivalent to a bosonic symmetry protected topological state made of local boson operators. The effect of this interaction influenced classification is estimated in experimental systems.

*Cenke Xu is supported by NSF Grant No. DMR-1920434, and the David and Lucile Packard Foundation. Chao-Ming Jian is supported by the Gordon and Betty Moore Foundations EPiQS Initiative through Grant No. GBMF4304.
Twisted Bilayer Graphene: Atomic Crystal Structure, Electronic Structure and Plasmonic Interactions* ZHONGWEI DAI (Presenter), Center for Functional Nanomaterials, Brookhaven National Laboratory, ZHAOLI GAO, Department of Physics and Astronomy, University of Pennsylvania, CALLEY EADS, SAMUEL TENNEY, Center for Functional Nanomaterials, Brookhaven National Laboratory, ALAN T JOHNSON, Department of Physics and Astronomy, University of Pennsylvania, JERZY T. SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory — Recent discovery of unconventional superconductivity in twisted bilayer graphene (tBLG) has triggered intensive discussions about the importance of interlayer coupling effects in commensurate tBLG, which was overlooked previously. Much of its macroscale properties, such as conducting electron behavior and light matter interactions in the commensurate tBLG systems remain unknown. Here we present study of the interlayer coupling effects in the twisted 30° bilayer graphene system using surface sensitive low energy electron microscopy (LEEM), Raman scattering and infra-red scattering near-field optical microscopy (IR-sSNOM). Strong crystal structure coupling between two graphene sheets was revealed by a sharp 12-fold symmetrical LEED diffraction pattern. Enhancement of interlayer light scattering was also observed by Raman spectroscopy. Most surprisingly, the plasmonic interaction was observed to be sharply quenched on 30° twisted bilayer graphene in contrast with enhanced plasmonic interaction on non-twisted, bilayer graphene.

*This research used resources of the Center for Functional Nanomaterials and the National Synchrotron Light Source II, which are U.S. Department of Energy (DOE) Office of Science facilities at Brookhaven National Laboratory, under Contract No. DE-SC0012704.

Filling-factor-dependence of the magnetoplasmon spectrum in graphene JORDAN PACK (Presenter), JORDAN RUSSELL, YASHIKA KAPOOR, JESSE BALGLEY, JEFF AHLERS, Washington University, St. Louis, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ERIK HENRIKSEN, Washington University, St. Louis — We present cyclotron resonance measurements of a graphite-gated, hexagonal boron nitride-encapsulated monolayer graphene device. We observe a remarkable progression of the CR lineshape as a function of the Landau level filling factor, \( \nu \), from a single peak at \( \nu=0 \) to four peaks at \( \nu=1 \) to two peaks for \( \nu>2 \), giving an unprecedented spectroscopic view of the evolution of the magnetoplasmon spectrum arising from the broken spin and valley symmetries in the \( N=0 \) Landau level. By comparing to many-particle theories of graphene CR, we extract precise values for the renormalized Fermi velocity and a Dirac mass due to sublattice-symmetry breaking by the hBN. A simple model of LL shifts due to interactions allows extraction of the effective \( g \) values for Zeeman gaps in the \( N=0 \) Landau level both at and below the Fermi energy. Additionally we find evidence for a small yet clear electron-hole asymmetry.
9:24AM W51.00008: Band Structures and Localized Graphene Surface Plasmons with Periodic Charge Doping*  MICHAEL SAMMON (Presenter), University of Minnesota, DIEGO RABELO DA COSTA, Physics, Universidade Federal do Ceará, TONY LOW, University of Minnesota — We present recent band structure calculations of artificial plasmonic crystals created by periodic doping. We focus on the Lieb and Kagome lattice, two lattices known to exhibit topological features. We show that within the Drude approximation of the conductivity and for neutral doping with alternating charges, the Kagome lattice exhibits both a flat band and a band gap with a large local density of states. Additionally, for doping of alternating, both lattices exhibit strong localization of the plasmon electric field intensity near the region of vanishing charge density. We discuss the effect of interband transitions on these properties.

*This work was supported by the National Science Foundation NSF/EFRI grant (#EFRI-1741660)

9:36AM W51.00009: Isotopic Effect of Carrier Relaxation in Graphene-hBN Heterostructures*  ALEXANDRA BRASINGTON (Presenter), Physics, University of Arizona, JAMES H. EDGAR, Chemical Engineering, Kansas State University, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, ARVINDER S SANDHU, BRIAN J LEROY, Physics, University of Arizona — In atomically thin systems, the choice of substrate plays an important role in the relaxation of photo-excited carriers. In previous work, hexagonal boron nitride (hBN) substrates have been shown to improve the thermal relaxation rates of carriers in graphene as compared to silicon oxide substrates. Naturally occurring boron contains a mixture of two isotopes with atomic masses 10 and 11 with abundances of 20% and 80% respectively. Theoretical studies have predicted a higher thermal conductivity with higher isotopic purity of hBN, due to reduced phonon scattering from isotopic defects. We utilize femtosecond pump-probe spectroscopy to observe the time dynamics of photo-excited carriers in graphene-hBN heterostructures for both natural and isotopically pure hBN.

*The work at the University of Arizona was supported by the U.S. Army Research Laboratory and the U.S. Army Research Office under Contract/Grant No. W911NF-14-1-0653.

9:48AM W51.00010: Evidence for excitonic solid states in double layer graphene  YIHANG ZENG (Presenter), QIANHUI SHI, ANNA OKOUNKOVA, Columbia Univ, KENJI WATANABE, TAKASHI TANIGUCHI, nims, JIA LI, physics, Brown Univ., CORY DEAN, Columbia Univ — Spatially indirect excitons can form when electron-doped and hole-doped 2D quantum wells are brought into close proximity. In the condition that interlayer separation is sufficiently large to suppress recombination and small enough that interlayer coulomb interactions are strong, the system can spontaneously condense into a superfluid-like macroscopically coherent state, termed an exciton condensate. In a double layer graphene system in the presence of magnetic field, upon decreasing the exciton density, we observe a sharp transition from an exciton superfluid to an exciton insulator, which shows insulating behavior in both charge transport and exciton transport measurement. At elevated temperature, the excitonic insulating state exhibits perfect coulomb drag, which is the signature of an exciton superfluid. Our data suggests a phase diagram consisting of a pinned excitonic Wigner crystal at lower exciton density, which transitions to a superfluid-like state at elevated temperature.
QIAOXIA XING (Presenter), Fudan Univ — Graphene plasmonics, allowing strong light-matter interactions, subwavelength light confinement and in situ tunability, has gained much attention due to the potential to develop new optoelectronic and photonic devices. Here, we experimentally demonstrate graphene split ring resonators with deep subwavelength confined magnetic dipole, quadrupole and electric dipole responses in terahertz regime. All modes can be tuned via chemical doping or stacking multiple graphene layers. Finite-element frequency domain simulations nicely reproduce experimental results. Our study demonstrates an example of tunable multiple resonances based on graphene, and shed new light on its application in tunable high-frequency magnetic metasurfaces.

DEEPAN KISHORE KUMAR (Presenter), NAI-CHANG YEH, Caltech — We have previously shown that our PECVD-grown, quasi-1D GNSPs exhibited perfect purity, high mobility [1] and strong broadband absorption [2]. Here we report broadband photoluminescence (PL) and ultra-long carrier lifetimes in GNSPs from time-resolved PL (TRPL) studies. GNSPs were deposited on quartz substrates to form uniform films with thicknesses of 5, 10, 20, 40 and 50 μm for the TRPL measurements. We used Nd:YAG laser at 355 nm with 10 ps pulse width and 0.1 mJ pulse energy under a repetition rate of 10Hz to carry out TRPL studies at temperatures from 15 K to 290 K. Detailed analysis of the TRPL data revealed two carrier lifetimes of $\tau_1 (~ 1 \text{ ns})$ and $\tau_2 (~ 10 \text{ ns})$, both were independent of either temperature or thickness, and the values were $\sim 10^3$ times longer than any lifetimes reported to date for graphene-based materials. We attribute the ultra-long lifetimes to the nanoscale quasi-1D nature of GNSPs, which breaks the global inversion symmetry so that photo-excited hot electrons and holes are rapidly separated due to their large differences in mobility, *a.k.a.* the photo Dember effect.


*This work is jointly supported by United Advanced Material and Army Research Office.

ZHIMING PAN (Presenter), RYUICHI SHINDOU, Peking Univ — Graphite in the quantum limit shows unconventional in-plane and out-of-plane transport behavior. To uncover its microscopic origin, we construct an interacting electron model with a pair of electron band and hole band with the valley degree of freedom. We use a fermionic renormalization group (RG) method and study a parquet RG equation of the model with screened Coulomb interaction. We found that, for strong screening region, the one-loop RG indicates a dominant instability of valley charge density wave (VCDW) with a finite pairing between the two valleys. We further construct an effective mean-field theory and clarify the in-plane transport behavior of the VCDW phase.
**W51.00014: Generation and Detection of Valley Current in Single and Double Layered Graphene through the Electron-Phonon Interaction**

ANKANG LIU (Presenter), ALEXANDER FINKELSTEIN, Department of Physics and Astronomy, Texas A&M University — We report a possible method to generate and detect the valley current carried by quasi-particles in both single and double layered graphene. We observe that the term in the collision integral originated from mixing the scalar and vector gauge-field-like vertices in the electron-phonon interaction turns current carriers of two different valleys in opposite directions. As a result, the electron-phonon collision produces a valley current. Finally, we show that the valley current carried by quasi-particles could be not only generated but also detected in a non-local resistance measurement through the inverse version of this mechanism. Our study proposes a new approach to manipulate the valley degrees of freedom in a pristine graphene or bilayer graphene sample without breaking the spatial inversion symmetry. The effect increases with temperature owing to a higher rate of collisions with phonons at higher temperatures.

**Friday, March 6, 2020 8:00 AM - 10:48 AM**

**Session W52 DCMP: Thin Film Coatings and Applications** Mile High Ballroom 1E - Daniel Dougherty, North Carolina State University

**8:00AM W52.00001: Growth of Conformal Thin Film Si Coatings on Terraced Substrates Using Subsequent Oblique Incidence Xe⁺ Ion Bombardment**

EMMETT RANDEL (Presenter), CARMEN SUSANA MENONI, RICHARD M BRADLEY, Colorado State University — Using a Si surface pre-patterned with a 500 nm pitch sinusoidal profile, it is demonstrated that ordered terraced topographies with sub-nanometer scale roughness on the facets develop under oblique incidence 1500 eV Xe⁺ broad beam ion bombardment. Bi-layers of SiO₂/Si were then deposited onto the terraced substrate using ion beam sputtering. Following the deposition of each Si layer, the oblique incidence Xe⁺ bombardment was repeated to restore the terraced structure. This work was performed in tandem with theory in an effort to refine models, showing agreement in selection of terraced slopes and the development of transverse roughness along the facets.

*Work supported by NSF Grant No. 1508745*
Amorphous oxides to improve the coatings of future gravitational wave detectors*  

GABRIELE VAJENTE (Presenter), Caltech, MARIANA FAZIO, Department of Electrical and Computer Engineering, Colorado State University Fort Collins, LE YANG, Department of Chemistry, Colorado State University Fort Collins, ALENA ANANYEVA, GARILYNN BILLINGSLEY, Caltech, ASHOT MARKOSYAN, RICCARDO BASSIRI, MARTIN M. FEJER, Edward L. Ginzton Laboratory, Stanford University, CARMEN SUSANA MENONI, Department of Electrical and Computer Engineering, Colorado State University Fort Collins — Amorphous oxides like tantala and titania-doped-tantala have been used as high index material for high reflectivity coatings in many applications, including the mirrors of current gravitational wave detectors. The sensitivity of those detectors is currently limited by coating Brownian noise, which is related to elastic energy loss in the coatings, as shown by the Fluctuation-Dissipation Theorem. This motivates a wide range search of an alternative amorphous material with lower mechanical loss, that could provide a substitute for the high refractive index currently used, namely titania-doped-tantala.

We characterized the optical and elastic properties of several oxides: yttria, hafnia, niobia, alumina, zirconia, zinc oxide, germania and doped germania. We also measured the mechanical loss at room temperature of all materials. Additionally, we performed several heat cycles and measured the changes induced in the mechanical loss.

We found interesting results for germania and doped germania: they exhibit room-temperature loss angles much lower than all oxides other than silica, making them a promising candidate for the high reflectivity coatings of future gravitational wave detectors.

*This work is supported by the National Science Foundation through grants No. 1708010 and 1710957.
8:24AM W52.00003: Wide survey of Ta$_2$O$_5$-based mixed oxide coatings for gravitational wave detectors* MARIANA FAZIO (Presenter), Department of Electrical and Computer Engineering, Colorado State University, LE YANG, Department of Chemistry, Colorado State University, GABRIELE VAJENTE, ALENA ANANYEVA, GARILYNN BILLINGSLEY, LIGO Laboratory, California Institute of Technology, ASHOT MARKOSYAN, RICCARDO BASSIRI, MARTIN M. FEJER, Department of Applied Physics, Ginzton Laboratory, Stanford University, CARMEN SUSANA MENONI, Department of Electrical and Computer Engineering, Department of Chemistry, Colorado State University — Thermal noise is a fundamental limitation in optical interferometry experiments as thermally driven fluctuations cause variations in the optical path. The sensitivity of gravitational wave detectors, such as Advanced LIGO and Advanced Virgo, is affected by the thermal noise in the high-reflectivity mirrors of the end masses. These mirrors are multilayer stacks of alternating layers of TiO$_2$:Ta$_2$O$_5$ and SiO$_2$, with the main source of thermal noise being the mechanical loss of TiO$_2$:Ta$_2$O$_5$. Towards the goal of identifying other potential dopants that can further decrease the thermal noise, we carried out an extensive study of Ta$_2$O$_5$ doped with different oxides: Al$_2$O$_3$, HfO$_2$, Nb$_2$O$_5$, Sc$_2$O$_3$, SiO$_2$, TiO$_2$, Y$_2$O$_3$, ZnO, and ZrO$_2$. Films were grown by reactive sputtering with a 20% dopant cation concentration. The influence of the dopant on the structure, optical properties, crystallization temperature and mechanical loss was evaluated. We found that oxides with the lowest Gibbs free energy of formation, such as Sc$_2$O$_3$, inhibit the complete oxidation of the Ta$_2$O$_5$ phase. We identify dopants for which the material crystallizes as a ternary compound, such as TiO$_2$ and ZnO, which can induce atomic mixing and reduce mechanical loss.

*Work supported by the Center for Coatings Research NSF award No.:1710957.

8:36AM W52.00004: Dielectrowetting of nematic liquid crystal films* ENSELA MEMA (Presenter), US Military Academy, LINDA CUMMINGS, LOU KONDIC, New Jersey Institute of Technology — We consider a mathematical model that describes the flow of a Nematic Liquid Crystal (NLC) film placed on a surface that contains interlaced electrodes (which generate an electric field that varies in the plane of the substrate). We assume that the NLC film is thin relative to the inter-electrode spacing. Under the usual long-wave scaling, a partial differential equation that describes the time evolution of the thin film is obtained. Due to the dielectric nature of NLC molecules, this equation is coupled to a boundary value problem that describes the interaction between the nematic director and the electric field potential. After validating our fully nonlinear simulations by linear stability analysis, we discuss the influence of an applied electric field on the stability of the NLC film.

*This work was supported in part by NSF Grant No. DMS-1815613
8:48AM W52.00005: Sound velocity study in multilayer ultrathin films using wavelet transform*  SAEED YOUSEFI SARRAF (Presenter), ROBBYN TRAPPEN, NAVID MOTTAGHI, ALAN BRISTOW, MIKEL HOLCOMB, West Virginia University — Ultrafast spectroscopy of thin films reveals mechanisms responsible for relaxation of charge carriers’ energy to lower energy states. In the case of a strong enough excitation pump pulse, a shock wave will travel with the sound velocity, longitudinally in the thin film. Due to the interference effect, the shock wave superimposes a sinusoidal wave on the transient reflectivity, which can be used to calculate the sound velocity. In lower thicknesses, this sinusoidal behavior is not analyzable by Fourier transforms. Wavelet transforms, which use scalable wavelets localized in time and space, are perfect tools to analyze these fast-vanishing oscillations. Wavelet analysis has been applied to the residual sinusoidal TR to extract information related to different oscillatory modes, in multilayer ultrathin films. This approach can isolate the location of various oscillatory modes with close energy ranges, at the surface, interface and in the bulk of the heterostructures. As a result, implementation of wavelet transforms provided information regarding the sound velocity and acoustic phonons in multilayer thin films.

*We acknowledge funding support from ACS (PRF #56642-ND10) for students, NSF (DMR-1608656) for growth, and DOE (DE-SC0016176) for optics supplies.

9:00AM W52.00006: Mixture and nanolamine – a pathway to understand coating mechanical loss* LE YANG (Presenter), MARIANA FAZIO, Colorado State University, GABRIELE VAJENTE, ALENA ANANYEVA, GARILYNN BILLINGSLEY, California Institute of Technology, ASHOT MARKOSYAN, RICCARDO BASSIRI, MARTIN M. FEJER, Stanford University, CARMEN SUSANA MENONI, Colorado State University — Composite oxides in the form of mixture and nanolamine are extensively used in optical coatings and as dielectric materials. Tunable properties accessible through mixing and nanolayering have drawn great attention to these composite thin films. TiO2-Ta2O5 mixture coating has been shown to reduce the mechanical loss compared to pure Ta2O5 coating thereby improving the sensitivity of the Advanced LIGO gravitational wave detector. In this work, reactive biased target ion beam deposition was used to grow mixture and nanolamine coatings of SiO2-Ta2O5 and TiO2-Ta2O5. Different mechanisms of mechanical loss reduction through heat treatment are observed. Ta2O5-SiO2 mixtures annealed at 750°C show diffraction only from the crystallized orthorhombic Ta2O5 phase, indicating an immiscibility of SiO2 in Ta2O5. Additionally, Ta2O5-SiO2 nanolayers remained separate by sharp interface after annealing. On the contrary, mixing identified by blurring of interfaces is observed in Ta2O5-TiO2 nanolamine after annealing at 650°C. This behavior resembles the mixture coating. This work brings out new understanding of the physical mechanism of coating mechanical loss reduction at room temperature.

*This work is supported by the National Science Foundation LIGO program through grant No. 1708010
Monitoring structural changes in steel thin films in electrolyte *in situ* by X-ray standing waves

DEBI GARAI (Presenter), Diamond Light Source Ltd, Amity Univ., ILARIA CARLOMAGNO, ELETTRA, AXEL WILSON, Diamond Light Source Ltd, CARLO MENEGHINI, Univ. Roma TRE, VLADYSLAV SOLOKHA, Diamond Light Source Ltd, JKU Linz, CHRISTIAN MORAWE, ESRF, AJAY GUPTA, Amity Univ., JORG ZEGENHAGEN, Diamond Light Source Ltd — Ultra-thin stainless steel films were deposited on Ru/B4C multilayers using DC magnetron sputtering and characterised by synchrotron X-rays. The X-ray standing wave (XSW) technique revealed the metal distribution with depth. Typical for stainless steel [1], the near surface region was free of nickel. The oxidation states of Cr, Ni and Fe were determined by X-ray near edge absorption structure (XANES) under XSW condition. Nickel was found to be largely metallic whereas Fe and Cr were oxidized in the surface region, forming an about 2 nm passive layer. Exposure to 0.1M KCl at cathodic potential of -0.6 V vs Ag/AgCl resulted in expansion of the steel film due to in-diffusion of hydrogen. Using XSW/XANES, structural and chemical changes of the steel film were further traced *in situ* as a function of electrode potential up to +0.8 V. Results will be presented in the talk.


Deformation profile and interface-mediated defect interaction in Cu/CuZr nanolaminates: An effective-temperature description

MICHAEL TONG (Presenter), University of Michigan-Ann Arbor, CHARLES LIEOU, Los Alamos National Laboratory, IRENE BEYERLEIN, University of California, Santa Barbara — Both simulations and experiments have suggested that Cu/CuZr nanolaminates are stronger and more ductile than their individual constituents due to interface-mediated interactions between plasticity carriers. We use the effective-temperature theories of dislocation and amorphous shear-transformation-zone (STZ) plasticity to study amorphous-crystalline interface (ACI)-mediated plasticity in Cu/CuZr nanolaminates under mechanical straining. The model is shown to capture reasonably well the measured deformation response when strained either in tension parallel to or in compression normal to the amorphous-crystalline interface. Our analysis indicates that increasing CuZr or decreasing Cu layer thickness increases the maximum flow stress for both perpendicular and parallel loading cases. In all slip strain analyses, maximum slip strain occurs at the ACI, thus indicating that plasticity carriers accumulate at the interface and are absorbed there. These findings indicate a significant anisotropy in strength with greater sensitivity to layer thickness for the case of tensile loading parallel to the ACI. Further findings signify that slip strain is more sensitive when the nanolaminate is compressed perpendicular to the ACI.
The next major upgrade to gravitational wave detector LIGO, called Advanced LIGO+ or A+, is planned to operate at room temperature and requires 4 times improvement in coating mechanical loss to meet its design sensitivity. The coatings are made up of alternating layers of high and low refractive index materials to make the mirrors highly reflective. The current coatings have amorphous silica as the low index layer and titania-doped tantala as the high index layer. The mechanical loss of high index layer dominates the coating loss and the thermal noise requirement for A+ could be met by finding a high index layer with low enough mechanical loss. In this talk, I will describe the research efforts aimed at finding such a coating. In particular, I will talk about how the atomic structure measurements and modeling of amorphous oxides are being used to guide the coating development process. I will highlight some interesting correlations in the structure and loss measurements and draw some empirical conclusions. Finally, I will discuss the thermally activated relaxation processes (TARP) in amorphous oxides based on atomic simulations of two-level systems (TLSs). TARP is believed to be the source of mechanical loss in amorphous materials.
9:48AM W52.00010: Addressing the Achilles’ Heels of Amorphous Carbon Overcoats with Doping: Mechanisms of Thermal and Oxidative Degradation  FILIPPO MANGOLINI (Presenter), University of Texas at Austin, BRANDON KRICK, Department of Mechanical Engineering and Mechanics, Lehigh University, TEVIS D.B. JACOBS, SUBARNA R. KHANAL, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, FRANK STRELLER, J. BRANDON MCCLIMON, Department of Materials Science and Engineering, University of Pennsylvania, JAMES HILBERT, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, SOMURI V. PRASAD, Sandia National Laboratories, THOMAS SCHARF, Department of Materials Science and Engineering, University of North Texas, JAMES OHLHAUSEN, Sandia National Laboratories, JENNIFER R. LUKES, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, W. GREGORY SAWYER, Department of Mechanical and Aerospace Engineering, University of Florida, ROBERT W CARPICK, Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania — Harsh environments pose materials durability challenges across different sectors. While amorphous carbon materials have been used as coatings in environmentally-demanding applications owing to their unique properties, their limited thermal stability and high reactivity in oxidizing environments have inhibited their use in many technologies. Silicon- and oxygen-containing hydrogenated amorphous carbon (a-C:H:Si:O) films are promising for several applications because of their higher thermal stability and lower residual stress compared to hydrogenated amorphous carbon (a-C:H). However, an understanding of their superior thermo-oxidative stability compared to a-C:H is lacking.

Here, we performed X-ray photoelectron/absorption spectroscopy experiments and molecular dynamics simulations to show how the introduction of silicon and oxygen in a-C:H enhances: 1) the stability at elevated temperatures in both vacuum and oxidizing environments; and 2) the resistance to degradation upon exposure to the harsh conditions of low Earth orbit (LEO) aboard the International Space Station. These findings provide a novel physically-based understanding of the superior stability of a-C:H:Si:O in harsh environments compared to a-C:H.

10:00AM W52.00011: capillarity-enhanced thin-film mineral coating in 3D-printed porous micromodel  HONGXIA LI (Presenter), AIKIFA RAZA, TIEJUN ZHANG, Mechanical Department, Khalifa University — In subsurface-related applications such as hydrocarbon recovery, carbon sequestration and water filtration, 3D-printed porous media, usually polymer-based material, are quite different from natural rocks. It is highly desireable to functionalize 3D-printed models in mimicking the surface chemistry of natural rocks. Here, we propose a surface-coating approach by seeding calcite nanoparticles (CalNPs) followed by in-situ growth of calcite crystals along the inner surfaces of as-printed 3D micromodels. Notably, surface coating inside porous media is quite challenging compared to the flat surfaces due to the capillary effect in the irregular pores/throats. To guarantee the coating uniformity, we tuned the properties of coating solutions for a lower surface tension, lower viscosity and higher volatility. In this way, we promote the formation of an ultra-thin liquid film in confined space of porous media. The stability of the coating layer, specifically the CalNPs, was also investigated using water-flush experiments. The capillary-rise enhanced nanoparticle stability is revealed from atomic force microscope (AFM) analysis. Through this work, we provide guidance on thin-film coating in porous media, where the effect of capillarity is a critical issue and requires careful attention.
10:12AM W52.00012: Effects of substrate bias on current for varying argon intensity in a low-pressure hydrogen/argon plasma in chemical vapor deposition. BHAVESH RAMKORUN (Presenter), KALLOL CHAKRABARTY, SUMNER B HARRIS, SHANE A CATLEDGE, Univ of Alabama - Birmingham — Studies have shown that in CVD, low substrate temperature often favors amorphous materials growth over crystalline. In a hydrogen/argon plasma acting on a negatively DC-biased silicon substrate, hydrogen alpha and bias current due to ion bombardment were monitored for temperature <1000°C. The temperature was controlled through microwave power of 0.6kW, and pressure of 10 – 30 torr. The flow rate of argon was varied between 0 sccm and 500 sccm, and hydrogen's was 500 sccm. Optical Emission Spectroscopy (OES) of hydrogen line was found to be influenced by argon flow rate. Current was recorded for several values of the applied bias voltage from 100V to 340V. A decrease in current with decreasing hydrogen emission for glow discharge systems has been reported in the literature. Our results substantiate these results, and further show a peak in current at 10 and 20 torr. OES data was used to estimate the plasma electron temperature to be constant at approximately 0.5 eV. This suggests that the observed peak in current may be due to variation in plasma density as Ar flow changes between 0 sccm and 500 sccm. These results may be used to correlate plasma emission characteristics with substrate bias conditions in order to better predict and control MPCVD grown materials.

10:24AM W52.00013: Measuring Local Electric Fields and Local Charge Densities at Electrode Surfaces using Graphene-enhanced Raman Spectroscopy (GERS)-based Stark-shifts* HAOTIAN SHI (Presenter), BOFAN ZHAO, STEVE CRONIN, Univ of Southern California — We report spectroscopic measurements of the local electric fields and charge densities at electrode surfaces using graphene-enhanced Raman spectroscopy (GERS) based on the Stark-shifts of surface-bound molecules (CuPc) and the G band frequency shift in graphene. The shifts in vibrational frequencies of the graphene G band and CuPc are obtained simultaneously and correlated. The 1531 cm⁻¹ peak exhibits Stark-shifts and can, thus, be used to report the local electric field strength at the electrode surface under electrochemical working conditions. Computational simulations using density functional theory (DFT) predict similar Stark shifts and provide a detailed atomistic picture of the electric field-induced perturbations to the surface-bound CuPc molecules.

National Science Foundation Grant CHE-1707657 (L.J.) and NRT-1449785. (M.B.)
10:36AM W52.00014: Ferroelectric polarization rotation through He irradiation induced uniaxial strain* ANDREAS HERKLOTZ (Presenter), ROBERT ROTH, KATHRIN DORR, NIRANJAN RAMAKRISHNEGOWDA, University of Halle-Wittenberg, YOGESH SHARMA, ALESSANDRO MAZZA, THOMAS ZAC WARD, Oak Ridge National Laboratory — The physical properties of ferroic thin films are typically dominated by their domain configurations and their responses to external fields. A central prerequisite to domain engineering and harnessing functionalities of ferroelectric thin films is thus the control of the polarization orientation. Historically, the direction of ferroelectric polarization in thin films has been mainly tailored by heteroepitaxial in-plane strain or a variation of growth conditions inducing defects.

Here, we deploy low-energy He implantation as an alternative approach. Ion implantation induces uniaxial out-of-plane strain, while the in-plane strain remains fixed due to coherent growth on the substrate. We show that this kind of uniaxial strain engineering effectively leads to polarization rotation from in-plane towards out-of-plane as the uniaxial strain is increasing. We find that this polarization rotation can be achieved via two different mechanisms: (i) via a sequence of phase transitions related to changes of crystal symmetries and (ii) via a continuous shift of the ferroelectric domain ratio towards out-of-plane oriented domains.

*This effort was supported by the DFG SFB 762 and the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), Materials Sciences and Engineering Division.

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W53 DMP: 2D Photonics and Optoelectronics Mile High Ballroom 1F -

Stephen Wu, University of Rochester - Tag(s): Focus
Two-dimensional ReS$_2$ for nonlinear photonics

BENJAMIN SMITH
(Presenter), Centre for Nanoscience and Nanotechnology, Department of Physics, University of Bath, KRISTINA RUSIMOVA, ANDRIY GORBACH, Centre for Photonics and Photonic Materials, Department of Physics, University of Bath, JUEJUN HU, SKYLAR DECKOFF-JONES, Department of Materials Science & Engineering, Massachusetts Institute of Technology, DANIEL WOLVERSON, Centre for Nanoscience and Nanotechnology, Department of Physics, University of Bath — The layered transition metal dichalcogenides (TMDs) have been the focus of increasing research in photonics, in part due to their large nonlinear optical (NLO) susceptibilities. Amongst the TMD family, the semiconducting rhenium dichalcogenides (ReX$_2$, where X = S or Se) are unusual due to their highly-anisotropic in-plane crystal structure. A Peierls distortion of the crystal lattice results in the formation of chains of Re atoms along one of the crystallographic directions. This structure leads to anisotropic optical, electrical and mechanical properties. Here, we demonstrate that this anisotropic crystal structure is highly useful for incorporating such 2D flakes within waveguides. It is shown that ReS$_2$ flakes preferentially cleave along the $a$ axis, producing flakes with long and narrow dimensions. This allows for waveguide integration with a long interaction length between the propagating light and the NLO material. ReS$_2$ flakes were exfoliated and characterised using Raman and atomic force microscopy (AFM). Waveguide devices incorporating these flakes were fabricated.

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THz Photoconductive Antennas Using Thin Black Phosphorus

M. HASAN DOHA (Presenter), AHMAD F. RAWWAGAH, JOSH P. THOMPSON, ARASH FEREIDOUNI, Physics, University of Arkansas, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, MIAOQING HUANG, Computer Science and Computer Engineering, University of Arkansas, MAGDA O. EL-SHENAWEE, Electrical Engineering, University of Arkansas, HUGH CHURCHILL, Physics, University of Arkansas — We report the fabrication and characterization of THz photoconductive antennas using thin (~50 nm) black phosphorus (BP) as the photoconductor and hexagonal boron nitride (hBN) as a capping layer to prevent oxidation of BP and enhance absorption. Dipole antennas were fabricated on oxidized high-resistivity silicon substrates, and BP and hBN flakes were picked up and transferred onto the antennas inside a nitrogen glovebox. BP flakes were aligned with the armchair axis along the anode-cathode gap of the antenna, with crystal orientation measured using reflection anisotropy. The transfer matrix technique was used to optimize the thickness of BP and hBN for maximum absorption. Photocurrent imaging under illumination with ~100 fs pulses at 1550 nm showed a bias-dependent maximum photocurrent near the anode side of the antenna gap with a responsivity at 50 kHz of about 0.2 mA/W at a source-drain bias of -100 mV. We will also report ongoing measurements to compare THz output power of these antennas with reference devices in which silicon is used as the photoconductor.
Defect and interface engineering for high-performance 2D photodetectors

ZHENHUA NI (Presenter), Southeast University — The performance of photodetectors based on two-dimensional (2D) materials is strongly influenced by defects and the interface [1]. The de-trap time of carriers from a deep trap could be prolonged by several orders of magnitude as compared to shallow trap, resulting in additional decay time of the device. We demonstrate that the trap states in 2D ReS$_2$ could be efficiently modulated by defect engineering through molecule decoration, and the both the response time and responsivity of the device is greatly improved [2]. We further elaborate that plasmon-induced hot electron transfer (HET) from tungsten suboxide nanocrystals to graphene is a sufficient fast process (<150 fs) to prevent carrier cooling and trapping processes. A fast near infrared (NIR) detector empowered by HET is demonstrated, and the response time is three-orders of magnitude faster than that based on common band-edge electron transfer [3]. Our results indicate that defect and interface engineering is a new strategy for implementation of efficient and high-speed photoelectric devices.

References:
Lithographic bandgap engineering of graphene on the 10 nm scale: the role of edges

LENÉ GAMMELGAARD, BJARKE SØRENSEN JESSEN, JOSE MANUAL CARIDAD, DTU Physics, Technical University of Denmark, MORTEN RISHØJ THOMSEN, Department of Physics, Ålborg University, TIMOTHY JOHN BOOTH, DTU Physics, Technical University of Denmark, TAKASHI TANIGUCHI, KENJI WATANABE, Research Center for Functional Materials, NIMS, JOACHIM DAHL THOMSEN, Materials Science and Engineering, Massachusetts Institute of Technology, DAVID MACKENZIE, Department of Electronics and Nanoengineering, Aalto University, THOMAS G PEDERSEN, Department of Physics, Ålborg University, MADS BRANDBYGE, ANTTI-PEKKA JAUHO, PETER BØGGILD (Presenter), DTU Physics, Technical University of Denmark — In the light of graphene's rich electronic properties and potentially high performance in applications, one of the most obnoxious roadblocks have been to pattern graphene on a small scale. Early theoretical work predicted that the bandstructure of graphene could be engineered by nanopatterning, such as nanoribbons and antidot lattices. Unfortunately, edge disorder and contamination associated with typical lithographic processes have strong detrimental effects on the transport properties. This has held back efforts to utilize quantum confinement in practical graphene devices as well as downscaling graphene components to a scale comparable to mainstream silicon electronics. The key is to control the chemistry and roughness of the edges, which has a striking impact on charge distribution and scattering in graphene, as illustrated by breakdown of the Quantum Hall Effect and ferroelectric behavior in graphene devices. By careful patterning through the hexagonal boron nitride encapsulation layer, we fabricated graphene devices with 35 nm pitch hole arrays and nm-scale edge roughness, yet exceptionally high carrier mobility. The distinct magnetotransport features are in quantitative agreement with zero-parameter tight-binding calculations and analytical models, including a ca. 150 meV bandgap. In addition we find that the subtle moiré-superlattice signatures associated with a small finite twist angle between the graphene and hexagonal boron nitride survives the aggressive lithographic patterning, suggesting that nanoscale circuits and components that exploit the novel properties of twisted 2D layers are feasible.

Graphene Double-Layer Heterostructure Photodetectors with Broadband, High and Fast Responsivity at Room Temperature*

HO VINH (Presenter), YIFEI WANG, ZACHARY HENSCHEL, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech, MICHAEL P. COONEY, NASA Langley Research Center, VINH Q NGUYEN, Department of Physics and Center for Soft Matter and Biological Physics, Virginia Tech — The hybrid semiconductor/graphene photodetectors have been intensively investigating due to their applications ranging from imaging, sensing to communications in the infrared region. Integration of colloidal semiconductor quantum dots with graphene can increase the responsivity of such photodetectors. However, the response time is in millisecond to second scale, caused by optical traps at interfaces between semiconductor quantum dots and graphene. Another limitation is that the operation bandwidth still has not expanded beyond near-infrared region due to the bandgap of semiconductor quantum dots. Here, we report photodetectors based on two graphene single-layers separated by a 5-nm Ti$_2$O$_3$ thin-film engineered by the e-beam evaporation method. The Ti$_2$O$_3$ barrier is utilized as a tunneling charge transport channel between two graphene layers to reduce the charge recombination, and also as a mean for light absorber. Our devices show a high responsivity together with a fast response time in the nano-second scale, and a broadband spectral response at room temperature.

*Supported by the Earth Science Technology Office (ESTO), NASA

Mismatch-free tunnel spin contacts by photo-induced molecular functionalization of single layer graphene*

NOEL NATERA CORDERO (Presenter), JESUS TOSCANO-FIGUEROA, VICTOR GUAROCHICO, DENIS BANDURIN, CHRISTOPHER ROBERT ANDERSON, IRINA GRIGORIEVA, IVAN JESUS VERA MARUN, Univ of Manchester — A major issue preventing efficient spin injection in graphene is the mismatch between the contact and the spin impedance of the channel. This is of particular relevance for ultra-thin (0.6 nm) alumina tunnel barriers. We overcame this problem by growing the alumina barriers on graphene functionalized with phenyl radicals. The functionalization is achieved by using a laser beam to catalyse a photochemical reaction in benzoyl peroxide. The sub-micron spatial resolution enabled by the focused laser beam allows a direct comparison of different functionalization levels within a single graphene flake. Raman spectroscopy and Atomic Force Microscopy showed a dependence of the roughness of the tunnel barrier on the level of functionalization with the roughness of the barrier on functionalized graphene, reduced to half of that on pristine graphene. This functionalization mitigates the impedance mismatch problem, leading to an order of magnitude increase in the spin valve response.

*Consejo Nacional de Ciencia y Tecnologia
High-performance WSe$_2$ lateral pn-homojunction achieved with oxygen plasma-treatment for broadband photodetector applications*  

SEKHAR BABU MITTA (Presenter), FIDA ALI, YANG ZHENG, WON JONG YOO, Sungkyunkwan Univ — 2D transition metal dichalcogenides have shown significant potential for developing future nanoscale optoelectronic devices, among them, bulk tungsten diselenide (WSe$_2$) with an indirect bandgap (1.2 eV) is a promising material for optoelectronic applications due to its tunable energy bands, fast charge transfer, and strong optical absorption. Here, we demonstrate the fabrication of WSe$_2$ lateral pn-homojunction via oxygen (O$_2$) plasma-doping for high-performance broadband photodetector applications. The WSe$_2$ pn-homojunction photodetectors display higher photoresponsivities of 250 mA/W and 2000 mA/W, EQE of 97 % and 420 %, and detectivity of 7.7 × 10$^9$ Jones and 7.2 × 10$^{10}$ Jones for visible (520 nm) and near IR (852 nm) laser illuminations, respectively at $V_g = 0$V and $V_d = 1$V. The O$_2$ plasma-doping enables an effective charge generation and separations at the junctions upon the laser illuminations and resulting in superior optoelectronic properties which aid us in the development of lateral pn-homojunction as promising broadband photodetectors.

*This work was supported by Global Research Laboratory (GRL) Program (2016K1A1A2912707) & Global Frontier R&D Program (2013M3A6B1078873), both funded by Ministry of Science, ICT & Future Planning via National Research Foundation of Korea (NRF)

Stamping of Naked and Suspended 2D Materials to Engineer Light Absorption  

ISRAEL REBOLLO (Presenter), FERNANDA CRISTINA RODRIGUES MACHADO, GARETH J MELIN, ALEXANDRE CHAMPAGNE, Department of Physics, Concordia University, Montreal, Canada — We present a nitrocellulose-based method to manipulate naked and suspended 2DM one by one. We make optical measurements on several heterostructures to demonstrate the ability to tune graphene light absorption by a factor of 20. We show spatially-deterministic micron-scale positioning of graphene, boron nitride, and MoS$_2$ naked crystals. Raman spectroscopy confirms the low defect density introduced upon transfer. We detail micro-Raman measurements on a suspended graphene heterostructure of about 12 µm$^2$ to test the validity of an exclusive absorption model based on first-principles calculations [1]. We build several other graphene heterostructures with 2 distinct geometries to engineer the exclusive graphene light absorption. Future applications include optical transducers where a small gate voltage moves a suspended 2DM to vastly enhance or suppress its exclusive light absorption. 

**9:48AM W53.00009: Novel Plasmonic Waveguides from Coulomb Engineered Two-Dimensional Materials**  ZHIHAO JIANG (Presenter), STEPHAN WOLFGANG HAAS, Univ of Southern California, MALTE ROESNER, Institute for Molecules and Materials, Radboud University — Plasmonic excitations in two-dimensional (2D) materials are strongly affected by the screening environment, which allows us to control them by the dielectric properties of the substrate. Here we present how these plasmonic excitations can be spatially confined within a homogeneous 2D material with the help of structured heterogeneous dielectric substrates. By using this environmentally-imprinted plasmonic confinement to spatially guide the propagating surface plasmons within the 2D material we can construct fundamentally new plasmonic waveguides. Our quantum mechanical random phase approximation calculations show that this plasmonic confinement can be induced in areas of in- or decreased substrate permittivities, depending on the excitation frequency. We study in detail how the spatial extend of the environmental dielectric pattern affects these novel plasmonic waveguides and find that sub nm plasmonic confinement can be achieved. Our proposal renders dielectric engineering a truly non-invasive way of imprinting plasmonic waveguide channels into otherwise homogeneous 2D materials with promising potential for quantum optics.

**10:00AM W53.00010: Enhanced resonant Raman spectrum of multilayer WS2 with thin film plasmonic cavity**  CHUN YUAN WANG (Presenter), Physics, University of Texas at Austin, MENG HSIEN LIN, HUNG YING CHEN, 2. Meta-SERS co. ltd, Taiwan, JIAMIN QUAN, JUNHO CHOI, XIAOQIN (ELAINE) LI, Physics, University of Texas at Austin, SHANGJR GWO, Physics, National Tsing Hua University, CHIH-KANG SHIH, Physics, University of Texas at Austin — Interactions of tightly bound electron-hole pairs (excitons) and the lattice vibration modes (photon) in two-dimension (2D) transition metal dichalcogenide (TMD) crystal is a subject of considerable current interest. Here, we report investigations of exciton resonance Raman spectroscopy assisted by plasmonic thin film cavity from single monolayer to tens of monolayers in WS2. Without the plasmonic cavity and under A exciton resonant excitation condition, the Raman response indeed shows strong enhancement relative to the no-resonance condition, as reported by others previously [1]. With plasmonic cavity, the Raman signal is enhanced further as anticipated [2]. However, we find the enhancement factor show dramatic dependence on the TMD layer thickness with an optimal thickness in the range of few nanometer. More specifically, we find that at this range of thickness, the Raman enhancement is more than 2 orders of magnitude higher than that for the monolayer case. Possible mechanisms will be discussed.


*We acknowledge funding from the AOARD FA-2386-18-1-4097 in US and MOST 108-2119-M-007-008 in Taiwan.*
10:12AM W53.00011: Optical temperature determination during laser annealing of graphite oxide*  
SHASHANK RAM NANDYALA (Presenter), JOSEPH R MURPHY, MICHAEL A SEAS, VIVEK JAIN, SUBASH KATTEL, JON M PIKAL, PATRICK A JOHNSON, JOHN ACKERMAN, WILLIAM RICE, Univ of Wyoming — Highly conductive, graphene-like, reduced graphite oxide (rGO) can be synthesized from graphite oxide (GO) via photochemical methods, solution chemistry, and high-temperature treatments. In order to develop intricate circuitry and conductive patterns out of rGO, controlled laser-based annealing of GO has been extensively developed. Here, we show that this laser-based technique creates a localized, optically induced thermal reaction in GO. We determine the local temperature at the irradiation spot by comparing the Stokes and anti-Stokes scattering intensities giving us a simultaneous measure of temperature during annealing. Using this technique, we compare the optically induced GO-to-rGO transition with standard induction furnace annealing. The optically created rGO patterns, which we show can be produced in air, argon, and vacuum environments, are characterized using electrical conductivity and Raman scattering. Our ability to generate conductive circuits using optical annealing of GO creates new opportunities for economical carbon-based electronics.

*The authors acknowledge support from the UW School of Energy Resources.

10:24AM W53.00012: Optical probe of the low doping regime in graphene: Comparison of Raman spectroscopy and transport measurements*  
ZHUOFA CHEN (Presenter), MOUNIKA VUTUKURU, ANNA K SWAN, Boston Univ — Identifying charge density fluctuations and impurities in graphene is vital for high-quality graphene-based devices. Here, we developed an optical probe to evaluate the doping level and charge fluctuation in the range from $10^{10}$ cm$^{-2}$ to $10^{12}$ cm$^{-2}$ by using the Raman 2D peak. We compare charge density estimated from Raman measurements with electrical transport measurement, the benchmark method for evaluating charge density fluctuations and other scattering mechanism. At low doping level(< $10^{12}$ cm$^{-2}$), the 2D Raman peak becomes asymmetric and can be fitted by two peaks, and the 2D peak-split(in cm$^{-1}$) correlates with charge density with high precision ($2\times10^{10}$ cm$^{-2}$ per 2D peak-split wavenumber). Our work provides a simple and non-invasive optical method to quantify the doping levels of graphene from $10^{10}$ cm$^{-2}$ to $10^{12}$ cm$^{-2}$, two orders of magnitude higher precision than previously reported optical methods [1]. The 2D peak-split method provides a platform for evaluating the quality of graphene before building high-quality graphene devices.

Reference:

*This work is supported by NSF DMR grant 1411008.
10:36 AM W53.00013: Probing strong light-matter interaction in the optically thin limit  
ERIC YUE MA (Presenter), TONY F HEINZ, Stanford Univ — Sharp and isolated resonances in condensed-matter systems yield pronounced signatures in dielectric function, which, in turn, are manifest in the reflectance and transmittance spectra. A canonical example is the Reststrahlen band, extended spectral bands with near-unity reflectance, known to occur in ionic crystals near their optical phonon frequencies in the mid-infrared. Although Reststrahlen bands in bulk materials have been extensively studied, their behavior in the optically thin limit has not been examined systematically. With the advent of 2D van der Waals materials, it has become possible to probe materials with precise thicknesses across several orders of magnitudes, with essentially no change to the dielectric function down to the few- or monolayer limit. Here we present a systematic study of Reststrahlen-like reflection bands when the material transitions from optically thick to optically thin. We describe, experimentally and theoretically, the evolution of the reflectance spectra and their relation to radiative and nonradiative rates.

Friday, March 6, 2020 8:00 AM - 10:00 AM

Session W54 DCMP: Topological Devices and Nanostructures Mile High Ballroom 2A

8:00 AM W54.00001: Robust axion insulator and Chern insulator phases in a two-dimensional antiferromagnetic topological insulator*  
CHANG LIU (Presenter), YONGCHAO WANG, HAO LI, YANG WU, YAOXIN LI, JIAHENG LI, KE HE, YONG XU, JINSONG ZHANG, YAYU WANG, Tsinghua University — Topology, magnetism, and two-dimensional materials are among the most actively-pursued fields in physics and material science. Here, we investigate the quantum transport behaviors of exfoliated MnBi$_2$Te$_4$, an antiferromagnetic topological insulator that hosts all three properties simultaneously. In the six septuple-layer crystal, we observe robust axion insulator state in zero magnetic field, over a wide field range, and at relatively high temperatures. A moderate magnetic field drives it into the Chern insulator state through a topological quantum phase transition. These results pave the road for realizing the topological magnetoelectric effect and axion electrodynamics in condensed matter systems.

*This work was supported by the Basic Science Center Project of NSFC under grant No. 51788104, MOST of China grant 2015CB921000, 2017YFA0302900. This work is supported in part by the Beijing Advanced Innovation Center for Future Chip (ICFC).
8:12AM W54.00002: Gate field effects on the topological insulator BiSbTeSe2 interface

SHUANGLONG LIU, University of Florida, YANG XU, Purdue University, YUN-PENG WANG, University of Florida, YONG CHEN, Purdue University, JAMES NATHAN FRY, HAI-PING CHENG (Presenter), University of Florida — Inspired by experimental efforts, we study interfacial processes between two slabs of BiSbTeSe2 (BSTS) via first principles calculations. Topological surface states are absent for the BSTS interface at its equilibrium separation, but our calculations show that they appear if the inter-slab distance is greater than 6 Å. More importantly, we find that topological interface states can be preserved by inserting two or more layers of hexagonal boron nitride between the two BSTS slabs. Using a first-principles based method that allows us to simulate a back gate, we observe that at low bias the extra charge induced by a gate voltage resides on the surface that is closest to the gate electrode, leaving the interface almost undoped. This explains the origin of the observed insensitivity of transport properties to back voltage at low bias. Our study resolves a few questions raised in experiment, which does not yet offer a clear correlation between microscopic physics and transport data.

*This work is supported by the US DOE BES, under Contract No. DE-FG02-02ER45995. Y. P. C. acknowledges partial support from NSF under Grant No. EFMA-1641101. Computations were done using the utilities of NERSC and UFRC.

8:24AM W54.00003: Controlling Strain Gradients in Weyl Semimetals

CARSTEN PUTZKE (Presenter), JONAS DIAZ-GOMEZ, Ecole Polytechnique Federale de Lausanne, RONI ILAN, Tel-Aviv University, DMITRY I. PIKULIN, Microsoft Station Q, University of California, ADOLFO G GRUSHIN, University Grenoble Alpes, NITYAN NAIR, University of California, Berkeley, CHANDRA SHEKAR, HORST BORRMANN, CLAUDIA FELSER, MPI-CPfS Dresden, JAMES ANALYTIS, University of California, Berkeley, PHILIP MOLL, Ecole Polytechnique Federale de Lausanne — Exposing Weyl semimetals to an external magnetic field leads to the quasiparticle chirality, which has attracted much attention over the past years. The magnetic field causes a shift in the node position and opens a new transport channel. The application of strong magnetic fields for future technological use of this phenomenon is technically impractical. An alternative path has been proposed theoretically. By using strain gradients in Weyl semi-metals it is possible to tune the position of the nodes in a spatially inhomogeneous manner, causing a similar effect as the application of a magnetic field, hence termed pseudo-magnetic field. In the Dirac semimetal Cd$_3$As$_2$ the application of the magnetic field leads to splitting into Weyl nodes with Fermi arcs only pointing along $k_z$, making this a good test candidate. We will show how the new concept of pseudo-magnetic fields is applied to Cd$_3$As$_2$. Using focused ion beam micro structuring we have been able to fabricate samples of Cd$_3$As$_2$ that can be deformed elastically by bending. Studying the coherent electron path composed of two Fermi arcs on opposing surfaces has allowed us to test the proposed pseudo-magnetic fields and to give an upper limit for its strength.

**8:36AM W54.00004: Spinful quantum dot coupled to the edge states of a topological insulator**

PARAMESHWAR PASNOORI (Presenter), NATAN ANDREI, Rutgers University, New Brunswick, COLIN RYLANDS, physics, university of maryland — Coupling a local quantum impurity to an interacting one dimensional system leads to striking strongly correlated effects. Here we study a spinful quantum dot coupled to the edge states of a topological insulator modeled by an interacting helical Luttinger liquid. We solve the model exactly using Bethe Ansatz and study the ground state properties of the system including the occupation number of the impurity and its density of states. Explicit expressions for the impurity magnetic susceptibility is derived at zero temperature.

**8:48AM W54.00005: Current-driven dynamics of spin textures on a surface of topological insulators**

DAICHI KUREBAYASHI (Presenter), NAOTO NAGAOSA, RIKEN CEMS — The application of topological properties has attracted research interest to more efficiently manipulate magnetization. For instance, at the interface of the topological insulator and the ferromagnetic insulator, the electrical control of magnetic textures, magnetization switching induced by electric current, and spin-charge conversion have been intensely studied theoretically and experimentally.

In this talk, we present analytical expressions of the spin-transfer torques on a surface of the magnetic topological insulator by including the higher-order contributions of momentum, k²-term and the hexagonal warping. We obtain six different types of the spin-transfer torque including both the field-like and the damping-like torques; the four of them appear only when the higher-order momentum contributions are included. In addition, we discuss the dynamics of magnetic skyrmions driven by the spin-transfer torques on the surface of the topological insulator. Unlike the skyrmion dynamics in conventional metals, we find that the dynamics significantly depends on the internal structure of magnetic textures.

*This work was supported by the RIKEN Special Postdoctoral Researcher Program, JST CREST Grant Number JPMJCR1874 and JP- MJCR16F1, and JSPS KAKENHI Grant Numbers 18H03676 and 26103006.*
9:00AM W54.00006: Nontrivial topology in ultrathin bismuth nanowires: An electronic transport study.*  
TITO HUBER (Presenter), Howard University, ALBINA NIKOLAEVA, Lises.Academy Sciences Moldova, LEONID KONOPKO, Academy of Sciences of Moldova — In the past, bismuth was considered to be topologically trivial on the basis of theoretical study of band inversions and angle resolved photoemission spectroscopy. However, the topological properties of bismuth are the subject of renewed study because of the observations of high mobility exhibited by Bi nanowires (suggesting topological protection) as well as the proposal of higher-order topology. We studied the magnetoresistance (MR) in samples of ultrathin nanowires of bismuth, diameter ~50 nm, that exhibit high mobility (Huber et al, Scientific Reports 7,15569 (2017)). The MR exhibits peaks for a sequence of orientations of the magnetic field B, including a coherence peak for B//(111), that can be interpreted in terms of Yamaji magic angles. Magic angles are observed in layered conductors with an open, corrugated, Fermi surface. In contrast, bulk bismuth does not display magic angles since the Fermi surface consist of small ellipsoids and is closed. We will discuss our interpretation of the observations in terms of inter-Bi bilayer coupling and hinge states.

*We acknowledge support by NSF-CIQM1231319, The Keck Foundation and The Boeing Company.

9:12AM W54.00007: Non-local Fermi level tuning of topological insulator Bi$_{2-x}$Sb$_x$Se$_3$ nanoplate devices*

YASEN HOU (Presenter), RUI XIAO, LUKE MCCLINTOCK, HENRY TRAVAGLINI, DONG YU, University of California, Davis — The spin-polarized topological surface states of a topological insulators (TIs) are attractive because of their potential applications in spintronics. A critical challenge of accessing the surface states is to reliably tune the chemical potential with respect to the bulk bands and Dirac point. Here we report non-local Fermi level tuning in Bi$_{2-x}$Sb$_x$Se$_3$ nanoplate devices. We found that applying a local electric field on a Bi$_{2-x}$Sb$_x$Se$_3$ nanoplate device induces a Fermi level shift hundreds of microns away. As temperature decreases to 77K, such a Fermi level shift is frozen, and the device stay in a different electronic state. Magnitude and direction of the Fermi level shift can be controlled by the applied electric field, which then tune the device conductance, field effect behavior and photo-generated carrier transport distance. The non-local Fermi level shift follows very well with a diffusion model and predicts a diffusion coefficient of $2 \times 10^{-6}$ cm$^2$/S at room temperature. Potential candidates for the diffusing carriers include vacancies of selenium and charge traps.

*This work was supported by National Science Foundation Grant DMR-1838532 and DMR-1710737
9:24AM W54.00008: Quantum spin Hall quantum point contacts  CHRISTOPH FLECKENSTEIN (Presenter), University of Wurzburg — Quantum spin Hall insulators (QSHIs) provide helical, time reversal protected edge modes. When strongly localized and thus considerably one-dimensional, these edge states may be described in terms of helical Luttinger liquids. In that respect, especially the formation of interaction induced gaps is particularly exciting. Although the formation of the underlying scattering terms might be demanding for isolated helical edges, the situation shifts when both edges of the QSHI are brought in proximity to each other. Then, the increased number of channels enables a variety of scattering terms, all of which relevant even for weak repulsive Coulomb interactions. Indeed, very recent transport experiments on QSHI quantum point contacts not only imply the existence of interactions at the helical edge, but also indicate the presence of two-particle scattering terms. This is especially interesting, since these terms, among proximity induced superconductivity, constitute one brick for the construction of parafermionic excitations in the same system.

9:36AM W54.00009: Giant and gate-tunable spin-galvanic effect in graphene-topological insulator van der Waals heterostructures at room temperature  DMITRII KHOKHRIAKOV (Presenter), MD ANAMUL HOQUE, BOGDAN KARPIAK, SAROJ DASH, Chalmers Univ of Tech — Unique electronic spin textures in topological states of matter are promising for emerging spin-orbit driven memory and logic technologies. However, there are several challenges related to the enhancement of their performance, electrical gate-tunability, interference from trivial bulk states, and heterostructure interfaces. We address these challenges by integrating graphene [1] with a 3D topological insulator (TI) in a van der Waals heterostructure [2] to take advantage of their remarkable spintronic properties and engineer strong proximity-induced spin-charge conversion phenomena. In these heterostructures, we experimentally demonstrate a giant spin-galvanic effect at room temperature due to an efficient conversion of a nonequilibrium spin polarization into a transverse charge current [3]. Importantly, we show a strong gate-tunability of the spin-galvanic signal, tracing its origin to the proximity-induced Rashba-Edelstein effect. These findings open interesting opportunities for exploring exotic physical phenomena and new device functionalities governed by topological proximity effects.

9:48AM W54.00010: Topological Sliding Moiré Heterostructure*  SHIZENG LIN (Presenter), YING SU, Los Alamos Natl Lab — We investigate the effect of sliding motion of layers in Moiré heterostructures on the electronic state. We show that the sliding Moiré heterostructure can generate nontrivial topology characterized by the first and second Chern number in the high dimensional manifold spanned by the physical dimensions and synthetic dimensions associated with the sliding displacement. The nontrivial topology implies a topological charge pumping caused by the sliding motion. We demonstrate the nontrivial topology and charge pumping explicitly in a one dimensional bi-chain model and the small-angle twisted bilayer graphene. Contrary to the conventional belief that the interlayer sliding in incommensurate Moiré Heterostructures does not affect the electronic structure, our results reveal that the sliding motion can generate nontrivial topology dynamically and hence cannot be neglected in the dynamical process.

*This work was carried out under the auspices of the U.S. DOE NNSA under contract No. 89233218CNA000001 through the LDRD Program, and was supported by the Center for Nonlinear Studies at LANL. This work was also supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, Condensed Matter Theory Program.

Friday, March 6, 2020 8:00 AM - 10:24 AM

Session W55 DCMP: Non-Hermitian Topological Phases Mile High Ballroom 2B

8:00AM W55.00001: Homotopical classification of non-Hermitian band structures  ZHI LI (Presenter), ROGER MONG, Univ of Pittsburgh — We proposed a framework towards the topological classification of non-Hermitian band structures. Different from previous K-theoretical approaches, our approach is homotopical, which enables us to see more topological invariants. Specifically, we considered the classification of non-Hermitian systems with separable band structures. We found that the whole classification set is decomposed into several sectors, based on the braiding of energy levels. Each sector can be further classified based on the topology of eigenstates (wave functions). Due to the interplay between energy level braiding and eigenstates topology, we found some torsion invariants, which only appear in the non-Hermitian world. We further proved that these new topological invariants are unstable, in the sense that adding more bands will trivialize these invariants.
8:12 AM W55.00002: Doubling theorem for Fermi points, degenerate points, and exceptional points in 2D non-Hermitian systems
CHING-KAI CHIU (Presenter), Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, ZHESEN YANG, Institute of Physics, Chinese Academy of Sciences, ANDREAS P SCHNYDER, Max-Planck Institute for Solid State Physics — Fermion doubling theorem, which is known as Nielsen-Ninomiya theorem, states that once a Weyl node with a non-zero topological charge is present in the 3D Brillouin zone, the node must be accompanied by at least one Weyl node to neutralize the total topological charge in the entire Brillouin zone. In 2D non-Hermitian systems, Fermi points, degeneracy points, and exceptional points can be protected by non-zero topological invariants in the absence of symmetries. We show that these three types of protected points obey the doubling theorem in the 2D Brillouin Zone in this talk.

8:24 AM W55.00003: Non-Hermitian exceptional Landau quantization in electric circuits*
XIAO-XIAO ZHANG (Presenter), MARCEL FRANZ, University of British Columbia — Alternating current RLC electric circuits form an accessible and highly tunable platform simulating Hermitian as well as non-Hermitian quantum systems. We propose here a realization of a time-reversal invariant pseudo-magnetic field, enabling the exploration of non-Hermitian physics under external magnetic field. Based on circuit realizations of non-Hermitian Dirac and Weyl systems under magnetic field, we identify the low-energy physics with a generic real energy spectrum from the non-Hermitian relativistic Landau quantization of exceptional points and rings, avoiding the non-Hermitian skin effect and providing a physical example of quasiparticles moving in the complex plane. Realistic detection schemes are designed that can be used to probe the flat energy bands, sublattice polarization, edge states protected by a non-Hermitian sublattice symmetry, and a characteristic nodeless probability distribution.

*Research described in this article was supported by NSERC and by CiFAR.

8:36 AM W55.00004: Topological invariants for non-Hermitian chiral-symmetric systems*
TIMO HYART (Presenter), WOJCIECH BRZEZICKI, Institute of Physics, Polish Academy of Sciences — We show that the topology of one-dimensional chiral-symmetric non-Hermitian systems is determined by a hidden Chern number described by an effective 2D Hermitian Hamiltonian $H_{\text{eff}}(k, \eta)$, where $k$ is the momentum and $\eta$ is the imaginary part of the energy [1]. This Chern number manifests itself as topologically protected in-gap end states at zero real part of the energy. We show that the bulk-boundary correspondence coming from the hidden Chern number is robust and immune to non-Hermitian skin effect. We introduce a minimal model Hamiltonian supporting topologically nontrivial phases in this symmetry class, derive its topological phase diagram and calculate the end states originating from the hidden Chern number. We discuss various generalizations and realizations of this model, and the corresponding topological invariants.


*The work is supported by the Foundation for Polish Science through the IRA Programme co-financed by EU within SG OP Programme.
8:48AM W55.00005: Non-Hermitian band theory of directional amplification  WENTAN XUE (Presenter), MING-RUI LI, FEI SONG, YU-MIN HU, ZHONG WANG, Tsinghua University — Owing to its open-system nature, amplification of electromagnetic and other signals is naturally described in terms of non-Hermitian operators. Recently, it has been shown that the non-Hermitian band theory is dramatically shaped by the non-Hermitian skin effect (NHSE), namely the exponential accumulation of eigenstates to the boundary of the system. In view of the NHSE, non-Bloch band theory based on the generalized Brillouin zone has been formulated to predict the topological edge modes. Here, we show that the non-Bloch band theory provides a natural framework for the intriguing phenomenon of directional amplification (or nonreciprocal amplification) that is useful in many applications. The magnitude of directional amplification is expressed in terms of the quantities of the generalized Brillouin zone. Our results provide a natural and quantitative theoretical formulation for the directional amplification.

9:00AM W55.00006: Non-Hermitian skin effect and chiral damping in open quantum systems* FEI SONG (Presenter), SHUNYU YAO, ZHONG WANG, Tsinghua University — One of the unique features of non-Hermitian Hamiltonians is the non-Hermitian skin effect, namely, that the eigenstates are exponentially localized at the boundary of the system. The non-Hermitian skin effect plays a crucial role in the non-Hermitian topology and bulk-boundary correspondence. For open quantum systems, a short-time evolution can often be well described by the effective non-Hermitian Hamiltonians, while long-time dynamics calls for the Lindblad master equations, in which the Liouvillian superoperators generate time evolution. In this Letter, we find that Liouvillian superoperators can exhibit the non-Hermitian skin effect, and uncover its unexpected physical consequences. It is shown that the non-Hermitian skin effect dramatically shapes the long-time dynamics, such that the damping in a class of open quantum systems is algebraic under periodic boundary conditions but exponential under open boundary conditions. Moreover, the non-Hermitian skin effect and non-Bloch bands cause a chiral damping with a sharp wave front.

References:

*This work is supported by NSFC under grant No. 11674189.
**9:12AM W55.00007: Observation of non-Hermitian topology and its bulk-edge correspondence***  
ANANYA GHATAK (Presenter), MARTIN BRANDENBOURGER, JASPER VAN WEZEL, CORENTIN COULAIS, Univ of Amsterdam — Topological edge modes and the bulk-edge correspondence has enabled the creation of robust electronic, electromagnetic and mechanical transport properties across a wide range of systems, from cold atoms to metamaterials, active matter and geophysical flows. Recently, in the advent of non-Hermitian topological systems novel topological phases have been introduced. However, whether such phases can be experimentally observed, and what their properties are, have remained open questions. Here, we discover and observe a novel form of bulk-edge correspondence for non-Hermitian topological phases. We find that a change in the bulk non-Hermitian topological invariant corresponds to a change of localization of the topological edge mode. Using a quantum-to-classical analogy, we create a mechanical metamaterial with non-reciprocal interactions, in which we observe experimentally the predicted bulk-edge correspondence, demonstrating its robustness. Our results have a major impact on the field of non-Hermitian topology and boost metamaterials by opening new avenues to manipulate waves in unprecedented fashions.


*The Netherlands Organization for Scientific Research (NWO) VENI and VIDI grants.

**9:24AM W55.00008: Symmetry and Topology in Non-Hermitian Physics**  
KOHEI KAWABATA (Presenter), Department of Physics, University of Tokyo, KEN SHIOZAKI, Yukawa Institute for Theoretical Physics, Kyoto University, MASAHITO UEDA, Department of Physics, University of Tokyo, MASATOSHI SATO, Yukawa Institute for Theoretical Physics, Kyoto University — Non-Hermiticity enriches topological phases beyond the existing framework for Hermitian topological phases. Here, we develop a general theory of symmetry and topology in non-Hermitian physics. We demonstrate that non-Hermiticity ramifies and unifies the celebrated Altland-Zirnbauer symmetry for insulators and superconductors, leading to 38-fold symmetry instead of the 10-fold one. Moreover, we reveal that two types of energy gaps are relevant for non-Hermitian systems because of the complex-valued nature of energy spectra, both of which constitute non-Hermitian topology. Based on these fundamental insights in non-Hermitian physics, we completely classify topological phases of non-Hermitian insulators and superconductors, as well as semimetals that support exceptional points. Our work paves the way toward unique phenomena and functionalities due to the interplay of non-Hermiticity and topology, such as symmetry-protected topological lasers and dissipative topological quantum computation.

Classification of Exceptional Points and Non-Hermitian Topological Semimetals

TAKUMI BESSHO (Presenter), Yukawa Institute for Theoretical Physics, Kyoto University, KOHEI KAWABATA, Department of Physics, University of Tokyo, MASATOSHI SATO, Yukawa Institute for Theoretical Physics, Kyoto University — Exceptional points are universal level degeneracies induced by non-Hermiticity. Whereas the past decades witnessed their new physics, the unified understanding has yet to be obtained. Here we present the complete classification of generic topologically stable exceptional points according to fundamental symmetries of charge conjugation, parity, and time reversal. This classification reveals unique non-Hermitian gapless structures with no Hermitian analogs and systematically predicts unknown non-Hermitian semimetals and nodal superconductors; a topological dumbbell of exceptional points in three dimensions is constructed as an illustration. Our work paves the way towards richer phenomena and functionalities of exceptional points and non-Hermitian topological semimetals.


Non-Hermitian physical aspects in disordered Weyl/Dirac semimetals

TAIKI MATSUSHITA (Presenter), Osaka Univ, YUKI NAGAI, JAEA, SATOSHI FUJIMOTO, Osaka Univ — Recently, the platform of non-Hermitian physics is extended to many-body or disordered systems where quasiparticles possess a finite lifetime. The realization of non-Hermitian topological defects in equilibrium systems attracts great interests because non-Hermitian nature makes topological classification very rich. For example, non-Hermitian perturbations in Weyl Hamiltonian lead to the realization of Weyl exceptional rings and flat bands.

Here, we show the non-Hermitian physics in disordered Weyl semimetals. In this presentation, we propose a general scheme for the generation of disorder-induced Weyl exceptional rings, a spectral collapse of Landau levels. Our scheme for a generation Weyl exceptional ring is applicable to almost all Weyl materials. Thus, Weyl exceptional rings in disordered Weyl semimetals are detectable by using photoemission or quasiparticle interference experiments. In addition, we propose that a new type of non-Hermitian effects in Weyl semimetals, the spectral collapse of Landau levels. We show that non-Hermitian perturbation leads to the collapse of Landau quantization which corresponds to non-Hermitian topological phase transition.

Taiki Matsushita was supported by a JSPS Fellowship for Young Scientists.

Non-Hermitian fractional quantum Hall states with 1/3 filling

YOSHIDA TSUNEYA (Presenter), KOJI KUDO, YASUHIRO HATSUGAI, Univ of Tsukuba — We elucidate the emergence of non-Hermitian fractional quantum Hall states (nHFQH) with 1/3 filling for cold atoms with two-body loss. We characterize the nHFQH states with the topological degeneracy under the periodic boundary condition and the total Chern number C_{tot}=1 for the ground state triplet. Furthermore, we point out that nHFQH states emerge even when the interaction is purely dissipative.

This work is partly supported by JSPS KAKENHI Grants No.JP16K13845, No.JP17H06138, and No.JP18H05842. A part of numerical calculations were performed on the supercomputer at the ISSP in the University of Tokyo.
10:12AM W55.00012: Appearance of a topological semimetal phase in 1D non-Hermitian systems
KAZUKI YOKOMIZO (Presenter), SHUICHI MURAKAMI, Tokyo Institute of Technology —
In our previous work, we establish a non-Bloch band theory in one-dimensional (1D) tight-binding non-Hermitian systems [1]. We show how to determine the generalized Brillouin zone \( C_\beta \) for the complex Bloch wave number \( \beta = e^{ik} \), \( k \in \mathbb{C} \). In contrast to Hermitian cases, where \( C_\beta \) is always a unit circle, in non-Hermitian systems \( C_\beta \) is a closed curve, not necessarily a unit circle. Furthermore, we find that \( C_\beta \) can have cusps, and its shape depends on system parameters. A byproduct of our theory is that one can prove the bulk-edge correspondence between the winding number defined from \( C_\beta \) and existence of topological edge states.

From the non-Bloch band theory, we show that in 1D non-Hermitian systems with both sublattice symmetry and time-reversal symmetry, a topological semimetal phase with exceptional points is stabilized, and this phase extends over a finite region on the phase diagram. This stems from unique features of the generalized Brillouin zone \( C_\beta \); as a system parameter changes, \( C_\beta \) also changes so as to keep the system gapless. Furthermore, we also find that the motion of the exceptional points within the topological semimetal phase is related to the change of the value of the winding number. [1] K. Yokomizo and S. Murakami, Phys. Rev. Lett. 123, 066404 (2019)

Friday, March 6, 2020 8:00 AM - 10:48 AM

Session W56 DCMP: Density Waves in Materials Mile High Ballroom 2C - Emma Cating-Subramanian

8:00AM W56.00001: Novel photoinduced charge density wave state and periodic lattice distortion in 17-TaSe\(_2\)
YINGCHAO ZHANG (Presenter), XUN SHI, WENJING YOU, ZHENSHEUNG TAO, YIGUI ZHONG, Department of Physics and JILA, University of Colorado, Boulder, PETER OPPENEER, Department of Physics and Astronomy, Uppsala University, MICHAEL BAUER, KAI ROSSNAGEL, Institute of Experimental and Applied Physics, Kiel University, HENRY KAPTEYN, MARGARET MURNANE, Department of Physics and JILA, University of Colorado, Boulder —

The amplitude mode in a charge density wave (CDW) material is the collective modulation of the relevant periodic lattice distortion (PLD). Here we use a femtosecond laser pulse to displacively excite the coherent amplitude mode in the CDW material 17-TaSe\(_2\). We then use time- and angle-resolved photoemission to track the dynamic evolution of the amplitude mode and electronic band structure – and in particular, the position and the width of the Ta 5\(d\) band. At sufficiently high fluences, and within a half-cycle of the amplitude mode oscillation, the PLD of 17-TaSe\(_2\) first relaxes to the position of the normal state, before overshooting to form an inverted CDW transient state. Moreover, the band width is maximum for the normal state, while it is reduced for both the ground CDW state and the inverted CDW state. Another important observation is that this inverted CDW state has larger density of states at the Fermi level than the normal state. Our observations are consistent with both density functional theory (DFT) and tight binding calculations. Our results show the possibility of using light to generate unique lattice distortions and electron correlations via ultrafast coherent phonon excitation.
8:12AM W56.00002: Suppression of charge density wave transitions in La(\textit{Ag}_{1-x}\textit{Au}_x)\textit{Sb}_2 (0 \leq x \leq 1) by pressure.\footnote{This work was supported by the Department of Energy, Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-07CH11358.} SERGEY L. BUD'KO (Presenter), LI XIANG, Ames Laboratory and Iowa State University, DOMINIC H RYAN, Department of Physics and Centre for the Physics of Materials, McGill University, PAUL C CANFIELD, Ames Laboratory and Iowa State University — LaAgSb$_2$ exhibits two CDW transitions at ambient pressure: at $T_1 \sim 207$ K a lattice modulation along the $a$-axis develops and upon further cooling, at $T_2 \sim 186$ K, an additional CDW ordering along the $c$-direction appears.\cite{1} Here, we report resistivity measurements on La(\textit{Ag}_{1-x}\textit{Au}_x)\textit{Sb}_2 (0 \leq x \leq 1) samples at ambient and high pressure that reveal suppression of both CDW transitions by pressure and Au substitution. By introducing simple pressure scale shifts for different $x$-values, the $T(P)$ data fall onto universal $T_1(P^*)$ and $T_2(P^*)$ curves. Results will be compared with and contrasted to the literature data on (La$_{1-x}$\textit{R}_x)AgSb$_2$ ($R$ = Ce, Nd).\cite{2}


8:24AM W56.00003: Emergence of charge density wave domain walls network in Pt doped TiSe$_2$\footnote{acknowledge support from DMREF 1629068} DAVIDE IAIA (Presenter), University of Illinois at Urbana-Champaign, KYUNGMIN LEE, Physics, The Ohio State University, JESSE CHOE, Physics, Rice University, JUNJING ZHAO, JUQIANG LI, Physics, University of Virginia, MING SHI, JUNZHANG MA, MENGYU YAO, Swiss Light Source, Paul Scherrer Institute, ZHENYU WANG, University of Illinois at Urbana-Champaign, MASAYUKI OCHI, Physics, Osaka University, RYOTARO ARITA, Applied Physics, University of Tokyo, UTPAL CHATTERJEE, Physics, University of Virginia, EMILIA MOROSAN, Physics, Rice University, VIDYA MADHAVAN, University of Illinois at Urbana-Champaign, NANDINI TRIVEDI, Physics, The Ohio State University — Charge density wave (CDW) incommensuration in the TiSe$_2$ family proceeds through the formation of domain walls (DWs). Previous scanning tunneling microscopy (STM) studies on Cu intercalated TiSe$_2$ have shown that DWs host an extra population of electrons and might play an important role in the emergence of superconductivity. Here we report a low temperature STM study of Pt-doped TiSe$_2$. A network of nanometer-thick DWs is observed and STM spectra reveal local inhomogeneity of the electronic properties which results in the emergence of pseudogaps of different size. In contrast to Cu intercalation, Pt substitution creates a network of 1D channels of low energy transport which subtract electrons from the bulk enhancing correlation effects. The interplay between electron correlation and disorder induced by DWs might be fundamental for the metal to insulator transition reported by previous transport measurements.
8:36AM W56.00004: Scanning Tunneling Microscopy of the Nearly-Commensurate and Incommensurate Charge Density Wave Phases of 1T-TaS$_2$*  MICHAEL BOYER (Presenter), MANOJ K SINGH, BISHNU SHARMA, BONING YU, Clark University — 1T-TaS$_2$ is an intensely-studied charge density wave (CDW) compound which hosts a wealth of interesting and diverse physics. At low temperatures, 1T-TaS$_2$ is in a Mott insulating, commensurate CDW state. At higher temperatures, the material can enter into triclinic, nearly-commensurate, and incommensurate CDW states. Studies across all four CDW states using multiple experimental techniques have been conducted, but considerable emphasis has been on the low-temperature commensurate CDW state. Here we present our scanning tunneling microscopy measurements on the higher-temperature nearly-commensurate and incommensurate CDW phases with a focus on domains, domain walls, and their changes with temperature.

*We acknowledge support from NSF Grant number DMR-1904918.

8:48AM W56.00005: Charge density wave (CDW) and magnetism in RNiC$_2$ family (R = rare earth metal)*  MARTA ROMAN (Presenter), KAMIL K. KOLINCIO, TOMASZ KLIMCZUK, Faculty of Applied Physics and Mathematics, Gdansk University of Technology — The ternary rare-earth nickel dicarbides RNiC$_2$ (R - rare earth metal) with a non-centrosymmetric, orthorhombic crystal structure offer a unique opportunity to tune the ground state with varying R atom. The charge density wave (CDW) has been found for most of the members of the RNiC$_2$ family (R = Pr – Lu) with the Peierls temperature scaling linearly with the unit-cell volume. LaNiC$_2$ compound is an unconventional superconductor, SmNiC$_2$ undergoes a ferromagnetic transition and the rest of the compounds (apart from nonmagnetic YNiC$_2$ and LuNiC$_2$ exhibiting large positive magnetoresistance and PrNiC$_2$ where only a weak magnetic anomaly is observed) order antiferromagnetically below 25 K.

In this presentation, the large diversity of physical phenomena occurring in the RNiC$_2$ family will be discussed in terms of relations between various types of ordering on the basis of magnetic, transport and galvanomagnetic measurements. The main emphasis will be put on the CDW mutually interacting with magnetism in the polycrystalline RNiC$_2$ and their solid solutions.

*The project was financially supported by the National Science Centre (Poland), Grant UMO-2015/19/B/ST3/03127.
9:00AM W56.00006: Core-level and Resonant Photoemission across the Charge Density Wave Transition in 1T-TiSe₂
ASHISH CHAINANI (Presenter), CHIEN-WEN CHUANG, Condensed Matter Physics, Natl Synchrotron Rad Res Ctr, Taiwan, YOSHIKAZU TANAKA, MASAKI OURA, RIKEN SPring-8 Center, Hyogo, Japan, KAI ROSSNAGEL, Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — We study the electronic structure of the charge density wave (CDW; \( T_{CDW} = 200 \) K) material 1T-TiSe₂, using core-level photoemission and valence band resonant photoemission spectroscopy (RESPES) across the Ti L-edge threshold. While 1T-TiSe₂ was extensively studied using various techniques including angle-resolved photoemission spectroscopy (ARPES)[1], time-resolved ARPES[2] and resonant inelastic X-ray scattering[3], the Ti L-edge RESPES has not been reported. The Ti 2p and Se 3d spectra show clear shifts across the CDW transition associated with band structure changes in the CDW phase. The Ti L-edge RESPES shows a clear resonance of Ti 3d character states and a Ti LVV Auger correlation satellite. Applying the Cini-Sawatzky method provides an estimate of the effective on-site Coulomb correlation energy between two holes, \( U_{dd} = -1.5 \) eV. The results are consistent with core level Auger spectra of 1T-TiSe₂[4], suggesting the effective attractive Coulomb correlation energy would favour a band Jahn-Teller based model for describing the CDW transition in 1T-TiSe₂.

References :
(3) C. Monney et al. PRL 109, 047401 (2012).

9:12AM W56.00007: High-temperature charge density wave in rare-earth tetratelluride
BAIQING LYU (Presenter), ALFRED ZONG, Massachusetts Institute of Technology MIT, DONG WU, International Center for Quantum Materials, Peking University, MAKOTO HASHIMOTO, DONGHUI LU, SLAC National Accelerator Laboratory, Stanford Synchrotron Radiation Lightsource, SU-DI CHEN, Stanford University, MAN LI, YA BOO HUANG, Shanghai Synchrotron Radiation Facility, NUH GEDIK, Massachusetts Institute of Technology MIT — Charge density waves (CDWs) are broken-symmetry ground states that are driven by the electron-phonon interaction in quasi one-dimensional (1D) or two-dimensional (2D) metals. The subject has generated considerable interest as it offers important insights into electron-phonon physics, its competition or coexistence with other ground states, as well as its potential role in the phase diagram of high-Tc cuprates. Recently, a CDW state was found in a newly synthesized quasi-2D compound, rare-earth tetratelluride. Here, by high-resolution angle-resolved photoemission spectroscopy, we demonstrate that in the CDW state, the Fermi surface is fully gapped but the gap size is momentum-dependent. Surprisingly, the CDW persists to above 400 K, providing a remarkable system for the room-temperature study of 2D semiconductors with collective electronic states.
**9:24AM W56.00008: Charge Density Wave Order in the Organic Metal α-(ET)$_2$ KHg(SCN)$_4$**

RAJU GHIMIRE (Presenter), BRET LARAMEE, OWEN GANTER, Clark University, ZAHIRUL ISLAM, ULRICH WELP, Argonne National Laboratory, JENNIFER NEU, National High Magnetic Field Laboratory, CHARLES C AGOSTA, Clark University — The family of crystalline organic metals α-(ET)$_2$ XHg(SCN)$_4$, with X=K, NH$_4$, Ti, or Rb are of interest because three of the compounds have a coexisting charge density wave (CDW) and metallic phase at low temperatures, while one (X = NH$_4$) has a superconducting ground state. They are all triclinic crystals and have a quarter filled conduction band. To find the nature of the density wave state we studied α-(ET)$_2$ KHg(SCN)$_4$ using elastic x-ray scattering at the Advanced Photon Source at Argonne National Laboratory. We will present preliminary scattering data at 4 K to search for incommensurate CDW, below the thermodynamic phase transition at 8K, and contrast it with data at 104 K. We encountered serious challenges of radiation damage to these organic materials and employed a mitigation scheme by using 18 keV x-rays with reduced incident flux for extended period of time. There seems to be a weak broadening of Bragg peaks below 8 K, which would indicate some structural anomaly at this temperature.

*We acknowledge funding from NSF, DMR-1905950.
Work at Materials Science Division of Argonne National Laboratory was supported by the US Department of Energy (DOE).This research used resources of the APS, User Facility operated by Argonne National Laboratory under Contract DE AC02-06CH11357.


JAN-HENDRIK PÖHLS (Presenter), MARGARETHA SANDOR, MARTIN OTTO, LAURENT RENÉ DE COTRET, MARK SUTTON, BRADLEY SIWICK, McGill Univ — Investigations of structural dynamics on the sub-picosecond timescale can provide a detailed fundamental understanding of the non-equilibrium properties of materials. While structural transformations are related to intensity changes in Bragg peaks, thermal diffuse scattering can reveal complete information on the underlying phonon modes. Because thermal diffuse scattering intensities are many order of magnitude lower than Bragg intensities, very sensitive measurements are required.

In this talk, I will present ultrafast electron diffuse scattering to directly observe electron-phonon interactions in charge-density wave (CDW) materials with a time resolution of ~100 fs. It was found that CDW materials and high-temperature superconductors (HTS) have a similar origin and hence, gaining deep insights in CDW materials is expected to enhance our understanding of HTS. Using a combination of density functional theory and experimental studies, the rich electron-phonon interactions of two CDW materials (*i.e.*, niobium diselenide and tantalum disulfide) were investigated. Measurements suggest photoexcitation significantly stiffens/softens acoustic modes only at certain wave-vectors, a phenomenon we have also investigated computationally.

*I would like to acknowledge the FRQNET PBEEE fellowship.*
**3D-ΔPDF analysis of three-dimensional CDW compound \((\text{Ca}_x\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}\)**

PUSPA UPRETI (Presenter), Physics (NIU) and Material Science Division (ANL), Northern Illinois University and Argonne National Lab, LEKHANATH POUDEL, NIST Center for Neutron Research, MATTHEW KROGSTAD, STEPHAN ROSENKRANZ, Material Science Division, Argonne National Laboratory, OMAR CHMAISSEM, Physics (NIU) and Material Science Division (ANL), Northern Illinois University and Argonne National Lab, RAYMOND OSBORN, Material Science Division, Argonne National Laboratory — A three-dimensional compound series \((\text{Ca}_x\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}\) has been identified as a promising system to understand the interplay between the charge-density-waves (CDW) and the superconductivity. The second order CDW transition temperature \(T^*\) in this family can be fully suppressed with the substitution of Ca for Sr, giving rise to a Quantum Critical Point at \(x\approx0.9\) at ambient pressure. For a comprehensive understanding of the lattice instability connected to this CDW transition and superconductivity, diffuse scattering measurements were performed on a single crystal doping series in \((\text{Ca}_x\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}\) with \((x=0, 0.1, 0.5, 0.6, 0.65, 0.7, 0.9)\) using x-ray diffraction. A 3D-ΔPDF analysis shows that there is an order-disorder transition at \(T^*\), with local distortions still present at higher temperature.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.*

**Optical Thermal Diffusivity Measurements in PdxErTe3**

ERIK KOUNTZ (Presenter), JOSHUA A STRAQUADINE, JIECHENG ZHANG, AHARON KAPITULNIK, IAN FISHER, Stanford Univ — PdxErTe3 is a quasi-2D metal with two stripe ordered charge density wave (CDW) orders with of Pd intercalated between the ErTe3 layers [1]. Increasing Pd intercalation increases disorder and suppresses the CDW transitions [1,2]. We use a photo-thermal microscope for high resolution thermal diffusivity and optical reflectivity measurements by measuring phase delay in local reflectivity. This is supplemented with resistivity and thermopower measurements. Our primary observation is a decrease of thermal diffusivity and the onset of anisotropy in all transport channels below the higher temperature CDW transition. We will further discuss the relation between thermal and charge transport, and the applicability of Wiedemann-Franz law through the two CDW transitions.

Density Wave Order in Superconducting Nb-Bi$_2$Se$_3$

Yanan Li (Presenter), Christian A Parsons, University of Wisconsin - Milwaukee, Sanath Ramakrishna, William Nelson, Ryan Baumbach, Arneil P Reyes, National High Magnetic Field Laboratory/Florida State University, Prasenjit Guptasarma, University of Wisconsin - Milwaukee

Topological Insulators such as Bi$_2$Se$_3$ and Bi$_2$Te$_3$, observed to have hexagonally deformed Fermi surfaces and strong nesting, have been proposed as potential candidates for the existence of density wave order. The presence of such order becomes particularly interesting in the context of superconductivity appearing in systems such as Cu-Bi$_2$Se$_3$ and Nb-Bi$_2$Se$_3$, and of possible intercalation-induced spontaneous symmetry breaking. So far, from experiments, we have some hints of density wave order, such as from electron diffraction and angle-resolved photoemission spectroscopy in Cu-Bi$_2$Se$_3$, and the observation of multiple Fermi surfaces in torque-magnetometry based quantum oscillations in Nb-Bi$_2$Se$_3$. However, there are no direct reports of Charge Density Wave order from resistivity. Here we report, for the first time, evidence for the coexistence of superconductivity with CDW order from transport measurements on single crystals of Nb$_x$-Bi$_2$Se$_3$ (0 < x < 0.25). We also report our studies of specific heat, magnetization, and $^{209}$Bi NMR. Based on our results, we argue that the Nb d orbital might not be responsible for the observation of multiple Fermi surfaces, and that such order could simply be induced by intercalants (Bi or Nb, or both). Further work is needed in this area.

Electronic Raman scattering spectra of various types of BEDT-TTF compounds


We measured Raman scattering spectra of various types of BEDT-TTF compounds such as a charge ordered material $\alpha$-(BEDT-TTF)$_2$I$_3$, a dimer-square lattice material $\beta$-(BEDT-TTF)$_2$I$_3$ and a quantum spin-liquid material $\kappa$-(BEDT-TTF)$_2$Ag$_2$(CN)$_3$. These three compounds show the broad Raman structures, which can be ascribed to the electronic Raman scattering. These structures correspond to charge excitation and magnetic excitation. Comparing these electronic Raman signals, we will discuss the electronic states of these compounds. For example, $\alpha$-(BEDT-TTF)$_2$I$_3$ shows a phase transition from charge ordered state to Dirac electron state. For clarification of the electronic state of $\alpha$-(BEDT-TTF)$_2$I$_3$, we focus on the charge excitation in the reflectivity and Raman spectra.
Alkali-metal-TCNQ salt, K-TCNQ, is a quasi-one-dimensional organic charge-transfer complex with segregated columns of alkali cations and TCNQ anion. The compound undergoes structural transition at Tc ~ 395 K as a result of strong electron-lattice interaction inherent in quasi-one-dimensional systems. Below Tc, an electric-induced transition from insulating to metallic phase is observed and contains two threshold behaviors in current-voltage characteristics, akin to charge density wave (CDW) systems. In CDW systems, the lower threshold is attributed to Coulomb blockade for soliton nucleation and the upper one is the depinning field. The upper threshold field follows an exponential temperature-dependence like in CDW systems implying collective charge dynamics near the transition. Low-frequency conductance noise spectroscopy is employed to understand charge carrier dynamics across both the thresholds. The power spectral density (PSD) of the measured current fluctuation increases by almost three orders around the lower threshold implying possible nucleation of phase solitons and on approaching the upper threshold field possible indications of CDW sliding are seen in the behavior of PSD. The existence and dynamics of CDW in these organic charge-transfer systems will be presented.
8:00AM W57.00001: Anomalous phonon vibrations of monolayer MoS$_2$ revealed by polarization degree of freedom of light* TENG-DE HUANG, KRISTAN BRYAN SIMBULAN, YANNWEN LAN, TING-HUA LU (Presenter), Department of Physics, National Taiwan Normal University — Light of linear and circular polarization is broadly used to explore interesting light-matter interaction in layered two-dimensional transition metal dichalcogenides (TMDs) such through Raman scattering and photoluminescence. Little attention has been given to the interaction of TMD materials and light with the elliptical polarization state. We applied elliptically polarized light in micro-Raman spectroscopy to observe variations in the relative intensity of the two most dominant Raman peaks of MoS$_2$. This provides an additional degree of freedom affecting the relationship between the two orthogonal components of the material's in-plane lattice vibrations. Different magnitudes of the in-plane lattice vibrations along two orthogonal directions were induced by varying the light from circularly polarized to elliptically polarized states. Besides, with changing the incident linear polarization angle, the out-of-plane $A_{1g}$ phonon mode red shifts, while the in-plane $E_{2g}$ phonon mode blue shifts. The anomalous lattice vibrations of monolayer MoS2 originate from the built-in strain introduced by the SiO$_2$/Si substrate. This work investigates the material's unexplored fundamental phonon property which may enlighten past and future studies.

*MOST 108-2112-M-003-009

8:12AM W57.00002: A first-principles study of the thermodynamic and vibrational properties of ReS$_2$ under pressure* NATALYA SHEREMETYEVA (Presenter), DAMIEN TRISTANT, ANTHONY YOSHIMURA, JASON GRAY, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, LIANGBO LIANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, VINCENT MEUNIER, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute — Two-dimensional layered materials (2DMs) are promising candidates for novel devices due to their tunable properties. The properties can be tuned by e.g. controlling the number of layers or applying external pressure on the structures. In order to control the (tuned) properties exactly, precise characterization of 2DMs' is needed. Here, the effect of hydrostatic pressure on the structural, energetic, electronic, and vibrational properties of layered bulk ReS$_2$ was studied using density functional theory. The electronic band gap of the 1T phase is shown to undergo a nearly-direct to indirect transition at about 9 GPa, while the 1T' phase is found to remain a robust nearly-direct band gap material under pressure. The computational analysis of the vibrational properties of both ReS$_2$ phases reproduced existing experimental Raman spectroscopy data for $\omega$ vs. $P$ trends and provided a path towards an accurate phase discrimination using infrared spectroscopy, inelastic neutron, and X-ray scattering.

*The authors gratefully acknowledge support by the NSF Grant EFRI 2-DARE (EFRI-1542707), the National Science Foundation (Award 1608171) and by the NY State Empire State Development's Division of Science, Technology and Innovation (NYSTAR) through Focus Center-NY–RPI Contract C150117.
8:24AM W57.00003: Van der Waals and Electron Stimulated Covalent Hydrogenation of Borophene  SHAOWEI LI (Presenter), University of California, Berkeley, MATTHEW S RAHN, QIUCHENG LI, MARK C HERSAM, Northwestern University — The recent experimental realization of atomically thin, crystalline boron sheets has opened a new direction in the study of synthetic 2D materials. Chemical modification of borophene could further enable fine-tuning of its band structure for nanoelectronic applications. Here, we present the first experimental study of both the non-covalent and covalent hydrogenation of borophene. Adsorbed hydrogen molecules are observed to form a triangular lattice on both $v_{1/6}$ and $v_{1/5}$ borophene polymorphs. The rotational excitation of H$_2$ is detected at 36 meV, indicating the adsorption of hydrogen is dominated by its van der Waals interaction with borophene. The formation of this H$_2$-borophene vertical heterostructure increases the work function of borophene. Moreover, covalent modification of borophene is achieved by inducing a hydrogen-borophene reaction at elevated tip bias voltage. This reaction significantly modifies the electronic structure of borophene and further increases its work function. Overall, this work illustrates the sensitivity of the electronic properties of borophene to chemical modification, which is expected to stimulate further exploration of boron-based chemistry in the two-dimensional limit.

8:36AM W57.00004: Native point defects and impurities in WSe$_2$*  DARSHANA WICKRAMARATNE (Presenter), United States Naval Research Laboratory — Tungsten diselenide (WSe$_2$) is being actively pursued for two-dimensional electronics and as a host for single-photon emitters. We have studied the properties of native defects and impurities in WSe$_2$ using density functional theory with a hybrid functional. We find that all native defects give rise to levels that are deep in the band gap, and thus will not contribute to conductivity. The defect chemistry of WSe$_2$ is likely dominated by common background impurities. In particular, substitutional oxygen, carbon, and transition metal impurities such as vanadium, are low energy defects. Our results allow us to comment on the origin of the frequently observed $p$-type conductivity and sub-band gap emission lines in as-grown WSe$_2$.

*This work was supported by a NRC associateship at the US NRL
8:48AM W57.00005: Discontinuous Evolution of the Structure of Stretching Polycrystalline Graphene.  FEDERICO D'AMBROSIO (Presenter), Univ of Utrecht, VLADIMIR JURIČIĆ, NORDITA, GERARD T. BARKEMA, Univ of Utrecht — Polycrystalline graphene has an inherent tendency to buckle, i.e. develop out-of-plane, three-dimensional structure, yielding a rich landscape of configurations. A force applied to stretch a piece of polycrystalline graphene influences the out-of-plane structure. In this talk, we show that if the graphene sheet is well-relaxed, as long as is not completely crystalline, this happens in non-linear fashion: occasionally, a tiny increase in stretching force induces a significant displacement, an avalanche-like event in which ridges and vertices are created and annihilated around the defects, which in turn can create vibrations in the surrounding medium [1]. We establish this effect in computer simulations: by continuously changing the strain, we follow the non-affine displacements of the atoms that turn out to exhibit a discontinuous evolution. Furthermore, the displacements exhibit a hysteretic behavior upon the change from low to high stress and back. Our results motivate further studies of dynamical elasticity of polycrystalline quasi-two-dimensional systems, and in particular the implications on their mechanical and thermal properties.


9:00AM W57.00006: Control of thermoelectric properties in MoSe$_2$ thin films by using He$^+$ irradiation  HYUK JIN KIM (Presenter), University of Seoul, VAN QUANG NGUYEN, THI HUONG NGUYEN, University of Ulsan, YANGJIN LEE, Yonsei University, SERA KIM, MAENG-JE SEONG, Chung-Ang University, KWANPYO KIM, Yonsei University, SUNGLAE CHO, University of Ulsan, YOUNG JUN CHANG, University of Seoul — Defect engineering have been widely used via chemical doping and ion irradiation techniques for modifying electrical and thermal properties. For increasing figure of merit, ZT=$\alpha^2 \sigma T/\kappa$ in thermoelectric materials, tuning of electrical and thermal characteristics plays an important role, where $\alpha$ is the Seebeck coefficient, $\sigma$ is the electrical conductivity, and $\kappa$ is the thermal conductivity. Here, we present our experimental control of both electrical conductivity and Seebeck coefficient of MoSe$_2$ thin films by irradiating high-energy He$^+$ ion beams. From different doses, we observed enhancement of electrical conductivity despite small decrease of Seebeck coefficient, which results in improvement of thermoelectric performance, i.e. power factor ($\alpha^2 \sigma$), for temperature range of 300K – 420K. To understand the irradiation-induced defects, we discuss complementary experimental analysis, such as X-ray diffraction, transmission electron microscopy and Raman spectroscopy.
9:12AM W57.00007: Shape - Composition - Defect Interplay in 2D Transition Metal Dichalcogenides* [Invited]  DAVID SROLOVITZ (Presenter), Materials Science and Engineering, City Univ of Hong Kong, JOEL M BERRY, Lawrence Livermore National Laboratory, SIMEON RISTIC, Materials Science and Engineering, University of Pennsylvania — We focus on the interplay of the 2D sheet shape via local variations in composition and/or variations in topological defect density through a combination of strain engineering and shape programming. This includes patterning composition and defect profiles via growth on non-flat substrates and patterning profiles via composition patterning. We implement these ideas theoretically and within phase field and finite element method computations. We then explore applications of these ideas to create a diverse set of composition, defect, and shape patterns and programming bilayer twist. We then exploit Janus structures to program bilayer twist and to actuate dynamic shape change.

*This work was funded by the Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by the United States Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under award no. DE-SC0012575 (DJS and JB) and through the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE-1845298 (SR).

9:48AM W57.00008: Study of the Shape Single Crystal Graphene Growth by Chemical Vapor Deposition on Copper Foil*  THARANGA NANAYAKKARA (Presenter), SAJITH WITHANAGE, U. KUSHAN WIJEWARDENA, ANNIKA KRIISA, RASANGA L SAMARaweera, RAMESH MANI, Georgia State University — The chemical vapor deposition (CVD) growth of single-crystal graphene on polycrystalline copper foils is a complex process affected by thermodynamics, kinetic, and growth parameters. Moreover, these factors lead to the diversity of island shapes of single-crystal graphene, including hexagons, flowers, squares, stars, dendrites, butterflies, hourglass, and lobes. Here, we present experimental observations of the different shapes of the micrometer-sized single-crystal graphene on copper foil obtained by the CVD technique. We applied Atomic Force Microscopy (AFM) and optical microscopy techniques to examine the diverse growth morphologies of the graphene shapes in different copper domains with various crystal orientations and the evolution of the nuclei shapes over the time.

*This work was supported by the NSF under Grant No. ECCS-1710302, and by the Army Research Office under Grants No. W911NF-14-2-0076 and No. W911NF-15-1-0433.
10:00AM W57.00009: Coupling of Quantum Valley Hall Edge States between CVD Bilayer Graphene Layer Stacking Domain Walls

QICHENG ZHANG (Presenter), University of Pennsylvania, SHENG WANG, University of California at Berkeley, ZHAOLI GAO, SEBASTIAN HURTADO PARRA, PAUL MASIH DAS, JOEL M BERRY, ZACHARIAH M ADDISON, WILLIAM PARKIN, MARIJA DRNDIC, JAMES MAKATO KIKKAWA, EUGENE JOHN MELE, University of Pennsylvania, FENG WANG, University of California at Berkeley, ZHENTANG LUO, Hong Kong University of Science and Technology, ALAN T JOHNSON, University of Pennsylvania — Quantum valley Hall (QVH) edge states are topologically protected in the absence of valley mixing. In addition to the long mean free path from the protection, their inter-wall coupling enables novel properties such as current partition and valley filtering, when arranged in specific configurations. Stacking order alternation across a boundary in Bernal stacking bilayer graphene creates a layer stacking wall (LSW) where QVH edge states are bound. However, the uncontrollable strain of LSWs upon their creation places a big challenge to study their inter-wall coupling. Here we use different strain mechanisms during chemical vapor deposition (CVD) and subsequent transfer processes to create well-separated LSWs and close packing LSW bundles, and report inter-wall coupling of QVH edge states in the latter case through electron transport measurements.

10:12AM W57.00010: Preferential hole formation in WSe$_2$ by electron beam irradiation

DONGHAN SHIN (Presenter), ANDREW O'HARA, Department of Physics and Astronomy, Vanderbilt Univ, JUNHAO LIN, Department of Physics, Southern University of Science and Technology, SOKRATES T PANTELIDES, Department of Physics and Astronomy, Vanderbilt Univ — In recent years, the trigonal-prismatic transition-metal dichalcogenides (TMDs) have been extensively studied due to a wide range of physical properties and applications. Scanning transmission electron microscopy (STEM) is a powerful tool for the investigation of material systems at the atomic level and the imaging of defect configurations. Moreover, STEM can be used to induce and modify defects. We will show that, using STEM, round multivacancy holes of various diameters and densities can be easily formed and stabilized in WSe$_2$, but not in other TMDs like WS$_2$. We report density-functional-theory (DFT) calculations to investigate the structure and stability of the observed defects in WSe$_2$. We construct a comprehensive model to explain how the observed stable defects form and grow in different TMDs by calculating formation energies, displacement thresholds, and electronic structures. The demonstrated control of high-density uniform multivacancies has potential for applications relating to molecular translocation.

*This work was supported by Department of Energy Grant DE-FG-02-09ER46554 and used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.
**10:24AM W57.00011: Structural Evolution of Many-Layer Epitaxial Graphene on 4H-SiC During Low-Energy Ion Implantation**  
*PAUL MICELI (Presenter), ALESSANDRO MAZZA, Univ of Missouri - Columbia, ANNA L MIETTINEN, Georgia Inst Tech, TIMOTHY R CHARLTON, THOMAS ZAC WARD, Oak Ridge National Laboratory, XIAOQING HE, ALEX A DAYKIN, SUCHISMITA GUHA, GUANG BIAN, Univ of Missouri - Columbia, EDWARD CONRAD, Georgia Inst Tech — The ability to modify graphene with defects and chemisorption is of interest for its potential to tailor graphene's physical properties, including induced p-orbital magnetism that could be useful for spintronics. As a pathway towards these goals, we have investigated the behavior of multilayer epitaxial graphene implanted by low-energy ions (360-2000 eV) of H, D and He. In situ x-ray scattering reveals that the ions expand the spacing between graphene layers, which depends on the type of ion, the fluence, as well as whether the range of the ion distribution resides at the buried interface or within the graphene. Neutron reflectivity measurements show that H remains chemisorbed in the graphene. We show that the apparently different behavior among the ions and their distributions can be understood by a single concept and by the appropriate scaling of the data.

*NSF grant no. DGE-1069091, DOE SCGSR, ORNL GO! Programs

**10:36AM W57.00012: Controlling Nanoscale Thermal Expansion of Monolayer Transition Metal Dichalcogenides by Alloy Engineering**  
*XUAN HU, ZAHRA HEMMAT, LEILY MAJIDI, Univ of Illinois - Chicago, JOHN CAVIN, Department of Physics, Washington University in St. Louis, ROHAN MISHRA, Washington University in St. Louis, SERDAR OGUT, AMIN SALEHI-KHOJIN, ROBERT KLIE (Presenter), Univ of Illinois - Chicago — Two dimensional materials, such as transition metal dichalcogenides (TMDs), graphene, boron nitride (BN) are seen as promising materials for future high power/high frequency electronics. However, the large difference in the thermal expansion coefficient (TEC) between many of these 2D materials could impose a serious challenge for the design of monolayer-materials-based nano-devices. To address this challenge, alloy engineering of TMDs is used to tailor their TECs. Here, in-situ heating experiments in a scanning transmission electron microscope are combined with electron energy-loss spectroscopy and first-principles modeling of monolayer Mo$_{1-x}$W$_x$S$_2$ with different alloying concentrations to determine the TEC. Significant changes in the TEC are seen as a function of chemical composition in Mo$_{1-x}$W$_x$S$_2$, with the smallest TEC being reported for a configuration with the highest entropy. This study provides key insights into understanding of nanoscale phenomena that control TEC values of 2D materials.

*X. H., Z. H., L. M. A. S. K., and R. F. K. were supported by the National Science Foundation (EFRI 2-DARE EFMA-1542864 and DMREF CBET-1729420). S.O. was supported by the National Science Foundation’s DMR-Ceramics program (DMR-1831406). JC and RM acknowledge support through NSF DMREF-1729787.
10:48AM W57.00013: Superelasticity and anomalous mechanical response of two-dimensional SiO2 under tensile and bending deformations*  RICARDO NUNES (Presenter), NESTOR REINA, HELIO CHACHAM, Physics, UFMG — Silica displays a rich phenomenology of mechanical response to deformations in its 3D form. It recrystallizes by dislocation creep and shows non-linear elastic behavior under large strains. In this study, we discuss results from first-principles calculations, that indicate that the recently synthetized 2D form of silica (2D-SiO2) displays as rich a response to mechanical deformations as its 3D counterpart. Under tensile uniaxial strain of up to 30% in both armchair (AC) and zigzag (ZZ) directions, 2D-SiO2 shows a non-linear elastic response, and the stress-strain curves do not display the plastic deformation platoo. At larger than 30% strains, the response is highly anisotropic: while in the AC direction the lattice breaks, in the ZZ direction it recovers the broken bonds and undergoes a process akin to a 15° rotation of the lattice. For even larger strains another effective rotation (by 30°) of the lattice takes place. The effective rotation is shown to occur also in the presence of vacancies in the SiO2 layer. Moreover, 2D-SiO2 shows an intrinsic non-linear response to bending deformations even for small deformations. We identify a metastable structure of a 2D-SiO2 layer that is connected with the anomalous bending response of 2D silica.

*CNPq, Fapemig, CAPES, INCT - NanoCarbono

Friday, March 6, 2020 8:00 AM - 9:48 AM

Session W58 DCMP: Exotic Features of Superconductors  Mile High Ballroom 3B

8:00AM W58.00001: Aharonov-Casher effect with vortices in an amorphous superconductor  ARNAB ROY (Presenter), AVIAD FRYDMAN, Bar Ilan Univ — A trajectory of a magnetic moment in an electric field results in the acquisition of a topological phase called the Aharonov-Casher (A-C) phase, analogous to the A-B phase acquired by a charged particle in a magnetic field. In condensed matter, experiments demonstrating the A-C effect are relatively few, the earliest being for superconducting vortices traversing a fabricated Josephson-junction array. In that regular geometry, a periodic response to induced charge was observed. In an irregular geometry, in analogy with universal conductance fluctuations, a complex quasi-periodic respinse may be expected.

An amorphous superconductor close to a superconductor-insulator transition (SIT) provides such a complex multiply connected region for superconducting vortices to interfere, as indicated by recent studies. In this study with amorphous indium oxide close to a disorder driven SIT, we introduce vortices in the system by applying a perpendicular magnetic field. The motion of these vortices around superconducting islands generates a complex interference pattern in the form of a spontaneous voltage that is tunable with both gate voltage and magnetic field. This effect is a demonstration of the quantum behavior of Josephson vortices which are present in the system close to the SIT.
8:12AM W58.00002: IDEAL DIAMAGNETIC RESPONSE OF A PRISTINE GRAPHENE-n-HEPTANE-PERMALLOY SYSTEM* SERAFIM TEKNOWIJOYO, Chapman Univ, YASUSHI KAWASHIMA, Tokai University, RAJENDRA DULAL, SARA CHAHID, ARMEN GULIAN (Presenter), Chapman Univ — We explored magnetic screening of milligauss fields in a system comprised of a single-layer graphene (on various substrates) wetted by n-heptane in the presence of a thin Fe-Ni foil parallel to the graphene layer. Our initial task was to confirm the results and find the origins of ideal diamagnetic screening reported previously in [Y. Kawashima, arXiv:cond-mat/1801.09376]. Indeed, we obtained ideal diamagnetic response. Also, in some cases “paramagnetic Meissner effect” has been obtained which in case of superconducting origin of observed facts can be associated with Wohlleben effect. At the same time, a crucial dependence of humidity and possibly other atmospheric factors on results has been observed which can be explained by chemisorption described in e.g. [T.L. Burnett et.al., arXiv:1204.3323]. These factors completely inhibit both normal and negative diamagnetism. To minimize this effect experiments were performed in Ar atmosphere. This may or may not be a footprint of superconductivity at room temperature. In both cases understanding the signal under different conditions may spread a light on a yet unknown phenomenon in condensed matter physics.

*This work was supported in part by the ONR Grants N00014-16-2269, N00014-17-1-2972, N00014-18-1-2636 and N00014-1901-2265.

8:24AM W58.00003: Odd Frequency Pairing in Superconducting Systems Using Renormalization Group Approach HENOC EJIGU (Presenter), University of California, Riverside — We investigate odd frequency pairing of electron-electron interaction on superconducting systems using the renormalization group method. Several experimental results induced by proximity effect have shown the feasibility of odd frequency pairing. Efforts have been made in the theoretical arena, since its first conception by Berezinskii, to understand this phenomenon, but many questions still remain unanswered. In our work, by considering a two-dimensional rotationally invariant Fermi surface and spinless system within the framework of renormalization group, we present a brief elucidation on the microscopic mechanism for odd frequency pairing, and show a self-contained derivation of the exact flow equation for the vertex functions and self energy that depend on the gradual evolution of the microscopic model action to the final effective action as a function of a continuously decreasing energy scale.
Local structure of the cuprate superconductors

ZACHARY ANDERSON (Presenter), DAMJAN PELC, University of Minnesota, MATTHEW KROGSTAD, Argonne National Lab, NIKOLAOS BINISKOS, BIQIONG YU, LIAM THOMPSON, JACK ZWETTLER, RICHARD SPIEKER, NINA G BIELINSKI, University of Minnesota, STEPHAN ROSENKRANZ, RAYMOND OSBORN, Argonne National Lab, MARTIN GREVEN, University of Minnesota — The cuprate superconductors have long been known to be electronically inhomogeneous at the nanoscale, although the nature and role of the inhomogeneity remain debated. Recent studies of superconducting fluctuations in cuprates have uncovered a universal inhomogeneity-driven regime in multiple compounds [1], and similar findings for other perovskite-derived superconductors point to universal underlying structural inhomogeneity [2]. Here we present complementary X-ray and neutron diffuse scattering studies of several cuprates, with the real-space local structure determined by the 3D ΔPDF method [3]. The experiments reveal intricate short-range correlated structural distortions, even in HgBa$_2$CuO$_{4+δ}$, which features a simple tetragonal average structure. We discuss the doping dependence of the local structure and correlations with the superconducting $T_C$.


*This work was funded by the DOE through the University of Minnesota Center for Quantum Materials under DE-SC-0016371.

Plasticity and stress engineering of cuprate superconductors

DAMJAN PELC (Presenter), ZACHARY ANDERSON, LIAM THOMPSON, School of Physics and Astronomy, University of Minnesota, MATTHEW KROGSTAD, Argonne National Laboratory, NIKOLAOS BINISKOS, BIQIONG YU, JACK ZWETTLER, RICHARD SPIEKER, NINA G BIELINSKI, School of Physics and Astronomy, University of Minnesota, STEPHAN ROSENKRANZ, RAYMOND OSBORN, Argonne National Laboratory, MARTIN GREVEN, School of Physics and Astronomy, University of Minnesota — Ceramic materials, including the cuprate high-temperature superconductors, are generally thought to be brittle at low temperatures due to their rigid ionic and covalent bonding. We present here the surprising discovery of room-temperature plasticity in the cuprates, observed with compressive stress perpendicular to the copper-oxygen planes. We further show that the electronic properties, in particular superconductivity, can be manipulated via plastic deformation. We discuss the origin of these effects and correlate them with structural changes as investigated by neutron and X-ray diffuse scattering measurements.

*This work was funded by the DOE through the University of Minnesota Center for Quantum Materials under DE-SC-0016371.
9:00AM W58.00006: Thermodynamic Evidence for a Multi-component superconducting order parameter in Sr$_2$RuO$_4$*

SAYAK GHOSH (Presenter), Cornell University, ARKADY SHEKHTER, National High Magnetic Field Laboratory, FABIAN JERZEMBECK, NAOKI KIKUGAWA, DMITRY SOKOLOV, ANDREW MACKENZIE, CLIFFORD W. HICKS, Max Planck Institute for Chemical Physics of Solids, BRAD J RAMSHAW, Cornell University — The unconventional superconductivity of Sr$_2$RuO$_4$ has remained a mystery for over 25 years, even though its normal metallic state is quite well-understood. Reaching a consensus on the bulk order parameter symmetry has been difficult primarily due to the contradictions that exist between several major experimental findings. We performed resonant ultrasound spectroscopy (RUS) measurements on Sr$_2$RuO$_4$, to measure its entire symmetry-resolved elastic tensor through T$_C$ ($\sim$1.43 K). Since different superconducting order parameters couple differently to shear and compressional sound modes, measurement of all elastic moduli places strong constraints on the order parameter symmetry, independent of microscopics. We observe a thermodynamic discontinuity in one of the shear moduli ($c_{66}$) at T$_C$, which requires a two-component superconducting order parameter ($E$ representation of $D_{4h}$). We discuss leading $E$-symmetry order parameters, and suggest that it may be necessary to go beyond the conventional "singlet/triplet" paradigm to finally resolve the mystery that is Sr$_2$RuO$_4$. We also measure an anomalous attenuation peak in compressional sound below T$_C$, possibly arising due to sound absorption into order parameter collective modes.

*Supported by the National Science Foundation under Grant No. DMR-1752784.

9:12AM W58.00007: Manipulating superconductivity in Sr$_2$RuO$_4$ thin films through epitaxial strain

HARI NAIR (Presenter), NATHANIEL SCHREIBER, JACOB RUF, LUDI MIAO, YAWEN FANG, YONGHUN LEE, Cornell University, MARIO BRÜTZAM, CHRISTO GUGUSCHEV, Leibniz-Institut für Kristallzüchtung, BRAD J RAMSHAW, KYLE M SHEN, DARRELL SCHLOM, Cornell University — Pushing the van Hove singularity in the $\gamma$ band of Sr$_2$RuO$_4$ towards the Fermi level can potentially raise the transition temperature, $T_c$, of this unconventional superconductor. To test this concept, we explore the effect of biaxial strains from –0.9% to +1.0% imposed by commensurate epitaxy on (NdAlO$_3$)$_{0.39}$–(SrAl$_{1/2}$Ta$_{1/2}$O$_3$)$_{0.61}$ (NSAT), NdGaO$_3$, (LaAlO$_3$)$_{0.29}$–(SrAl$_{1/2}$Ta$_{1/2}$O$_3$)$_{0.71}$ (LSAT), LaGaO$_3$, and SrTiO$_3$ substrates on the superconducting $T_c$ and upper critical field $H_{c2}$ of Sr$_2$RuO$_4$ thin films. These biaxial strain studies are distinct from and compliment the existing uniaxial strain studies on Sr$_2$RuO$_4$ single crystals. Mean free paths up to 144 nm are observed in Shubnikov-de Haas oscillation measurements on these thin films and $T_c$s range from 1 K to 1.8 K for films with similar residual resistivities. The measured mean free paths in combination with the coherence lengths, determined from upper critical field measurements, established that all films are superconducting in the clean limit.
9:24AM W58.00008: Spectroscopic study of doped strontium ruthenates compositions

RAJENDRA DULAL (Presenter), VAHAN NIKOGHOSSYAN, Chapman Univ, BORIS GORSHUNOV, ELENA ZHUKOVA, Moscow Physical-Technical University, YURI ALESCHENKO, ANDREY MURATOV, Moscow P.N. Lebedev Physical Institute, SERAFIM TEKNOWJJOYO, SARA CHAHID, ARMEN GULIAN, Chapman Univ — Extraordinary properties of Sr$_2$RuO$_4$ have attracted much attention since the discovery of superconductivity in this material in [Y. Maeno et.al., Nature 372, 532 (1994)]. This material are isostructural to the high T$_c$ cuprate superconductors which motivated extensive search of physically and chemically modified ruthenates [Gulian, et.al., Quantum Stud. Math. Found., 5, 161 (2018)]. One of the compositions Sr$_2$Ru$_{1-x}$Re$_x$O$_3$Se, revealed feature, which most naturally fitted into the pattern of presence of a small fraction of superconducting phase in a multiphase sample with the dominant ferromagnetic phase, almost masking out this superconductivity at ~30 K. We present compositional, morphological, structural, magnetotransport, heat capacity, magnetic susceptibility, Raman and terahertz spectroscopy data to facilitate theoretical analysis of metamagnetism vs. superconductivity in this material.

*This work was supported in part by the ONR Grants N00014-16-2269, N00014-17-1-2972, N00014-18-1-2636, and N00014-1901-2265.

9:36AM W58.00009: μSR study on the antiperovskite oxide supercondctor Sr$_{3-x}$SnO

ATSUTOSHI IKEDA (Presenter), Department of Physics, Kyoto University, ZURAB GUGUCHIA, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, SHUN KOIBUCHI, Department of Physics, Kyoto University, MOHAMED OUDAH, Stewart Blusson Quantum Matter Institute, University of British Columbia, SHINGO YONEZAWA, Department of Physics, Kyoto University, HUBERTUS LUETKENS, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, YOSHITERU MAENO, Department of Physics, Kyoto University — Antiperovskite (inverse perovskite) oxides are the materials crystallizing in the same structure as the ordinary perovskite oxides but with the inverted positions of the metal element and oxygen. Some of these materials are theoretically suggested to be topological crystalline insulators based on the first-principles calculations [1, 2]. We discovered the first superconductivity among this group of oxides in Sr$_{3-x}$SnO [3]. Reflecting the topology of the electronic band structure in the normal state, a topological superconductivity is theoretically proposed in this compound [3, 4]. In order to investigate the nature of the superconducting state, we performed the muon spin rotation (μSR) experiment. Under small magnetic fields, we successfully observed increase of the relaxation rate of μ$^+$ below the transition temperature and confirmed the bulk superconductivity. The ratio between the relaxation rate and transition temperature $\sigma/T_c$ is much smaller than those of the conventional superconductors and close to the values known for unconventional ones.


Friday, March 6, 2020 8:00 AM - 10:48 AM
**8:00AM W59.00001: Topological Surface States of Cadmium Arsenide Thin Films**  
LUCA GALLETTI (Presenter), DAVID KEALHOFER, TIMO SCHUMANN, MANIK GOYAL, SALVA SALMANI REZAIE, SUSANNE STEMMER, University of California, Santa Barbara — Thin films of the topological semimetal cadmium arsenide (Cd$_3$As$_2$) can host different types of topological surface states, depending on their crystallographic orientation$^1$. Here we elucidate the nature of these surface states by comparing films grown in (112) and (001) orientations, respectively. For (112) thin films Weyl orbits$^2$, involving Fermi arcs on opposite surfaces, have been predicted, which should exhibit a thickness-dependent phase in quantum oscillations. We compare quantum transport in films of varying thickness at apparently identical gate-tuned carrier concentrations and find no clear dependence of the relative phase of the quantum oscillations on the sample thickness$^3$. Small variations in carrier densities, difficult to detect in low-field Hall measurements, lead to shifts in quantum oscillations that are commensurate with previously reported phase shifts. By contrast, measurements of the quantum Hall effect in (001)-oriented thin films show evidence of topological insulator-like states at bottom and top interfaces. Quantum oscillation measurements in different geometries are used to determine interactions between the surfaces.


**8:12AM W59.00002: Large Thermal Hall effect observed in Bi$_{89}$Sb$_{11}$ topological insulator and Weyl Semimetal**  
DUNG VU (Presenter), Department of Mechanical Engineering, Ohio State Univ - Columbus, NANDINI TRIVEDI, Department of Physics, Ohio State Univ - Columbus, JOSEPH P C HEREMANS, Department of Mechanical Engineering, Ohio State Univ - Columbus — Bi$_{89}$Sb$_{11}$ alloy, a topological insulator, becomes a Weyl semimetal in a magnetic field above a critical value $H_C$ applied along the trigonal direction (001). We measured a Bi$_{89}$Sb$_{11}$ single crystal sample along the trigonal axis in a longitudinal magnetic field $H>H_C$. We observed large field-induced increases in the longitudinal electronic thermal conductivity along (001), which is mostly linear in field and maximal for $35K<T<200K$, attributed to the thermal chiral anomaly [1]. We report a large thermal Hall effect in the sample for the same temperature range: magnetic field applied along (001), heat flux along (010); transverse temperature gradient measured along (100), longitudinal gradient along (010). peaks at 0.07 in the temperature range $160K<T<200K$. We will present the field dependence of the sample's transport properties including thermopower, Nernst thermopower, Hall and electrical resistivity, and thermal conductivity, and discuss possible connections of this large thermal Hall effect to conveyor-belt entropy transport mediated by topologically protected Fermi arc surface states in Weyl semimetals [2].


*Funding: Center for Emergent Materials, NSF-DMR-1420451.
8:24AM W59.00003: Spin Zero Effect in Dirac Semimetal ZrTe$_5$*  JINGYUE WANG (Presenter), JINGJING NIU, BAOMING YAN, XINQI LI, RAN BI, Peking Univ, YUAN YAO, Institute of Physics CAS, DAPENG YU, South University of Science and Technology of China, XIAOSONG WU, Peking Univ — One of the characteristics of topological materials is their non-trivial Berry phase. Experimental determination of this phase largely relies on a phase analysis of quantum oscillations. We study the angular dependence of the oscillations in a Dirac material ZrTe$_5$ and observe a striking spin zero effect, i.e., vanishing oscillations accompanied with a phase inversion. This indicates that the Berry phase in ZrTe$_5$ remains non-trivial for arbitrary field direction, in contrast with previous reports. The Zeeman splitting is found to be proportional to the magnetic field based on the condition for the spin zero effect in a Dirac band. Moreover, it is suggested that the Dirac band in ZrTe$_5$ is likely transformed into a line-node other than Weyl points for the field directions at which the spin zero occurs. The results underline a largely overlooked spin factor when determining the Berry phase from quantum oscillations.

*This work was supported by National Key Basic Research Program of China (No.2016YFA0300600, No.2013CBA01603 and No. 2016YFA0300903) and NSFC (Project No. 11074007, No. 11774009, No. 11222436, and No. 11234001).

8:36AM W59.00004: Electric modulation of the Fermi arc spin polarization of a Dirac semimetal nanowire*  BENCHUAN LIN (Presenter), SHUO WANG, Southern University of Science and Technology, ANQI WANG, Peking Univ, KE XIA, DAPENG YU, Southern University of Science and Technology, ZHI-MIN LIAO, Peking Univ — The spin polarization of the exotic topological surface states of Dirac/Weyl semimetals, namely Fermi arcs, were predicted to exist but never accessed in a simple transport structure. Here we report the direct access of the Fermi arc spin polarization through the electromagnetic transport experiment. The net spin polarization was manifested as a voltage of the ferromagnetic contact, which was induced by applying a charge current via spin momentum locking property of the Fermi arc in the Cd$_3$As$_2$ nanowire. Moreover, a gate voltage controlled topological phase transition of the surface states is demonstrated to be able to switch on/off the spin signals. Thus a topological field-effect transistor is proposed.

*This work was supported by National Key Research and Development Program of China (No. 2016YFA0300802), and NSFC (No. 11774004 and No. 61825401).
Large in-plane Hall/Nernst effect generated by Berry curvature in Weyl semimetallic phase of indium doped $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$  

CHENGLONG ZHANG, TIAN LIANG (Presenter), YOSHINORI TOKURA, RIKEN — The Hall/Nernst effects have led to interesting phenomena in modern physics such as Berry curvature. The conventional Hall/Nernst signals appear only when the magnetic field is applied perpendicular to the sample because the conventional Lorentz force vanishes when the magnetic field is applied in the plane.

Interestingly, in the Weyl semimetallic phase of indium doped $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$, large in-plane Hall/Nernst signals are observed. This suggests the existence of large Berry curvature coming from the Weyl nodes. When no magnetic field is applied, the time reversal symmetry requires the Weyl nodes to distribute such that Hall/Nernst signals vanish completely. As the magnetic field is turned on, the Weyl nodes move in the momentum space and generate the finite value of Hall/Nernst signals, even when the magnetic field is applied in the plane. The implication of the experimental data will be discussed.

Magnetic electron lensing in the 3D Dirac semi-metal $\text{Cd}_3\text{As}_2^*$

XIANGWEI HUANG, CARSTEN PUTZKE, CHUNYU GUO, JONAS DIAZ, Ecole Polytechnique Federale de Lausanne, MARKUS KOENIG, HORST BORRMANN, Max-Planck-Institute for Chemical Physics of Solids, NITYAN NAIR, JAMES ANALYTIS, University of California, Berkeley, PHILIP MOLL (Presenter), Ecole Polytechnique Federale de Lausanne — While electrons moving perpendicular to a magnetic field are confined to cyclotron orbits, they can move freely parallel to the field. This simple fact leads to complex current flow in clean, low carrier density semi-metals, such as current jets along the magnetic field when currents pass through point-like constrictions. Occurring accidentally at imperfect current injection contacts, “current jetting” plagues the research of longitudinal magnetoresistance. We demonstrate the controlled generation of tightly focused electron beams in a new class of microdevices machined from crystals of the Dirac semi-metal $\text{Cd}_3\text{As}_2$. The current beams can be guided by tilting an in-plane magnetic field and their range tuned by the field strength. Finite element simulations quantitatively capture the voltage induced at faraway contacts when the beams are steered towards them, supporting the picture of controlled electron jets. These experiments demonstrate the first direct control over the highly non-local signal propagation unique to 3D semi-metals in the current jetting regime.

*This project was funded by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (“MiTopMat” - grant agreement No. 715730).
Higher harmonics of quantum oscillations uncover Dirac Fermions in LaRhIn$_5$

ARIS ALEXANDRADINATA (Presenter), University of Illinois at Urbana-Champaign, CHUNYU GUO, CARSTEN PUTZKE, Institute of Material Science and Engineering, Ecole Polytechnique Federale de Lausanne, FENGREN FAN, Max Planck Institute for Chemical Physics of Solids, SHENGNAN ZHANG, QUANSHENG WU, OLEG V. YAZYEV, Institute of Material Science and Engineering, Ecole Polytechnique Federale de Lausanne, KENT SHIRER, MAJA BACHMANN, Max Planck Institute for Chemical Physics of Solids, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory, CLAUDIA FELSER, YAN SUN, Max Planck Institute for Chemical Physics of Solids, PHILIP MOLL, Institute of Material Science and Engineering, Ecole Polytechnique Federale de Lausanne — Quantum oscillations are commonly used to experimentally diagnose the band topology of a semimetal. When the cyclotron orbit encloses a topological defect, it is often presumed that the nontrivial Berry phase results in a $\pi$-phase shift of the fundamental harmonic. However, this presumption neglects how spin-orbit coupling renders the Berry phase a continuously varying quantity, and ignores the Zeeman interaction with the spin-orbit-induced magnetic moment. Here, we overcome these shortcomings and demonstrate how to rigorously identify three-dimensional Dirac fermions from the higher harmonics of quantum oscillations. Applying this method to the intermetallic LaRhIn$_5$, we unambiguously identify the nontrivial Berry phase of a topological Fermi pocket with a small frequency $\approx 7T$, despite the presence of large, trivial Fermi pockets which dominate transport by orders of magnitude. Our analysis identifies LaRhIn$_5$ as a 3D Dirac-point metal, revising a previous proposal of LaRhIn$_5$ as a nodal-line semimetal by Mikitik et. al. [Phys. Rev. Lett. 93, 106403 (2004)]. The electronic similarity of LaRhIn$_5$ to the prototypical heavy-fermion superconductors Ce(Co,Rh,Ir)In$_5$ further suggests them as prime candidates for strongly-correlated Dirac systems.

α-Sn Magnetotransport Devices

OWEN VAIL (Presenter), US Army Rsch Lab - Adelphi, YU HAO CHANG, SEAN HARRINGTON, Materials Department, University of California, Santa Barbara, PATRICK AUBREY FOLKES, PATRICK TAYLOR, BARBARA NICHOLS, GEORGE J DE COSTER, US Army Rsch Lab - Adelphi, CHRIS J PALMSTROM, Materials Department, University of California, Santa Barbara — α-Sn, the diamond-cubic phase of tin, is of significant scientific interest due to its topological band structure and single-element nature. Consistent high-quality growth on insulating CdTe opens the doors to unconventional electronics using a widely available material. After verifying epitaxial growth of our films, we perform transport measurements to characterize the electronic carriers in the material. We identify two-channel transport and attribute the n-type transport to a semimetallic channel that tentatively suggests Dirac behavior, while the p-type component corresponds to growth impurities resulting from the CdTe substrate. We apply a field effect gate voltage in order to map out the charge neutrality point and modulate the channel between majority n-type and majority p-type carriers. Careful preparation of the CdTe surface before growth is considered crucial to attain a low dopant density and accessible topological states on an insulating substrate. This work readily lends itself to the development of topologically enabled devices for fieldable applications such as low power electronics in order to achieve a high level of computation at the edge.

*Office of the Under Secretary of Defense for Research and Engineering: Laboratory University Collaboration Initiative
Cadmium arsenide ($\text{Cd}_3\text{As}_2$) is a three-dimensional Dirac semimetal that also hosts exotic surface states connecting the projections of the Dirac nodes. Probing the electronic properties of thin films of $\text{Cd}_3\text{As}_2$ requires tuning of the Fermi level close to the Dirac nodes. Conventional gate dielectrics, such as $\text{Al}_2\text{O}_3$, must be deposited at low temperatures that do not exceed the stability limit of $\text{Cd}_3\text{As}_2$, which introduces a high density of (near) interface trap states that limit the modulation of carrier densities that can be achieved [1]. To address this problem, here we report on the use of hexagonal boron nitride (hBN) towards high-quality $\text{Cd}_3\text{As}_2$ devices. In addition to protecting the $\text{Cd}_3\text{As}_2$ channel from photoresist, the high breakdown voltage of hBN also allows us to tune the carrier density up to a larger range allowing us to explore new quantum states.

MoTe$_2^*$ [Invited] JOHN SCHNEELOCH (Presenter), YU TAO, Univ of Virginia, CHUNRUO DUAN, Physics, Rice University, JUNJIE YANG, Physics, New Jersey Institute of Technology, SACHITH DISSANAYAKE, Physics, Duke University, FENG YE, ADAM ACZEL, JAIME A. FERNANDEZ-BACA, Neutron Scattering Division, Oak Ridge National Laboratory, GUANGYONG XU, Neutron-Condensed Matter Science Group, National Institute of Standards and Technology, MASAKI MATSUDA, Neutron Scattering Division, Oak Ridge National Laboratory, DESPINA LOUCA, Univ of Virginia — Neutron scattering has a proud history of elucidating certain kinds of structural phase transitions, but sliding layer transitions such as those in MoTe$_2$ have been relatively neglected. On cooling, the monoclinic 1T'-MoTe$_2$ transitions into the orthorhombic T$_d$-MoTe$_2$, which has received much attention since it was reported to be a Weyl semimetal and to exhibit extreme magnetoresistance. MoTe$_2$ structures can, to a good approximation, be built from sequences of two symmetry-equivalent stacking operations, with transitions occurring via layer sliding between different stackings. Thus, a wide variety of nearly-degenerate structures are conceivable, and our elastic neutron scattering studies show that changes in stacking with temperature in MoTe$_2$ are, indeed, complex. Both order-to-order and order-to-disorder transitions exist along the T$_d$-1T' thermal hysteresis loop. A pseudo-orthorhombic T$_d^*$ phase with a four-layer unit cell appears only on warming. T$_d^*$ is centrosymmetric, and the order-to-order transitions between T$_d$ and T$_d^*$ may make a more convenient topological switch than the disordered transitions to and from 1T'. The kink in resistivity vs. temperature on warming is primarily due to the onset of T$_d^*$, and the residual hysteresis in the resistivity toward the temperature extremes is likely related to changes in the presence of 1T'- or T$_d$-phase twin domain boundaries. Changes in stacking have a subtle effect on low-energy shear phonon modes, as seen from inelastic neutron scattering. A multitude of ways of influencing these transitions are known; we will discuss how both W-substitution and pressure drive the transition toward a simpler phase coexistence behavior, though with opposite effects on transition temperature or the 1T' $\beta$ angle. We will discuss changes in band structure with pressure and strain. Finally, we will discuss open questions concerning the cause of the transition.

*This work is supported by the Department of Energy, grant number DE-FG02-01ER45927.
10:36AM W59.00012: Quantitative analysis of chiral anomaly induced negative magnetoresistance in nodal-line semimetal SrAs$_3$
MINHAO ZHAO (Presenter), FAXIAN XIU, Fudan Univ — Recently, three-dimensional topological nodal-line semimetals has been reported frequently as a new class of quantum materials. In nodal-line semimetals, the conduction and the valence bands contact with each other. The band crossing points around the Fermi level form a closed loop. Chiral anomaly is one of the property of nodal-line semimetal. The phenomenon of chiral anomaly in transport measurement is negative magnetoresistance (NMR) when current is parallel with magnetic field. The electronic conductivity induced by chiral anomaly is:
$$\sigma_{zz}=\frac{e^2}{4\pi^2 \hbar c} \nu c \left((eB)^2 \nu^2/\mu^2 \tau\right)$$
[1]. The $\nu$ is fermi velocity; $\mu$ is chemistry potential and $\tau$ is scattering time. The $\tau$ depends on the magnetic field and temperature. When the magnetic is higher than the quantum limit, the $\tau$, the NMR will saturate.

Among the predicted nodal-line semimetals[2], SrAs$_3$ has high mobility and low fermi energy, which makes this material an ideal platform to research the behavior of NMR with magnetic field and temperature. Under 31.5 T, we observed the process from NMR appeared to saturated. And analyzed the behavior of NMR quantitatively. Combined with the result from PPMS, we also got the temperature dependence of $\tau$.

W59.00013: Observation of a Thermoelectric Hall Plateau in the Extreme Quantum Limit*
WENJIE ZHANG (Presenter), Peking Univ, PEIPEI WANG, Southern University of Science and Technology of China, BRIAN SKINNER, Ohio State University, RAN BI, Peking Univ, VLADYSLAV KOZII, Massachusetts Institute of Technology, CHANG-WOO CHO, Southern University of Science and Technology of China, RUIDAN ZHONG, JOHN SCHNEELOCH, Brookhaven National Laboratory, DAPENG YU, Southern University of Science and Technology of China, GENDA GU, Brookhaven National Laboratory, LIANG FU, Massachusetts Institute of Technology, XIAOSONG WU, Peking Univ, LIYUAN ZHANG, Southern University of Science and Technology of China — The thermoelectric Hall effect is the generation of a transverse heat current upon applying an electric field in the presence of a magnetic field. Here we demonstrate that the thermoelectric Hall conductivity $\alpha_{xy}$ in the three-dimensional Dirac semimetal ZrTe$_5$ acquires a robust plateau in the extreme quantum limit of magnetic field. The plateau value is independent of the field strength, disorder strength, carrier concentration, or carrier sign. We explain this plateau theoretically and show that it is a unique signature of three-dimensional Dirac or Weyl electrons in the extreme quantum limit. We further find that other thermoelectric coefficients, such as the thermopower and Nernst coefficient, are greatly enhanced over their zero-field values even at relatively low fields.

*National Key Basic Research Program of China (No. 2016YFA0300600) and NSFC (No. 11574005, No. 11774009). Guangdong Innovative and Entrepreneurial Research Team Program (No. 2016ZT06D348), NFSC (11874193) and Shenzhen Fundamental subject research Program (JCYJ20170817110751776) and Innovation Commission of Shenzhen Municipality (Grant No. KQTD2016022619565991). DOE Office of Basic Energy Sciences Award DE-SC0018945. NSF STC No. DMR-1231319. U.S. Department of Energy under Contract No. DE-SC0012704.

Friday, March 6, 2020 8:00 AM - 10:36 AM
8:00AM W60.00001: Planar Hall effect in thin films of the 3D Dirac semimetal Cd$_3$As$_2$

MANIK GOYAL (Presenter), TIMO SCHUMANN, DAVID KEALHOFER, SUSANNE STEMMER, University of California, Santa Barbara — Cd$_3$As$_2$ is a 3D Dirac semimetal with doubly degenerate band crossings at isolated points in the bulk Brillouin zone. It can also host gapless surface states. In Dirac and Weyl semimetals, a giant planar Hall effect (PHE) has been predicted to be associated with the chiral anomaly. In this talk, we will discuss our measurements of the PHE in (001) and (112) oriented epitaxial thin films of Cd$_3$As$_2$ having a wide range of film thicknesses. We show that the PHE depends sensitively on the Fermi level. Studies of films of different thickness allow us to distinguish the contributions of bulk and surface states. We will discuss the different mechanisms that give rise to the PHE in these films.

8:12AM W60.00002: NMR Investigation of Field-Induced Energy Gap in Topological Node-Line Semimetal ZrGeSe

GUOQING WU (Presenter), SHENGTANG WAN, RONGXING CAO, JIAN HU, XIANGHUA ZENG, YAFANG XU, JINBO ZHANG, Yangzhou Univ, LIN WANG, Beijing High Pressure Science Center, QIULIANG WANG, Chinese Academy of Science, LEI GUO, Southeast University, RENKUI ZHENG, Chinese Academy of Science, BING WU, fayetteville state university — The discovery of topological semimetals provides opportunities to explore the exotic properties of relativistic fermions in condensed matter. Among those materials, the nodal-line semimetal represents a new type of topological quantum state which displays Dirac cones along a one-dimensional line or a closed circle protected by combined symmetry of inversion and time-reversal, in contrast with the Dirac or Weyl semimetals with discrete Dirac or Weyl cones. Here we report NMR investigation of field-induced energy gap in topological nodal-line semimetals of ZrGeSe single crystals, with high magnetic field up to 16 T and high hydrostatic pressure up to 50 GPa. We found that the opening of the energy gap is driven by the magnetic field-induced anti-ferromagnetic (AFM) order, and the gap opening is highly restricted under high pressure.

*NSF of China #61474096, # 51477167, and # 41527802. NSF of Jiangsu # BK20180889, and BK20180890

8:24AM W60.00003: Violation of Ohm`s law in a Weyl metal

DONGWOO SHIN (Presenter), JEEHOON KIM, Pohang Univ of Sci & Tech — Weyl metal is one of the topological non-trivial materials holding Weyl fermions which are massless and have a chirality. The Weyl metal has been described in terms of axion electromagnetism rather than in Maxwell electromagnetism, and has peculiar properties such as chiral anomaly, the presence of magnetic monopole in the reciprocal lattice space and negative longitudinal magneto resistance. In this presentation, by transportation experiment besides negative longitudinal magneto resistance, we observed ohm’s law was broken in the Weyl metal and carried experimental and theoretical analysis of the violation of ohm`s law [1].

REFERENCES:
8:36AM W60.00004: Interplay of Dirac Nodes and Volkov-Pankratov Surface States in Compressively Strained HgTe  
DAVID MAHLER (Presenter), JULIAN-BENEDIKT MAYER, PHILIPP LEUBNER, LUKAS LUNCZER, DOMENICO DI SANTE, GIORGIO SANGIOVANNI, RONNY THOMALE, EWELINA M HANKIEWICZ, HARTMUT BUHMANN, CHARLES GOULD, LAURENS W MOLENKAMP, University of Wurzburg — With the advent of topological materials, the Weyl fermion, a massless particle once proposed to describe neutrinos, can now be investigated in condensed matter systems as Weyl semi-metals, and their close cousins Dirac semi-metals. The HgTe material system, as a prototypical topological insulator for transport studies, is ideally suited, as the tunability of the details of its band structure through strain engineering, and its Fermi level by gating provide unparalleled control for the investigation of Weyl/Dirac semi-metals [1].
We can clearly disentangle surface and bulk contributions by using gate voltage to tune the Fermi energy precisely to the Weyl/Dirac nodes and thus convincingly identify the chiral anomaly. We find no evidence for Fermi-arcs, but topological surface states, that are responsible for the transport in the electron regime. These states are created by the same band inversion leading to the formation of the Dirac/Weyl nodes, and therefore must always be present. Additionally, in the hole regime surface states induced by the electric field, so called massive Volkov-Pankratov states [2, 3], are observed.


8:48AM W60.00005: Exploring broken time-reversal symmetry in Cd$_3$As$_2$/(Ga,Mn)Sb Dirac semimetal/ferromagnetic semiconductor heterostructures*  
ARPITA MITRA (Presenter), RUN XIAO, NITIN SAMARTH, Pennsylvania State University — Cd$_3$As$_2$ has attracted attention as a canonical Dirac semimetal. In this study, we aim to break time reversal symmetry (TRS) in Cd$_3$As$_2$ by interfacing with a ferromagnetic semiconductor, (Ga,Mn)Sb. We have grown epitaxial Cd$_3$As$_2$/(Ga,Mn)Sb bilayers using molecular beam epitaxy on GaSb (111) buffer layers deposited on GaAs (111)B substrates. High-resolution x-ray diffraction shows good crystalline quality of GaSb and Cd$_3$As$_2$ layers with full width half maximum of rocking curves, 0.04° and 0.11°, respectively. Atomic force microscopy shows smooth surfaces of (Ga,Mn)Sb and Cd$_3$As$_2$ with root mean square roughness ~ 1.3 nm. SQUID magnetometry reveals that (Ga,Mn)Sb films are ferromagnetic, while low temperature magnetoresistance data show that they are highly resistive for the Mn composition used. We report the temperature dependent magneto-transport properties in these Cd$_3$As$_2$/(Ga,Mn)Sb heterostructures and investigate the magnetic proximity effect by varying the thickness of the Cd$_3$As$_2$ layer. We are also exploring interfacing Cd$_3$As$_2$ with other ferromagnetic semiconductors in order to find an efficient material for breaking TRS in Cd$_3$As$_2$.

*Supported by the Institute for Quantum Matter under DOE EFRC grant DE-SC0019331
9:00AM W60.00006: Negative longitudinal magnetoresistance, anisotropic magnetoresistance, and planar Hall effect in epitaxial thin films of elemental Bismuth*

EUGENE ARK (Presenter), DESHUN HONG, TERENCE BRETZ-SULLIVAN, CHANGJIANG LIU, SHULEI ZHANG, Materials Science Division, Argonne National Laboratory, LEENA AGGARWAL, VIDYA MADHAVAN, Physics, University of Illinois at Urbana-Champaign, ANAND BHATTACHARYA, Materials Science Division, Argonne National Laboratory — Observations of negative longitudinal magnetoresistance (NLMR), anisotropic magnetoresistance (AMR), and the planar Hall effect (PHE) under an in-plane magnetic field are often used as indications of non-trivial topology in non-magnetic material systems. We show NLMR, AMR, and PHE in crystalline epitaxial thin films (< 50 nm) of elemental Bismuth (111) grown by molecular beam epitaxy on intrinsic GaAs (111) substrates. Films were characterized in-situ using scanning tunneling microscopy to confirm topography and density of states. Furthermore, the thickness and temperature dependence of these phenomena are investigated, demonstrating a high degree of tunability. We posit that these observations may be due to the Rashba effect in the surface states of Bi (111), rather than any non-trivial topological effects.

*All work at Argonne was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. The use of facilities at the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. Department of Energy, Basic Energy Sciences under contract No. DEAC02-06CH11357. Work at the University of Illinois was supported by MRSEC Seed Grant number NSF DMR 17-20633 COOP ANTC.

9:12AM W60.00007: Quantum Hall effect due to surface states in (001)-plane cadmium arsenide thin films

DAVID KEALHOFER (Presenter), Physics, UC Santa Barbara, LUCA GALLETTI, TIMO SCHUMANN, Materials, UC Santa Barbara, ALEXEY SUSLOV, National High Magnetic Field Laboratory, SUSANNE STEMMER, Materials, UC Santa Barbara — We report transport studies of gated Hall bar structures fabricated from (001)-oriented epitaxial thin films of cadmium arsenide, a three-dimensional Dirac semimetal, in magnetic fields up to 45 T. This orientation does not host Fermi arc-type surface states because the Dirac nodes project onto the same point in the surface Brillouin zone. Recent developments in the growth of these layers have resulted in films with quantum mobilities exceeding 4,000 cm²/Vs. We explain the quantum Hall effect, which prominently features plateaus at even and odd filling factors across a range of carrier density, in terms of a surface state different from the Fermi arc-type states thought to exist on other surfaces, underlining differences between these measurements and those in the more widely studied (112)-plane films.
9:24AM W60.00008: Anomalous Hall Effect induced by extremely low field in ultra pure ZrTe$_5$  
JOSHUA MUTC (Presenter), PAUL MALINOWSKI, QIANNI JIANG, ZHAOYU LIU, University of Washington,  
DI XIAO, Physics, Carnegie Mellon University, JIUN-HAW CHU, University of Washington —  
ZrTe$_5$ has gathered interest in recent years due to its non-trivial topology. In monolayer form, it is  
predicted to be a quantum spin hall insulator. In bulk, it is predicted to reside extremely close to  
a phase transition between a strong and weak topological insulator, with a 3D Dirac semimetal  
state at the boundary between these two phases. We report detailed measurements of the  
anomalous hall effect (AHE) in ultra-pure, high mobility bulk ZrTe$_5$. We find the hall resistance  
saturates at an extremely low magnetic field (B $\ll$ 1T), and remains at the saturation value for  
fields up to 32T. This AHE is present despite no evidence of magnetism in ZrTe$_5$. We investigate  
the AHE effect in ZrTe5 as a function of temperature, magnetic field angle, strain, and doping,  
and discuss the origins of this effect.

*This work is supported as part of Programmable Quantum Materials, an Energy Frontier  
Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy  
Sciences (BES), under award DE-SC0019443.

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supported by the National Science Foundation Cooperative Agreement No. DMR-1644779, the  
State of Florida and the United States Department of Energy

9:36AM W60.00009: Epitaxial Growth and in-situ magneto-transport of Na$_3$Bi – a 3D Dirac semimetal  
DANA PEIRCE (Presenter), IGOR PINCHUK, RYAN MUZZIO, SIMRANJEET SINGH, JYOTI KATOCH, Carnegie Mellon Univ —  
3D topological Dirac semimetals (TDS) such as Na$_3$Bi and Cd$_3$As$_2$ possess Dirac nodes located outside the time-reversal invariant momentum points in the Brillouin zone. Recent theoretical and experimental work shows that quantum confinement of 3D TDS can open a tunable bulk bandgap and give rise to thickness-dependent alternate transitions between trivial and quantum spin Hall insulator states. In this talk, we will present our results on ultra-thin growth of Na$_3$Bi films on insulating substrates using molecular beam epitaxy (MBE). We will also discuss our efforts towards angle-dependent high-field in-situ magnetotransport measurements on back-gated thin films of Na$_3$Bi.
9:48AM W60.00010: Evolution of the electronic structure of the Weyl semimetal TaAs under pressure  ZUZANA MEDVECKA (Presenter), MARCEL NAUMANN, MARCUS P. SCHMIDT, VICKY SÜSS, HELGE ROSNER, MICHAEL NICKLAS, ELENA HASSINGER, Max Planck Institute for Chemical Physics of Solids — Weyl semimetals provide ideal condensed matter platform to study Weyl fermions. When current and magnetic field are parallel in such systems, the chiral anomaly is expected to induce a negative longitudinal magnetoresistance. To observe this special feature the Fermi level must be close to the band crossing points (Weyl nodes) where quasiparticles behave like Weyl fermions [1].

We studied whether hydrostatic pressure can tune the Weyl node energy in TaAs closer to the Fermi level by the Shubnikov-de Haas effect at pressures up to 2.5 GPa. Analysis of the quantum oscillations (QO) showed that the big electron and hole Fermi surface pockets in TaAs are shrinking in size by 40% while the small electron pocket does not. Therefore some of the Weyl nodes are moving closer to the Fermi level with pressure.

Two-band model fits of the magnetoconductivity reveal that the electron and hole densities and mobilities in TaAs do not show a significant evolution with pressure. This seeming disagreement with QO can be explained by the smaller electron pocket being probably the main contributor to the magnetoresistance in TaAs. Our experimental data are further supplemented by theoretical calculations.


10:00AM W60.00011: The chiral qubit: quantum computing with chiral anomaly* [Invited]
QIANG LI (Presenter), Brookhaven National Laboratory — The quantum chiral anomaly enables a nearly non-dissipative current in the presence of chirality imbalance. We propose to utilize the chiral anomaly for the designs of qubits potentially capable of operating at THz frequency and at room temperature with a coherence time to gate time ratio of about $10^4$. The proposed “Chiral Qubit” is a micron-scale ring made of a Weyl or Dirac semimetal, with the $|0\rangle$ and $|1\rangle$ states corresponding to the symmetric and antisymmetric superpositions of chiral currents circulating along the ring clockwise and counter-clockwise. A fractional magnetic flux through the ring induces a quantum superposition of the $|0\rangle$ and $|1\rangle$ quantum states. The entanglement of qubits can be implemented through the near-field THz frequency electromagnetic fields (EMF). We show that the Hamiltonian of the chiral qubit is similar to that of the superconducting qubit. This means that quantum gates can be implemented in a traditional way, and the algorithms developed for superconducting quantum processors will apply. Light-driven (THz) ultrafast topology switching, demonstrated experimentally in Dirac/Weyl semimetal recently, will be discussed.

The author is grateful for collaborations with Dmitri Kharzeev and Jigang Wang.

*This work is supported by the US Department of Energy, Office of Basic Energy Science, Materials Sciences and Engineering Division, under contract #DE-SC0012704.
**8:00AM W61.00001: Electronic structure and ferroelectricity of multiferroic Lu\(_{0.5}\)Sc\(_{0.5}\)FeO\(_3\)**

JEONG KYU KIM (Presenter), Pohang Univ of Sci & Tech, BONGJAE KIM, Department of Physics, Kunsan National University, Gunsan 54150, Korea, DONGHWAN KIM, KYOO KIM, Pohang Univ of Sci & Tech, YOUNGHAK KIM, Pohang Accelerator Laboratory, Pohang 37673, Korea, YAZHONG WANG, SANG-WOOK CHEONG, R-CEM & Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, JAE-HOON PARK, KYUNG-TAE KO, Pohang Univ of Sci & Tech — We investigated the electronic structure of a multiferroic Lu\(_{0.5}\)Sc\(_{0.5}\)FeO\(_3\) single crystal using x-ray absorption spectroscopy, cluster model calculation, and ab initio analysis. X-ray linear dichroism measurement reveals that the A-site ion hybridizes strongly with O ions, where the hybridization strength of Lu is nearly twice larger than that of Sc. In addition, the anisotropic hybridization of Lu is larger, that results in the wider splitting of \(a_{1g}\) states from \(e_g\pi\) states. The difference affects the energetic landscape of ferroelectric transition which is captured in ab initio calculation. Interestingly, the Born effective charge of planar O ions exhibits small deviation from a nominal valence instead of the anisotropic bonding, while that of apical O ion shows large value. Our observation suggest that the electronic contribution of \(e_g\pi\) and \(e_g\sigma\) bonds to six apical O ions in AO\(_8\) cage should be counted in to describe a ferroelectric instability in h-A(Mn,Fe)O\(_3\)

*This work is supported by Study for Nano Scale Optomaterials and Complex Phase Materials (2016K1A4A4A01922028) through NRF funded by MSIP of Korea. PAL is supported by MSIP of Korea. B. K. acknowledges support from NRF (grand No. 2018R1D1A1A02086051). K. K. acknowledges support from NRF (grand No. 2016R1D1A1B02008461).

**8:12AM W61.00002: Competing magnetic orders and anisotropic transport in quantum critical Sr\(_3\)Ru\(_2\)O\(_7\)**

ADITYA PUTATUNDA (Presenter), GUANHUA QIN, Univ of Missouri - Columbia, WEI REN, Dept of Physics, Univ of Shanghai, DAVID SINGH, Univ of Missouri - Columbia — We investigated Sr\(_3\)Ru\(_2\)O\(_7\), the classic example of a quantum critical metal known to show a metamagnetic quantum phase transition as well as electronic nematicity, through first-principles calculations. The density functional calculations predict a ferromagnetic ground state in contrast to its experimentally observed paramagnetic character. This raises the question whether there exists competing magnetic orders that suppresses its ferromagnetism and if so, then what are those? We performed a thorough search to identify such low energy antiferromagnetically ordered metastable states. We indeed obtain such an (almost) doubly degenerate state with a striped order and calculated its associated transport properties within Boltzmann transport theory. Our results indicate significant transport anisotropy which have been discussed in context of strong spin fluctuations present in this material.

*Work at the University of Missouri was supported by the Department of Energy Award No. DE-SC0019114
Dynamical simulation of spin-orbit insulator and application to bilayer iridate

HIDEMARO SUWA (Presenter), Department of Physics, University of Tokyo, GIA-WEI CHERN, Department of Physics, University of Virginia, KIPTON BARROS, Theoretical Division and CNLS, Los Alamos National Laboratory, CRISTIAN BATISTA, Department of Physics and Astronomy, The University of Tennessee — Spin-orbit insulators emerge in 5d electron systems with strong spin-orbit interaction, which can be described by a Hubbard model in the intermediate coupling regime of intra-atomic Coulomb repulsion (U) comparable to the dominant hopping amplitude (t). A reliable calculation in this regime is theoretically challenging because of the lack of a small parameter. We have developed a new numerical approach that enables large-scale numerical simulations (on finite lattices of more than 10,000 sites) of dynamical correlation functions at finite temperatures in a broad range of U/t values. The simulation of the self-consistent density matrix dynamics is combined with sampling from the Boltzmann distribution. As a relevant application of the newly developed method, we have calculated the dynamical spin structure factor of the bilayer iridate Sr$_3$Ir$_2$O$_7$. Our approach gives an excellent account of the experimental observations. The present method can be applied not only to iridates but also to various systems without any restrictions on the hopping amplitudes, lattice geometry, or electron filling fraction.


Infrared Spectroscopic Study on Doping Evolution of the Electronic Response of Sr$_3$(Ir$_{1-x}$Ru$_x$)$_2$O$_7$

GIHYEON AHN (Presenter), Hanyang Univ, JULIAN L SCHMEHR, STEPHEN WILSON, Materials Department, University of California, Santa Barbara, SOONJAE MOON, Hanyang Univ — We investigate the electronic response of the spin-orbit-coupled Sr$_3$(Ir$_{1-x}$Ru$_x$)$_2$O$_7$ system over a wide doping range by using infrared spectroscopy. Our data show that the electronic ground state evolves from the effective total angular momentum $J_{\text{eff}} = 1/2$ Mott state to a correlated metallic state with Ru doping. We observe that the Ru-doping-driven insulator-metal transition occurs only above a critical Ru concentration of $x_c \approx 0.35$. The low-energy optical response of the compound located at the insulator-metal transition boundary shows a peculiar behavior that might be associated with the spin-lattice coupling. Our data also suggest that the effect of the spin-orbit coupling in the electronic response may persist even in the metallic compounds with high Ru concentration. We will discuss the changes in the electronic structure associated with the insulator-metal transition.
Temperautre dependence of the low-energy electronic structure of Ca$_3$Ru$_2$O$_7$ IGOR MARKOVIC (Presenter), Univ of St Andrews, MATTHEW D. WATSON, Diamond Light Source, OLIVER J CLARK, FEDERICO MAZZOLA, Univ of St Andrews, EDGAR ABARCA MORALES, DMITRY SOKOLOV, ANDREW P. MACKENZIE, Max Planck Institute for Chemical Physics of Solids, PHIL KING, Univ of St Andrews — We use angular-resolved photoemission spectroscopy (ARPES) and ab initio calculations to study the low-energy electronic band structure of a bilayer ruthenate system, Ca$_3$Ru$_2$O$_7$, across a wide temperature range. Ca$_3$Ru$_2$O$_7$ is a bad metal which undergoes two magnetic transitions [1]: a Néel ordering at 56 K and a spin-reorientation with a coupled structural transition at 48 K. At low temperatures we find it to be a compensated semimetal, in general agreement with previous ARPES [2] and de Haas-van Alphen [3] experiments. Our measurements across the 48 K transition, however, reveal dramatic changes in the low-energy electronic structure in terms of the shape and size of the Fermi surface. This is accompanied by a significant increase in the scattering rate, and our temperature-dependent ARPES suggests new insights into the unusual transport properties of this system in its “bad metal” phase. We further explore the role of crystal structure, magnetism, and spin-orbit coupling in the evolution of the electronic structure across the 48 K phase transition.


Hydrodynamic electron flow in PdCoO$_2$: in-plane microwave spectroscopy JAMES DAY (Presenter), GRAHAM BAKER, University of British Columbia, SEUNGHYUN KHIM, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, DOUGLAS ANDREW BONN, University of British Columbia — Hydrodynamic electron flow—in which electronic viscosity affects transport properties—has been observed in the DC resistance of PdCoO$_2$ [1]. Predictions that hydrodynamic effects also influence the AC electromagnetic response of a metal exist [2, 3], but confirming experimental evidence is lacking. In these proposals, the electronic viscosity affects the gradient of the induced current density, thereby influencing the diffusion of electromagnetic fields into the sample. Here we report results of microwave spectroscopy measurements of PdCoO$_2$ aimed at testing these predictions.

In the measurements reported here, a microwave magnetic field was applied parallel to the $ab$ plane. The induced response has two components. First, flow along a high-mobility ($a/b$) direction, with a velocity gradient along the low-mobility $c$ direction. Second, flow along the low-mobility $c$ direction, with a velocity gradient along a high-mobility ($a/b$) direction. The latter is favorable to observing nonlocal electrodynamics. We see the onset of the anomalous skin effect.

Graham Baker (Presenter), James Day, University of British Columbia, Seunghyun Khim, Andrew Mackenzie, Max Planck Institute for Chemical Physics of Solids, Douglas Andrew Bonn, University of British Columbia — Hydrodynamic electron flow—in which electronic viscosity affects transport properties—has been observed in the DC resistance of PdCoO$_2$ [1]. Predictions that hydrodynamic effects also influence the AC electromagnetic response of a metal exist [2,3], but confirming experimental evidence is lacking. In these proposals, the electronic viscosity affects the gradient of the induced current density, thereby influencing the diffusion of electromagnetic fields into the sample. Here we report results of microwave spectroscopy measurements of PdCoO$_2$ aimed at testing these predictions.

In the measurements reported here, a microwave magnetic field was applied parallel to the $c$ axis. The induced flow is always along a high-mobility ($a/b$) direction, with a velocity gradient along the other high-mobility ($b/a$) direction. This geometry is favorable to observing the effect of viscosity. The results appear to be inconsistent with existing predictions.


9:24AM W61.00008: Suppression of ferromagnetic spin correlation in the filled skutterudite superconductor SrOs$_4$As$_{12}$ revealed by $^{75}$As NQR-NMR*  
Yuji Furukawa (Presenter), Qing Ping Ding, Iowa State University, K Nishine, Jun-Ichi Hayashi, Yukihiro Kawamura, Chihiro Sekine, Muroran Institute of Technology — Recently new filled-skutterudite compounds Sr$_T$$^4$As$_{12}$ ($T$ = Fe, Ru, Os) have been synthesized, which provides a new opportunity of systematic studies of the effects of different $d$ electron of 3$d$, 4$d$ and 5$d$ in the systems [1]. Motivated by the recent observation of ferromagnetic spin correlations in the 3$d$ compound SrFe$_4$As$_{12}$ [2], we have carried out nuclear quadrupole resonance (NQR) and nuclear magnetic resonance (NMR) measurements to investigate the role of magnetic fluctuations in the newly discovered superconductor 5$d$-compound SrOs$_4$As$_{12}$ which exhibits a superconducting transition at $T_c$ = 4.8 K [3]. From the temperature dependence of Knight shift $K$ and nuclear spin lattice relaxation time $T_1$, we found that no obvious ferromagnetic spin correlations in SrOs$_4$As$_{12}$. Furthermore, the temperature dependence of $1/T_1$ in the superconducting state evidences a conventional $s$-wave superconductivity in SrOs$_4$As$_{12}$.

*USDOE under Contract No. DE-AC02-07CH11358.
9:36AM W61.00009: First Principles Studies of Fe-intercalated NbS₂*  SOPHIE WEBER
(Presenter), University of California, Berkeley, JEFFREY B NEATON, Kavli Energy Nanoscience Institute at Berkeley — Layered transition metal dichalcogenides (TMDs) can allow for the intercalation of magnetic ions, resulting in novel magnetic and electronic properties which can be tuned by altering intercalant species and concentration. Recent experiments on Fe₁/₃NbS₂, a bulk antiferromagnet with a Néel temperature of 42K, have shown that an applied current can reversibly switch the magnetic order, which is read out in the resistivity*. It is hypothesized that the magnetoelectric response to the current is due to a redistribution of magnetic domains**. To shed light on these findings, we examine the ground state structure and magnetic properties of Fe₁/₃NbS₂ using density functional theory calculations. We compute energetics of different experimentally proposed magnetic orderings, and the corresponding band structures and Fermi surfaces. Implications of our calculations for the reported switching behavior and resistivity response are discussed.

* Nair et al., arXiv:1907.11698 (2019)
** Little et al., arXiv:1908.00657 (2019)

*This work is supported by the Department of Energy through the EFRC for Novel Pathways to Quantum Coherence in Materials. Computational resources provided by NERSC.

9:48AM W61.00010: Theory of magneto-elastoresistance and application to WTe₂: exploring electronic structure and extremely large magnetoresistance under strain*  PETER ORTH
(Presenter), NA HYUN JO, Iowa State University, LIN-LIN WANG, Ames Laboratory, SERGEY L. BUD'KO, PAUL C CANFIELD, Iowa State University — The application of uniaxial stress to is a promising route to probe and control the properties of quantum materials. One crucial step is to quantify the effects of strain on the electronic band structure, carrier density and mobility. Here, we demonstrate that much information can be obtained by exploring a novel experimental observable: magneto-elastoresistance (MER), which refers to magnetic field-driven changes of the elastoresistance. We apply this powerful approach to study the combined effect of strain and magnetic fields on the semi-metallic transition metal dichalcogenide WTe₂, and discover a large and temperature non-monotonic elastoresistance (ER) that can be tuned by magnetic field. We report on our theoretical analysis of these observations based on semi-classical Boltzmann transport theory combined with input from first-principles calculations. We highlight how MER can generally yield new insights beyond the zero field ER. For WTe₂ specifically we derive an effective low-energy three-band model that can account for the salient experimental features.

*This work was supported by the U.S. DOE (BES, DMSE and EFRC CATS) funded through Ames Laboratory, Contract No. DE-AC02-07CH11358, and by the Gordon and Betty Moore Foundation’s EPiQS Initiative through Grant GBMF4411.

10:00AM W61.00011: Photoelectrical imaging and coherent spin-state readout of single nitrogen-vacancy centers in diamond [Invited]  FEDOR JELEZKO (Presenter), Ulm University — Selected by Focus Topic Organizer (Xuedan Ma)
10:36AM W61.00012: Nonequilibrium Orbital Transitions via Applied Electrical Current in Calcium Ruthenate

BING HU (Presenter), HENGDI ZHAO, University of Colorado, Boulder, FENG YE, CHRISTINA HOFFMANN, Neutron Scattering Division, Oak Ridge National Laboratory, ITAMAR KIMCHI, GANG CAO, University of Colorado, Boulder — Simultaneous control of structural and physical properties via applied electrical current poses a key, new research topic and technological significance. Studying the spin-orbit-coupled antiferromagnet Ca$_2$RuO$_4$, and its derivative with 3% Mn doping to alleviate the violent first-order transition for more robust measurements, we find that a small applied electrical current couples to the lattice by significantly reducing its orthorhombicity and octahedral rotations, concurrently diminishing the 125K antiferromagnetic transition and inducing a new orbital order below 80K. The phase diagram reveals a critical regime near a current density of 0.15A/cm$^2$ that separates the vanishing antiferromagnetic order and the new orbital order. Further increasing current density (> 1A/cm$^2$) enhances competitions between relevant interactions in a metastable manner, leading to a peculiar glassy behavior above 80K. The coupling between the lattice and nonequilibrium driven current is interpreted theoretically in terms of $t_{2g}$ orbital occupancies. The current-controlled lattice is the driving force of the observed novel phenomena. Finally, we note that current-induced diamagnetism is not discerned in pure and slightly doped Ca$_2$RuO$_4$.

*This work is supported by NSF via grants DMR 1712101 and DMR 1903888

10:48AM W61.00013: Quantum liquid from strange frustration in the trimer magnet Ba$_4$Ir$_3$O$_{10}$

HAO ZHENG (Presenter), HENGDI ZHAO, YIFEI NI, CHRISTOPHER POCS, YU ZHANG, University of Colorado, Boulder, FENG YE, CHRISTINA HOFFMANN, XIAOPING WANG, Neutron Scattering Division, Oak Ridge National Laboratory, MINHYEA LEE, MICHAEL A HERMELE, ITAMAR KIMCHI, GANG CAO, University of Colorado, Boulder — We present the experimental observation of a new kind of frustrated quantum liquid arising in an unlikely place: the magnetic insulator Ba$_4$Ir$_3$O$_{10}$ where Ir$_3$O$_{12}$ trimers form an unfrustrated square lattice. Experimentally we find a quantum liquid state persisting down to 0.2 K that is stabilized by strong antiferromagnetic interaction with Curie-Weiss temperature -766 K. The astonishing frustration parameter of 3800 is beyond any known iridate thus far. Heat capacity and thermal conductivity are both linear at low temperatures, a familiar feature in metals but here in an insulator pointing to an exotic quantum liquid state; a mere 2% Sr substitution for Ba produces long-range order at 130 K and destroys the linear-T features. Although the Ir$^{4+}$(5d$^5$) ions in Ba$_4$Ir$_3$O$_{10}$ appear to form Ir$_3$O$_{12}$ trimers of face-sharing IrO$_6$ octahedra, we propose that intra-trimer exchange is reduced and the lattice recombines into an array of coupled 1D chains with additional spins. An extreme limit of decoupled 1D chains can explain most but not all of the striking experimental observations, indicating that the inter-chain coupling plays an important role in the novel frustration mechanism leading to this quantum liquid.

*This work is supported by NSF via grants DMR 1712101 and DMR 1903888
8:00AM W62.00001: Exciton Transport in the Electron-hole System $\text{Ta}_2\text{NiSe}_5$  

AKITOSHI NAKANO (Presenter), Physics, Nagoya University, TAKAYUKI NAGAI, Materials Research Center for Element Strategy, Tokyo Institute of Technology, NAOYUKI KATAYAMA, HIROSHI SAWA, Applied Physics, Nagoya University, HIROKI TANIGUCHI, ICHIRO TERASAKI, Physics, Nagoya University — A ternary transition metal chalcogenide, $\text{Ta}_2\text{NiSe}_5$ has been recently proposed as a candidate of the Excitonic insulator (EI). An extremely flattened band dispersion in a single particle excitation spectrum observed by an angle resolved photoemission spectroscopy is regarded as evidence of the EI phase in this compound[1]. However, macroscopic physical property to evidence the spontaneously generated electron-hole pairs in $\text{Ta}_2\text{NiSe}_5$ have not been found yet. 

In this time we focus on the dielectric constant and thermopower of single crystals of $\text{Ta}_2\text{NiSe}_5$. The dielectric constant characterizes the charge response upon an ac field that rocks an electron-hole pair. In particular, when the electron-hole pairs are tightly bound, they can behave as permanent electric dipoles and should exhibit a peculiar ac response. Similarly a temperature gradient couples to excitons. 

The dielectric constant below 50 K shows relaxor-like relaxation, implying the existence of randomly distributed electric dipoles. Furthermore, a large thermopower of 600 $\mu$V/K at 100 K suddenly drops toward zero down to 50 K. We ascribe these highly unconventional transport properties in $\text{Ta}_2\text{NiSe}_5$ at low temperatures to exciton transport.

Time-resolved ARPES signatures of pump driven normal-to-excitonic insulator transition

* ENRICO PERFETTO (Presenter), Physics Department, Univ of Roma, DAVIDE SANGALLI, ANDREA MARINI, ISM, CNR, GIANLUCA STEFANUCCI, Physics Department, Univ of Roma — We consider a ground-state band insulator turning into a nonequilibrium excitonic insulator (EI) when pumping it at sub-gap frequencies slightly larger than the excitonic energy. The macroscopic polarization in the non-equilibrium EI phase is characterized by self-sustained oscillations with a frequency depending on the absorbed energy. We show that during the pump-driving the excitonic ARPES structure undergoes a convex-to-concave shape transition and concomitantly the system goes through a BEC-BCS crossover. Furthermore attosecond pulses shone after the pump-driving at different times \( t_{\text{delay}} \) generate a photocurrent which oscillates in \( t_{\text{delay}} \). This phenomenon is related to the AC response of an exotic Josephson junction.

*1) RISE Co-ExAN (Grant No. GA644076)
2) European Union project MaX Materials design at the eXascale H2020-EINFRA-2015-1, Grant Agreement No. 676598
3) Nanoscience Foundries and Fine Analysis-Europe H2020-INFRAIA-2014-2015, Grant Agreement No. 654360
4) MIUR PRIN Grant No. 20173B72NB

Dynamics of an order parameter coupled phonon in an excitonic insulator

HONGLIE NING (Presenter), OMAR MEHIO, MICHAEL BUCHHOLD, Institute for Quantum Information and Matter, California Institute of Technology, TAKASHI KURUMAJI, JOSEPH G CHECKELSKY, Department of Physics, Massachusetts Institute of Technology, GIL REFAEL, DAVID HSIEH, Institute for Quantum Information and Matter, California Institute of Technology — An impulsively stimulated Raman active phonon can be suppressed or amplified using two optical pulses tailored to be period-matched with this certain mode. \( \text{Ta}_2\text{NiSe}_5 \) is an excitonic insulator candidate which exhibits multiple coherent phonons in transient reflectivity. We conducted double-pump coherent phonon spectroscopy measurements on \( \text{Ta}_2\text{NiSe}_5 \) to understand the interaction between the phonon and the excitonic order parameter. We further developed theoretical methods to simulate the dynamics of the order parameter coupled phonon.
8:36AM W62.00004: Imaging and Spectroscopy of an Exciton Condensate* SUBHRADEEP MISRA (Presenter), Department of Condensed Matter Physics, Weizmann Institute of Science, MICHAEL STERN, Physics Department and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, VLADIMIR UMANSKY, ISRAEL BAR-JOSEPH, Department of Condensed Matter Physics, Weizmann Institute of Science — We study the spatial and spectral properties of the photoluminescence of an exciton liquid at low temperatures and show that it evolves from a disordered liquid to a homogenous Bose-Einstein condensate, extending over a few hundred microns and covering the entire area of the mesa. The appearance of the condensate is marked by the emergence of a narrow PL peak, which gains strength as the temperature is reduced, and as the power is increased. We suggest that this peak is a result of the dark condensate formation and its interaction with the bright thermal exciton population.

*This work is funded by the Israeli Science Foundation (ISF).

8:48AM W62.00005: Bardasis-Schrieffer polaritons in excitonic insulators* ZHIYUAN SUN (Presenter), ANDREW MILLIS, Columbia Univ — Bardasis-Schrieffer (BS) modes in superconductors are fluctuations of order parameters corresponding to subdominant pairing channels, e.g., d-wave fluctuations in a s-wave superconductor. We generalize the notion of BS mode to excitonic insulators and show that in s-wave excitonic insulators, a p-wave BS mode exists at energies below the gap energy, has a non-vanishing optical matrix element with light and moreover hybridizes strongly with photons to form Bardiasis-Schreiffer polaritons, which are observable in both far-field and near-field optical experiments. We also show that strong driving of the BS mode by an intense light pulse can convert an s-wave excitonic insulator to a p-wave insulator and trap it there.

*This work is supported by the DOE under Grant DE-SC0019443.
9:00AM W62.00006: Discrete breaking of symmetry in the excitonic phase of Ta$_2$NiSe$_5$

GIACOMO MAZZA (Presenter), College de France, MALTE ROESNER, Radboud University, LUKAS WINDGAETTER, SIMONE LATINI, ANGEL RUBIO, Max Planck Institute for Structure and Dynamics of Matter, ANTOINE GEORGES, College de France — Ta$_2$NiSe$_5$ (TNS) is an excitonic insulator candidate material. Condensation of excitons is supposed to originate from particle-hole pairs formed across valence and conduction bands which weakly overlap at the Fermi level. Yet clear cut signatures of such a phase together with its possible origins remain open questions. Here we report on the understanding of the symmetry principles underlying an instability of the excitonic type in TNS.

By means of ab-initio calculation we uncover a set of discrete symmetries in the high-temperature phase of TNS with significant effect to its low-energy band structure. We derive a minimal electronic model consistent with these symmetries and present evidence of an electronic phase transition related to a spontaneous breaking of these symmetries. The breaking of such discrete symmetries is intrinsically coupled to a lattice instability, which drives the high-temperature orthorhombic structure to the low-temperature triclinic one. Our results open new perspectives on the interpretation of a phase characterized by the condensation of excitons hosted by this material.

9:12AM W62.00007: Cluster mean-field analysis of the finite-temperature properties of the one-dimensional extended Falicov-Kimball model*

MASAHIRO KADOSAWA (Presenter), Physics, Chiba Univ, SATOSHI NISHIMOTO, Institute for Theoretical Solid State Physics, IFW-Dresden, KOUDAI SUGIMOTO, Physics, Keio Univ, YUKINORI OHTA, Physics, Chiba Univ — Motivated by a recent finding that Ta2NiSe5 is in a strong-coupling excitonic insulator state [1], we study finite-temperature properties of the one-dimensional extended Falicov-Kimball model (EFKM), the simplest lattice model for the excitonic insulator state. Here, we use the cluster mean-field method with a sine-square deformation and calculate the finite-temperature phase diagrams of the model, which are compared with the results of a previous study at zero temperature [2]. Moreover, we calculate the optical conductivity spectra of the model at finite temperatures and find that the temperature dependence of the spectral features observed in experiment [3] are well reproduced by our calculations.


*This work was supported in part by SFB 1143 of the Deutsche Forschungsgemeinschaft, by Grants-in-Aid for Scientific Research from JSPS (Projects No. JP17K05530 and No. JP19K14644), and by Keio University Academic Development Funds for Individual Research.
9:24AM W62.00008: Global Spin Current in Excitonic Phases of the Two-Band Hubbard Model* \textsc{Shunsuke Yamamoto} (Presenter), \textsc{Hisao Nishida}, Physics, Chiba University, \textsc{Koudai Sugimoto}, Physics, Keio University, \textsc{Yukinori Ohta}, Physics, Chiba University — It has recently been pointed out that the k-space spin texture may emerge in the doped excitonic phase of a two-orbital Hubbard model containing the cross-hopping terms with certain symmetry [1-3]. Thanks to the spontaneous breaking of the inversion symmetry by the excitonic phase transition, the global spin current perpendicular to the applied electric field is induced by the spin-dependent off-diagonal component of the Drude weight. The mechanism is quite different from the conventional one originated from the spin Hall effect where a spin-orbit coupling plays an essential role, and thus our result gives a new route to generate a spin current.


*This work was supported in part by Grants-in-Aid for Scientific Research from JSPS (Projects No. JP17K05530 and No. JP19K14644) and by Keio University Academic Development Funds for Individual Research.

9:36AM W62.00009: Sign-Free Determinant Quantum Monte Carlo Study of the Bilayer Hubbard and Two-Orbital Hubbard-Kanamori Models \textsc{Xuxin Huang} (Presenter), Applied Physics, Stanford University, \textsc{Martin Claassen}, Center for Computational Quantum Physics, The Flatiron Institute, \textsc{Brian Moritz}, SLAC National Accelerator Laboratory and Stanford University, SSRL Materials Science Division, \textsc{Thomas Devereaux}, Materials Science and Engineering, Stanford University — Two-band Hubbard models, as prototypes for various strongly correlated systems, have attracted intense research interest over the past few decades. Determinant Quantum Monte Carlo (DQMC), an unbiased finite-temperature numerical technique well suited to study such models, generically suffers from the fermion sign problem. However, for some variations, e.g. the bilayer Hubbard model with symmetric electron-hole doping and the half-filled two-orbital Hubbard-Kanamori model, particle-hole symmetry can be utilized to perform sign-problem-free studies. Here, using DQMC we show that the bilayer Hubbard model possesses a Berezinskii–Kosterlitz–Thouless (BKT) transition to an inter-layer biexciton condensate at intermediate coupling and finite electron-hole doping. For the Hubbard-Kanamori model, we treat the full rotationally invariant interaction, including the Hubbard and Hund's coupling terms, using a decoupling scheme which involves a 12-state auxiliary field per site, and present the magnetic correlation and phase transition results obtained from DQMC.
**9:48AM W62.00010: Novel states of charge-imbalanced polariton condensates**  
ARTEM STRASHKO (Presenter), Center for Computational Quantum Physics, Flatiron Institute, Simons Foundation, FRANCESCA MARCHETTI, Departamento de Fisica Teorica de la Materia Condensada & Condensed Matter Physics Center (IFIMAC), Universidad Autonoma de Madrid, ALLAN MACDONALD, Department of Physics, The University of Texas at Austin, JONATHAN KEELING, SUPA, School of Physics and Astronomy, University of St Andrews — Polariton condensation is a well-established phenomenon featuring all the signatures of an ordinary condensate. However, in the context of polariton condensation, almost exclusively balanced systems, with equal densities of electrons and holes, have been studied. This misses a whole class of potential exotic imbalanced condensed states like an FFLO or a breached-pair state.

Inspired by pioneering works on imbalanced electron-hole systems in TMDC monolayers strongly coupled to a cavity photon, using variational mean-field theory, we explore whether a combination of strong matter-light coupling and electric field biasing promotes novel condensed states, which do not exist otherwise.

On top of a balanced polariton and a dark imbalanced FFLO condensates, we find novel imbalanced polaritonic states with coexisting polariton condensate and unpaired electrons with either isotropic or anisotropic Fermi surface depending on applied bias voltage. These states arise due to combination of strong matter-light coupling and long-range Coulomb potential.

**10:00AM W62.00011: π-ton contributions to optical conductivity in correlated electron systems**  
ANNA KAUCH (Presenter), PETRA PUDLEINER, KATHARINA ASTLEITHNER, PAUL WORM, CLEMENS WATZENBÖCK, Vienna Univ of Technology, PATRIK THUNSTRÖM, Uppsala University, TIN RIBIC, KARSTEN HELD, Vienna Univ of Technology — The interaction of light with solids gives rise to new bosonic quasiparticles, with the exciton being the most famous of these polaritons. While excitons are the generic polaritons of semiconductors, we show that for strongly correlated systems another polariton is prevalent [1] -- originating from the dominant antiferromagnetic or charge density wave fluctuations in these systems. As these are usually associated with a wave vector \((\pi, \pi, \ldots)\) or close to it, we call the derived polaritons \(\pi\)-tons.

These \(\pi\)-tons yield the leading vertex correction to the optical conductivity in all correlated models studied:

- the Hubbard
- the extended Hubbard model
- the Falicov-Kimball
- the Pariser-Parr-Pople model

both in the insulating and in the metallic phase.


*This work was supported by the European Research Council under the European Union's Seventh Framework Program (FP/2007-2013) through ERC Grant No. 306447, the Austrian Science Fund (FWF) through project P 30997-N32 and Doctoral School ```Building Solids for Function```
10:12AM W62.00012: Quantum nematicity in EuB$_6$  
GABRIELLE BEAUDIN (Presenter), ANDREA BIANCHI, WILLIAM WITCZAK-KREMPA, Universite de Montreal — Our experimental discovery of a quantum nematic phase in the colossal magneto resistive material EuB$_6$ constitutes a breakthrough in quantum material research. Unlike the quantum nematics in the cuprate and arsenide superconductors, there is no nearby lattice instability complicating the interpretation, making EuB$_6$ a clean model system for studying electronic nematicity. Interestingly, the nematic appears in the same region of the temperature-magnetic field phase diagram where experiments indicate magnetic polarons. This not only indicates a new understanding of nematicity but also paves the way for obtaining novel magneto resistive transistor action in spintronic devices.

10:24AM W62.00013: Strong polaron–spin fluctuations drive the insulator–semimetal transition in low-density electron gases  
ANDREA BIANCHI (Presenter), GABRIELLE BEAUDIN, ALEXANDRE DÉSILETS-BENOIT, Universite de Montreal, STAVROS SAMOTHRAKITIS, KILIAN STENNING, School of Metallurgy and Materials, University of Birmingham, MICHAEL NICKLAS, MPI-CPFS, SIMON GERBER, NIKOLA EGETENMEYER, JORGE GAVILANO, MICHEL KENZELMANN, LNS, PSI, ROBERT CUBITT, CHARLES DEWHURST, Institut Laue Langevin, MARK LAVER, Physics, University of Warwick — One of the outstanding questions in physics is the formation of magnetic moments in metallic systems of low carrier density. For the design of materials for spintronic applications, we need to understand the physics in a regime where mobile charge carriers couple strongly to the magnetic moments. One way to realise such a strong interaction is to work with materials with a low carrier density where two competing electronic ground states are close in energy. Switching between these different electronic ground states then leads to large effects in the electronic transport. What makes the physics in these colossal magnetoresistance (CMR) materials fascinating is that the CMR effects stem from an electronic phase separation at the nanometre scale, despite the fact that these materials are chemically homogeneous. "Magnetic polarons" are thought to be responsible for the CMR effects in some materials. Here we present results of a small angle neutron scattering (SANS) study showing the dramatic influence of magnetic polarons on ferromagnetic fluctuations in EuB$_6$, giving clear evidence for their involvement in the insulator-to-metal transition as the result of large scale magnetic fluctuations.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W63 DCMP: STM on twisted 2D heterostructures  
Mile High Ballroom 4D - Jairo Velasco Jr., University of California, Santa Cruz
Recent experiments on magic-angle twisted bilayer graphene (MATBG) have shown various intriguing low-temperature electronic phases induced by filling of the moiré flat bands [1][2]. These phases, including correlated insulator and superconducting phases, are derived from a high-temperature “parent phase,” which is currently not well understood. Previously, there have been scanning tunneling microscopy and spectroscopy (STM/STS) measurements of this parent phase that have shown signatures of strong electronic correlations [3]. In this talk, we report on new, higher resolution STM/STS studies of this phase. Our experimental results reveal new distinct filling-dependent spectroscopic features that reflect key information on the nature of many-body correlations in MATBG. We have found that these features can be compared to a model of strongly interacting electrons in the flat bands allowing us to determine the microscopic origin of these features as well as extract an estimate of the strength of electronic correlation in MATBG.


*This work has been supported by the Moore Foundation and the DOE.
Magic-angle twisted bilayer graphene (MATBG) has a complex gate-accessible electronic phase diagram characterized by a variety of exotic insulating, superconducting, and topological phases. Using a homebuilt dilution-fridge scanning tunneling microscope (STM), we probe the spectroscopic properties of MATBG to gain insight into the underlying mechanisms of its phases. At partial filling of the flat bands, consistent with previous studies, our measurements at high temperatures (< 12K) show significant deviations from the single-particle density of states (DOS), indicating the presence of strong electronic interactions [1]. We extend these STM measurements to millikelvin temperatures, where we explore how the “parent phase” develops into correlated insulating and superconducting phases. Our measurements have uncovered a series of gate-dependent energy gaps in the DOS at the Fermi level corresponding to electron fillings at which electrical transport measurements reveal these phases. These spectra, along with their magnetic field and spatial dependencies, provide key information about the microscopic origin of each energy gap and their connection to the various electronic phases in MATBG.


*This work is supported by the Moore Foundation and the DOE.
Spectroscopy with scanning tunneling microscopy (STM) in a high magnetic field can be used to probe the quantization of the density of states into Landau levels (LL), which provides important information on electronic properties such as the relevance of broken symmetries and the presence or absence of Dirac cones. We apply this technique to study gated magic-angle twisted bilayer graphene (MATBG) devices, for which recent magnetotransport studies have reported transitions in the LL fan diagrams as a function of the filling of electrons in MATBG’s flat bands [1-3]. These reported changes correlate with the appearance of various correlated insulating, magnetic, and superconducting phases. Our STM measurements are carried out in a dilution-fridge system allowing us to resolve the energy of the LL with high resolution and to probe MATBG devices as a function of filling of its flat band. We will describe these measurements, their connection to the magnetotransport studies, and their interpretations in terms of microscopic properties of MATBG as a function of electron density.


*This work is supported by the Moore Foundation and the DOE.
8:36AM W63.00004: Atomic-scale structure and electronic properties of twisted double bilayer graphene  

CARMEN RUBIO VERDÚ (Presenter), SIMON ELI TURKEL, LARRY SONG, Physics Department, Columbia University, DANTE KENNES, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, LEDE XIAN, Max Planck Institute for the Structure and Dynamics of Matter, HECTOR OCHOA, Physics Department, Columbia University, ANGEL RUBIO, Center for Computational Quantum Physics (CCQ), The Flatiron Institute, ABHAY PASUPATHY, Physics Department, Columbia University — The fundamental properties of 2D materials are dramatically modified when they are brought next to each other to form a vertical heterostructure. The electronic characteristics of such van der Waals materials can be further controlled by the twist angle degree of freedom, inducing electronic flat bands that lead to emergent phases such as correlated insulating (CI) and superconducting (SC) states in twisted bilayer graphene. Such phenomenology is expected in higher order heterostructures where the vertical stacking order plays a major role. Recent works showed that double bilayer graphene (tDBG) at a twist angle of ~1.3° hosts displacement field tunable CI and SC states, as well as ferromagnetic order. We show real-space imaging of tDBG moiré superstructure by means of Scanning Tunneling Microscopy/Spectroscopy (STM/STS). STS reveals the presence of van Hove singularities whose spatial distribution within the moiré unit cell is determined by the inequivalent stacking sites. Tuning carrier density and displacement field reveals long-range broken symmetries that emerge when the Fermi level is brought in the vicinity of such flat bands. Our results shed light into the underlying mechanisms behind electron-electron correlations in tDBG and the emergent ferromagnetic order.

8:48AM W63.00005: Identifying the effect of hBN alignment on twisted bilayer graphene using scanning tunneling microscopy*  

CHENG-LI CHIU (Presenter), XIAOMENG LIU, YONGLONG XIE, BERTHOLD JAECK, Princeton University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ALI YAZDANI, Princeton University — When two graphene layers are stacked with a small twist angle, a moiré superlattice arises that modifies the electronic band structure. Specifically, at the magic angle (~1.1deg), the bands become flat. In these flat bands, various correlated electronic states emerge. In some samples, correlated insulating behaviors are observed at integer fillings, accompanied by superconducting states upon doping. In other samples, the quantum anomalous Hall effect replaces the correlated insulator at ¾ filling while superconductivity is absent. Despite the lack of direct experimental evidence, it has been suggested that the latter phase is produced by the alignment between graphene and the hBN substrate. Using a scanning tunneling microscope (STM), we extract the hBN alignment information from graphene-hBN moire lattice superimposed on the graphene-graphene moire lattice. Comparing spectra from different samples, we explore the effect of hBN alignment on the electronic properties of twisted bilayer graphene.

*This work is supported by Moore Foundation, DOE, NSF-MRSEC.
**9:00AM W63.00006: Imaging moiré superlattices in twisted bilayers of 2D materials**

LEO MCGILLY (Presenter), ALEXANDER KERELSKY, NATE FINNEY, Columbia University, KOSTANTIN SHAPOVALOV, Institute of Materials Science of Barcelona, AUGUSTO GHIOTTO, EN-MIN SHIH, YIHANG ZENG, SAMUEL MOORE, WENJING WU, YUSONG BAI, Columbia University, LIN ZHOU, Nanjing University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, JAMES C HONE, XIAOYANG ZHU, DMITRI BASOV, CORY DEAN, CYRUS DREYER, ABHAY PASUPATHY, Columbia University — Two-dimensional materials stacked into van der Waals (vdW) heterostructures form moiré superlattices as a result of a relative rotational misalignment between layers as well as a lattice mismatch between two dissimilar materials. The resulting physics of the vdW heterostructures can be dominated by the large scale periodicity of the moiré superlattice which is generally substantially larger than the atomic scale lattice. In this work we outline a method to visualize the real-space moiré superlattices in a variety of twisted vdW heterostructures utilizing piezoresponse force microscopy which locally measures an electromechanical sample surface deformation. Its origin is suggested to arise due to the flexoelectric effect wherein electric polarization is induced through strain gradients present within moiré superlattices.

*Swiss National Science Foundation project P400P2_186744*

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**9:12AM W63.00007: Flat bands in small angle twisted bilayer WSe$_2$**

ZHIMING ZHANG (Presenter), Physics Department, University of Arizona, YIMENG WANG, Department of Electrical and Computer Engineering, The University of Texas at Austin, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, KEIJI UENO, Department of Chemistry, Saitama University, EMANUEL TUTUC, Department of Electrical and Computer Engineering, The University of Texas at Austin, BRIAN J LEROY, Physics Department, University of Arizona — The discovery of superconductivity in magic angle twisted bilayer graphene has ignited great interest in exploring flat bands in two-dimensional van der Waals heterostructures. We demonstrate for the first time the existence of flat bands in the electronic structure of a 3° twisted bilayer WSe2 sample using low temperature scanning tunneling microscopy and spectroscopy. Using variable height spectroscopy, we observe sharp peaks in the density of states near the valence band edge related to the flat bands. By decay constant measurements, we assign various peaks in the density of states to different locations in the Brillouin zone. By direct spatial mapping of the wavefunctions at the flat band energy, we have found that the flat band is localized in the form of a hexagonal network, which is in excellent agreement with first-principle density functional theory calculations.

*Work at the University of Arizona was supported by the National Science Foundation under grants DMR-1708406 and EECS-1607911 and the Army Research Office under Grant No. W911NF-18-1-0420.*
Effect of Spin-orbit Coupling in Twisted Bilayer and Double Bilayer Transition Metal Dichalcogenides

SUDIPTA KUNDU, MIT NAIK, MANISH JAIN (Presenter), Center for Condensed Matter Physics, Department of Physics, Indian Institute of Science — Since the discovery of flat bands at magic angles in twisted bilayer graphene, the formation of flat bands has been predicted for several other twisted bilayers, especially twisted transition metal dichalcogenides (TMDs). The effect of spin-orbit coupling is quite prominent in TMDs such as WSe$_2$. Using a multiscale approach, based on classical force-fields for structural relaxation and density functional theory calculations for electronic structure, we investigate the influence of spin-orbit coupling on the flat bands in twisted TMD systems. Owing to spin-valley coupling, spin-orbit interaction affects the flat bands of the twisted bilayer TMDs with twist angle close to 0$^\circ$ differently than those near 60$^\circ$. The spin-orbit splitting of bands near valence band edge decreases with smaller twist angle. We study wavefunction localization near valence and conduction band edges in these bilayers and extend our studies to twisted double bilayer TMDs as well.

*We thank Supercomputer Education and Research Centre, IISc for providing the computational facilities.

Tunable Moiré Superlattice of Artificially Twisted Monolayers

YI-CHENG CHIANG (Presenter), PO YEN CHEN, XIN-QUAN ZHANG, YING-YU LAI, CHUN-AN CHEN, ERH-CHEN LIN, Materials Science and Engineering, National Tsing Hua University, SYU YOU GUAN, Physics, Academia Sinica, SHANGJR GWO, Physics, National Tsing Hua University, CHIA-SENG CHANG, Physics, Academia Sinica, LIH JUANN CHEN, YI-HSIEN LEE, Materials Science and Engineering, National Tsing Hua University — Twisting between two stacked monolayers modulates periodic potentials and forms the Moiré electronic superlattices, which offers an additional degree of freedom to alter material property. Considerable unique observations, including unconventional superconductivity and quantized interlayer excitons are correlated to the electronic superlattices but further study requires reliable routes to study the Moiré in real space. Scanning tunneling microscopy (STM) is ideal to precisely probe the Moiré superlattice and correlate coupled parameters among local electronic structures, strains, defects, and band alignment at atomic scale. Here, a clean route is developed to construct twisted lattices using synthesized monolayers for fundamental studies. Diverse electronic superlattices are experimentally confirmed with STM at room temperature.
9:48AM W63.00010: Unsupervised learning of nematic order from scanning tunneling spectroscopy on twisted bilayer graphene* SAMUEL LEDERER (Presenter), Cornell University, YOUNGJOON CHOI, Caltech, PAVEL ISMAILOV, Cornell University, ANDREW WILSON, NYU, STEVAN NADJ-PERGE, Caltech, EUN-AH KIM, Cornell University — Moiré materials such as magic angle twisted bilayer graphene (TBG) provide an exciting platform for the study of novel states of matter, but their large unit cells present significant difficulties for atomic resolution probes such as scanning tunneling microscopy (STM). We therefore develop an automated method to extract salient physical quantities from STM data on moiré materials, and apply it to measurements on TBG that visually suggest the breaking of rotational symmetry (i.e. nematic order). We apply the machine learning technique of Gaussian mixture modeling to this data to classify the STM images at different bias voltages into several categories in an unbiased fashion. This classification yields evidence for a nematic order that manifests itself in a manner strongly dependent on bias voltage. In addition to providing evidence for spatial symmetry breaking in TBG, our techniques can be applied in the future to overcome the intrinsic challenges of exploiting STM in the burgeoning field of moiré materials.

*This work was partially supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1719875), as well as NSF grant 1934714.

10:00AM W63.00011: Moiré superlattice of a charge transfer Kondo monolayer and its interplay with superconductivity* SHUANGZAN LU, Wuhan University, HYEONGDO NAM, PENGHAO XIAO, University of Texas at Austin, YANPING GUO, Wuhan University, MENGKE LIU, University of Texas at Austin, YUSONG BAI, Wuhan University, ZHENGBO CHEN, University of Texas at Austin, HAITAO ZHOU, Chinese Academy of Sciences, GRAEME HENKELMAN, University of Texas at Austin, GREGORY A FIETE, Northeastern University, H.-J. GAO, Chinese Academy of Sciences, ALLAN MACDONALD, University of Texas at Austin, CHENDONG ZHANG (Presenter), Wuhan University, CHIH-KANG SHIH, University of Texas at Austin — Moiré pattern formation has emerged as a powerful tool to create controllable two-dimensional electronic superlattices. Moiré superlattices can exhibit remarkable properties such as unconventional superconductivity and Mott insulators in twisted graphene bilayers, and moiré exciton bands in transition metal dichalcogenide heterobilayers. Here, we report on the observation of a moiré superlattice formed between an organic monolayer and a s-wave superconductor. Although the organic molecule does not contain magnetic atoms, the interlayer charge transfer from the superconductor to the p-orbitals creates a local moment leading to the co-existence of Kondo screening and Cooper pair formation, and to an interplay between superconductivity and the Kondo effect. More specifically, the moiré pattern leads to a strong modulation of the “local” Kondo temperature by a factor of three. In addition, the interplay of Kondo screening and Cooper pair formation leads to a modulation of the pairing gap by about 30%. We show that the periodicity of these superlattices is tunable by the twist angle, making it possible to tailor the properties of this heterostructure.

*Work supported by NSF-MRSEC-DMR-1720595, Welch F-1672, National Key R&D Program of China (No. 2018FYA0305800).
10:12AM W63.00012: Scanning tunneling microscopy and spectroscopy of graphene on in-plane anisotropic rhenium disulfide*  RYAN PLUMADORE (Presenter), JUSTIN BODDISON-CHOUINARD, SAMANTHA SCARFE, ADINA A LUICAN-MAYER, Univ of Ottawa — Van der Waals heterostructures made of graphene placed on top of other 2D materials have been shown to affect the band structure of graphene and lead to proximity-induced novel phenomena. In this talk, we focus on a system that has graphene placed on top of the in-plane anisotropic semiconductor ReS$_2$. Using scanning tunneling microscopy and spectroscopy, we characterized the changes at the atomic scale in the structure and electronic properties of Dirac electrons placed in the longitudinal periodic potential of ReS$_2$.

*The authors acknowledge funding from the National Sciences and Engineering Research Council (NSERC) Discovery Grant RGPIN-2016-06717. We also acknowledge the support of the National Sciences and Engineering Research Council of Canada (NSERC) through Strategic Project STPGP 521420.

10:24AM W63.00013: Transition Metal Adatoms on Graphyne: Electronic Structure and Thermoelectric Properties*  ANDREA LATGE (Presenter), PEDRO VENEZUELA, DEBORA RODRIGUES, Instituto de Física, Niterói, RJ Brazil, Universidade Federal Fluminense — Thermoelectricity is the advantageous property of some materials to convert waste thermal energy into electricity. The research interest of achieving high thermoelectric efficiency increased in the recent years, specially promoted by the demand for eco-friendly energy harvesting technology. It is known that 2D systems provide much higher thermoelectric conversion than bulk materials, due to enhancement of Seebeck coefficient and reduction of phonon thermal conductivity. Therefore, graphene nanostructures and other 2D sp-sp2 carbon allotropes such as graphynes and graphdiynes are promising candidates to thermoelectric applications and spin caloritronics, an emerging technology combining spintronics and thermoelectronics.

Here we investigated structural and electronic properties of Mn and Fe adatoms adsorbed on Graphyne (Gy) using density functional theory. We verified that the band structure of Gy sheets, strongly depends on the adatom distance to the plane. To explore the effects of quantum confinement, we also discuss the functionalization of Gy nanoribbons. Finally, we focus on the electronic transport and thermoelectric quantities with the perspective of spin caloritronics nanodevices.

*We thank the INCT de Materiais de carbono, CAPES, CNPq, and FAPERJ E-23/202.953/2016.
10:36AM W63.00014: Electronic structure of carbon nanotubes on graphene substrates
BENEDETTA FLEBUS (Presenter), ALLAN MACDONALD, University of Texas at Austin — Allotropes of carbon, including one-dimensional carbon nanotubes and two-dimensional graphene sheets, continue to draw attention as promising platforms for probing the physics of electrons in lower dimensions. Recent research has shown that the electronic properties of graphene multilayers are exquisitely sensitive to the relative orientation between sheets, and in the bilayer case exhibit strong electronic correlations when close to a magic twist angle. Here, we investigate the electronic properties of a carbon nanotube deposited on a graphene sheet by deriving a low-energy theory that accounts both for rotations and rigid displacements of the nanotube with respect to the underlying graphene layer. We show that this heterostructure is described by a translationally invariant, a periodic or a quasi-periodic Hamiltonian, depending on the orientation and the chirality of the nanotube. Furthermore, we find that, even for a vanishing twist angle, rigid displacements of a nanotube with respect to a graphene substrate can alter its electronic structure qualitatively. Our results identify a promising new direction for strong correlation physics in low dimensions.

10:48AM W63.00015: Q-Valley Quasiparticle Interference in Few-Layer Transition Metal Dichalcogenides*
PATRICK CHEUNG (Presenter), YAN-FENG ZHOU, FAN ZHANG, University of Texas at Dallas — Quantum transport experiments have provided compelling evidence for the threefold flavors of the Q-valley electrons in few-layer transition metal dichalcogenides (TMD). We study the quasiparticle interference (QPI) due to Q-valley electrons scattering off localized impurities, which modifies the local density of states. In the quantum Hall regime, all the TMD odd-layers thicker than bilayer exhibit Landau level triplets. When a Landau level triplet is one-third filled or empty, the flavor SU(3) symmetry is broken in the ferroelectric nematic ground states tunable by an in-plane electric field and an out-of-plane magnetic field. We show the QPI patterns of such flavor states, which can be probed by scanning tunneling spectroscopy.

*This theoretical work at UTD is supported by Army Research Office under Grant No. W911NF-18-1-0416 and Natural Science Foundation under Grant No. DMR-1921581 through the DMREF program.

Friday, March 6, 2020 8:00 AM - 10:00 AM

Session W65 DCMP: Superlattices and Nanostructures IV: Polaritons and Plasmons Mile High Ballroom 4F - GuangXin Ni, Columbia Univ
8:00AM W65.00001: Calibration of long-lifetime polariton structures* JONATHAN BEAUMARIAGE (Presenter), ZHENG SUN, Physics and Astronomy, University of Pittsburgh, MARK STEGER, National Renewable Energy Laboratory, DAVID M MYERS, Polytechnique Montreal, SHOUVIK MUKHERJEE, DAVID WAYNE SNOKE, Physics and Astronomy, University of Pittsburgh, LOREN PFEIFFER, KENNETH WEST, Electrical Engineering, Princeton University — In short-lifetime polariton samples both the upper and lower polariton branches can be resolved through white light reflectivity. However, in long-lifetime polariton samples the linewidths are so narrow that they can not be resolved through typical spectroscopy. Additionally, photoluminescence from the upper polaritons can often not be seen at relevant detunings, as the upper polaritons quickly drop down to lower polariton states. As such, the calibration of long-lifetime polariton samples is uniquely challenging compared to short-lifetime polariton samples. In this work, we will show various measurements which demonstrate the cavity lifetime is 100 ps or more, and use this collective set of information to create an accurate calibration of the long-lifetime polariton samples.

*University of Pittsburgh: the Army Research Office (W911NF-15-1-0466)

8:12AM W65.00002: Dynamics of an Exciton-Polariton Condensate in a Tilted Ring Microcavity* SHOUVIK MUKHERJEE (Presenter), Univ of Pittsburgh, VALERII K. KOZIN, ANTON V. NALITOV, IVAN A. SHELYKH, University of Iceland, ZHENG SUN, Univ of Pittsburgh, DAVID M MYERS, Engineering Physics, Polytechnique Montreal, BURCU OZDEN, Penn State Abington, JONATHAN BEAUMARIAGE, Univ of Pittsburgh, LOREN PFEIFFER, KENNETH WEST, Princeton University, ANDREW DALEY, University of Strathclyde, DAVID WAYNE SNOKE, Univ of Pittsburgh — We have created polariton condensates in a semiconductor microcavity with a lifetime greater than the equilibration time scale for the system at cryogenic temperature (below 10 K). By etching the microcavity into ring micro-channels of width 15 μm we confined the condensate to flow in a circular trap. We have directly imaged the motion of the condensate in the ring using time-resolved optical microscopy techniques. We study both the dynamical and the steady-state regime and present quantitative bounds on the strength of the interactions between polaritons in this system. We also measure the spatial coherence of the condensate in these micro-channels leading to important implications for scaling such networks of micro-channels for simulating NP-hard problems.

*Authors acknowledge funding from ARO (W911NF-15-1-0466), Gordon and Betty Moore Foundation (GBMF-4420) and by the NSF MRSEC program (DMR-0819860).
8:24AM W65.00003: Pushing Photons with Electrons: Observation of the Polariton Drag Effect*  QI YAO (Presenter), Univ of Pittsburgh, DAVID M MYERS, Polytechnique Montreal, BURCU OZDEN, Pennsylvania State University, JONATHAN BEAUMARIAGE, Univ of Pittsburgh, LOREN PFEIFFER, KENNETH WEST, Princeton University, DAVID WAYNE SNOKE, Univ of Pittsburgh — Exciton-polaritons are quasiparticles that are a superpositions of excitons and photons. In a microcavity, exciton-polaritons have an effective mass and can form a Bose-Einstein condensate (BEC). Experimentally, this condensate can be generated by pumping light into a microcavity structure with quantum wells at the antinodes of the light field, and then we can measure the the energy, real-space and momentum-space distributions of the polaritons using the light they emit, using conventional optical methods.

In our experiment, we observed a change in the angle of emission of the photons when injecting electrons to the system, which indicates that the interaction of electrons with the polaritons changes the momentum of the polariton condensate. The condensate flow was accelerated when electrons flow with the same direction, while the condensate was slowed down when electrons flow in the opposite direction. Because the experiment is a photon-in, photon-out system, this is equivalent to steering photons using a DC electrical current.

*University of Pittsburgh: the Army Research Office (W911NF-15-1-0466)
Princeton: the Gordon and Betty Moor Foundation (GBMF-4240) and the National Science Foundation MRSC program through the Princeton Center for Complex Materials (DMR-0819860)

8:36AM W65.00004: Observation of the amplitude mode in a microcavity polariton condensate driven by quantum fluctuations*  MARK STEGER (Presenter), National Renewable Energy Laboratory, RYO HANAI, ALEXANDER EDELMAN, PETER B LITTLEWOOD, James Franck Institute and Department of Physics, University of Chicago, DAVID WAYNE SNOKE, JONATHAN BEAUMARIAGE, Physics and Astronomy, University of Pittsburgh, BRIAN FLUEGEL, National Renewable Energy Laboratory, KENNETH WEST, LOREN PFEIFFER, Electrical Engineering, Princeton University, ANGELO J MASCARENHAS, National Renewable Energy Laboratory — We directly observe emission into the amplitude mode from an exciton-polariton condensate: the signature of this mode being the ghost-branch photoluminescence at energies below the condensate. This amplitude mode, the number-fluctuation variant of the Goldstone mode, appears in many forms of condensed matter; however, the polariton system gives a unique way to passively monitor this mode in the steady-state system without driving the population far out of equilibrium. This mode is predicted to manifest as an excitation of condensed particles into the upper-polariton state. Here we present experimental results in agreement with our theoretical analysis. Additionally, we present a family of ghost-branch modes that require an expanded theory to capture.

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**8:48AM W65.00005: Hyperbolic phonon polaritons in calcite for nanoscale infrared confinement**  
VANESSA BRESLIN (Presenter), National Research Council, United States Naval Research Laboratory, DANIEL RATCHFORD, ALEXANDER GILES, ADAM DUNKELBERGER, JEFFREY OWRUTSKY, United States Naval Research Laboratory — Phonon-polaritons are collective oscillations resulting from the coupling of photons with optical phonons in polar materials and are supported within a material-specific spectral region called the Reststrahlen band, which is bounded by the transverse and longitudinal optical phonons. In this region, the material behaves optically like a metal due to the negative real part of the permittivity, resulting in the incident light being strongly reflected. When polar materials are nanostructured, phonon-polaritons can enable a variety of near-field optical effects such as sub-diffraction light confinement. Interestingly, a polar material which supports phonon-polaritons can also have anisotropic optical properties, such that different components of its permittivity tensor have opposite signs. These materials are referred to as hyperbolic as they behave optically like a dielectric in one direction and like a metal in the other. Here, we report on the observation of hyperbolic phonon-polaritons (HPhPs) in calcite nanopillar arrays, demonstrate the aspect ratio dependence of the HPhP resonance frequencies, and verify our results through comparison to an analytical model. Calcite is an ideal low-loss material for studying HPhPs that could find applications in mid-IR nanophotonic devices.

**9:00AM W65.00006: Creation of partially rotating vortex of polariton condensate by non-resonant Laguerre-Gaussian optical excitation in semiconductor microcavity**  
DAEGWANG CHOI, MIN PARK, BYOUNG YONG OH, MIN-SIK KWON, Department of Physics, KAIST, SUK IN PARK, HANG KYU KANG, SOOSEOK KANG, JIN DONG SONG, Center for Opto-Electronic Convergence Systems, KIST, HYOU NGSOON CHO, YONG-HOON CHO (Presenter), Department of Physics, KAIST — An exciton-polariton is a bosonic quasi-particle formed by a strong coupling between a quantum well exciton and a cavity photon in a semiconductor microcavity. Its bosonic nature offers the ground state condensation and superfluidity that hosts quantized vortices generated by various optical excitation methods. Here, we observed a new method for creating quantized vortices in the polariton superfluid whose vorticity is determine by the orbital angular momentum of a non-resonant Laguerre-Gaussian optical excitation.[1] Moreover, the polariton condensate is found to be in two different energy states, a vortex carrying excited state and the irrotational ground state, which is confirmed by the tomographic interferometer.[2] As a result, only a part of superfluid is found to be rotating with a vortex core and the fraction of the rotating superfluid can be controlled by changing the excitation beam size or the pumping power. This striking observation will be helpful for improving our understanding of relaxation process and non-equilibrium physics in semiconductor and non-equilibrium superfluid.  

*National Research Foundation of Korea (NRF2019R1A2B5B03070642)
Topological Surface-plasmon-polariton Modes on Biharmonic Metal-dielectric Gratings

THOMAS SMITH (Presenter), ALESSANDRO PRINCIPI, Physics and Astronomy, University of Manchester — The area of topological plasmonics is a relatively new and rather unploughed field. The majority of progress thus far has been in constructing crystal structures whose atomic sites take the form of an array of metallic nanoparticles. Such nanoparticles are capable of hosting localised plasmon-polariton modes, which form the basis upon which a tight-binding model may be generated. Through this model, the topological character of the lattice may be probed. A similar result may be arrived at by considering surface-plasmon-polariton resonances on biharmonic metal-dielectric gratings. In such a case, provided that the surface is smooth and has a parabolic profile, the amplitude of the SPP mode may be described by an emergent 1D Schrödinger equation. This equation may then be made to mimic the SSH model through a suitable manipulation of the physical parameters of the system. Then topological states may be observed within the basic scattering formalism, whose existence and character are then confirmed through a tight-binding model.

*This work was made possible through the support of the EPSRC with the Ph.D. studentship grant EP/N509565/1 and the Royal Society International Exchange grant IES\R3\170252.

Photonic crystal for graphene plasmons

LIN XIONG (Presenter), CARLOS FORSYTHE, Columbia Univ, MINWOO JUNG, Cornell University, ALEXANDER MCLEOD, YUTAO LI, SHUAI ZHANG, YINAN DONG, SONG LIU, Columbia Univ, MICHAEL M FOGLER, University of California San Diego, JAMES H. EDGAR, Kansas state university, GENNADY SHVETS, Cornell University, CORY DEAN, DIMITRI BASOV, Columbia Univ — Graphene surface plasmon polaritons (SPPs) are hybrid excitations of electrons and photons which can be controlled by the optical properties of graphene. Periodically varying the optical properties results in a photonic crystal for graphene SPPs. Here we utilize cryogenic near-field optical microscopy to study the band structure induced by a graphene photonic crystal consisting of a high-mobility graphene atop a patterned SiO₂ dielectric layer [Xiong, Nat. Commun. 10: 4780 (2019)]. Gating through the dielectric provides a periodic field effect that spatially modulates local carrier densities [Forsythe, Nat. Nanotech. 13, 566–571 (2018)] and the propagation of plasmon polaritons through the graphene. A full plasmonic bandgap and characteristic SPP propagation properties are revealed. Selective engineering of domain wall in the middle of the photonic crystal produces localized SPP modes propagating strictly along the domain wall. These findings signify a new route towards designer-engineered band-structures to route and manipulate highly confined plasmons within high mobility graphene devices.
9:36AM W65.00009: Plasmon resonance shift and near electric field of silver nanoparticles: Theoretical analysis of size, shape, and aggregation effects. MASAFUYU MATSUI (Presenter), HISAO NAKAMURA, AIST — We develop theoretical method to analyze optical response of nanoparticles by combining with discrete dipole approximation. To clarify microscopic level mechanism of plasmon resonance and near field effect, the induced dipole is decomposed into contributions from the electric field by incident light (an incident light term) and that by the induced dipole oscillations (a dipole-dipole interaction term). We examine our theoretical approach to silver nanoparticles and analyze size, shape-dependence of optical response as well as effect of aggregation. The analysis quantitatively reveals that the incident light term dominates the plasmon resonance along the direction of the small diameter whereas the dipole-dipole interaction term is dominant in that of the large diameter. To show effect of aggregation to optical response, we calculate total optical response of interacting two nanospheres. The plasmon resonance along the direction, on which two spheres are aligned, is caused by an interparticle interaction, resulting in the similar behavior to the prolate nanospheroid. These results indicate usefulness of modeling of the optical response of multi-nanoparticles by that of a shape-anisotropic nanoparticle.

9:48AM W65.00010: Size tunable passive cloaking platform using self-assembled plasmonic nanostructures. Imran Khan,1 Arnold Kim,2 and Sayantani Ghosh1 1Department of Physics, University of California, Merced, CA 95343 USA 2Department of Applied Mathematics, Univ* IMRAN KHAN (Presenter), Physics, University of California, Merced, ARNOLD D.KIM, Applied Mathematics, Univ of California - Merced, SAYANTANI GHOSH, Physics, University of California, Merced — Plasmonic cloaking works by suppressing dominant scattering harmonics radiated from the cloaked object. A shell made of plasmonic nanoparticles (NPs), in combination with the cloaked object as a core, creates the complete plasmonic cloaking structure. In this study, we present the design and fabrication of spherical nano- to micron-scale shell structures via molecular self-assembly of gold NPs, with the goal of reduced scattering and therefore, cloaking, in the VIS-NIR spectral range. Scattering suppression range is varied by tuning the critical parameters of the effective medium, such as core to shell radius ratio and the filling fraction of the NPs in the shell wall. In addition to experimental work, we have also developed a multiscale simulation platform that explicitly models multiple scattering by the gold NPs and their multiple interactions with the core. Simulation results shows that the nano-assembled spheres yield suppressed visibility in the desired spectral range.

*This research was supported by NSF CREST grant no. HRD-1547848

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W66 DCMP: Quantum Many-Body Scars Four Seasons 1 - Nicolas Regnault, Ecole Normale Superieure - Tag(s): Invited
Quantum many-body scars: a new form of weak ergodicity breaking in constrained quantum systems* [Invited] ZLATKO PAPIC (Presenter), Univ of Leeds — Recent experiments on large chains of Rydberg atoms [1] have demonstrated the possibility of realising one-dimensional, kinetically constrained quantum systems. It was found that such systems exhibit surprising signatures of non-ergodic dynamics, such as robust periodic revivals in global quenches from certain initial states. This weak form of ergodicity breaking has been interpreted as a manifestation of "quantum many-body scars" [2], i.e., the many-body analogue of unstable classical periodic orbits of a single particle in a chaotic stadium billiard. Scarred many-body eigenstates have been shown to exhibit a range of unusual properties which violate the Eigenstate Thermalisation Hypothesis, such as equidistant energy separation, anomalous expectation values of local observables and subthermal entanglement entropy. I will demonstrate that these properties can be understood using a tractable model based on a single particle hopping on the Hilbert space graph, which formally captures the idea that scarred eigenstates form a representation of a large SU(2) spin that is embedded in a thermalising many-body system. I will show that this picture allows to construct a more general family of scarred models where the fundamental degree of freedom is a quantum clock [3]. These results suggest that scarred many-body bands give rise to a new universality class of constrained quantum dynamics, which opens up opportunities for creating and manipulating novel states with long-lived coherence in systems that are now amenable to experimental study.


*This work was supported by EPSRC grants EP/P009409/1 and EP/R020612/1.

Quantum many-body scars: connections to integrability and stability* [Invited] ANUSHYA CHANDRAN (Presenter), Boston Univ, VEDIKA KHEMANI, Stanford University, CHRISTOPHER LAUMANN, Boston Univ, CHENG-JU LIN, Perimeter Institute for Theoretical Physics, OLEXEI I MOTRUNICH, Caltech — Quantum many-body scar states are exceptional finite energy density eigenstates in an otherwise thermalizing system that do not satisfy the eigenstate thermalization hypothesis. Recent atomic array experiments in the Rydberg blockaded regime suggests that the simplest blockaded Hamiltonian, the PXP Hamiltonian, has such scars in its spectrum. In this talk, I will discuss the connections between integrability and quantum scars by identifying a proximate integrable point at which the non-thermal signatures of the scar states become more pronounced. I will further discuss the stability of quantum scars to generic perturbations. Although the scar states hybridize with the other states in the spectrum upon perturbation, their nonthermal properties survive for a parametrically long time in quench experiments.

*This work was supported by National Science Foundation (NSF) through Grants No. DMR-1619696, PHY-1656234 and DMR-1752759. The work was also supported by the Sloan Foundation through the Sloan Research Fellowship and by the Perimeter Institute for Theoretical Physics.
We study the spin-1 XY model on a hypercubic lattice in d dimensions and show that this well-known nonintegrable model hosts an extensive set of anomalous finite-energy-density eigenstates with remarkable properties. Namely, they exhibit subextensive entanglement entropy and spatiotemporal long-range order, both believed to be impossible in typical highly excited eigenstates of nonintegrable quantum many-body systems. While generic initial states are expected to thermalize, we show analytically that the eigenstates we construct lead to weak ergodicity breaking in the form of persistent oscillations of local observables following certain quantum quenches—in other words, these eigenstates provide an archetypal example of so-called quantum many-body scars. This work opens the door to the analytical study of the microscopic origin, dynamical signatures, and stability of such phenomena.
9:48AM W66.00004: Phenomenology and mechanisms of Quantum many-body scarring*

[Invited] WEN WEI HO (Presenter), Harvard University, SOONWON CHOI, University of California, Berkeley, CHRISTOPHER J TURNER, University of Leeds, HANNES PICHLER, Harvard University, ALEXIOS MICHAELIDIS, IST Austria, SAMBUDDHA CHATTOPADHYAY, Harvard University, ZLATKO PAPIC, University of Leeds, MAKSYM SERBYN, IST Austria, DMITRY ABANIN, University of Geneva, MIKHAIL LUKIN, Harvard University — A central postulate of statistical mechanics is ergodicity -- a generic interacting, quantum many-body system initialized out of equilibrium is expected to explore its allowed phase phase and eventually thermalize. Known exceptions to this behavior include strongly disordered, many-body localized (MBL) systems, and finely-tuned integrable systems. In this talk, I will discuss a different mechanism pertaining to a weak form of ergodicity breaking: Quantum many-body scarring (QMBS) [1]. Motivated by recent quench experiments with Rydberg atom arrays [2] which observed surprisingly slow thermalizing dynamics from certain simple initial states, QMBS is tied to the presence of special, eigenstate thermalization hypothesis(ETH)-violating eigenstates in the many-body spectrum. I will first discuss how a variational description of the many-body dynamics seen in the experiments, using the time-dependent variational principle (TDVP) over a manifold of entangled matrix-product states, can capture this non-thermalizing dynamics and furthermore provide some insight into the connection to the similarly named phenomenon of quantum scars in single-particle chaos in terms of isolated, unstable, periodic orbits [3]. I will also discuss a complementary approach in which the scarred states can be understood as arising from an embedded su(2) symmetric subspace [4]. More generally, I will discuss physical mechanisms giving rise to QMBS in other settings that can be analytically understood, such as from the idea of embedded Hamiltonians [5] and from the dynamics of virtual entangled pairs [6].


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10:24AM W66.00005: Integrability, Thermalization, and Quantum Scars in a Constrained Hamiltonian [Invited] SANKHYA MOUDGALYA (Presenter), Physics, Princeton University, ABHINAV PREM, Princeton Center for Theoretical Sciences, Princeton University, RAHUL NANDKISHORE, Physics, University of Colorado, Boulder, NICOLAS REGNAULT, Ecole Normale Superieure, ANDREI BERNEVIG, Physics, Princeton University — We study the quantum dynamics of a simple translation invariant, center-of-mass preserving model of interacting fermions in one dimension, which arises in multiple experimentally realizable contexts. We show that this model exhibits a Hilbert space that fractures into exponentially many dynamically disconnected Krylov subspaces. Each of the exponentially large Krylov subspaces can either be integrable or non-integrable. We analytically find examples of several integrable subspaces, and show evidence for the validity of Eigenstate Thermalization Hypothesis (ETH) restricted to each non-integrable subspace. This model thus exhibits phenomenology associated with quantum scars, i.e. the fate of an initial product state under time-evolution depends on the properties of the Krylov subspaces it has weights in. In addition, some of the non-integrable Krylov subspaces show conventional quantum scars, which manifest as revivals and slow thermalization of certain charge density wave configurations.

Friday, March 6, 2020 8:00 AM - 11:00 AM

Session W67 DCMP: Strange Metal Physics

8:00AM W67.00001: Theories of Planckian dissipation in strongly correlated systems [Invited] AAVISHKAR PATEL (Presenter), Physics, University of California, Berkeley, SUBIR SACHDEV, Physics, Harvard University — The apparently universal value, $2\pi k_B T/h$, of the transport scattering rate observed experimentally in a wide variety of non-Fermi liquid metals with $T$-linear resistivity has been a longstanding mystery in condensed matter physics; this phenomenon is called 'Planckian dissipation'. We present a lattice model of fermions with $N$ flavors and random interactions that describes a non-Fermi liquid metal at low temperatures $T \to 0$, in the solvable limit of large $N$. We begin with quasiparticles around a Fermi surface with effective mass $m^*$, and then include random interactions that lead to fermion spectral functions with frequency scaling with $2\pi k_B T/h$. The resistivity $\rho$ obeys the Drude formula $\rho = m^*/(ne^2\tau_{tr})$, where $n$ is the density of fermions, and the transport scattering rate is $1/\tau_{tr} = f 2\pi k_B T/h$; we find $f$ to be of order unity and essentially independent of the strength and form of the interactions, hence 'universal'. The random interactions are a generalization of the Sachdev-Ye-Kitaev models; it is assumed that processes nonresonant in the bare quasiparticle energies only renormalize $m^*$, while resonant processes are shown to produce Planckian dissipation. We point out some predictions of this theory that are, in principle, testable in photoemission experiments. We further present some other large $N$ models that can also give rise to Planckian dissipation under certain conditions.


*This research was supported by the U.S. Department of Energy under Award No. DE-SC0019030, and by the Miller Institute for Basic Research in Science.
The perfectly linear temperature dependence of the resistivity observed as $T \rightarrow 0$ in a variety of metals close to a quantum critical point (QCP) is a major puzzle of condensed matter physics. I will present resistivity measurements supporting that $T$-linear resistivity as $T \rightarrow 0$ is a generic property of cuprates, associated with a universal scattering rate [1]. We measured the low-$T$ resistivity of the bi-layer cuprate Bi2212 just above its pseudogap critical point $p^*$ and found that it exhibits a $T$-linear dependence with the same slope as in the single-layer cuprate Nd-LSCO close to its own $p^*$, despite their very different Fermi surfaces and structural, superconducting and magnetic properties. We then showed that the $T$-linear coefficient (per CuO$_2$ plane), noted $A$, for various cuprates presenting this phenomenon, is given by a universal relation implying a specific scattering rate for charge carriers in all these samples: $1/\tau = h/2\pi k_B T$, where $h$ is the Planck constant and $k_B$ is the Boltzmann constant. This specific scattering rate corresponds to what is called the Planckian limit, and works not only for hole-doped cuprates but also for electron-doped cuprates, despite the different nature of their QCP and strength of their electron correlations.


In collaboration with: Siham Benabib, Wojciech Tabis, Baptiste Vignolle, Laboratoire National des Champs Magnetiques Intenses,; Francis Laliberte, Maxime Dion, Maude le Lizaire, Universite de Sherbrooke
9:12AM W67.00003: Strange Metals and Anomalous Dimensions for Conserved Currents

[Invited] PHILIP PHILLIPS (Presenter), University of Illinois at Urbana-Champaign — The unsaturating resistivity exceeding the Ioffe-Regel-Mott bound in the strange metal phase of the cuprates implies that electrons are not the propagating degrees of freedom. The search for new degrees of freedom has led some to conclude that not only does the relevant gauge field that describes the interactions with electromagnetic radiation have an anomalous dimension but so does the current. This conclusion flies in the face of the well known result in quantum field theory that conserved quantities do not acquire anomalous dimensions under any amount of renormalization. My talk will focus on demistifying the claim of anomalous dimensions of conserved quantities. I will show that Nother’s Second Theorem[1,2] actually allows for electromagnetisms in which the conserved current and gauge field can actually have arbitrary dimensions. Specific models are constructed which exhibit such anomalies[1,2]. I will show that the resulting Aharonov-Bohm effect deviates strongly from the standard result and hence can be used a sharp test of anomalous dimensions in the strange metal phase of the cuprates.


*We thank DMR19-19143 for partial funding.


10:24AM W67.00005: Strange metallicity in the doped Hubbard model [Invited] THOMAS DEVEREAUX (Presenter), Stanford Univ — Strange or bad metallic transport, defined by its incompatibility with conventional quasiparticle pictures, is a theme common to strongly correlated materials and ubiquitous in high temperature superconductors. The Hubbard model represents a minimal starting point for modeling strongly correlated systems. Here we demonstrate strange metallic transport in the doped two-dimensional Hubbard model using determinantal quantum Monte Carlo calculations. Over a wide range of doping, we observe resistivities exceeding the Mott-Ioffe-Regel limit with linear temperature dependence. The temperatures of our calculations extend to as low as 1/40 the non-interacting bandwidth, placing our findings in the degenerate regime relevant to experimental observations of strange metallicity. Our results provide a foundation for connecting theories of strange metals to models of strongly correlated materials.
Organic electrochemical transistors (OECTs) have gained considerable interest for applications in bioelectronics, power electronics, circuits and neuromorphic computing. Their defining characteristic is the bulk-modulation of channel conductance owing to the facile penetration of ions into the (semi)conducting polymeric channel. For this reason, their device scaling relies on film thickness, and often relaxes the stringent demands of clean and controlled interfaces required in traditional FETs. Despite recent progress and a rapidly expanding library of new materials, the understanding of stability and transport/coupling of ionic and electronic carriers remain largely unexplored. We highlight recent synthetic and processing approaches used to tailor device properties and stability, as well as new opportunities enabled by such advances. Our understanding of critical processes in electrochemical devices further requires us to study these materials in device-relevant conditions, considering the effects of ions and solvent on microstructure and transport. To this end, we report on recent efforts using ex situ as well as operando scattering and spectroscopy to build a more device-relevant picture of structure-transport relations.
Visualizing charge transfer across length scales in printable, conductive polymer electrodes* [Invited] ERIN RATCLIFF (Presenter), Univ of Arizona — Organic electrochemical transistors leverage the unique hybrid electrical/ionic conduction mechanism of conductive polymers when interfaced with mobile electrolyte species. Understanding the underlying structure-function properties of charge transport and transfer is critical to new technological development. Specifically, semicrystalline conductive polymers exhibit a heterogeneous spatial landscape of sub-populations of different electronic and physical properties at nanometer length scales. Each of these sub-populations is expected to have different potential-dependent electrical and ionic charge transport properties, but these behaviors are difficult to resolve at nanometer length scales. This talk will cover a tool suite of spectroelectrochemical methodologies that enables resolution of sub-population behaviors in conductive polymer electrodes, including measurement of potential-dependent ion diffusion coefficients. New nanoscale characterization approaches to measure localized charge transfer rates and structures will also be discussed.

*This research was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award DE-SC0020208 (diffusion coefficients), by the National Science Foundation (NSF) under Award # DMR-1608289 (scanning probe approaches). This research used resources of the Advanced Light Source, which is a DOE Office of Science User Facility under contract no. DE-AC02-05CH11231. SINS data was collected on beamline 5-4 under the assistance of Hans A. Bechtel. Use of the Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515.
Monitoring plant physiology with organic electrochemical transistors

ELENI STAVRINIDOU (Presenter), Linkoping University — Plants are the basis of food, providers of oxygens and regulators of the ecosystem. Plants convert solar energy into chemical energy with the process of photosynthesis where carbon dioxide is converted to sugar molecules. Sugars are not only the energy source in plants but also important signalling molecules, involved in regulation of physiology including stress responses. Currently there are no methods that allow real time monitoring of sugar transport in plants. Sugar detection is based on enzymatic assays, chromatography and/or mass spectrometry; all of these methods require sample collection and preparation. Organic electrochemical transistors (OECTs) are ideal tools for interfacing with organisms, since they can translate complex biological input to an electronic readout signal. OECT sensors can operate in complex media and they can directly detect products from the biological unit. In my group we are developing sugars sensors based on the organic electrochemical transistor for monitoring plant processes in-vitro and in-vivo. In a first example we measure the export of glucose in real time, from isolated chloroplasts, with a temporal resolution of 1min. The OECT based platform is able to distinguish the metabolic phase of the chloroplast prior isolation from the plant. In another example we are developing implantable OECT-based sugar sensors for in-vivo, real time monitoring of sugar transport in trees. The OECTs sensors show high device to device reproducibility, stability during the operation in the in-vivo environment and most importantly they do not cause a significant wound response from the plant. The sensors reveal kinetics of sugars transport that were not observed before. Our work benchmarks the OECT-based sensors as powerful tools for monitoring processes in plants, in real time both, in-in vivo and in-vitro systems.

Electrolyte-Gated Transistors for Fundamental Physics and Applications

C. DANIEL FRISBIE (Presenter), University of Minnesota — Electrolyte-gated transistors (EGTs) constitute a general class of devices in which an electrolyte is employed as the gate insulator; the very large capacitance of the electrolyte results in low voltage operation, high gate-induced carrier densities, and consequently high transconductance. These devices are divided into two broad categories, either the electric double layer transistor (EDLT) or the electrochemical transistor (ECT), depending on the mechanism of operation. This talk will begin with a general description of EGTs using a solid state electrolyte or ion gel, including typical fabrication methods, principles of operation (i.e., electrochemical vs double-layer charging), and quasi-static and dynamic performance. Applications of EGTs in printed electronics and biosensing will be briefly described, and then the discussion will move to use of EGTs to explore transport physics in novel materials at high carrier density. Specific examples include double layer gating of organic semiconductor single crystals such as rubrene and C60, and 2D materials, such as tellurene. In the case of tellurene, we are able to access the insulator-to-metal transition.

*This work was primarily supported by the MRSEC program of the National Science Foundation at the University of Minnesota under Award DMR-1420013.
Adapting organic electronics to biology (and not vice versa)!*

RÓISÍN OWENS (Presenter), Chemical Engineering and Biotechnology, University of Cambridge — In vitro models of biological systems are essential for our understanding of biological systems. In many cases where animal models have failed to translate to useful data for human diseases, physiologically relevant in vitro models can bridge the gap. Many difficulties exist in interfacing complex, 3D models with technology adapted for monitoring function. Polymeric electroactive materials and devices can bridge the gap between hard inflexible materials used for physical transducers and soft, compliant biological tissues. An additional advantage of these electronic materials is their flexibility for processing and fabrication in a wide range of formats. In this presentation, I will discuss our recent progress in adapting conducting polymer devices, specifically the Organic Electrochemical Transistor (OECT), to integrate with 3D cell models. We go further, by generating 3D electroactive scaffolds capable of hosting and monitoring cells. I will also highlight recent research using biomimetic models of cell membranes interfaced with organic electronic electrodes and transistors for drug discovery.

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Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X01 DAMOP: Dissipative and Far-From-Equilibrium Quantum Dynamics in AMO Systems 103
11:15AM X01.00001: Theory of non-Hermitian fermionic superfluidity subject to inelastic collisions in ultracold atoms  KAZUKI YAMAMOTO (Presenter), Department of Physics, Kyoto University, MASAYA NAKAGAWA, Department of Physics, University of Tokyo, KYOSUKE ADACHI, BDR, RIKEN, KAZUAKI TAKASAN, Department of Physics, UC Barkeley, MASAHITO UEDA, Department of Physics, University of Tokyo, NORIO KAWAKAMI, Department of Physics, Kyoto University — In recent years, non-Hermitian (NH) quantum systems have been actively studied [1,2]. However, since most of the previous studies dealt with single-particle physics, understanding of many-body physics in NH systems is yet in its infancy.

Motivated by recent experimental advances in ultracold fermionic atoms, we analyze a non-Hermitian (NH) BCS Hamiltonian with complex-valued interactions arising from inelastic scattering between fermions [3]. We develop a mean-field theory to obtain a NH gap equation for order parameters, which are similar to but different from the standard BCS ones because of the inequivalence of left and right eigenstates in the NH physics. We find unconventional phase transitions unique to NH systems: the superfluidity breaks down and reappears with increasing dissipation, featuring exceptional points for weak attractive interactions. As for strong attractive interactions, the superfluid gap never collapses but is enhanced by dissipation due to an interplay between the BCS-BEC crossover and the quantum Zeno effect.


11:27AM X01.00002: The Threefold Way in Non-Hermitian Random Matrices*  RYUSUKE HAMAZAKI (Presenter), KOHEI KAWABATA, NAOTO KURA, MASAHITO UEDA, Physics, University of Tokyo — Non-Hermitian random matrices have been utilized in diverse scientific fields such as dissipative and stochastic processes, nuclear physics, and neural networks. However, the only known universal level-spacing statistics are those of the Ginibre ensemble characterized by complex-conjugation symmetry. In this talk, we report our discovery of two distinct universality classes characterized by transposition symmetry [1]. We find that transposition symmetry alters repulsive interactions between two neighboring eigenvalues and deforms their spacing distribution, which is not possible with other symmetries including Ginibre's complex-conjugation symmetry which can affect only nonlocal correlations. Our results complete the non-Hermitian counterpart of Dyson's threefold classification of Hermitian random matrices and serve as a basis for characterizing nonintegrability and delocalization in open quantum systems with symmetry [1,2].


*R. H. was supported by the Japan Society for the Promotion of Science through Program for Leading Graduate Schools (ALPS) and JSPS fellowship (JSPS KAKENHI Grant No. JP17J03189).
The effective non-hermitian Hamiltonian (ENH) in strongly-correlated electron systems (SCES), which is introduced by H. Shen and L. Fu (PhysRevLett.120.146402), is derived by the spectral function, and the non-hermitian physics is now studied eagerly.

However, the essential questions, "Is this ENH the same one as the ENH in the context of open quantum system?" and "Why is the post selection not necessary to derive the ENH in SCES?", still remain. In this paper, we prove that the ENH in each context, OQS and SCES, corresponds to each other and clarify why the post selection is not necessary in SCES by treating the model in SCES as in OQS. Moreover, we propose the method to detect the non-hermitian properties in OQS without post selection, which is the great obstacle to experimental detection.

The Lindblad equation is a well-known quantum master equation that describes the evolution of open quantum systems. In general, the Lindblad equation is more challenging to analyze than the Schrödinger equation for closed systems, as one has to deal with the space of operators rather than the Hilbert space. One approach to this difficulty is to construct exactly solvable models. However, very few exact results are available for open many-body systems, although many such examples are known in closed many-body systems.

In this talk, we construct a solvable example of a quantum Ising model with bulk dissipation [1]. By vectorizing the density matrix, its Liouvillian is mapped to a non-Hermitian analog of the Ashkin-Teller model, further reducing to the staggered XXZ chain with pure-imaginary anisotropy parameters. Using this mapping, we show that the steady states are doubly degenerate and these two are unique. Moreover, we obtain the exact formula for the Liouvillian gap, the inverse relaxation time, for a particular set of parameters corresponding to a uniform XXZ chain. The result implies a kind of phase transition for the first decay mode.


*JSPS KAKENHI Grant No. 18K03445 and Institute for Physics of Intelligence
12:03PM X01.00005: Effects of dipole-dipole interaction in atomic vapors probed by two-dimensional coherent spectroscopy*  DANFU LIANG (Presenter), Department of Physics, Florida International University, SHAOGANG YU, State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, YIFU ZHU, Department of Physics, Florida International University, XIAOJUN LIU, State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, HEBIN LI, Department of Physics, Florida International University — Neutral atoms without permanent dipole moments can interact due to transition-induced dipole moments. Dipole-dipole interactions (DDIs) can lead to an energy shift of the atomic energy level and a change in the dephasing rate. The DDIs are usually detected by measuring the energy shift which might be difficult for weak DDIs, while the dephasing rate change has been largely overlooked. Optical two-dimensional coherent spectroscopy (2DCS) is extremely sensitive to DDIs and able to reveal the dephasing rate change due to DDIs. We implemented photon-echo, 1Q-2Q and double-quantum optical 2DCS to probe the effect of DDIs in the rubidium atomic vapor. From these spectra, we retrieved the decay rate change due to DDIs for the hyperfine levels of $^87\text{Rb}$ or $^85\text{Rb}$'s D2 lines. The results show that the change in dephasing rate is the primary effect, compared to the energy shift, of DDIs in dilute atomic vapors. This technique allows us to detect weak DDIs and measure the effects in both energy shift and dephasing rate due to DDIs.

*This research is based on work supported by the National Science Foundation (PHY-1707364)

12:15PM X01.00006: Effects of a dissipative coupling to the momentum of a particle in a double well potential*  DOMINIK MAILE (Presenter), Department of Physics, University of Konstanz, SABINE ANDERGASSEN, Department of Theoretical Physics, University of Tübingen, GIANLUCA RASTELLI, Department of Physics, University of Konstanz — Double well potentials offer the possibility of coherent state preparation and therefore constitute important building blocks in the analysis of quantum information and quantum engineering devices. Here we present a study of the coherent tunneling in a parabolic double well potential in presence of different dissipative interactions. Specifically, we investigate the effects of an environmental coupling to the momentum and/or to the position of a particle in the potential. Using the semiclassical approximation to calculate instanton paths in Euclidean time, we find that momentum dissipation greatly enhances the coherent tunnel splitting. In presence of both types of dissipation, the momentum dissipation shifts the critical coupling strength of the dissipative phase transition induced by the position dissipation.

*We acknowledge financial support from the Deutsche Forschungsgemeinschaft (DFG) through ZUK 63 and the Zukunftskolleg, and by the MWK-RiSC program.
Symmetry Breaking and Phase Transition in a Driven-Dissipative Kerr Oscillator

X. H. H. ZHANG (Presenter), HAROLD U BARANGER, Duke University — We show that quantum many-body effects can appear in a single non-linear oscillator that is driven by an external field in the presence of dissipation. This simple system is a paradigmatic example of open quantum many-body systems in which there has been great interest recently due to recent experimental advances such as quantum simulation. Here, weak non-linearity plays the role of the thermodynamic limit. Using both analytical and numerical methods, we demonstrate $\mathbb{Z}_2$ symmetry breaking and the corresponding phase transition.


Open quantum systems approach to Bose polaron problems with applications

MIGUEL GARCIA-MARCH (Presenter), Univ Politecnica de Valencia, MOHAMMAD MEHBOUDI, CHRISTOS CHARALAMBOUS, ICFO - The Institute of Photonics Sciences, ANIELLO LAMPO, Internet Interdisciplinary Institute (IN3), LUIS A. CORREA, University of Exeter, MACIEJ A LEWENSTEIN, ICFO - The Institute of Photonics Sciences — We discuss the dynamics of one and two quantum impurities immersed in a homogeneous or trapped Bose-Einstein condensate (BEC) in the framework of the quantum Brownian motion model [1-4]. When the impurities are untrapped, we show that the long-time behavior is superdiffusive. For the trapped impurities, we discuss the realistic conditions for the final state to be squeezed or to present entanglement in the two impurities case. We discuss two applications: i) for quantum non-demolition thermometry in a BEC [5]; and ii) to construct a system that permits a heat current between two BECs, and evaluate this system as a thermal diode [6].


12:51PM X01.00009: Universality in the decay and revival of Loschmidt Echoes  MYUNG-JOONG HWANG (Presenter), Division of Natural Sciences, Duke Kunshan University, BO-BO WEI, Physics department, The Chinese University of Hong Kong, Shenzhen, SUSANA HUELGA, MARTIN PLENIO, Institute of Theoretical Physics, Ulm university — Understanding non-equilibrium quench dynamics through a quantum phase transition is an important theoretical task. It has long been observed that a sudden quench dynamics near a quantum phase transition characterised by the Loschmidt echo exhibits a critically enhanced decay. In this contribution, we present the dynamical scaling laws that govern the decay and revival of the Loschmidt echo completely characterised by equilibrium critical exponents of a critical point. We reveal such dynamical scaling laws by analyzing relevant perturbations to the Loschmidt echo cast in a scaling invariant form. We will show the validity and the generality of the predicted dynamical scaling laws using numerical calculation of a diverse range of critical models such as Ising spin models with a short and long range interaction, a finite-component system phase transition, and a topological phase transition. Our finding promotes the Loschmidt echo to a quantitative non-equilibrium probe of criticality and allows for quantitative predictions on the role of criticality on various physical scenarios where the Loschmidt echo is central to describing non-equilibrium dynamics.

1:03PM X01.00010: Analytical Study of Decoherence in Rydberg Atom Qubits  ANANT KALE (Presenter), MANUEL ENDRES, Caltech — Individually trapped neutral atoms are a promising candidate for use in quantum computing and simulation applications. Entanglement can be generated between these atoms via strong dipole-dipole interactions by driving them to highly excited Rydberg states (n>20). However, the fidelity of single qubit operations as well as 2 qubit entangling gates is limited by several decoherence channels of which the dominant ones are finite temperature effects, laser frequency noise and intensity noise. Here we present an analytical (perturbative) expression for the effect of these noise sources on the rabi oscillations of a single atom and a pair of atoms in the Rydberg blockade regime. We derive this result in terms of the power spectral density (PSD) of the noise sources and use it to predict the maximum achievable single qubit and 2-qubit gate fidelities. Using this analytical result, we can appropriately adjust the driving laser’s locking parameters in experiments to modify its PSD and increase coherence time as well as gate fidelities. This work provides crucial insight for upcoming experiments aiming to entangle two alkaline-earth atoms for the first time.

1:15PM X01.00011: Non-Hermitian topological light steering  HAN ZHAO, XINGDU QIAO, TIANWEI WU (Presenter), BIKASHKALI MIDYA, University of Pennsylvania, STEFANO LONGHI, Dipartimento di Fisica, Politecnico di Milano, LIANG FENG, University of Pennsylvania — Photonic topological insulators provide a route for disorder-immune light transport, which holds promise for practical applications. Flexible reconfiguration of topological light pathways can enable high-density photonics routing, thus sustaining the growing demand for data capacity. By strategically interfacing non-Hermitian and topological physics, we demonstrate arbitrary, robust light steering in reconfigurable non-Hermitian junctions, in which chiral topological states can propagate at an interface of the gain and loss domains. Our non-Hermitian–controlled topological state can enable the dynamic control of robust transmission links of light inside the bulk, fully using the entire footprint of a photonic topological insulator.
**1:27PM X01.00012: Quantum Quenches in Coupled Luttinger Liquids: Truncated Spectrum Approach vs Semi-Classics**

ROBERT KONIK (Presenter), CMPMSD, Brookhaven National Laboratory, ANDREW JAMES, Physics, Open University, ANDREW HALLAM, Physics, University of Ghent — We consider a quantum quench of multiple Luttinger liquids. Here we initialize the system by supposing the Luttinger liquids are in their ground state. At t=0 we turn on a tunnel coupling between the liquids. We then study the subsequent time evolution of quantities such as the mode occupation numbers. We show that there are discrepancies between the results as determined by the truncated spectrum approach and a semi-classical treatment. We argue that this difference is real through unitary perturbation theory which is exact at short times. We comment on the relevance of these results for experimental quantum quenches on two coupled Luttinger liquids.

*We acknowledge support by the Office of Basic Energy Sciences, Material Sciences and Engineering Division, US Department of Energy (DOE) under Contract No. DE-SC0012704.

**1:39PM X01.00013: Non-equilibrium dynamics of the Pokrovsky-Talapov model**

VALENTIN KASPER (Presenter), ICFO, JAMIR MARINO, University of Mainz, SICONG JI, JOERG SCHMIEDMAYER, TU Vienna, EUGENE DEMLER, Harvard University — The unprecedented control in AMO systems allows us to study paradigmatic models of solid-state and high-energy physics. In particular AMO systems give us the unique opportunity to study the non-equilibrium physics of systems of closed quantum systems which is difficult or impossible in a solid state or high energy context. In this work we study the non-equilibrium physics of the Pokrovsky-Talapov model which is effectively realized by two Raman tunnel-coupled one-dimensional Bose gases. In particular, we study two quench protocols: a quench from the commensurate to incommensurate phase and vice versa. In particular, we compute the short and medium time dynamics of density and phase fluctuations and comment on the dynamics of emergent defects in this system.

**1:51PM X01.00014: New exact eigenstates in the Lesanovsky model, proximity to integrability and the PXP model, and approximate scar states**

DANIEL MARK (Presenter), Department of Physics, Caltech, CHENG-JU LIN, Perimeter Institute for Theoretical Physics, OLEXEI I MOTRUNICH, Department of Physics, Caltech — Cold Rydberg atoms have received significant recent attention. We study a model of Rydberg atoms in a nearest-neighbor Rydberg blockaded regime, introduced by Lesanovsky in Phys. Rev. Lett. 108, 105301 (2012). This many-body model (which has one parameter $z$) has an exactly known gapped, liquid ground state, and two exactly known low-lying excitations. We discover two new exact low-lying eigenstates. We also discuss behavior of the model at small parameter $z$ and its proximity to an integrable model. Lastly, we discuss connections between the PXP and Lesanovsky models at intermediate $z$. The PXP model describes a recent experiment that observed unusual revivals from a charge density wave initial state, which are attributed to a set of many-body "scar states" which do not obey the eigenstate thermalization hypothesis. We discuss the possibility of scar states in the Lesanovsky model.

Friday, March 6, 2020 11:15 AM - 1:39 PM
11:15AM X02.00001: Modeling and experimental studies of neat and metal-doped stishovite, coesite, and quartz under high pressure.*  ISKANDER BATYREV (Presenter),
MICHAEL C GOLT, ROSARIO C SAUSA, CCDC Army Research Laboratory —
The results of a comparative study of neat and doped silicon dioxide polymorphs (Fe, Ni or Cu) obtained by density functional theory (DFT) at 0 K and at ambient pressure, 10 GPa, and 20 GPa are presented. The metal atoms are introduced at substitutional and octahedral interstitial sites of the crystal, and the relaxed structures are analyzed and ranked according to total energy. Changes in the enthalpy of the neat and doped crystals are estimated at selected temperatures using quantum mechanics molecular dynamics (DFT-MD). We report the modeled enthalpy of the neat and doped crystals, as well as the dependency of the unit-cell parameters, band gaps, and Raman-active modes on pressure, and compare some of these results to those obtained experimentally using a diamond anvil cell. In addition, we present our search results of the high-pressure phases of silicon dioxide using DFT-based evolutionary simulations and report on the stability of the silica phases, as evaluated by convex-hull construction.

*This work was supported in part by a grant of computer time from the DOD High Performance Computing Modernization Program at the ARL, Navy, AFRL, and ERDC DoD Supercomputing Resource Centers.

11:27AM X02.00002: Dynamics of the High-Pressure Phase Transition in 2,4,6-triamino-1,3,5-trinitrobenzene (TATB)*  BRAD STEELE (Presenter), MATTHEW KROONBLAWD, I-FENG W KUO, Lawrence Livermore Natl Lab — Understanding the sensitivity and performance of energetic materials (EMs) requires information on how they respond under extreme conditions. TATB is an insensitive crystalline EM with graphitic-like layers and a resilient 2D intermolecular hydrogen bonded network. Recent static compression diamond anvil cell experiments combined with first-principles calculations found evidence it undergoes a high-pressure phase transition that involves sliding of its graphitic layers. Layer sliding alters the stacking motif and leads to a transition from a triclinic to monoclinic unit cell. In this work, the dynamics of the phase transition under pressure are investigated using density functional theory and a classical force field. Assessments of the thermodynamic drivers and kinetic barriers for the transition are discussed.

*This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344. Thanks to the Laboratory Directed Research and Development Program at LLNL for supporting this study under 18-SI-004.
11:39AM X02.00003: Pseudopotentials for simulations of materials at extreme conditions*

D HAMANN (Presenter), Physics and Astronomy, Rutgers University, Piscataway, NJ and Mat-Sin Research LLC, Murray Hill, NJ, JOHN PASK, Physics Division, Lawrence Livermore Nat. Lab., Livermore, CA — The ONCVPSP approach [1] has been extended to permit deep core electrons to be active and to accurately reproduce atomic scattering properties to high energies. The basic principles of generalized norm conservation and systematic convergence optimization have been preserved. The original algorithms have been revised to permit consistent optimization of multiple pseudo wave functions for each angular momentum. Ground-state benchmark performance with active deep levels is comparable to that for the original 1 and 2 projector valence plus shallow-core potentials. A confined-atom model has been developed to compare pseudo and all-electron atoms at extreme temperatures and pressures, and verifies the accuracy of the extended potentials up to temperatures which ionize deep core electrons. The open-source oncvpsp-4.0.1 code incorporating these advances for scalar- and fully-relativistic treatments is now available.


*This work was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

11:51AM X02.00004: Chemical Potential of Nitrogen at High Pressure and High Temperature: Application to Phase Diagram Calculations of Nitrogen-Rich Compounds*

HANOF ALKHALDI (Presenter), PETER KROLL, University of Texas at Arlington — High-pressure research of nitrogen-rich compounds is driven by a quest for hard materials and compounds with high energy density, but also has implications for planetary science. To predict the formation of nitrogen-rich compounds at high pressure and high temperature, knowledge of the chemical potential of nitrogen at extreme conditions is an indispensible ingredient. Here, we provide models together with intelligible data for the chemical potential of molecular nitrogen at temperature and pressure conditions relevant for experiments in the diamond anvil cell. In combination with first-principles calculations, we derive pressure−temperature phase diagrams readily accessible to guide experimental efforts. We demonstrate the validity of our approach for characteristic systems, including pure nitrogen and nitrogen-rich metal nitrogen phases that have already been discovered at pressures above 50 GPa. We then provide predictions for new metal-nitrogen compounds awaiting their synthesis at high pressure and high temperature.

*This work was supported by the National Science Foundation (award OISE-1743701). The computational work was done by the Texas Advance Computing Center, and by the High Performance Computing facilities at UTA. H.A. is supported by the government of Saudi Arabia.
Finite-Temperature Dynamics of Elemental Electrides Under Extreme Conditions

REETAM PAUL (Presenter), SUXING HU, VALENTIN KARASIEV, Laboratory for Laser Energetics, University of Rochester, NY, STANIMIR BONEV, Lawrence Livermore National Laboratory, CA — Crystalline alkali metals generally exhibit near free-electron behavior at ambient conditions. For sodium at high pressures of above 200GPa, a deviation from such a metallic behavior was found in the insulator hP4 electride phase[1]. We investigated the temperature-induced changes in such systems using density functional theory. For the solid phase, the closure of the band gap with increasing temperature was explored through a comparison between the time scales for electron–phonon and phonon–phonon interactions. However, the more-intriguing aspect has been the observation of a metallic state, upon melting of Na-hP4, with coalescent dynamic electron bubbles rather than a conventional uniform electron gas. In essence, the emphasis of this work is to highlight the differences between the dynamics of the electride phases of pure elements, e.g., Na-hP4, vis-à-vis non-electride phases, e.g. Na-tI19, under thermal effects.


This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856.

A first-principles study on the phase stability of Mg$_{1-x}$Fe$_x$N alloys: the unconventional rock-salt occurrence under high pressure

MARIBEL NUNEZ VALDEZ (Presenter), Goethe University Frankfurt, JOHANNES WAGNER, Helmholtz-Zentrum Potsdam (GFZ) — Due to the large atomic radius difference of Mg and Fe, alloys between them cannot be synthesized at ambient pressure. However, using a combination of high pressure and nitrogen incorporation, Serghiou et al [1] reported a rock-salt (RS) solid solution formation between MgN and FeN. The potential of these materials for applications in spintronics and their structural analog condition to Mg$_{1-x}$Fe$_x$O, one of the most abundant phases of the Earth's interior, require knowledge of their properties. Therefore, we employ ab initio electronic structure calculations based on density functional theory (DFT) to investigate the field stability, structural and magnetic properties of bulk Mg$_{1-x}$Fe$_x$N. Our results provide insights to understand the interplay between pressure and composition to stabilize the RS structure and the rise/suppression of magnetism in the solid solution.


M. Núñez Valdez is also at the Helmholtz-Zentrum Potsdam (GFZ).

*This work is funded by the Helmholtz Association. The authors gratefully acknowledge the computing time granted by the John von Neumann Institute for Computing (NIC) and provided on the supercomputer JUWELS at Jülich Supercomputing Centre (JSC) under Project ID AblInitioModMatsGeo.
**Local Hydrodynamic Pressure for Strongly Inhomogeneous States**

JAMES DUFTY (Presenter), JEFFREY WRIGHTON, Physics, University of Florida, KAI LUO, Geophysical Laboratory, Carnegie Institution for Science —

Continuum descriptions of complex systems, both classical and quantum, are increasingly adopted as alternatives first principles many-body analyses. The macroscopic momentum balance equation has its origin in the underlying exact conservation law, with a precisely defined operator for the associated momentum flux. Its average in a local equilibrium ensemble provides the basis for a hydrodynamic description. In particular, a local pressure is defined in terms of the trace of the average momentum flux. Other definitions for a local pressure are possible, such as a local virial pressure or a thermodynamic pressure obtained from the grand potential for local equilibrium. It is shown that all three local pressures have the same global pressure but differ locally, except for weakly inhomogeneous states. For uniform temperature, the trace of the momentum flux agrees with the local thermodynamic pressure even for strong density inhomogeneity.

This provides an important connection to density functional methods for hydrodynamic applications. For non-uniform temperatures and strong inhomogeneities there is no simple relationship among the different definitions of the local pressure, so the proper choice is that from the average momentum flux.

*Supported by US DOE Grant DE-SC0002139.

**32 Ages of the universe in just 2 weeks: High-speed Shock-waves in DFT**

JACOB WILKINS (Presenter), Oxford e-Research Centre, University of Oxford, MATT I. J. PROBERT, Department of Physics, University of York — To date, the ab initio exploration of materials in extreme conditions has focused on equilibrium studies. However, this fails to capture the dynamic effects commonly seen in the shock-waves used to reach extreme conditions experimentally. In order to more accurately reproduce these mechanisms, we have developed a partially fire-and-forget approach to induce a series of independent shocks into the medium, to determine the shock response of the material.

We have also used optimisations of the Hugoniostat[1] approach tailored to ab initio calculation, so that we can use DFT-based methods to accurately calculate a complete Hugoniot in a single calculation. Using the series of isolated shocks and a predictor algorithm to approach the target pressure in uniform steps. From this, we can extract an ideal coupling parameter, reducing the calculation time, even for extreme compressions.

These two distinct improvements make it feasible to perform ab initio shock studies with high accuracy in DFT. We demonstrate these capabilities with simulations of shocks in quartz.

12:51PM X02.00009: Study of compaction, preheating and strength in shock compressed porous silica  JASON KOSKI (Presenter), KEITH A JONES, TRACY JOHN VOGLER, J MATTHEW D LANE, Sandia National Laboratories — The shock response of porous silica is investigated using molecular dynamics. We develop Hugoniot curves of amorphous SiO$_2$ as a function of initial preheat temperature for $T = 300K$ to $T = 600K$ and a range of porous states ranging from full density (2.2 g/cc) down to aerogel densities (0.22 g/cc). We focus on relatively low shock pressures (under 6.0 GPa) where the compaction state changes significantly in this regime. We show peak and residual shear stress plots as a function of pressure for this system. We find that the overall strength is dependent on the compaction state of the material, which is a function of both the initial temperature and initial porosity.


1:03PM X02.00010: Accelerating the characterization of energy landscapes with swarm intelligence and machine learning*  LI ZHU (Presenter), RONALD COHEN, TIMOTHY A STROBEL, Carnegie Inst of Washington — The prediction of reaction pathways for solid-solid transformations remains a key challenge. Here, we develop a pathway sampling method via swarm intelligence and graph theory and demonstrate that our PALLAS method is an effective tool to help understand phase transformations in solid-state systems. The method is capable of finding low-energy transition pathways between two minima without having to specify any details of the transition mechanism a priori. We benchmarked our PALLAS method against known phase transitions in cadmium selenide (CdSe) and silicon (Si). PALLAS readily identifies previously-reported, low-energy phase transition pathways for the wurtzite to rock-salt transition in CdSe and reveals a novel lower-energy pathway that has not yet been observed. In addition, PALLAS provides detailed information that explains the complex phase transition sequence observed during the decompression of Si from high pressure. We also introduce a computationally efficient approach based on machine learning techniques, allowing us to map the energy landscapes efficiently. The PALLAS methodology represents a promising tool for materials by design with valuable insights for novel synthesis.

*This work was supported by DARPA under Grant No. W31P4Q1310005.
1:15PM X02.00011: Anomalies in thermal properties of ferromagnesite \((\text{Mg}_{1-x}\text{Fe}_x)\text{CO}_3\) across the spin transition*

HAN HSU (Presenter), CHRISTIAN CRISOSTOMO, National Central University, Taiwan, WENZHONG WANG, ZHONGQING WU, University of Science and Technology of China — Ferromagneiste \((\text{Mg,Fe})\text{CO}_3\) is considered as a major carbon carrier in the Earth’s lower mantle. Thorough knowledge of this mineral at high pressure \((P)\) and temperature \((T)\) can thus provide valuable insights to the Earth's deep carbon cycle. With \(\text{Fe}^{2+}\) substituting \(\text{Mg}^{2+}\) in the octahedral site, \((\text{Mg,Fe})\text{CO}_3\) undergoes a spin transition from the high-spin \((\text{HS}, S = 2)\) to the low-spin \((\text{LS}, S = 0)\) state at 45–50 GPa. Previous static calculations [1] adopting the local density approximation + self-consistent Hubbard \(U\) (LDA+U_\text{sc}) method have successfully explained the spin transition and accompanying volume/elastic anomalies observed in room-temperature experiments. Here, by combining LDA+U_\text{sc} with lattice dynamics, we compute the thermal properties of \((\text{Mg,Fe})\text{CO}_3\) at high-\((P,T)\) conditions. Our results indicate that nearly all thermal properties, including thermal expansion, Grüneisen parameter, heat capacity, and thus thermal conductivity, are significantly changed by spin transition. Geophysical and geochemical consequence of spin transition in \((\text{Mg,Fe})\text{CO}_3\) can thus be expected.


*The work is primarily supported by the Ministry of Science and Technology of Taiwan under Grants No. MOST 107-2112-M-008-022-MY3 and 107-2119-M-009-009-MY3.

1:27PM X02.00012: Shock compression of dry Air*

NILANJAN MITRA, SUBHADEEP PAL (Presenter), Indian Institute of Technology Kharagpur — A molecular dynamics based shock compression study is presented for dry air. Dry air is modeled to consist of 78.08% of Nitrogen, 20.95% of Oxygen and 0.97% of Carbon-dioxide. Shock Hugoniot curves are developed for air under various initial temperature and pressure conditions simulating air at various mean-sea-level altitudes. Reactive potentials have been used for the simulations and possibilities of dissociation and ionization of the gaseous molecules along with chemical reactions between the gasses have been investigated. Equation of state parameters are also derived from the MD simulations for use in continuum simulations.

*Research funded by ONR-Global

Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X08 DQI: Qubit Coherence and Noise Characterization 104 - Kevin Young, Sandia National Laboratories
11:15AM X08.00001: Anomalous Charge Noise in Superconducting Qubits  CHRIS WILEN (Presenter), BRADLEY CHRISTENSEN, ALEXANDER M OPREMCKA, AMEYA RISWADKAR, LARA FAORO, LEV B IOFFE, ROBERT F MCDERMOTT, University of Wisconsin - Madison — We describe experiments to probe fluctuations in offset charge in weakly charge-sensitive superconducting qubits that depart from the transmon regime. We explore a range of device geometries to elucidate the surprising scale dependence of charge noise in these qubits, and we describe experiments to investigate possible spatial correlation in charge fluctuations in neighboring devices. Since quantum error correction schemes such as the two-dimensional surface code rely on the assumption of uncorrelated noise, these studies could have implications for scale-up towards fault-tolerant superconducting qubit arrays.

11:27AM X08.00002: Phonon traps reduce the quasiparticle density in superconducting circuits  FRANCESCO VALENTI (Presenter), FABIO HENRIQUES, THIBAULT CHARPENTIER, MARC LAGOIN, CLEMENT GOURIOU, Karlsruhe Institute of Technology, MARIA MARTÍNEZ, Universidad de Zaragoza, LAURA CARDANI, MARCO VIGNATI, INFN-Sezione di Roma, LUKAS GRUENHAUPT, DARIO GUSENKOVA, JULIAN FERRERO, SEBASTIAN T. SKACEL, WOLFGANG WERNSDORFER, ALEXEY V. USTINOVI, Karlsruhe Institute of Technology, GIANLUIGI CATELANI, Forschungzentrum Jülich, OLIVER SANDER, IOAN-MIHAI POP, Karlsruhe Institute of Technology — Out of equilibrium quasiparticles (QPs) are a main source of decoherence in high impedance superconducting quantum circuits. Despite significant progress in the understanding of QP dynamics, pinpointing their origin and decreasing their density remain outstanding tasks. The cyclic process of recombination and generation of QPs implies the exchange of phonons between the superconducting film and the underlying substrate. Reducing the number of substrate phonons with frequencies above the spectral gap of the superconductor should result in a reduction of QPs [1]. Indeed, we demonstrate that surrounding high impedance resonators made of granular aluminum (grAl) with lower gapped thin film aluminum islands increases the internal quality factors of the resonators in the single photon regime, suppresses the noise, and reduces the rate of observed QP bursts [2]. The aluminum islands are positioned far enough from the resonators to be electromagnetically decoupled, thus not changing the resonator frequency, nor the loading. We therefore attribute the improvements observed in grAl resonators to phonon trapping at frequencies close to the spectral gap of aluminum, well below the grAl gap.

11:39AM X08.00003: Photon-assisted charge-parity switches in superconducting qubits*
KYLE SERNIAK (Presenter), Yale University, MANUEL HOUZET, Univ. Grenoble Alpes, CEA, INAC-Phelips, Grenoble, France, GIANLUIGI CATELANI, JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Germany, SPENCER DIAMOND, MAX HAYS, VALLA FATEMI, MICHEL H. DEVORET, LEONID GLAZMAN, Yale University — Here we identify a mechanism by which stray photons, with energy large enough to break Cooper pairs, can cause decoherence in superconducting qubits. Similar to decoherence induced by steady-state nonequilibrium quasiparticles, these photon-assisted tunneling (PAT) processes are associated with a change in the charge parity of the qubit. This enables the separation of these quasiparticle-related processes from other contributions to decoherence. Our theory predicts similar rates of PAT-induced relaxation and excitation of the qubit, in agreement with recent experiments. This talk will detail the similarities and differences between PAT processes and decoherence induced by nonequilibrium quasiparticle tunneling.

*Work supported by: ARO, NSF, ANR, and AFOSR

11:51AM X08.00004: Microscopic charging and in-gap states in superconducting granular aluminum*
FANG YANG, Institute for Nanoelectronic Devices and Quantum Computing, Fudan University Shanghai, TIM STORBECK, THOMAS GOZLINSKI, LUKAS GRUENHAUPT (Presenter), IOAN-MIHAI POP, WULF WULFHEKEL, Physikalisches Institut, Karlsruhe Institute of Technology — Granular aluminum (grAl) is a viable material for high-impedance quantum circuits [1], thanks to its high kinetic inductance, low microwave frequency losses [2], and fabrication by deposition of pure aluminum in an oxygen atmosphere. The material’s microstructure – pure aluminum grains in non stoichiometric aluminum-oxide – can be modeled as a Josephson junction array [3], in which the oxide thickness is controlled by the oxygen partial pressure during deposition. Here we present scanning tunneling microscope measurements of the local electronic structure of superconducting grAl and we confirm an increased superconducting gap in the grains of films with $\rho \approx 300 \, \mu\Omega\text{cm}$ and $\rho \approx 2000 \, \mu\Omega\text{cm}$. In the high resistivity film, we find Coulomb charging effects, a first indication for grain decoupling, and in-gap states on individual grains, which could contribute to flux noise and dielectric loss not only in devices employing grAl, but also in pure aluminum circuits, where such states could form in Josephson junctions or in oxidized aluminum surfaces.


*This work was supported by the Deutsche Forschungsgemeinschaft and the Alexander von Humboldt Foundation.
**12:03PM X08.00005: Probing non-equilibrium quasiparticle populations in superconducting quantum circuits.**

JAMES FARMER (Presenter), DARIAN HARTSELL, HAIMENG ZHANG, EVANGELOS VLACHOS, ELI M LEVENSON-FALK, Univ of Southern California — Non-equilibrium quasiparticle (QP) populations in superconducting quantum circuits are a limiting source of decoherence. When properly phase biased, nanobridge Josephson junctions provide sub-gap bound states for QPs and so function as QP traps [1]. The occupation of a trap state by a QP alters the inductive contribution of the junction to its host circuit. Thus, the population of QPs trapped in the junction can be directly measured by probing the resonance of a capacitively shunted nanobridge with standard superconducting qubit hardware. By measuring QP trapping in real time and performing statistical analyses, one can infer information about the QP generation, annihilation, and trapping mechanisms. We discuss these single-shot fidelity measurements of QPs trapping in the junctions of a nanobridge SQUID embedded in a superconducting resonator. We further discuss the use of our device as a tool for measuring QP properties and for testing methods of QP mitigation. [1] E. M. Levenson-Falk, F. Kos, R. Vijay, L. Glazman, and I. Siddiqi, Phys. Rev. Lett. 112, 047002 (2014).

*This work was supported by the AFOSR Young Investigator Program grant FA9550-19-1-0060 and by the NSF grant DMR-1900135.

**12:15PM X08.00006: Improved material loss measurement using cryogenic resonator testbed**

HAOZHI WANG (Presenter), COREY RAE MCRAE, KEEGAN MULLINS, University of Colorado, Boulder, JOSH MUTUS, DAVID FORK, Google, DAVID PAPPAS, NIST Boulder — Loss measurements are critical for the superconducting qubit community as the coherence of quantum systems are limited by loss through energy relaxation. The standard procedure for measuring loss is to design and fabricate resonators that incorporate the material-under-test and measure the temperature, power, and geometry dependence. By analyzing the transmission $S_{21}$ data on complex plane, it is possible to extract the internal quality factor, $Q_i$, i.e. the inverse of the loss tangent of the material. However, there are several variations of experimental set-up, measurement and fitting algorithms used in the field. This results in uncertainty when comparing $Q_i$ values between research groups. In this talk, we will compare the results of different measurement configurations, especially for input and output line filtering and isolation, and quantify the accuracy of loss measurement in order to identify best practices for resonator measurement and setup procedures.

**12:27PM X08.00007: Detection of non-equilibrium quasiparticles in charge sensitive transmons**

CIHAN KURTER (Presenter), MARTIN O SANDBERG, VIVEKANANDA ADIGA, ZLATKO MINEV, AARON FINCK, IBM Tj Watson Research Center, ANDREW EDDINS, ROBERT M SHELBY, IBM Almaden Research Center, MARKUS BRINK, JERRY M. CHOW, IBM Tj Watson Research Center — Non-equilibrium quasiparticles are considered possible sources causing decoherence in superconducting qubits. Thus, exploring the dynamics of quasiparticles is crucial to understand their mechanism and how to minimize their presence in superconductors. Here, we study charge parity fluctuations in 2D transmon qubits with sufficiently strong coupling and low $E_J/E_C$ ratio. We will show measurements of density of quasiparticles on various qubits to discuss impact on coherence.
12:39PM X08.00008: Experimental study of flux noise in nanowire transmons subject to an applied magnetic field*  
THIJS STAVENGA (Presenter), Delft University of Technology, FLORIAN LUTHI, Intel Corporation, ELMORE VAAL, OLUWATUMININU ALUKO, Delft University of Technology, PETER KROGSTRUP, Niels Bohr Institute, University of Copenhagen, LEONARDO DICARLO, Delft University of Technology — Flux noise is generally the dominant dephasing mechanism in transmon qubits using SQUID loops as a tunable inductive element. Continuing experimental research ambitions to elucidate the microscopic origin and mitigation of flux noise. In this work, we experimentally investigate flux noise using an unconventional knob for circuit QED: an applied magnetic field. We first present various changes introduced to our circuit QED system to further extend the field compatibility of resonators and nanowire transmons beyond 70 mT. Next, we use standard coherence measurements and sensitivity analysis on and off flux sweetspots to investigate the dependence of flux noise on field applied along the axis of the two constituent nanowire junctions.

*Research funded by the ERC Synergy Grant QC-lab, Microsoft Corporation, and the Danish National Research Foundation.

12:51PM X08.00009: Surface spin induced 1/f flux noise dependent on SQUID geometry (1)*  
LEON DING (Presenter), JOCHEN BRAUMUELLER, ANTTI VEPSALAINEN, YOUNGKYU SUNG, MORTEN KJAERGAARD, Research Laboratory of Electronics, Massachusetts Institute of Technology, TIM MENKE, Harvard University; Research Laboratory of Electronics, Massachusetts Institute of Technology, RONI WINIK, Research Laboratory of Electronics, Massachusetts Institute of Technology, DAVID K KIM, BETHANY NIEDZIELSKI, ALEXANDER MELVILLE, JONILYN YODER, CYRUS F. HIRJIBEHEDIN, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, WILLIAM OLIVER, Department of Electrical Engineering and Computer Science, Department of Physics, Massachusetts Institute of Technology; MIT Lincoln Laboratory — Magnetic flux noise is the dominant source of dephasing in tunable superconducting qubits. While the mechanism behind this 1/f flux noise is poorly understood, it has been proposed that it originates from random fluctuations of spin impurities located on the surface of SQUIDs. A previously proposed microscopic model predicts that flux noise increases with the perimeter and decreases with the wire width of the SQUID loop. Here, we demonstrate the validity of this model by measuring the flux noise amplitudes of about 50 capacitively shunted flux qubits over a wide range of geometric SQUID parameters. Our results show good agreement with the proposed model assuming independent spins, and may therefore serve as a guide on how to improve SQUID designs to minimize 1/f flux noise.

*This research was funded in part by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), and the Department of Defense (DoD) via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the ODNI, IARPA, the DoD, or the U.S. Government.
Surface spin induced 1/f flux noise dependent on SQUID geometry (2)*
JOCHEN BRAUMUELLER (Presenter), LEON DING, ANTTI VEPSALAINEN, YOUNGKYU SUNG, MORTEN KJAERGAARD, TIM MENKE, RONI WINIK, Massachusetts Institute of Technology MIT, DAVID K KIM, BETHANY NIEDZIELSKI, ALEXANDER MELVILLE, JONILYN YODER, CYRUS F. HIRJIBEHEIDIN, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, WILLIAM OLIVER, Massachusetts Institute of Technology MIT — The dominant source of decoherence in frequency tunable superconducting qubits is 1/f flux noise, presumably originating from local magnetic spin impurities located at the surface of their SQUID loops. Here, we measure the flux noise amplitudes of capacitively shunted flux qubits and study their dependence on geometric parameters of their SQUID loops. Our data show good agreement with a previously presented microscopic model for independent spin impurities which has so far eluded experimental verification. We discuss limitations of the proposed model for superconducting films of finite thickness and provide numerical simulations of the current distribution in our SQUIDs, which can refine the considered model. Finally, we apply and confirm our results by observing consistently low flux noise amplitudes in samples with optimized SQUID parameters – small perimeters and large wire widths.

*This research was funded in part by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), and the Department of Defense (DoD) via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. Opinions, interpretations, conclusions, and recommendations are those of the authors and are not necessarily endorsed by the US Government.

Characterizing non-classical non-Gaussian noise: photon shot noise fluctuations*
YUXIN WANG (Presenter), AASHISH CLERK, University of Chicago — Understanding how to accurately describe environmental noise is of crucial importance for designing control protocols that enable high-fidelity quantum operations. While standard approaches often assume classical Gaussian noise, going beyond these assumptions is important in many settings. Here, we consider both the non-classical and non-Gaussian nature of photon number fluctuations in a driven dissipative quantum resonator; such fluctuations can be a significant limitation on the performance of superconducting qubits. We extend the Keldysh approach for characterizing this quantum noise [1,2] to calculate its frequency-resolved third cumulant, the so-called bispectrum. We discuss how the quantum noise bispectrum directly reveals features of non-classicality and non-equilibrium bath dynamics. We also show how this quantum bispectrum could be measured using standard experimental tools in circuit QED.


*This work was supported as part of the Center for Novel Pathways to Quantum Coherence in Materials, an EFRC funded by the US DOE, Office of Basic Energy Sciences.
1:27PM X08.00012: Identifying Noise Sources via Multi-level Quantum Noise Spectroscopy*
YOUNGKYU SUNG (Presenter), ANTTI VEPSALAINEN, JOCHEN BRAUMÜLLER, FEI YAN, JOEL WANG, MORTEN KJAERGAARD, RONI WINIK, PHILIP KRANTZ, ANDREAS BENGTTSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology MIT, DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, MOLLIE SCHWARTZ, JONILYN YODER, MIT Lincoln Laboratory, TERRY PHILIP ORLANDO, SIMON GUSTAVSSON, WILLIAM OLIVER, Research Laboratory of Electronics, Massachusetts Institute of Technology MIT — Identifying dominant sources of noise and mitigating or eliminating them is crucial for engineering robust quantum devices. Although existing quantum noise spectroscopy (QNS) protocols provide insight into noise sources by measuring the noise power spectral density, they do not directly identify the physical origin of the noise process. Here, we develop and experimentally validate a multi-level QNS protocol using a superconducting transmon qubit as a spectrometer. This technique has two notable implications: First, it expands the applicability and spectral range of a qubit spectrometer beyond the two-level approximation. Second, it can be applied to higher excited levels, which enables us to extract and identify the noise contributions from multiple noise sources.

*This research was funded by the ARO grant No. W911NF-14-1-0682; and by the Department of Defense via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government.

1:39PM X08.00013: Measuring effective temperatures of qubits using correlations
ANATOLY KULIKOV (Presenter), ROHIT NAVARATHNA, ARKADY FEDOROV, The University of Queensland — Initialization of a qubit in a pure state is a prerequisite for quantum computer operation. Qubits are commonly initialized by cooling to their ground states through passive thermalization or by using active reset protocols [1, 2]. To accurately quantify quality of the initialization and to shed light on origin of spurious excitation one requires an accurate tool to measure the excited state population [3]. We propose a new technique of finding the excited state population of a qubit using measurement correlations in time. We experimentally implement the proposed method using a circuit QED platform and compare its performance with previously developed techniques [4]. The method does not rely on having high-fidelity measurement or the higher energy levels. We measure the spurious qubit population with accuracy of up to ≈0.01% and discuss its possible sources.

Photon Shot Noise Limited Charge Sensitivity in a Hybrid Quantum System

SISIRA KANHIRATHINGAL (Presenter), MILES BLENCOWE, BENJAMIN BROCK, ALEXANDER J RIMBERG, Dartmouth Coll — Hybrid mesoscopic quantum systems serve as essential building blocks for quantum information and metrology devices. One such system that displays a rich variety of behavior in the quantum-classical regime is a Cooper pair transistor embedded in a quarter wave cavity (cCPT). As one application, this device can act as a highly sensitive charge detector, and form the basis for an optomechanical system in the single photon strong coupling regime. We present a theoretical analysis of the photon shot noise limited charge sensitivity of the device, assuming a low average photon number drive. This lower bound is difficult to achieve using conventional detection approaches, owing mainly to the low frequency noise caused by the coupling of thermally activated two-level-fluctuators to the cCPT. The effects of this interaction are observed as 1/f noise in the microwave cavity fundamental resonance frequency. Using careful calibration of a feedback mechanism called Pound-Drever-Hall (PDH) locking, we should be able to observe this noise near the low photon limit. Moreover, a modified PDH scheme may possibly suppress this noise, and achieve charge sensitivity close to our theoretical, minimum shot noise prediction.

*This work was supported by the NSF under Grant Nos. DMR-1807785, DMR-1507400.

Characterization of noise correlations in superconducting quantum circuits

TENGHUI WANG (Presenter), FENG WU, JINGWEI ZHOU, HAO DENG, GENGYAN ZHANG, XUN JIANG, WENLONG YU, HSIANG-SHENG KU, CHUNQING DENG, Alibaba Quantum Laboratory, Alibaba Group — Superconducting quantum circuits have been an important platform to realize a scalable quantum computing system. Qubit decoherence, which is caused by the fluctuations of its environment, remains a main obstacle to realize fault-tolerant quantum computing. To reduce decoherence, it is important to identify the source of fluctuations by precisely characterizing its correlations. Prevalent methods only consider the second order correlation under the Gaussian approximation. However, environment with higher order correlations is not uncommon in mesoscopic quantum systems. Based on a weak measurement scheme [1], we present an experiment to detect high-order correlations in a superconducting circuit. We verified the scheme by reconstructing the noise power spectral density and compared the results with that obtained from dynamical decoupling. We also demonstrated the characterization of higher-order correlation of the environment.

Reference:

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X16 DQI: Superconducting Qubits: 3D Integration and Cryogenic Packaging 201 - Josh Mutus, Google Inc.
11:15AM X16.00001: Scalable packaging for superconducting qubits with vertical wiring*
SHUHEI TAMATE (Presenter), YUTAKA TABUCHI, Research Center for Advanced Science and Technology, The University of Tokyo, LASZLO SZIKSZAI, KOICHI KUSUYAMA, KUN ZUO, Center for Emergent Matter Science, RIKEN, YUJI HISHIDA, WEI QIU, HIROTAKA TERAI, National Institute of Information and Communications Technology, MASAHIRO UKIBE, GO FUJII, KAZUMASA MAKE, NAOYA WATANABE, KATSUYA KIKUCHI, National Institute of Advanced Industrial Science and Technology, YASUNOBU NAKAMURA, Research Center for Advanced Science and Technology, The University of Tokyo — Superconducting quantum circuits are one of the most promising platforms for realizing a large-scale quantum computer. To implement realistic quantum error correction codes, such as surface codes, we aim at integrating a two-dimensional array of superconducting qubits in a scalable way. Therefore, a natural strategy for the chip packaging is to use the third dimension for the wiring. Here we demonstrate a packaging scheme for a qubit chip, where coaxial cables for the control and readout of qubits are vertically connected to the backside of the chip. The electrical contacts between the superconducting circuits and coaxial cables are provided by spring probes and superconducting through-silicon via. We will present the design and performance of the chip and package.

*This work was supported by JST ERATO (Grant No. JPMJER1601) and MEXT Q-LEAP (Grant No. JPMXS0118068682).

CHAN U LEI (Presenter), LEV KRAYZMAN, SUHAS GANJAM, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Yale University — Superconducting quantum circuits provide a promising platform for quantum information processing. Resonant modes found in superconducting enclosures can be engineered to offer superior coherence and a better electromagnetic environment than their planar analogs. Here, we will discuss the Multilayer Microwave Integrated Quantum Circuit (MMIQC). This platform combines the high coherence of 3D superconducting enclosures with the lithographic precision and versatility of existing MMIC (Monolithic Microwave Integrated Circuit) technology to realize quantum modules that are both scalable and highly coherent. In this talk, we will present an overview of the MMIQC architecture and the ability to realize modular quantum networks.

*US Army Research Office grant W911NF-18-1-0212.
Multilayer Microwave Integrated Quantum Circuits: Part 2*

LEV KRAYZMAN (Presenter), CHAN U LEI, SUHAS GANJAM, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Yale University — Superconducting quantum circuits provide a promising platform for quantum information processing. Resonant modes found in superconducting enclosures can be engineered to offer superior coherence and a better electromagnetic environment than their planar analogues. Here, we will discuss the Multilayer Microwave Integrated Quantum Circuit (MMIQC). A crucial component of the MMIQC is the realization of a high quality superconducting enclosure. The ability to make such a component necessitates the production of a high quality superconducting seam. In this talk, we will present an indium bump-bonding approach to produce superconducting seams with RF conductance exceeding $10^{10}/\Omega m$.

*US Army Research Office grant W911NF-18-1-0212

Multilayer Microwave Integrated Quantum Circuits: Part 3*

SUHAS GANJAM (Presenter), CHAN U LEI, LEV KRAYZMAN, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Yale University — Superconducting quantum circuits provide a promising platform for quantum information processing. Resonant modes found in superconducting enclosures can be engineered to offer superior coherence and a better electromagnetic environment than their planar analogs. Here, we will discuss the Multilayer Microwave Integrated Quantum Circuit (MMIQC). A crucial component of the MMIQC is the realization of a high quality superconducting enclosure. In this talk, we will demonstrate on-chip microwave resonant cavities with low-power quality factors exceeding 300 million. In addition, we will describe their power and temperature dependence. Finally, we will discuss factors that may limit the performance of these cavities by placing bounds on intrinsic loss mechanisms.

*US Army Research Office grant W911NF-18-1-0212
Superconducting qubits are amongst the most promising platforms towards building near term, practical quantum information processors. As the number of qubits per device increases, package design becomes an increasingly important aspect enabling efficient qubit control. Multiple, often interrelated factors such as spurious modes, conduction losses, and crosstalk impose challenges that require a comprehensive approach to package design. Here, we provide an overview of our recent work aimed at addressing these challenges, including chip-to-board interconnect design, interposer design, and material choices. We present results from simulations of these elements and corresponding physical measurements on a newly designed package.

*This research was funded in part by the ARO grant No. W911NF-18-1-0411; and by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.
12:15PM X16.00006: 3D Integration with Protected Qubits*  ANJALI PREMKUMAR (Presenter), ANDRAS GYENIS, PRANAV MUNDADA, ANDREW HOUCK, Princeton University — Large-scale quantum computation will require 3D integrated architectures to achieve all-to-all connectivity, individual qubit addressability, and protection against crosstalk and decoherence channels. A central challenge in 3D quantum hardware is ensuring that additional materials and structures (such as dielectrics) do not suppress qubit lifetimes. Thus far, 3D integration schemes have typically involved a vacuum region between the qubit and other structures to avoid dielectric loss [1,2,3]. In this talk, we propose to use intrinsically protected qubits for 3D integration: resistance to dielectric loss allows for simple layered structures similar to classical 3D architectures. We show that disjoint support in fluxonium qubits leads to relaxation times \(\sim 10\text{ms}\), even when low-quality-factor SiN is deposited on top. We demonstrate a two-layer fluxonium device fabricated with techniques common in single-layer processing. The ideas explored here will allow for simple, repeatable fabrication processes for 3D quantum processors based on protected qubits.


*This research was supported by the NSF GRF and the ARO.

12:27PM X16.00007: Quantifying the impact of a caps and vias architecture for superconducting qubits  KEITH JACKSON (Presenter), ANDREW BESTWICK, SHANE A CALDWELL, MATTHEW J REAGOR, Rigetti Quantum Computing — Scaling high-fidelity superconducting quantum processors to hundreds of qubits requires low on-chip crosstalk at both DC and microwave frequencies, control of the microwave environment seen by each qubit, and accurate coupling strengths between specific modes. To enable this, we describe a chip architecture that combines superconducting caps with recessed cavities bump bonded to a quantum IC with superconducting vias. We describe measurements showing the impact of both caps and vias across a 16+ qubits, including data that enable us to separate out the effects of caps, vias, and the placement of the cap indium bumps on device crosstalk.

12:39PM X16.00008: Design Considerations for Near-term Quantum Processors  ANNA STOCKKLAUSER (Presenter), Rigetti Quantum Computing — Progress in the development of quantum computing systems based on superconducting qubits brings more and more near-term applications within reach. Accelerating this progress requires improvements in the reliability and manufacturability of quantum chips and other specialized components as quantum processors approach 100+ qubits. This talk will address challenges and solutions in the design and fabrication of superconducting qubit-based quantum processors related to scaling, 3D integration, and device operation. We will discuss how these improvements support progress towards demonstrating practical near-term applications with variational algorithms on hybrid quantum-classical machines.

The presented work is the result of a cross-team effort at Rigetti Computing.
Cryogenic Thermalization Measurements of Microwave Attenuators*
ANIKET MAITI (Presenter), VIJAY JAIN, LUIGI FRUNZIO, ROBERT SCHOELKOPF, Yale University — Dephasing due to residual thermal photons in readout cavities is a leading factor in limiting the coherence of superconducting qubits. This thermal noise originates from strong cavity drives and poor thermalization of microwave attenuators. It has been shown that cold attenuators could allow one to approach the qubit decoherence limits imposed by $T_1$ [1]. We thus study the thermalization of cryo-attenuators by using a coaxial stub cavity over-coupled to a microwave input line for absolute temperature measurement. In particular, we look at the power dependence and the time constant for the temperature of a few attenuator designs, and discuss strategies for improvement.


*We acknowledge support from the U.S. Army Research Office Grant Nr. W911NF-18-1-0212

Dilution-equivalent solid-state chip refrigeration* ALBERTO RONZANI (Presenter), JANNE LEHTINEN, EMMA MYKKANEN, ANTTI KEMPPINEN, LEIF GRÖNBERG, ANTTI MANNINEN, MIKA PRUNNILA, VTT Micro & Nanoelectronics — Cooling below 100 mK is an operative prerequisite in several quantum technology applications. It is typically achieved in expensive He3/He4 dilution refrigerators, where massive thermal payloads are cooled to very low temperatures over the course of tens of hours. Yet, in several quantum devices, only few miniaturized active elements are required to reach such low temperature levels.

Here we present a multi-stage thermionic cooler, targeting the 1.5K to 100 mK range. Its core concept consists in suspending silicon substrates with semiconductor-superconductor tunnel junctions, providing both phonon isolation and efficient electron cooling of chip-level payloads.

Compared to dilution refrigeration, our approach reduces sub-kelvin cooldown times to few seconds and benefits from intrinsically maintenance-free operation. Furthermore, the negligible system mass and footprint are optimally suited to compact turnkey systems and are especially ideal for space-borne applications.


*We acknowledge H2020 programme projects EFINED and MOS-QUITO (766853, 688539), Academy of Finland projects Centre of Excellence QuMOS, ETHEC (312294, 288907, 287768, 322580).
1:15PM X16.00011: Hot electron measurements below 100 mK for quantum devices*

ZACHARY STEFFEN (Presenter), SUDEEP DUTTA, RUI ZHANG, YIZHOU HUANG, KUNGANG LI, FREDERICK C WELLSTOOD, BENJAMIN PALMER, University of Maryland, College Park — Recently, the electron-phonon coupling constant of the resistive alloy material nichrome (NiCr) was estimated as $\Sigma_{\text{NiCr}} = (5 \times 10^8) \text{ Wm}^{-3}\text{K}^{-5}$ from measurements of the dephasing rate of a superconducting transmon qubit coupled to a NiCr attenuator [1]. In this talk, we will discuss ongoing measurements to more directly measure the electron temperature and find the electron-phonon coupling constant of NiCr. In particular, we have fabricated NIS junctions consisting of NiCr/AlOx/Al structures and measured the current voltage characteristics at temperatures down to 20 mK. These measurements will be used to extract the electron temperature of the NiCr material which can be compared to the previously reported value, allowing for more accurate thermal modeling of future NiCr devices.


*F. C. Wellstood and S. K. Dutta were supported by the Maryland Quantum Materials Center and the Joint Quantum Institute.

1:27PM X16.00012: Extending Superconducting Qubits Out of Plane (Part 1): Qubits with Air Bridge Crossovers in Multi-Tier Stacks*

JONILYN YODER (Presenter), JUSTIN MALLEK, DAVID K KIM, DONNA-RUTH YOST, GREG CALUSINE, RABINDRA DAS, ALEXANDRA DAY, ALEXANDER MELVILLE, BETHANY M NIEDZIELSKI, DANNA ROSENBERG, MIT Lincoln Laboratory, GABRIEL ORR SAMACH, MIT Lincoln Laboratory, Massachusetts Institute of Technology, MOLLIE SCHWARTZ, STEVEN WEBER, MIT Lincoln Laboratory, WILLIAM OLIVER, MIT Lincoln Laboratory, Massachusetts Institute of Technology — Out-of-plane connectivity within superconducting quantum circuits enables increased complexity and wiring density. We are developing heterogeneous 3D integration of a qubit tier combined with an interposer with high-aspect-ratio superconducting through-silicon vias and a superconducting multi-chip module. In part 1 of this talk, we will focus on circuit complexity within the superconducting qubit tier, including implementation of air bridge crossovers (1) to increase mutual inductance by directly embedding them within qubit and coupler loops, (2) to improve connectivity of the ground plane, and (3) as a method for routing wires and circuit elements past each other.

*This research is funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the U.S. Government.
1:39PM X16.00013: Extending Superconducting Qubits Out of Plane (Part 2): Through-Silicon Vias*  JUSTIN MALLEK (Presenter), JONILYN YODER, DONNA-RUTH YOST, RABINDRA DAS, ALEXANDRA DAY, DANNA ROSENBERG, GREG CALUSINE, MATTHEW COOK, EVAN GOLDEN, DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, MOLLIE SCHWARTZ, COREY STULL, SERGEY TOLPYGO, WAYNE WOODS, WILLIAM OLIVER, MIT Lincoln Laboratory — Addressing complex arrays of high coherence qubits is a necessary capability for the construction of a quantum processor. To enable high connectivity of superconducting qubits we are utilizing heterogeneous 3D integration of a qubit tier, an interposer with high-aspect-ratio superconducting through-silicon vias (TSVs), and a superconducting multi-chip module. In part 2 of this talk we will focus on the fabrication of TSVs within the interposer tier and their implementation within multi-tier stacks.

*This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

1:51PM X16.00014: Quantifying Losses in Transmon Qubits*  GREG CALUSINE (Presenter), WAYNE WOODS, ALEXANDER MELVILLE, KYLE SERNIAK, DAVID K KIM, JONILYN YODER, WILLIAM OLIVER, MIT Lincoln Lab — Reducing losses in superconducting qubit circuits is critical for enabling the development of large-scale quantum computing architectures. This task is especially challenging in the face of variability resulting from device-to-device differences and fluctuating device properties. We apply statistical characterization of sets of superconducting resonators and transmon qubits to overcome variability and quantify loss contributions from a variety of sources such as surface and bulk dielectrics, packaging, and nonequilibrium quasiparticles. As part of this approach, we develop the fabrication processes and EM modeling techniques necessary for accurately modeling dielectric losses. Through this study, we seek to develop a model of qubit losses that allows for iterative improvement in device coherences and consistency.

*This material is based upon work supported by the Department of Defense under Air Force Contract No. FA8721-05-C-0002. Any opinions, findings, conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the Department of Defense.
Effects of surface treatments and packaging on transmon qubits
MATTHIAS MERGENTHALER (Presenter), CLEMENS MÜLLER, MARC GANZHORN, STEPHAN PAREDES, PETER MÜLLER, STEFAN FILIPP, ANDREAS FUHRER, IBM Research - Zurich — The last two decades have seen significant advances in the coherence times of superconducting qubits. However, further progress in transmon coherence times seems to require substantial effort in understanding the remaining limitations due to material interfaces and imperfections, which give rise to two level fluctuators [1-3]. Often, ion milling is an integral part of Josephson junction fabrication and possibly damages the material surface, but its impact on qubit coherence is not well understood and needs experimental investigation.
Here, we present our work towards understanding decoherence mechanisms in flux-tunable transmon qubits. We study the effects of qubit packaging under UHV and controlled atmospheres on the qubit coherence. In addition, we analyze the impact of surface treatments, such as UV light exposure and ion milling, on the qubit parameters. For further insight, qubit coherence and parameter fluctuations are investigated by tracking the coherence times and transition frequencies of multiple qubits over several hours. The resulting noise spectra for different packaging and treatment methods are then compared.


Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X17 DQI: Fabrication of Silicon Qubits 203 - Eleanor Crane, London Center Nanotechnology

State-of-the-art Quantum Dot devices from a full 300mm process line: towards scalable spin qubit devices
HUBERT C GEORGE (Presenter), STEPHANIE BOJARSKI, RAVI PILLARISETTY, BRENNEN MUELLER, LESTER LAMPERT, THOMAS WATSON, FLORIAN LUTHI, ROMAN CAUDILLO, DAVID J MICHALAK, ERIC HENRY, OTTO ZIETZ, JEANETTE MARIE ROBERTS, Components Research, Intel Corporation, ANNE-MARIJE ZWERVER, TOBIAS KRÄHENMANN, GERTJAN EENINK, GIORDANO SCAPPUCCI, MENNO VELDHORST, LIEVEN M VANDERSYPEN, QuTech and Kavli Institute of Nanoscience, JIM CLARKE, Components Research, Intel Corporation — Intel continues with its efforts towards the fabrication of spin qubit devices in a full 300mm process line. Significant progress has been achieved on the fin-based process flow that yields QD devices with performance comparable to academic's state-of-the-art devices. Among other important milestones of this work is the implementation of fin-to-fin charge sensing which is needed to operate in the single electron regime. We will also present updates on wide linear array devices as well as the current status of spin qubit device fabrication; both are key to the long-term implementation of scalable spin qubit devices in silicon for quantum computing technology.
11:27AM X17.00002: The impact of using palladium gates for silicon quantum dot fabrication: defect densities and strain  RYAN STEIN (Presenter), ZAC BARCIKOWSKI, University of Maryland, College Park, JOSHUA POMEROY, MICHAEL DAVID STEWART, National Institutue of Standards and Technology —
Quantum dots (QD) in the silicon MOS system benefit from the use of palladium or platinum for gate materials because the small grain size of these metals compared to aluminum aids in shrinking the gate and dot dimensions. However, it is not clear what differences arise with respect to process-induced defect density and homogeneous strain. Here, we present measurements of oxide defect densities (fixed charge and interface trap density) as a function of forming gas anneal temperature for three different gate metals: Al, Ti/Pd, and Ti/Pt. We also investigate the concomitant effect of these anneals on the mechanical properties of the gate material, such as the intrinsic film stress, coefficient of thermal expansion, and bi-axial modulus. Our initial results indicate that Ti/Pd and Ti/Pt result in much higher fixed charge density and higher, though comparable, interface trap densities when compared to Al. These results provide guidance on adjusting QD fabrication for these gate materials.

11:39AM X17.00003: Revising the point-charge model for dopants in Si and applications to atomic-scale system simulations  KEYI LIU (Presenter), University of Maryland, College Park, PIOTR T. ROZANSKI, MICHAL ZIELINSKI, Institute of Physics, Nicholaus Copernicus University, GARNETT BRYANT, Nanoscale Device Characterization Division, National Institute of Standards and Technology —
Dopants in silicon are strong candidates for qubits in scalable solid-state quantum systems. Tight-binding (TB) theory has been used to provide a good atomic-scale model with reasonable precision when a central cell correction is adjusted to fit to experimental binding energies for one choice of the bulk Si TB parameters. However, this simple model fails to predict the correct dopant level energy degeneracies for many other well-established bulk Si TB models. We argue that the point-charge dopant model with a simple central cell correction is missing vital contributions from the dopant potential that must be included to encapsulate the underlying physics. We have developed a dopant model that includes several new corrections that are obtained explicitly using atomic orbitals to evaluate the appropriate dopant matrix elements rather than by fitting to experiment. We find that these new corrections play a critical role in defining the dopant physics, as all bulk Si TB parameters predict the correct ordering of dopant levels in our new model. Results are discussed to show the effect on interdopant exchange coupling and the level structure of dopant clusters. Finally, we discuss how these models can be utilized to effectively simulate many-body physics in atom chains and arrays.
11:51AM X17.00004: Low-frequency electron spin-qubit detuning noise in highly purified $^{28}\text{Si}/^{28}\text{SiGe}$

TOM STRUCK, ARNE HOLLMANN, RWTH Aachen University, FLOYD SCHAUER, ANDREAS SCHMIDBAUER, Universität Regensburg, VEIT LANGROCK, Forschungszentrum Jülich, OLESIY FEDORETS, RWTH Aachen University, KENTAROU SAWANO, Tokyo City University, HELGE RIEMANN, NIKOLAY V ABROSIMOV, Leibniz-Institut für Kristallzüchtung, LUKASZ CYWINSKI, Polish Academy of Sciences, DOMINIQUE BOUGARD, Universität Regensburg, LARS SCHREIBER (Presenter), RWTH Aachen University — The manipulation fidelity of a single-electron spin qubit gate-confined in a $^{28}\text{Si}/^{28}\text{SiGe}$ quantum dot has recently been drastically improved by nuclear isotope purification [1]. Here, we characterize a $^{28}\text{Si}/^{28}\text{SiGe}$ device with an embedded nanomagnet, a large valley splitting (> 0.2 meV [2]), and a remaining $^{29}\text{Si}$ concentration of only 60 ppm in the strained silicon quantum well layer, which is grown by molecular beam epitaxy. We identify the combination of charge noise and gradient magnetic field as the dominant source of low frequency qubit detuning noise. The power spectral density (PSD) of the charge noise explains the frequency-dependence of the detuning noise PSD, as well as the observation of a decreasing time-ensemble spin dephasing time with increasing measurement time over several hours [3]. We also comment on the role of the remaining nuclear spins in the SiGe barrier on the qubit dephasing and the origin of the observed large valley splitting.


*DFG projects BO 3140/4-1, 289786932; BMBF Contract No. FKZ: 13N14778; QuantERA ERA-NET Cofund in Quantum Technologies implemented within the European Union’s Horizon 2020 Programme.

12:03PM X17.00005: Single-electron control in a foundry-fabricated 2D array of silicon quantum dots

FABIO ANSALONI (Presenter), ANASUA CHATTERJEE, HEORHII BOHUSLAVSKYI, FERDINAND KUEMMETH, Univ of Copenhagen — Two-dimensional quantum dot arrays constitute a useful platform for spin-qubit processors and condensed matter simulations. With the advent of foundry-fabricated silicon qubits [1], larger CMOS quantum dot arrays become increasingly promising for implementing multi-qubit devices. We use a 2x2 array of quantum dots, fabricated fully at CEA-LETI using industrial silicon-on-insulator technology, to reconfigure the array as single, double, triple, or quadruple dots, and use dispersive charge sensing to deplete all dots down to the last electron. Combining high-frequency reflectometry with pulsed-gate techniques, we tune tunneling rates and demonstrate the shuttling of individual electrons within the two-dimensional array.


*We thank Louis Hutin, Silvano De Franceschi and Maud Vinet for providing the LETI FDSOI samples, funded by European Union's Horizon 2020 research and innovation programme under grant agreement No. 688539.
Spin Qubits Confined to a Silicon Nano-Ridge

JAN KLOS (Presenter), BIN SUN, JACOB BEYER, SEBASTIAN KINDEL, LENA HELLMICH, JOACHIM KNOCH, LARS SCHREIBER, RWTH - Aachen — Electrostatically defined quantum dots (QDs) in silicon are an attractive platform for quantum computation based on electron spin qubits. Si qubit devices have been demonstrated by the modification of industrial FinFETs [1]. We propose a scalable qubit device fabricated by industry-compatible processes such as damascene and spacer processes [2]. The device consists of a double array of QDs formed along a silicon nano-ridge. We implement TiN side-gates, a global back-gate and a dense metallic top-gate array for controlling the QDs potentials. In order to minimize potential fluctuations caused by interface roughness and charged defects at the Si/SiO₂ interface, the nano-ridge is anisotropically etched and exhibits atomically flat {111} facets. We characterized its interface roughness and the defect density of the Si/SiO₂ interface. The most relevant process modules are experimentally demonstrated including local oxidation of the silicon nano-ridge, side-gate formation and top-gate fabrication using a low-pitch self-aligned spacer process.


Silicon spin qubit development in a 300 mm integrated process

NARD DUMOULIN STUYCK (Presenter), KU Leuven, imec, ROY LI, STEFAN KUBICEK, FAHD A MOHIYADDIN, BOGDAN GOVOREANU, IMEC, ASSER ELSAYED, MOHAMED SHEHATA, KU Leuven, imec, JULIEN JUSSOT, BT CHAN, IULIANA RADU, IMEC, MARC HEYNS, KU Leuven, imec — Semiconductor spin qubits are developing at a rapid pace with increasing qubit coherence times and quantum gate-fidelities over the last years [1]. This progress has resulted in multiple proposals for large-scale spin qubit-arrays [2-4]. However, scaling up existing qubit prototypes to several qubit arrays require advanced fabrication techniques.

We address this challenge by employing a state-of-the-art 300mm fabrication process [5-6]. In this talk, we present the integration of Si-MOS spin qubit devices in an hybrid integration scheme, which combines e-beam and optical lithography. This enables fast turn-around times while still offering the necessary qubit design flexibility. Furthermore, industrial-scale characterization allows for the room temperature statistical extraction of key device and material parameters. This data and its correlation to low temperature device performance will be discussed, along with the main challenges for further development.


*N. D.S. acknowledges FWO-Vlaanderen for a SB research grant*
12:39PM X17.00008: Industrial quantum dot arrays for spin-qubit quantum computation by all-optical 300mm lithography  TOBIAS KRÄHENMANN (Presenter), ANNE-MARIJE ZWERVER, QuTech and Kavli Institute of Nanoscience, TU Delft, The Netherlands, STEPHANIE BOJARSKI, HUBERT C GEORGE, BRENNEN MUELLER, JIM CLARKE, Components Research, Intel Corporation, Hillsboro, OR, USA, LIEVEN M VANDERSYPEN, QuTech and Kavli Institute of Nanoscience, TU Delft, The Netherlands — Using quantum dot arrays fabricated in a 300mm process line, we demonstrate well-controlled single and double quantum dots formed in an isotopically enriched $^{28}$Si-MOS substrate. These devices are fully fabricated with optical lithography, plasma etching, and chemical-mechanical polishing techniques for patterning, compatible with state of the art industrial fabrication. In the many-electron regime independent tunnel-barrier control is shown, a prerequisite for high-fidelity two-qubit control. Data driven process improvements of the quantum dots have led to a significant increase in charge-sensing sensitivity capable of single shot read-out. Using state of the art charge detection methods, we are able to observe single-electron occupation of these quantum dot arrays. The few-electron regime shows stable device behavior, with dots forming both under the plunger and barrier gates. The occurrence of spurious dots is analyzed. Here, we will show our latest results on utilizing these quantum dot arrays as spin-qubits.

12:51PM X17.00009: Pauli spin blockade for holes in a hot silicon FinFET* SIMON GEYER (Presenter), LEON CAMENZIND, RICHARD J. WARBURTON, DOMINIK ZUMBUHL, ANDREAS V. KUHLMANN, Department of Physics, University of Basel — Quantum information can be encoded in the spin state of a single electron or hole confined to a semiconductor quantum dot (QD) (Loss and DiVincenzo, PRA57, 120 (1998)). Silicon is a particularly promising platform for scalable spin-based quantum computing due to its fully developed, industrial manufacturing processes. Furthermore, a nearly nuclear-spin-free environment can be engineered by means of isotopic purification. Holes in silicon are of particular interest, since they are subject to a strong spin-orbit-interaction, allowing for fast, all-electrical spin manipulation (Maurand et al., Nature Comm. 7, 13575 (2016)). We define single and double QDs in a FinFET-like device architecture. A second gate layer, which is fabricated in a self-aligned process, allows for in-situ adjustments of the tunnel couplings and makes these devices highly tunable. In addition, conventional impurity-doped source and drain contacts are replaced in an overlapping-gate structure by a metallic silicide. We observe Coulomb blockade and, furthermore, Pauli spin blockade for both electrons and holes. The large singlet-triplet splitting allows spin blockade for holes to be observed at temperatures as high as 10 K, paving the way for a hot spin-qubit. 

*Supported by SNSF, SNF, EMP and G H Endress Foundation
Crossbar architecture with individually addressable single electron transistors* PETER BAVDAZ (Presenter), GERTJAN EENINK, JOB VAN STAVEREN, CARMINA ALMUDEVER, FABIO SEBASTIANO, MENNO VELDHORST, GIORDANO SCAPPUCCI, Delft University of Technology — Achieving sublinear scaling of interconnects between room temperature equipment and cryogenic hardware is essential in engineering a practical spin based quantum computer. This requirement is equally present in high throughput characterization for the device fabrication-measurement cycle. In addition to cryogenic multiplexing, the lines into the cryostat can be further reduced at the qubit plane. Here, a sparse crossbar architecture of single electron transistors (SETs) is presented, allowing for the formation of a quadratic number of unique SETs with linearly increasing control lines. We show experimental effort toward realizing crossbars which are operated using a CMOS multiplexer consisting of commercial components at 50 mK capable of supporting up to 648 SETs. These structures provide insight into shared control, enable statistical characterization of substrate uniformity and serve as a platform for device design optimization. Furthermore, by evolving the unit cell, such structures can act as stepping-stones towards proposed fully-coupled crossbar qubit architectures and integration of cryogenic electronics.

*This work is part of the research programme OTP with project number 16278, which is (partly) financed by NWO. M.V. acknowledges support from the NWO Vidi Program.

Silicon quantum dot fabrication with subtractive processing THOMAS MCJUNKIN (Presenter), EVAN R MACQUARRIE, MARK ALAN ERIKSSON, University of Wisconsin - Madison — The overlapping aluminum gate design for silicon quantum dot qubits has shown success in the formation of one and two qubit systems. However, charge noise and device consistency are still major points of concern for silicon quantum systems. Here, we present an alternative approach to silicon quantum dot fabrication, utilizing negative-tone e-beam lithography and subtractive processing to replicate the typical three-layer aluminum gate structure with two layers of palladium gates. Using high-precision HSQ e-beam resist, all plunger, barrier/tunnel, and accumulation gates can be fabricated as a single layer. This eliminates overlay issues and ensures barrier gates, typically written as the third layer, have large action on the dots. The self-oxidation of the three aluminum gate layers is replaced with a single layer of deposited dielectric. Progress towards the realization of a well-controlled, lower noise quantum dot system using etched palladium gates will be presented.
Charge and Hybrid Qubits in 22nm FDSOI process  

ELENA BLOKHINA (Presenter), PANAGIOTIS GIOUNANLIS, School of Electrical and Electronic Engineering, UCD, DIRK R LEIPOLD, IMRAN BASHIR, MIKE ASKER, Equal1 Labs, ALI ESMAILIYAN, HONGYING WANG, TEERACHOT SIRIBURANON, ANDRII SOKOLOV, R. BOGDAN STASZEWSKI, School of Electrical and Electronic Engineering, UCD — A number of recent studies report the achievements of silicon-based qubits. Furthermore, the benefits of nanometer-scale CMOS technologies boost the potential of miniaturization, scalability and full system integration for quantum computers. This abstract presents the recent development of a quantum system-on-a-chip utilizing quantum structures fabricated in 22nm FDSOI. The main challenge of achieving deep cryogenic operation for the mixed-signal classic circuit controlling the quantum core was surpassed by using programmable local heating DACs that slightly boost the local temperature of the die, which needs to be maintained around 4 K. A staged multi-phase operation was adopted for the digital core in order to minimize the quantum decoherence originated in digital noise injection.

We show that the fabricated quantum structures can be used to realize charge and/or hybrid qubits. The theoretical analysis and modeling of qubits are based on a Hubbard model in the tight-binding limit. Different types of qubits (for instance, spin, charge or hybrid) have been examined. Various topologies of interacting qubits are investigated exhibiting maximally entangled states. Preliminary experimental results are also presented.

Improving Gate Dielectrics for Reducing Charge Noise in Si/SiGe Quantum Dots  

NATHAN HOLMAN (Presenter), JOHN DODSON, EVAN MACQUARRIE, University of Wisconsin - Madison, LISA F EDGE, HRL, ROBERT F MCDERMOTT, SUSAN NAN COPPERSMITH, MARK G FRIESEN, MARK ALAN ERIKSSON, University of Wisconsin - Madison — We report on the materials development of a novel low temperature SiO$_2$ gate dielectric for use in Si/SiGe quantum dot devices. X-ray Photoemission Spectroscopy (XPS) measurements show nitric acid oxidation of silicon (NAOS) or silicon-germanium alloys produces a more stoichiometric and thicker silicon oxide over other low temperature techniques [1]. Using this approach, we create a ~1.7 nm SiO$_2$ gate dielectric over the active region of a Si/SiGe quantum dot device coupled to a Nb microwave resonator for charge state readout. By measuring the current noise in a quantum dot we observe a 1/f power spectral density of chemical potential noise with an amplitude of 0.203 μeV$^2$/Hz at 1 Hz which compares favorably to similar devices using ALD Al$_2$O$_3$ and native SiO$_2$ [2]. Further, we demonstrate low frequency Landau-Zener spectroscopy of a double dot charge qubit and discuss cavity-charge coupling experiments [3,4].

References:
Electron spins in silicon have long coherence times and are a promising qubit platform. However, electric field noise in semiconductors poses a challenge for most single- and multi-qubit operations in quantum-dot spin qubits. Here, we investigate the dependence of low-frequency charge noise spectra on temperature and aluminum-oxide gate dielectric thickness in Si/SiGe quantum dots with overlapping gates. We find that charge noise increases with aluminum oxide thickness. Additionally, we observe strong dot-to-dot variations in the temperature dependence of the noise magnitude and spectrum. These findings suggest that each quantum dot experiences noise caused by a distinct ensemble of two-level systems, each of which has a non-uniform distribution of thermal activation energies. Taken together, our results suggest that charge noise in Si/SiGe quantum dots originates at least in part from a non-uniform distribution of two-level systems near the surface of the semiconductor.

*Research was sponsored by ARO grant numbers W911NF-16-1-0260 and W911NF-19-1-0167. We gratefully acknowledge Lisa F. Edge of HRL Laboratories, LLC. for the epitaxial growth of the SiGe material.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X18 GSNP: The Statistical Physics of Real-world Networks II
11:15AM X18.00001: The statistical physics of real-world networks: standing on Jaynes’ shoulders* [Invited]  FABIO SARACCO (Presenter), Networks Unit, IMT School For Advanced Studies Lucca —

In 1957 Jaynes proposed an Information Theory approach to derive the statistical ensembles of Statistical Mechanics: the maximisation of the Shannon entropy, after constraining the energy of the system, returns exactly the probability distributions of the canonical ensemble. Otherwise stated, Jaynes’ approach consists in fixing some crucial information regarding the description of the system (i.e. the energy) and then maximising the “ignorance” about the unconstrained degrees of freedom.

Recently, the same approach was extended to the study of complex networks. Analogously, the constraints represent some - local or global - informative quantities for the description of the real system, while all other observables are left completely random. This approach provides a reliable benchmark for the analysis of complex networks, to reconstruct a network from a limited information or to highlight the role of local constraints in the ensemble non equivalence. In the present seminar I will review the definition and the evolution of such framework and introduce some of its last applications in different fields, as online social networks, economic and financial systems, biological networks.

* I acknowledge support from the EU project SoBigData (Grant No. 654024) and from the Italian “Programma di Attivita’ Integrata” (PAI), project “TOol for Fighting FakEs” (TOFFEe) funded by IMT School for Advanced Studies Lucca.

11:51AM X18.00002: Complex networks with complex nodes* [Invited]  RAISSA D'SOUZA (Presenter), University of California, Davis — The statistical physics perspective has provided a wealth of understanding about the structure and function of massive networks including phase transition behaviors, non-trivial network structures such as modularity and heterogeneous degree distributions, and the analysis of the dynamics unfolding on networks. It reveals the massive implications that network structure has on network function and resilience. Yet, complementary to this perspective of complex networks, simple networks of nonlinear nodes have been studied extensively in fields of dynamical systems and control theory. Real world networks -- from brain networks to social networks to critical infrastructure networks -- lie at the interface of both, with nonlinear nodes and highly non-trivial network structures. We are at a point in time when there is opportunity for these fields to come together. This talk will survey results of a recent project at three different scales on the complex node versus complex network spectrum, from synchronization in nanoscale oscillations to hierarchy and stability in multilayered social systems of macaque monkeys.

* The speaker gratefully acknowledges support from the US Army Research Office MURI Award No. W911NF-13-1-0340 and DARPA Award No. W911NF-17-1-0077.
12:27PM X18.00003: Percolation in real interdependent networks* [Invited] FILIPPO RADICCHI (Presenter), Indiana Univ - Bloomington — The function of a real network depends not only on the reliability of its own components, but is affected also by the simultaneous operation of other real networks coupled with it. Robustness of systems composed of interdependent network layers is generally framed and characterized in terms of percolation models. In this talk, I will consider three different percolation models that provide different insights on the robustness of real-world interdependent networks. I will first consider the ordinary percolation model and illustrate a theoretical approach consisting in a system of heuristic equations able to approximate the phase diagram for arbitrary networks. Second, I will introduce and characterize the redundant percolation model, a genuine model for interdependent networks where the addition of new layers boosts system robustness by creating redundant interdependencies among network layers. Third, I will generalize the problem of optimal percolation from single-layer to multi-layer networks, and present several algorithms for finding approximate solutions to the problem.

*National Science Foundation (CMMI-1552487) and U.S. Army Research Office (W911NF-16-1-0104).

1:03PM X18.00004: Structure, phase transitions, and message passing in sparse networks [Invited] MARK NEWMAN (Presenter), Univ of Michigan - Ann Arbor — Most networks and graphs encountered in empirical studies, including the Internet and the World Wide Web, social networks, and biological and ecological networks, are very sparse. Standard spectral and linear algebra methods perform poorly when applied to such networks. Message passing methods, such as belief propagation, offer an alternative that can deliver better performance as well as new analytic insights. This talk will introduce the message passing method through a progressive series of examples and illustrate how the method can be used for a wide range of calculations of network structure and function. Among other things, the talk will touch upon the calculation of percolation thresholds, graph spectra, and community structure, the deep connections between message-passing fixed points and structural phase transitions in networks, and a new solution to the long-standing problem of message passing on networks with a high density of short loops.

1:39PM X18.00005: A Networks View on Functional Brain Dynamics: timeseries, behavior and beyond [Invited] TOMMASO GILI (Presenter), Networks Unit, IMT School for Advanced Studies Lucca — Most of what we know about brain functioning comes from the time dependent investigation of its activity through the registration of specific proxies. Neurovascular and electrophysiological timeseries have been vastly used to associate the brain functional segregation with specific behavioral outcomes. In this presentation I will show the networks perspective of brain functioning by highlighting the state-of-the-art of graph embedding in human neuroscience and the fundamental role of functional topology in supporting human behavior in healthy subjects and in neuropsychiatric patients.

Friday, March 6, 2020 11:15 AM - 2:15 PM
Session X19 DBIO: Frontiers in Actomyosin Stress Sensing and the Dynamics of the Cytoskeleton 207 - John Crocker, University of Pennsylvania - Tag(s): Invited

11:15AM X19.00001: Elementary contractile unit and collective motor behavior [Invited]  
JACQUES PROST (Presenter), Curie Institute Paris and MechanoBiology Singapore, CNRS/NUS — After introducing the main features characterizing an elementary contractile unit in cells as studied in M Sheetz lab in Singapore and Columbia New-York, I will recall theoretical results concerning motor collections obtained over the years. In particular I will show how a symmetry breaking transition, emergent feature of a large number of molecular motor collection, underpins a number of biological functions such as muscle oscillations. I will then show how a simple modification of the theoretical framework allows to understand all experimental observations including force build-up followed by a relaxation and the existence of half integer steps in the contraction/relaxation curve, which is a resurgence of a nanoscopic scale in a mesoscopic system.

Myosin filaments reversibly generate large forces in cells  

11:51AM X19.00002: Julie Theriot Invited Talk [Invited] —

12:27PM X19.00003: Dissecting fat-tailed fluctuations in the cytoskeleton with active micropost arrays* [Invited]  
DANIEL REICH (Presenter), Johns Hopkins University — The actomyosin cytoskeleton is critical to a wide range of cellular mechanobiology and mechanotransduction. However, the understanding of the connections between molecular-scale processes and cell-scale mechanical phenomena is not complete. Using active micropost array detectors containing magnetic actuators, we have characterized the mechanics and fluctuations of cells’ actomyosin cortex and stress fiber networks in detail. Both structures show consistent power law viscoelastic behavior and highly intermittent fluctuations with fat-tailed amplitude distributions. In the cortex, the dynamics are dominated by occasional large events, similar to what is seen in earthquakes or systems with avalanches. We have observed this behavior across multiple cell types and substrate stiffnesses, and the regular arrays of microposts enable measurement of the largest events’ symmetry and extent (up to several micrometers), revealing spatiotemporal dynamics resembling that seen in plastic solids. These results suggest that actomyosin components may self-organize into marginally stable plastic networks that give cells their unique biomechanical properties.

*Supported in part by NIH grant HL-127087.
1:03PM X19.00004: How immune cells respond to physical cues – the role of cytoskeletal dynamics* [Invited] ARPITA UPADHYAYA (Presenter), University of Maryland, College Park — The activation of lymphocytes, an essential step in the adaptive immune response, involves the binding of specialized receptors with antigens. This results in large-scale dynamics and re-structuring of the cytoskeleton, and movement of receptors into sub-micron clusters, which are critical for immune cell activation. Antigen presenting surfaces possess a wide variety of physical attributes, which influence cytoskeletal organization and receptor mobility, but how cells respond to these physical cues is not well understood. I will summarize our recent studies that examine how immune cells respond to physical cues such as surface mobility and topography. Regulation of membrane receptor mobility is important in tuning cellular response to external signals, such as during B cell signaling following the binding of B cell receptors (BCR) to antigen. We have used single molecule imaging to examine BCR movement and machine learning techniques to relate receptor trajectories to their signaling states. We find that the dynamic actin network fine-tunes receptor mobility and receptor-ligand interactions, thereby modulating B cell signaling. In vivo, B cells encounter surfaces of antigen presenting cells that are highly convoluted with a wide range of curvatures. We have used nanotopographic surfaces that allow systematic variation of geometric parameters to show that surface features on a subcellular scale influence B cell signaling and actin dynamics. Nanotopography-induced actin dynamics requires BCR signaling, actin polymerization, and myosin contractility. The topography of the stimulatory surface also modulates the distribution of BCR clusters and calcium signaling in activated B cells. Active cytoskeletal control of receptor diffusion may be a general feature that directs how diverse cell types respond to physical stimuli and transduce external signals into internal chemical signals.

*This work was funded by the grants NIH AI122205, NSF PHY 1607645 and NSF PHY 1806903.

1:39PM X19.00005: Cells in microgels: 3D printed microtissues and three-dimensional cell migration [Invited] TAPOMOY BHATTACHARJEE (Presenter), Princeton University, THOMAS ANGELINI, University of Florida — In most natural settings, cells thrive in 3D complex environments. The demand of studying cells in 3D has led to the development of many 3D growth media and various bio-printing techniques. Most 3D growth media use bio-degradable polymer networks; during 3D bio-printing cell-loaded polymeric filaments are spatially arranged that solidify during the printing process to preserve the shape. However, the spatial variation in network structure and the transience of degradable gels make quantitative cell behavior studies in these materials extremely challenging. Moreover, the general approaches of 3D bio-printing rely on intimate interactions between cells and specialized materials. Instead, we have developed a 3D growth medium from the jammed system of granular polyelectrolyte microgels that allows for 3D culture of cells. We find that single cell motility can be altered by varying inter-microgel pore spacing in 3D growth media. The self-healing nature of this growth media allows creation of highly precise tissue like structures by direct injection of cells inside the sacrificial 3D media. Finally, we have characterized the macroscopic rheological behaviors of this 3D medium and related them to the classic polyelectrolyte physics scaling laws that control single-microgel elasticity This work provides a revised approach of 3D cell culture and bio-printing and yields principles for predicting cellular migration and creating complex structures of cells with direct implications for tissue-engineering.
11:15AM X20.00001: Statistical Physics of Noninteracting Bacterial Populations* [Invited]
FARSHID JAFARPOUR (Presenter), University of Pennsylvania — Genetically identical bacterial cells in identical environments display significant variability in their phenotypic behavior; they grow at different rates, divide at different sizes, and have different generation times. With recent advances in single-cell technologies, now we can measure not only the distributions of these quantities but also the subtle correlations between these variables both within and across generations. These statistical descriptions have paved the way for the phenomenological models of cellular growth and division. In this talk, I will take these phenomenological models as the microscopic dynamics of individual cells to quantitatively predict the macroscopic properties of populations both in batch and chemostat settings. In particular, I derive the growth rate of the population, the rate at which a population approaches its steady state, and the rate of neutral genetic drift from the single-cell variables.

*This material is based upon work supported by the National Science Foundation under Grant No. NSF-DMR-1506625.

11:51AM X20.00002: Optimal segregation of key proteins in microbes
JISEON MIN (Presenter), ARIEL AMIR, Harvard University — Asymmetric segregation of key proteins at cell division has been observed in various unicellular organisms, including E. coli and budding yeast. It is often assumed to enhance the fitness of the population. We study the population growth in the presence of asymmetric segregation and find, generically, a phase transition occurring between a regime where asymmetry is beneficial to one where it is detrimental. We investigate the nature of this phase transition in the presence of asymmetry in cell division, stochasticity and multiple key proteins, each of which can be beneficial or deleterious, segregating in different proportions.
Understanding Cell Size Homeostasis and Phenotypic Switching Dynamics during Bacterial Filamentation

YANYAN CHEN (Presenter), JAVIER BUCETA FERNANDEZ, Lehigh University — Colonies of bacteria undergoing filamentation present a noticeable phenotypic diversity in terms of their size and yet homeostasis is achieved. While the mechanism for achieving size homeostasis at a normal size scale is clear, the following questions remain in the context of filamentation. How do filamentous strains achieve size homeostasis? What is the dynamics underlying phenotypic switching? To answer these questions, we have modeled the bacterial growth and division processes during filamentation and performed analyses of experimental phenotypic lineage trees. Our model reveals how making compatible the observed adder-like correlations at the collective level and sizer properties at the individual cell level. We further show that size homeostasis is independent on the division pattern (i.e. what septa are eventually selected for cell cleavage in filamentous cells). Also, our analyses of lineage trees combined with mathematical models suggest that changes in the phenotypic composition of colonies mainly derive from a switch of the growth/division mode. Altogether, our work sheds light on the dynamics of filamentation and helps to understand the transition from a regular to a filamentous phenotype.

Effect of non-genetic inheritance dynamics on the variation in cellular traits [Invited]

HARSH VASHISTHA, MARYAM KOHRAM, HANNA SALMAN (Presenter), Univ of Pittsburgh — Isogenic cell populations exhibit large phenotypic heterogeneity even when experiencing homogenous environmental conditions. The evolution of this heterogeneity is limited in part by the inheritance of cellular traits from one generation to the next. In this talk, we will introduce a new experimental technique based on trapping sister bacterial cells in microfluidic channels immediately after they separate from a single mother. Our new setup allows us to follow the sister cells growth and gene expression dynamics for up to ~100 generations while both cells experience identical environmental conditions. This in turn, provides a quantitative measurement of how identical cells become different over time, which reflects the non-genetic inheritance effects, and reveals their contribution to restraining the variability of cellular traits. Our results show that the inheritance dynamics vary significantly among different cellular traits, and its effects, can extend up to ~10 generations.
12:51PM X20.00005: A large deviation principle linking lineage statistics to fitness
ETHAN LEVIEN (Presenter), SEAS, Harvard University, TREVOR GRANDPRE, Physics department, UC Berkeley, JANE KONDEV, Physics department, Brandeis University, ARIEL AMIR, SEAS, Harvard University — In exponentially proliferating populations of bacteria, a population may double at a rate greater than or less than the average doubling time of a single-cell, depending on the variability and heritability of generation times at the single-cell level. Previous studies have shown that the distribution of generation times obtained from an isolated lineage is, in general, insufficient to determine the population’s doubling time or growth rate, both of which are proxies for fitness. This poses a fundamental challenge for experimentalists who wish to probe the fitness effects of physiological perturbations using single-cell tracking data. Using a large deviation approach, we present a procedure for inferring a population’s fitness from lineage statistics that is independent of the model specifics. Interestingly, the Large deviation structure underlying the population dynamics imposes a fundamental constraint on the accuracy to which one can infer a population’s fitness from finite lineage data.

*Funding was provided by NSF Grant DMS-1902895 (EL), Californian Alliance Research Exchange with NSF Grants 1647273/1742065/1306595/1306683/1306747/1306760 (TG), MRSEC at Brandeis University DMR-1420382 (JK), and NSF CAREER 1752024 (EL,AA)

1:03PM X20.00006: A Sensitivity Analysis of Growth Rate to Perturbations in Essential Gene Expression
PAOLA BARDETTI (Presenter), ENRIQUE ROJAS, New York Univ NYU — Cell growth is one of the most fundamental physiological processes that bacteria perform, yet the mechanisms by which cells achieve specific growth rates are unknown. To elucidate the genetic basis for cell growth, we performed an essential genome-wide stability analysis of single-cell growth rate upon CRISPRi-mediated perturbation in gene expression. We used mechanistic mathematical modeling to interpret our data. We found that acute transcriptional inhibition of expression of a ribosomal subunit resulted in a growth rate decay that could be predicted by the linear correlation between ribosome concentration and growth rate previously reported. While this confirms that ribosome concentration is rate-limiting with respect to growth, transcriptional inhibition of several other genes involved in various processes resulted in much more rapid growth decay. Overall, decay times were heterogeneous even among genes in the same metabolic pathway. Genes whose inhibition yields fast growth-rate decay times represent key regulators of cellular growth rate. We found that the proteolysis of these proteins is critical for their ability to efficiently mediate growth-rate kinetics in response to nutrient shifts.
CHUNG YIN LEUNG (Presenter), ROGELIO RODRIGUEZ-GONZALEZ, GUANLIN LI, YORAI WARDI, JOSHUA WEITZ, Georgia Inst of Tech — The spread of antibiotic-resistant pathogens is a global threat to public health. As such, there is growing interest in alternative antimicrobials including phage, or viruses that only infect bacteria. However, phage therapy has shown inconsistent efficacy in clinical trials, possibly due to heterogeneity in the host immune response. By combining nonlinear population models and animal experiments, we have shown that host immunity can work synergistically with phage to cure an acute respiratory infection. Nonetheless, phage therapy could still fail when phage resistance is high. In such cases, we consider two strategies proposed to enhance the robustness of phage therapy: combining phage with antibiotics and combining different strains of phage (phage cocktail). Our model predicts that host immunity is also required for the efficacy of phage-antibiotic combinations. Finally, we discuss applications of optimal control theory to optimize the dosing and composition of single phage and phage cocktail therapy, and opportunities to extend findings to application of phage therapy to complex spatial environments.

*The work was supported by the Army Research Office grant W911NF-14-1-0402, National Science Foundation grant PoLS 1806606, and National Institutes of Health grant 1R01AI146592-01.

SUCKJOON JUN (Presenter), University of California, San Diego — Bacterial physiology is a branch of biology that aims to understand overarching principles of cellular reproduction. Many important issues in bacterial physiology are inherently quantitative, and the field is currently enjoying its second Renaissance due to physicists. In this talk, I will focus on cell-size control and homeostasis, a fundamental problem that has been rapidly transforming just in the past few years. I will introduce some of the long-standing questions, and explain the answers that experimentalists and theorists have provided so far. Collectively, the emerging picture is likely to answer a general class of problems in biology beyond bacteria, i.e., how individual cells can converge to their average state without invoking any apparent feedback mechanisms.

*Paul G. Allen Frontiers Group, Pew Charitable Trusts, NSF CAREER (MCB-1253843), NIH (R01 GM118565).
11:15AM X21.00001: Reactive Modeling of Silica Synthesis*  ROLAND FALLER (Presenter), Chemical Engineering, University of California, Davis — Reactive Molecular Dynamics can describe complex problems where quantum approaches are too slow and do not properly take into account environmental effects and on the other hand classical molecular dynamics is not capable of describing reactions. ReaxFF is a good model for such systems but it needs to be properly trained for the system at hand. In this study we train a ReaxFF model for silica synthesis as an industrially important question is to characterize silica gels and organo-silicon surface coatings. These are formed by reactive condensation of organo-silicon precursors. The morphologies of silica gels obtained from alkoxy silanes can then be determined using our newly trained models and improved simulation techniques. It is found that the gels obtained from trialkoxysilanes are more loosely bonded, and that the chemistry of the headgroup is important to the gel morphology. We furthermore can describe the chemisorption of alkoxy silanes with organic headgroups to hydroxylated silica surfaces. This approach can also be applied to zeolite synthesis.

*This project was partially supported by Lam Research Corporation.

This project is partially supported by the National Science Foundation under grant 1911267.

11:27AM X21.00002: Evolution of Amorphous Calcium Sulfate Nanoparticles into Crystalline Phases and Development of Short Range Order  CAIYUN JIA (Presenter), Zhejiang University, JAMES J DE YOREO, Pacific Northwest National Lab, BAOHONG GUAN, Zhejiang University — The involvement of amorphous precursors in crystal nucleation remains an important but poorly understood phenomenon in materials science. In particular, the mechanisms by which amorphous precursor evolves to crystalline phase is typically unclear. By maintaining calcium sulfate at a low supersaturation to slow the nucleation rate, we captured amorphous calcium sulfate (ACS) nanoparticles of distinct sizes and shapes, and observed several stages of its evolution. The ACS nanoparticles grow by fusion accompanied by internal structural evolution and gradually develop a layered morphology. Aggregation of the growing ACS particles gives birth to bulk ACS material exhibiting a more compact structure within which crystalline domains form and develop into the gypsum structure. Structural characterization reveals the ACS nanoparticles have a proto-gypsum property ranging from short-range order to medium-range order and that the ACS nanoparticles are hydrous within which elimination of H2O molecules from the first to the second coordination shell of Ca facilitates ions transport and therefore formation of nanocrystalline domains within the amorphous precursors. This finding provides new insights into the evolution of amorphous precursors and their role in multi-stage crystallization.
11:39AM X21.00003: Using neutral atoms to study in situ damage on organic materials
GEORGIOS STRATIS (Presenter), JORDAN D. ZESCH, Physics, The University of Texas at Austin, HENRY PAN, LAUREN J. WEBB, Chemistry, The University of Texas at Austin, MARK G RAIZEN, Physics, The University of Texas at Austin — We use helium atoms excited in a metastable state to characterize in real-time damage induced on organic materials due to electron impact. More specifically, we used a self-assembled monolayer of 11-bromo-1-undecanethiol on gold-coated silicon exposed to 30 eV electron beam. After each electron beam exposure, we probed the sample using helium atoms in $^3S_1$ state that is 19.8 eV above the ground state. Once the helium atoms encounter the sample's surface, they de-excite and the excess energy causes electron emission from the surface. By measuring the kinetic energies of the emitted electrons we can determine chemical changes that occurred between each electron beam exposure. Due to the fact that metastable helium atoms barely damage our sample while being probed, this technique ensures that any chemical changes we observe are solely due to the electron beam impact. This project is part of a broader effort to develop a neutral atom microscope.

11:51AM X21.00004: Quantitatively Accurate Theory to Predict Adsorbed Configurations of Surfactants on Metal Surfaces
SUMIT SHARMA (Presenter), XUEYING KO, ohio univ — We have developed a theoretical model to predict adsorbed configurations of linear surfactant molecules on metal surfaces. Our coarse-grained simulations of adsorption of surfactants show that our theoretical model is quantitatively accurate in predicting adsorbed configurations. We show that depending on the relative interaction strengths of the polar group and the alkyl tails with the metal surface, the linear surfactant molecules either adsorb by lying parallel to the surface to form stripes or adsorb perpendicular to the surface to form a monolayer. In the case of monolayer formation, our theory predicts that adsorbed surfactant molecules will undergo an orientational transition. This orientational transition is seen in simulations and have also been reported in experiments.

*NSF CBET # 1705817

12:03PM X21.00005: Prospects for polarized neutron scattering from substrate molecules prepared via Signal Amplification by Reversible Exchange
GEORGE THURSTON (Presenter), MICHAEL KOTLARCHYK, Rochester Institute of Technology — We calculate and simulate absolute polarized neutron scattering cross sections for prototypical substrate molecules that have been proven to acquire nuclear spin hyperpolarization via Signal Amplification by Reversible Exchange (SABRE), such as pyridine. Because of the dramatic spin-dependence of polarized neutron scattering, combined with degrees of hyperpolarization that can be orders of magnitude in excess of thermal polarizations, such molecules will exhibit scattering cross sections that provide for potentially useful probes of molecular conformation and solution structure. We examine cross-sections for the neutron spin-flip and no-spin-flip cases. Experiments that combine these cross-sections can yield useful partial structure factors, including direct measurements of distances between chosen nuclei. We explore protocols that yield potentially useful signals proportional both to the first and second powers of the degree of nuclear spin hyperpolarization, and address considerations needed for practical implementation.
12:15PM X21.00006: Development of Angle-Dependent Phase Field Crystal Model for Vapor-Liquid-Solid Transitions

ZI-LE WANG (Presenter), State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University, ZHI-RONG LIU, College of Chemistry and Molecular Engineering, Peking University, ZHI FENG HUANG, Department of Physics and Astronomy, Wayne State University, DUAN WENHUI, State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University — As an efficient and fast-developing continuum modeling approach, the phase field crystal (PFC) method is able to resolve systems on atomic length and diffusive timescales. It can well describe system elasticity, plasticity and other important properties by introducing a free energy functional of a conserved atomic density field. However, what is lacking in majority of PFC models is the interaction or coexistence between vapor and condensed phases, an important factor for many physicochemical processes. Here we present a new PFC model based on the angle-adjustable density field formulation we developed before, which incorporates bond-angle dependence of anisotropic interparticle interactions. The relative stability of vapor, liquid and solid phases, the coexistence and transitions between them, and the corresponding interfacial dynamics can be well described by the model. The pressure-temperature phase diagram for pure substance has been obtained, with results consistent with those of some real material systems. Our new PFC model could serve as an effective tool to model realistic experimental processes such as chemical vapor deposition and vapor-liquid-solid growth.

12:27PM X21.00007: Combining Optical Tweezers and Laser Induced Nucleation to Get Liquid Phase Separation and Polymorphically Selective Crystals*

OMAR GOWAYED (Presenter), TASFIA TASNIM, JANICE ABER, BRUCE ALLEN GARETZ, JOSÉ FUENTES-RIVERA, NYU Tandon Sch of Engr — A laser-induced phase-separated (LIPS) solution droplet formed by tightly focusing a continuous-wave, near-infrared laser beam at the glass/solution interface of a mm-thick layer of glycine in D$_2$O was irradiated with a single unfocused ns near-IR laser pulse in order to study the effect of nonphotochemical laser-induced nucleation (NPLIN) on the droplet, as well as to help characterize the behavior of the LIPS droplet. This revealed that NPLIN could nucleate crystals within a LIPS droplet and that the LIPS droplet was observed to be more labile to spontaneous nucleation than the control for the first 40 min of relaxation. The resulting crystals were analyzed using powder X-ray diffraction, and 100% of crystals formed within the LIPS droplet induced by NPLIN and by spontaneous nucleation were α-glycine. The results indicate that the LIPS droplet and the surrounding solution are not equilibrium phases of aqueous glycine, but phases in which gradient optical forces have induced a partitioning of large and small solute clusters.

*This work was supported primarily by the MRSEC Program of the National Science Foundation (NSF) under Award Number DMR-1420073. The authors are grateful for shared facilities provided through the MRSEC program of the NSF under Award Number DMR-1420073.
Separation of Carbon Dioxide from Mixed Vapors by Blockage of Methane in Graphene Nanoribbons* SILVINA GATICA (Presenter), HIND H ALJADDANI, Howard University —
We study numerically the adsorption of a mixture of CO2 and CH4 on a graphite substrate covered by graphene nanoribbons (NRs). The NRs are flat and parallel to the graphite surface, at a variable distance ranging from 0.6 nm to 1.4 nm. We show that the NRs-graphite substrate acts as an effective filter for CO2. Our study is based on Molecular Dynamics (MD) simulations. Methane is considered a spherical molecule and carbon dioxide is represented as a linear rigid body. Graphite is modeled as a continuous material, while the NRs are approached atomistically. We observe that when the NRs are placed 0.6 nm above the graphite surface, methane is blocked out, while CO2 molecules can diffuse and be collected in between the NRs and the graphite surface. Consequently, the selectivity of CO2 is extremely high. We also observe that the initial rate of adsorption of CO2 is much higher than CH4. Overall we show that the filter can be optimized by controlling the gap between NRs and the NRs-graphite separation.

*This work used the Extreme Science and Engineering Discovery Environment (XSEDE) through allocation TG-DMR180036.

On-surface synthesis of graphene nanostructures on non-metallic substrates* MAREK KOLMER (Presenter), Oak Ridge National Laboratory, ANN-KRISTIN STEINER, Friedrich Alexander University Erlangen-Nuremberg, RAFAL ZUZAK, LUKASZ ZAJAC, Jagiellonian University in Krakow, MADS ENGELUND, Espeem S.A.R.L, SZYMON GODLEWSKI, Jagiellonian University in Krakow, WONHEE KO, MIGUEL ANGEL FUENTES-CABRERA, JINGSONG HUANG, AN-PING LI, Oak Ridge National Laboratory, MAREK SZYMONSKI, Jagiellonian University in Krakow, KONSTANTIN AMSHAROV, Friedrich Alexander University Erlangen-Nuremberg — On-surface synthesis of atomically precise carbon-based nanostructures has generated enormous expectations about their potential applications. However, so far selected noble metals have been mostly used as substrates catalyzing the on-surface reactions strongly limiting this perspective.

Here, we will present a method to tackle this long-standing challenge of on-surface synthesis of predesigned carbon nanostructures directly on non-metallic substrates [1]. We will show that thermally triggered intra-molecular C-C coupling is effectively realized on a model transition metal oxide substrate via selective activation of C-F bonds and corresponding cyclodehydrofluorination reactions. Our low temperature STM, XPS and mass spectroscopy experiments prove that flexible oligophenylene chains can be transformed into predesigned nanographene molecules. Finally, we will discuss a strategy to combine C-F bond activation with previous reports on the inter-molecular C-C bond formation [2,3].

[1] M. Kolmer et al., Science, 363, 57-60 (2019);

*Part of work was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a DOE Office of Science User Facility.
1:03PM X21.00010: Anisotropic Ti ionic diffusion giving the anisotropic photo-reactivity in rutile TiO$_2$: A Diffusion Monte Carlo Study  TOM ICHIBHA (Presenter), Materials Science and Technology division, Oak Ridge National Laboratory, ANOUAR BENALI, Computational Science Division, Argonne National Laboratory, KEN'TA HONGO, Research Center for Advanced Computing Infrastructure, JAIST, RYO MAEZONO, School of Information Science, JAIST — Self-diffusion of Ti interstitials is essential for TiO$_2$ photo-catalysts, because it works for maintaining the surface stoichometry and keeping the photo-reactivity. We revisited ab initio evaluations of the barrier energies along the possible diffusion paths of Ti interstitials in rutile TiO$_2$ bulk using diffusion Monte Carlo method. Our calculation predicted that Ti interstitials diffuse faster in parallel to c-axis, reasonably explaining why rutile TiO$_2$ has a superior photo-activity on (001) surface to (110). Our prediction does not support the previous GGA-DFT works, and this discrepancy can be explained by the poor cancellation of the self-interactions in GGA-DFT.

1:15PM X21.00011: Unraveling the mechanism of catalytic water oxidation via de novo synthesis of reactive intermediate*  ALIREZA KARBAKHSH RAVARI (Presenter), Department of Physics and Astronomy, Purdue University — Artificial photosynthesis has the potential to provide carbon-free fuel. The current systems are limited by the lack of understanding of multi-electron water oxidation catalysts (WOC). Trial and error is the only way that new catalysts are being discovered. A thorough spectroscopic analysis of the prototypical [(tpy)(bpy)Ru(H$_2$O)]$^{2+}$ -which is the parent complex in the largest family of WOCs- is presented in this study and will give us a clear understanding of dynamics of this catalyst family. This understanding would help to design a catalyst rationally. De novo synthesis of the reactive intermediate with 2,2'-bipyridine-N-oxide, resulted in a hundredfold catalytic activity compare to the parent compound. In situ Raman spectroscopy along with electrolysis of parent and enriched intermediate shed light on the mechanism of the catalysts. Finally, the redox potential of the ligand was shown to be correlated with the rate of O$_2$production.

*This work was supported by the National Science Foundation, Division of Chemistry CHE-1900476 (Y.P.). Access to EPR was provided by the Amy Instrumentation Facility, Department of Chemistry under the supervision of Dr. Michael Everly.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X22 DBIO: Robophyscis IV and Animal Behavior 303 - Kaushik Jayaram,
University of Colorado, Boulder
Controlling robot dynamics via environmental deformations

HUSSAIN GYNAI (Presenter), SHENGKAI LI, YASEMIN OZKAN-AYDIN, Georgia Inst of Tech, CAMILA DOMINGUEZ, Central Florida University, ENES AYDIN, PABLO LAGUNA, DANIEL I GOLDMAN, Georgia Inst of Tech — In an effort to construct a robophysical analog gravity system, we previously studied the dynamics of a 200-gram differential wheeled robot driving on a deformable spandex membrane (d=2.4m) with a static central depression (Li et al., 2019). The system displays rich dynamics, including precessing orbits reminiscent of those in general relativity. Remarkably, the vehicle-membrane system can be mapped to the dynamics of a test particle in a fiducial spacetime. To take the next step and study how the vehicle dynamics can be manipulated via dynamic non-local changes in membrane curvature, we developed an automated gantry system that can control the position of a spherical object which creates a local deformation on the membrane. From experiments implementing a closed, circular object trajectory, the translating depression can capture the locomoting car from specific initial conditions, depending on initial orientation and position of the car and object trajectories. We explore how feedback from internally based measurements of the vehicle’s tilt and acceleration can enhance capture rates.

Modeling and simulation of complex dynamic musculoskeletal architectures

XIAOTIAN ZHANG (Presenter), FAN KIAT CHAN, TEJASWIN PARTHASARATHY, MATTIA GAZZOLA, University of Illinois at Urbana-Champaign — Natural creatures, from fish and cephalopods to snakes and birds, combine neural control, sensory feedback and compliant mechanics to effectively operate across dynamic, uncertain environments. In order to facilitate the understanding of the biophysical mechanisms at play and to streamline their potential use in engineering applications, we present here a versatile and robust numerical approach to the simulation of musculoskeletal architectures. It relies on the assembly of heterogeneous, active and passive Cosserat rods into dynamic structures that model bones, tendons, ligaments, fibers and muscle connectivity. We demonstrate its utility in a range of problems involving biological and soft robotic scenarios across scales and environments: from the engineering of millimeter-long bio-hybrid robots to the synthesis and detailed reconstruction of complex musculoskeletal systems. The versatility of our methodology offers a powerful framework to aid forward and inverse bioengineering designs as well as fundamental discovery in the functioning of living organisms.

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ONR MURI N00014-19-1-2373
Strategic Research Initiatives (SRI) program of the University of Illinois at Urbana-Champaign
11:39AM X22.00003: Chrono: A multi-physics engine for simulation of robophysical systems

MILAD RAKHSHA (Presenter), RADU SERBAN, DAN NEGRUT, Mechanical Engineering, University of Wisconsin-Madison — Early-stage computer analysis of robophysical systems informs critical design decisions, where systematic study of the design-space via experiment can be challenging and expensive. We present the latest capabilities of a multi-physics platform, called Chrono, that allows for computer modeling and simulation of such systems. The term multi-physics is used herein as a broad umbrella for rigid body dynamics with frictional-contact, flexible body dynamics, fluid dynamics, and fluid-solid interaction. This paradigm is critical in many robophysical systems since locomotion of rigid/flexible robots in conjunction with rigid, granular, and fluid substrates is ubiquitous. The simulation platform supports applications that range from locomotion of robotic agents over non-trivial geometries and on gravel, to underwater robotics. Furthermore, we describe how these simulations can be used as episodes of deep reinforcement learning models for training smart agents who can learn efficient locomotion pathways through machine learning. This is important because (i) fine-tuning the optimum design parameters can be laborious, and (ii) training agents in a virtual environment instead of the real world reduces the time and risks of the operation.


ASHER ELMQUIST (Presenter), RADU SERBAN, DAN NEGRUT, University of Wisconsin - Madison — We present here a simulation infrastructure designed to allow for safe, low-cost, and rapid development, testing, and evaluation of robot control strategies particularly in scenarios that are difficult or impossible to test in reality. The software platform provides (a) simulated dynamics to support interaction between the robots and the environment, (b) simulated sensing to provide the robots with a realistic perspective of the environment, (c) simulated communication to support inter-robot communication used for collaboration and coordination. Support of dynamics allows the exploration of physics-limited scenarios such as slip, collisions, non-linear flexibility, or interaction with fluid. Combining the dynamic simulation with virtual sensing allows us to enhance the capability of the control strategies by exploring sensing limited scenarios such as low light or inclement weather. In addition to dynamics and sensing, simulated communication in the virtual environment allows for coordination that may be used in multi-robot scenarios. These complex scenarios that include dynamics, sensing, and communication are parallelized in this simulation framework such that hundreds of variations can be performed to probe difficult or impossible to test edge-cases.
12:03PM X22.00005: Learning to locomote in the presence of symmetry  SCOTT KELLY (Presenter), Univ of North Carolina - Charlotte — Deep reinforcement learning algorithms provide a paradigm whereby a biomorphic robot can refine a strategy for efficient locomotion based on judicious trial and error, exploiting a biologically inspired architecture for the storage of experiential knowledge. An important feature of this paradigm is its applicability to systems for which accurate mathematical models are unavailable, so that behavioral policies must be constructed directly from sensor feedback. It's commonly the case that even when a mathematical model is unavailable for a system's dynamics, fundamental considerations ensure that symmetries underlie these dynamics. Practical reinforcement learning in a physical setting requires a parsimonious approach to data collection and representation. This talk will discuss the use of symmetry to improve the economy with which a physical robot can learn to locomotive efficiently.

12:15PM X22.00006: Nonlinear distance and velocity estimation from optic flow  FLORIS VAN BREUGEL (Presenter), University of Nevada, Reno — Vision is widely used by animals and robots for position and velocity estimation. Robots typically use stereopsis or feature recognition to extract distance from image data. Stereopsis, however, requires 2 calibrated cameras positioned at a sufficiently large distance, and feature based methods require computationally expensive image processing. These limitations preclude small animals and robots from estimating distance in this manner. What alternative solutions exist? I will review a nonlinear estimation method for separating distance and velocity information from optic flow generated by a single dynamically moving camera. Unfortunately, this approach requires calculating the time derivative of optic flow, a notoriously noisy signal. To overcome this limitation, we use a new neural network optic flow estimator, flownet2, and total variation regularization methods to estimate smooth derivatives. These steps allow us to independently measure distance and velocity from a single dynamically moving camera. We propose that this approach to integrating multiple sensory modalities during dynamic motion, which we refer to as idiokinemetry, is likely a general feature of how animals perceive the world, and may inspire the development of smaller and more robust robotic systems.
Raising head facilitates antenna cleaning in a honey bee*  WEI ZHANG (Presenter), JIANING WU, ZHIGANG WU, School of Aeronautics and Astronautics, Sun Yat-Sen University — Antennae are arguably of significance for honey bees to engage in olfaction, foraging, flying and other physiological behaviors. Contamination on the hairy antennae by dust and pollen is an ineluctable problem. Honey bees have a special structure, namely the antenna cleaner on their forelegs, to clean their antennae with. The antenna cleaner is composed of a deep notch on the ventral surface of the proximal end of the basitarsus and a large spur, which is movable, inserted at the inner angle of the distal end of the tibia. To maintain cleanliness, a honey bee grooms antennae frequently by swinging forelegs with the elaborate antenna cleaner. By high-speed imaging, we find that the honey bee raises its head while grooming antennae by forelegs. By theoretical and experimental combined study, we demonstrate that the head-raising behavior accelerates relative speed by 310% and increases friction force by 70%, which facilitates a swift and efficient grooming stroke. This behavior may inspire next-generation cleaning devices applied in microelectromechanical systems.

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Large scale quantitative phenotyping of aversive behaviour and habituation in C. elegans*  LUIGI FERIANI (Presenter), IDA BARLOW, ADAM MCDERMOTT-ROUSE, ANDRE BROWN, Imperial College London — The nematode C. elegans has been influential in the development of the physics of behaviour, especially in methods for representing and analysing postural dynamics. To apply these methods in the context of genetic and drug screens, we need to be able to record behaviour with high resolution and throughput. We have combined robotic liquid handling, multi-camera imaging systems, and tracking software in a high-throughput pipeline that can record from about 500 samples simultaneously. Quantitative analysis of the spontaneous locomotion of C. elegans already yields a multidimensional phenotype that allows us to detect even subtle drug treatment-induced changes in its behaviour. We have added a wide-area, intense blue LED illumination to our recording system to increase the dimensionality of the explored phenotype space by both analysing the response elicited by a single stimulus, and studying simple of forms of learning such as habituation to repeated stimulations.

*ERC-2016-STG
Using robotics and physics to understand the evolution of novel functional morphologies

BROOKE FLAMMANG (Presenter), Biology, New Jersey Institute of Technology, KAELYN GAMEL, AUSTIN GARNER, University of Akron — Remoras are fishes that attach to other swimming organisms via an adhesive disc evolved from dorsal fin elements. However, the factors driving the evolution of remora disc morphology are poorly understood. Fortunately, the fundamental physics of suction and friction are mechanically conserved through time. Using a morphologically relevant bioinspired remora disc, we experimentally investigated the performance of hypothetical evolutionary intermediates. Herein, we translated fundamental biological principles into engineering design rules and show that a passive model system can autonomously achieve adhesive forces measured in live remoras in any environment. Our experimental results show that an increase in lamellar number resulted in an increase in shear adhesive performance, supporting the phylogenetic trend observed in extant remoras. The greatest pull-off forces measured for our model were on surface roughness on the order of shark skin and exceeded those measured for live remoras attached to shark skin by almost 60%. Overall, relative to fossil remoras and their closest ancestor, extant remoras exhibit a morphology indicative of selection for enhanced shear adhesive performance.

Electrically Programmable Micro-Scale Shape Memory Devices*

QINGKUN LIU (Presenter), WEI WANG, MICHAEL REYNOLDS, MARC MISKIN, MICHAEL CAO, DAVID MULLER, PAUL L MCEUEN, ITAI COHEN, Cornell University — We demonstrate microscale shape memory devices capable of achieving micrometer bending radius with a holding time of several tens of hours. The core of these devices consists of a nanometer-thin platinum layer capped on one side by titanium. Under application of potentials in the range of 1 volt, ions oxidize the platinum, create a differential in stress between the two sides, and cause the structure to bend. Using thick panels we can localize the bending and readily create 3D shapes and patterns that can be reversibly erased and rewritten by short electrical pulses. This electrical programmability can be harnessed to make sequential and bidirectional folding. We demonstrate several reconfigurable 3D patterns, kirigami, and origami motifs. As such these micro-scaled shape memory devices enable a variety of applications in fields ranging from mechanical memory storage to microscopic robots.

*This work was supported by the Army Research Office (ARO W911NF-18-1-0032), the Cornell Center for Materials Research (DMR-1719875), the Air Force Office of Scientific Research (MURI: FA9550-16-1-0031), and the Kavli Institute at Cornell for Nanoscale Science. This work was performed in part at Cornell NanoScale Facility, an NNCI member supported by NSF Grant NNCE-1542018.
1:15PM X22.00011: The radical pair mechanism can provide a sensitive and robust magnetic compass for birds. SHAWN STRAUSSER (Presenter), THORSTEN RITZ, University of California, Irvine — Many adult birds can travel 5,000km or more with a precision of centimeters. Earth's magnetic field provides an omnipresent source of information that aides in this navigation. The mechanism by which animals sense the Earth's magnetic field remains one of the most important problems in sensory biology. The radical pair mechanism (RPM) proposes that the Earth’s magnetic field influences a chemical pathway via electron spins in a radical pair. Recently it has been shown that a so called “quantum needle” radical pair model can be extraordinarily sensitive to directional changes, thus potentially providing the basis for a highly sensitive magnetic. However, it has also been shown that many compass systems are fragile, i.e. that even small, naturally occurring, variations in parameters can abolish effects that are observed in models without considering such noise. Here, we ask what effects noise has on a quantum needle compass system. Rather than reducing the quantum needle, noise is found to either leave the needle intact or even enhance it in some systems. This suggest that a quantum needle based compass may not only be distinguished by a high sensitivity, but also by being unusually robust to noise, making it a highly optimized system for magnetoreception.

1:27PM X22.00012: Breathing from Underground: Diurnal Variability in the Ventilation Mechanism of Termite Mounds SAURABH SAXENA (Presenter), NEDA YAGHOOBIAN, Florida State Univ — Termites are social insects that build massive porous mounds for creating a habitable environment for their colony. These structures exhibit intricate architectures that can effectively harness natural wind, solar energy, and colony’s metabolic heat to produce controlled microclimates in termite nests. Based on experimental studies, several mechanisms have been proposed to explain the ventilation and gas exchange process in termite mounds, such as, metabolism-driven convection, the impact of external wind, and formation of thermal gradients due to diurnal variation of the mound surface temperature. This study investigates the underlying physics of the ventilation mechanisms in termite mounds. Computational fluid dynamics (CFD) modeling is used to simulate flow past and through the porous bodies of termite mounds. For this purpose, the Navier–Stokes equations are modified in a Direct Numerical Simulation using the Darcy-Brinkman-Forchheimer model to represent the porosity. The effect of the diurnally variable surface temperatures is considered through the dynamic coupling of the CFD model with an energy balance-based model that simulates the spatiotemporally variable surface temperatures in high resolution.
1:39PM X22.00013: Specialisation and plasticity in a primitive social insect  
SOLENN PATALANO, BSRC Alexander Fleming, ADOLFO ALSINA, Max Planck Institute for the Physics of Complex Systems, WOLF REIK, The Babraham Institute, STEFFEN RULANDS (Presenter), Max Planck Institute for the Physics of Complex Systems — Biological systems rely on an influx of energy from the environment to build and maintain complex spatio-temporal structures in noisy environments. It has recently become evident that they also have the remarkable capacity to break up and rebuild such structures, exemplified by the capability of differentiated cells to reprogram after injury. Here we use primitive societies of *Polistes* wasps as a model system where we experimentally perturb the nest and follow the re-establishment of the social steady state. We combine a unique experimental strategy correlating measurements across vastly different spatial scales with a theoretical approach to show that *Polistes* integrates antagonistic processes on different scales to simultaneously achieve plasticity and robust specialisation. We show that stability of the nest relies on epigenetic DNA modifications that suppress transcriptional noise. Such dynamics provide a general principle of how both specialization and plasticity can be achieved in biological systems.

1:51PM X22.00014: Hydrodynamics of sheep herds  
RAPHAEL SARFATI (Presenter), University of Colorado, Boulder, MARINE DE MARCKEN, University of Washington, ORIT PELEG, University of Colorado, Boulder — The collective motion of living entities, from cells to wildebeests, is a fascinating and aesthetic phenomenon which continues to intrigue physicists as well as any curious observer. Over the past decade, many compelling findings have come out of the rigorous study of systems such as bird flocks and mosquito swarms, where individuals are scattered and interact remotely. In parallel, slowly-moving aggregates of grasping individuals, such as ants and bees, have been successfully investigated from a material perspective. A third category of interest is now surfacing, in which individuals move collectively while remaining in a near-jamming state. This includes for example crowds of humans, or herds of sheep, which are the focus of this presentation. By employing optical flow methods to measure the velocity field of dense sheep herds, we construct a hydrodynamics framework to study the collective motion of living systems flowing like liquids. The proposed methods are versatile and can be adapted to other flocking systems, such as flamingoes, penguins, etc.

2:03PM X22.00015: The decision-making and mechanics of honey bee swarm formation  
GARY NAVE (Presenter), ORIT PELEG, University of Colorado, Boulder — In late spring and early summer, honey bee colonies may begin the process of swarming, in which the colony will send two-thirds of its population, including the mother queen, to form a new hive. The bees assemble themselves into a temporary hanging cluster for anywhere from a few hours to several days, protecting the queen and young bees while scouts identify a new nest location. While the house-hunting process has been studied, the process of formation has remained overlooked. In this work, we present both experimental results and computational modeling on the process of swarm formation to address questions of decision-making as bees join the swarm and the mechanical properties of bees within the swarm. Using agent-based modeling methods, we identify local decision-making rules that reproduce the experimentally observed behaviors in swarm formation. Understanding the behavior of honey bees during swarming lays the groundwork for improved control strategies for multi-agent robotic systems.
11:15AM X23.00001: The role of physical forces in cortical morphogenesis* [Invited] MARIA HOLLAND (Presenter), University of Notre Dame — Between individuals and across species, brain morphology is strikingly consistent in some significant ways. One example is a characteristic pattern of cortical thickness in gyrencephalic, or folded, brains - thick outer folds, or gyri, and thin inner folds, or sulci. This raises the question: which factors (genetic, biochemical, physical, and/or others) lead to this morphological consistency? In a recent combined theoretical, numerical, and experimental study, we found that the physical forces generated by buckling instabilities were sufficient to generate physiological gyral-sulcal thickness ratios. We now consider the more complex, fully three-dimensional pattern of cortical thickness in the brain, and investigate the role of physical forces in its evolution, consistency, and variability.

*NSF CRII grant: IIS-1850102

11:51AM X23.00002: New directions for the animal shape analysis VASYL ALBA (Presenter), JAMIE CARTHEW, MADHAV MANI, RICHARD CARTHEW, Northwestern University — We used a new precise tool to address a question of quantitative description of the morphological traits in biological systems. We found that directions of natural variation are related to the directions of well-known mutations. We studied a population of fruit flies that were under developmental pressure as well as different species. We found some conserved features in the ensemble variability and identified features that are associated with environmental conditions and with genetic variation.
Surface Stresses Drive Morphological Changes in Three-Dimensional Microtissues

ERIK MAILAND (Presenter), Institute of Mechanical Engineering and Bioengineering, Ecole Polytechnique Federale de Lausanne, BIN LI, Department of Mechanical and Aerospace Engineering, Cornell University, JEROEN EYCKMANS, Department of Biomedical Engineering, Boston University, NIKOLAOS BOUKLAS, Department of Mechanical and Aerospace Engineering, Cornell University, MAHMUT SELMAN SAKAR, Institute of Mechanical Engineering and Bioengineering, Ecole Polytechnique Federale de Lausanne

The formation and maintenance of tissue boundaries is vital for morphogenesis and homeostasis as groups of cells with distinct functions must often be kept physically separated. Cells organize into sheets on the tissue surfaces by forming intercellular mechanical connections directly or through the ECM. The collective dynamics of boundary regulation have been extensively studied with micropatterned epithelial monolayers, whose behavior has been captured using physical models based on nematic liquid crystals. However, less is known about surface effects in 3D fibrous tissues and their contribution to tissue architecture. We developed a high-throughput biomimetic platform for the study of morphogenesis in multilayered 3D microtissues. We performed local mechanical perturbations using a robotic microsurgery system and selective optochemical manipulations using a programmable projector. We show both experimentally and by using computer simulations that cells at the tissue boundary develop surface stresses and, together with contractile cells residing in the core, drive macroscale deformation. We demonstrate that targeted elimination of cells at the tissue surface induces a local stress gradient that leads to tissue morphogenesis.

Mechanoregulation of Valvular Morphogenesis

JONATHAN BUTCHER (Presenter), Cornell University

Defective heart valve morphogenesis is a major cause of preterm fetal death and premature postnatal tissue failure. While much has been learned over the past 30 years regarding the genetic and molecular agents engaged in valve morphogenesis, much less is known about how these networks contribute to cellular and tissue level responses essential for sculpting initially amorphous globular cushions into elongated, thin, and striated leaflets that are competent for long term biomechanical function. Recent studies from our group and others have highlighted that the local mechanical environment within the fetal heart are essential mediators of proper, and when perturbed defective, valvular growth and maturation. We here clarify the embryonic and fetal mechanical environment and elaborate how these mechanical signals coordinate and integrate both canonical valvulogenic signaling programs and previously understudied cellular migration and traction generating programs towards maturation. As this field deepens in its understanding, new opportunities to engineer molecular therapies to harness mechanotransduction and/or mechanosensation could help rebalance disturbed valvulogenic programming, improve anatomical outcomes at birth, and ultimately extend valve performance.

*European Research Council ROBOCHIP (714609).

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Organ Size Coordination by Chemical Signaling

OJAN K DAMAVANDI

Presenter, Syracuse University, DAVID LUBENSKY, University of Michigan — A profound open question in biology is how animals ensure that their body parts have the correct relative proportions given that development is often noisy. For instance, wings of the same fruit fly do not differ in size by more than about 1% in normal conditions. More interestingly, knocking out a single gene (dilp8) responsible for a hormone secreted by the organs in fly larvae leads to increased size asymmetry of 2-3% between left and right wings. Inspired by this example, we model noisy growth of bilaterally symmetric organs and investigate different mechanisms of organ size coordination using a single coordination signal secreted by the organs. We find that generally feedback can help coordinate organs during growth, thus suppressing variability and speeding development, but that no mechanism with a single signal can robustly coordinate final organ sizes. Finally, we show that a particularly appealing mechanism is proportional feedback on growth rate, which best matches the available data on the biological signatures of dilp8 in flies. Our work suggests that while inter-organ feedback is beneficial to development, organs must additionally employ autonomous size specification mechanisms to ensure low asymmetry at the end of growth.

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Generating Cell Fate Patterns via Mechanical Stress in Stem Cell Colonies

HAYDEN NUNLEY (Presenter), XUFENG XUE, JIANPING FU, DAVID LUBENSKY, Univ of Michigan - Ann Arbor — Embryonic development depends on fate specification events in which a field of initially equivalent cells differentiates in a spatially controlled manner. A key example is neural induction in which a strip of cells differentiates into the neural plate, flanked by the neural plate border (NPB). Classic studies of neural induction have confirmed the role of diffusible chemical signals from neighboring tissues; the role of mechanical signals in fate patterning events like neural induction remains poorly understood.

Recent experiments in stem cell colonies on micropatterned substrates demonstrated that neural induction can be recapitulated without exogenous morphogen gradients [1]. We propose a mechanical model for neural induction in which cell fate determines active contractility and in which mechanical stress biases cell fate. This model reproduces a key experimental observation, that the concentric width of the NPB domain is approximately independent of colony size. The model also predicts a non-monotonic dependence of the NPB domain width on substrate stiffness. Preliminary experimental results are consistent with model predictions.


NSF DGE 1256260, NSF CMMI 1917304, NSF-Simons Center for Quantitative Biology Pilot Grant
1:15PM X23.00007: How can proteins take derivatives? MANON WIGBERS (Presenter), Ludwig Maximilian University of Munich, TZER HAN TAN, MIT, FRIDTJOF BRAUNS, TOBIAS HERMANN, Ludwig Maximilian University of Munich — Many cellular processes, such as cell division and cell motility, rely crucially on the dynamic localization of proteins in space and time. These localization patterns emerge collectively from local molecular interactions of proteins. To analyze how the interplay of diffusion and protein interactions on a nanometer scale influence the protein patterns on the cellular scale, the framework of reaction-diffusion models has proven useful. The study of such systems goes back to Turing, who showed how patterns can emerge from a homogenous steady state when two reactive components have different diffusivities. However, in nature, systems typically develop in a heterogeneous and temporally evolving environment and from one pattern into another, rather than from a homogeneous steady state into a pattern.

Here, we study how protein localization patterns arise in heterogeneous systems. We show how localization patterns of upstream regulators dynamically control pattern formation. In particular, we identify concrete mechanisms through which downstream systems can effectively take spatial or temporal “derivatives” of the upstream protein concentration profile. Such mechanisms allow the cell to precisely and robustly control spatial protein organization.

1:27PM X23.00008: Hierarchical “buckling without bending” and brain shape* JENNIFER SCHWARZ (Presenter), MAHESH CHANDRASEKHAR GANDIKOTA, Syracuse University, TYLER ENGSTROM, Physics, William and Hobart Smith College, TENG ZHANG, Syracuse University — While studies of brain shape development have focused on the cerebrum, the cerebellum, otherwise known as the little brain, typically houses more neurons than the cerebrum and has a distinct morphology with 8-10 primary lobes that subsequently branch into smaller lobes. A recent “buckling without bending” model quantifies the onset of shape change in the developing cerebellum. It consists of an inner incompressible core of cells and an outer fluid-like cortical layer of dividing cells encased by a basement membrane. Additionally, there are two types of fibrous cells—ones spanning the cerebellum and ones spanning the cortical layer. The onset of shape change is a consequence of mechanical constraints on the outer fluid-like cortical layer as it proliferates. This model is now generalized beyond the onset of shape change to predict shape development at later stages. In particular, a hierarchical version of the model is implemented to predict subsequent branching of the smaller lobes. Predictions are compared with various mammalian cerebella exhibiting varied counts of branching generations. We also explore how some aspects of “buckling without bending” may lead to a new level of detail for characterizing shape change in the developing cerebrum.

*NSF-DMR-1832002
1:39PM X23.00009: Mechanomorphogenesis of bacterial biofilms*  JING YAN (Presenter), Yale University — Surface-attached bacterial communities called biofilms display a diversity of morphologies. Although structural and regulatory components required for biofilm formation are known, it is not understood how these essential constituents promote biofilm surface morphology. Here, using *Vibrio cholerae* as our model system, we combine mechanical measurements, theory and simulation, quantitative image analyses, surface energy characterizations, and mutagenesis to show that mechanical instabilities, including wrinkling and delamination, underlie the morphogenesis program of growing biofilms. We also identify interfacial energy as a key driving force for mechanomorphogenesis because it dictates the generation of new and the annihilation of existing interfaces. Finally, we discover feedback between mechanomorphogenesis and biofilm expansion, which shapes the overall biofilm contour. The morphogenesis principles that we discover in bacterial biofilms, which rely on mechanical instabilities and interfacial energies, should be generally applicable to morphogenesis processes in tissues in higher organisms.

*Jing Yan holds a Career Award at the Scientific Interface from the Burroughs Wellcome Fund.

1:51PM X23.00010: Quantifying mechanochemical coupling in the actomyosin cortex during early development in vivo  MELIS TEKANT (Presenter), ALEXANDRU BACANU, YOON JUNG, JORN DUNKEL, NIKTA FAKHRI, Massachusetts Institute of Technology MIT — Spatiotemporal symmetry-breaking transitions in biochemical patterns are essential in triggering morphological changes during the development of all life forms, both at the unicellular and multicellular level. The realization of cell and tissue-scale deformations is achieved through intra-cellular force networks that translate localized biochemical signals into effective mechanical stresses that determine the global shape dynamics. However, the mechanochemical coupling between the biochemical patterns, force network activity and the resulting stresses is not well understood. Here, we quantify the local coupling between membrane-bound Rho-GTP and the mechanical deformations of the actomyosin cortex in the starfish oocytes during meiosis. We generate various Rho-GTP dynamic patterns and map the resulting stress patterns via tracking endogenous tracer particles embedded in the cell cortex. This method provides a novel approach to probe the local coupling between biochemistry and mechanics and the resulting morphological changes.
2:03PM X23.00011: The role of environment, material, and function in the morphological diversity of termite mounds  TADEU FAGUNDES (Presenter), JUAN ORDONEZ, NEDA YAGHOOBIAN, Florida State Univ — Several species of termites across the globe construct mound architectures that are of several orders of magnitude larger than themselves. These superstructures exhibit distinctive structural designs that range widely in size and shape. There are several studies exploring the function of termite mound structures, but only a few works explore reasons behind the morphological variety observed in them. To explain this diversity, the present work introduces a computational model that couples the mound’s environment, material, and thermal function to its shape. Using the fundamentals of heat transfer, the model captures the main features observed in termite mounds, such as the mound orientation and spire tilt. The influence of each environmental agent over the mound structure is analyzed, revealing a strong correlation between the mound structure and the combined effects of the environmental forces. The proposed methodology can be used in the prediction of the effect of environmental forces on the thermal performance and architecture of any natural structure for which structural and environmental information can be obtained. As such, this framework provides a broader view of the factors that are effective in the form and function of naturally made structures.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X25 GSNP: Pattern Formation, Chaos, Nonlinear Dynamics III

402 - Thomas Witten, University of Chicago

11:15AM X25.00001: Operator scrambling, hypersensitivity, and quantum Lyapunov spectrum*  BIN YAN (Presenter), NIKOLAI SINITSYN, WOJCIECH HUBERT ZUREK, Los Alamos National Laboratory — This work presents a model study of the quantum inverted harmonic oscillator (IHO), an archetype example for quantum chaotic systems. It is shown that the IHO exhibits hypersensitivity to perturbations, i.e., the Loschmidt echo decays as a double exponential. A quantum Lyapunov spectrum has been introduced to detect the exponential operator growth in chaotic systems. The IHO is demonstrated to possess a quantum Lyapunov spectrum that is identical to the classical one.

*This research was supported in part by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, Condensed Matter Theory Program. BY acknowledges partial support from the Center for Nonlinear Studies at LANL.
11:27AM X25.00002: Non-equilibrium Renormalization Group Fixed-Points of the Quantum Potts Chain*  YANTAO WU (Presenter), Princeton University — We devise a renormalization group recursion relation of the Loschmidt amplitude of the quantum Potts chain. The non-equilibrium fixed-points of the renormalization procedure determine the dynamical phases of the system, giving rising to a dynamical quantum phase transition. We will also discuss how there fixed-points affect the dynamical phase transition of the disordered Potts chain and the Loschmidt amplitude of the excited states.

*DOE Award DE-SC0017865

11:39AM X25.00003: Laminar Chaos in a Mackey-Glass feedback circuit with Variable Time-Delay*  DAVID JIN (Presenter), Grinnell College, JUAN PABLO SPEER, University of Alabama, Birmingham, JOSEPH HART, YANNE CHEMBO, THOMAS E. MURPHY, RAJARSHI ROY, Institute for Research in Electronics and Applied Physics, University of Maryland, College Park — Laminar chaos is a newly discovered chaotic behavior theoretically predicted in 2018 [1], which can be characterized by steady-state phases separated by short and irregular burst-like transitions. It has been observed experimentally in an optoelectronic variable time-delay feedback system implemented with a field-programmable gate array (FPGA) [2]. The Mackey-Glass model, developed to simulate the physiological mechanism of red blood cells, is a common time-delay system that can yield a wide range of periodic and chaotic dynamics. We report here the observation of laminar chaos in an electronic Mackey-Glass feedback circuit, the first observation of its kind, implemented with an Arduino board to produce variable time delays. This unique system implementation allows us to easily create audio signals from laminar chaos that contrast with signals generated by a system with a constant time delay.


*We would like to acknowledge the contributions of Evan Dowling, Don Schmadel, and Daniel Serrano. We would also like to recognize the NSF for funding the TREND REU program (1756179) at the University of Maryland, College Park.
Theory of gating in recurrent neural networks

KAMESH KRISHNAMURTHY (Presenter), Dept. of Physics and Princeton Neuroscience Institute, Princeton University, TANKUT CAN, Initiative for the Theoretical Sciences, The Graduate Center, CUNY, DAVID SCHWAB, Initiative for the Theoretical Sciences, The Graduate Center, CUNY and Facebook AI Research —

Understanding the emergent dynamics of networks of neurons is a central challenge in theoretical neuroscience. Most of the work in understanding the dynamics of these networks has focused on models with `additive interactions', where the input to a neuron is a weighted sum of the output of the rest of the network. However, there is ample evidence from neurophysiology that neurons can have gating or multiplicative interactions, where e.g. one neuron can dynamically decide whether another neuron is influenced by the rest of the network. Such gating interactions lead to qualitatively different behavior of single neurons, and are likely to have even more dramatic effects on the collective behavior of a network. Furthermore, researchers in machine learning have found that gating interactions facilitate training of model neural networks. Thus, gating can have significant implications for information processing. We leverage tools from the field theory of disordered systems to develop a theory of gating in a canonical neural network model. Our theory allows us to elucidate the dynamical aspects of gating which are important for the network's information processing capabilities.

*CV Starr Fellowship (KK); NSF PHY-1734030 (KK, DS); NIH 5R01EB026943, Simons Investigator in the MMLS (DS)

Short-term forecasting of hyperchaotic time series by noisy echo state network

TAKAYA MIYANO (Presenter), AREN SHINOZAKI, Ritsumeikan Univ, YOSHIHIKO HORIO, Research Institute of Electrical Communication, Tohoku University — We have applied a noisy echo state network, wherein pseudorandom numbers subject to uniform distribution are input to the reservoir nodes, to the short-term forecasting of a hyperchaotic time series generated by a star network of nonidentical Lorenz subsystems. The chaotic dynamics have five positive Lyapunov exponents with a Lyapunov dimension exceeding 12. Although the predictive model incurs a large prediction error, it is capable of reproducing the geometric structure of the hyperchaotic attractor with sufficient fidelity. We discuss these results in terms of Ueda's view of chaos, wherein chaotic dynamical behavior is recognized as a piecewise deterministic process with intervening stochastic processes such as numerical round-off errors and perturbations caused by experimental measurements.

*This study was partly supported by JSPS KAKENHI Grant No. 18H03307.
12:15PM X25.00006: Critical branching processes in digital memcomputing machines

SEAN BEARDEN (Presenter), FORREST C SHELDON, MASSIMILIANO DI VENTRA, University of California, San Diego — Memcomputing is a novel computing paradigm that employs time non-locality (memory) to solve combinatorial optimization problems. It can be realized in practice by means of non-linear dynamical systems whose point attractors represent the solutions of the original problem. It has been previously shown that during the solution search digital memcomputing machines go through a transient phase of avalanches (instantons) that promote dynamical long-range order. By employing mean-field arguments we predict that the distribution of the avalanche sizes follows a Borel distribution typical of critical branching processes with exponent $\tau=3/2$. We corroborate this analysis by solving various random 3-SAT instances of the Boolean satisfiability problem. The numerical results indicate a power-law distribution with exponent $\tau=1.51\pm0.02$, in very good agreement with the mean-field analysis. This indicates that memcomputing machines self-tune to a critical state in which avalanches are characterized by a branching process, and that this state persists across the majority of their evolution. [1]


*Work supported in part by CMRR, DARPA, NSF Graduate Reasearch Fellowship, and the Alfred P. Sloan Foundation.

12:27PM X25.00007: Connecting Dynamics and Trainability in Recurrent Neural Networks

TANKUT CAN (Presenter), Initiative for the Theoretical Sciences, The Graduate Center, CUNY, KAMESH KRISHNAMURTHY, Dept. of Physics and Princeton Neuroscience Institute, Princeton University, DAVID SCHWAB, Initiative for the Theoretical Sciences, The Graduate Center, CUNY and Facebook AI Research — Recurrent neural networks (RNNs) are well-suited for complex sequential learning tasks, but are notoriously difficult to train due to the problem of exploding or vanishing gradients (E VG) of the cost function. Local switch-like multiplicative “gates” were introduced to address this issue by modulating inter-neuron interactions and selectively updating the state of the network, promoting longer time scales. As such, these "gated" RNNs seem to mitigate the EVG, making training tractable. However, the specific role of each gate type on dynamics and training remains unclear. We take a dynamical systems perspective to study these questions for two popular gated RNN architectures: the Gated Recurrent Unit (GRU) and Long Short-Term Memory (LSTM). Using random matrix theory, we elucidate how gating enriches the repertoire of dynamical behavior expressed by these networks. Our approach furthermore sheds light on how gating is able to overcome the EVG by shaping asymptotic stability. Finally, we connect the intrinsic dynamics upon random parameter initialization to the subsequent ease of training GRUs and LSTMs.

*KK: CV Starr Fellowship, CPBF Fellowship (NSF PHY-1734030);
DS: CPBF NSF-PHY-1734030, NIH 5R01EB026943, Simons Investigator in the MMLS
12:39PM X25.00008: Misalignment-induced frequency locking in lasers  
NIKETH NAIR (Presenter), YEHUDA BRAIMAN, Oak Ridge National Lab — We study arrays of heterogeneous single-mode semiconductor lasers coupled through an external cavity with facet misalignments. This system can be modeled mathematically as a set of coupled nonlinear delay-differential equations. The heterogeneity, in the form of frequency detuning, is represented as parametric disorder between the oscillators, and the facet misalignments is represented by a small disordering of the time-delays in the coupling terms. In this system, we show that the introduction of time-delay disorder induces perfect frequency locking in a system that otherwise is unable to frequency-lock due to heterogeneous natural frequencies, as well as chaotic behavior.

12:51PM X25.00009: Self-beating*  
KUAN-REN CHEN (Presenter), JIAN-SHIUNG HONG, Department of Physics, National Cheng Kung University, ALEXANDER CHEN, School of Electrical Engineering and Computer Science, The Pennsylvania State University — There are two kinds of nonlinear mechanism. Beat is typical for the kind involving two or more frequencies. The other kind involves only one frequency due to large wave amplitude or weak media. Considering only linear materials and processes, we discover a new mechanism of self-beating to produce a wave function that does not appear to be linear. During a pulsed light being transmitted through a plasmonic slit, a portion of the light pulse transmits as a sub-pulse, while the rest is reflected at the exit interface, propagates a round-trip, and then reaches the exit again. These linear processes repeat. The superposition of transmitted sub-pulses with a phase delay in-between produces a periodic light that beats its original light frequency. Together with the plasma effects of non-uniform dispersion and sub-pulse spreading, self-beating can explain intrigue phenomena observed. The analytical model explains the complicated simulation results.

*Ministry of Science and Technology, Taiwan, and National Center for High-performance Computing

1:03PM X25.00010: Chaotic Dynamics Enhance the Sensitivity of Inner Ear Hair Cells  
JUSTIN FABER (Presenter), DOLORES BOZOVIC, University of California, Los Angeles — Hair cells of the auditory and vestibular systems can detect sounds that induce sub-nanometer vibrations of the hair bundle, below the stochastic noise levels of the surrounding fluid. Hair cells of certain species are known to oscillate without external stimulation. These spontaneous oscillations are believed to be a manifestation of an underlying active mechanism and may play a role in signal detection. We previously demonstrated experimentally that the spontaneous oscillations exhibit chaotic dynamics. We propose that the instabilities giving rise to chaotic dynamics are responsible for the extreme sensitivity of hair cells. We will present experimental measurements of spontaneous and driven hair bundle oscillations. By varying the conditions of the surrounding fluid, we were able to modulate the degree of chaos observed in the hair cell dynamics. We found that the hair bundle is most sensitive to small-amplitude stimulus when it is poised in the weakly chaotic regime. Further, we found that the response time to a force step decreases as the level of chaos is increased. These results agree well with our numerical simulations of a chaotic Hopf oscillator and suggest that chaos may be responsible for the extreme sensitivity and temporal resolution of hair cells.
1:15PM X25.00011: Nonlinear Coherent Perfect Absorbers*  YAQIAN TANG (Presenter), DO HYEOK JEON, TSAMPIKOS KOTTOS, Physics, Wesleyan University — Coherent perfect absorber (CPA) is a resonant mechanism in which a cavity with a minimal amount of losses can completely absorb incident radiation with an appropriately tailored waveform. The cavity acts as an interferometric trap that confines the incident light for long times and thus amplifies the net absorption. Although in current studies, it was assumed that the medium inside the cavity is linear, there are realistic scenarios where nonlinear mechanisms are engaged.

Here we develop the theoretical framework for the design of CPA waveforms under nonlinear conditions. As an example, we use a photonic circuit consisting of an array of coupled resonators with a nonlinear target embedded in the array. A general solution for the design of the incoming waveform is proposed, and a plethora of CPA frequencies that depend on the intensity of the incident radiation is found—a feature that was not present in linear CPAs. Furthermore, we have demonstrated that under appropriate conditions one can realize a CPA degeneracy, which resembles an exceptional point singularity.

*Office of Naval Research via grant N00014-19-1-2480.

1:27PM X25.00012: Recent advances on non-normalizable Boltzmann-Gibbs statistics and infinite-ergodic theory  EREZ AGHION (Presenter), Max Planck inst. for physics of complex systems, DAVID A KESSLER, ELI BARKAI, Bar Ilan Univ — The equilibrium state of a thermal system, in the presence of a strongly confining potential, is given by the famous Boltzmann-Gibbs distribution. This, along with the ergodic hypothesis, are hallmarks of statistical physics. If the potential is weakly confining, the Boltzmann factor is non-normalizable and the particle packet is constantly expanding. This gives rise to many questions. Among them: can we still infer the shape of the potential landscape, by observing the spatial distribution of the diffusing particles? How do we obtain ensemble and time-averaged observables in this case? And what is the entropy-energy relation in this system?

We show that the non-normalizable Boltzmann state is obtained from an entropy maximization principle, in the spirit of the canonical ensemble from standard thermodynamics, as well as from the ground state of the effective Hamiltonian of the system. The ergodic properties of important physical observables, like energy and occupation times in the system, are given by the Aaronson-Darlin-Kac theorem, and a generalized virial theorem is derived. Thus, our work extends the standard thermodynamic theory to a new class of potentials, and provides further strong evidence to the physical significance of infinite-ergodic theory.
Experimental Observation of a Non-Normalizable Boltzmann State

CARSTEN DIETVORST (Presenter), DIEGO KRAPF, Colorado State University — The probability density function of a particle in equilibrium suspended in a fluid follows a Boltzmann distribution, \( P(x) = \exp(-V(x)/k_BT)/Z \), where \( V \) is the potential energy, \( k_BT \) is thermal energy, and \( Z \) is the normalizing partition function. However, there are cases where the Boltzmann distribution is not normalizable and the system cannot reach thermodynamic equilibrium. It has recently been shown theoretically and via simulations that, in many instances, a particle coupled to a heat bath approaches in the long time a non-normalizable Boltzmann state, such that \( P_t(x) = \exp(-V(x)/k_BT-x^2/4Dt)/Z_t \), where \( D \) is the diffusion coefficient and \( Z_t \sim t^{-\alpha} \) [1]. These systems violate the ergodic hypothesis, i.e. the time average of an observable does not converge to the ensemble average in the long time limit. Here, we test these predictions using functionalized polystyrene beads near a charged surface in liquid. The electrostatic potential \( V(x) \sim \exp(-x/\lambda_D) \), with Debye length \( \lambda_D \), yields a non-normalizable Boltzmann distribution. We track charged particles in 3D near surfaces bearing different surface charge densities. Our experiments reveal a non-normalizable Boltzmann state and ergodicity breaking in agreement with theoretical predictions.


Experimental Search for Supradegeneracy*

DANIEL SHEEHAN (Presenter), Univ of San Diego — Recently a new statistical mechanical phenomenon has been formally identified that turns some thermodynamic intuitions on their heads: supradegeneracy [1]. Normally, population inversion (as in lasers) requires nonequilibrium conditions, but supradegenerate systems are predicted to exhibit inversion at equilibrium. If realized, this phenomenon might help lead to improved photovoltaics and to new types of thermophotovoltaics and batteries [2]. Although supradegenerate systems do not appear in Nature, it seems likely that manmade ones can be realized. This talk reviews the current laboratory search for supradegeneracy in condensed matter systems, specifically, in semiconductors and concentration-graded ionomer membranes.


*This research was partially funded by the Laney and Flora Thornton Foundations.
Lacunarity exponents in chaotic systems

MARC PRADAS (Presenter), MICHAEL WILKINSON, School of Mathematics and Statistics, The Open University, UK, GREG HUBER, Chan Zuckerberg Biohub, ALAIN JACK PUMIR, Physics, ENS-Lyon — Many physical processes result in very uneven, apparently random, distributions of matter, characterised by fluctuations of the local density varying over orders of magnitude. Examples include the distribution of stars within galaxies, distribution of debris floating on fluids, distribution of human population, and the distribution of small inertial particles in a turbulent flow. Many of these systems can be described by chaotic dynamical systems and the existence of a power-law describing the high-density regions is consistent with the notion that chaotic systems can have fractal invariant measures. However, the distribution of density in the sparse regions can also have a power-law distribution, with an exponent that we refer to as lacunarity exponent, and which is not related to the fractal properties of the system. Here, we discuss a robust mechanism that explains the wide occurrence of these power laws and gives analytical expressions for the lacunarity exponent in some cases of interest, including simple chaotic models and the problem of particles advected by fluid flow.

*We acknowledge financial support from the Engineering and Physical Sciences Research Council of the UK, grant EP/R041954/1, and from the National Science Foundation, grants PHY11-25915 and PHY17-48958.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X27 DBIO: Physics of Neural Systems

Unifying criticality and the neutral theory of neural avalanches

SAKIB MATIN (Presenter), THOMAS TENZIN, W. KLEIN, Boston Univ — The interest in the question of criticality in the brain has been prompted by experiments which show that the collective firing of neurons (neural avalanches) follow power-law distributions. Three proposed explanations of this emergent scale-free behavior are criticality, neutral theory, and self-organized criticality. We study a model of the brain for which the dynamics are governed by neutral theory and find that the scale-free behavior is controlled by the proximity to a critical point. Our results unify the neutral theory of neural avalanches with criticality, which requires fine tuning of control parameters, and rule out self-organized criticality. We use tools from percolation theory to characterize the critical properties of the neural avalanches and identify the tuning parameters, which are consistent with experiments. The scaling hypothesis provides a unified explanation of the power laws which characterize the neural avalanches. We discuss how our results can motivate future empirical studies of criticality in the brain.
11:27AM X27.00002: Spontaneous spatial symmetry breaking in excitatory neuronal networks and its effects in sparsely connected networks. MIHAI BIBIREATA (Presenter), VALENTIN SLEPUKHIN, ALEX LEVINE, University of California, Los Angeles — We explore the dynamics of the preBötzinger complex, the mammalian central pattern generator with N \sim 10^3 neurons, which produces a collective metronomic signal that times the inspiration. Our analysis is based on a simple firing-rate model of excitatory neurons with dendritic adaptation (the Feldman Del Negro model [Nat. Rev. Neurosci. 7, 232 (2006), Phys. Rev. E 82, 051911 (2010)]) interacting on a fixed, directed Erdős–Rényi graph. In the all-to-all coupled variant of the model, there is a type of spontaneous symmetry breaking in which some fraction of the neurons become stuck in a high firing-rate state, while others become quiescent. This separation into firing and non-firing clusters persists into more sparsely connected networks, but is now determined by k-cores in the directed graphs. It produces a number of features of the dynamical phase diagram that violate the predictions of mean-field analysis. In particular, we observe in the simulated networks that stable oscillations do not persist in the large-N limit, in contradiction to the predictions of mean-field theory. Moreover, we observe that the oscillations in these sparse networks are remarkably robust in response to killing neurons, surviving until \sim 20% of the network remains. This is consistent with experiment.

11:39AM X27.00003: A model for oscillatory gating of information flow between neural circuits as a function of local recurrence MIKAIL KHONA (Presenter), ILA R FIETE, Massachusetts Institute of Technology MIT — Physical connections between neurons are hardwired on the timescale of seconds, but information and signals must be routed flexibly for computation on the same timescales. Many species exhibit circuit-level oscillations with systematic phase relationships between spikes and the regional oscillation. We present a mechanistic neural model of communication, regulated by oscillations. If one or more networks (the “transmitters”) drives a second (the “receiver”) and both network states are periodically modulated, what relationships in their oscillations will allow the transmitter to optimally drive the receiver? As the receiver network moved parametrically from a ‘sensory’ regime to a ‘memory’ regime, we show that the optimal phase offset depends on its operating mode. A sensory network responds optimally when cells are maximally depolarized, or when the transmitter-receiver pair have zero phase offset, while a network with strong recurrent weights, external inputs are drowned out by local contributions when cells are maximally depolarized, and a phase offset of 90 degrees is optimal. Our results generalize to networks with global inhibition, asynchronous inputs and to networks with discrete fixed points in the strong coupling regime.
11:51AM X27.00004: Quasicriticality or Criticality in the brain?* LEANDRO FOSQUE (Presenter), JOHN BEGGS, GERARDO ORTIZ, Indiana Univ - Bloomington, RASHID WILLIAMS-GARCIA, Mathematics, University of Pittsburgh —
Recent experimental studies (Fontenele et. al. 2019) show that critical exponents for size and duration distributions of avalanches in cortical activity are scattered across, clustering around a dynamical critical scaling relation line. Had one assumed these samples were in critical states and all brains, across species, belong to the same universality class, then we should have only observed one point on that scaling line. So, why do experiments show a spread of points along the scaling line, even within the same species? The quasicriticality hypothesis (Williams-Garcia et al. 2014) states that the brain operates in a quasicritical state, which allows optimal information processing, given external stimulus. We conjecture that those experimental results are consistent with quasicriticality. We further show evidence, by performing numerical simulations of our cortical branching model (CBM), of quasicriticality. Thus, the quasicriticality hypothesis is consistent with the observed scattered data along the dynamical critical scaling relation line.

*1513779 NSF Robust Intelligence Program.

12:03PM X27.00005: Compression as a path to simpler models of collective neural activity* LUISA RAMIREZ (Presenter), Univ Fed de Minas Gerais, WILLIAM S BIALEK, princeton university —
Experiments now make it possible to observe, simultaneously, the electrical activity of hundreds or even thousands of neurons in a small region of the brain. But making models that capture the behavior of these real neural networks easily leads to a combinatorial explosion of complexity and we need explicit strategies for simplification. In many condensed matter systems, interactions are local, but this is not an effective guide for neurons. More abstractly, interactions may be compressible, so that the influence of the whole system on each degree of freedom can be represented by just a few bits of information. We test this idea, analyzing experiments from the vertebrate retina and the mouse hippocampus. Data sets are large enough to provide reliable sampling of activity patterns in subgroups of neurons, and within these groups we find, for example, that the influence of eight neurons on one neuron can be captured almost completely with just ten states, much less than the 256 possible states. This compression can be iterated, providing a path to describing the influence of the whole network on each neuron with a much reduced number of parameters.

*Travel grant support.
12:15PM X27.00006: Effects of local excitations on large-scale brain network dynamics: Insights from coupled Wilson-Cowan oscillators under perturbative stimulation
EVANGELIA PAPADOPOULOS (Presenter), CHRISTOPHER LYNN, University of Pennsylvania, DEMIAN BATTAGLIA, Aix-Marseille University, DANIELLE BASSETT, University of Pennsylvania — Composed of many coupled dynamical units, the brain is a canonical example of a complex network. At the macroscale, it consists of large neuronal populations that generate time-varying activity and that interconnect via a web of anatomical links. However, despite recent progress, we still lack a mechanistic understanding of how large-scale brain networks shape system-wide dynamics, and specifically, how local changes in neural activity affect functional interactions across the brain as a whole. Motivated by a vast literature suggesting that synchronization of activity underlies the coordination of distinct brain areas, we combine structural connectivity data and biophysical modeling to study how regional excitations of activity modulate network-wide synchrony. By employing computational modeling, we examine how the impacts of excitations depend on the location of the perturbation, and, crucially, on the baseline state of the system. Furthermore, we uncover state-specific relationships between brain network properties and the effects of local excitations on the coherence of network dynamics. As a whole, this work provides insight into how local changes in neural activity can propagate via structural links to cause distributed alterations to inter-regional communication patterns.

12:27PM X27.00007: Robust simplicity in the multimodal sensory control of insect flight.
SIMON SPONBERG (Presenter), VARUN SHARMA, Georgia Inst of Tech — Animal movement combines many physiological and physical systems to enable agility and robust behavior. Frequently the behavior that’s manifest can be described, at least in specific experimental contexts, by relatively low order, and often linear, dynamical systems. How does this simplicity arise from the component systems and are the emergent dynamics preserved in the face of changes of context? Insect flight is a challenging task with unstable mechanics and control requirements on the order of a single wingstroke. Using an agile hawk moth, Manduca sexta, tracking a robotic flower during foraging behavior we have shown that the underlying frequency response is linear, time invariant on the scale of 10’s of seconds, and relies on the linear superposition of vision and touch (via the moth’s long proboscis). However, as light levels drop the dynamics of the visual system adjusts, producing slower responses and reduced visual-motor gains. Does the simple emergence remain? We show that the mechanical, touch response to the flower also adjust correspondingly to produce a robust linear superposition of the two cues across contexts. In high and low light cases the two sensory system partition the frequency domain and this partition shifts as light levels dim.
12:39PM X27.00008: Scalable maximally informative dimensions analysis of deep neural networks  JIMMY KIM (Presenter), Northwestern University, DAVID J. SCHWAB, Institute for Theoretical Science, CUNY Graduate Center — Maximally informative dimensions (MID) is a technique in neuroscience used to analyze neural responses to natural stimuli. It assumes that neurons are only sensitive to a low-dimensional subspace within the high-dimensional stimulus space and extracts those relevant dimensions by maximizing the mutual information between the neural response and stimulus projections. Despite its advantages, MID suffers from scalability issues of the optimization. As such, in practice, no more than a handful of dimensions can be found. Here, we present a method based on variational lower bounds of mutual information that allows for the efficient extraction of large number of informative dimensions. We demonstrate this method by studying a deep neural network trained on CIFAR-10, and suggest possible applications towards the information-theoretic view of deep learning as well as a new, principled method of visualizing multiple different facets of a neuron.

12:51PM X27.00009: Inferring structure-function relationships in neural networks from geometric features of their error landscapes*  JAMES FITZGERALD (Presenter), TIRTHABIR BISWAS, Janelia Research Campus — Neural computation in biological and artificial networks relies on nonlinear synaptic integration. The synaptic connectivity between neurons in these networks is a critical determinant of overall network function. However, what features in connectivity are specifically required to generate measurable network-level computations are largely unknown. Here we introduce a geometric framework for calculating and analyzing connectivity constraints in nonlinear recurrent neural networks of rectified linear units. We focus on network-level functions defined by steady-state responses to a finite set of input conditions. By analytically determining how well any network approximates the responses, we show that error landscapes typically have degenerate global minima with several flat and semi-flat dimensions. The latter emerges from the rectifying nonlinearities. Further, at increasing noise or error levels, topological transitions occur where the space of admissible solutions changes suddenly and drastically. This is reminiscent of sudden changes associated with phase transitions in physical systems. These results allow us to develop a formalism for extracting rigorous insights into neural network structure and function from the geometries and topological transitions of error surfaces.

*HHMI
1:03PM X27.00010: An olfactory pattern generator for functional neural circuit analysis in *Drosophila larva*  
GUANGWEI SI (Presenter), JACOB BARON, YU FENG, ARAVINTHAN SAMUEL,  
Harvard University — For physical stimuli, it is straightforward to engineer patterns to stimulate the sensory circuits and probe the functional properties. However, this framework is generally not applicable to olfaction, since olfactory stimuli lack a well-defined space. The typical olfactory stimuli, fixed odor panels of pure chemicals, natural scents or mixtures, lack the capability to systematic sample the olfactory sensory periphery. Here, we present a stimuli method that project activity pattern directly onto the olfactory receptor neurons. This method is based on the flexible and precise mixing of an optimized set of primary odors using microfluidics. The primary odors were derived for the *Drosophila larva* to separately target each free variable in the olfactory code, the activity of an individual olfactory receptor neuron type. Our device allows us to program and deliver any mixture of primary odors from all combinatorial possibilities during an experiment, allowing selection of any receptor neuron activity combination on demand. We combine this stimulus method with imaging the olfactory representations in the *Drosophila larva* from receptor neurons to interneurons of the antennal lobe and Kenyon Cells of the mushroom body.

*This work was supported by an NSF grant (NSF-IOS-1556388).

1:15PM X27.00011: Sequential and efficient neural-population coding of complex task information  
SUE ANN KOAY (Presenter), Princeton Neuroscience Institute, Princeton University, STEPHAN Y THIBERGE, Bezos Center for Neural Dynamics, Princeton University, CARLOS BRODY, DAVID TANK, Princeton Neuroscience Institute, Princeton University — A crucial component of cortical computation is context: variables that indicate the external state of the world, and the internal state of the animal. However, the need to simultaneously represent many pieces of information in neural activity can also pose computational challenges for neural systems to overcome. We recorded from large neural populations in posterior cortices as mice performed a complex, dynamic task involving multiple interrelated variables. How are these variables represented together without crosstalk, and what of their time-dependent relationships to each other? We found that the neural encoding implied that correlated task variables were represented by uncorrelated modes in an information-coding subspace, which can in theory enable optimal decoding directions to be insensitive to neural noise levels. Across posterior cortex, principles of efficient coding thus applied to task-specific information, with neural-population modes as the encoding unit. Remarkably, this encoding function was multiplexed with rapidly changing, sequential neural dynamics, yet reliably followed slow changes in task-variable correlations through time. We can explain this as due to a mathematical property of high-dimensional spaces that the brain might exploit as a temporal scaffold.
Heterogeneity of timescales in random networks with bistable units

NICOLAE ISTRATE (Presenter), Department of Physics, Institute of Neuroscience, University of Oregon, MERAV STERN, Department of Applied Mathematics, University of Washington, LUCA MAZZUCATO, Departments of Biology and Mathematics, Institute of Neuroscience, University of Oregon — Recent experiments reveal that neural circuits operate in a regime with simultaneous presence of multiple timescales. Such heterogeneity of timescales was observed not only across different brain areas (Murray JD et al 2014) but also across neurons within the same circuit (Cavanagh SE et al 2016) during periods of ongoing activity, suggesting that it may be an intrinsic dynamical property of recurrent circuits. Here we investigate which neural mechanisms may support this heterogeneous distribution of timescales. We show that random neural networks with bistable units (Stern M et al 2014) naturally exhibit large heterogeneity of timescales across neurons in the presence of a distribution of self-couplings. We provide a biophysical interpretation for the bistable units in our rate network in terms of Hebbian assemblies. We show that, in recurrent spiking networks where excitatory and inhibitory neurons are arranged in assemblies, one can achieve a heterogeneous distribution of timescales when assembly sizes are unequal. We thus interpret the rate network self-couplings as potentiated synaptic couplings between neurons within the same assembly. Our results establish a novel theoretical framework to investigate the observed heterogeneity of intrinsic neuronal timescales.

Recurrence Neural Networks Learn Simple Computations on Complex Time Series through Examples*

JASON KIM (Presenter), ZHIXIN LU, DANIELLE BASSETT, University of Pennsylvania — A hallmark of artificial and biological neural networks is their ability to represent and generalize complex information. Artificial neural networks generate novel images of cats after seeing many pictures of cats. Conference attendees generate creative new future research directions after carefully listening to a talk. How do neural networks represent, manipulate, and extrapolate complex information given only examples? Previous methods such as FORCE learning have demonstrated the ability of a neural network to replicate complex, and even chaotic, patterns of observed outputs in response to specific patterns of driving inputs. Here, we explain how a neural network further learns the underlying computations performed on the observed outputs. Specifically, we demonstrate that a neural network trained to output slightly translated or rotated chaotic manifolds in response to small driving inputs can extrapolate this output to generate largely translated or rotated chaotic manifolds in response to large driving inputs. We conclude with an analytic understanding of how this extrapolation occurs, yielding design principles for creating neural networks that can generalize knowledge.

*JZK acknowledges funding from the NSF GRFP No. DGE-1321851, and DSB from the NSF CAREER PHY-1554488.
1:51PM X27.00014: Universal scaling laws of interaction time distribution in honeybee and human social networks*  
SANG HYUN CHOI (Presenter), VIKYATH D RAO, TIM GERNAT, ADAM HAMILTON, GENE ROBINSON, NIGEL GOLDENFELD, University of Illinois at Urbana-Champaign — Compared to the heavy-tailed inter-event time distribution which reflects collective emergent properties, the duration of interaction events has received less attention but may reflect the variability in the interaction behavior. Here we report measurements of trophallaxis and face-to-face event durations of honeybees show that its distribution is heavy-tailed as in human face-to-face interactions. We derive the power-law form by viewing the termination of an interaction as a particle escaping over an energy barrier. The variability within the population is represented by the distribution of barrier heights determined by extreme value theory. We find a universal scaling law connecting the exponent in the interaction time distribution to that in the barrier height distribution, which is verified by both honeybee and human data. Although less prominent than in humans, individual differences in honeybee interactivity, which are usually overlooked, are confirmed. Our work shows how individual differences can lead to universal patterns of behavior that transcend species and specific mechanisms of social interactions.

*This work was partially supported by National Institutes of Health Grant R01GM117467.

2:03PM X27.00015: Social inhibition maintains adaptivity and consensus of honey bees foraging in dynamic environments  
SUBEKSHYA BIDARI (Presenter), ZACHARY KILPATRICK, ORIT PELEG, University of Colorado, Boulder — To effectively forage in natural environments, organisms must adapt to changes in the quality and yield of food sources across multiple timescales. How do individuals foraging in groups use private observations and the opinions of their neighbors in changing environments? We address this problem in the context of honey bee colonies whose inhibitory social interactions promote adaptivity and consensus needed for effective foraging. Individual and social interactions within a mathematical model of collective decisions shape the nutrition yield of a group foraging from feeders with temporally switching quality. Social interactions improve foraging from a single feeder if temporal switching is fast or feeder quality is low. When the colony chooses from multiple feeders, the most effective form of social interaction is direct switching, whereby bees flip the opinion of nestmates foraging at lower yielding feeders. Model linearization shows that effective social interactions increase the fraction of the colony at the correct feeder and the rate at which bees reach that feeder. Our mathematical framework allows us to compare a suite of social inhibition mechanisms, suggesting experimental protocols for revealing effective colony foraging strategies in dynamic environments.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X28 DCMP: Quantum Nanomechanics  
405-407 - Mark Dykman, Michigan State Univ - Tag(s): Invited
Superconducting qubits are an excellent system for building quantum computing systems, due to their good individual qubit performance metrics, the availability of a high fidelity two-qubit entangling gate, and their easy lithographic scaling to large qubit numbers. In addition, these qubits provide unique opportunities as testbed systems for quantum communication as well as developing hybrid quantum systems. One compelling opportunity is provided by the ability to use superconducting qubits to control and measure acoustically-active structures, structures that can potentially serve to link these qubits to other two-level systems or to e.g. optical signals. I will describe our recent progress in coupling superconducting qubits to surface acoustic waves. In one experiment we have demonstrated the quantum control of a single microwave-frequency mechanical mode in a surface acoustic wave (SAW) resonator [1]. In a second experiment [2], we have launched and received itinerant phonons in a 2 mm long acoustic Fabry-Perot resonator, and generated a phonon-mediated entanglement between two qubits.


*Support provided by the AFOSR MURI program, ARL (W911NF-15-2-0058), UChicago MRSEC (NSF DMR-1420709) and NSF SHyNE (NSF NNCI-1542205) as well as LDRD funds (ANL) and DOE.
Quantum acoustics: creation and control of multi-phonon Fock states

ROBERT SCHOELKOPF (Presenter), Yale University — Quantum states of mechanical motion can be important resources for quantum information, metrology, and studies of fundamental physics. There have recently been several new demonstrations that advance our ability to generate, control, and measure individual quanta of motion. In our approach, we combine a superconducting qubit with a piezoelectric transducer, which can couple to high quality factor bulk acoustic resonators [1]. In analogy with cavity QED, this system allows for strong coupling between the electrical excitations of the qubit and single Gigahertz phonons trapped in a single-crystal substrate, opening new capabilities for manipulation of mechanical degrees of freedom in the quantum domain. First, we show that a single excitation can be controllably swapped back and forth between the qubit and the acoustic resonator. Next, by employing a flip-chip geometry and a phononic “supercavity” made by curving one side of the substrate, we observe increased phonon lifetimes approaching 100 microseconds, comparable to state-of-the-art qubit coherence times. Using this system, we can then carry out a protocol to climb the phonon ladder, creating multi-photon Fock states or superpositions of Fock states, and measuring the Wigner function of the results using the qubit. I will talk about the prospects of using these mechanical degrees of freedom as multi-mode memories and as probes of the fundamental mechanisms of decoherence in quantum systems.

This work performed in collaboration with Yiwen Chu, Peter Rakich, Taekwan Yoon, Vijay Jain, and Prashanta Kharel.


*This research was supported by US Army Research Office, ONR YIP, NSF MRSEC, and the Packard Fellowship for Science and Engineering.
Mechanical resonators based on carbon nanotubes feature a series of truly exceptional properties. Carbon nanotubes are the lightest resonators fabricated thus far. The mechanical vibrations are enormously sensitive to the electrons flowing through the nanotube, and vice versa. Taking advantage of this coupling, we developed a novel detection method that allows us to measure the mechanical vibrations of nanotube resonators with an unprecedented sensitivity [1]. In this talk, I will discuss our efforts to cool the amplitude of the thermal vibrations to a few quanta [2]. Cooling is achieved using a simple yet powerful method, which consists in applying a constant (DC) current of electrons through the suspended nanotube in a dilution fridge. I will also present results where we strongly couple mechanical vibrations to the two electron states involved in single-electron tunnelling (SET). It effectively creates a highly nonlinear potential for mechanical vibrations despite the relatively low quanta population (about 80 quanta). This enables us to demonstrate the polaronic nature of charge transport through a nanoelectromechanical device.

Nitroxide Radical Polymer-Solvent Interactions and Solubility Parameter Determination  

ALEXANDRA EASLEY (Presenter), Materials Science and Engineering, Texas A&M University, LILLIAN VUKIN, DYLAN HOWARD, JOSE L PENA, Artie McFerrin Department of Chemical Engineering, Texas A&M University, JODIE LUTKENHAUS, Artie McFerrin Department of Chemical Engineering and Materials Science and Engineering, Texas A&M University — Nitroxide radical polymers such as poly(2,2,6,6-tetramethylpiperidinyloxy-4-ylmethacrylate) (PTMA) are electrode materials of interest for organic batteries. They exhibit a reversible capacity (111 mAh/g theoretical), high redox potential (3.6 V vs Li/Li⁺), and rapid charging. One major consideration for the design and processing of organic batteries is the interaction between the polymer and solvent, such as the electrolyte. For example, linear PTMA may dissolve in the electrolyte solution, which leads to capacity fade during long-term cycling. To predict these polymer-solvent interactions, the Flory-Huggins interaction parameter, the Hildebrand and Hansen solubility parameters of PTMA are determined using group contribution calculations and experimental methods. Using calculated and measured solubility parameters, the Flory-Huggins interaction parameter for PTMA is estimated for common battery electrolyte systems. Membrane osmometry is used to confirm the PTMA Flory-Huggins interaction parameter. Once confirmed, the PTMA Flory-Huggins interaction equation is used to recommend new electrolyte solvents to improve battery performance.

Shape Engineering of Monodispersed Cone-Shaped Particles by Tuning Blend Structure of AB Diblock Copolymer and C-Type Copolymer within Emulsion  

EUN JI KIM (Presenter), JAE MAN SHIN, KANG HEE KU, YONGJOO KIM, HONGSEOK YUN, BUMJOON KIM, KAIST — Precise control of the shape and nanostructure of block copolymer (BCP) particles are of great interest for their shape-dependent physical properties. Here, we exploit the blend of poly(styrene-block-1,4-butadiene) (PS-b-PB) BCP and poly(methylmethacrylate-statistical-(4-acryloylbenzophenone)) (P(MMA-stat-4ABP)) sCP within the colloidal confinements to develop a series of particles with different symmetry. The key strategy for tuning the particle shape is to systematically control the incompatibility between the BCP and sCP by varying the mole fraction of 4ABP in sCPs (Φ₄ABP) and the volumetric ratio of sCPs in total blend (fₛCP). The particles were produced by membrane emulsification method to have monodisperse particle size and shape, and the particle shape can be tuned sequentially from striped ellipsoid to Janus-sphere, to cone-shaped with the increase of Φ₄ABP and fₛCP. In particular, the shape-anisotropy of cone-shaped particles was systematically controlled by varying the size and Janusity, which is supported by quantitative calculation from the modified theoretical model. Furthermore, the importance of the shape control of monodispersed cone-shaped particles was demonstrated by investigating the colloidal coating property of these particles.
11:51AM X32.00004: Aqueous Solution Behavior of Poly(ethylene oxide) in Presence of Complex Ions*  DAVID HOAGLAND (Presenter), SATYAM SRIVASTAVA, ZACHARY FINK, Univ of Mass - Amherst, ELIZABETH BURNS, GCP Applied Technologies — Poly(ethylene oxide) (PEO) in aqueous solutions has often been studied by experiment and modeling, but despite widespread use, questions about solution properties remain. Motivated by PEO's potential to reduce CO2 emissions as a strength-building concrete additive, chain conformation was examined in solutions containing complex ions present during concrete curing. Ion-induced changes for linear 100,000 g/mol PEO were mostly unremarkable and consistent with past reports, the hydrodynamic radius by dynamic light scattering or intrinsic viscosity depressed slightly as ion concentration grows. Trends for aluminum-containing ions [at neutral and basic pH monovalent anion Al(OH)4 predominates] were different, with radius by dynamic light scattering approximately 50% larger than by intrinsic viscosity. We hypothesize weak ion-mediated coupling between hydroxyl end groups disruptable by shearing. In support, hydrodynamic radius by dynamic light scattering fell to the value by intrinsic viscosity when hydroxyl end groups were converted to methoxy end groups. The chemistry of the ion-induced chain association remains unclear.

*GCP Applied Technologies

12:03PM X32.00005: Quantitatively Determining of Population Ratios in Bimodal Polymeric Solutions by Neutron Scattering*  GUAN-RONG HUANG (Presenter), KUNLUN HONG, CHI-HUAN TUNG, DONGSOOK CHANG, CHRISTOPHER N LAM, CHANGWOO DO, YUYA SHINOHARA, Oak Ridge National Lab, SHOU-YI CHANG, National Tsing Hua University, YANGYANG WANG, WEI-REN CHEN, Oak Ridge National Lab — Association of amphiphilic polymers in aqueous solutions is of fundamental importance. The coexistence of unimers and aggregates over a broad range of phase regions has been widely reported. Although scattering technique has been employed to identify the structure of micellar aggregates and free unimers as well as its time-evolution processes, the determination of their relative population of unimer and aggregate itself is still challenging. Here, using small angle neutron scattering, we present a comprehensive SANS study of n-dodecyl-PNIPAm. By adjusting the deuterium/hydrogen ratio of water, the intra-micellar polymer and water distributions are obtained. The micellar aggregation number and number density are further determined. Most importantly, the distributions of unimers and micellar aggregations at different temperatures are obtained quantitatively for the first time.

*SANS experiment was carried out on EQ-SANS at SNS and polymer synthesis and characterization was performed at CNMS; both are DOE Office of Science User Facilities. part of the research (data analysis) was supported by the Laboratory Directed Research and Development Program at ORNL.
12:15PM X32.00006: Role of Miscibility in the Shape Memory Properties of Polymer Blends
SURBHI KHEWLE (Presenter), PRATYUSH DAYAL, Chemical Engineering, Indian Inst of Tech Gandhinagar — Shape Memory Polymers (SMPs) are smart materials capable of transforming back to their intended shape and therefore, are used to replicate biomimetic functionalities in artificial materials. Here, we demonstrate that unlike chemical synthesis, polymer blending can be used as an effective technique to design SMPs. In our work, we consider partially miscible crystalline and amorphous polymer blends, to represent the hard and soft segments of SMPs, respectively. To determine the miscibility of blend we construct equilibrium phase diagram by combining Flory-Huggins and phase-field theories that account for both, amorphous-amorphous and crystal-amorphous interactions. We incorporate the effect of these interactions into standard viscoelastic model and determine thermo-mechanical behaviour of SMP blend, using composition dependent viscoelastic properties calculated from Equivalent Box Model. Finally, via simulations, we determine shape fixity and recovery ratios and demonstrate that our calculations are in excellent agreement with the experimental results for PCL-SBS blends. We believe that our findings can not only be utilized to design SMP blends with tailored properties but also be used to establish their structure-property relationships.

*The authors thank IIT Gandhinagar for funding.

12:27PM X32.00007: Dynamic interfacial trapping of Janus nanorod aggregates in polymer blends
FELIPE LEIS PAIVA, MICHAEL HORE, Department of Macromolecular Science ad Engineering, Case Western Reserve University, ARGIMIRO SECCHI, COPPE Graduate Program in Chemical Engineering, Universidade Federal do Rio de Janeiro, VERONICA CALADO, School of Chemistry, Universidade Federal do Rio de Janeiro, JOAO M MAIA (Presenter), SHAGHAYEGH KHANI, Department of Macromolecular Science ad Engineering, Case Western Reserve University — Taking advantage of both shape and chemical anisotropy on the same nanoparticle offers rich plasmonic and self-assembly possibilities for nanotechnology. Combining Dissipative Particle Dynamics and Discrete Dipole Approximation calculations, the directed assembly of Janus nanorod aggregates in polymer blends has been assessed, along with the optical properties resulting thereof. Janus rods become kinetically-trapped and exhibit either parallel or antiparallel alignment with respect to their long axis. This depends on several factors that can be precisely tuned. Ultimately, two different aggregate structures result from rod tumbling that are not observed under quiescent conditions: monolayer-like aggregates exhibiting trapped rods with antiparallel configuration; and stacked nanorod arrays similar to superlattice sheets. Hence, the present study offers fundamental insight into relevant parameters governing the directed assembly of Janus nanoparticles at an interfacial level as well as an assessment of the potentially novel optical applications deriving from the resulting aggregate structures, such as peculiar displays and sensors.

*This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001.
Tuning Diblock Copolymer Micelles by Cosolvent Effects: A Simulation Study

DONG MENG (Presenter), JING ZONG, Mississippi State Univ — A powerful method to manipulate the micellar structures formed by amphiphilic diblock copolymers (DBC) in a selective solvent is by addition of a cosolvent. Unlike the single-solvent case, few simulation studies on DBC micellization in solvent mixtures have been reported due to high computational cost associated with the necessity of treating solvents explicitly. Here, the Field-Accelerated Monte Carlo simulation is employed for the task under the expanded grand canonical ensemble. We investigate the effects of introducing a cosolvent on the critical micelle concentration, micellar morphology, and aggregation number. Specifically, we consider two types of solvent pair: interacting-solvent and cononsolvent pairs. It is found that the interacting-solvent pair promotes morphology transition from micelles to vesicles. In the case of cononsolvent pair with respect to the corona block, aggregation number of micelles increases significantly as the result of maximizing contact between polymers and the minor amount of cosolvent. Our study reveals the competing and cooperative interplays of solvent pairs in determining the DBC micellar structures, pointing out the necessity of considering solvent explicitly in simulations as oppose to the conventional "effective-single-solvent" approach.

Efficient sampling of polymer conformations using Brownian Bridges

VIVEK NARSIMHAN (Presenter), SHIYAN WANG, DORAISWAMI RAMKRISHNA, Purdue Univ — In this talk, we introduce a mathematical concept known as a stochastic bridge, and describe how it can be utilized in many areas of polymer physics. A stochastic bridge is a random process whose start and end regions in phase space are specified. Such processes naturally find utility in situations when one wants to sample polymer conformations with a given topology and/or energy. In the first part of the talk, we expand upon our previous work and discuss how one can systematically generate bridge processes for continuous polymer chains described by a stochastic differential equation. We will then discuss how to use such ideas to generate polymer conformations of a given topology (e.g., rings, polymers with fixed winding or twist, etc.). We will then study a canonical problem – a polymer under an external field – and show how a bridge formulation allows one to exactly sample polymer conformations in a given range of total energy. This methodology thus allows one to sample rare events (i.e., high energy) efficiently, or conversely most probable configurations (i.e., low energy). We will conclude on how to scale these ideas to larger dimensional systems, and discuss some advantages and disadvantages of using bridge processes compared to other biased sampling strategies.
1:03PM X32.00010: Investigation of polymer diffusion in confined geometries using differential dynamic microscopy techniques  EMMANUEL HITIMANA (Presenter), SVETA MOROZOVA, Macromolecular Science and Engineering, Case Western Reserve University — The fundamental understanding of polymer diffusion in confined geometries is important for industrial as well as broader applications such as transport in cell-like environments, improved drug delivery, and filtration. However, the study of polymer diffusion in such environments is often challenging due to the nanometer size scales of polymers and to the inhomogeneous geometry of the landscape. We have developed differential dynamic microscopy (DDM) techniques to investigate the dynamics of fluorescein tagged poly-l-lysine chains in confined environments in any arbitrary direction along textured surfaces. Using a curved surface, we can control the local confinement. The role of polymer molecular weight, concentration, confinement, and local geometry on polymers dynamics will be discussed.

1:15PM X32.00011: Direct visualization of branched polymer dynamics using single molecule studies*  SHIVANI PATEL (Presenter), CHARLES M SCHROEDER, University of Illinois at Urbana-Champaign — We study the dynamics of single branched polymers in dilute and non-dilute solutions using single-molecule fluorescence microscopy. In particular, we use a hybrid enzymatic-synthetic approach to synthesize DNA-based branched polymers such as comb polymers that contain a long backbone with multiple side branches grafted at various positions. Following synthesis, we directly study the dynamics of single branched polymers, particularly in non-dilute solutions in extensional flow, and compare them to the dynamics of linear polymers. We further study the effects of background concentration and polymer topology on branched polymer dynamics in order to elucidate the non-equilibrium behavior of topologically complex polymers. For instance, our work on comb polymer dynamics has shown that contrary to dilute solutions and melts, the addition of branches on to a linear backbone speeds up the relaxation of comb polymers compared to their linear analogs in semi-dilute solutions. Overall, our work shows that single polymer dynamics can be used to provide a direct link between polymer microstructure and bulk rheological properties.

*Funding for this research was provided by NSF CBET 1254340.
1:27PM X32.00012: Additive Driven Morphological Transition of Block Copolymer Particles: Elongation, Transformation and Disassembly of Single Domain  
SEONGHAN LEE (Presenter), JAE MAN SHIN, KANG HEE KU, BUMJOON KIM, KAIST — Particles with controllable shape and internal morphology received great attention as a promising colloidal material. Here we report co-assembly of polystyrene-\(b\)-poly(2-vinylpyridine) (PS-\(b\)-P2VP) diblock copolymer (BCP) and bromoalkyl based small molecule additives confined in evaporative emulsion droplet. The presence of additives with varying volume fraction (\(\varphi\)) resulted in (1) significant increase of aspect ratio of prolate particles from 2.4 to 4.5 (\(\varphi<0.40\)), (2) unique transformation of domain structure from conventional lamellar stacks into spherical shaped, multi-layered lamellar (\(0.40<\varphi<0.45\)), and (3) disassembly of single lamellar domains into micellar spheres (\(0.45<\varphi\)). Investigation on the morphological evolution of particle demonstrated that the favorable interaction with P2VP and bromine-containing additives allows quaternization and significant swelling of P2VP domains, which is further assisted with the presence of external aqueous phase. This additive induced morphological transformation was further systematically controlled by incorporation various types of additives to achieve control over the degree of P2VP domain swelling.

1:39PM X32.00013: Single molecule visualization of single ring polymers in the flow-gradient plane of shear flow*  
MICHAEL TU (Presenter), Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, RAE M ROBERTSON-ANDERSON, Department of Physics, University of San Diego, CHARLES M SCHROEDER, Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign — The lack of free ends on ring polymers yields a unique topology that has fascinated polymer physicists and chemists for decades. Despite recent progress, we still lack a clear understanding of the molecular-level dynamics of ring polymers. Here, we use single-molecule imaging to directly visualize individual ring polymers in shear flow. We have built a custom shear flow apparatus to be used in conjunction with single-molecule fluorescence microscopy to study the dynamics of individual ring polymers in the flow-gradient shear flow. Using this device, we are able to characterize the fractional extension and orientation angle of ring polymers under steady shear, and compare the responses to their linear counterparts. We report the steady-shear fractional extension, orientation angle, and temporal-averaged spatial conformations of ring polymers in shear flow as a function of the applied dimensionless flow strength (\(Wi\), Weissenberg number), and compare the results to their linear polymer counterparts. We also report observations of tumbling and tank-treading-like behavior of ring polymers in shear flow. Overall, these results provide new molecular-level insights into the dynamics of ring polymers in flow.

*NSF CBET-1604038
Phase behavior of diblock copolymer-homopolymer ternary blends containing an asymmetric diblock copolymer*  

BO ZHANG (Presenter), SHUYI XIE, FRANK S BATES, TIMOTHY LODGE, University of Minnesota — Lifshitz points (LPs) are predicted to exist in symmetric A/B/A-B ternary blends in the mean-field limit, where A and B are homopolymers and A-B is the corresponding diblock copolymer. At finite molecular weights, the LP is replaced by a channel of bicontinuous microemulsion (BμE) due to fluctuation effects. A recent study of symmetric ternary blends, where A is poly(cyclohexylethylene) (PCHE) and B is poly(ethylene) (PE), demonstrated that the BμE is bracketed by a line of congruent lamellar-disorder transitions and a Scott line of critical points, at homopolymer content near the predicted LP value. In this work, we investigated the phase behavior of a similar PCHE/PE/PCHE-PE ternary blend but with a compositionally asymmetric diblock copolymer. The phase behavior, which was determined using small angle X-ray and neutron scattering and optical transmittance measurements, revealed that the line of congruent transitions is decoupled in composition from the line of critical points. Additionally, a wide range of phase space between the compositions associated with the congruent condition and Scott line was identified as containing the BμE morphology.

*Office of Basic Energy Sciences (BES) of the U.S. Department of Energy (DoE), under Contract No. DE-FOA-0001664

Interactions between Colloidal Particles Mediated by Nonadsorbing Polymers: Casimir and Anti-Casimir Effects  
PENGFEI ZHANG, Center for Advanced Low-Dimension Materials, State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, Donghua University, QIANG WANG (Presenter), Colorado State University — Using a lattice self-consistent field (SCF) theory and the corresponding lattice Monte Carlo (MC) simulations combined with our recently proposed Z method (Zhang, P.; Wang, Q. Soft Matter, 2015, 11, 862), we examined homopolymer solutions confined between two parallel and nonabsorbing surfaces and in equilibrium with a bulk solution, and accurately calculated the effective interaction between the two surfaces. Close to the critical point of the bulk solution, we found for the first time the Casimir effect with long-range attractive intersurface potential $W<0$ extending to $D/R_e \approx 10$, where $D$ denotes the intersurface separation and $R_e$ the root-mean-square chain end-to-end distance in the bulk solution. On the other hand, by directly comparing our MC results with SCF predictions based on the same model system, we were able to quantitatively and unambiguously distinguish the mean-field and the fluctuation contributions to $W$, and found for the first time the fluctuation-induced repulsion $W>0$ between the two surfaces at intermediate $D=R_e$ (i.e., the anti-Casimir effect) predicted by Semenov and Obukhov (Obukhov, S. P.; Semenov, A. N. Phys. Rev. Lett. 2005, 95, 038305), which is about one order of magnitude stronger than that due solely to the finite chain length given by the SCF theory.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X33 DPOLY DSOFT DMP: Polymer Crystals and Crystallization II  
505 - Toshikazu Miyoshi, Univ of Akron - Tag(s): Focus
11:15AM X33.00001: Controlling the Mechanical Behavior of Hydrogenated Polynorbornene*  
JARED KLEIN (Presenter), RICHARD REGISTER, Princeton University —  
Hydrogenated polynorbornene (hPN) synthesized via ring-opening metathesis polymerization is a semi-crystalline polymer even while atactic, as it is able to accommodate stereodefects within the crystal. We have previously shown control over phase behavior in hPN via epimerization of the cyclopentylene ring in the backbone structure. The polymorphic transition temperature into a rotationally-disordered state, \( T_{cc} \), is strongly affected by epimerization, while epimerization has only a minor effect on the melting temperature, \( T_m \), and no appreciable effect on the total crystallinity (J. P. Klein and R. A. Register, J. Polym. Sci. B, 57, 1188 (2019)). In this talk, the effect of epimerization on both the stress-strain behavior and dynamic mechanical thermal properties are discussed. Epimerization causes a decrease in both the Young's modulus and the yield strength of the polymer, and it also reduces the breadth of the modulus-vs.-T plateau region (above \( T_g \)) significantly, in line with the decrease in \( T_{cc} \). hPN-based polymers with a pyrene endgroup show a strong fluorescence sensitivity to melting/crystallization, and work is underway to evaluate their utility in probing other hPN transitions.

*NSF Polymers Program (DMR 1402180) and NSF MRSEC Program through PCCM (DMR 1420541)

11:27AM X33.00002: What happens upon annealing of pre-drawn semicrystalline polymers?  
TRAVIS SMITH (Presenter), SHIQING WANG, Univ of Akron — As part of efforts to understand mechanical behavior semicrystalline polymers under large deformation, we investigate what happens to predrawn semicrystalline polymers upon annealing at elevated temperatures. For instance, LLDPE drawn at room temperature will neck to its characteristic draw ratio around 5.5 and will shrink by 10% when unloaded but will remain in this highly stretched state for many years. Such predrawn PE samples will either exhibit various levels of retractive stress when held at a fixed length or shrink by different amounts, depending on the annealing temperature. The physical meaning of this characteristic will be explored experimentally, first mechanically and eventually by in situ WAXS and SAXS measurements. Specifically we will search for evidence to support our concept that there is partial melting upon annealing due to the chain tension produced by the pre-cold-drawing, at temperatures well below the melting temperature. The universality of the phenomenology and its molecular interpretation is explored by making a similar investigation of a second semicrystalline polymer, poly(ethylene terephthalate), drawn above its glass transition temperature \( T = 70 \) Celsius.

*This work is supported by NSF (DMR-1905870).
Entanglement Effect on Chain-Folding Structure in Semicrystalline Polymer Blends

FAN JIN (Presenter), TOSHIKAZU MIYOSHI, Univ of Akron — Entanglement effect on chain-folding structure of semicrystalline polymers is not clearly understood over the past decades. Very recently, we demonstrated that Poly(Lactic Acids) chains with three different molecular weights of 46K, 90K, and 320K g/mol do not change adjacent re-entry structure under different supercoolings. It was suggested that entanglement of polymer chains limit adjacent re-entry number in the melt-grown crystals. In this study, we isothermally crystallize polymer blend samples consisting of long and short Poly(Lactic acid) chains from the melt state. Only long polymer chains are labeled by $^{13}$C. $^{13}$C-$^{13}$C double quantum (DQ) spectroscopy is applying to study local chain-folding structure of PLLA as a function of blending ratio and as a function of molecular weight of short PLLA chains.

Flow-Induced Crystallization of Polymers during Multi-Axial Deformation

LIANGBIN LI (Presenter), University of Science and Technology of China — Flow- or stretch-induced crystallization (FIC/SIC) is believed to be mainly responsible for the excellent mechanical properties of polymers during real processing. The development of synchrotron radiation (SR) X-ray scattering techniques with high time resolution has been a mainstream research tool to study the structural evolution of polymers under complex external fields. The FIC behaviors of polymers during multi-axial deformation like biaxial stretching, film blowing and service of sounding balloon has been systematically studied with the combination of in-situ SR X-ray scattering and the custom-built devices. Considering the phenomenon of frustrating SIC for natural rubber during biaxial stretching, we proposed a new model for SIC based on the results of theoretical calculation and the in-situ X-ray scattering, which decoupled the free energy contributions of chain orientation from that of conformational entropy reduction. This model is also suitable for the crystallization of polymers under other flow fields.

References


*This work is supported by the National Natural Science Foundation of China (51633009).
Homogeneous crystal nucleation – Nucleation kinetics and thermal stability of nuclei*  
CHRISTOPH SCHICK (Presenter), RUSLAN ADRIANOV, TIMUR MUKHAMEZTYANOVA, Butlerov Institute of Chemistry, Kazan Federal University, RENE ANDROSCH, Interdisciplinary Center for Transfer-oriented Research in Natural Sciences, Martin Luther University Halle-Wittenberg — Crystal nucleation in polymer melts at common laboratory cooling rates (< 10 K/s) is typically heterogeneous. Studying homogeneous crystal nucleation in bulk samples requires bypassing the low-supercooling temperature range of pre-dominant heterogeneous nucleation. This became possible with the availability of fast scanning chip calorimetry. The strategy for studying homogeneous nucleation kinetics by fast scanning calorimetry will be introduced [1]. We will discuss the temperature dependency of the rate of homogeneous nucleation and its relation to the glass transition. We describe a method allowing to investigate the ability of nuclei to stabilize/grow on heating to the crystallization temperature [2] and, finally, to determine the thermal stability of homogeneous nuclei in polymers.


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Are Spherulites Spherical? 3D Visualization of Semicrystalline Polymer Morphology Using Optical Tomography*  
SHU-GUI YANG, ZHEN-ZHEN WEI, Univ of Sheffield, GORAN UNGAR (Presenter), School of Materials Science and Engineering, Xian Jiaotong University, PANTEA KAZEMI, Univ of Sheffield, HUI-JIE XIE, Physics Department, Zhejiang Sci-Tech University, LILIANA CSEH, School of Materials Science and Engineering, Xian Jiaotong University, HINA SABA, Physics Department, Zhejiang Sci-Tech University — Spherulites, shish-kebab, cylindrites and other morphological features of bulk semicrystalline polymers have been studied for decades using methods such as polarized optical microscopy, TEM or AFM. For these studies either thin films or thin sections were used, giving 2D but not 3D pictures. The organization in the 3rd dimension has been implied rather than directly observed. Attempts at 3D imaging have been made with varying success using approaches, notably electron tomography (TEM) and some other methods. Most studies focussed on polymer blends and block copolymers, relying on contrast produced by the chemically different components, although some remarkable images of crystal lamellae were obtained by TEM. However 3D images of microstructure on the crucial 10-1000 micron scale, especially of single-component polymers or their nanocomposites, are still missing. Here we present first such images obtained by confocal microscopy using appropriate sample preparation and image processing. Already rather unsuspected features of 3D morphology are emerging, previously being hidden by the limitations of the conventional techniques.

*Supported by NSFC grant 21674099.
12:51PM X33.00007: Advanced Polymeric Particles Templated by Polymer Crystallization at Curved Liquid/Liquid Interface  
MARK STAUB (Presenter), CHRISTOPHER LI, Drexel Univ —  
Polymeric micro/nanoparticles have attracted significant interest in the past few decades due to their relevance in a number of fields. The methods commonly employed tend to provide particles that have simple morphology of spheres or cylinders that are inherently fluidic and dynamic due to the long chain nature of macromolecules. As more complex particles, in function and structure, are emerging as solutions to a variety of problems, simple and versatile methods to obtain them are a necessity. Towards this aim, our group has developed a miniemulsion crystallization process where polymer single crystal-like growth is confined to a dynamic liquid/liquid interface. This process produces unique hollow polymer capsules termed “crystalsomes” that have excellent mechanical properties compared to their amorphous counterpart the polymersome. This talk will focus upon using blends of amphiphilic block co-polymers in the miniemulsion process to template hierarchically structured crystalsomes. The block co-polymers serve as macromolecular surfactant along with the hydrophobic segment acting as the crystalline motif. It will be shown by altering the hydrophobic monomeric unit, its degree of polymerization, and the particle size a variety of crystalsomes with tunable porosity can be obtained.

1:03PM X33.00008: Phenomenological Theory of Prefreezing at the Solid-Melt Interface  
OLEKSANDR DOLYNCHUK (Presenter), MUHAMMAD TARIQ, THOMAS THURN-ALBRECHT, Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg —  
Crystallization of liquids is usually initiated at the interface to a solid. The underlying process can be either heterogeneous nucleation or the recently observed process of prefreezing. The latter is the reversible and abrupt formation of a crystalline layer at the interface melt-solid at temperatures higher than the bulk melting point. We present a phenomenological theory of prefreezing and derive such equilibrium properties as the temperature dependent thickness of the prefrozen layer, the prefreezing temperature $T_{\text{max}}$, and the mesoscopic jump of thickness at $T_{\text{max}}$. The theory provides a clear thermodynamic explanation of the abrupt formation of a crystalline layer as a result of the interplay of the interfacial energies $\gamma_{\text{sub,cry}}$, $\gamma_{\text{cry,melt}}$, and $\gamma_{\text{sub,melt}}$. The prefreezing temperature $T_{\text{max}}$ was found to depend on all three interfacial energies and bulk parameters. However, we show that the difference of the interfacial energies $\Delta \gamma = \gamma_{\text{sub,melt}} - (\gamma_{\text{sub,cry}} + \gamma_{\text{cry,melt}})$ acts as a driving force for prefreezing, as $T_{\text{max}}$ tends to increase with increasing $\Delta \gamma$. The analytical outcomes are in accordance with recent experimental results for polyethylene and poly(ε-caprolactone) crystallized on graphite and MoS$_2$ via prefreezing.

1:15PM X33.00009: Role of flow-induced nematic order in polyethylene nucleation*
WENLIN ZHANG (Presenter), RONALD LARSON, Univ of Michigan - Ann Arbor — We employ united-atom molecular dynamics (MD) simulations to quantify the role of nematic order in polyethylene (PE) nucleation. In our simulations, stretched periodic PE chains are blended with free PE chains of the length of 500 and 1000 backbone carbons (C500 and C1000). These bidisperse systems are the simplest realizations of real polymer samples, in which only polymers with long branches or high molecular weights are stretched by flows. By simulating isothermal nucleation and performing mean-first-passage time analysis for the growth of the largest nucleus in our simulations, we show that the nucleation rate of PE increases exponentially with increasing average nematic order of monomers. We also validate the predicted quiescent nucleation rates by computing the crystallization half-time at various temperatures using the crystal growth velocity, sampled from simulations of isothermal crystallization of chains near crystalline slabs, and the Avrami equation. The predicted crystallization half-times agree with experiments, suggesting our predicted nucleation rates are reasonable.

*We are grateful for the funding of this work by Dow under a University Partnership grant and the computational resources provided by the Extreme Science and Engineering Discovery Environment (XSEDE).

1:27PM X33.00010: Crystallization and liquid crystallinity in heptadecanylcarbazole-dithienylbenzothiadiazole (PCDTBT) conjugated polymers*
RYAN FAIR (Presenter), Materials Science and Engineering, Pennsylvania State University, ENRIQUE GOMEZ, Chemical Engineering, Pennsylvania State University — Conjugated polymers exhibit rich phase behavior including liquid crystalline and crystalline phases. Conflicting reports of one such polymer, poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)] (PCDTBT), have claimed the material to be amorphous or semicrystalline. We use oscillatory shear rheology to demonstrate that PCDTBT exhibits liquid crystallinity by identifying the nematic to isotropic temperature. We also find a crystalline phase when annealed at high temperatures, which is likely due to the high $T_g$, near 120 °C, that is identified also through rheology. We corroborate the phase behavior using X-ray diffraction, differential scanning calorimetry, and polarized optical microscopy. High resolution transmission electron microscopy reveals the consequences of annealing in the amorphous or liquid crystalline phase prior to crystallization, and yields images of the crystalline morphology that are produced under these different conditions.

*NSF Grant# 1905550
1:39PM X33.00011: Analyzing morphological and optical properties of poly(3-hexylthiophene) (P3HT) via emitted light's polarization  
HUAN NGUYEN (Presenter), PAULO TARAUJO, Univ of Alabama - Tuscaloosa — With the improvement in synthetic methodologies, polythiophenes and specifically poly(3-hexylthiophene) (P3HT) have become forerunners in the field of conjugated polymers. We study P3HT's morphological and optical properties via measurements of absorption and polarization-resolved photoluminescence via Stokes spectroscopy. Our recent results show that P3HT's aggregation behaviors change drastically when using chloroform stabilized and non-stabilized by amylene. Specifically, P3HT drop-cast films made from stabilized chloroform presented H-aggregates, while similar samples using non-stabilized chloroform exhibited J-aggregates. Here, we hypothesize that the amylene from stabilized chloroform induces a higher probability for the stacked coupling of isolated chains via weak van-der-Waals force leading to the formation of H-aggregates. To rule the influence of amylene out, we are currently performing a set of analyses and experiments consisting of temperature-dependent measurements, thermal annealing, various P3HT chain sizes, and blended MeOH@Chloroform solvents.

1:51PM X33.00012: Computational Model for End-On LCEs*  
JAMES WATERS (Presenter), ANNA BALAZS, Univ of Pittsburgh —  
In main-chain liquid crystalline elastomers (LCE’s), and in side-chain LCE’s where mesogens are attached to the polymer backbone at their midpoint, the polymer chains comprising the elastomer align with the mesogens when they are in the nematic state. For the case of side-chain mesogens attached at one end, though, ordering of the mesogens can induce alignment of the polymer backbone either parallel or orthogonal to the nematic director. We incorporate a theory of side-chain LCE’s into a constitutive model for elastomers to describe these competing effects. We compare simulation results against experiment, and show how an end-on attachment scheme can create elastomers with bidirectional responses, meaning as temperature is varied, a single structure can be made to bend or twist in different directions. We anticipate that this can dramatically increase the possibilities for soft robotic systems.

*U.S. Department of Energy  
Army Research Office

2:03PM X33.00013: WITHDRAWN ABSTRACT  
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Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X34 DPOLY: Organic Electronics III: Electrochemical Transistors and Doping  
506 - Dean DeLongchamp, National Institute of Standards and Technology
11:15AM X34.00001: Charge and Ion Transport in Radical Polymer-based Organic Electrochemical Transistors  BRYAN BOUDOURIS (Presenter), HO JOONG KIM, Davidson School of Chemical Engineering, Purdue Univ — Radical polymers are composed of a non-conjugated macromolecular backbone with open-shell sites that are present on the side chains of each repeat unit. Previously, we have demonstrated that this macromolecular design motif alters the route by which charge is transported in solid-state electronic devices when compared with the more common conjugated polymers utilized in organic electronics. Here, we report on the application of a specific high-performance radical polymer, poly(4-glycidyloxy-2,2,6,6-tetramethylpiperidine-1-oxyl) (PTEO), as the active layer component in an electrolyte-gated organic electrochemical transistor (OECT) device structure. Specifically, we establish the differences in charge and ion transport (i.e., mixed conduction) in these inherently glassy radical polymer systems relative to many oft-used OECT semicrystalline macromolecular materials. Moreover, we highlight the unique synergies that exist between mixed conduction that exist in non-conjugated radical polymer systems. Finally, we manipulate the degree of crosslinking within the radical polymer thin films after casting of the film (i.e., through the use of photoinitiated crosslinking) in order to demonstrate a mechanically-stable, solvent-robust OECT that achieves high device performance as well.

11:27AM X34.00002: Quantifying the Energetics of Ion Injection into Mixed Ionic/Electronic Conductors*  LUCAS FLAGG (Presenter), CONNOR BISCHAK, RAMSESS JAVIER, DAVID S GINGER, Chemistry, University of Washington — Organic electrochemical transistors (OECTs) rely on the electrochemical doping of an organic semiconductor to modulate the conductivity of the channel. This doping process requires electronic charge injection into the polymer from the metal contacts, as well as charge compensation by an ion provided by the electrolyte. Numerous factors have been shown to affect the ease and speed of ion injection including polymer side chain, polymer crystallinity, ion type, pH, solvent, etc. Here we use kinetics derived from temperature dependent spectroelectrochemistry measurements to extract the activation energy of ion injection into a polymer semiconductor. We compare the energetics of injection in a variety of different polymers, salts, and solvents to quantify the contribution of each of the factors controlling ion injection. A deeper understanding of the relative importance of each factor will help with future design of mixed ionic/electronic conductors.

*This work was primarily supported by the National Science Foundation (NSF DMR-1607242) and the NSF DMREF (award number 1629369).
11:39AM X34.00003: Counter-ion exchange as a tool to modulate polaron delocalization and temperature stability of doped polymeric semiconductors* ELAYNE THOMAS (Presenter), KELLY A PETERSON, DAKOTA RAWLINGS, RACHEL A SEGALMAN, MICHAEL L. CHABINYC, University of California, Santa Barbara — The design of high-performance doped semiconductors requires an understanding of the coupling between ionic and electronic carriers. We utilize a method of counter-ion exchange using the polymeric semiconductor PBTTT-C_{14} to deconvolute the effects of ionic/polaronic interactions with the electrical properties of doped semiconducting polymers. Here, the dopant NOPF_{6} is used followed by the exchange of counter-ions ranging from 5 to 11 Å in diameter. The long-range order of the polymeric crystallites is not affected with this exchange process while effectively modifying the counter-ion distance to the charge carrier. Doped films achieve electrical conductivity of 320 S/cm and is not sensitive to an increased ion-polaron distance. We posit that other factors dominate the electrical properties at a device scale, such as the morphology and presence of domain boundaries. Interestingly, the temperature stability of the doped film can be drastically improved with the use of counter-ions containing less labile bonds. This platform serves as a unique way to retain the morphology of polymeric thin films while studying charge interactions at the local scale.

*DOE Office of Basic Energy Sciences (DE-SC0016390)
The Advanced Light Source (DE-AC02-05CH11231)
NSF Graduate Fellowship (DGE-1650114)

11:51AM X34.00004: The role of counter ion structure on the spatial distribution and molecular configuration of charge carriers in solid state electrochemically doped conjugated polymers DAKOTA RAWLINGS (Presenter), RACHEL A SEGALMAN, MICHAEL L. CHABINYC, University of California, Santa Barbara — In a chemically doped or electrochemically doped conjugated polymer, electronic charge carriers are inherently associated with a countercharge in the form of a molecular or atomic counterion. It is expected that the structure of the counter ion will affect its distribution in the polymer film along with that of associated electronic charge carriers. Furthermore, the effect of counter ion structure on the charge storage configuration (i.e. polaron vs. bipolaron) is unknown. Here, we quantify the charge configuration and the distribution of charge carriers between aggregated and amorphous domains as a function of the counter ion structure in semicrystalline conjugated polymer films. We employ an organic electrochemical transistor with a cation tethered polymeric ionic liquid (PIL) as the gate dielectric, where the size and structure of the mobile anionic counterion in the PIL can be varied to modulate the counterion that is associated to charge carriers in the semiconductor. Operando electron paramagnetic resonance and in situ device measurements reveal the polaron to bipolaron ratio as a function of the gate bias for a range of counter ions. This is paired with in situ optical spectroscopy to determine the distribution of charge carriers between amorphous and aggregated domains.
12:03PM X34.00005: Understanding the Working Mechanism of Organic Electrochemical Transistors* VIKASH KAPHLE, PUSHPA PAUDEL, BJORN LUSSEM (Presenter), Kent State Univ - Kent — The organic electrochemical transistor (OECT) is a key element for the field of organic bioelectronics [Nat. Rev. Mat. 3, 17086, 2018]. OECTs are versatile and can be functionalized for a wide range of analytes, including various metabolites, hormones, or neurotransmitters.

Operation of OECTs is often described by a 1D model based on standard TFT theory [Adv. Func. Mat. 17, 3538, 2007]. Still, although the model is successful in explaining general trends of device operation, a quantitative analysis is still challenging.

In this presentation, limits of current OECT device models are discussed. It is argued that the current model implicitly neglects lateral ion migration inside the transistor channel, which leads to non-equilibrium solution. To address this problem, a 2D numerical simulation is presented that solves the continuity equation of holes and cations consistently. It is argued that cations accumulate at the drain electrode, which leads to an additional potential drop at the contacts. This potential drop can be explained by an additional contact resistance, which increases with applied gate potential. The model predictions are confirmed experimentally by measuring the channel potential and the contact resistance of OECTs.

*Funding from the NSF (EECS #1750011) is acknowledged.

12:15PM X34.00006: Bio-Sensors Based on Organic Electrochemical Transistors* PUSHPA PAUDEL (Presenter), VIKASH KAPHLE, DRONA DAHAL, RAJ KISHEN RADHA KRISHNAN, BJORN LUSSEM, Kent State Univ - Kent — Organic Electrochemical Transistors (OECTs) are capable of sensing a wide variety of biomolecules such as Glutamate, Acetylcholine [1], Lactic acids [2], or Glucose [3]. However, despite this success, the precise sensing mechanisms is still under discussion. This lack of understanding precludes a targeted design of OECT applications and currently limits the sensitivity of these devices. Here, we study the working mechanism of OECT based neurotransmitter (Acetylcholine and Glutamate) and Glucose sensors. We discuss the selectivity of these sensors, and study the influence of channel dimensions on their sensitivity. Finally, approaches to increase the spatial and temporal resolution of these transistors are presented.

References:

*NSF Career #1750011
A flexible complementary logic circuit built from two identical organic electrochemical transistors. LORENZO TRAVAGLINI, ADAM P MICOLICH, CLAUDIO CAZORLA, ERICA ZEGLIO, School of Materials Science and Engineering, Univ of New South Wales, ANTONIO LAUTO, School of Science, Western Sydney University, DAMIA MAWAD (Presenter), School of Materials Science and Engineering, Univ of New South Wales — Organic electrochemical transistor (OECT) with a conjugated polymer as the electrically active channel is the basic unit in organic bioelectronic devices. Increased functionalities can be further achieved by building complementary logic circuits combining more than one OECT in different architectures. The simplest circuit can be built by connecting one p-type and one n-type organic semiconductors in series. In this study, we build a complementary logic circuit on a flexible substrate with two OECTs having one material as the active channel. We demonstrate its DC operation with a gain of ~ 7 and its AC response within a frequency range suitable for physiological applications. Our approach to use one single material as an active channel in both OECTs simplifies the manufacturing process and eliminates the need to source different materials with similar electrical performances.

References:

Humidity-Dependent Mixed Ionic-Electronic Conduction in Polythiophene-Derived Polyelectrolytes. GARRETT GROCKE (Presenter), BAN DONG, SHRAYESH PATEL, University of Chicago — Conjugated polyelectrolytes that can conduct both ionically and electronically are attractive candidates for next-generation electrochemical devices. Importantly, the ability to transport both electronic and ionic charge carriers is intimately linked to processing conditions and morphology. This work reports the influence of humidity on the structure and conduction of a series of poly[3-(potassium-n-alkanoate) thiophene]s in the thin film regime. These materials were found to be highly resistive under anhydrous conditions but exhibited mixed ion-electron conduction as a function of increasing relative humidity. UV-Vis-NIR measurements provide evidence for water-assisted formation of alkanoate-stabilized polythiophene polaron states and thus generation of charge carriers for electronic conduction, wherein dissociation of potassium-alkanoate bonds leads to the enhanced ionic conductivity. Additionally, in-situ humidified synchrotron X-ray scattering experiments reveal the resiliency of the underling semicrystalline morphology to increasing relative humidity, which balances the extent of both electronic and ionic conductivity. Our results show the strong influence of humidity on mixed ion-electron conduction characteristics of conjugated polyelectrolytes in self-doped conditions.
12:51PM X34.00009: Charge Transport, Morphological Properties and Cooling Performance of Functionally Graded Semiconducting Polymer Thin Films as Organic Thermoelectrics
TENGZHOU MA (Presenter), BAN DONG, University of Chicago, JOSEPH WALTER STRZALKA, Argonne National Laboratory, SHRAYESH PATEL, University of Chicago — Molecularly doped semiconducting polymers have demonstrated great potential in organic thermoelectrics (TEs) for thermal energy management. While functionally graded materials (FGMs) where transport properties are spatially controlled have been proven to improve TE device performance, experimentally fabricating FGMs has been a challenging task. In this work, we utilize the facile processability to modulate electronic properties through molecular doping of conjugated polymers to fabricate and characterize FG thin films. We leverage sequential vapor doping of poly[2,5-bis(3-tetradecylthiophen-2-yl)thieno[3,2-b]thiophene] (PBTTT) with 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F₄TCNQ) to fabricate one form of FGMs: continuously graded thin films. We observe the presence of a 5mm gradient across which doping level and transport properties vary continuously. We predict TE cooling performance based on our experimental results where cold side temperature ($T_c$) and coefficient of performance are calculated through linear constitutive relations coupled with conservation of charge and energy. The results demonstrate that $T_c$ of graded samples are significantly improved compared to that of uniform profile. This study provides guidelines to further development on more complex FGMs.

1:03PM X34.00010: Modulating Spin Concentrations in Self-Doped Organic Molecules
DANIEL POWELL (Presenter), LUISA WHITTAKER-BROOKS, University of Utah — N-type doping methods in organic systems typically combine small ionizable species with a semiconductor scaffold in solution before casting the pair into films. How dopants distribute within the cast semiconductor is unpredictable. The distribution of dopants, which vary from small to very large in their relative sizes, may affect semiconductor continuity, grain boundaries, morphology and packing of the semiconductor, electronic state distribution near the Fermi-energy, and yield topological variations in the electronic structure. Direct comparisons between different doping concentrations can therefore be rather nebulous, making the selection of the proper dopant for a given organic semiconductor highly convoluted. These challenges may be mitigated using self-dopants, where the electron source is covalently attached to the semiconductor. We have investigated the effects of steric hindrance, counterions, and dopant/semiconductor proximity on the efficiency of self-doping in a variety of perylene diimides. We believe our findings offer design considerations for the fabrication of effective self-dopants in n-type organic semiconductors.
1:15PM X34.00011: Bio-sourced Eumelanin Pigments: Charge Transport Properties and Beyond

MANUEL REALI (Presenter), ABDELAZIZ GOUDA, CLARA SANTATO, Ecole Polytechnique de Montreal — Green electronics recently opened new research avenues to use bio-sourced, biocompatible materials to limit the environmental footprint of electronics\textsuperscript{1-3}. Within bio-sourced carbon-based materials, eumelanin, a black-brown conjugated biopigment, emerged as an excellent candidate for green electronics.

Eumelanin features fascinating properties (e.g. broadband optical absorption\textsuperscript{4,5}, metal-ion chelation\textsuperscript{6}, mixed ionic/electronic conductivity\textsuperscript{7-9}) and biocompatibility\textsuperscript{1,10}. Its conjugated sp\textsuperscript{2} backbone suggests that it would be a naturally occurring semiconductor. The amorphous semiconductor model (ASM) for eumelanin, proposed in the 70s after the observation of an electrical resistive switching of wet melanin pellets\textsuperscript{11}, has been recently questioned by proposing mixed electronic/protonic and proton membrane models\textsuperscript{8,9,12}.

Herein, we report for the first time the electrical resistive switching response of dry eumelanin pellets, as opposed to previous studies indicating dry eumelanin as an insulating material\textsuperscript{11,13}. Wet pellets show a reversible and reproducible resistive switching, in agreement with McGinness et al\textsuperscript{11}. These findings rather suggest that dry pellets would be predominant electronic conductors.

1:27PM X34.00012: Evaluation of environmental effects on the performance of 2,8-difluoro 5,11-bis(triethylsilylethynyl) anthradithiophene thin-film transistors*

ZAFRULLAH JAGOO (Presenter), Univ of NC - Chapel Hill, ZACHARY LAMPORT, OANA D. JURCHESCU, Wake Forest University, LAURIE MCNEIL, Univ of NC - Chapel Hill — The electrical performance of organic transistors has been known to suffer from exposure to high moisture and oxygen levels. Reduction of the carrier mobility, threshold voltage shifting to more negative gate voltages and appearance of a hysteresis loop when scanning the gate voltage in the forward direction and then backwards are all manifestations of transistor deterioration. The worst possible outcome would be that the transistor is not longer functional after prolonged exposure to air. The study was conducted using a bottom-gate bottom-contact transistor with 2,8-difluoro 5,11-bis(triethylsilylethynyl) anthradithiophene (diF-TES ADT) as the active layer. The top surface of the semiconductor was uncovered and the device characteristics were measured at different oxygen and humidity levels. We found out that the organic thin-film transistor performed better electrically in the absence of water vapor and oxygen. Moreover, the degradation was reversible if the source of water vapor and oxygen was removed. This demonstrate the importance of encapsulation in organic semiconductor devices.

*NSF Award NSFDMR-1708379
1:39PM X34.00013: Bio-sourced, potentially biodegradable materials for fast response moisture sensors  
ABDELAZIZ GOUDA (Presenter), MANUEL REALI, CLARA SANTATO, Ecole Polytechnique de Montreal — Humidity is a very important physical parameter that plays an imperative role in technology and human activity. Researchers are paying more attention to develop moisture-responsive materials with outstanding characteristics such as high sensitivity, wide humidity detection range, fast response and short recovery times to keep pace with the ongoing development in technology. Abundant, bio-sourced and biodegradable organic materials, such as melanin, are needed to enable the development of eco-designed technologies that alleviate the environmental footprint of the electronics sector. Melanin is a ubiquitous biomacromolecule with diverse functions including hydration dependent electrical response [1], photoresponse [2], antioxidant [3], metal chelation [4], and free radical scavenging [5]. Melanin originates from the oxidative polymerization of (5,6)-dihydroxindole (DHI) and (5,6)-dihydroxindole 2-carboxyl acid (DHICA) building blocks [6]. DHI-melanin features ordered, conjugated structure with better electrical conductivity with respect to DHICA-melanin [5]. Herein, we investigate DHI-melanin and DHI-DHICA melanin thin films, spin coated and polymerized on technologically relevant and potentially biodegradable substrates, as active layers for fast response moisture sensors.

1:51PM X34.00014: Effects of Molecular Weight and Annealing on Charge Carrier Concentration in Thin PANI-CSA Films  
ARUN KUMAR AGARWAL (Presenter), SIDDHARTHA PANDA, Materials Science Programme, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India — PANI-CSA thin films have shown promising results like higher temperature sensitivities (Ahmad et al, J. Appl. Polym. Sci. 2013) and overcoming limitations of Wiedemann-Franz law (Jin et al, J. Phys. D: Appl. Phys. 2010) hence, can be used in flexible wearable sensors, thermoelectric devices. However, charge transport in PANI-CSA thin films is not very well understood. Effect of doping on electrical conductivity ($\sigma$) in PANI-CSA, effect of molecular weight ($M_W$) on mobility ($\mu$) in RR-P3HT (Zhang et al, Jour. of Amer. Chem. Soc. 2006) and change in grain size on annealing in P3HT:PCBM (Beal et al, Macromolecules 2010) have been reported. However, there is no study on effect of $M_W$ on charge carrier concentration ($n$) in annealed PANI-CSA thin films. PANI-CSA thin films (~50-70nm) were fabricated with different $M_W$ of PANI-EB. Their $\sigma$ was checked before and after annealing which showed a strong dependence on $M_W$. Annealing decreased $\sigma$ for all films but effect was more prominent at lower $M_W$. AFM was done to map morphological changes with $M_W$ and annealing. DC Hall measurements were done to measure $\mu$ but were inconclusive due to low $\mu$ (Yamada et al, Synth. Met. 2019) hence, AC Hall measurements were done which indicated that the change in $\sigma$ has two contributors; change in $\mu$ and change in $n$. 
Effects of concentration and local structure on charge trapping in polymer electrets with amine-based substituents.* EVAN PLUNKETT (Presenter), QINGYANG ZHANG, CHEN CHI, HOWARD EDAN KATZ, DANIEL REICH, Johns Hopkins University — Thin film polymer dielectrics with controllable electronic properties are of considerable interest for applications in organo-electronic systems. We use amine-based moieties in thin film polystyrene dielectrics to modify electron and hole trap states and densities. When chemically bound to polymers and also when introduced as free additives, these moieties induce changes in static potential differences that modify the behavior of adjacent electronic materials. For example, N,N'-diphenyl-N,N'-di-p-tolybenzene-1,4-diamine in polystyrene exhibited threshold voltage shifts up to \( \Delta V_{th} = O(50V) \) after application of static electric fields as measured in pentacene-based OFETs. Films with free additive concentration in the range of 1-3% showed a strongly concentration dependent stability in \( V_{th} \), in contrast to polystyrene systems with tethered amines. Stability is higher at lower amine concentrations suggesting clustering of additives is an important effect in these systems.

*Supported by U.S. DOE grant DE-FG02-07ER46465

Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X35 DPOLY DSOFT: Kinetics and Aggregation of Polymers in Complex Fluids and Geometries 507 - Jeffrey Ethier, Illinois Institute of Technology

Network Centrality of Heterogeneous Elastomers for Describing Mechanical Property  YOSHIFUMI AMAMOTO (Presenter), KEN KOJIO, ATSUSHI TAKAHARA, Kyushu Univ, YUICHI MASUBUCHI, Nagoya University, TAKAAKI OHNISHI, The University of Tokyo — There have been a lot of attempts to describe structure-property relationships of heterogeneous elastomers. However, it is hard to evaluate the heterogeneity quantitatively. In this presentation, we report the network structure of the elastomers in terms of connectivity was evaluated based on centrality, one of indicators utilized in complex network science, and its effect for the mechanical property was investigated. A construction and a uniaxial elongation of elastomers were performed with coarse-grained molecular dynamics simulation. End-to-end distance of partial chains, which strongly affect stress in entropy elasticity was evaluated. We found that the end-to-end distance increased with increasing the network centrality. Furthermore, network centrality incorporating initial end-to-end distance could be a unified indicator for the mechanical property of the heterogeneous elastomers. We think the complex network could be one of the suitable approaches to reveal structure-property relationships of materials.
11:27AM X35.00002: Understanding aggregation and growth in a cross-linked polymer film*

TINE CURK (Presenter), ERIK LUIJTEN, Northwestern University — Oil paints, used by celebrated artists such as Rembrandt, Picasso, Dalí and others, are composite materials consisting of pigment nanoparticles and polymerized drying oil. Dissociation of the pigment results in metal ions that react with the oil, yielding an insoluble metal soap. Over time scales of decades to centuries, these metal soaps aggregate, forming visible clusters and thus tainting the original work of art.

Lack of understanding of the aggregation and growth processes that occur in a cross-linked film hinders the conservation efforts aimed at preserving traditional works of art. To understand this degradation process, we propose a theoretical model combining existing models of nucleation and growth, as well as Ostwald ripening, with the elasticity and creep behavior of cross-linked polymers. Our model predicts the growth rates of clusters spanning nanoscopic to macroscopic length scales. The analytical results are supported by Monte Carlo simulations.

*This research was supported in part by the Andrew W. Mellon Foundation via the Center for Scientific studies in the Arts at Northwestern University.


CARLOS LOPEZ (Presenter), ANDREA SCOTTI, MONIA BRUGNONI, STEFFEN BOCHENEK, JEROME CRASSOUS, WALTER RICHTERING, Physical Chemistry, RWTH Aachen University — Soft, adaptive microgels are potential building blocks for smart materials with precisely controlled viscoelastic properties that are highly responsive to environmental conditions. We compare the flow properties of different PNIPAM microgels: regularly crosslinked and ultra-low crosslinked (ULC) microgels. We show that the flow properties of ULC microgels reveal a colloid-to-polymer transition with increasing solution concentration. At low concentrations, the viscoelastic properties and phase behaviour of ULC microgels are identical to those of regularly crosslinked microgels. With increasing concentration, the viscosity and plateau modulus display a much weaker increase for ULC relative to regularly cross-linked systems. Oscillatory rheology in the linear viscoelastic region reveals that for regularly crosslinked microgels in concentrated solution, the flow properties are determined by the highly cross-linked core, while for ULC microgels the brush-like interaction is dominant.

*A.S. thanks the Alexander von Humboldt Foundation for financial support. The authors acknowledge financial support from the SFB 985 "Functional Microgels and Microgel Systems" of DFG, Projects A3 and B8 and from the IHRS BioSoft.
11:51AM X35.00004: Electrostatics and Rheology of Unentangled Semidilute Polyelectrolyte Solutions  GUANG CHEN (Presenter), ANTONIO PERAZZO, HOWARD A STONE, Princeton University — Polyelectrolytes (PE) are charged polymers in polar solvents. Classical scaling theory suggests that the viscosity $\eta$ for salt-free semidilute unentangled PE solutions in $\Theta$ solvents obeys the empirical Fuoss law $\eta \sim c^{1/2}$ in the higher polymer concentration ($c$) regime, and $\eta \sim c^{5/4}$ in the lower $c$ regime. However, recent experiments have also reported $\eta \sim c^{0.68}$ and $\eta \sim c^{0.91}$, which are at odds with the classical scaling theory. To rationalize the four distinct scaling laws, we probe the electrostatic energy per monomer under the influence of salt and their contributions to the viscosity of PE solutions. We identify four consecutive regimes dependent on the magnitude of the ratio of the polymer concentration over the salt concentration, which capture the unexplained observations and classical PE solution theories, and provide physical insights for the effects of salt contamination and added salt on the properties of both weakly and strongly charged semidilute unentangled PE solutions.

12:03PM X35.00005: Patterned fluorescence photobleaching recovery on multicomponent sodium polystyrene sulfonate solutions to investigate temporal aggregate formation.*  PAUL BALDING (Presenter), PAUL RUSSO, RACHEL BORRELLI, Georgia Institute of Technology — Patterned fluorescence photobleaching recovery was used to investigate multicomponent mixtures of sodium polystyrene sulfonate (NaPSS) to further understand translational diffusion and formation of temporal aggregates observed in dynamic light scattering (DLS) of charged macromolecules. Mixtures consisted of fluorescein isothiocyanate labeled NaPSS probe and an unlabeled NaPSS matrix in salt concentrations that exceeded $C_p/C_s = 5.7$. In an effort to entrain single polymers into temporal aggregates, the matrix concentration was increased for several molecular weight probe polymers. If dilute probes enter matrix polymer aggregates then probe diffusion would be dictated by the aggregate, independent of probe molecular weight. But measured self-diffusion depended on probe molecular weight, evidence against probe aggregate inclusion. Further, probe diffusion depended on matrix molecular weight, at least above the entanglement concentration, suggesting that probes do not become entrained in the temporal aggregates, but respond to the presence of matrix polymer. Diffusion in unimodal NaPSS systems obeyed theoretical scaling laws of $D \sim C^{-0.5}$ but did not exhibit bi-exponential decay behavior as would be expected for diffusers in and outside temporary aggregates.

*Georgia Tech Hightower Family
12:15PM X35.00006: Simulating Surface-Grafted Polymers in Solvent Mixtures: Effects of Cononsolvency  JING ZONG (Presenter), DONG MENG, Chemical engineering, Mississippi State Univ — One puzzling phenomenon about polymer conformations in a mixture of solvents is the cononsolvency effect -- polymers in a good solvent undergo reentrant coil-to-globule-to-coil transition upon addition of a good cosolvent. Recent studies have suggested the generic nature of the cononsolvency effect independent of chemically specific details of the polymer and solvents. In this study, we first reinforce such claim by showing that a coarse-grained soft model frequently used in studying polymers is able to reproduce the reentrant transition at the single-chain level, provided that solvents are treated explicitly. In our Monte Carlo simulations, the coil-to-globule-to-coil transition occurs as the chemical potential of polymers in solution decreases upon increasing the cosolvent fraction, ruling out increasingly worse solvent quality as the cause of collapse. To further our microscopic understanding, we apply the soft model to studying conformational responses of surface-grafted polymers under the cononsolvency effect. By analyzing the inter-polymer density correlations, we illustrate the highly correlated nature of polymer clustering mediated by the cosolvents. Conformational responses of high grafting density brushes will also be discussed in the context of smart sensor surfaces.

12:27PM X35.00007: Humidity- and surfactant-accelerated aging in poly(vinyl alcohol)-based thin films*  KATARZYNA MAJERCZAK (Presenter), ZHENYU JASON ZHANG, Univ of Birmingham — This work aims to understand how relative humidity (RH) and chemical composition influence the diffusion of guest molecules in formulated polymer films replicating packaging materials for detergent products. Surface morphology of thin poly(vinyl alcohol) films containing glycerol and surfactants of various headgroup chemistry was examined using Atomic Force Microscopy under controlled RH conditions (15% – 55% RH). Diffusion was found to be controlled by both surfactant “blooming” from the polymer matrix and RH, leading to changes in film morphology. Anionic surfactants bloomed in the films at low concentration (1 wt%) above a threshold of 35% RH. Higher concentrations (above 3 wt%) were required for blooming of cationic surfactant, while nonionic surfactants showed no changes in film morphology regardless of concentration or RH. It is likely that chemical compatibility and charge-pairing effects are the main driving forces for these changes. Increased RH and presence of glycerol could enhance the free volume within the polymer matrix, accelerating diffusion and therefore achieving equilibrium (surfactant blooming), as confirmed by Dynamic Vapour Sorption measurements.

*This research was funded by EPSRC (grant number EP/P007864/1) and University of Birmingham.
Simulations of symmetric diblock copolymer melts have shown that the order-disorder transition (ODT) is given by \((\chiN)_{ODT} = 10.495 + 41\tilde{N}^{-1/3} + 123\tilde{N}^{-0.56}\), where \(\tilde{N}\) is the invariant polymerization index. This result, however, is specific to monodisperse molecules, whereas there is always some degree of polydispersity in experiments even when the molecules are synthesized by anionic polymerization. Using simulations, the polydispersity correction to the ODT is evaluated for the small degrees of polydispersity characteristic of anionic polymerization. We find that polydispersity reduces \((\chiN)_{ODT}\) for large \(\tilde{N}\), but increases \((\chiN)_{ODT}\) for small \(\tilde{N}\). These corrections should allow experimentalists to estimate the Flory-Huggins \(\chi\) parameter with greater accuracy.

*This work was supported by NSERC of Canada and Compute Canada

The thermodynamics of the binding of a charged dendrimer [poly(amidoamine)] to an uncharged graphene sheet is investigated through simulations and a mean-field theory. A non-monotonicity that is observed in the degree of binding of the dendrimer as a function of pH is explained through potential of mean force (PMF) calculations and the Flory-Huggins-Debye-Huckle type mean field theory, by analyzing the electrostatic and non-electrostatic interactions between the pairs of dendrimer, graphene, and water molecules and ions. The simulation trends are satisfactorily reproduced by the theoretical results. In addition to the van der Waals interactions between the dendrimer and the graphene sheet, it is found that the presence of the solvent ions and counterions too has a major influence on these trends.

*DST, India; CSIR, India; MHRD, India;
1:03PM X35.00010: Complex Viscosity of Helical and Doubly Helical Polymeric Liquids from General Rigid Bead-Rod Theory  JOURDAIN PIETTE, A. JEFFREY GIACOMIN (Presenter), MONA KANSO, Queen's University — With general rigid bead-rod modelling, we recreate shapes of complex macromolecular structures with beads, by rigidly fixing bead positions relative to one another. General rigid-bead rod theory attributes the elasticity of polymeric liquids to the orientation that their macromolecules develop during flow. For oscillatory shear flow, the frequency dependencies of both parts of the complex viscosity are predicted correctly. In this paper, we use general rigid-bead rod theory for the most complex macromolecular architectures to date. We thus explore the role of helix geometry on the complex viscosity of a helical polymeric liquid. Specifically, we investigate the effects of helix radius, flight length, helix length and the number of beads per flight on the complex viscosity function, the fluid relaxation time, the zero-shear values of the steady shear viscosity and of the first normal stress coefficient. As a worked example, we examine specifically deoxyribonucleic acid (DNA). Using general rigid bead-rod theory, we dissect the DNA to see how the first helix, second helix, and then the base pairs, each contribute to the complex viscosity. We next explore the rheological implications of gene replication to find that the unzipping of DNA into a pair of single strands is viscostatic.

1:15PM X35.00011: The tail free discotic liquid crystal 1,2,3,4,7-pentafluorotriphenylene: a study in structural variations*  MITCH POWERS (Presenter), BRETT ELLMAN, JOHN PORTMAN, Physics, Kent State University, ZHE LI, Advenchen Laboratories, KUNLUN WANG, PARIKSHIT GURAGAIN, ROBERT J TWIEG, SCOTT BUNGE, Chemistry, Kent State University, LEWIS L SHARPNACK, DENA MAE AGRA-KOOIJMAN, Physics, Kent State University, SATYENDRA KUMAR, SUNY-Albany — Discotic liquid crystals are disc shaped molecules that self assemble into long columns of cofacial molecules while still maintaining some liquid-like properties. They are typically formed by rigid aromatic molecular cores surrounded by a number of flexible tails. The tails play an important role, as they separate the columns and provide a source of entropy which inhibit crystallization. In this contribution, we describe a tail free discotic liquid crystal 1,2,3,4,7-pentafluorotriphenylene (7F-TFT). We will explore the nature of this tail free mesophase by comparing this compound with a number of closely related compounds based on tetrafluorotriphenylene. By varying the position and chemical species of the fifth substituent, we will see the effects that molecular structure have on this unusual mesogen.

*We gratefully acknowledge support from the NSF (award 1809536). This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562. Specifically, it used the Bridges system, which is supported by NSF award number ACI-1445606, at the Pittsburgh Supercomputing Center (PSC), through allocation TG-DMR190030.
1:27PM X35.00012: Effects of Boundary Conditions and Alignment Methods on Liquid Crystal Performance in Microwave Devices  JASON NOBLES (Presenter), OLHA MELNYK, ANATOLIY GLUSHCHENKO, ROBERT CAMLEY, ZBIGNIEW J CELINSKI, University of Colorado, Colorado Springs — Microwave devices are ubiquitous in our daily lives; cell phones, satellite communications, automobile safety radars all depend on microwaves. We are working on a technology, a merger of microwave science with liquid crystal physics, that has the potential to revolutionize microwave technology by reducing the size and cost of these devices by a factor of 100. As part of this effort, we are investigating a variety of the techniques used to control the initial state of the liquid crystal in a device to determine the optimum method to use with this emerging microwave technology. From our work, we see that a treated thin film of polyimide provides the best results. However, our work also demonstrates that, if a specialized liquid crystal known as dual frequency liquid crystal is used, the initial state of the liquid crystal does not significantly impact the performance of the device. This discovery reduces the number of steps necessary to manufacture microwave devices, saves on chemical and treatment costs, and eliminates several manufacturing challenges unique to liquid crystal based microwave devices. These benefits add up to a significant savings in time and cost during the design and manufacture of microwave components based on liquid crystal technology.

1:39PM X35.00013: Fast Water Transport in Polyelectrolyte Brush Functionalized Nanochannels*  VISHAL SANKAR SIVASANKAR (Presenter), SAI ANKIT ETHA, HARNOOR SINGH SACHAR, SIDHARTHDA SACHAR, Mechanical Engineering, University of Maryland, College Park — The need for enhanced transport and enhanced separation in nanochannels is prevalent across disciplines of fluid mechanics, material science, bio-medicine, nanotechnology, etc. In this study, we show that the functionalization of nanochannel with pH-responsive polyelectrolyte (PE) brushes, which we model using newly formulated augmented Strong Stretching theory, can lead to fast electroosmotic (EOS) transport of water. We observe that the presence of PE brushes results in enhanced flux when compared to brush free nanochannel. This is because of the localization of the EDL charge density away from the flow retarding wall. The enhanced flux obtained in brush functionalized nanochannels tends to be comparable to graphene-based state-of-the-art nanostructures which indicate that such a system could be used for fast transport of water. Moreover, we also witness a large gradient in the flow profiles, for certain conditions of the solvent, which suggests that these brush functionalized nanochannels could also be useful in size-based separation of particles.

*This work has been supported by the Department of Energy Office of Science grant DE-SC0017741.
Mechanisms of Surfactant Adsorption and Interfacial Tension Lowering for Enhanced Oil Recovery (EOR) Applications

JAEYUB CHUNG (Presenter), BRYAN BOUDOURIS, ELIAS I FRANSES, Chemical Engineering, Purdue Univ — The robust evaluation of aqueous surfactant formulations depend on their ability to lower the interfacial tensions (IFTs) of oil/water interfaces for mobilizing oil. For a formulation to be most effective, the IFT of an oil/water interface should be ultralow (<0.01 mN/m). We have discovered that there are two types of relevant equilibrium IFTs (EIFTs). The un-pre-equilibrated EIFT (EIFT$_{up}$) is established when primarily the surfactants have equilibrated across the interface, and applies to the early stages of the EOR process. The pre-equilibrated EIFT (EIFT$_{p}$) is established when the oil and aqueous components are also equilibrated, and is applied to the later stages. The two EIFTs can be different due to the preferential partitioning of the various surfactant components usually present in commercial surfactants. Such partitioning can change drastically the chemical potentials and the partition coefficients of these surfactant components, and causes an IFT shift to a more stable value as the oil and aqueous phases components equilibrate also at longer times. The results have significant implications for understanding the effect of the surfactant concentration and composition on the EIFT.

*The authors are grateful for the financial support from Pioneer Oil Company (Vincennes, IN).

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X36 DPOLY: Fantastic Polyelectrolytes and How They Behave in Coacervates

601/603 - Michael Rubinstein, University of North Carolina at Chapel Hill - Tag(s): Invited
**11:15AM X36.00001: Structure and Dynamics of Polyelectrolyte Solutions and Coacervates**

[Invited] RALPH COLBY (Presenter), Pennsylvania State University — The shear rate dependence of viscosity is used to evaluate the concentration dependences of specific viscosity, relaxation time and terminal modulus for several polyelectrolytes in three solvents: deionized water, ethylene glycol and glycerol. Small-angle X-ray scattering determines the correlation length of these polyelectrolyte solutions from a peak in their scattering function, which changes as expected with solvent dielectric constant. In semidilute unentangled solutions, dynamics are described by the Rouse model and combined with the correlation length in different ways to determine the number density of chains, which allows calculation of the number-average molecular weight using a robust method that is insensitive to the presence of salt. The high viscosity glycerol solvent allows characterization of the viscoelastic response of high molecular weight polyelectrolytes over a wide range of frequency, showing Rouse character in unentangled solutions and a clear rubbery plateau in strongly entangled solutions.

A simple way to make a polyampholyte gel is to mix oppositely charged polyelectrolytes, which precipitate to form a sediment that is termed a coacervate. Hydrophilic coacervates (with roughly 70 % water in them) are reversible gels with labile ionic interactions and their dynamics are described by a sticky Rouse model. In both examples, while not everything is understood for these complicated forms of condensed matter, polymer physics can be used to gain important insights.

*This work was supported by the NSF Chemistry Division.

**11:51AM X36.00002: Phase Behavior and Viscoelasticity of Polyelectrolyte Coacervates at High Salt Concentrations**

[Invited] JENNIFER LAASER (Presenter), FRANCES J MORIN, MARISSA PUPPO, LEXI KNIGHT, Chemistry, University of Pittsburgh — Separating the salt and polymer volume fraction-dependent dynamics of complex coacervates is challenging because changing the salt concentration of the sample typically also changes the polymer concentration in the polymer-rich phase. Here, we describe a way to address this challenge using a “salt-addition” method for preparation of complex coacervates that allows us to increase the salt concentration of the coacervate without significantly changing the polymer volume fraction. Using this method, we investigate the rheology of polystyrenesulfonate (PSS)/poly(diallyldimethylammonium chloride) (PDADMAC) coacervates at salt concentrations near and above the critical salt concentration. We find that the dependence of the relaxation times on salt concentration is similar to that observed in previous studies, but that the relaxation times scale significantly more strongly with polymer volume fraction than previously assumed. Additionally, we identify a second critical salt concentration above which the coacervates separate at high salt concentrations, and use thermogravimetric analysis to characterize the phase behavior of these materials in the high-salt regime. These results demonstrate that the salt addition method is a powerful approach for exploring and identifying new behaviors of coacervates in the high salt limit.

*Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for partial support of this research.
12:27PM X36.00003: Fantastic Entanglements between Polyelectrolytes in Solutions [Invited]
CARLOS LOPEZ (Presenter), Physical Chemistry, RWTH Aachen University — We study the entanglement properties of flexible and semiflexible polyelectrolytes sodium polystyrene sulfonate and sodium carboxymethyl cellulose. In dilute salt-free and excess-salt solutions these polymers adopt rod-like and expanded coil conformations respectively. The solvent’s ionic strength has a large impact on the conformation of polyelectrolytes, and the number of binary interchain contacts, quantified through the intrinsic viscosity and osmotic pressure respectively. While adding salt leads to a large decrease in polymer size, it does not affect their entanglement density and entanglement crossover. This contradicts packing models of polymer entanglement and suggests that the density of binary contacts in solution is not affected by the solvent quality. Based on this observation, we work out the reptation dynamics of polyelectrolytes in salt-free solution, which differ appreciably from earlier models.

1:03PM X36.00004: Structure and rheology of polyelectrolyte complex coacervates [Invited]
AMANDA MARCIEL (Presenter), Rice Univ, SAMANVAYA SRIVASTAVA, University of California, Los Angeles, MATTHEW TIRRELL, The University of Chicago — Polyelectrolyte complexes are highly tunable materials that span from low-viscosity liquids (coacervates) to high-modulus solids with high water content, making them attractive as surface coating, membrane purification and bioadhesive materials. However, most of their properties and their effects with salt, pH, polymer ratio and temperature have only been qualitatively described. Here, we present an investigation of the structure and chain conformations, and rheological properties of polyelectrolyte complex (PEC) coacervates comprising biomimetic model polyelectrolytes. Systematic studies using small-angle X-ray scattering (SAXS) of the structure and chain behavior in liquid PEC coacervates revealed a physical description of these materials as strongly screened semidilute solutions of polyelectrolytes comprising oppositely charged chains. At the same time, solid PECs were found to be composed of hydrogen-bonding driven stiff ladder-like structures with large correlation lengths. While the liquid complexes behaved akin to semidilute polyelectrolyte solutions upon addition of salt, the solids were largely unaffected by it. Terminal relaxations of the chains in PEC coacervates were explored by rheology measurements. Excellent superposition of the dynamic moduli data was achieved by a time-salt superposition.

1:39PM X36.00005: Fantastic Saloplastic* [Invited] JOSEPH SCHLENOFF (Presenter), MO YANG, ZACH DIGBY, KHALIL AKKAOUI, Florida State Univ — Oppositely-charged polymers spontaneously assemble into amorphous complexes or coacervates, driven mainly by the release of counterions. Macromolecules within these polyelectrolyte complex/coacervates, PECs, are well blended due to pairing of oppositely-charged repeat units Pol⁺ and Pol⁻. These charge pairs can be quickly and reversibly broken by the addition of salt to the solution in which PECs are immersed, reducing their bulk modulus. This reversible doping by salt, termed saloplasticity, controls all of the physical and mechanical properties of PECs. This talk will illustrate the concept and origin of saloplasticity and show how a “stick association” theory of polymers can be extended to PECs to predict their dynamics as a function of salt doping.

*This work was supported by the National Science Foundation, Division of Materials Research.
11:15AM X37.00001: Finite speed of quantum scrambling with long range interactions
[Invited] ANDREW LUCAS (Presenter), University of Colorado, Boulder — In a locally interacting many-body system, two isolated qubits, separated by a large distance r, become correlated and entangled with each other at a time $t \geq r/v$. This finite speed v of quantum information scrambling limits quantum information processing, thermalization and even equilibrium correlations. Yet most experimental systems contain long range power law interactions -- qubits separated by r have potential energy $V(r) \propto r^{-\alpha}$. Examples include the long range Coulomb interactions in plasma ($\alpha=1$) and dipolar interactions between spins ($\alpha=3$). In one spatial dimension, we prove that the speed of quantum scrambling remains finite for sufficiently large $\alpha$. This result parametrically improves previous bounds, compares favorably with recent numerical simulations, and can be realized in quantum simulators with dipolar interactions. Our new mathematical methods lead to improved algorithms for classically simulating quantum systems, and improve bounds on environmental decoherence in experimental quantum information processors.

11:51AM X37.00002: Emergent locality in systems with power-law interactions*
[Invited] YEVGENY BAR LEV (Presenter), Ben-Gurion University of the Negev — In generic systems with local interactions transport is diffusive and information propagates inside a quasicausal "light-cone" parametrized by a constant velocity known as the Lieb-Robinson velocity. Introducing long-range interactions, should intuitively enhance transport by long-range hops, and deform the linear "light-cones," into a superballistic form. Using two numerically exact techniques I will show that this is not the case for a number of generic one-dimensional systems. All studied systems, for sufficiently short-range interactions, show universal behaviour of asymptotically emergent locality and a unique composite transport comprised of diffusive and superdiffusive features.

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National Science Foundation Grant No. CHE-1464802
Binational Science Foundation Grant No. 2019644

12:27PM X37.00003: Locality and Digital Quantum Simulation of Power-Law Interactions
[Invited] MINH CONG TRAN (Presenter), University of Maryland, College Park — The propagation of information in non-relativistic quantum systems obeys a speed limit known as a Lieb-Robinson bound. We show that Lieb-Robinson bounds provide tighter estimates for the gate count in quantum algorithms for simulating power-law interacting Hamiltonians. In addition, we prove new Lieb-Robinson bounds using techniques from quantum simulation algorithms. This brings the analysis full circle, revealing a deep connection between Lieb-Robinson bounds and digital quantum simulation.

1:03PM X37.00004: Dominic Else Invited Talk [Invited] —
1:39PM X37.00005: Signaling and scrambling for strongly long-range interacting quantum systems [Invited]  ZHEXUAN GONG (Presenter), Colorado School of Mines, ANDREW GUO, MINH C TRAN, ANDREW CHILDS, University of Maryland, ALEXEY V GORSHKOV, National Institute of Standard and Technology — Strongly long-range interacting quantum systems—those with interactions decaying as a power-law $1/r^\alpha$ in the distance $r$ on a D-dimensional lattice for $\alpha \leq D$—have received significant interest in recent years. They are present in leading experimental platforms for quantum computation and simulation, as well as in theoretical models of quantum information scrambling and fast entanglement creation. Since no notion of locality is expected in such systems, a general understanding of their dynamics is lacking. As a first step towards rectifying this problem, we prove two new Lieb-Robinson-type bounds that constrain the time for signaling and scrambling in strongly long-range interacting systems, for which no tight bounds were previously known. Our first bound applies to systems mappable to free-particle Hamiltonians with long-range hopping, and is saturable for $\alpha \leq D/2$. Our second bound pertains to generic long-range interacting spin Hamiltonians, and leads to a tight lower bound for the signaling time to extensive subsets of the system for all $\alpha < D$. This result also lower-bounds the scrambling time, and suggests a path towards achieving a tight scrambling bound that can prove the long-standing fast scrambling conjecture.

Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X38 DQI: Superconducting Qubits: Circuit Theory, Hamiltonian Analysis and Design Tools 607 - Arne Grimsmo, Univ of Sydney

11:15AM X38.00001: QuCAT: superconducting quantum circuit analyzer tool in Python*
MARIO GELY (Presenter), GARY STEELE, Delft University of Technology — Quantum circuits constructed from Josephson junctions and superconducting electronics are key to many quantum computing and quantum optics applications. Designing these circuits involves calculating the Hamiltonian describing their quantum behavior. In this talk, we present QuCAT, or "Quantum Circuit Analyzer Tool", an open-source framework to help in this task. This open-source Python library features an intuitive graphical or programmatical interface to create circuits, the ability to compute their Hamiltonian, and a set of complimentary functionalities such as calculating dissipation rates or visualizing current flow in the circuit.

*This work was supported by the European Research Council under the European Union’s H2020 program [grant numbers 681476-QOM3D, 732894-HOT, 828826-Quromorphic]
MATTHEW WEIPPERT (Presenter), KRISTINA COLLADAY, DAVID FERGUSON, RYAN J EPSTEIN, Northrop Grumman - Mission Systems — We report on efficient quantum simulation of large superconducting circuits using matrix product states (MPS) and the density matrix renormalization group (DMRG) technique. We analyze a circuit containing a chain of Josephson junctions, forming a superinductor, with a flux-tunable compound center junction. Kuzmin et al. explored similar circuits experimentally, achieving super strong coupling in circuit electrodynamics [1]. We obtain the lowest-lying eigenstates and energies for a chain length of 40 Josephson junctions with derived error bounds. Using these tensor network techniques we investigate the offset charge sensitivity of the circuit as a function of compound junction flux, which is not amenable to classical analysis and is intractable via exact diagonalization.


This research was supported by the Army Research Office under contract W911NF-17-C-0024.

AGUSTIN DI PAOLO (Presenter), THOMAS BAKER, ALEXANDRE FOLEY, DAVID SENECHAL, ALEXANDRE BLAIS, Institut quantique and Departement de Physique, Universite de Sherbrooke — We introduce a tensor-network method tailored to the simulation of large-scale superconducting quantum circuits. We leverage information unavailable to other state-of-the-art numerical techniques to produce first-principles coherence-time estimates for the fluxonium qubit. In particular, we study the charge dispersion of this qubit due to coherent quantum phase slip processes. Taking advantage of this novel approach, we present direct numerical evidence of the validity of the effective theory introduced in [V. E. Manucharyan et. al, PRB 85, 024521 (2012)].

This work was undertaken thanks in part to funding from NSERC and the Canada First Research Excellence Fund.

DAVID FERGUSON (Presenter), DAVID J. CLARKE, RYAN J EPSTEIN, MOE S KHALIL, Northrop Grumman - Mission Systems, DANIEL WEISS, JENS KOCH, Northwestern University — Many superconducting qubits, such as transmons, are naturally described in terms of Cooper-pair charges hopping on and off of the nodes of the superconducting circuit. Others, such as flux qubits, are naturally described via superconducting vortices hopping in and out of the loops of the superconducting circuit. This talk describes a method to transform the Hamiltonian of a superconducting circuit from the Cooper-pair number basis to the dual vortex-number basis. In contrast to other methods that also accomplish this transformation, our method is non-perturbative and isospectral. It provides a useful framework to compare and evaluate the novel properties of qubits of the flux-qubit type such as nonstoquasticity and decreased sensitivity to environmental noise.

This research was supported by the Army Research Office under contract W911NF-17-C-0024.
12:03PM X38.00005: Designing Better Superconducting Qubits using First-Principles Calculations and Theory  
SINEAD GRIFFIN (Presenter), Lawrence Berkeley National Laboratory — Superconducting qubits have emerged as one of the leading candidates for scalable quantum computing, despite suboptimal coherence times and resonantor quality factors. In this work, we combine first-principles calculations and effective models to describe key performance losses in niobium-based superconducting qubits. We find that defects play a decisive role in their operational efficiency, and that careful control of stoichiometry can significantly improve their performance. We compare our theoretical predictions with recent experiments confirming the importance for defects for understanding decoherence pathways in qubits and quantum materials.

12:15PM X38.00006: Design and Analysis of Multi-Qubit Superconducting Chips for Extensible Surface Coding*  
NADIA HAIDER (Presenter), QuTech and TNO, The Netherlands, ALESSANDRO BRUNO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands, MARC BEEKMAN, PIOTR KAMINSKI, QuTech and TNO, The Netherlands, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands — We present an effective numerical method to analyze qubit-qubit avoided crossings and two-qubit gate times in a superconducting multi-qubit chip. Our hybrid simulation approach, combining finite element and circuit simulation, is a convenient tool to investigate complex chip layouts with limited computational resources. The simulation method has been applied to design and investigate a new multi-qubit chip layout. This new chip design and improved fabrication process have allowed us to also reduce mode hybridization between qubits and resonators and to increase qubit coherence time.

*Research funded by Intel Corporation.

12:27PM X38.00007: Design and quantization of superconducting circuits*  
ZLATKO MINEV (Presenter), THOMAS G MCCONKEY, FIRAT SOLGUN, JERRY M. CHOW, JAY M GAMBETTA, DAVID MCKAY, IBM TJ Watson Research Center — Quantum information processing using superconducting circuits has steadily developed into a large and diverse field. The success of building larger devices emphasizes the need to more efficiently and accurately design and quantize the distributed microwave structures, including non-linear elements, such as Josephson tunnel junctions, which comprise these devices. In this talk, we review some recent results on the comparison between several of the commonly used quantization and design approaches.

*IBM Research
12:39PM X38.00008: Derivation of the Hamiltonian of a flux qubit-LC oscillator circuit using the circuit variables*  FUMIKI YOSHIHARA (Presenter), National Institute of Information and Communications Technology, SAHELI ASHHAB, Qatar Environment and Energy Research Institute, TOMOKO FUSE, KOUICHI SEMBA, National Institute of Information and Communications Technology — We derive the Hamiltonian of a single-Josephson-junction flux qubit-LC oscillator circuit using the standard quantization procedure [1]. The derived Hamiltonian consists of terms related to the LC oscillator, the flux qubit (and its higher energy levels), and the product of the two flux variables. This Hamiltonian is similar to that of the quantum Rabi model, where a two-level atom and a harmonic oscillator are coupled by a dipole-dipole interaction. Therefore, it is not surprising that the observed transmission spectra of a flux qubit-LC oscillator circuits can be well fitted by the quantum Rabi Hamiltonian [2]. We also find that the simple picture that models the coupling using a common inductor shared by the LC oscillator and the flux qubit needs only a minor modification. We thank Michel Devoret and Motoaki Bamba for stimulating discussions.

*This work was supported by Japan Society for the Promotion of Science Grant-in-Aid for Scientific Research (Grant No. JP19H01831), and Japan Science and Technology Agency Core Research For Evolutionary Science and Technology (Grant No. JPMJCR1775)

12:51PM X38.00009: Efficient Hamiltonian Parameter Estimation with Sequential Monte Carlo Technique*  JÉRÉMY BÉJANIN (Presenter), CAROLYN EARNEST, MATTEO MARIANTONI, Department of Physics and Astronomy and Institute for Quantum Computing, University of Waterloo, YUVAL R SANDERS, Department of Physics and Astronomy and ARC Centre of Excellence for Engineered Quantum Systems, Macquarie University — As quantum computers grow in size the task of calibrating them becomes more complex. There are many parameters to optimize for and the resulting performance of the qubits depends strongly on how well various quantities are measured. For example, knowledge of the coupling to neighboring qubits or resonators is necessary for two-qubit gates. In addition, it is preferable if qubits are located far away in frequency from harmful systems like Two-Level State defects.

By utilizing a frequency tunable qubit as a probe, we can measure the parameters of a resonance, namely the frequency and coupling strength, and use this information to calibrate gates or improve coherence times. Because these parameters fluctuate over time, this calibration should be repeated regularly. It is therefore important that it runs quickly. Using tunable transmon superconducting qubits, we demonstrate a method to efficiently measure the parameters of these resonant couplings. Initially, these parameters are estimated from a state of zero knowledge with a method based on Hamiltonian dynamics. Subsequently, a Sequential Monte Carlo technique can quickly refine and improve the accuracy of that estimate.

*This research was undertaken thanks in part to funding from the Canada First Research Excellence Fund (CFREF).
ANDREY KLOTS (Presenter), University of Wisconsin - Madison, LEV B IOFFE, Google.; University of Wisconsin - Madison, ROBERT F MCDERMOTT, University of Wisconsin - Madison — We propose a mathematical formalism and software that allow to express Hamiltonian of any superconducting circuit in a standardized way. The process allows for efficient/quick diagonalization of Hamiltonians of complex circuits. With vastly increasing number of various complicated qubit designs (0-pi qubits, gmoms,...) it becomes necessary to be able to describe various LCJ circuits analytically and model them numerically. Normally, this requires thorough study of different degrees of freedom in the circuit in order to decide which variables are essential to understanding the properties of a circuit and which are secondary. Proposed formalism automatically classifies different degrees of freedom of a circuit based on their essential properties (charge quantization, mode frequencies) and role in the circuit. Hamiltonian of any qubit circuit can be automatically obtained and the generalized coordinates can be quantized in a most natural way: through charge number operators for charge islands and photon number operators for oscillatory circuit modes. This, in turn allows us to automatically and efficiently find eigenstates of various quantum qubit circuits. We show how the formalism is used for advancing practical qubit applications.

*We thank ARO HiPS W911NF-18-1-0106
Quantum landscape engineering of superconducting circuit ground states for higher-order coupler design* TIM MENKE (Presenter), Harvard Department of Physics, MIT Research Laboratory of Electronics, MIT Department of Physics, Harvard University, Massachusetts Institute of Technology, CYRUS F. HIRJIBEHEDIN, STEVEN WEBER, MIT Lincoln Laboratory, JOCHEN BRAUMÜLLER, ANTTI VEPSALAINEN, RONI WINIK, Research Laboratory of Electronics, Massachusetts Institute of Technology, GABRIEL ORR SAMACH, MIT Research Laboratory of Electronics, MIT Department of Electrical Engineering and Computer Science, MIT Lincoln Laboratory, Massachusetts Institute of Technology, DAVID K KIM, ALEXANDER MELVILLE, BETHANY NIEDZIELSKI, DANNA ROSENBERG, MOLLIE SCHWARTZ, JONILYN YODER, MIT Lincoln Laboratory, ALAN ASPURU-GUZIK, Department of Chemistry and Department of Computer Science, Vector Institute for Artificial Intelligence, CIFAR Senior Fellow, University of Toronto, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, ANDREW JAMES KERMAN, MIT Lincoln Laboratory, WILLIAM OLIVER, Research Laboratory of Electronics, Department of Electrical Engineering and Computer Science, Department of Physics, MIT Lincoln Laboratory, Massachusetts Institute of Techn — The response of the ground state energy of a superconducting circuit to external magnetic flux can be shaped by design to engineer quantum devices including artificial spin couplers. We propose a methodology for adding higher-order polynomial terms into the ground state energy versus flux by strongly coupling a series of rf SQUIDs. The fundamental instance of two rf SQUIDs generating a ground state with 4th-order terms is implemented experimentally. Probing this circuit with a sensor flux qubit, the qubit’s transition frequency maps the derivative of the quartic ground state in accordance with simulation. Modest levels of qubit coherence are maintained despite the relatively strong inductive coupling. These results demonstrate the viability of this design for use as a 4-local coupler and show promise for extending to higher polynomial order.

*This research is funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002.
The Hodgkin-Huxley model describes the conduction of the nervous impulse through the axon, whose membrane’s electric response can be described by multiple connected electric circuits containing capacitors, voltage sources, and conductances. These conductances depend on previous depolarizing membrane voltages, which can be identified with a memory resistive element called memristor. Inspired by the recent quantization of the memristor, the Hodgkin-Huxley model has been studied in the quantum regime. The circuit obtained in this model is proposed as the building block for the construction of quantum neurons networks which can process quantum information. Hence, we study two such circuits connected in series, coupled to a quantized source. Since the main quantum contribution on these systems comes from the second moment of the voltage, we study correlations such as degree of coherence, between voltage and conductance in both circuits, proving they are quantum variables. This study paves the way for advances in hardware-based neuromorphic quantum computing, as well as quantum machine learning, which might be more efficient resource-wise.

*The authors acknowledge support from the EU Flagship projects QMiCS and OpenSuperQ, as well as the U.S. Department of Energy project ERKJ333.

The manipulation and the measurement of any system made of superconducting qubits rely on the use of often strong microwave drives. Current experiments show that the standard Lindblad Master Equation commonly used to describe these driven systems breaks down even for moderate drive strength. We developed a corrected numerical implementation of the Floquet-Markov Master Equation that exactly takes into account the effects of drives and apply it to study more accurately the dissipative dynamics of superconducting qubits.

*This work was undertaken thanks in part to funding from NSERC and the Canada First Research Excellence Fund. This research was funded in part by the ARO grant No. W911NF-18-1-0411.
1:51PM X38.00014: Lifetime renormalization of driven transmon qubits and the classification of mechanisms for drive-induced energy relaxation*  
HAKAN TURECI  
(Presenter), Princeton University, ALEXANDRU PETRESCU, Département de Physique, Université de Sherbrooke, MOHAMMAD MOEIN MALEKAKHLAGH, IBM Thomas J. Watson Research Center — Recent experiments in superconducting qubit systems have shown an unexpectedly strong dependence of the qubit relaxation rate on the readout drive power. This phenomenon limits the maximum measurement strength and thus the achievable readout speed and fidelity. In two recent papers [1,2] we have shown that the leading mechanism responsible for the enhancement of energy relaxation times of weakly anharmonic qubits is the presence of number non-conserving terms in the Josephson potential, which activate additional multi-photon and qubit-cavity correlated relaxation channels in the presence of drives. We address here a realistic experimental setup and account for the joint effects of radiative (Purcell) decay at finite temperature and dephasing.


*This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Award No. DE-SC0016011.

Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X41 GMAG DMP: Novel Magnetic Materials 707 - Christopher Safranski, IBM TJ Watson Research Center
Crystal growth and characterization of the magnetic properties of intercalated transition metal dichalcogenides

KANNAN LU (Presenter), University of Illinois at Urbana-Champaign, DEEPAK SAPKOTA, The University of Tennesse, Knoxville, ADAM ACZEL, LISA DEBEER-SCHMITT, YAN WU, Oak Ridge National Lab, DAVID MANDRUS, The University of Tennesse, Knoxville, GREG MACDOUGALL, University of Illinois at Urbana-Champaign

The intercalated transition metal dichalcogenide (TMDC) Cr$_{1/3}$NbS$_2$ has attracted significant interest in recent years due to reports of a magnetic soliton lattice in this material in finite fields. This novel topological state of matter is understood to result from competing Zeeman, Dzyaloshinskii-Moriya and ferromagnetic exchange terms in the spin Hamiltonian. Despite this theoretical understanding, there are few other experimental realizations of soliton lattice materials beyond the singular compound Cr$_{1/3}$NbS$_2$. With this motivation in mind, we have undertaken a concerted effort at Illinois to grow large single crystals of additional intercalated TMDCs, and characterize them with a series of techniques, including magnetization, heat capacity, x-ray and neutron scattering. In this talk, I will report on these data and their implications for the magnetic ground states for each of the materials studied. In particular, I will report on our use of powder x-ray diffraction and magnetization to infer information about the centrosymmetry of the structure in these materials, and thus the potential for DM interactions. I will supplement with neutron diffraction from single crystals to comment on ordered ground states, and their potential to contain soliton phases in finite fields.

Vestigial Potts nematicity in a triangular lattice magnet

JÖRN VENDERBOS (Presenter), Drexel Univ, RAFAEL FERNANDES, Physics, University of Minnesota

Motivated by recent experimental evidence for spontaneous rotational symmetry breaking in the hexagonal antiferromagnet Fe$_{1/3}$NbS$_2$, this talk discusses the general theory of nematic order in magnetic system with hexagonal symmetry, focusing in particular on the possibility of a vestigial nematic phase. In stark contrast to tetragonal systems, such as the iron-pnictides, nematic order in hexagonal systems is described by the 3-state Potts model. We develop the general theory of (single-q) magnetic order at degenerate symmetry-related wave vectors, and show that distinct magnetic phases can be elegantly captured by composite order parameters: bilinears of the primary magnetic order parameters which transform irreducibly under the symmetry group. Singling out the composite nematic order parameter, we extend the Landau-type mean field theory with magnetic fluctuations and show that a vestigial nematic phase, i.e., a non-magnetic phase with broken rotation symmetry, can exist. We discuss experimental signatures and interpret our results in light of the reported measurements on Fe$_{1/3}$NbS$_2$. 
Effect of Confinement on Magnetism and Skyrmionic Properties of CoSi Nanoparticles

RABINDRA PAHARI (Presenter), BALAMURUGAN BALASUBRAMANIAN, AHSAN ULLAH, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, ROHIT PATHAK, ARTI KASHYAP, School of Basic Sciences, Indian Institute of Technology Mandi, RALPH SKOMSKI, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, GEORGE C HADJIPANAYIS, Department of Physics and Astronomy, University of Delaware, DAVID SELLMYER, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska — Quantum-confinement and surface effects often result in unusual magnetic ordering, modified ordering temperatures, and different spin structures in nanoparticles as compared to the corresponding bulk alloys [1, 2]. In sharp contrast to non-magnetic bulk equiatomic CoSi, we show a magnetic ordering at room temperature with a net magnetic moment \( m = 0.11 \mu_B/Co \) for CoSi nanoparticles. The nanoparticles have an average size of 11.6 nm, and crystallize in the cubic B20 structure, which supports spin spirals and skyrmions with broken helicity caused by non-zero Dzyaloshinskii-Moriya (DM) interactions [3]. DC susceptibility and anomalous Hall resistivity measurements are used to discuss the effect of confinement within the small diameter of CoSi nanoparticles on the room-temperature skyrmionic properties, which are essential for exploiting these complex spin structures for practical applications.

References

*This research is supported by the U.S. Department of Energy (DE-FG02-04ER46152 and DE-FG02-04ER4612), NSF-NNCI (1542182), and NCMN-NRI.
New magnetic orderings in elemental Neodymium

HASITHA SURIYA ARACHCHIGE (Presenter), Department of Physics & Astronomy, University of Tennessee, Knoxville, LISA DEBEER-SCHMITT, Neutron Scattering Science Division, Oak Ridge National Laboratory, DAVID PARKER, ANDREW MAY, Materials Science & Technology Division, Oak Ridge National Laboratory, MARKUS BLEUEL, Center for Neutron Research, National Institute of Standards and Technology, GANESH POKHAREL, Department of Physics & Astronomy, University of Tennessee, Knoxville, WEI TIAN, Neutron Scattering Science Division, Oak Ridge National Laboratory, CRISTIAN BATISTA, Neutron Scattering Division and Shull-Wollan Center, Oak Ridge National Laboratory, DAVID MANDRUS, Department of Materials Science & Engineering, University of Tennessee, Knoxville, ANDREW D CHRISTIANSON, Materials Science & Technology Division, Oak Ridge National Laboratory — The element neodymium is one of the most magnetically complex elements. Previous reports find a myriad of magnetic phases as a function of temperature and field below the antiferromagnetic transition temperature of 19.9 K [1-3]. Here we present a small angle neutron scattering (SANS) study of neodymium to probe whether the complex magnetic interactions on the double hexagonal closed packed (DHCP) crystal structure of neodymium can host novel spin textures. The SANS measurements reveal several new features. Firstly, the measurements establish regions in the HT phase diagram where scattering patterns characteristic of a skyrmion lattice are present. Additionally, we find new low field phase boundaries and pockets that bear some semblance to existing phase diagrams of skyrmion materials.

References


*This work was supported by U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division and the Gordon and Betty Moore Foundation’s EPiQS Initiative as the funding agencies.
12:03PM X41.00005: Magnetic textures in single crystals of Ni$_{1-x}$Fe$_x$Br$_2$* BINOD RAI (Presenter), Materials Science and Technology Division, Oak Ridge National Laboratory, HASITHA SURIYA ARACHCHIGE, GANESH POKHAREL, Physics and Astronomy, The University of Tennessee, YAOHUA LIU, Neutron Scattering Division, Oak Ridge National Laboratory, SHIZENG LIN, Theoretical Division, Los Alamos National Laboratory, CRISTIAN BATISTA, Physics and Astronomy, The University of Tennessee, DAVID MANDRUS, Materials Science and Engineering, The University of Tennessee, ANDREW D CHRISTIANSON, ANDREW MAY, Materials Science and Technology Division, Oak Ridge National Laboratory — Recently, frustrated systems with finite easy axis anisotropy have been proposed as a route to realize topological spin textures. In this context, Ni$_{1-x}$Fe$_x$Br$_2$ has been predicted to host a field-induced skyrmion phase. This presentation will discuss the magnetic properties of Ni$_{1-x}$Fe$_x$Br$_2$ single crystals and the magnetic field-temperature phase diagram. NiBr$_2$ crystallizes in the centrosymmetric CdCl$_2$ structure type. It exhibits a commensurate antiferromagnetic phase below $T_N = 48$ K and an incommensurate helimagnetic phase below $T_{IC} = 22$ K, both with easy plane anisotropy. The helimagnetic structure of Ni$_{1-x}$Fe$_x$Br$_2$ is tuned as a function of composition and applied magnetic field, as demonstrated using bulk measurements and neutron scattering. A change in magnetic anisotropy from easy plane to easy axis is observed around $x = 0.07$, which is expected as a key feature to realize a skyrmion phase in this system.

*U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division

12:15PM X41.00006: Imaging skyrmions in B20 epitaxial thin films grown on Si substrates using variable temperature Magnetic Force Microscopy (MFM) CAMELIA SELCU (Presenter), TAO LIU, DENIS PELEKHOV, ROLAND BENNETT, BINBIN WANG, NURIA BAGUES SALGUERO, JACOB REPICKY, JOSEPH P CORBETT, BRENDAN MCCULLIAN, Ohio State Univ - Columbus, YUNQIU (KELLY) LUO, Laboratory of Atomic and Solid State Physics (LASSP), Cornell University, SHUYU CHEN, ADAM S AHMED, P CHRIS HAMMEL, MOHIT RANDERIA, JAY A GUPTA, DAVID W. MCCOMB, ROLAND KAWAKAMI, Ohio State Univ - Columbus — In the search for the next-generation magnetic storage, tuning the size of the skyrmions with high Curie temperatures ($T_C$) promotes the possibility to use them for such application. We have successfully grown Fe-rich Fe$_{1.2}$Ge thin films using Molecular Beam Epitaxy (MBE) with a $T_C$ higher than the room temperature. Furthermore, we have observed skyrmions in the Fe-rich Fe$_{1.2}$Ge thin films at room temperature. Here, we report the first time imaging of the skyrmions in FeGe and Fe rich Fe$_{1.2}$Ge epitaxial thin films grown on Si substrates using Magnetic Force Microscopy (MFM). Based on the MFM images, skyrmions were observed in temperatures and magnetic fields consistent with the topological Hall measurements for the FeGe thin films. Additionally, the topological Hall resistance scales down with the density of skyrmions at lower temperatures in these films. Also, we observed skyrmion motion and annihilation which might be driven by the stray field of the MFM tip probably due to the defects in the FeGe films.
Skyrmions are a topologically protected magnetic texture that attracts attention both for its interesting physics, and for potential spintronics applications. Central to the realization of applications is the requirement to have small skyrmions. Recently, skyrmions have been reported to exist in two new materials, Gd$_2$PdSi$_3$ [1] and Gd$_3$Ru$_4$Al$_{12}$ [2]. The skyrmions in these materials are reportedly extremely small (2.3 – 3 nm compared to 20 – 60 nm in other materials), and, in contrast to most known skyrmion materials, are thought to be stabilized by frustration, rather than by the antisymmetric Dzyaloshinskii-Moriya interaction.

In this talk, we will present measurements of resonant X-ray scattering on Gd$_2$PdSi$_3$ and muon spin rotation on Gd$_2$PdSi$_3$ and Gd$_3$Ru$_4$Al$_{12}$. These measurements reveal interesting new features about the magnetic structures in these materials, as well as the dynamics surrounding these magnetic states.


*This work was funded by the UK Skyrmion Project EPSRC Programme Grant (EP/N032128/1). M. N. Wilson acknowledges the support of the Natural Sciences and Engineering Research Council of Canada (NSERC).
Lattice dynamics of antiperovskite manganese nitrides exhibiting large negative and positive thermal expansion*  
SHEENA PATEL (Presenter), STJEPAN B HRKAC, JEFFREY BROCK, NELSON HUA, University of California, San Diego, HAIDAN WEN, Argonne National Laboratory, OLEG SHPYRKO, ERIC FULLERTON, University of California, San Diego — Antiperovskite manganese nitrides Mn$_3$AN (where A is a metal or semiconducting element) have strong charge-spin-lattice interactions resulting in magnetovolume effects such as large positive (PTE) and negative thermal expansion (NTE) over transitions between their ferrimagnetic, antiferromagnetic, and paramagnetic phases [1]. We grow films of Mn$_3$Cu$_{1-x}$Ge$_x$N with x = 0.1 to 0.5, which exhibit tunable NTE coefficients over a 50 K region, occurring anywhere from around 100 K to around 400 K depending on x. We also grow films of Mn$_3$Cu$_{1-x}$Ni$_x$N with x = 0.09 to 0.10, which have a first order hysteretic PTE of 1-1.5% near 100 K and exhibit NTE for a total lattice contraction of roughly 0.5% over a 25 K range around 175 K. These regions are linked to transitions in magnetic phases. To probe the coupling of the structure and magnetism, we have measured the X-ray diffraction following photoexcitation within and through the interesting regions at the Advanced Photon Source. We present the complex lattice dynamics and discuss the spin-lattice coupling driving their response.


*Work at UCSD was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contracts No. DE-SC0018237 and DE-SC0001805.

Non-periodic magnetic structure in chiral helimagnet Mn$_{1/3}$NbS$_2$*  
SUNIL KARNA (Presenter), Department of Physics and Astronomy, Louisiana State University, Baton Rouge, MICHALIS CHARILAOU, Department of Physics, University of Louisiana at Lafayette, ANDRAS KOVÁCS, Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, LISA DEBEER-SCHMITT, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, DAVID P YOUNG, JOHN DITUSA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge — We have investigated the magnetic state of Mn$_{1/3}$NbS$_2$ through $ac$-magnetic susceptibility, Small-angle Neutron Scattering (SANS), Lorentz Transmission Electron Microscopy (LTEM) and micromagnetic simulations. The $ac$ susceptibility displays temperature, field, and frequency dependencies which define a complex phase diagram below the critical temperature for magnetic ordering, $T_C = 45$ K. SANS reveals a streak of magnetic scattering along the c-axis near $Q = 0$ appearing below $T_C$, demonstrating a disordered ferromagnetic (FM) or helical spin ordering in this system. The width of this streak shortens and becomes more intense near $T_C$ and is gradually suppressed by the application of $H$ along the beam. Micromagnetic simulations of thin lamella are in agreement with LTEM images of Mn$_{1/3}$NbS$_2$ where extended FM regions result from a shape anisotropy in thin samples that are separated by the chiral domain walls.

*This material is based upon the work supported by the U.S. Department of Energy under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents.
1:03PM X41.00010: Local structural distortions and magnetism in lacunar spinel compounds* JULIA ZUO (Presenter), EMILY C SCHUELLER, RAM SESHADRI, STEPHEN WILSON, University of California, Santa Barbara — Lacunar spinels $AB_4Q_8$ ($A=$Al, Ga, Ge; $B=$V, Nb, Mo, Ta; $Q=$S, Se) display a variety of novel phenomena including skyrmion lattices and pressure-induced insulator-metal transitions and superconductivity. The high temperature structure features unique tetrahedral transition-metal clusters with $S=1/2$ moments on an FCC lattice. Low temperature distortions of these clusters are crucial to the properties of lacunar spinels. In skyrmion hosts GaV$_4$S$_8$ and GaV$_4$Se$_8$, a low temperature rhombohedral distortion allows for polar and magnetic order. In GaNb$_4$Se$_8$ and GaTa$_4$Se$_8$, antiferromagnetic interactions lead to geometric frustration and a magnetic transition associated with a tetragonal distortion. We present results of local structural characterization on lacunar spinels in connection to their magnetic properties.

*This work was supported primarily by the NSF through the DMREF program DMR 1729489. The use of shared facilities from the Materials Research Science and Engineering Center (MRSEC) is gratefully acknowledged. The MRL Shared Experimental Facilities are supported by the MRSEC Program of the NSF under DMR 1720256; a member of the NSF-funded Materials Research Facilities Network (www.mrfn.org).

1:15PM X41.00011: Magnetic texture evolution within uniaxial kagome ferromagnets immediately below Curie temperature AKIRA SUGAWARA (Presenter), TETSUYA AKASHI, Center for Exploratory Research, Hitachi Ltd, MOHAMED A KASSEM, Department of Physics, Assiut University, YOSHIKAZU TABATA, TAKESHI WAKI, HIROYUKI NAKAMURA, Department of Materials Science and Engineering, Kyoto University — Magnetic textures such like skyrmion and skrmionic bubbles attracts attention in connection with topology of electronic structures. Such texture formation usually occurred slightly below Curie temperature ($T_C$) due to competition of micromagnetic parameters that change rapidly with approaching $T_C$. We examined magnetic texture within two uniaxial kagome ferromagnets: Co$_3$Sn$_2$S$_2$ ($T_C=176$ K) studied extensively as a Weyl-semimetal and Fe$_3$Sn$_2$ ($T_C= 657$ K) interested for its massive Dirac fermions. In-situ Lorentz microscopy was performed during cooling across $T_C$ under zero field. In Co$_3$Sn$_2$S$_2$, nucleation of bubble domains followed by their spontaneous reorganization occurred in narrow temperature range immediately below $T_C$, whereas the domain wall motion was mostly frozen below 160 K. The morphology of the domains also depended on cooling rate through domain wall creep associated with thermal depinning. The magnetic phase diagram is influenced by slow spin dynamics also, hence is not determined uniquely as a function of field and temperature. In contrast such creep motion did not occur in Fe$_3$Sn$_2$ immediately below $T_C$, whereas domain wall motion occurred continuously in wide temperature range down toward room temperature.
Hexagonal ferrites such as PbFe$_{12}$O$_{19}$, SrFe$_{12}$O$_{19}$, BaFe$_{12}$O$_{19}$ show interesting magnetic and ferroelectric properties at low temperatures. The magnetic ordering temperature of these compounds can be tuned by random site dilution replacing Fe ions by Ga ions, for example in PbFe$_{12-x}$Ga$_x$O$_{19}$. According to recent experiments, the critical temperature of these compounds varies as $T_c \propto (1 - x/x_c)^{2/3}$, where $x_c$ is very close to the percolation threshold of the lattice [1]. Motivated by these results, we re-examine the shape of the magnetic phase boundary over the entire $x$ range from 0 to $x_c$. We perform large scale Monte-Carlo simulation of diluted XY and Heisenberg models for both cubic lattices and lattices representing the crystal structure of the hexaferrites. In particular, we study the critical behavior of the percolation transition and width of the critical region.

References:

We report the observation of a chemical-substitution driven phase transition from a gapped quantum paramagnetic phase to one with long range order in Cs$_{1-x}$Rb$_x$FeCl$_3$. The $x = 0$ compound in this series of triangular-lattice antiferromagnets has a spin-singlet ground state due to strong easy-plane magnetic anisotropy. In contrast, the $x = 1$ material orders magnetically in a 120° structure [1]. Calorimetric and magnetic experiments performed on a series of samples with $0 \leq x \leq 1$ reveal that in the low-temperature limit magnetic order appears at $x \sim 0.35$. Inelastic neutron scattering experiments show that this coincides with the closure of the gap in the spin excitation spectrum. It appears that disorder effects in this material are more pronounced than those in the only other known phase transition of this type, namely in DTNX [2].


*This work was supported by Swiss National Science Foundation under Division 2
Intrinsic stability of magnetic anti-skyrmions in the tetragonal inverse Heusler compound Mn$_{1.4}$Pt$_{0.9}$Pd$_{0.1}$Sn

RANA SAHA, ABHAY KANT SRIVASTAVA, TIANPING MA (Presenter), JAGANNATH JENA, PETER WERNER, Nano-Systems from ions, spins and electrons, Max Planck Institute of Microstructure Physics, VIVEK KUMAR, CLAUDIA FELSER, Solid State Chemistry, Max Planck Institute for Chemical Physics of Solids, STUART PARKIN, Nano-Systems from ions, spins and electrons, Max Planck Institute of Microstructure Physics — Magnetic anti-skyrmions [1] are one of several chiral spin textures that are of great current interest both for their topological characteristics and potential spintronic applications. Anti-skyrmions were recently observed in the inverse tetragonal Heusler material Mn$_{1.4}$Pt$_{0.9}$Pd$_{0.1}$Sn. Here we show, using Lorentz transmission electron microscopy, that anti-skyrmions are found over a wide range of temperature and magnetic field in wedged lamellae formed from single crystals of Mn$_{1.4}$Pt$_{0.9}$Pd$_{0.1}$Sn for thicknesses ranging up to ~250 nm [2]. The temperature-field stability window of the anti-skyrmions varies little with thickness. Using micromagnetic simulations we show that this intrinsic stability of anti-skyrmions can be accounted for by the symmetry of the crystal lattice which is imposed on that of the Dzyaloshinskii-Moriya exchange interaction. These distinctive behaviors of anti-skyrmions makes them particularly attractive for spintronic applications.


Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X42 GMAG: Structured Materials

Vacancies in artificial spin ice*

PABLO DÍAZ (Presenter), FELIPE BREVIS, EUGENIO VOGEL, Univ de La Frontera — We study artificial spin-ice systems (in the form of square arrays of islands of magnetic materials) from the numerical point of view. Typical Permalloy elongated and anisotropic islands [1] occupy the positions completely filling a layer L×L, with variable L; several equivalent layers are then piled up. We focus on the vertices (that are the convergence points of islands) as the internal layers are diluted upon introducing vacancies (lack of islands). This is both a random and controlled process for a single internal layer; the uppermost and lower-most layers remain without vacancies. The introduction of vacancies generated several new types of vertices that can be characterized according to their distribution depending of vacancy concentration. We found that a small amount of vacancies has strong influence on the vertex distributions. Moreover, we considered a code based format for the different vertices and found that is possible to write on each layer complete and robust messages. The propagation of information in a transverse way (from top to lower layer) is also explored.


*Chilean sources: Fondecyt 1190036, Cedenna (Conicyt FB0807)
11:27AM X42.00002: Field-tunable correlations in perpendicular artificial spin ice arrays
SUSAN KEMPINGER (Presenter), North Central College, YU-SHENG HUANG, PAUL EDWARD LAMMERT, Penn State University, MICHAEL VOGEL, JOHN PEARSON, Argonne National Lab, AXEL HOFFMANN, University of Illinois, VINCENT CRESPI, Penn State University, PETER E SCHIFFER, Yale University, NITIN SAMARTH, Penn State University — Artificial spin ice (ASI) provides an effective platform for the study of custom designed frustration and its relationship with geometry, interaction, and stochasticity. Perpendicular ASI is particularly useful in this context, as the state of each element in a lattice is readily accessed using Kerr microscopy and the microstate of the entire lattice can be characterized through an applied field protocol. Unfortunately, studies of perpendicular ASI have been limited by weak interactions between elements. We have overcome this limitation by fabricating perpendicular ASI systems from Pt/Co islands on a soft-magnetic Ni_{80}Fe_{20}(Py) underlayer to increase interactions. In the simplest case, the Py is saturated and serves to break the lateral symmetry in the arrays. We show that this configuration leads to a highly tunable system with unusual properties such as directionally-tunable interactions, preferred next-nearest neighbor coupling, and in situ adjustable coordination number. This project was funded by the US Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under Grant No. DE-SC0010778

11:39AM X42.00003: Competition between topological order and long range order in Santa Fe spin ice
AYHAN DUZGUN (Presenter), CRISTIANO NISOLI, Los Alamos National Laboratory — Artificial spin ices are two-dimensional arrays of interacting single-domain ferromagnetic nano-islands [1,2]. Santa Fe Ice is a newly proposed and recently realized artificial spin ice lattice whose vertex-frustrated [3,4] spin ensemble can be described by strings of topologically protected excitations. We have investigated numerically Santa Fe Ice in and out of equilibrium. Depending on structural parameters, its ground state can either be a disordered topological phase [5,6] or an ordered, anti-ferromagnetic state. In the latter case, however, the topological phase is still present and can trap the system, delaying or preventing the relaxation to the ordered state either after quenches or even after a slow annealing when in the neighborhood of the structural transition.

11:51AM X42.00004: Shape transformations of flexible ferromagnetic ribbons

KOSTIANTYN YERSHOV (Presenter), Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01171 Dresden, Germany, VOLODYMYR P. KRAVCHUK, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany, DENIS D. SHEKA, Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine, JEROEN VAN DEN BRINK, Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01171 Dresden, Germany, YURI GAIDIDEI, Bogolyubov Institute for Theoretical Physics of National Academy of Sciences of Ukraine, 03143 Kyiv, Ukraine — We propose a minimal extension of the anisotropic 2D Heisenberg model in order to describe flexible magnetic systems with coupled magnetic and mechanical subsystems[1,2]. The coupling between the magnetic and mechanical subsystems is driven by uniaxial anisotropy with the easy-axis normal or tangential to the magnetic film and by the Dzyaloshinskii--Moriya interaction (DMI). We show that the presence of DMI results in a spontaneous deformation of a flexible magnetic ribbon. The final state is characterized by the geometrical chirality whose sign is determined by the sign of the DMI constant. Depending on the mechanical, magnetic, and geometric parameters of the system one can obtain two different states: a twisted-state with zero curvature of the central line is typical for small DMI constants and narrow ribbons, while a DNA-like state with nonzero curvature of its central line is preferable for large DMI constants and wider ribbons. All these states can be efficiently controlled by magnetic fields opening new possibilities in the development of nanorobots in the context of organicelectronics and spintronics.


12:03PM X42.00005: A New Approach of Constructing Shape-controlled Nanowire Arrays

FEI CHEN (Presenter), RUWEN PENG, MU WANG, Nanjing Univ — Magnetic nanowires with controlled morphology and crystallinity are enabling devices with novel functionalities. The fabrication of the nanowires with specific shapes such as standing U-shaped nanowires and helical nanowires is still challenging, especially on a rough and bumpy surface. Here we demonstrate a unique way to fabricate cobalt nanowire arrays on an arbitrarily-shaped surface by electrodeposition. When the pH of the electrolyte is around 2.3, the deposit shows monocrystalline hcp structure with the c-axis perpendicular to the long-axis of the nanowire arrays. On the other hand, when the pH is around 4.5, the deposit shows polycrystalline hcp structure. Counter intuitively, here the growth direction of nanowire is perpendicular to its longitudinal axis, and the specific geometry of nanowires can be achieved by introducing specially designed shaped substrate. The spatial separation and the width of the nanowires can be tuned by voltage, electrolyte concentration and temperature in electrodeposition. By taking cobalt nanowire array as an example, we show that head-to-head and tail-to-tail magnetic domain walls can be easily introduced and modulated in the nanowire arrays, which is enlightening to construct new devices such as domain wall racetrack memory.
We experimentally observe both U- and S-shaped zero-field magnetic configurations in single square permalloy dots, with a dot's configurational state dependent on field history and temperature. Magnetization of 170 nm x 170 nm x 7 nm dots is probed using 4-terminal anisotropic magnetoresistance (AMR) measurements. Room temperature field sweeps parallel to the dot edge yield AMR curves characteristic of both a U-shaped state [1], and of a previously unreported S-shape, for identical field sweep parameters. The S-shape sweep pattern is not observed at low T, implying the state is thermally activated, a result confirmed by micromagnetic simulations. The S-state also occurs when sweeping the field off-axis by several degrees, consistent with minimizing Zeeman interaction energy. The existence of multiple zero-field configurations precludes use of the Stoner-Wolfarth model typically used at this scale, instead necessitating a more complicated configurational picture as dot size decreases.


This work supported in part by NSF Grant No. DMR 1609782. Portions of this work conducted in the Minnesota Nano Center, which is supported by the NSF through the National Nano Coordinated Infrastructure Network, Award Number NNCI -1542202.
In-tissue embedded magnetic nanoparticle (MNPs) detection is one of the most interesting cases for biomedical applications. Biological (especially tumor) tissues present a variety of morphologies. Ferrogels (FG) are magnetic composites that are widely used in the area of biomedical engineering and biosensing. We propose to substitute biological samples and use synthetic ferrogel to mimic main properties of the living systems at the stage of the development of magnetic biosensor prototypes. Natural tissue requires tight protocol of storage/testing but synthetic hydrogels are less demanding to test conditions. In order to make FG widely available there is a need in the development of synthesis techniques with enhanced size of a batch. Electrophysical techniques of electric explosion of the wire or laser target evaporation (LTE) are suitable for this objective. We have developed magnetic biosensor prototype for the detection of mesoscopic distributions of magnetic nanoparticles using magnetoimpedance phenomenon. Prototypes with FeNi/Ti or FeNi/Cu multilayered elements were designed and the stray fields of embedded LTE MNPs were measured. A model for MI response based on a solution of Maxwell equations was developed. We discuss the possibility of creation of a new generation of drug delivery systems for magnetic field assisted delivery, positioning and biosensing.


*RSF 18-19-00090 and MAT2017-83631-C3-R grants
**1:03PM X42.00008: Tunability of magnetism in Heusler Mn$_3$Ga: Crossover between cubic and tetragonal phase upon Co-substitution**

THI QUYNH ANH NGUYEN (Presenter), HUYNH THI HO, SOON CHEOL HONG, SONNY H. RHIM, Univ of Ulsan — Structural and magnetic properties of Co substituted Mn$_{3-x}$Co$_x$Ga ($x = 0$-$1$) is investigated using *ab initio* calculations. Ferrimagnetic Mn$_3$Ga possesses two inequivalent Mn sites, octahedral Mn-I and tetrahedral Mn-II, where Co prefers Mn-II site, which leads to intriguing physics. Notably, structural transition, from tetragonal to cubic phase, occurs around $x=0.6$. Unlike other Co compounds, local moment of Co nearly vanishes in tetragonal phase, which results in decreasing total moment with Co concentration. In contrast, in cubic phase Co retains usual moment: Magnetic moment increases linearly with $x$ obeying Slater-Pauling rule of cubic Heusler, $M = N_V - 24$, where $M$ is the magnetization, $N_V$ is numbers of valance electrons. In particular, the integral $M$, a signature of half-metallicity, emerges in cubic phase for $x=0.5$ and $1.0$. Furthermore, the vanishing moment of Co for tetragonal phase is analyzed phenomenologically using Heisenberg model, where the exchange coefficients of two Mn sites tends to compensate.

*(NFR-2015M3D1A1070465)
(NRF 2018R1A4A1020696)
(NRF-2019R111A3A01059880)

**1:15PM X42.00009: Deconvoluting Magnetic contributions in BiFeO$_3$ NPs using First Order Reversal Curves**

ALEXANDER CARDONA RODRÍGUEZ (Presenter), EDWIN ER RAMOS, NICOLÁS VERGARA, DIEGO CARRANZA, ANDREAS REIBER, JUAN RAMÍREZ, University of the Andes — BiFeO$_3$ (BFO) in bulk is ferroelectric (FE) and antiferromagnetic (AF) at room temperature. Additional it also possesses a Dzyaloshinski-Moria (DM) anisotropy that produces a 62 nm wavelength spin spiral. Therefore, in nanostructured BFO systems, a complex ferromagnetism-like behavior appears that depends on the balance between size and magnetic length scales. Furthermore, it is known that the physical properties in perovskites in general, and BFO in particular, are very sensitive to changes in their crystal structure. Hence, one can exploit such effects to control their degrees of freedom. Here we present first-order reversal curves (FORC) as a reliable method to deconvolute the BFO magnetic contributions that appear when nanostructured in the form of nanoparticles with sizes below and above the wavelength spin spiral. We use FORC to obtain coercivity distributions for different nanoparticles sizes. Our results suggest two main contributions to BFO magnetism that can be related to an intrinsic core-shell structure that forms due to strain relaxation.

Magnetorheological elastomers (MREs) are polymers with embedded micron or submicron ferromagnets. MREs are a promising platform for studying cell responses to dynamic mechanical changes in their environment, as the shear modulus is tunable via an applied magnetic field [1]. MREs deform under applied magnetic fields, including visible twisting. In this work, we used a multi-scale approach to model the magnetic reversal and field-dependent deformations. Ferromagnetic particles in the polymer interact via dipolar coupling, but are also permitted to move; the balance of dipole, elastic energies, and Zeeman energy dictates the deformations of MREs. A point-dipole based model was used to study the behavior of a collection of particles in an elastomer matrix, and micromagnetic simulation results for a ferromagnetic sphere provided the susceptibilities used as input parameters. Volume-preserving in- and out-of-plane deformations were incorporated in the model, as well as, twisting of the matrix as observed in experiments. Modelling results will be presented and compared to experimental hysteresis measurements.

References

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Ferromagnetic Liquid Droplets

Ferrofluids are dispersions of ferromagnetic or superparamagnetic nanoparticles in carrier fluids and are paramagnetic liquids that become magnetized in the presence of an external magnetic field but completely lose the magnetization at remanence when the field is removed. We have found a route to reversibly transform these paramagnetic droplets into ferromagnetic droplets by the formation, assembly and jamming of a magnetic nanoparticle-surfactants at the interface of the droplet with a surrounding immiscible fluid that encapsulates the magnetic nanoparticle dispersion. These liquid droplets have a coercivity and remanent magnetization at room temperature. They couple features of liquids, including versatile and reversible control of shape, and translational and rotational degrees of freedom, but preserve a magnetic moment, enabling remote manipulation by an external magnetic field. The droplets were shaped into cylinders, made buoyant in the surrounding liquid, and, in response to a rotating permanent magnet, rotated at an increasing angular velocity that reached a size-dependent maximum velocity. Assemblies of multiple liquid magnets form switchable, dynamic self-organized patterns, similar to those of Mayer's floating magnets. The ability to shape and manipulate the ferromagnetic liquid droplets opens possibilities for magnetically actuated sensors, all-liquid magnetic storage medium and magnetically driven 3D-printed robotic systems. These findings represent a new concept where soft matter, nanotechnology and magnetism meet, establishing a platform for a new generation of all-liquid devices. In collaboration with N. Kent, A. Ceballos, R. Streubel, Y. Jiang, Y. Chai, J. Forth, S. Shi, D. Wang, B. A. Helms, P. D. Ashby, P. Fischer and T. P. Russell.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X43 DCOMP DMP: Computational design and discovery of novel materials VII: Machine learning and high throughput computing

702 - Feng Zhang, Ames Lab
11:15AM X43.00001: Density Functional Theory Calculations on Surface Oxygen Vacancy Formation in Metal Oxides  
YOYO HINUMA (Presenter), Chiba Univ, TAKASHI TOYAO, Hokkaido University, TAKASHI KAMACHI, Fukuoka Institute of Technology, ZEN MAENO, SATORU TAKAKUSAGI, SHINYA FURUKAWA, Hokkaido University, ICHIGAKU TAKIGAWA, RIKEN, KEN-ICHI SHIMIZU, Hokkaido University — Properties of materials may be significantly changed from intrinsic ones by making small physical and chemical changes in the form of defects. As a result, various point and extended defects are intentionally introduced to govern their chemical reactivity, catalytic, electrical, optical, and mechanical properties. One mechanism important in catalysis is the Mars-Van Krevelen mechanism that is frequently encountered. An example is where O vacancy sites on a metal oxide catalyst surface acts as the reaction site.

Accurate calculation of the surface vacancy formation energy based on first principles calculations require calculation of a surface model and is much more computationally expensive than a bulk calculation. Catalysts typically require a certain physical quantity to be within a certain range, hence rapid judgement of whether a candidate material is viable or not based on quantities (descriptors) that are easy to calculate can significantly accelerate the screening process. We report on correlations between descriptors that can be calculated at low cost and the O vacancy formation energy of various insulating binary oxide materials [Hinuma et al., J. Phys. Chem. C 2018, 122, 29435] as well as spinel oxides containing zinc.

11:27AM X43.00002: Genarris 2.0: A Random Structure Generator for Molecular Crystals  
RITHWIK TOM (Presenter), TIM C ROSE, IMANUEL BIER, HARRIET O’BRIEN, Carnegie Mellon University, ALVARO VAZQUEZ-MAYAGOITIA, Argonne National Lab, NOA MAROM, Carnegie Mellon University — Genarris 2.0 is an open-source Python code, parallilized with mpi4py, that performs configuration space screening of molecular crystals by random structure generation. It may be used for generating initial populations to seed other structure search algorithms (such as genetic algorithms) or for generating datasets to train machine learning models. The target unit cell volume is estimated from the single molecule structure by a machine-learned model trained on data from the Cambridge Structural Database (CSD). Crystal structures are then generated in all space groups compatible with the requested number of molecules per cell (Z) with one molecule in the asymmetric unit (Z’=1), including those with special Wyckoff positions. To avoid unphysically close intermolecular distances, structures undergo a cascade of three increasingly rigorous checks. Special settings are applied for strong hydrogen bonds, which are automatically detected. Once an initial dataset of several thousand structures is generated, a smaller dataset may be selected based on quality and diversity criteria via user-defined workflows. For clustering Genarris uses the affinity propagation machine learning algorithm with a relative coordinate descriptor (RCD) or a radial symmetry function (RSF) representation.
Exploring the quantum chemical space of small molecules: QM7-X database

JOHANNES HOJA, LEONARDO MEDRANO SANDONAS, Physics and Materials Science Research Unit, University of Luxembourg, BRIAN ERNST, Department of Chemistry and Chemical Biology, Cornell University, ALVARO VAZQUEZ-MAYAGOITIA (Presenter), Argonne Leadership Computing Facility, Argonne National Laboratory, ROBERT DISTASIO, Department of Chemistry and Chemical Biology, Cornell University, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, University of Luxembourg — Robust and extensive databases of molecular properties are required to enable rational exploration of chemical space. Most databases created so far either include only equilibrium structures of molecules or do not use sufficiently high level of quantum mechanics. Here, we introduce the QM7-X database created with the goal of sampling the vast chemical space for small organic molecules. As basis for QM7-X, we used all molecules within the GDB7 database. All possible enantiomers and diastereomers were also added. Then, to have a sufficient sampling of the potential energy surface, we have considered 100 non-equilibrium conformations around every conformer of a molecule, producing a database of approximately 4.2 million structures in total. Several physicochemical properties were subsequently computed by performing quantum mechanics calculations using FHI-AIMS code at the PBE0-MBD level of theory. As a first attempt for predicting molecular properties, we have applied neural networks in the form of the SchNet package. We also demonstrate that the exploration of the QM7-X chemical space breaks traditional textbook notions of chemical correlations and enables building robust and transferable machine learning models for molecular property prediction.

Matching Crystal Structures Atom-to-Atom: Applications to Phase Transitions and Interface Structures*

FELIX THERRIEN (Presenter), Colorado School of Mines, PETER GRAF, National Renewable Energy Laboratory, VLADAN STEVANOVIC, Colorado School of Mines — Finding an optimal match between two different crystal structures underpins many important materials science problems including describing solid-solid phase transitions, developing models for interface and grain boundary structures, finding suitable substrates and their orientation, etc. We designed and implemented an algorithm that tackles this problem by finding the atom-to-atom map and alignment that minimizes a chosen distance function. We demonstrate its capacity to describe transformation pathways of several solid-solid transformations. In particular we show its ability to seamlessly predict important experimentally observed characteristics of the martensitic transformation of steel. Next, we study several interfaces and show our method's relevance in predicting interfacial planes and their orientation relationships. Finally, from our findings, we define a rigorous metric for measuring distances between crystal structures and use it as a tool to screen the Inorganic Crystal Structure Database.

*This work was supported as part of the Center for the Next Generation of Materials by Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.
12:03PM X43.00005: Predicting h-BCN Geometric Structures Using Clustering and Regression Methods* 
SONALI JOSHI (Presenter), DAVE AUSTIN, DUY LE, TALAT S. RAHMAN, Univ of Central Florida — Despite the fact that hexagonal graphene-like boron–carbon–nitrogen (h-BCN) monolayer, a synthesized material that has received a great deal of attention thanks to its intriguing properties and its potential application, there is no consensus on its geometric structure. We report here results of our machine learning approach that utilizes clustering and neural networks to find the lowest energy structure of h-BCN. Our dataset consists of 300 randomly generated h-BCN structures, optimized using density functional theory based calculations. To characterize the atomic environment of the atoms, a pattern recognition scheme based on neighbors was developed. We found that our model accurately predicts the total energy of h-BCN structure with a R-squared score as high as 0.85, depending on the number of k-means clusters used. We will also discuss the improvement of our predictions using a deep neural network.

*Work supported in part by DOE grant DE-FG02-07ER15842

12:15PM X43.00006: Towards a Crystalline Organic Superconductor Database* 
OWEN GANTER (Presenter), CHARLES C AGOSTA, Clark University — A database of layered organic crystalline materials containing structural information, experimentally determined properties, and electronic band structure is proposed. Layered organic crystals have a rich electronic phase diagram and exhibit numerous electronic ground states including traditional and unconventional superconductivity, charge and spin density waves, Dirac points, and spin liquid states. The proposed database will be a versatile tool for scientists studying quantum materials and will pave the way towards new discoveries and materials via machine learning methods. We will present a computer algorithm for analyzing the crystal structure of layered organic crystals and storing the extracted structure parameters in the database. The algorithm analyzes molecular conformation, dimerization, packing types, and intermolecular interactions of cations that form the conductive layer of these materials. We will discuss the challenges of inputting experimentally determined material properties from scientific articles into the database, and the best methods to do it. We will also show a Python based system for automatically initializing, executing, and analyzing WIEN2k DFT calculations for materials in the database.

*We acknowledge the support Grant# DMR-1905950 from the NSF
12:27PM X43.00007: Accelerated enumeration of derivative structures using zero-suppressed binary decision diagram  KOHEI SHINOHARA (Presenter), ATSUTO SEKO, Kyoto Univ, TAKASHI HORIZIYAMA, Hokkaido Univ, MASAKAZU ISHIHATA, NTT Communication Science Laboratories, JUNYA HONDA, The Univ of Tokyo, ISAO TANAKA, Kyoto Univ — The enumeration of “derivative structures” [1], which are unique substitutional atomic configurations derived from a given parent lattice, plays an essential role in searching for the ground states in multi-component systems. The possible size of supercells to enumerate the derivative structures, however, is limited because the number of the derivative structures increases exponentially as the number of sites in a substitutional lattice increases. In the present study, we apply a compressed data structure of the zero-suppressed binary decision diagram (ZDD) [2] to enumerate the derivative structures much more efficiently. We also employ an efficient procedure [3] to build the ZDD representing the derivative structures without listing all substitutional structures. The present study shows simple applications of the procedure to enumerate the derivative structures for the face-centered cubic and hexagonal close-packed parent lattices in binary, ternary, and quaternary systems. The present procedure with the ZDD should significantly contribute to computational approaches based on the derivative structures.


12:39PM X43.00008: Multifidelity Learning and Statistical Analysis of Material Properties*
ABHIJITH GOPAKUMAR (Presenter), MOHAN LIU, Northwestern University, RAMAMURTHY RAMPRASAD, Georgia Institute of Technology, CHRISTOPHER MARK WOLVERTON, Northwestern University — There are many examples of materials data where the coexistence of two types of datasets occur: a smaller, higher-fidelity (higher accuracy) dataset, and a larger, lower-fidelity dataset. Here, we investigate a statistical modeling approach for materials properties in these cases of varying fidelity. Kriging based multi-fidelity learning is an approach suited to these cases, and we demonstrate its usefulness by applying it to model and predict the chemical properties of compounds in the Open Quantum Materials Database (OQMD). Specifically, we focus datasets of DFT-calculated bandgaps, and consider a case of high-fidelity data from computationally expensive hybrid HSE calculations and low-fidelity PBE GGA calculations. The multifidelity model is trained on a database containing 1100 HSE bandgaps and combined with results from the OQMD which contains a much larger set of PBE bandgaps. We demonstrate the utility of this multifidelity approach in predicting HSE bandgaps for all materials in OQMD, analyze the predicted results for various material classes, and compare the multifidelity approach with multiple single-fidelity machine learning models trained on the same dataset.

*Toyota Research Institute (TRI) Accelerated Materials Design and Discovery program
12:51PM X43.00009: Symbolic Regression in Materials Science* YIQUN WANG (Presenter), JAMES RONDINELLI, Northwestern University — One of the fundamental research objectives of materials science is to design new materials with optimal performance. Typical machine learning models could be powerful predictors but not ideal in terms of interpretability. Here we present on an alternative to machine-learning models: symbolic regression (SR), which simultaneously searches for the optimal form of a function and set of parameters to the given problem, and is a powerful regression technique when little if any a-priori knowledge of the data distribution is available. We present how SR can learn the Landau free energy expansion describing the structural phase transition in LaNiO$_3$ using existing computational data [1]. Our model is able to capture the coupling of the temperature and order parameter, and we successfully predicted the structural phase transition at high temperature. We encourage materials scientists to utilize SR to open challenges in materials research, which could potentially unearth hidden governing laws in materials science from a data-driven approach.


*This work was supported by the NSF DMREF program under grant numbers DMR-1729303.

1:03PM X43.00010: DFT-45B---a fertile soil (data) for your seeds (machine learning algorithms)* CHANDRAMOULI NYSHADHAM (Presenter), CHRISTOPH KREISBECK, Kebotix, Inc., Cambridge, MA 02139, USA., GUS HART, Brigham Young Univ - Provo — Machine-learning (ML) models have become the new paradigm in computational materials science for predicting properties of materials with the accuracy of quantum mechanics at a fraction of the cost. Accurate data (fertile soil) is crucial and helps us to build better ML models (healthier plants) using any ML algorithms (seeds). The inconsistencies in the materials data extracted from existing material repositories---less than a few hundred calculations for each alloy system, varied sizes of prototypes, and varying k-point density for different cell sizes---make it challenging to develop effective ML models. We created a DFT-based materials dataset (DFT-45B) consisting of 45 binary alloys (all binary combinations of 10 different elements---Ag, Al, Co, Cu, Fe, Mg, Nb, Ni, Ti, and V) with over 71775 calculations free of such inconsistencies. Each alloy system includes all possible enumerated crystal structures until 8 atoms for fcc, bcc and hcp crystal types. As the data encompasses the space of 10 elements and all their binary combinations, it is helpful to understand the similarity between various elements and alloys. In this talk, we present the methodology and heuristics of the dataset.

*ONR (MURI N00014-13-1-0635)
1:15PM X43.00011: Bayesian Machine Learning in Metamaterial Design: Fragile Becomes Supercompressible  
MIGUEL BESSA (Presenter), PIOTR GLOWACKI, MICHAEL HOULDER, Delft University of Technology — Designing future-proof materials goes beyond a quest for the best. The next generation of materials needs to be adaptive, multipurpose, and tunable. This is not possible by following the traditional experimentally guided trial-and-error process, as this limits the search for untapped regions of the solution space. Here, a computational data-driven approach is followed for exploring a new metamaterial concept and adapting it to different target properties, choice of base materials, length scales, and manufacturing processes. Guided by Bayesian machine learning, two designs are fabricated at different length scales that transform brittle polymers into lightweight, recoverable, and supercompressible metamaterials. The macroscale design is tuned for maximum compressibility, achieving strains beyond 94% and recoverable strengths around 0.1 kPa, while the microscale design reaches recoverable strengths beyond 100 kPa and strains around 80%. The data-driven code is available to facilitate future design and analysis of metamaterials and structures (https://github.com/mabessa/F3DAS).


1:27PM X43.00012: A roadmap for machine learning in alloy modeling*  
GUS HART (Presenter), Brigham Young Univ - Provo, TIM MUELLER, John Hopkins University, CORMAC TOHER, STEFANO CURTAROLO, Duke University — Years before the data science craze, ideas of modern machine learning played an essential role in alloy modeling. Genetic algorithms (for both searching materials space and model construction), statistical learning methods based on Bayesian ideas, dimensionality reduction approaches (cluster expansion, compressive sensing, interatomic potentials, etc.) have contributed to a rich heritage of innovation in the field. Recent developments in data science, and the affordability of generating unprecedented volumes of high-quality training data, open up further avenues. New materials informatics approaches, machine-learned interatomic potentials (GAP, SNAP, MTP, genetic programs, atomic cluster expansion, and others), new thermodynamic approaches such as nested sampling, etc., provide unrivaled opportunities in computational alloy modeling and discovery. We highlight past successes and spotlight promising new approaches.

*Office of Naval Research (MURI N00014-13-1-0635)
Leveraging machine learning to determine nanoscale structures from theory and experiments* VENKATA SURYA CHAITANYA KOLLURU, SPENCER HILLS, ERIC SCHWENKER, NOBUYA WATANABE, FATIH G SEN, ARUN KUMAR MANNODI KANAKKITHODI, MICHAEL STERNBERG, MARIA CHAN (Presenter), Argonne Natl Lab — Determining the atomistic details of nanoscale structures is a fundamental problem. Although there are both experimental and computational methods to determine these nanoscale structures, they both possess limitations. We develop the FANTASTX code (Fully Automated Nanoscale To Atomistic Structure from Theory and eXperiment) to overcome the limitations of either by combining both experimental and computational data using machine learning techniques. We demonstrate the effectiveness of FANTASTX by determining the structures of nanoparticles and solid interfaces from x-ray and electron microscopy data combined with atomistic and first principles energies, using multi-objective optimization and a variety of canonical and grand canonical sampling algorithms.

*We acknowledge funding from the USDOE: Center for Electrochemical Energy Science EFRC, Argonne National Laboratory LDRD program, and the Center for Nanoscale Materials under Contract No. DE-AC02-06CH11357; computational resources of the National Energy Research Scientific Computing Center under Contract No. DE-AC02-05CH11231.

Machine learning for novel and improved inorganic scintillators ANJANA TALAPATRA (Presenter), CHRISTOPHER STANEK, BLAS PEDRO UBERUAGA, GHANSHYAM PILANIA, Los Alamos National Laboratory — Scintillators are detector materials with a wide range of applications, from medical imaging to radiation detection. These materials convert a fraction of the energy deposited by high energy radiation into visible or ultraviolet photons. An ideal scintillator may have high light output, fast response time, and emission at suitable wavelengths. However, no single scintillator is ideal for all uses; there is a need to design custom scintillators optimized for each application. Currently, the discovery and design of new scintillators relies on a laborious, time-intensive approach, yielding little physical insight and leaving a vast space of potentially revolutionary materials unexplored. To accelerate the discovery of optimal scintillator materials, we are developing a closed loop machine learning driven adaptive design framework based on literature data, experiments and calculations. This talk presents an overview of this framework, focusing on the screening of complex chemistries with high band-gaps to identify promising materials amenable to band-gap/band-edge engineering to yield custom scintillation properties. The framework is general and is expected to prove useful for applications beyond scintillator discovery such as photovoltaic and semi-conductor materials.
2:03PM X43.00015: Exploring Information Density in Crystalline and Amorphous Configurations using Deep Neural Networks  SHYAM DWARAKNATH (Presenter), Lawrence Berkeley National Laboratory, WISSAM A SAIDI, Mechanical Engineering & Materials Science, University of Pittsburgh — Predicting the properties of amorphous systems is one of the grand challenges for computational material science. Deep neural network potentials (DNP) promise to recreate the chemical fidelity of DFT while scaling to much larger systems, enabling more realistic simulations of amorphous materials. DNPs also provide a tool to analyze large quantities of DFT data by selective training and evaluation. We trained a DNP on the crystalline polymorphs for SiO2 from the Materials Project. This DNP successively predicted the total energies of several DFT computed quasi-amorphous configurations suggesting that the local atomic environments encoded in amorphous compounds are also present in the potential energy space covered by polymorphism. More importantly, a DNP trained on just the amorphous configurations was able to predict the energies of polymorphs, including the ground state configuration over 100 meV/atom below the lowest included amorphous configuration. This suggests that DNPs trained on quasi-amorphous configurations may be an effective means of identifying ground state configurations as well as polymorphism in never before explored systems.

Friday, March 6, 2020 11:15 AM - 1:51 PM

Session X45 GMAG: Magnetic Anisotropy: Hard and Soft Materials 706 - Scooter Johnson, U.S. Naval Research Laboratory - Tag(s): Focus
11:15AM X45.00001: First-principles calculations on the surfaces and interfaces of SmFe$_{12}$*
TOMOHARU SHIOZAWA (Presenter), YUTA AINAI, Department of Materials Science and Engineering, Tokyo Institute of Technology, YASUTOMI TATETSU, University Center for Liberal Arts Education, Meio University, YOSHIHIRO GOHDA, Department of Materials Science and Engineering, Tokyo Institute of Technology — Nd-Fe-B sintered magnets are currently used in a wide range in industry. However, it is seriously problematic that the coercivity of Nd-Fe-B sintered magnets significantly decreases at high temperatures. In contrast, a new magnetic compound SmFe$_{12}$ has a higher magnetic anisotropy than Nd$_2$Fe$_{14}$B which is the main phase of Nd-Fe-B sintered magnets. Therefore, SmFe$_{12}$-based magnets can be expected as a preferable alternative of existent magnets. The performance of magnets is strongly influenced by microstructural interfaces. However, there are few studies about interfaces including SmFe$_{12}$.

We performed first-principles calculations on the surfaces and interfaces of Nd$_2$Fe$_{14}$B and SmFe$_{12}$, and analyzed the structural stability and magnetic properties. The surface energies of SmFe$_{12}$ and Nd$_2$Fe$_{14}$B are examined to find the most stable surfaces. Then, the interface of SmFe$_{12}$ with a subphase is constructed using the most stable surface structures. For stable interface structures, the magnetic properties are examined, where the magnetic moment of Fe is enhanced around the interface of SmFe$_{12}$/SmCu. We will also present the results on the magnetic anisotropy and the magnetic coupling at SmFe$_{12}$-based interfaces.

*This work was partially supported by ESICMM funded by MEXT (Grant No. 12016013).

11:27AM X45.00002: Additive manufacturing of PPS bonded NdFeB magnets to design a Halbach array for polarized neutron reflectivity experiments*
TEJ LAMICHHANE (Presenter), Oak Ridge National Lab — Additive manufacturing (AM) is a layer by layer material printing technology which is found to be very useful in permanent magnet (PM) manufacturing. In bonded PM, the mechanical strength and the loading volume fraction of magnetic materials can be increased by mechanical extrusion of optimally magnetic particle loaded polymer composites. AM process reduces the price of magnet production by reducing the waste of magnetic materials via net-shaped printing and avoiding the cost of expensive complex molding tools needed for small scale industrial production. AM printed isotropic polyphenylene sulfide (PPS) bonded Nd-Fe-B magnets were used to design a cylindrical Halbach array for polarized neutron reflectivity measurements. We will discuss in detail about the challenges associated in developing the prototype Halbach ring magnet and validate the concept of variable magnetic contrast in neutron measurements.

*This research was supported by the Laboratory Directed Research and Development (LDRD) program of Oak Ridge National Laboratory and Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.
11:39AM X45.00003: First-principles Study on Crystalline Nd-Fe alloys as Candidate Structures for Grain-Boundaries in Nd-Fe-B Sintered Magnets*  
YUTA AINAI (Presenter), Department of Materials Science and Engineering, Tokyo Institute of Technology, YASUTOMI TATETSU, University Center for Liberal Arts Education, Meio University, ASAKO TERASAWA, YOSHIHIRO GOHDA, Department of Materials Science and Engineering, Tokyo Institute of Technology — Due to technological progress in industry, the coercivity enhancement of Nd-Fe-B sintered magnets at high temperatures is highly demanded. It has been identified that the grain-boundaries (GBs) are known as Nd-Fe alloys with fcc diffraction patterns. However, the detailed atomic arrangement on the atomic scale is still unclear. Therefore, in this study, we investigated Nd-rich alloys with Fe as a candidate structures for GBs. 
First, we performed first-principles calculations for cuprite, fluorite, half-Heusler, and sphalerite Nd-Fe alloys in a wide range of the Fe composition ratio in order to determine the most stable fcc Nd-Fe alloy. We found that only the fluorite Nd-Fe alloy keeps the high crystallinity in a range of around 65 to 100 at.%. In contrast, cuprite, half-Heusler, and sphalerite alloys become amorphous-like structures after optimizing structures. 
Second, we added metallic elements such as Al, Co, Cu, and Ga into the fluorite Nd-Fe alloys and optimized the structures in order to check the stability. Only the formation energies of the fluorite Nd-Fe-Ga alloys show the negative values. These results indicate that Ga promotes the stabilization of Nd-Fe alloys more than any other metallic elements.

*This work was support in part by MEXT as the ESICMM (Grant No. 12016013).

11:51AM X45.00004: Low-Dimensional Hard Magnetic Materials [Invited]  
J LIU (Presenter), University of Texas at Arlington — Ferromagnetism is a size-dependent physical phenomenon. Although the size dependence has been studied in theory for decades, nanoscale ferromagnetic materials especially hard magnetic nanostructures and materials with controllable size and shape are not available till recently. We have worked at bottom-up approaches to preparation of low-dimensional hard magnetic materials including nanoparticles and nanowires/nanorods. By adopting newly developed “salt-matrix annealing”, “surfactant-assisted milling” and improved chemical solution techniques, we have successfully synthesized monodisperse hard magnetic FePt and SmCo nanoparticles as well as FeCo, CoNi, CoCx and Co based nanowires/nanorods. These first-ever-available nanoscale ferromagnets display various hard and soft magnetic properties at room temperature which are found to be strongly size and shape dependent. A systematic study on size dependent Curie temperature of the L1₀ structured FePt ferromagnetic nanoparticles with size from 2 to 15 nanometers reveals the finite size effect in the tiny ferromagnets. In case of the Co nanowires with controlled diameter and length, coercivity up to the theoretical limit has been achieved that renewed our understanding of the Brown’s Paradox. The ferromagnetic nanocrystals can be used as building blocks for advanced bulk and thin film magnets, and can be also applied in biomedicine and ferrofluid technologies.
12:27PM X45.00005: High-throughput search for rare-earth free permanent magnets*
ALENA VISHINA (Presenter), OLGA VEKILOVA, HEIKE HERPER, OLLE ERIKSSON, Uppsala Univ — High performance permanent magnets are needed for a large number of applications, such as electric motors, wind mills. At the same time most high performance magnets contain rare-earth (RE) materials which makes them expensive.
We propose to apply a high-throughput approach to the search of RE free permanent magnets. Going through a large number of known structures from ICSD [1], and using a full-potential LMTO method with relativistic formulation as implemented in the RSPt code [2] to calculate magnetic anisotropy and Tc, we are looking for the materials with magnetization >1 T, uniaxial anisotropy >1 MJ/m³, and Tc>300 K to identify the suitable replacement for rare-earth containing materials. Starting with the materials containing 3d+5d+1 extra elements of the periodic table to test the method, we have found several candidates that have characteristics suitable for a good permanent magnet, such as Pt₂FeCu, Pt₂FeNi, W₂FeB₂, etc. Based on the search result we have also proposed two new materials, not existing in ICSD - Pt₂FeCo and Pt₂CoNi [3].

*We acknowledge financial support of the SSF and SNIC for the computation resources.

12:39PM X45.00006: Development of magnetic hardness in melt-spun Mn₅₀Bi₅₀₋ₓMₓ alloys (M = Mg, In, Sn, Sb, Bi) subjected to magnetic-field annealing* ALEXANDER GABAY, GEORGE C HADJIPANAYIS (Presenter), Univ of Delaware — The theoretical maximum energy product (BH)ₘ of the MnBi compound, 20 MGOe, perfectly fits the "gap" between the inexpensive hard ferrites and the supply-critical rare-earth magnets. Decades of R&D efforts focused on consolidation of fine MnBi single crystals could only produce MnBi magnets exhibiting (BH)ₘ of 5–8 MGOe. A different approach relying on a melt-spinning, followed by compaction and magnetic-field annealing avoids the highly reactive single crystals, but it does not develop coercivity Hₐ in the binary MnBi alloys. Here, we report how alloying with M = Mg, In, Sn and Sb affects the phases, the texture and the hard magnetic properties of field-annealed magnets prepared from the melt-spun Mn₅₀Bi₅₀₋ₓMₓ alloys. Sn delays the formation of the MnBi phase while further decreases the already low Hₐ. 1.5 at.% In decreases the solidus temperature and slightly increases the Hₐ. In melt-spun alloys modified with 1.5 at.% Sb, a transient metastable phase ensures a submicron size of MnBi grains and leads to a Hₐ > 7 kOe, but suppression of the texture limits the (BH)ₘ to 5.4 MGOe. Alloing with Mg increases the Hₐ without undermining the texture; a breakthrough (BH)ₘ of 9.8 MGOe was realized in the Mn₅₀Bi₄₇Mg₃ magnet.

*Work supported by DOE through DE-FG02-90ER45413 and EE0007794.
Tuning of spin reorientation temperature of SmFeO$_3$: Role of exchange interaction between 4f & 3d electrons

AZAM KHAN ( Presenter), ANJU AHLAWAT, SRINIBAS SATAPATHY, AK KARNAL, Raja Ramanna Centre for Advanced Technology — Emergent technologies based on spintronics demand the unprecedented control on magnetic anisotropy. Here we present the control on magnetic anisotropy of SmFeO$_3$ by the means of Tm$^{3+}$ doping at Sm$^{3+}$ site.

A series of nano particles of Sm$_{1-x}$Tm$_x$FeO$_3$ (X=0, 0.3, 0.5, 0.7, 1) orthoferrite have been synthesized by sol-gel auto-combustion method and phase purity was confirmed by the X-ray diffraction pattern. The crystallographic information obtained from Rietveld refinement and Raman spectroscopy confirmed the changes in oxygen octahedra with the change in doping percentage of Tm$^{3+}$ ion in SmFeO$_3$. Temperature dependent dc magnetization measurement implies the tuning of spin reorientation temperature from 480 K to 80 K as a function of Tm$^{3+}$ ion doping concentration. The room temperature magnetic isotherm confirms the canted antiferromagnetic character of nano particles. Sm$_{0.7}$Tm$_{0.3}$FeO$_3$ shows the spin reorientation at room temperature which might be used in room temperature spintronics devices.

References

*Funding will be received by Department of Atomic energy, India
Self-biased nanocrystalline barium hexaferrite thick films formed by aerosol deposition for microwave devices

Scooter Johnson (Presenter), United States Naval Research Laboratory, Dong-Soo Park, Korean Institute of Material Science, Sanghoon Shin, Syed B Qadri, United States Naval Research Laboratory, Pavel Kabos, Kevin Coakley, National Institute of Standards and Technology, Edward P Gorzkowski, United States Naval Research Laboratory — High-frequency devices utilizing magnetic materials such as barium hexaferrite (BaFe$_{12}$O$_{19}$, BaM) are critical for many electronics. One promising route to forming these materials is aerosol deposition (AD), a process that creates thick 95% dense films by room-temperature impact consolidation*. AD utilizes high-velocity impact to fracture and mechanically and chemically bonds solid particles together.

We use AD to deposit BaM in a non-magnetically biased (NMB) and in a 4 kOe bias field (MB). We report results of these films as-deposited and sintered from 700C to 1000C.

The best films were deposited under MB and annealed at 1000C and show a clear OOP orientation (23 % improvement compared to NMB). Properties include, magnetic saturation: 62 emu/g (72 emu/g bulk) and remanence: 43 emu/g. FMR results give an anisotropy field of 15 kOe (16 kOe bulk), linewidth of 1.8 kOe, and damping factor of 4x10$^{-4}$. Films deposited under NMB show comparably poorer values. XRD results suggest good crystallinity and phase uniformity overall. Sintering increases the crystallite size from about 10 nm to 25 nm.

The overall results suggest that depositing the films with AD under MB significantly increases the magnetic orientation of the film.

Investigation of fabrication method of $L1_0$-FeCo multilayer film

HISAAKI ITO (Presenter), TAKUYA MIYASHITA, TAKUYA KUMAGAI, Sci Univ of Tokyo, TOSHIO MIYAMACHI, FUMIO KOMORI, The Univ of Tokyo, TOMOYUKI KOGANEZAWA, TAKUO OHKOCHI, JASRI, MASATO KOTSUGI, Sci Univ of Tokyo — The $L1_0$-type FeCo ordered phase exhibits large magnetic anisotropy, large magnetic moment, and high Curie temperature. Since $L1_0$-FeCo does not contain rare-earth elements, it is a potential candidate as a high-performance magnetic material [1]. On the other hand, the $L1_0$-FeCo system is at a non-equilibrium state, and its fabrication has been a challenge so far [2]. To overcome the problem, we inserted periodic buffer layers between the FeCo layers to maintain the $L1_0$ (fcc) structure [3]. For establishing the fabrication method of $L1_0$-FeCo, we here investigated the growth temperature ($T_s$) dependence of (7 ML-FeCo/3 ML-Ni buffer)$_3$ films fabricated by pulsed laser deposition.

The formation of the stable B2 (bcc) structure was suppressed at $T_s = 450°C$ or lower. Although the formation of the fcc structure was confirmed, the $L1_0$-ordering was not recognized. Unfortunately, the spontaneous easy axis of magnetization in all the specimens was still the in-plane direction. However, the in-plane magnetization decreased at $T_s = 300$ and 450°C, and the magnetocrystalline anisotropy showed the maximum value for $T_s = 300°C$.


Influence of W thickness on Perpendicular Magneto-crystalline Anisotropy of Pt/Co/W(111) Superlattices

HUYNH THI HO (Presenter), SANGHOON KIM, SONNY H. RHIM, SOON CHEOL HONG, Univ of Ulsan — Tri-layer superlattice with reflection asymmetry in the spirit of Rashba effect has been explored in spintronics. Pt/Co/W (111) superlattice is investigated by employing first-principles calculations to clarify experimental results, where perpendicular magnetocrystalline anisotropy (PMA) depends on W thickness. Moreover, the enhancement of PMA with respect to Pt/Co due to non-magnetic W is examined. Our calculation results show that the thickness dependence of PMA is evident, whose maximum occurs when W is three monolayers, where the orbital hybridization at interfaces with W is responsible for PMA. Surprisingly, W contributes to PMA with appreciable orbital magnetic anisotropy, which follows the so-called Bruno relation, $E_{PMA} \sim m_{orb}^+ - m_{orb}^-$. To clarify the physics origin, PMA is analyzed in the framework of second-order perturbation theory, where $\langle m=-2 | L_z | m=+2 \rangle$ dominates. In addition, $k$-resolved PMA demonstrates that contribution is from the $\Gamma$ with $d$ orbitals of $m = \pm 2$, where $m$ is the magnetic quantum number.

*National Research Foundation of Korea(NRF) (NRF-2018R1A4A1020696)
Creative Materials Discovery Program through the NRF of Korea (NRF-2015M3D1A1070462)
BK21+
1:39PM X45.00011: An efficient model for modelling Barkhausen noise in PMA thin films
AUDUN SKAUGEN (Presenter), LASSE LAURSON, Computational Physics Laboratory, Tampere University
and Helsinki Institute of Physics — The motion of domain walls in thin films with perpendicular
magnetic anisotropy (PMA) is of great interest due to their technological applications in spintronic devices, as well as the critical phenomenon of Barkhausen noise due to the domain wall pinning to quenched disorder. However, current numerical studies of domain walls, using micromagnetic discretized solvers on the entire system, are limited to small system sizes by the expensive computation of the far-field forces between every pair of spins. As a result, the statistical signature of Barkhausen noise has strong finite size effects in such studies.

We present an efficient, principled numerical model which reduces the description of the PMA thin film to a single one-dimensional domain wall, by integrating over the coordinate perpendicular to the domain wall. The full nonlocal demagnetizing field is included in the computation, but formulated as an integral over the remaining dimension along the wall. This allows for numerical studies of Barkhausen noise in large systems, while still including physical effects such as Walker breakdown and nonlocal interactions.

Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X46 GMAG DMP: 3D Frustrated Magnets: Other Geometries 708 -
Jeremy Carlo, Villanova Univ - Tag(s): Focus
11:15AM X46.00001: Frustrated Magnetism in Mott Insulating V$_2$O$_3$ [Invited] HARALD JESCHKE
(Presenter), Okayama University — The phase diagram of V$_2$O$_3$ as function of transition metal
doping and temperature is famous for showing transitions between metallic and insulating and
between paramagnetic and antiferromagnetic phases. In particular, the Mott metal-insulator
transition which is induced by a few percent of chromium doping has been studied intensively.
Using a combination of density functional theory calculations and inelastic neutron scattering
experiments, we study the magnetic interactions in the chromium-stabilized antiferromagnetic
and paramagnetic insulating phases as function of temperature [1]. The calculations based on an
energy mapping technique [2] are performed for low temperature monoclinic and high
temperature rhombohedral structures. Both calculations and INS cross sections reveal significant
magnetic frustration and degeneracy of the paramagnetic insulating phase which is relieved by
the rhombohedral-to-monoclinic transition at $T_N$=185 K. Magnetic frustration can be shown to be
present in rhombohedral (V$_{1-x}$Cr$_x$)$_2$O$_3$ for a large range of dopings. This suggests that magnetic
frustration plays an important role in suppressing the magnetic long-range-ordering temperature
and thereby exposing a large phase space for the paramagnetic Mott metal-insulator transition.

D. Lumsden, J. Hong, O. Delaire, W. Bao, C. L. Broholm


11:51AM X46.00002: Magnetic Field Induced Phase Transition in Spinel GeNi$_2$O$_4$*
TATHAMAY BASU (Presenter), TAO ZOU, Z DUN, Michigan State Univ, CLARINA RELOJ DELA CRUZ,
TAO HONG, HUIBO CAO, Oak Ridge National Laboratory, MENGZE ZHU, Michigan State Univ,
HAIDONG ZHOU, University of Tennessee, XIANGLIN KE, Michigan State Univ — Cubic spinel GeNi$_2$O$_4$
exhibits intriguing magnetic properties with two successive antiferromagnetic phase transitions
(~12 and 11 K) in the absence of structural distortion. By means of heat capacity and magnetic
susceptibility measurements, we have revealed a new magnetic phase in presence of magnetic
field field ($\geq$ 4 T) along the [111] direction, which is not observed when the magnetic field is
applied along the [100] and [110] directions. Neutron powder diffraction measurements confirm
such a field-induced phase transition and suggest it be ascribed to a spin reorientation in
presence of magnetic field. We will discuss the potential mechanisms regarding such a peculiar
magnetic anisotropy in this cubic system.

*Work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy
Sciences, Materials Sciences and Engineering Division, under Award No. DE-SC0019259.
12:03PM X46.00003: Characterization of the crystal field scheme of a new family of geometrically frustrated rare earth spinels.* DALMAU REIG-I-PLESSIS (Presenter), GREG MACDOUGALL, University of Illinois, ADAM ACZEL, Oak Ridge National Lab, ALEXANDRA COTE, SEAN VAN GELDERN, University of Illinois — The pyrochlore lattice is known for having a large variety of exotic, frustration-driven phases, the specifics of which are determined by the symmetry of the local moments and their interactions. Here we present on a new family of compounds MgRE$_2$Se$_4$ (RE = Ho, Tm, Er, and Yb), which form in the spinel structure, were the rare earth atoms are a pyrochlore sublattice. In this presentation we will show inelastic neutron scattering measurements of the crystal electric field (CEF) excitations. We fit this neutron data to find the most likely CEF Hamiltonian for each compound in the family and comment on the possible consequences of the result. We show that MgTm$_2$Se$_4$ has a spin singlet ground ground state with a low lying signlet excited state, similar to an Ising moment in a transverse field. MgHo$_2$Se$_4$ has an Ising ground state with several additional thermally accessible levels. MgEr$_2$Se$_4$ is shown to have Ising moments and is a spin ice compound. MgYb$_2$Se$_4$ is shown to be an effective spin 1/2 system with strong spin anisotropy.

*I acknowledge support from National Science Foundation, under grant number DMR-1455264-CAR, as well as from U.S. D.O.E., Office of Science, Office of Workforce Development for Teachers and Scientists, Office of Science Graduate Student Research (SCGSR) program.

12:15PM X46.00004: Update on the Magnetic and Structural Properties of the Solid Solutions CuAl$_{2(1-x)}$Ga$_{2x}$O$_4$* THOMAS BULLARD (Presenter), MICHAEL SUSNER, UES, Inc., KEITH TADDEI, Oak Ridge National Lab, JACILYNN BRANT, Nature Communications, TIMOTHY HAUGAN, RQQM, Air Force Research Lab — Magnetic frustration continues to be an area of interest due to its association with the emergence of novel magnetic ground states such as spin glasses. Two systems that have been identified as spin glasses are the spin ½ antiferromagnetic spinels CuAl$_2$O$_4$ and CuGa$_2$O$_4$. In this research we examine the solid solution between these two end members, CuAl$_{2(1-x)}$Ga$_{2x}$O$_4$. The solution displays magnetic glassy properties such as bifurcation in the FC - ZFC DC susceptibility, a frequency dependence of the freezing temperature, memory effects, and slow relaxation. Whether the system is better classified as a cluster glass or insulator spin glass will be discussed. Further, we observe an increase in the magnetic frustration as Ga$^{3+}$ is replaced with Al$^{3+}$. We have examined the atomic occupancy of the even members of the solid solution via neutron and synchrotron diffraction. As Ga$^{3+}$ is replaced with Al$^{3+}$ we find an increase in frustration as the magnetic Cu$^{2+}$ ion shifts from the octahedral to the tetrahedral sublattice.

*Funding for this work was provided by the Air Force Office of Scientific Research (AFOSR) under LRIR #15RQCOR215, #18RQCOR100, and the Aerospace Systems Directorate (AFRL/RQ)
Mean field theory for cooperative magnetism in non-Kramers garnets

BRUNO TOMASELLO (Presenter), Institut Laue - Langevin, RAFAŁ WAWRZYNIAK, Max Planck Institute for Chemical Physics of Solids, GÖRAN NILSEN, ISIS neutron source, STFC, TOM FENNELL, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, TIM ZIMAN, Institut Laue - Langevin — Kramers’ theorem entails a fundamental symmetry valid only for odd-electron systems, i.e. any eigenstate and its time-reversed counterpart belong to the same spectrum. Notwithstanding, the magnetic states of non-Kramers ions, which have even number of electrons, can be constrained because of time-reversal symmetry. Indeed, if the low-lying singlets of a crystal of such ions are well gapped from the eigenstates at higher energies, then the magnetic moments at low-temperatures can only be axially anisotropic and only magnetostriction can account for low energy fluctuations. Rare-earth garnets are a suitable playground for studying the competition of magnetic frustration, magneto-elasticity, induced magnetic ordering, and the role of nuclear moments. This talk presents our current theoretical understanding of the non-Kramers garnet Tb$_3$Ga$_5$O$_{12}$, benefitting from state of the art neutron scattering experiments for the crystal-field and magnetic structure – PRB, 100, 094442(2019). The discussion highlights the mean-field theory proposed in the 70s by Hammann & Manneville for the induced magnetic ordering found in both Tb$_3$Ga$_5$O$_{12}$ and Ho$_3$Ga$_5$O$_{12}$. We contrast our study to the work of Paddison et al. on the magnetic ordering and excitations of the non-Kramers Ho$_3$Ga$_5$O$_{12}$ – arXiv:1908.03530(2019).

Absence of long-range magnetic ordering in the S=1/2 frustrated system Ca$_3$Cu$_2$GeV$_2$O$_{12}$

CHRISTOPHER WIEBE (Presenter), Univ of Edinburgh, JOEY A. LUSSIER, Dept. of Chemistry, University Of Winnipeg, BROOKE RICHTIK, COLE D MAUWS, Dept. of Chemistry, University of Manitoba, JEFFREY LYNN, NIST — Quantum spin liquids can be found in materials with a combination of geometric frustration along with low spin. Due to its spin of S=1/2, the copper (II) ion is often present in the discussion of new spin liquid candidates. The solid state compound Ca$_3$Cu$_2$GeV$_2$O$_{12}$ is a material that crystallizes in the garnet structure (space group #230, Ia-3d), where 3-dimensional frustration from competing exchange interactions is known to occur. Heat capacity measurements have shown a lack of sharp ordering transitions in this compound down to 0.35 K, which is confirmed with a lack of long-range magnetic order via neutron diffraction measurements to 0.07 K. This system displays a Weiss temperature of -0.93(1) K indicating net antiferromagnetic interactions and significant $J_1$-$J_2$ competition causing frustration. Using both neutron and X-ray diffraction along with heat capacity and magnetometry, the work presented here shows that Ca$_3$Cu$_2$GeV$_2$O$_{12}$ has potential as a new spin liquid candidate.

*We are grateful for funding of this project through NSERC (Discovery Grant and Canada Research Chair program), the CFI, and the Leverhulme Trust.
Magnetic order and single-ion anisotropy in Tb$_3$Ga$_5$O$_{12}$ rare-earth garnet. RAFAL WAWRZYNCZAK (Presenter), BRUNO TOMASELLO, Institut Laue-Langevin, PASCAL MANUEL, DMITRY KHALYAVIN, DUC LE, TATIANA GUIDI, ISIS Facility, Rutherford Appleton Laboratory-STFC, ANTONIO CERVELLINO, Paul Scherrer Institut, TIM ZIMAN, MARTIN BOEHM, Institut Laue-Langevin, GÖRAN NILSEN, ISIS Facility, Rutherford Appleton Laboratory-STFC, TOM FENNELL, Paul Scherrer Institut — Terbium gallium garnet (TGG), Tb$_3$Ga$_5$O$_{12}$ exhibits complex low-temperature magnetism, that involves frustration, single-ion anisotropy and induced-moment type ordering. Tb$^{3+}$ magnetic ions form two interpenetrating half-garnet lattices – three-dimensional arrangements of corner-sharing triangles. The low-symmetry local environment of Tb$^{3+}$ sites provides a complete lifting of the degeneracy within the lowest crystal electric field (CEF) manifold. The resulting ground-state observed with inelastic neutron scattering is a quasidoublet comprised of two closely-lying singlets. The spectroscopic data allowed for refinement of the CEF Hamiltonian parameters and retrieval of its eigenstates. Despite the singlet ground-state TGG orders magnetically at $T_N=0.25$ K, much lower than $|\theta_{CW}|=8$ K given by the bulk susceptibility. Neutron powder diffraction has shown the ordered structure to be of a multiaxial antiferromagnet type with strong single ion anisotropy. The results of powder magnetization measurements are in good agreement with values based on the CEF model down to 20 K, where the onset of magnetic correlations is seen. Also, a strong temperature-dependence of the quasidoublet ground-state is found. These observations suggest existence of a correlated paramagnet regime of unknown nature.

Field dependence of magnetic order in frustrated diamond-like antiferromagnet LiYbO$_2$* MITCHELL BORDELON (Presenter), LORENZO J POSTHUMA, University of California, Santa Barbara, ERIC M KENNEY, Physics, Boston College, NICHOLAS BUTCH, CRAIG BROWN, NIST Center for Neutron Research, ARNAB BANERJEE, Neutron Scattering Division, Oak Ridge National Laboratory, MICHAEL JOHN GRAF, Physics, Boston College, STEPHEN WILSON, University of California, Santa Barbara — Frustrated magnetism is a hotbed for searching for new electronic phases of matter. This can theoretically lead to states such as the spiral spin liquid where coplanar degenerate spiral states contain coherently fluctuating spins. One proposed venue for this state has been in the cubic diamond lattice arising from frustration in a J$_1$-J$_2$ Hamiltonian. Here we propose a new materials system where spiral spin liquids may potentially be observed based upon a tetragonally-elongated diamond lattice. This is exemplified by effective J = 1/2 moments within LiYbO$_2$ via a combination of low-energy inelastic neutron scattering, crystalline electric field analysis, and linear spin wave theory. Magnetic order and its evolution under magnetic field will be discussed.

*This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-SC0017752 and National Science Foundation Graduate Research Fellowship Program under grant no. 1650114.
A breathing pyrochlore lattice has alternating tetrahedra of different sizes, in which there exist different interactions. The competition of these interactions could lead to some interesting phenomena, for example, magnetic frustration and magnetoelastic coupling [1]. The breathing pyrochlore material LiGaCr$_4$S$_8$ has been measured to have a negative thermal expansion from 10 K to 110 K [1]. We performed THz transmission spectroscopy measurements in this temperature range on a polycrystal sample. An absorption at around 0.3 THz was found, which is possibly an excitation of the Cr$^{3+}$ ion. We also observed a strong absorption above 0.6 THz likely due to lattice vibrations.


*This research is supported by the Center for Emergent Materials, an NSF MRSEC under award number DMR-1420451. GP, DM, ADC are supported by the Gordon and Betty Moore Foundation's EPIQS Initiative and U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
1:27PM X46.00010: Single Crystal Growth and Magnetic-Thermal Characterization of a Rare-Earth Based Breathing Pyrochlore Family  

RABINDRANATH BAG (Presenter), LALIT YADAV, ZHENZHONG SHI, SACHITH DISSANAYAKE, Department of Physics, Duke University, Durham, North Carolina, USA, DAVID E GRAF, EUN SANG CHOI, Department of Physics, National High Magnetic Field Laboratory, Florida State University, Florida, USA, FRANZ LANG, Department of Physics, University of Oxford, Oxford, UK, CATALINA SALAZAR MEJIA, ELIZABETH GREEN, Department of Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany, STEPHEN BLUNDELL, Department of Physics, University of Oxford, Oxford, UK, SARA HARAVIFARD, Department of Physics and Department of Mechanical Engineering & Materials Science, Duke University, North Carolina, USA — The Breathing Pyrochlore (BP) lattice, which consists of three dimensionally corner sharing tetrahedra with alternating sizes, has recently attracted much attention due to presence of frustrated or competing interactions. BP system has also been proposed to host of many intriguing phenomena such as Quantum Spin Liquid, Quantum Spin Ice and Weyl magnons, due to anisotropic spin-spin interactions [1-3]. Large and high quality single crystals of BP compounds are highly needed, in order to advance these hypotheses experimentally. We have successfully grown single crystals of a rare-earth BP family, using the uniquely modified travelling solvent floating zone techniques. Additionally, we have performed specific heat, thermal conductivity, AC/DC magnetic susceptibility, magnetization, magneto-dielectric, μSR and X-ray diffraction measurements to probe the physical properties of these new compounds. In this talk I will present the results of our single crystal growth and characterization efforts.

References:
1:39PM X46.00011: Field Dependent Neutron Scattering Studies of Breathing Pyrochlore

$\text{Ba}_3\text{Yb}_2\text{Zn}_5\text{O}_{11}$

SACHITH DISSANAYAKE (Presenter), WILLIAM STEINHARDT, ZHENZHONG SHI, STEPHEN J KUHN, Department of Physics, Duke University, JEFFREY RAU, Department of Physics, University of Windsor, NICHOLAS BUTCH, Center for Neutron Research, National Institute of Standards and Technology, MATTIAS D FRONTZEK, ANDREY PODLESNYAK, Neutron Scattering Division, Oak Ridge National Laboratory, YIMING QIU, Center for Neutron Research, National Institute of Standards and Technology, WANGCHUN CHEN, National Institute of Standards and Technology, DAVID E GRAF, National High Magnetic Field Laboratory, Florida State University, TAO HONG, Neutron Scattering Division, Oak Ridge National Laboratory, CASEY MARJERRISON, Department of Physics, Duke University, MICHEL J P GINGRAS, Department of Physics and Astronomy, University of Waterloo, SARA HARAVIFARD, Department of Physics and Department of Mechanical Engineering & Materials Science, Duke University

Breathing pyrochlore systems are composed of corner-sharing tetrahedra of different sizes pointing in opposing directions, leading to different intra- and inter-tetrahedra exchange interactions and the emergence of the Dzyaloshinskii-Moriya interaction due to loss of inversion symmetry. They are predicted to host exotic physics including quantum spin ice, quantum spin liquid, and field-tunable Weyl magnons. In this talk we will present single-crystal field-dependent unpolarized and polarized inelastic neutron scattering measurements on Yb-based breathing pyrochlore system, as well as a theoretical model that can effectively describe some of our experimental findings.

1:51PM X46.00012: Neutron Scattering Studies of Rare-Earth Based Breathing Pyrochlore System.

LALIT YADAV (Presenter), RABINDRANATH BAG, SACHITH DISSANAYAKE, ZHENZHONG SHI, Department of Physics, Duke University, GUANGYONG XU, HUI WU, CRAIG BROWN, NICHOLAS BUTCH, Center of Neutron Research, National Institute of Standards and Technology, FRANZ LANG, STEPHEN BLUNDELL, Department of Physics, University of Oxford, SARA HARAVIFARD, Department of Physics and Department of Mechanical Engineering & Materials Science, Duke University

Breathing Pyrochlore materials have emerged as a promising candidate to study frustrated magnetism and topological phenomena, such as Weyl and Dirac magnons. We have initiated design and synthesize of rare-earth based Breathing Pyrochlore compounds. Further, we have been using neutron diffraction and inelastic scattering techniques to probe the static and dynamic properties of these compounds. In this talk, we are going to present our latest experimental results.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X47 GMAG DMP DCOMP: Multiferroics and Magnetoelectricity in Complex Oxides

Natalia Perkins, University of Minnesota - Tag(s): Focus
THz spectroscopy of BiFeO$_3$ in the magnetic-field-induced canted AFM state. * JOHAN VIIROK (Presenter), LAUR PEEDU, URMAS NAGEL, TOOMAS ROOM, National Institute of Chemical Physics and Biophysics, DÁVID SZALLER, Institute of Solid State Physics, Vienna University of Technology, Austria, VILMOS KOCSIS, SANDOR BORDACS, Department of Physics, Budapest University of Technology and Economics, Hungary, ISTVAN KEZSMARKI, Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, HANS ENGELKAMP, DIMA KAMENSKY, High Field Magnet Laboratory, Radboud University, The Netherlands, KOMALAVALLI THIRUNAVUKKARASU, MYKHAYLO OZEROV, DMITRY SMIRNOV, JUREK KRZYSTEK, National High Magnetic Field Laboratory, Tallahassee, FL, YUKIHIRO OZAKI, TOSHIMITSU ITO, YASUHIDE TOMIOKA, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan, TRINANJAN DATTA, Department of Chemistry and Physics, Augusta University, Augusta, GA, RANDY FISHMAN, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN — BiFeO$_3$ is a well-known room temperature multiferroic material where the cycloidal magnetic order induces electric polarization in addition to existing polarization. The cycloidal order is transformed by strong magnetic fields into a canted antiferromagnetic (AFM) order above B=18T and the cycloidal modes are replaced by excitations of the canted AFM structure [U. Nagel et al., Phys. Rev. Lett., 110:257201, (2013)].

Here we present the THz spectroscopy results for three different magnetic field orientation, parallel to hexagonal c axis, perpendicular and parallel to a axis, measured on the single FE domain crystals grown by the laser-diode heating floating-zone method [T. Ito et al., Cryst. Growth Des. 11 (2011) 5139]. The dependence of mode frequencies as a function of magnetic field were studied up to 35T at liquid He temperatures. In light of these experimental results, a microscopic model is proposed for the canted AF phase.

*Part of the research was supported by the by the Estonian Ministry of Education and Research Grant IUT23-3 and by the European Regional Development Fund project TK134.
11:27AM X47.00002: Magnetoelectric spectroscopy of spin excitations in LiCoPO$_4$*  
TOOMAS ROOM (Presenter), JOHAN VIROK, LAUR PEEDU, URMAS NAGEL, National Institute of Chemical Physics and Biophysics, Estonia, SANDOR BORDACS, Department of Physics, Budapest University of Technology and Economics and MTA-BME, Hungary, ISTVAN KEZSMARKI, Experimental Physics 5, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany, VILMOS KOCSIS, YUSUKE TOKUNAGA, YASUJIRO TAGUCHI, YOSHINORI TOKURA, Center for Emergent Matter Science (CEMS), RIKEN, Japan — In this work [V. Kocsis et al., PRB 100, 155124 (2019)] we study optical magnetoelectric (ME) effect using optical directional anisotropy as measured by the THz absorption spectroscopy of spin resonances in LiCoPO$_4$. The antiferromagnetic domains are selected by ME poling and their population is measured by directional anisotropy [V. Kocsis et al., PRL 121, 057601 (2018)]. Here we demonstrate that the directional anisotropy can also be used to investigate the form and the spectral dependence of the ME susceptibility tensor and hence to identify different spin-multipolar orders responsible for the ME effect. From the spectrum of the directional anisotropy one can determine the static ME coupling via the ME susceptibility sum rule. We conclude, for the poling magnetic field direction along the local electric polarization, the observed ME spin resonances are responsible for the static ME effect and the symmetric part of the ME tensor with zero diagonal elements dominates over the antisymmetric components.

*Part of the work was supported by The Estonian Ministry of Education and Research under Grant No. IUT23-03, and the European Regional Development Fund project TK134.

11:39AM X47.00003: Model for the Spin Dynamics of the Multiferroic (NH$_4$)$_2$FeCl$_5$ (H$_2$O)*
RANDY FISHMAN (Presenter), WEI TIAN, JAIME FERNANDEZ-BACA, Oak Ridge National Lab, JANICE L MUSFELDT, University of Tennessee, JUN HEE LEE, MINSEONG LEE, Ulsan National Institute of Science and Technology, JOHN SINGLETON, National High Magnetic Field Lab, Los Alamos — The multiferroic behavior of any material sensitively depends on the microscopic interactions between the spins. We evaluate the magnetic interactions in the multiferroic erythrodsiderite (NH$_4$)$_2$FeCl$_5$ (H$_2$O) by comparing inelastic neutron scattering spectra of a single crystal sample with a simple Heisenberg model containing five exchange interactions and an easy-plane anisotropy. The cycloidal spin state in every bc plane is produced by two competing exchange interactions. Using the observed wavevector of this cycloidal spin state is used as a constraint, excellent agreement is found between the observed and predicted spectra. The resulting exchange and anisotropy parameters are compared with the predictions of first-principle calculations.

OMAR CHMAISSEM (Presenter), KAMAL CHAPAGAIN, Physics, Northern Illinois University, BIANCA HABERL, Neutron Scattering Division, Oak Ridge National Lab, JEFFREY LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology, SAUL LAPI DUS, X-ray Science Division, Advanced Photon Source, Argonne National Lab, CURTIS KENNEY-BENSON, HPCAT, X-ray Science Division, Advanced Photon Source, Argonne National Lab, BOGDAN M DABROWSKI, Institute of Physics, Polish Academy of Sciences, STEPHAN ROSENKRANZ, Materials Science Division, Argonne National Lab — Multiferroic oxides have recently emerged as key materials with the potential to tackle the exploding demand for systems that enable efficient energy usage and enhance the functionality of spintronic devices. In this talk, I will discuss the recent development of single-site manganese-based multiferroic perovskite materials, Sr$_{1-x}$Ba$_x$Mn$_{1-y}$Ti$_y$O$_3$, with ferroelectric transition temperatures boosted to ~430 K. Using a series of temperature-dependent scattering experiments at various pressures, we demonstrate the tunable character of coupling between the magnetic and ferroelectric order parameters and show that ferroelectricity could be easily manipulated through the application of either external or chemical pressures. Measurements of the magnetic and structural properties under pressure allowed the construction of a detailed P-T phase diagram in which the diverse phases are delineated. Impressive spontaneous polarization values of ~30 $\mu$C/cm$^2$, in agreement with Ti-free Sr$_{1-x}$Ba$_x$MnO$_3$, are calculated using an empirical c/a-based equation or derived from a point charge model with bond-lengths and angles determined by neutron diffraction.

*Work at MSD at ANL (scattering and analysis) was supported by the U.S. DOE, Office of Science, Materials Sciences and Engineering Division.*
12:03PM X47.00005: Insights into the coupled phenomena in molecular multiferroic (ND$_4$)$_2$[FeCl$_5$(D$_2$O)] via inelastic neutron scattering studies*  WEI TIAN (Presenter), RANDY FISHMAN, HUIBO CAO, GABRIELE SALA, DANIEL M. PAJEROWSKI, TAO HONG, LUKE L. DAEMEN, YONGQIANG CHENG, JAIME A. FERNANDEZ-BACA, Oak Ridge National Lab — (ND$_4$)$_2$[FeCl$_5$(D$_2$O)] is a rare molecular magnet exhibiting direct coupling between magnetism and electric polarization as well as a very rich magnetic field versus temperature phase diagram[1-3]. In order to gain a deep understanding of the emergent coupled phenomena, we performed inelastic neutron scattering experiments to investigate the dynamics in this material. Our data analysis shows the spin dynamics can be described by a Heisenberg Hamiltonian model with an easy-plane anisotropy that captures the key observations. Our inelastic neutron scattering results also reveal the role the ion played in the intriguing properties observed in (NH$_4$)$_2$[FeCl$_5$(H$_2$O)].

References

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12:15PM X47.00006: Magnetization reversal by electric field in Co substituted bismuth ferrite thin film  MASAKI AZUMA (Presenter), Tokyo Institute of Technology and Kanagawa Institute of Industrial Science and Technology, KEISUKE SHIMIZU, Tokyo Institute of Technology, KEI SHIGEMATSU, Tokyo Institute of Technology and Kanagawa Institute of Industrial Science and Technology, HAJIME HOJO, Kyushu University — Electric field manipulation of magnetization is intensively investigated because of potential application in low-power-consumption non-volatile magnetic memory devises. Ferroelectric BiFeO$_3$ has a cycloidal space-modulated spin structure with a periodicity of 62 nm superimposed on the G-type antiferromagnetic structure. The presence of cycloidal ordering prohibits the appearance of net ferromagnetic magnetization due to spin canting and a linear magnetoelectric effect. We have observed a spin structure transition from low-temperature cycloidal one to high-temperature collinear one at ~200 K using Mössbauer spectroscopy in rhombohedral BiFe$_{0.1}$Co$_{0.9}$O$_3$ thin films fabricated by PLD on SrTiO$_3$ (STO) (111) substrate. Spontaneous magnetization of 0.03 u$_B$/f.u. confined in a magnetic easy plane perpendicular to the electric polarization is generated by Dzyaloshinskii-Moriya interaction. Films fabricated on GdScO$_3$ (110) substrate has out-of-plane component of magnetization which can be observed by MFM. It is demonstrated that the out-of-plane magnetization can be reversed by electric polarization reversal using PFM at room temperature.
12:27PM X47.00007: Spin-liquid-like state in ferroelectric TbInO$_3$ with a nearly triangular lattice* [Invited] VALERY KIRYUKHIN (Presenter), Rutgers University — Quantum spin liquids (QSL) have been continuously attracting attention since Anderson’s seminal work in 1970’s. As most visionary ideas, QSLs have been found to be relevant to many diverse branches of physics, ranging from superconductivity to quantum computing applications. Known QSL candidate compounds are typically based on geometrically frustrated magnetic lattices, such as the kagome and triangular (TL) lattices. After decades of activity, their properties are still enigmatic, and the number of strong QSL candidates is limited. We describe a recently-discovered QSL candidate TbInO$_3$, containing nearly-triangular layers of non-Kramers Tb$^{3+}$ ions. No signs of static magnetic order are found down to the temperatures two orders of magnitude smaller than the effective interaction energy, by a variety of complementary techniques. Inelastic neutron scattering studies reveal a broad continuum of magnetic excitations located at the TL Brillouin zone boundary that can be described in the framework of the uncorrelated nearest-neighbor valence bonds model. TbInO$_3$ is also ferroelectric, containing atomically-sharp domain boundaries that could host exotic states. These observations make TbInO$_3$ a rather unique QSL candidate, in which fluctuating quantum magnetic state is combined with ferroelectricity.

*Supported by the US Department of Energy (DOE) under Grant No. DOE: DE-FG02-07ER46382.

1:03PM X47.00008: An annealing study of CaMn$_2$O$_4$-d, a possible multiferroic candidate* MELISSA GOOCH (Presenter), Texas Center for Superconductivity, Univ of Houston, HUNG-CHENG WU, Physics, National Sun Yat-sen University, LIANGZI DENG, Texas Center for Superconductivity, Univ of Houston, HUNG-DUEN YANG, Physics, National Sun Yat-sen University, PAUL C. W. CHU, Texas Center for Superconductivity, Univ of Houston — Manganese oxides have experienced a considerable increase in research interest due to their rich and complex phase diagrams. Ca-Mn-O is an excellent example, whose rich phase diagram contains phases that have been theoretically predicted to be multiferroic and CaMn$_2$O$_4$ to date is still not well understood and a hopeful candidate. Polycrystalline samples were synthesized and annealed with two different growth environments to further investigate the effect of oxygen deficiencies. Therefore, argon as well as oxygen gas flows were utilized. From initial dc magnetization and $C_p$ measurements, the previously report $T_N$ ~ 220 K was observed for both samples. However, a spontaneous polarization ($P_S$) was observed at ~ 253 K for the oxygen annealed sample with no applied field while no $P_S$ was observed up to 7 T and temperatures down to 2 K for the argon annealed sample. Anomalies above 260 K were detected in both samples, which were not only time-, but also field-dependent. Measurements are ongoing to gain greater insight into this complex system.

*The work performed at Houston is supported by USAFOSR Grant FA9550-15-1-0236, TLL Temple Foundation, JJ&R Moores Endowment, and State of Texas through TCSUH.
1:15PM X47.00009: Pressure effect on multiferroics investigation with neutron scattering*
YAN WU, WEI TIAN, HUIBO CAO (Presenter), Oak Ridge National Lab — Multiferroics have attracted tremendous research interests with their rich physics and potential in constructing next-generation multifunctional devices. The type-II multiferroics have magnetic phase related ferroelectricity. In a system where the magnetic phase is closely correlated with crystal lattice, compressing the unit cell with high pressure would lead to distinct magnetic phase transitions and then tune the ferroelectricity. We studied systems mainly with neutron scattering techniques in identifying their magnetic phase transitions under pressures to provide understanding for change of the ferroelectric properties in the system.

*The research was supported by the U.S. DOE, Office of Science, Early Career Research Program Award KC0402010 and used the DOE User Facility operated by the ORNL.

1:27PM X47.00010: Magnetostructural domain wall patterning in ferrimagnetic spinels*
LAZAR KISH (Presenter), University of Illinois at Urbana-Champaign, ADAM ACZEL, LISA DEBEER-SCHMITT, ALEXANDER N. THALER, Oak Ridge National Laboratory, DALMAU REIG-I-PLESSIS, University of British Columbia, ALEXANDER ZAKRZEWSKI, GREG MACDOUGALL, University of Illinois at Urbana-Champaign —
The ferrimagnetic spinels Mn3O4 and MnV2O4 are known for their anomalous magnetoresponsive behavior, including strong magnetoelastic and magnetodielectric couplings. Mechanically strained samples of these materials show a real-space separation of the volume into stripe-like regions of alternating magnetization on the nanometer lengthscale. I will show small angle neutron scattering data associating these features with known first order magnetic transitions in these materials, and their control via applied magnetic field. I will then draw a direct connection to bulk magnetic measurements, and demonstrate how these domains can lead to anomalous magnetization behaviors.

*Research was supported by National Science Foundation under NSF DMR 1455264

1:39PM X47.00011: Large and highly anisotropic magnetocaloric effects in disordered-perovskite RCr0.5Fe0.5O3 single crystals (R = Gd, Er) HYUNJUN SHIN (Presenter), JONGHYUK KIM, DONGGUN OH, YOUNG JAI CHOI, NARA LEE, Yonsei University — We have successfully synthesized the disordered-perovskite RCr0.5Fe0.5O3 (R=Gd, Er) single crystals which crystallize in an orthorhombic Pbmn structure, and investigated anisotropic magnetic and magnetocaloric properties. In GdCr0.5Fe0.5O3, the isotropic nature of large Gd3+ moments leads to a tremendously large entropy change of ~50 J/kg K for both ab and c axes. On the other hand, ErCr0.5Fe0.5O3 exhibits a highly anisotropic magnetocaloric effect which results in a rotational entropy variation of ~21 J/kg K at the ordering temperature of Er3+ moments, TEr = 6 K. Our findings suggest the important roles of magnetic anisotropy of rare-earth magnetic ions and enrich fundamental and applied research on magnetic materials in view of distinct magnetic characteristics in disordered perovskites.
An ab initio Study of Oxygen Vacancies in Ba$_2$CuO$_4$ and Sr$_2$CuO$_4$

MATTHEW MATZELLE (Presenter), CHRISTOPHER LANE, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern University — Oxygen vacancies play a key role in providing a fertile environment for superconductivity to emerge in the Ba$_2$CuO$_4$ and Sr$_2$CuO$_4$ family of novel superconductors. However, there is considerable debate as to whether or not the vacancies reside in the CuO$_2$ plane or at the apical sites. Using state-of-the-art ab initio techniques, we systematically examine the energy landscape and electronic structure of oxygen vacancies in Ba$_2$CuO$_4$ and Sr$_2$CuO$_4$. A number of different configurations involving single and multiple vacancies are considered. Planar vacancies are found to yield lower energies, and materials with apical vacancies display exotic band structures. Finally, we will briefly connect our results to recent experiments.

THz spectroscopy of spin excitations in magnetoelectric LiCoPO$_4$ in high magnetic fields

Laur Peedu (Presenter), Toomas Room, Johan Viirok, Urmas Nagel, National Institute of Chemical Physics and Biophysics, Sandor Bordacs, Budapest University of Technology and Economics, Vilmos Kocsis, Yusuke Tokunaga, Yasujiro Taguchi, Yoshinori Tokura, Riken, Hans Engelkamp, Uli Zeitler, High Field Magnet Laboratory, Radboud University, Istvan Kezsmarki, University of Augsburg — LiCoPO$_4$ belongs to the family of magnetoelectric lithium-orthophosphates. In these compounds the cross-coupling between magnetization and electric polarization leads to variety of spin excitations that have entangled dynamic electric and magnetic properties. In this work THz spectroscopy was used to measure absorption spectra of spin excitations in LiCoPO$_4$ single crystal below antiferromagnetic ordering temperature and in magnetic field up to 32 T. Three spin flop transitions for the magnetic field parallel to the magnetic easy axis were identified from the magnetic field dependence of spin excitations and from the magnetic field dependence of magnetization. Using polarized light and ME poling to create a single ME domain [V. Kocsis et al. PRL121, 057601 (2018), PRB100, 155124 (2019)], the selection rules of spin excitations were determined. Several magnetic-, electric-dipole active and magnetoelectric resonances were found.

*Part of the work was supported by The Estonian Ministry of Education and Research under Grant No. IUT23-03, and the European Regional Development Fund project TK134.
Disorder Effects on Superconducting Island Arrays Proximity-Coupled to Graphene*  
RITA GARRIDO MENACHO (Presenter), VINCENT HUMBERT, NADYA MASON,  
University of Illinois at Urbana-Champaign — Two-dimensional superconductors have been extensively studied due to the presence of quantum phase transitions (QPT) in these systems at millikelvin temperatures. One of the most investigated QPT is the Superconductor-(Metal)-Insulator Transition (SMIT). However, in the presence of disorder, the nature of transport across the SMIT is not well understood, largely because disorder is difficult to controllably tune in 2D superconducting films. To overcome this difficulty, we have developed arrays of superconducting Sn islands proximity-coupled to graphene with controllable island point disorder and graphene disorder. We studied the SMIT in these devices as a function of magnetic field and analyzed the transport signatures using scaling. Depending on the amount of point disorder, graphene disorder, and device geometry, we observed an evolution in the critical exponents from diffusive to percolative transport. We additionally performed Hall measurements, in which we observed peaks in the transverse resistance corresponding to pinning and depinning of magnetic field-induced vortices. These transport signatures suggest unusual behavior as a function of disorder near the Quantum Critical Point (QCP).

*This work was supported by the National Science Foundation (NSF) under DMR 17-10437.

The effects of charge carriers, organic solvents and magnetic ions on the superconductivity of doped 1T-SnSe₂  
HANLIN WU (Presenter), SHENG LI, DANIEL PEIRANO PETIT, BING LV, Physics, University of Texas at Dallas — We reported bulk superconductivity up to 7.6 K through careful manipulation of the charge carrier density and basal spacing \(d\) in the chemically intercalated two dimensional CdI₂-type 1T-SnSe₂ phase. We found out the very unusual scaling behaviour of \(T_C\) with the basal spacing distance caused by different organic co-intercalation, meanwhile the \(T_C\) appears to be almost independent with the alkali metal concentration. In this presentation, we focus on more chemical doping studies that close to the insulator-superconducting transition regime, more precisely-controlled doping level and various organic molecules have been tested through soft chemical methods. In addition, intercalation of the magnetic molecules are also carried out to study the interplay of superconductivity, magnetism, and possible charge density wave transition in these intercalated system. The details of the results will be presented with their physics origins being further elaborated.
**11:39AM X48.00003: Uniaxial strain effect on superconductivity in 1D and 2D LaAlO$_3$/SrTiO$_3$ channels**

XINYI WU (Presenter), MEGAN BRIGGEMAN, JOSEPH ALBRO, JIANAN LI, Univ of Pittsburgh, JUNG-WOO LEE, HYUNGWOOD LEE, CHANG-BEOM EOM, Univ of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — We investigate the effects of uniaxial strain on superconductivity of nanowires in LaAlO$_3$/SrTiO$_3$. The interface of LaAlO$_3$ and SrTiO$_3$ has a high-mobility 2D electron gas which can be superconducting at sub-Kelvin temperatures. We are able to create 1D conducting channels at the interface using conductive atomic force microscope lithography [1]. Superconductivity in the system is associated with ferroelastic domain boundaries [2] and therefore is in 1D regimes. Application of an external uniaxial stress is expected to displace the ferroelastic domain boundaries. Our experiments indicate that uniaxial stretching of the nanowire in the parallel direction completely suppress the superconducting state, while reversal of the applied strain restores superconductivity. We will discuss implications of possible electron-pairing mechanism in the 1D superconductor.


*JL acknowledges a Vannevar Bush Faculty Fellowship (ONR N00014-15-1-2847), and the Office of Naval Research (N00014-16-1-3152). The work at University of Wisconsin-Madison was supported by the National Science Foundation under DMREF Grant No. DMR-1629270, AFOSR FA9550-15-1-0334 and AOARD FA2386-15-1-4046.

**11:51AM X48.00004: Effect of quantum fluctuations on the critical supercurrent through a mesoscopic normal-metal island**

VLADIMIR BUBANJA (Presenter), Callaghan Innovation — We consider the transport properties of a single-electron transistor consisting of a diffusive normal-metal island and superconducting electrodes. We show that the interplay of a dissipative impedance of the gate electrode, a weak magnetic field, and a charging energy of the island causes a suppression of the critical supercurrent of the transistor. When the device is voltage biased, pumping of single electrons can be achieved by a periodic modulation of the gate voltage [1-3]. We derive the analytic expressions for the error rates and show that they are suppressed by the applied magnetic field [4].

**12:03PM X48.00005: Low Temperature Terahertz Nano-Imaging of BSCCO High Temperature Superconductor**  
RAN JING (Presenter), ROCCO VITALONE, MICHAEL BERKOWITZ, GUANGXIN NI, Columbia University, The Department of Physics, BRIAN S Y KIM, Columbia University, The Department of Mechanical Engineering, DMITRI BASOV, Columbia University, The Department of Physics — Terahertz (THz) near-field imaging and nano-spectroscopy is a capable tool to research nano-scale low energy electromagnetic phenomena. Of particular interest are high-temperature superconductors (HTSC) whose characteristic energy scale exists in the THz regime. We discuss our recent development of a cryogenic, scanning near-field microscope suitable for nano-scale imaging and spectroscopy throughout the THz frequency range. We report THz near-field measurements of optimally doped and over-doped BSCCO-2212 thin film devices above and below their superconducting transition temperatures. Near-field can measure the c-axis Josephson plasma resonance (JPR) spectroscopically. Further, the large anisotropy between the in and out of plane plasma frequency caused by JPR also contributes to a hyperbolic polariton modes in the bulk of a thin film which can be detected by near-field imaging [1][2].


**12:15PM X48.00006: Electric Field Effects in Mesoscopic Metal Superconductors**  
LOREN ALEGRIA (Presenter), CHARLOTTE BOETTCHER, AMIR YACOBY, Harvard University — The superconducting state of metals is typically thought to be negligibly affected by the presence of externally applied electric fields, given sub-nanometer screening lengths. But recent studies of mesoscopic metallic superconducting channels at millikelvin temperatures observe a reduction of the superconducting critical current under applied gate voltage [1]. We extend these measurements of Ti and Al nanowires and find revealing effects, including voltage tuned oscillations in the critical current as a function of magnetic field. We present possible explanations and experiments underway to evince the origin of the effect.


*This research was supported by an appointment to the Intelligence Community Postdoctoral Research Fellowship Program at Harvard University, administered by Oak Ridge Institute for Science and Education through an interagency agreement between the U.S. Department of Energy and the Office of the Director of National Intelligence.*
**12:27PM X48.00007: Quasiparticle Poisoning of a Superconducting Island by Nonequilibrium Phonons**

ELSA T MANNILA (Presenter), OLIVIER MAILLET, Aalto University, VILLE F MAISI, Lund University, JUKKA P PEKOLA, Aalto University — Quasiparticle excitations are detrimental to the operation of various superconducting devices. The density of quasiparticles should be exponentially suppressed at low temperatures, but commonly a quasiparticle density many orders of magnitude larger than the thermal expectation is observed. Phonons with energy greater than twice the superconducting gap can break Cooper pairs to form quasiparticles, and conversely two quasiparticles recombining to form a Cooper pair will emit such phonons. In our experiment, we demonstrate how the superconducting island of a single-electron transistor is poisoned with quasiparticles and the parity effect is consequently destroyed, when another heated superconducting island is used as an emitter of nonequilibrium phonons, while a thermal phonon emitter, a similarly heated normal metal island, creates much fewer quasiparticles.

**12:39PM X48.00008: InAs nanowire Josephson junctions with in-situ grown full shell Al**

IJU CHEN (Presenter), MARTIN BJERGFELT, THOMAS KANNE NORDQVIST, DAMON JAMES CARRAD, THOMAS SAND JESPERSEN, KASPER GROVE-RASMUSSEN, JESPER NYGÅRD, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen — Superconductor-semiconductor hybrid nanowires are ideal material systems for studying various quantum transport phenomena such as Andreev and Majorana bound states. For quantum information technologies based on these quantum phenomena, it is highly desirable to develop hybrid nanowires with high-quality superconductor-semiconductor interfaces and ballistic transport in the semiconductor. In this study, we use shadow mask structures on the growth substrate to grow full shell Al-InAs-Al Josephson junction nanowires in situ. The in-situ grown junction can be free from surface damage and over-etching associated with the Al etching process. Electrical characterization of the Josephson junctions shows a hard superconducting gap. We observe multiple Andreev reflections in the open-channel regime and sub-gap states in the tunnel coupled regime. Furthermore, as a result of fluxoid quantization in the Al shell, the superconductivity is modulated by the magnetic flux and its effect on the Josephson junction is investigated.
12:51PM X48.00009: Theory of superconductivity in an ultra-dilute fermionic liquid in the proximity of a quantum phase transition. Piotr Chudzinski (Presenter), School of Mathematics and Physics, Queens Univ Belfast — We study the problem of superconductivity in an extremely weakly doped narrow gap semiconductor, driven by electron-phonon coupling in a non-adiabatic regime. We derive an analytic theory analogue to Eliashberg equations that shall allow us to determine the critical temperature. In the first stage, based on our recent correlated electron-ion dynamics study, we obtain the effective non-adiabatic electron-phonon coupling function. We then add long-range Coulomb type interactions to derive propagators for the emergent collective state. Since the electron-phonon coupling is highly anisotropic, in the second step we test whether coupling to cooperons is able to induce a thermodynamic phase transition. Finally, we discuss transport properties of the emergent superconducting condensate, in particular (magneto-)thermoelectricity driven by vortex states. Our study is applicable in various classes of novel superconducting phases in materials with extremely small carrier concentrations such as doped SrTiO, but also a mysterious case of elementary bismuth.

*SFI-DfE NI Investigators Programme Partnership #15/IA/3160

1:03PM X48.00010: Suppression of quantum metallic state in disordered Ta thin films with the addition of artificial periodic pinning centers Eunseong Kim (Presenter), Junghyun Shin, Sun-gyu Park, Suhyeon Noh, Korea Adv Inst of Sci & Tech — We studied the low temperature transport properties of perforated superconducting Ta films with periodic triangular array of holes to investigate the role of pinning effect on superconductor-insulator transition. Magnetic field and temperature dependence of transport characteristics in 7 perforated Ta thin film samples with uniform thickness but different densities of holes are investigated and compared with a reference sample without holes. High density artificial periodic pinning centers increase activation energies for motion of vortices and induce cusp-like magnetic field dependence of resistance due to commensurate matching effect of interstitial vortices between holes as well as trapped vortices inside holes. As hole density increases, matching effects is observed up to higher field. Besides Resistance of field cooling decreases as Arrhenius form of thermal activated model up to higher magnetic field and, zero-temperature limit metallic state is more suppressed.
**1:15PM X48.00011: Thickness dependent study of superconducting behavior and contact dynamics in atomically thin Fe(\text{Te}_{0.7}\text{Se}_{0.3}) Flakes**  
ANDREW STEELY (Presenter), CHUNLEI YUE, YUN LING, ABIN JOSHY, Tulane Univ, ZHIQIANG MAO, Pennsylvania State University, JIANG WEI, Tulane Univ — We present evidence of thickness dependent superconducting behavior in strain-free Fe(\text{Te}_{0.7}\text{Se}_{0.3}) flakes. Due to non-uniform Te/Se spatial distribution, we find that R(T) behavior in flakes <10nm can be explained and confirmed using the BKT transition for inhomogeneity model, as well as finite state effects (FSE). For >10nm flakes we find a systematic suppression of the superconductivity and broadening of the superconducting phase transition. Additionally, we present a self-heating model at the metal-superconductor-metal (MSM) interface to explain unusual observed switching behavior in I-V characteristics for flakes thinner than 10nm. We propose a 2D network of superconducting paths connecting superconducting islands within Fe(\text{Te}_{0.7}\text{Se}_{0.3}) thin flakes to describe the thickness-dependent behavior of this natural percolating system.

*This work was supported by the DOE under grant DESC0014208 and by the Board of Regents Support Fund (BoRSF) under grant LEQSF(2015-18)-RD-A-23.*

**1:27PM X48.00012: Gaussian state superposition ansatz for quantum impurity problems: Numerical methods and applications**  
SAMUEL BOUTIN (Presenter), BELA BAUER, Station Q, Microsoft Quantum — Recent work of Bravyi and Gosset [1] demonstrated that superposition of Gaussian states can approximate efficiently the ground state of gapped quantum impurity problems. We introduce an efficient numerical method for finding the ground state approximation in this variational manifold. As a benchmark, we first apply our method, based on imaginary time evolution, to the Anderson impurity model. We then study a generalization of this approach to models of superconducting islands in the Coulomb blockade regime.

Two-dimensional superconductors have attracted growing interest because of their scientific novelty, structural tunability, and useful properties. Studies of their magnetic responses, however, are often hampered by difficulties to grow large-size samples of high quality and uniformity. We report here an imaging method that employed NV$^-$ centers in diamond as sensor capable of mapping out the microwave magnetic field distribution on an ultrathin superconducting film of micron size. Measurements on a 33nm-thick film and a 125nm-thick bulk-like film of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ revealed that the ac Meissner effect set in at 78K and 91K, respectively; the latter was the superconducting transition temperature ($T_c$) of both films. The unusual ac magnetic response of the thin film presumably was due to thermally excited vortex-antivortex diffusive motion in the film. Spatial resolution of our ac magnetometer was limited by optical diffraction. The technique could be extended with better detection sensitivity to extract local ac conductivity/susceptibility of ultrathin or monolayer superconducting samples as well as ac magnetic responses of other two-dimensional exotic thin films of limited lateral size.

*National NSF of China Grants (No.11874123) and the National KRDP of China (No. 2016YFA0300902).
11:15AM X49.00001: Phase Diagram of Spin Triplet Superconductor UTe$_2$ Under Pressure and Magnetic Field  

WEN-CHEN LIN (Presenter), DANIEL J CAMPBELL, University of Maryland, College Park, DAVID E GRAF, Florida State University, SHENG RAN, NICHOLAS BUTCH, National Institute of Standards and Technology, JOHNPIERRE PAGLIONE, University of Maryland, College Park — The heavy fermion superconductor UTe$_2$ has recently drawn much attention due to several exotic properties. It exhibits two reentrant superconducting states under extremely high magnetic fields that appear correlated with ferromagnetic interactions [1-2], and has been proposed as a candidate three-dimensional topological superconductor [3-4]. Here, we report details of the field-temperature-pressure phase diagram of UTe$_2$ under pressures up to 18.8kbar and high magnetic fields. Electrical resistivity and tunnel diode oscillator (TDO) measurements were performed under external magnetic field along the crystallographic b axis (hard axis), revealing a systematic progression of the superconducting and field-polarized phases that have relations to those observed at ambient pressure [2][5]. We will discuss our observations and their relevance on the interplay between ferromagnetism and superconductivity in this rich system.


11:27AM X49.00002: Anomalous heat capacity of spin triplet superconductor UTe$_2$  

IAN HAYES (Presenter), TRISTIN METZ, YUN SUK EO, SHENG RAN, University of Maryland, College Park, NICHOLAS BUTCH, National Institute of Standards and Technology, JOHNPIERRE PAGLIONE, University of Maryland, College Park — The recently discovered superconducting state in uranium ditelluride is a playground of exotic phenomena, including field-reentrant superconductivity up to sixty tesla and spin-triplet pairing.[1, 2] In addition this system shows a large residual density of states at zero temperature, suggesting that about half of the electrons fail to condense, and an apparent violation of entropy balance across the superconducting transition.[1, 3] This talk will present millikelvin specific heat data on UTe2 as a function of magnetic field applied along multiple crystallographic axes. The specific heat shows an upturn at the lowest temperatures. The form of the upturn in temperature and its evolution in magnetic field suggest that it has its origin in critical ferromagnetic fluctuations, supporting the idea that UTe2 is the paramagnetic end member of the series of uranium-based ferromagnetic superconductors. Furthermore, subtracting this upturn restores entropy balance to the superconducting transition. The talk will conclude with a discussion of the implications of these observations for the triplet pairing scenario.

**11:39AM X49.00003: NMR Study of the Spin-triplet Superconductor UTe$_2$**

(QING-PING DING (Presenter), Ames Laboratory and Dept. of Phys. and Astro., Iowa State University, SHENG RAN, NICHOLAS BUTCH, NIST Center for Neutron Research, National Institute of Standards and Technology, YUJI FURUKAWA, Ames Laboratory and Dept. of Phys. and Astro., Iowa State University — Recently, spin-triplet superconductivity has been discovered in nearly ferromagnetic (FM) heavy fermion UTe$_2$ [1]. Here, we report the $^{125}$Te nuclear magnetic resonance (NMR) studies of UTe$_2$ in both the normal and superconducting (SC) states. The magnetic fluctuations in the normal state, and the SC gap information in the SC state has been revealed. We will also discuss the relationship between FM spin fluctuations and superconductivity in UTe$_2$.


*The research was supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Ames Laboratory is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358.

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**11:51AM X49.00004: The electronic fluid in cuprate superconductors and NMR**

(JUERGEN HAASE (Presenter), Univ Leipzig — Nuclear magnetic resonance (NMR) is a powerful technique to explore quantum fluids in solids. Recently it was found that a number of early conclusions derived with NMR about the cuprates were flawed, as is easily seen from an overview of all cuprate planar copper shifts [1] and relaxation data [2,3]. For example, there is no evidence for special electronic spin fluctuations [2,3], and, the uniform magnetic response above Tc shows hitherto unknown behaviour [1,2]. The latter implies a large spin shift below Tc for one direction of the external magnetic field, while the nuclear relaxation ceases completely for all cuprates [3]. This must have consequences for the pairing. To shed more light on this peculiar behaviour, we discuss data for other nuclei and their relation to the local charge symmetry, which sustains the existence of this unusual spin shift.

12:03PM X49.00005: Identify the Chiral Superconductivity in 4Hb-TaS2 through Magnetic-Spectral Responses  XUEJIAN GAO (Presenter), KAM TUEN LAW, Department of Physics, Hong Kong University of Science and Technology, PATRICK A LEE, Department of Physics, Massachusetts Institute of Technology — Chiral superconductivity, which breaks time-reversal symmetry spontaneously, is an alternative ingredient to cook up a topological superconductor holding the Majorana fermions that can be used to perform fault-tolerant quantum computation. A recent experiment [1] showed signatures of time-reversal symmetry breaking in superconducting 4Hb-TaS2 which abruptly appeared at the critical temperature Tc, implying possibility for the existence of chiral superconductivity. Through group theory analysis, we argue that only a chiral and a non-chiral superconducting states are allowed by the crystalline symmetry and strong Ising-type spin-orbital coupling in 4Hb-TaS2, both of which are mixed singlet-triplet states. It is further shown that the non-chiral superconducting state is more susceptible to an in-plane magnetic field and can be magnetically driven to a nodal superconducting phase, while the chiral one does not share this property. According to their different magnetic-spectral responses, an experimentally feasible way concerning the measurement of specific heat is proposed to identify the chiral superconductivity from the non-chiral one for this particular material.


12:15PM X49.00006: Mixed-parity superconductivity near Lifshitz transitions in strongly spin-orbit-coupled metals* MATTHEW TROTT, CHRISTOPHER HOOLEY (Presenter), School of Physics and Astronomy, SUPA, University of St Andrews, UK — We consider a strongly spin-orbit-coupled metal, one of whose Fermi surfaces is close to a Lifshitz (topological) transition. Via a renormalization group analysis of the square-lattice Hubbard model with strong Rashba spin-orbit coupling, we show that such a metal is generically unstable to the formation of mixed-parity superconductivity with a helical triplet component.

*This work has been funded by the Engineering and Physical Sciences Research Council (UK) under grant numbers EP/L015110/1 (Trott) and EP/R031924/1 (Hooley).
12:27PM X49.00007: Superconductivity mediated by ferroelectric fluctuations: anisotropic gap structure and possible application to SrTiO$_3$  MARIA NAVARRO GASTIASORO, University of Minnesota, THAIS VICTA TREVISAN (Presenter), Ames Lab, RAFAEL FERNANDES, University of Minnesota — SrTiO$_3$ is a semiconducting oxide that undergoes a phase transition to a superconducting state upon electron doping. Although such superconducting phase was first observed more than 50 years ago, its nature and origin remain an unsettled puzzle. Interestingly, recent experimental and theoretical works suggest an interplay between ferroelectricity and superconductivity in this material. Motivated by these studies, we study superconductivity mediated by odd-parity ferroelectric modes. We consider a Rashba-like coupling between the electrons and the ferroelectric fluctuations, which is possible due to the presence of spin-orbit coupling. We derive the effective pairing interaction and solve the resulting linearized gap equation away from quantum criticality. We find that the effective coupling, which is attractive in the singlet channel, is dominated by the soft transverse optical mode. Moreover, the superconducting gap is shown to develop an anisotropy that grows as the system approaches the ferroelectric phase. Finally, we discuss the competition with other even-parity superconducting channels and the possible application of our results to SrTiO$_3$.

12:39PM X49.00008: Enhancement of superconductivity mediated by antiferromagnetic squeezed magnons* EIRIK ERLANDSEN (Presenter), AKASHDEEP KAMRA, ARNE BRATAAS, ASLE SUDBO, Norwegian Univ Tech (NTNU) — We theoretically investigate magnon-mediated superconductivity in a heterostructure consisting of a normal metal and a two-sublattice antiferromagnetic insulator. The attractive electron-electron pairing interaction is caused by an interfacial exchange coupling with magnons residing in the antiferromagnet, resulting in p-wave, spin-triplet superconductivity in the normal metal. Our main finding is that one may significantly enhance the superconducting critical temperature by coupling the normal metal to only one of the two antiferromagnetic sublattices employing, for example, an uncompensated interface. Employing realistic material parameters, the critical temperature increases from vanishingly small values to significantly larger values than 1 K as the interfacial coupling becomes strongly sublattice-asymmetric. We provide a general physical picture of this enhancement mechanism based on the notion of squeezed bosonic eigenmodes.

*We acknowledge financial support from the Research Council of Norway Grant No. 262633 ` Center of Excellence on Quantum Spintronics", and Grant No. 250985, ` Fundamentals of Low-dissipative Topological Matter".
**12:51PM X49.00009: Nonlinear optical effects in inversion-symmetry-breaking superconductors**

TIANRUI XU (Presenter), Physics, University of California, Berkeley, TAKAHIRO MORIMOTO, Applied Physics, The University of Tokyo, JOEL MOORE, Physics, University of California, Berkeley — We study nonlinear optical responses in superconducting systems with inversion ($I$) symmetry-breaking order parameters. We first show that any superconducting system with $I$ and time-reversal ($T$) symmetries requires an $I$-breaking order parameter to support optical transitions between particle-hole pair bands. We then use a 1D toy model of an $I$-breaking superconductor to numerically calculate linear and nonlinear conductivities, including shift current and second harmonic generations (SHG) responses. We find that the magnitude of the signal is significantly larger in shift current/SHG response than in the linear response due to the matrix element effect. We also present various scaling behaviors of the SHG signal, which may be relevant to the recent experimental observation of SHG in cuprates[1]. Finally, we confirm the generality of our observations regarding nonlinear responses of $I$-breaking superconductors, by analyzing other models including a 1D three-band model and 2D square lattice model.


*The Ultrafast Materials Science Program, U.S. Department of Energy*
1:03PM X49.00010: Energy-scale relationship between magnetic excitations and superconductivity in Hg-family of high-$T_c$ cuprates

LICHEN WANG (Presenter), Solid State Spectroscopy, Max Planck Institute for Solid State Research, GUANHONG HE, International Center for Quantum Materials, Peking University, ZICHERN YANG, Solid State Spectroscopy, Max Planck Institute for Solid State Research, MIRIAN GARCIA-FERNANDEZ, ABHISHEK NAG, KEJIN ZHOU, I21 Inelastic X-ray Scattering, Diamond Light Source, MATTEO MINOLA, Solid State Spectroscopy, Max Planck Institute for Solid State Research, MATTHIEU LE TACON, Institute for Solid State Physics, Karlsruhe Institute of Technology, BERNHARD KEIMER, Solid State Spectroscopy, Max Planck Institute for Solid State Research, YINGYING PENG, YUAN LI, International Center for Quantum Materials, Peking University — High-temperature superconductivity in the cuprates is realized upon doping antiferromagnetic parent compounds, in which spin excitations have a band width of a few hundred meV. At such high energies, paramagnons and two-magnon excitations are known to persist well into and beyond the superconducting doping range [1,2,3], but it remains unclear to what extent they contribute to Cooper pairing [4] or how the magnetic and superconducting energy scales are related to each other. We have used resonant inelastic X-ray scattering and Raman scattering to study the first two members of the Hg-family of cuprates, HgBa$_2$CuO$_{4+d}$ and HgBa$_2$CaCu$_2$O$_{6+d}$, which have nearly identical crystal structure in the charge-reservoir layers but different electronic environment in the quintessential Cu-O layers. We find that the latter compound, which has higher $T_c$ and larger superconducting gap, also has considerably higher magnetic excitation energies.


1:15PM X49.00011: Hidden Spin-Momentum Texture in High Tc Cuprate Superconductor

CHIU-YUN LIN (Presenter), KENNETH GOTLIEB, University of California, Berkeley, MAKSYM SERBYN, Institute of Science and Technology, Austria, WENTAO ZHANG, Physics and Astronomy, Shanghai Jiao Tong University, CHRISTOPHER SMALLWOOD, Physics and Astronomy, San Jose State University, CHRIS JOZWIAK, ZAHID HUSSAIN, Advanced Light Source, Lawrence Berkeley National Lab, ASHVIN VISHWANATH, Physics, Harvard University, ALESSANDRA LANZARA, University of California, Berkeley — Cuprate superconductor is one of the most well studied compounds. Even so, experiments discover new results after thirty years of intense study by the community. Spin-orbit coupling (SOC) in cuprate superconductors was not a focus of condensed matter research due to the negligible SOC value of the conducting orbitals comparing with the strong electronic correlations and its centrosymmetric crystal structure. However, using spin- and angle-resolved photoemission spectroscopy, we directly probed the spin-momentum entangled texture in Bi2Sr2CaCu2O8+x. The unexpectedly strong spin asymmetry in such globally inversion-symmetric crystal highlights the importance of the local environment that carriers see, meanwhile, poses the intriguing question of how the high-temperature superconducting state emerges in the presence of this nontrivial spin texture.
1:27PM X49.00012: NCCO: Examining antiferromagnetic hotspots and spin texture comparison with Bi-based cuprates*  KAYLA CURRIER (Presenter), Physics, University of California, Berkeley — Recent work on cuprate Bi2212 has revealed a nontrivial spin texture with a rashba-like spin orbit coupling. This texture has been attributed to local inversion symmetry breaking that causes a local electric field within the material. Theory suggests that this property is due to the specific structure of the layers in Bi2212. We examine the spin texture in single-layer electron-doped cuprate NCCO and show how it fits in with the proposed theory. In addition, equilibrium data taken on different dopings of NCCO are compared to recent work showing fermi surface reconstruction. Here we focus on the antiferromagnetic hotspots along the zone boundary. Overall we show part of the picture of how NCCO fits in with the current understanding of cuprates and some of their properties.

*Funding for this project was provided by the Department of Energy as part of the Ultrafast Materials program.

Friday, March 6, 2020 11:15 AM - 1:51 PM

Session X50 DCMP: Correlated 2D Materials and Models Mile High Ballroom 1C -

Shenglong Xu, University of Maryland, College Park

11:15AM X50.00001: Temperature dependence of the Mott gap in single-layer 1T-TaSe2 revealed by scanning tunneling spectroscopy  WEI RUAN (Presenter), YI CHEN, University of California, Berkeley, JINWOONG HWANG, Lawrence Berkeley National Laboratory, SHUJIE TANG, Stanford, RYAN LEE, HSIN-ZON TSAI, SALMAN ABDUL GAFFAR KAHN, FRANKLIN LIOU, ANDREW AIKAWA, University of California, Berkeley, ZHIXUN SHEN, Stanford, SUNG-KWAN MO, Lawrence Berkeley National Laboratory, MICHAEL F CROMMIE, University of California, Berkeley — A key to unraveling the high-temperature superconductivity mechanism in cuprates is to understand the Metal-insulator transition in Mott insulators that can be induced by either doping charge or raising temperature. While the doping dependence of the Mott gap in cuprates has been studied extensively, it is difficult to explore the gap’s temperature dependence in these systems due to its large size (typically 1~2 eV) and the resulting high temperature scale required to melt the Mott-state. Here we use scanning tunneling microscopy/spectroscopy to investigate the temperature dependence of the electronic structure of the single-layer Mott insulator 1T-TaSe2 which has a much more modest Mott gap of ~ 0.1 eV. We observe that the gap closes rapidly at a temperature scale that is significantly smaller than the gap size. This is accompanied by changes in the exotic orbital texture of the upper Hubbard band that are consistent with reduced screening at elevated temperatures. This phenomenon is unique among strongly correlated systems and is compatible with recent theoretical predictions where spin fluctuations are responsible for the rapid gap closing.
Manipulation of electron-phonon energy transfer pathways in 2D transition metal dichalcogenides through ultrafast excitation

EMMA CATING-SUBRAMANIAN (Presenter), CHRISTIAN GENTRY, XUN SHI, YINGCHAO ZHANG, WENJING YOU, SINEAD RYAN, JILA, University of Colorado Boulder, BALDWIN AKIN VARNER, Norfolk State University, KAI ROSSNAGEL, Christian-Albrechts-Universitat zu Kiel, HENRY KAPTEYN, MARGARET MURNANE, JILA, University of Colorado Boulder — The complex phase landscape of quantum materials provides tremendous opportunity for design, manipulation, and coherent control of material properties using light. Understanding that complexity also poses a significant challenge, and multiple techniques are needed to map and exploit the rich phase space of strongly correlated materials. For example, using ultrafast electron calorimetry via time- and angle-resolved photoemission (ARPES), a bi-directional energy transfer between strongly-correlated electron and phonon modes in a material has been observed for the first time - in this case a charge density wave (CDW) material \( \Gamma - \text{TaSe}_2 \).

Here we use visible pump-probe spectroscopy to further explore and manipulate the couplings between the electron and phonon systems. By varying the pump fluence, we can alter the relative coupling strength of multiple phonon modes, demonstrating the use of light to control material properties and select available vibrational relaxation pathways in quantum materials.

Negative Parabolic Magneto-resistance in a strongly interacting 2D Hole system in GaAs/AlGaAs

ARVIND SHANKAR KUMAR (Presenter), CHIEH-WEN LIU, SHUHAO LIU, Case Western Reserve University, LOREN PFEIFFER, KENNETH WEST, Princeton University, XUAN GAO, Case Western Reserve University — Electron-electron interactions are believed to be an important factor in the origin of the 2D Metal-Insulator Transition observed in strongly correlated 2D electron/hole systems. In the weakly interacting (Fermi Liquid) regime, these interactions can be shown to cause a negative parabolic correction to the magneto-resistance of the 2D electron/hole system. In the strongly interacting regime (\( \omega_c \tau > 1 \)) for a strongly interacting 2D hole liquid (\( r_s = 20-30 \)) in a GaAs/AlGaAs quantum well at low temperatures (\( T = 0.09 - 1 \) K), in a hole density range (\( p = 0.98-1.98 \times 10^{10} / \text{cm}^2 \)) close to the critical density for the 2D Metal-Insulator transition, where the temperature dependence of resistivity is non-monotonic. We study the extracted hole-hole interaction correction to Drude conductivity in this regime and compare its temperature dependence to conventional Fermi Liquid theories. This study gives insight on the validity of a Fermi Liquid picture in the strongly interacting regime and explores whether this conventional picture of interacting electron systems can be used to explain the origin of the 2D metallic state.

*The work was funded by NSF (DMR-1607631) (CWRU), The Gordon and Betty Moore Foundation and NSF MRSEC (Grant# 1420541) (Princeton University).
11:51AM X50.00004: Theory of Strain Effects on Extremely Correlated Metals in Two-dimensions*  
MICHAEL ARCINIAGA (Presenter), University of California, Santa Cruz, PEIZHI MAI, Oak Ridge National Laboratory, B SRIRAM SHASTRY, University of California, Santa Cruz — We study the strain dependence of anisotropic resistivity [1] within the t-t'-J model, applicable to cuprate superconductors. This model is treated using the recently developed extremely correlated Fermi liquid theory (ECFL). We obtain the temperature, density and strain dependence of the anisotropic resistivity. We compute the strain response functions in different geometries for comparing with planned experiments [1]. We also study the strain dependence of the optical weight and the local density of states (LDOS) at low T. Our results provide quantitative predictions of these quantities for experimental tests on strongly correlated materials such as high-Tc materials.


*The work at UCSC was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award DE-FG02-06ER46319. The work at ORNL was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. DOE, Office of Science, Advanced Scientific Computing Research and BES, Division of Materials Sciences and Engineering.

12:03PM X50.00005: Construction and classification of point group symmetry protected topological phases in 2D interacting fermionic systems*  
JIANHAO ZHANG (Presenter), Institute for Advanced Study, Tsinghua University, QING-RUI WANG, Department of Physics, The Chinese University of Hong Kong, SHUO YANG, Department of Physics, Tsinghua University, YANG QI, Department of Physics, Fudan University, ZHENGCHENG GU, Department of Physics, The Chinese University of Hong Kong — The construction and classification of symmetry protected topological (SPT) phases in interacting bosonic and fermionic systems have been intensively studied in the past few years. Very recently, a complete classification and construction of space group SPT phases were also proposed for interacting bosonic systems. In this paper, we attempt to generalize this classification and construction scheme into interacting fermion systems systematically. In particular, we construct and classify point group SPT phases for 2D interacting fermion systems via lower-dimensional block-state decorations. We discover several intriguing fermionic SPT states that can only be realized in interacting fermion systems (i.e., no free-fermion and bosonic SPT realizations). Moreover, we also verify the recently conjectured crystalline equivalence principle for 2D interacting fermion systems. Finally, a potential experimental realization of these new classes of point group SPT phases in 2D correlated superconductors is also addressed.

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Hong Kong's Research Grants Council (GRF No.14306918, ANR/RGC Joint Research Scheme No. A-CUHK402/18)
NSFC (Grant No. 11804181)
National Key R&D Program of China (Grant No. 2018YFA0306504)
12:15PM X50.00006: The Non-Gaussian Exact Diagonalization Method and Its Application to the 2D Hubbard-Holstein Model*  
YAO WANG (Presenter), ILYA ESTERLIS, Harvard University, TAO SHI, Institute of Theoretical Physics, Chinese Academy of Sciences, JUAN IGNACIO CIRAC, Max-Planck-Institut für Quantenoptik, EUGENE DEMLER, Harvard University — We propose a novel numerical method that embeds the variational non-Gaussian wavefunction approach with exact diagonalization, allowing for efficient treatment of correlated systems with both electron-electron and electron-phonon interactions. Using a generalized polaron transformation, we construct a variational wavefunction that minimizes the entanglement between electrons and phonons; exact diagonalization is then used to treat the electronic part of the wavefunction exactly, thus taking into account high-order correlation effects beyond the Gaussian level. Keeping the full electronic Hilbert space, the complexity is increased only by a polynomial factor relative to the exact diagonalization calculation for pure electrons. As an example, we use this method to study ground-state properties of the two-dimensional Hubbard-Holstein model, providing evidence for the existence of intervening phases between the spin and charge-ordered states.

*This work is supported by the MPHQ fellowship, Harvard-MIT CUA, and AFOSR-MURI grant (Award No. FA9550-14-1-0035 and Award No. FA9550-16-1-0323).

12:27PM X50.00007: Electro-magnetic duality in 2D topological orders with gapped boundaries  
HONGYU WANG (Presenter), YINGCHENG LI, Fudan University, YUTING HU, Department of Physics and Institute for Quantum Science and Engineering, South University of Science and Technology, YIDUN WAN, Fudan University — We generalize the Electro-magnetic (EM) duality and the mapping to the Levin-Wen (LW) model of the quantum double (QD) model to the case of topological orders with gapped boundaries. To achieve our goal, we Fourier transform the extended QD model defined on the lattice with boundaries. The input data of the model is finite group $G$ and the boundary condition is characterized by subgroup $K \subseteq G$. After the Fourier transform, we find while the bulk degrees of freedom become $\text{rep}_G$, the boundary condition is now characterized by Frobenius algebra $((\mathds{C}[G]/\mathds{C}[K])^*)$, the quotient of the group algebra of $G$ over that of $K$. We also show that our Fourier-transformed extended QD model can be mapped to an extended LW model on the same lattice via enlarging the Hilbert space of the extended LW model. Moreover, our Fourier transform of the extended QD model provides a visualizable explanation of the phenomenon of splitting and partial condensation of anyons.
**12:39PM X50.00008: Catastrophe theory classification of Fermi surface topological transitions in two dimensions**

ANIRUDH CHANDRASEKARAN (Presenter), Boston Univ, OLEKSANDR SHTYK, Quantlab Group, JOSEPH BETOURAS, Physics, Loughborough University, CLAUDIO CHAMON, Boston Univ — We classify all possible singularities in the electronic dispersion of two-dimensional systems that occur when the Fermi surface changes topology, using catastrophe theory. For systems with up to seven control parameters (i.e., pressure, strain, bias voltage, etc), the theory guarantees that the singularity belongs to one of seventeen standard types. We show that at each of these singularities the density of states diverges as a power law, with a universal exponent characteristic of the particular catastrophe, and we provide its universal ratio of amplitudes of the prefactors of energies above and below the singularity. We further show that crystal symmetry restricts which types of catastrophes can occur at the points of high symmetry in the Brillouin zone. For each of the seventeen wallpaper groups in two-dimensions, we can list which catastrophes are possible at each high symmetry point.

*This work is supported by the DOE Grant No. DE-FG02-06ER46316 (A.C. and C.C.), the EPSRC grant No. EP/P002811/1 (J.J.B.) and the Royal Society (J. J. B. and C.C.).

**12:51PM X50.00009: Symmetry protected long-lived excitations and tomographic dynamics in 2D electron fluids**

PATRICK LEDWITH (Presenter), HAOYU GUO, Harvard University, LEONID LEVITOV, Massachusetts Institute of Technology — We will discuss the peculiar collective behavior in two-dimensional Fermi gases arising from head-on carrier-carrier collisions. These collisions dominate at cold temperatures, $T \ll T_F$, due to the combined effects of Pauli blocking and momentum conservation. Odd-parity harmonics are protected from these collisions and hence have anomalously long lifetimes. They instead slowly relax via small angle scattering which leads to a strange "superdiffusive" behavior. These long-lived modes give rise to a "tomographic" transport regime dominated by fermionic jets with an unusual hierarchy of time scales and scale-dependent transport coefficients with nontrivial fractional scaling dimensions. We will also discuss proposals for experimental realizations and implications for ongoing studies of electron hydrodynamics.

References:


*Patrick Ledwith was supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate (NDSEG) Fellowship Program.*
1:03PM X50.00010: Hydrodynamic electron flow in 2D semiconductor heterostructures*
AYDIN KESER (Presenter), DAISY QINGWEN WANG, University of New South Wales & FLEET ARC, OLEH KLOCHAN, UNSW Canberra, ADFA, FLEET ARC, DEREK HO YEW HUNG, SHAFFIQUE ADAM, Physics, Yale NUS College, DOMITRIE CULCER, ALEX HAMILTON, OLEG SUSHKOV, University of New South Wales & FLEET ARC — We propose simple geometries to directly test hydrodynamic flow in 2D electron systems by longitudinal resistance measurements. We model the boundaries of the electron fluid as `slippery', i.e. supporting no longitudinal stress, hence, we show that the viscous component of resistance depends significantly on the geometric features while it vanishes along the straight featureless sections. Moreover, since the viscous resistance increases quadratically with the inverse scale of the system, we show that channels in which the viscous and Ohmic effects are comparable can be manufactured with current technology. Elementary, bent or nozzle/diffuser type channels show significant departure from their diffusive counterparts in the hydrodynamic regime.

*This research was supported by the Australian Research Council Centre of Excellence in Future Low-Energy Electronics Technologies (Project No. CE170100039) and funded by the Australian Government. This work was performed in part at the NSW Node of the Australian National Fabrication Facility.

1:15PM X50.00011: Atypical Behavior of Collective Modes in Two-Dimensional Fermi Liquids
MATTHEW GOCHAN (Presenter), JOSHUAH TIMOTHY HEATH, KEVIN SHAWN BEDELL, Boston College — Since its development by L.V. Landau sixty years ago, Fermi liquid theory continues to serve as a formidable model for interacting Fermi systems in addition to providing the standard which all other models are held to. Of the numerous accomplishments of Fermi liquid theory, the calculation of various transport properties is of particular interest. In this talk we apply the Landau kinetic equation to a two-dimensional Fermi liquid and discuss the consequences of the reduced dimensionality on the behavior of the collective modes. As a function of the usual dimensionless parameter $s = \omega/\nu_F$, we find expected behavior in addition to new results for the behavior of the zero sound mode $c_0$. Additionally, we investigate the effect of a Coulomb interaction on the system resulting in an expression for plasmon frequency $\omega_p$ in 2D with a crossover as a function of $q$ to the zero sound mode.

1:27PM X50.00012: A determinantal quantum Monte Carlo study of deconfined quantum criticality*
CHAO WANG (Presenter), YONI SCHATTNER, STEVEN KIVELSON, Stanford Univ — We study an interacting electron-dimer model on the square lattice using the determinantal quantum Monte Carlo technique. We present evidence for a deconfined quantum critical point between antiferromagnetic and columnar valence-bond solid phases and examine the properties of the critical point.

*This work was supported in part by the Department of Energy, Office of Basic Energy Sciences, under contract no. DE-AC02-76SF00515 at Stanford. YS was also supported by the Zuckerman STEM Leadership Program.
Among various ground states of rare earth monotelluride, bulk GdTe is metallic with antiferromagnetic order (AFM) at low temperature. We grow GdTe thin films by molecular beam epitaxy (MBE) and study their properties by scanning tunneling microscopy (STM) and magnetic property measurement. Density of states (DOS) obtained by STM exhibits insulating gap, which can be closed by magnetic field for certain film thicknesses, indicating a transition from insulator to metal. The gap size can be as large as 30 meV and closed by relatively weak magnetic field of 2.6 T for 6 layers of GdTe. We attribute the observed effects to the exchange interaction between d and f electrons.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X51 DCMP: Transport in Graphene Systems Mile High Ballroom 1D - Gregory Stephen, Laboratory for Physical Sciences

11:15AM X51.00001: Flat-Band Magnetism and Half-Metallicity in Twisted Bilayer Graphene* ALEJANDRO LOPEZ BEZANILLA (Presenter), Los Alamos National Laboratory — Evidence of flat-band magnetism and half-metallicity in compressed twisted bilayer graphene is provided with first-principles calculations. We show that dynamic band-structure engineering in twisted bilayer graphene is possible by controlling the chemical composition with extrinsic doping, the interlayer coupling strength with pressure, and the magnetic ordering with external electric field. By varying the rotational order and reducing the interlayer separation an unbalanced distribution of charge density results in the spontaneous apparition of localized magnetic moments without disrupting the structural integrity of the bilayer. Substitutional doping shifts the chemical potential of one spin distribution and leads to half-metallicity.

*This work was supported by the U.S. DOE Office of Basic Energy Sciences Program E3B5.
11:27AM X51.00002: Evidence for a three-layer-coherent quantum Hall state in graphene triple layers  
ANNA OKOUNKOVA (Presenter), YIHANG ZENG, CORY DEAN, JAMES C HONE, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science — Heterostructures consisting of two graphene monolayers separated by a thin BN spacer provides a rich platform in which to study correlated states driven by strong interlayer interactions. In the quantum Hall effect regime, tuning this system to total filling fraction $\nu_{\text{tot}} = 1$ (i.e. half filling of the lowest Landau level in each layer) results in a spontaneously formed interlayer coherent state believed to be a Bose-Einstein condensate of indirect excitons or a pseudo spin ferromagnet. Here we report the first realization of a triple layer system where three monolayer graphene layers are strongly coupled via coulomb interaction while maintaining negligible interlayer tunneling. We demonstrate independent control of the density in each layer, giving access to the entire phase space of this system. Tuning the relative filling fraction between all three layers allows us to effectively shift the exciton condensate between different layer pairs and then probe this phase with the third layer. When the total filling factor of all three layers equals 1, we observe simultaneous quantization of Hall resistance in the drive and drag layer and vanishing longitudinal resistance, suggesting a generalized exciton condensate phase with macroscopic phase coherence across all three layers.

11:39AM X51.00003: Nonlocal transport in twisted double bilayer graphene*  
SUBHAJIT SINHA (Presenter), PRATAP ADAK, SURYA KANTHI R. S., L. D. VARMA SANGANI, Tata Institute of Fundamental Research (TIFR), KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Tsukuba, MANDAR M DESHMUKH, Tata Institute of Fundamental Research (TIFR) — In the spectrum of 2D materials, superlattices have emerged as a promising platform to modulate band structure. In graphene, it does the job of breaking the inversion symmetry between the K and K' points. In the case of bilayer graphene, spatial inversion symmetry can also be broken by applying a transverse electric field, which opens up a gap at CNP. Both these ways result in the generation of a valley current via the valley Hall effect. This shows up as non-local resistance, away from the path of charge current.
We integrate both these ways of valley current generation and implement it on dual gated twisted double bilayer graphene device, where the two copies of bilayer graphene have been rotated by 1.18°. We observe large non-local resistance few microns away from local probes. We further demonstrate its tunability with electric field and with charge density. One can thus explore this additional valley degree of freedom to transmit information coherently over distances of few microns in graphene. This may open up new avenues in the emerging field of valleytronics.

*We acknowledge funding from Department of Atomic Energy, India and Department of Science and Technology, India.
XI ZHANG (Presenter), KAN-TING TSAI, YUJIE LUO, KE WANG, University of Minnesota — Ballistic Dirac-Fermion transport across gate-defined PN junctions exhibits strong dependence on incident angle due to the linear dispersion relationship. Multiple experiments have been performed utilizing the angle-dependence of Klein tunneling, in which novel electron-optics concepts including electron collimation [1] and Veselago lensing [2][3] have been demonstrated. Here we demonstrate preliminary experimental observations of quantum interferences based on these concepts. Preliminary transport data across carefully-engineered PN junctions will be presented and quantitative analysis based on Klein-tunneling probability will also be discussed.


NARGESS ARABCHIGAVKANI (Presenter), RATCHANOK SOMPHONSANE, HARHIREA RAMAMOORTHY, GUANCHEN HE, JUBIN NATHAWAT, SHENCHU YIN, BILAL BARUT, State Univ of NY - Buffalo, JONAS FRANSSON, Physics and Astronomy, Uppsala University, JONATHAN P BIRD, State Univ of NY - Buffalo — The transport properties of bilayer graphene are known to be affected by weak localization at low temperatures. In this study, we use differential conductance mapping to explore the transport properties in bilayer graphene at low temperatures, under conditions for which they are influenced by the proximal of the graphene to a ferromagnet (Co). The low-temperature differential conductance is measured around the Dirac point, with the floating Co “gate” both included in, and absent from, the current path. In the latter case the differential conductance shows the characteristic dip that is known to provide a signature of weak localization. With the Co gate in the current path, however, the differential conductance shows a zero-bias anomaly, implying the suppression of the weak localization at certain energies that are insufficient to cause dephasing of the carriers. The presence and the magnitude of the zero-bias anomaly is depending on the carrier concentration in graphene, making it gate controllable.

*National Science Foundation
United States Department of Energy
12:15PM X51.00006: Mini-Dirac cones in AB-stacked graphene in perpendicular electric fields
RYUTA YAGI (Presenter), KOTA HORII, RYOYA EBISUOKA, SHINGO TAJIMA, Graduate School of Advanced Sciences of Matter, Hiroshima University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science — AB-stacked multilayer graphene with number of layers shows semi-metallic band structure arising from the overlap of bilayer-like bands. By conducting low temperature magnetotransport experiments using encapsulated graphene samples with a top and a bottom gate electrode, we observed that mini-Dirac cones are formed in a perpendicular electric field. In zero perpendicular electric fields, Landau level near the charge neutrality point showed structures which are characteristic of semi-metallic band structures. The structure showed significant variations in perpendicular electric fields. The variations of the Landau level structure were interpreted as a formation of levels arising from mini-Dirac cones from numerical calculations of dispersion relations and the Landau levels. The mini-Dirac cones originate from a trigonal warping in the band structure. The perpendicular electric field opens energy gaps between bilayer-like band, and the trigonal warping closes the gaps locally, thereby mini-Dirac cones form.

12:27PM X51.00007: Anomalous Quantum Hall States in Bilayer Graphene*
JUNG-JUNG SU (Presenter), Natl Chiao Tung Univ, CHUN NING LAU, Ohio State University, ALLAN MACDONALD, Physics, University of Texas at Austin — Bernal stacked bilayer graphene has a collection of competing broken symmetry states characterized by flavor-dependent spontaneous valley polarization.[1] The possible states include polarized and unpolarized orbital magnets and various quantum anomalous Hall states. By carefully evaluating the orbital magnetizations of the competing states, we find that the phase diagram is profoundly altered by a B field by favoring states of which its natural filling factor $\nu_N = \sigma_H/(e^2/h)$ is close to the actual filling factor $\nu$, increasingly so as the B field strengthens. We have explored how coupling of orbital magnetization to external B fields is manifested in the dependence of ground state properties on weak gate $V_g$ and magnetic fields $B$ that favor particular states. We construct the ground-state phase diagram of this system, vs. $V_g$ and $B$ at fixed $\nu$, and vs. $V_g$ and $\nu$ at fixed $B$, and obtain excellent agreement with two-point conductivity measurements. This work explains why the $\nu_N = \pm 4$ quantum Hall Effect in bilayer graphene is stable to anomalously weak B fields, and suggests that $\nu_N = \pm 2$ anomalous quantum Hall effects could occur in the absence of a B field in samples of sufficiently high quality.

[1] PRL 106 (15), 156801

*Work in Austin was supported by DOE grant DE- FG02-02ER45958.
12:39PM X51.00008: Electronic Thermal Conductance Suppression in Lightly Doped Bilayer Graphene Measured via Johnson Noise Thermometry*  ARTEM TALANOV (Presenter), JONAH WAISSMAN, MARINE ARINO, Harvard University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, PHILIP KIM, Harvard University — Systems with strongly interacting and correlated electrons can exhibit exotic new physics, such as the hydrodynamics regime, where particles' behavior is best collectively described as a viscous fluid rather than as individual particles. Several such systems have recently been both predicted and shown experimentally to have thermal conductivity enhanced or reduced relative to the near-universal Lorentz value expected from Wiedemann-Franz Law. Bilayer graphene presents a strong candidacy for quantum criticality and hydrodynamics at charge neutrality, where the carrier-carrier Coulomb energy dominates the kinetic energy of quasiparticles. We explore such behavior by measuring the electronic thermal conductivity of bilayer graphene encapsulated in boron nitride and gated by dual graphite gates, with residual density below $3 \times 10^{10}$ cm$^{-2}$. We use our high-frequency Johnson noise thermometry technique to measure the electronic cooling of the electron system, extracting out the thermal conductivity. We observe a large reduction of the thermal conductivity below the Wiedemann Franz Law at electron doping slightly away from charge neutrality. We discuss these results in the context of hydrodynamics.

*NDSEG Fellowship

12:51PM X51.00009: Designing transport properties of graphene nanoribbon junctions*  KRISTIANS CERNEVICS (Presenter), OLEG V. YAZYEV, Ecole Polytechnique Federale de Lausanne — Graphene nanoribbons (GNRs) have recently emerged as promising candidates for next-generation electronic devices, including the realization of all-graphene nanocircuitry. Junctions connecting two or more GNRs are the elementary components of GNR circuits. We systematically address the electronic transport properties of 60°- and 120°-angled junctions connecting a pair of GNR leads of identical width and chirality utilizing tight-binding model calculations. An exhaustive exploration of GNR junctions carried out by screening over 50,000 configurations allows us to formulate general guidelines into engineering transport properties GNR circuits. For instance, we find that 120°-angled junctions with sublattice imbalance have a perfect transmission via a resonant state occurring at zero energy, and thus identified as ideal GNR interconnects.

*Swiss National Science Foundation (grant No. 172534)
1:03PM X51.00010: In-situ TEM observation of suspended graphene during Joule heating process

DONG HOON SHIN, EWHA Woman's Univ, JUN-HEE CHOI, Surface Technology Division, Korea Institute of Materials Science (KIMS), HEENA INANI, KIMMO MUSTONEN, Physics, University of Vienna, HYUNJEONG JEONG, EWHA Woman's Univ, JANI KOTAKOSKI, Physics, University of Vienna, SANG WOOK LEE (Presenter), EWHA Woman's Univ — Dynamic surface modification of suspended graphene at high temperature was observed using in-situ transmission electron microscope (TEM) measurement. The suspended graphene were prepared on top of the SiN membrane with hole substrate so that TEM observation was conducted under Joule heating processes. Current-voltage characteristics of suspended graphene devices inside of TEM chamber were measured to monitor and control the high temperature condition of graphene surface by estimating electrical power on the devices. During the in-situ TEM observation, it was found that residual materials, previously remained on the graphene surface, were removed at high temperature. Dynamic movement of residue on the graphene surface and shrinkage of atomic distance of graphene were also observed while the Joule heating process.

*This work was supported by NRF, FWF, and HFSP

1:15PM X51.00011: Excitonic Condensate Phase in Hybrid double-layer structures

XIAOXUE LIU (Presenter), Department of Physics, Brown University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, CORY DEAN, Department of Physics, Columbia University, JIA LI, Department of Physics, Brown University — In this talk I will present Coulomb transport measurement of exciton condensate phase in a hybrid double-layer structure, where twisted bilayer graphene (tBLG) and monolayer graphene (MLG) are separated by a thin insulating barrier. With a large twist angle, the lowest Landau level in twisted bilayer graphene features eight-fold degeneracy, where each broken symmetry state in the quantum Hall effect regime is described by Landau wavefunction with orbital index N=0 [1]. As such, excitonic pairing across the insulating barrier is expected to be robust over a large phase space, characterized by filling fractions \(n_{\text{MLG}}\) and \(n_{\text{tBLG}}\), along with perpendicular electric field \(D\). Using Coulomb drag measurement, we discovered multiple copies of fully developed exciton condensate phase in both the electron-electron and electron-hole quadrants of the phase space. Over a large filling fraction range, -5 < \(n_{\text{total}}\) < 5, the value of quantized Hall resistance plateaus varies with total filling fraction \(n_{\text{total}}\). Most interestingly, the strength of exciton pairing is shown to be tunable with layer polarization in tBLG. This tunability adds an extra dimension to the phase space, which allows us to investigate the behavior of exciton condensate in a three-component system with three layers of graphene.
1:27PM X51.00012: High-order fractal quantum oscillations in highly doped graphene/BN superlattices* WU SHI (Presenter), SALMAN KAHN, Lawrence Berkeley National Lab and UC Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, MICHAEL F CROMMIE, ALEX ZETTL, Lawrence Berkeley National Lab and UC Berkeley — High temperature quantum oscillations have been reported in graphene/BN superlattices beyond secondary Dirac points both for electron and hole doping [1,2]. These so-called Brown-Zak (BZ) oscillations originate from periodic emergence of delocalized Bloch states in high magnetic field. However, the BZ oscillations is much less visible for hole doping than for electron doping due to strong electron-hole asymmetry. Here, we employed a newly developed electron beam doping technique to induce high electron and hole carrier densities in graphene/BN superlattices while maintaining high mobilities. Enhanced BZ oscillations are observed beyond the third-generation neutrality points at high temperatures. High-order magnetic Bloch states are also seen even for hole doping, demonstrating the effectiveness of our doping technique. Theoretical simulation of the magnetotransport provides qualitative agreement of the carrier density dependence of BZ oscillations with our experimental results.

References:

*This work was supported in part by the U.S. Department of Energy under Contract No. DE-AC02-05-CH11231, within the sp2-Bonded Materials Program (KC2207).

1:39PM X51.00013: Proximity-induced spin-orbit coupling in bilayer graphene/WSe₂ heterostructures probed by quantum Hall measurements DONGYING WANG (Presenter), SHI CHE, GUIXIN CAO, Department of Physics, The Ohio State University, RUI LYU, Department of Physics and Astronomy, University of California, Riverside, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, CHUN NING LAU, MARC W BOCKRATH, Department of Physics, The Ohio State University — The physical properties of 2D materials are highly sensitive to the interface in a van der Waals heterostructure [1], leading to intensive studies into the resulting proximity effects. In particular, significant effort has been made to increase the spin-orbit coupling (SOC) in graphene by coupling it to transition metal dichalcogenides [2]. However, it remains challenging to study high-quality quantum Hall signatures, which acts as a precise probe of SOC strength [3]. Here we report a direct observation of SOC in a bilayer graphene/WSe₂ heterostructure in quantum Hall measurements [4]. A distinct Landau level (LL) crossing pattern emerges when tuning the charge density and displacement field, originating from a layer-selective SOC proximity effect. By analyzing the LL structure, we simultaneously estimate both Ising (~2.2 meV) and Rashba SOC (~15 meV) energy scales, which are consistent with the theoretical predictions of interlayer twist angle dependence. Our study provides a high mobility system with potential to realize novel topological electronic states and manipulate spin in nanostructures.

1:51PM X51.00014: Atypical Quantized Hall Resistances in Millimeter-Scale Epitaxial Graphene $p$-$n$ Junctions  
ALBERT RIGOSI (Presenter), National Institute of Standards and Technology, DINESH PATEL, National Taiwan University, MARTINA MARZANO, INRIM, MATTIAS KRUSKOPF, HEATHER M. HILL, HANBYUL JIN, JIUNING HU, ANGELA HIGHT WALKER, National Institute of Standards and Technology, CHI-TE LIANG, National Taiwan University, MASSIMO ORTOLANO, Politecnico di Torino, LUCA CALREGARO, INRIM, DAVID B NEWELL, National Institute of Standards and Technology — Epitaxial graphene (EG) on silicon carbide (SiC), which grows on hexagonal SiC at high temperatures, can be nearly defect-free on the centimeter scale and exhibits properties that make it suitable for large-scale and high-current applications. We have demonstrated the millimeter-scale fabrication of monolayer epitaxial graphene $p$-$n$ junction devices using simple ultraviolet photolithography, thereby significantly reducing device processing time compared with electron beam lithography typically used for obtaining sharp junctions. This work presents the resulting experimental data obtained from these devices when introducing multiple current inputs in several different configurations. Furthermore, the LTspice circuit simulator is used to examine the various rearrangements of the electric potential in the device when injecting current at up to three independent sites. These measurements yield nonconventional, fractional multiples of the typical quantized Hall resistance at the $v=2$ plateau ($R_H = 12.9$ kΩ) that take the form: $a/b * R_H$. Here, $a$ and $b$ have been observed to take on values such 1, 2, 3, and 5 to form various coefficients of $R_H$. These results support the potential for drastically simplifying device processing time and may be used for many other two-dimensional materials.

2:03PM X51.00015: Spin waves in canted antiferromagnet of bilayer graphene  
HAILONG FU (Presenter), KE HUANG, Pennsylvania State University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, JUN ZHU, Pennsylvania State University — Antiferromagnets are promising candidates for spintronics applications thanks to their high-frequency dynamics and insensitivity to external magnetic field perturbations. The $\nu=0$ quantum Hall state in bilayer graphene supports a canted antiferromagnetic (CAF) phase when a small electric field is applied perpendicular to the plane. This state is predicted to support dissipationless spin transport through a superfluidity mechanism [1]. Previous experiments showed that spin waves can be excited by a finite dc bias on one side of a quantum Hall region and detected on the other side using a non-local transport setup [2, 3]. Here we report on spin wave transport through the $\nu=0$ CAF state of bilayer graphene. In our devices, we observe spin wave excitations with non-zero dc bias thresholds similar to what’s reported [2]. We also observe, in certain measurement setups, strong non-local signals with a dc bias threshold close to zero, only when the $\nu=0$ state is in the CAF phase. We present the temperature, magnetic field, and electric field dependence of the zero-threshold signal and discuss potential origins.

11:15AM X52.00001: Spin Relaxation Times of Copper Phthalocyanine (CuPc) Qubits diluted in Diamagnetic Zinc Phthalocyanine (ZnPc) Host Matrices*  
CHANDLER MERRILL (Presenter), HENNA POPLI, HANS MALISSA, Physics and Astronomy, University of Utah, RYAN STOLLEY, JOEL MILLER, Chemistry, University of Utah, VALY VARDENY, CHRISTOPH M BOEHME, Physics and Astronomy, University of Utah — We report on electron paramagnetic resonance (EPR) measurements of powder CuPc prepared in a solid-state complex, ZnPc. The free electron spin of CuPc constitutes a two-state quantum system that may potentially be a candidate as a quantum bit (qubit) for quantum computing applications [1]. We test whether the CuPc electron spin increases its spin dephasing time, $T_2$, when the exchange interactions between adjacent CuPc qubits is reduced by diluting CuPc molecules in a zinc phthalocyanine (ZnPc) host matrix [2] at concentrations of 0%, 1%, 5%, and 10%, which modifies the average distance between CuPc molecules. ZnPc is a diamagnetic molecule that nominally does not exhibit an EPR signal and, also, the dominant Zn isotopes are I=0. We study the system using continuous wave and pulsed EPR, and we find similar results to previous studies on CuPc in liquid host matrices, $T_2$ on the order of 1 µs observed for both, CuPc as well as another yet unidentified paramagnetic center that is likely due to an admixture to the ZnPc matrix. We also study the temperature dependence of the EPR signals between 5 K and room temperature. [1] M.Warner et. al, Nature, 503, 504(2013). [2] S.Seelan, et. al, Journal of Molecular Catalysis A: Chemical, 168, 61(2001).

*National Science Foundation, NSF-#1836989

11:27AM X52.00002: First Principles Studies of the Structural Evolution of a Dicyanobenzene Molecular Junction with Gold Electrodes  
MO LI (Presenter), JOSHUA YOUNG, New Jersey Inst of Tech, MANUEL SMEU, Physics, Binghamton University — Molecular electronics have attracted attention due to their potential in decreasing the size of transistors to the molecular scale. We present our first principles studies of the structural and electronic properties of a single-molecule dicyanobenzene junction with gold electrodes. Density functional theory (DFT) was used to simulate the formation process of the dicyanobenzene molecular junction by elongating a gold nanowire with a dicyanobenzene molecule placed above a thin gold wire. As the wire was stretched and broken, we found four significant stages of system rearrangement. The molecule first rotated (the first stage) and then gradually slipped into the junction and bonded to the gold atomic tips in three stages. For each stage, we performed calculations using the non-equilibrium Green's function combined with the DFT (NEGF-DFT) method to obtain the electronic transport pathway and the conductance of the molecular junction. We found that after the main transmission channel switches from via the gold bridge to via the molecule, the conductance increases while the junction is elongated, which is due to an interesting alignment between the frontier molecular levels and the Fermi energy of the electrodes.
11:39AM X52.00003: Scanning tunneling microscopy study of atomistic energy level engineering in donor-acceptor molecules  GIANG DUC NGUYEN (Presenter), GARY TOM, Stewart Blusson Quantum Matter Institute, University of British Columbia, CHRISTOPHER M TONGE, ZACHARY M HUDSON, Department of Chemistry, University of British Columbia, SARAH A BURKE, Stewart Blusson Quantum Matter Institute, University of British Columbia — Donor-acceptor materials show highly tunable electronic properties via exchange of the donor and acceptor units, making them appealing for light-harvesting and light-emitting applications. While ab-initio calculations can be used for guidance in molecular design of these complexes, there has been little microscopic characterization of the donor-acceptor electronic interaction at the molecular level. Here we present atomistic energy level engineering in N-heterotriangulence derivatives functionalized with different acceptor units. Individual isolated molecules deposited on Ag(111) substrate were studied with scanning tunneling microscopy (STM). The bond-resolved STM (BRSTM) technique was performed to confirm the molecular structure. We performed STM spectroscopy to obtain the molecular energy levels with the spatial distribution mapping of molecular orbitals respectively. Our STM results are corroborated by density function calculations and macroscopic optical absorption/emission measurements.

11:51AM X52.00004: Temperature and Pressure Dependent Properties of A3Ti2O7* SIZHAN LIU (Presenter), New Jersey Inst of Tech, ELI STAVITSKI, ZHENXIAN LIU, Brookhaven National Laboratory, SUYIN WANG, YU-SHENG CHEN, Argonne National Laboratory, BIN GAO, JAEOOK KIM, SANG-WOOK CHEONG, Rutgers University, SANJIT GHOSE, Brookhaven National Laboratory, TREVOR TYSON, New Jersey Inst of Tech — Theoretical models of the A3Ti2O7 system suggest that electric polarization is due to the combination of the coherent TiO6 octahedral rotation and tilting, both being nonpolar. For the doped A3Ti2O3 systems, different size atoms enable the possibility of site-selective substitution in A’ or A site to tune the TiO6 octahedral rotation and tilting. In this work, a structural study over a broad range of temperatures and pressures has been conducted by x-ray diffraction, Raman spectroscopy, x-ray absorption spectroscopy, x-ray pair distribution function measurements and DFT modeling. The long-range and local symmetries and local atomic and electronic structural changes will be discussed and compared with previous work.

*This work is supported by NSF Grant No. DMR-1809931.
12:03PM X52.00005: Characterizing Cellulose Crystallographic Texture in Plant Cell Walls Using Grazing Incidence X-ray Scattering* SINTU RONGPIPI (Presenter), DAN YE, Department of Chemical Engineering, Pennsylvania State University, WILLIAM JOHN BARNES, SARAH KIEMLE, Department of Biology, Pennsylvania State University, ARTHUR WOLL, Cornell University, Cornell High Energy Synchrotron Source, CHENHUI ZHU, Advanced Light Source, Lawrence Berkeley National Laboratory, CHARLES ANDERSON, DANIEL COSGROVE, Department of Biology, Pennsylvania State University, ESTHER WINTER GOMEZ, ENRIQUE D GOMEZ, Department of Chemical Engineering, Pennsylvania State University — Cellulose, the most abundant biopolymer on earth, is a versatile material with tuneable properties. It exists as semi-crystalline microfibrils in plant cell walls. This crystalline structure is important for plant growth and determines properties of cellulosic materials. However, several aspects of this crystalline structure remain elusive - one of them being orientation of cellulose crystallites. We studied the structure of cellulose in plant primary cell walls through grazing incidence wide angle X-ray scattering (GIWAXS). GIWAXS of cell wall reveal strong texturing of cellulose. The degree of texturing is determined through pole figures constructed from combination of GIWAXS and XRD rocking scans. We find that cellulose texturing depends on developmental age of tissue. GIWAXS of cell wall mutants reveals interactions between wall polysaccharides. We find that cellulose texture is disrupted in pectin and cellulose mutants but not in xyloglucan mutants. These findings provide insights on cellulose crystalline structure which can help design cellulose-like materials and efficient biomass conversion process.

*The work was supported as part of The Center for Lignocellulose Structure and Formation, an Energy Frontier Research Center funded by the U.S. Department of Energy

12:15PM X52.00006: Redesign and Develop Effective Liposomal Formulation for Prodrug Delivery Through Synchrotron X-ray Studies of Molecular Interactions* TIEP PHAM (Presenter), PAOLA LEON-PLATA, PIN ZHANG, CHANG LIU, Chemical Engineering, University of Illinois at Chicago, WEI BU, BINHUA LIN, Institute of Molecular Engineering, University of Chicago, YING LIU, Chemical Engineering, University of Illinois at Chicago — Liposomal formulations may provide advantages for drug delivery to overcome high dose and toxicity issues of anticancer chemotherapy prodrugs such as capecitabine. However, because of the enormous combination and the unique molecular structure of the prodrug, it is difficult to prepare liposomal-capcitabine formulations with high drug loading and long-term stability based on empirical trials.

In this study, we synthesized a capecitabine analogue by conjugating a carbon chain of cetyl chloroformate with 5-fluorouracil (5FU) (5FU-PAL). We optimized the liposomal formulation of 5FU-PAL for prolonged blood circulation and sustained release based on the understanding of molecular packing and interactions of 5FU-PAL and phospholipids at the gas-water interface by employing synchrotron X-ray reflectivity (XR) and grazing incidence X-ray diffraction (GIXD) integrated with a Langmuir trough. It was found that 5FU-PAL interacts strongly with positively charged lipid in the head group region. The studied could precisely quantify the maximum drug loading in the liposomal formulations. It is also found that 5FU-PAL at the air-water interface folded into highly-ordered multiple layer structures.

*NSF
Long-Term Performance Prediction of Mixed Matrix Membranes at Different Adsorbent Dose and Operating Conditions*  
RAKA MONDAL (Presenter), Chemical Engineering, Indian Institute of Petroleum and Energy, Vizag — Mixed matrix membranes (MMMs) with nanoparticles showing adsorption property of small sized solute can find wide application in large-scale water purification. The breakthrough behavior of the membrane dictates its life indicating need for regeneration or eventual replacement. A two-dimensional transient model was developed using equations of continuity, motion and convective-diffusive-adsorption based solute transport. The governing partial differential equations has been solved using finite element method by COMSOL v5.3® software package. The model was verified for adsorptive removal of chromium(VI) from synthetic solution using graphene oxide incorporated MMM hollow fibers. The model parameters were evaluated using experimental data of long-term filtration the solution with respect to throughput and rejection characteristics. The validated model was extended for simulation of large-scale filter interrelating feed concentration, adsorbent dose, trans-membrane pressure drop and cross flow rates. From the simulation, at a fixed operating condition, a performance curve was generated linking and breakthrough volume of the MMMs. It can be extended for design of any large-scale hollow fiber MMM based filtration system.

*Indian Institute of Petroleum and Energy, Visakhapatnam, India

Time-dependent mechanical response of ice adhesion on metal substrates*  
MARINA MACHADO DE OLIVEIRA (Presenter), Chemical Engineering, University of Wyoming, JOSEPH R MURPHY, WILLIAM RICE, Physics, University of Wyoming, JOHN ACKERMAN, VLADIMIR ALVARADO, Chemical Engineering, University of Wyoming — Ice adhesion on aerospace-relevant materials is both complex and poorly understood. Measuring and understanding the underlying physics requires reliable testing techniques that can yield multifaceted datasets. The latter includes surface morphology (i.e., roughness and its spatial correlation structure), resolving substrate-induced strain, and direct mechanical testing of adhesion. Our initial creep test data using a stress-controlled rheometer showed an apparent adhesion dependence on both surface roughness and temperature: namely, that the adhesion strength is higher for rougher surfaces and seems to increase with temperature. To shed light on these initial findings, we performed time-dependent stress ramps from -20 to -7°C to determine the dynamical stress relaxation mechanism. Additionally, we investigated the spatial correlation surface roughness maps for aluminum specimens. Stress-ramp results confirmed a connection between surface roughness and apparent adhesion. Moreover, the creep-test behavior appears to represent an upper bound of the time-dependent adhesive behavior of ice. These results take us a step forward to understanding ice adhesion mechanisms.

*We acknowledge funding support from NASA Grant WY-80NSS17M0049
12:51PM X52.00009: Electrical Measurement of Water Assisted Ion Desorption and Solvation on Isolated Carbon Nanotubes  PATRICK EDWARDS (Presenter), BO WANG, Physics, University of Southern California, STEVE CRONIN, Electrical Engineering, University of Southern California, ADAM W. BUSHMAKER, Physical Sciences Laboratories, The Aerospace Corporation — With continued reduction in the feature size of device structures we are quickly approaching the one-dimensional limit of electrical conduction. In this regime it becomes increasingly important to study the effects of individual dopants and defects on device performance. Recent studies on the electrical properties of suspended carbon nanotube field-effect transistors (CNT-FETs) have revealed extreme sensitivity in device conductivity in the presence of individual gaseous ions adsorbed at the nanotube surface. We will present an investigation on the mean residence time of gaseous ions adsorbed on the surface CNT-FETs with and without native surface water layers that exist in atmospheric conditions. Devices dehydrated by various methods were all found to have substantially higher mean ion residence times. We propose that native water molecules in ambient conditions provide a reduction pathway for incoming gaseous ions, yielding Hydronium ions ($\text{H}_3\text{O}^+$). We characterize the interaction between these ions with the CNT-FET surface via large switching events in device conduction and compare to measurements taken on desiccated devices.

1:03PM X52.00010: Enhancing Superionic Conductivity in Cluster-Based Sodium-Rich Antiperovskites  HONG FANG (Presenter), PURUSOTTAM JENA, Virginia Commonwealth Univ — Sodium (Na) superionic conductors are the key to developing next-generation solid-state batteries with safety and low cost. However, most of the known Na-conductors exhibit limited ionic conductivities at room temperature (RT), hindering their practical applications. To meet the challenge, a series of Li- and Na-rich antiperovskite superionic conductors based on cluster ions (e.g. $\text{BH}_4^-$ and $\text{BCl}_4^-$) have been theoretically developed [e.g. Fang et al. PNAS 114, 11046, 2017; ACS App. Mat. Inter. 11, 963, 2018]. These materials exhibit superior properties as solid electrolytes with greatly enhanced ionic conductivities at RT. One cluster-based solid electrolyte of such, $\text{Na}_3\text{O(BH)}_4$, has been successfully synthesized for the first time most recently and its measured RT ionic conductivity is well above $10^{-3}$ S/cm which is four orders of magnitude higher than that of its halogen counterparts Na$_3$OX (X = Cl, Br, I) [Sun et al. J. Am. Chem. Soc. 141, 5640, 2019]. In this work, we aim to further enhance the ionic conductivity of the Na-superionic conductor by using chemical mixing according to the size effect. The study further shows the advantage of utilizing cluster ions as building blocks, introducing additional degrees of freedom into tuning the properties of superionic conductors.

1:15PM X52.00011: Absorption spectra and density of states of cubic Frenkel exciton system with Gaussian diagonal disorder*  ABDELKRIM BOUKAHIL (Presenter), Physics Department, University of Wisconsin - Whitewater, NOUREDINE ZETTILI, Department of Physical and Earth Sciences, Jacksonville State University — We used the coherent potential approximation to investigate the density of states and the optical absorption of Frenkel exciton systems in cubic lattices with nearest neighbor interactions and a Gaussian diagonal disorder. Our results for the simple cubic are in good agreement with previous investigations using finite-array calculations.

*A.B. acknowledges support from the University of Wisconsin-Whitewater.
Flexible bimodal photoemission electron source based on Au-coated fiber optic nanotips

SAM KERAMATI (Presenter), University of Nebraska - Lincoln, ALI PASSIAN, Oak Ridge National Laboratory and University of Tennessee, VINEET KHULLAR, Oak Ridge National Laboratory, JOSHUA BECK, CORNELIS UITERWAAL, HERMAN BATELAAN, University of Nebraska - Lincoln — Ultrashort laser-driven coherent electron sources based on nanotip needles have been studied motivated by their desired properties for ultrafast electron diffraction and microscopy, electron point projection microscopy, etc. While the conventional schemes require focusing the fs laser beam on or near the apex of a nanotip, which is prone to misalignment and unwanted scattering, we demonstrate and characterize a nanotip electron source based on tapered optical fibers coated with Au on one end. Our theoretical analysis followed by detailed experiments at a range of visible wavelengths confirm that the observed nonlinear electron emission is assisted by surface plasmon excitation in the metallized fiber taper. Fiber tips leverage over the conventional tips in two major ways: 1) They are alignment-free by end-fire coupling, 2) They emit not only using ultrashort pulsed lasers but also by low-power CW diode lasers in the long wavelength regime. The fiber tips are useful where back-illumination or raster scanning an electron source is needed as in electron nanolithography using a single fiber or a bundle for parallel processing.

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Investigation of multicolored and white light emission from IR-excited nano-particles

LIDONG MA (Presenter), BALDASSARE DI BARTOLO, Boston College — The search for multicolored light produced by some IR laser-excited luminescent nano-powders has revealed, for laser power exceeding a threshold value, the emission of white light (WL) with black-body characteristics. We are directing our research to the study of the physical parameters that may influence the threshold power of the laser and the efficiency of the WL emission.

A typical compound that we are investigating consists of nano-powders of SrZrO3 doped with Yb. The parameters of relevance include Yb concentration, pressure, temperature, size of nano-crystals, exciting power and wavelength of the laser, dynamical parameters such as decay and build-up patterns.

The aim of this research is both theoretical and experimental: theoretical for I will try to uncover the mechanism of the WL production and experimental for the possible application as efficient light sources of systems similar to the ones that we will investigate (oxide nano-powders doped with lanthanide or transition metal ions).

The “new” light sources in the market (fluorescence lights sources, and LED lamps) beat the Edison bulbs in efficiency, but they do not produce the black-body emission of the Edison bulbs that is most pleasing to the eye.
On-and-off chip magnetic cooling for semiconductor nanostructures below 1 mK*  

DOMINIK ZUMBUHL, MOHAMMAD SAMANI (Presenter), University of Basel — Magnetic cooling has the potential to make the regime beyond dilution refrigerators and below 1 mK accessible to experiments, to investigate interesting novel physics such as exotic quantum phases, new (topological) quasi particles and unprecedented quantum coherence, e.g. in quantum transport. In Basel, the strategy is to cool each of the sample wires with its own, separate demagnetization refrigerator and to simultaneously provide on-chip cooling. This approach reduces external heat leaks (off-chip cooling) and provides local cooling (on-chip) where it’s most effective.

This strategy has proven highly successful in metallic Coulomb blockade thermometers, where temperatures below 1 mK were recently demonstrated. Efforts in semiconductors such as 2D gases and nanostructures are underway, integrating ideas such as large metallic reservoirs on low-resistance ohmic contacts and metallic back gates for on-chip cooling. Semiconductor noise of typical micro-eV scale (corresponding to 10s of mK) presents a serious obstacle for on-chip thermometry. We are exploring methods which are insensitive to charge-noise and employ these as integrated on-chip microkelvin thermometers.

*Supported by Swiss NSF, Swiss Nanoscience Institute SNI, and the European Microkelvin Platform (EMP).

A realistic dimension-independent approach for charged defect calculations in semiconductors  

HUI-XIONG DENG (Presenter), JUN-WEI LUO, Institute of Semiconductors, SUHUAI WEI, Beijing Computational Science Research Center — First-principles calculations of charged defects have become a cornerstone of research in semiconductors and insulators by providing insights into their fundamental physical properties. But current standard approach using the so-called “jellium model” has encountered computational difficulty for low-dimensional semiconducting materials. In this presentation, we propose a physical, straightforward, and dimension-independent universal model to calculate the formation energies of charged defects in both three-dimensional (3D) bulk and low-dimensional semiconductors. This realistic model reproduces the same accuracy as the traditional jellium model for most of the 3D semiconducting materials, and remarkably, for the low-dimensional structures, it is able to cure the divergence caused by the artificial long-range electrostatic energy introduced in the jellium model, and hence gives meaningful formation energies of defects in charged state and transition energy levels of the corresponding defects. Our realistic method, therefore, will have significant impact for the study of defect physics in all low-dimensional systems including quantum dots, nanowires, surfaces, interfaces, and 2D materials.

Friday, March 6, 2020 11:15 AM - 1:51 PM

Session X53 DCMP: Superconducting, Electronic and Chemical Properties of 2D Materials Mile High Ballroom 1F - Amber McCreary, National Institute of Standards and Technology
11:15AM X53.00001: Andreev Reflection in Pseudospin-1 System*  XIAOLONG FENG
(Presenter), YING LIU, YEE SIN ANG, SHENGYUAN YANG, Singapore University of Technology and Design — An incoming electron can be reflected as a hole at a normal-metal (N)/superconductor (S) interface, known as Andreev reflection. And a perfect Andreev reflection is predicted at two-dimensional metal/s-wave superconductor interface. Compared with previous models in which the N sides are of two-dimensional electron gas and graphene, we find a perfect Andreev reflect with a larger incident angle allowed at pseudospin-1 metal/s-wave superconductor interface. Additionally, an all-angle perfect Andreev reflection occurs in the limits. To support our discoveries, we study the differential conductance which can be observed directly in experiments.

*This work was supported by Singapore Ministry of Education Academic Research Fund Tier 2 (Grant No. MOE2017-T2-2-108).

11:27AM X53.00002: Tunneling spectroscopy as a probe of fractionalized excitations in RuCl3/graphene stacks*  ALESSANDRO PRINCIPI (Presenter), Physics and Astronomy, University of Manchester, MATTEO CARREGA, NEST, Istituto Nanoscienze, Consiglio Nazionale delle Ricerche — Recent studies of alpha-RuCl3 have spurred a significant deal of interest. This material is predicted to well approximate a Kitaev quantum spin liquid, a topologically-ordered state that supports fractionalized spin excitations. Several experimental studies have focused on large bulk samples, while few of them have dealt with lateral transport in proximity to thin multilayers finding unexpected results. In this work, we model the electron tunnelling through thin alpha-RuCl3 samples encapsulated with graphene and study signatures of fractionalised excitations in spin-unpolarized tunnelling currents. Since such devices can be produced by several labs in the world, our aim is to validate tunnelling spectroscopy as a tool to address the intriguing physics at play in thin alpha-RuCl3 multilayers.

*A.P. and M.C. acknowledge support via the Royal Society International Exchange IES\R3\170252
11:39AM X53.00003: On-Chip Strain Enhanced Superconductivity in 1T'-MoTe₂* TARA PENA (Presenter), WENHUI HOU, AHMAD AZIZIMANESH, Electrical and Computer Engineering, University of Rochester, CARLA WATSON, Physics and Astronomy, University of Rochester, ARFAN SEWAKET, STEPHEN M WU, Electrical and Computer Engineering, University of Rochester — Two-dimensional transition metal ditellurides have been found to have unique electronic/structural phase transitions with respect to strain. Bulk Weyl semimetal 1T'-MoTe₂ has been shown to exhibit enhanced superconductivity from the nominal value of 100 mK up to 7 K under applied hydrostatic pressure. In this work, we explore the use of on-chip thin film stress capping layers to achieve the same effect from in-plane strain on exfoliated 1T'-MoTe₂. These stress capping layers are analogous to the SiNₓ capping layers used in industrial strained silicon processes. We examine 1T'-MoTe₂ channels under various thin film stressors and observe superconducting onsets at temperatures as high as 4 K. Devices are sensitive to both geometry and stressor layer composition. Control devices eliminate the potential of this effect arising from defect formation or unintended doping. Challenges related to low-temperature thin film strain transfer, and thermal matching of the stressor layers will be explored. Upon further optimization and standardization, this technique can be used to explore the superconducting phase diagram of MoTe₂ with respect to strain, temperature, and thickness.

*Work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE-1939268.

11:51AM X53.00004: Unconventional Superconductivity in Semiconductor Artificial Graphene* TOMMY LI (Presenter), Freie Univ Berlin, HARLEY SCAMMELL, Harvard University, JULIAN P INGHAM, Boston University — Unconventional superconductivity featuring large pairing energies has attracted immense interest, yet tractable microscopic theories have proven elusive. A major breakthrough has been the advent of twisted bilayer graphene (TBG), which serves as a simple model system to `look under the hood' of unconventional superconductivity. We propose a new model, within current experimental reach, to investigate the microscopics of strong-binding superconductivity. Our proposed device is semiconductor artificial graphene, a two dimensional electron gas overlaid with a periodic potential. We demonstrate that this system realises a new mechanism for pairing, whereby the topology of the Dirac points gives rise to an attraction in the \( p + ip \) channel. The pairing interaction, which originates from charge dynamics on the interlocking sublattices, dominates due to antiscreening, and -- in contrast to graphene -- can be strongly enhanced through device engineering. The unconventional superconducting gap provides a realisation of a Fulde-Ferrell-Larkin-Ovchinnikov state. The pairing strength is similar to TBG, and within the accuracy of our calculations we find \( T_c \) up to 20 K for InAs heterostructures.

*This work was funded by the Danish National Research Foundation and Microsoft Station Q.
12:03PM X53.00005: Structural, Topological, and Superconducting Properties of 2D Tellurium Allotropes from \textit{ab initio} Predictions*  
CHUNYAO NIU (Presenter), CHUNXIANG ZHAO, Zhengzhou University, Zhengzhou 450001, China, XIAOLIN CAI, Henan Polytechnic University, Jiaozuo 454000, China, YU JIA, Zhengzhou University, Zhengzhou 450001, China, ZHENYU ZHANG, University of Science and Technology of China, Hefei 230026, China — 2D Tellurium, will extended the realm of two-dimensional (2D) materials to group-VI elements beyond the discovery of graphene, phosphorene, and borophene, and it will provide new candidates for next-generation electronic and optoelectronic device applications. Through the particle-swarm optimization searches combined with \textit{ab initio} calculations, we further predict 31 novel stable 2D tellurium allotropes with various geometric structures which sorted by different thickness of atomic layers (termed as M-α, B-α, T-α, T+α, and so on). Their thermodynamic stabilities have been carefully verified by the phonon modes calculations. We show that four (the B-α, B-β, B-γ, and B-η phases) exhibit topological insulators, and three (B-β, B-ε and T-κ phases) are intrinsic superconductors with Tc ~8 K. Interestingly, B-β phase possesses both topological and superconducting properties, which is the 2D monolayer material that have such intrinsic properties and may provide an appealing platform for exploring topological superconductivity in 2D systems.

*This work was supported by NSF of China (Nos. 11504332 and 11774078).

12:15PM X53.00006: Proximity induced spin-orbit splitting in graphene nanoribbons on transition metal dichalcogenides*  
ENRICO ROSSI (Presenter), SATRIO GANI, ERIC J WALTER, Physics, William & Mary — We study the effect of transition metal dichalcogenides (TMD) on the electronic structure of graphene nanoribbons (GNRs) from first-principles. We consider both semiconducting TMDs and metallic TMDs and different stacking configurations. We find that when the TMD is semiconducting the effects on the band structure of the GNRs are small. In particular the spin-splitting induced by proximity on the GNR's bands is only of the order of few meV irrespective of the stacking configuration. When the TMD is metallic, such as NbSe2, we find that the spin-splitting induced in the GNRs can be very large and strongly dependent on the stacking configuration. For optimal stacking configurations the proximity-induced spin-splitting is of the order of 20 meV for armchair graphene nanoribbons, and as high as 40 meV for zigzag graphene nanoribbons. This results are encouraging for the prospect of using GNR-TMD heterostructures to realize quasi one-dimensional topological superconducting states.

*Work supported by NSF Grant No. DMR-1455233 CAREER, ONR Grant No. ONR-N00014-16-1-3158, ARO Grant No. W911NF-18-1-0290, and BSF Grant No. 2016320.
12:27PM X53.00007: Electron-electron interactions, valleys, and band nesting in gated MoS$_2$ quantum dots. LUDMILA SZULAKOWSKA (Presenter), University of Ottawa, MACIEJ BIENIEK, Wroclaw University of Science & Technology, PAWEL HAWRYLAK, University of Ottawa. We report on the effect of valley, spin and band nesting on the many-electron properties of gated MoS$_2$ quantum dots. We start with single electron atomistic calculation for a computational box with periodic boundary conditions containing up to $10^6$ atoms, using a tight binding model developed from ab-initio methods for MoS$_2$ [1,2]. The effect of the metallic gates is modelled as a parabolic lateral confining potential. We find a twofold degenerate energy spectrum of confined electrons originating from the two non-equivalent valleys K and -K as well as a sixfold degenerate ladder of states associated with six secondary conduction band minima Q [3]. These electronic states up to 5 K-derived shells are then populated with up to 6 electrons and electron-electron interactions are turned on. We demonstrate that the large intra-valley exchange interaction determines the many-electron ground state of these QDs. As a consequence, with varying QD size and confining potential, a valley-polarized and spin-polarised broken symmetry ground states emerge.


12:39PM X53.00008: Ultra-thin van der Waals crystals as semiconductor quantum wells* JOHANNA ZULTAK (Presenter), SAMUEL MAGORRIAN, VLADIMIR FAL’KO, ROMAN GORBATCHEV, Univ of Manchester. Control over the electronic spectrum at low energy is at the heart of the functioning of modern advanced electronics which highly relies on meticulous engineering of the size quantization of electrons in quantum wells. This avenue hasn’t yet been explored in 2D materials. Here we transfer this concept onto the van der Waals heterostructures which utilize few-layers films of InSe as quantum wells. Precise control over the energy of the subbands and their uniformity guarantees extremely high quality of the electronic transport in such systems. Using novel tunnelling and light emitting devices, we reveal the full subbands structure by studying resonance features in the tunnelling current, photoabsorption and light emission. [1]


*This work was supported by the European Graphene Flagship Project (696656) and European Quantum Technology Flagship (820378) and the Royal Society.
Observation of tunable plasmons in large area type-II Weyl semimetal films*  CHONG WANG (Presenter), SHENYANG HUANG, QIAOXIA XING, GUOWEI ZHANG, FANJIE WANG, YANGYE SUN, YUANGANG XIE, YUCHEN LEI, ZHENGZONG SUN, HUGEN YAN, Fudan Univ — The observation of the highly tunable and confined plasmons in Graphene has stimulated the exploration of plasmons in other 2D materials. Here, for the first time, plasmonic resonance modes are observed in CVD-grown large area films of WTe$_2$, which is known as a type-II Weyl semimetal, by far-infrared absorption spectroscopy. Plasmon-phonon hybridization is revealed by mapping the plasmon dispersion on Si/SiO$_2$ substrates. The plasmon frequency is tunable by changing the temperature and film thickness. Moreover, the plasmon modes are still observable with film thickness down to 8 nm, indicating the potential for tuning by gate. Our results represent a first look at the plasmon in large area CVD-grown Weyl semimetal films and suggest a practical platform to experimentally study the topological plasmons.

*the National Natural Science Foundation of China (Grant No. 11704075) and China Postdoctoral Science Foundation.

The Origin of Hydrophilicity on 1T'-MoS$_2$  LAURA NICHOLS, XIAO SHEN (Presenter), Univ of Memphis — Single-layer MoS$_2$ has been shown to excel in many applications like as a catalyst, supercapacitor, transistor, and biosensor. It has been shown that there is a correlation between the catalytic activity and the metallic character of the surface. Consequently, the metallic phase of MoS$_2$ has been shown to surpass the performance of the semiconducting phase. However, the metallic phase is less energetically favorable than the semiconducting 2H phase, and it is unstable in air. Recently, it has been shown that a metallic phase of MoS$_2$ is stable in water. This metallic phase is also found to be hydrophilic which provides additional advantages in applications as a supercapacitor or biosensor. We attribute this metallic phase to 1T'-MoS$_2$ and investigate the origin of the hydrophilic behavior. Through first-principles calculations, we found that, with a sulfur vacancy on the surface, dissociative adsorption of a water molecule is favorable only on the 1T' surface. The water dissociation on the surface not only increases the hydrophilicity of the surface, but it also explains the enhanced stability of 1T'-MoS$_2$ in water by reducing the energy difference between the 1T' and 2H phases.
**1:15PM X53.00011: Metal-based nanomats as catalysts for self-oscillating Belousov-Zhabotinsky reactions**

**VISHESH SHARMA** (Presenter), **KABEER JASUJA**, **PRATYUSH DAYAL**, Indian Inst of Tech Gandhinagar — Chemical reactions exhibiting self-sustained oscillations have been used to replicate “life-like” characteristics in various synthetic systems. Belousov-Zhabotinsky (BZ) reactions are such reactions that exhibit a periodic color change of the solution, facilitated by oxidation and reduction of the metal-ion catalyst. Recently, we have shown that by using 0D-2D heterostructures as catalytic mats, specifically graphene-based nanosheets decorated with Ce or Ru nanoparticles, the frequency of oscillations for the BZ reactions are significantly enhanced. Here, however, we establish that bare metal nanosheets can also be used to catalyze BZ reactions. In particular, we show that when bare Ceria and Ru nanosheets are used as catalysts for BZ reactions, the oscillations change depending upon the presence of oxy-functional groups. Also, we designed hybrid 0D-2D metal catalysts, decorating Ce and Ru NPs on respective Ru and Ce nanosheets. Our experiments reveal that the frequency of oscillations is dependent on the conductivity of the bare metal nanosheets and the NP loading. Although our work focusses on BZ reactions, our findings open up new avenues to tune characteristics of dynamical systems through the use of catalytic nanomaterials.

*DST-SERB, Project No. EMR/2016/007778* for funding.

**1:27PM X53.00012: Stable out-of-plane piezoelectric group-IV monochalcogenide monolayers with a buckled honeycomb structure**

**SHIVA POUDEL** (Presenter), **SALVADOR BARRAZA-LOPEZ**, Physics, Univ of Arkansas-Fayetteville — We used DFT to study 12 group-IV monochalcogenide monolayers MX (M=Si, Ge, Sn, Pb and X =S, Se, Te) with a 2-fold degenerate honeycomb structure. The exchange of M and X atoms yields a two-fold degenerate structure and the bucking of atoms in the unit cell provides a thickness Δz and an out-of-plane electric polarization. A 2D structural phase transformation is discussed from the perspective of elastic energy barriers J \[1,2,3,4\]; J is the smallest energy required to change the buckled unit cell (Δz>0) onto a planar unit cell (Δz=0). These materials will not undergo a 2D phase transformation. For comparison, silicene has a similar structure and a lower J and undergoes the 2D structural transformation \[5\]. This study increases the understanding of relationships among the structure, ferroelectric behavior, and structural phase transformations in 2D materials with structural degeneracies.

References:
2. T. Bishop et al., *PRL* 122, 015703 (2019)
4. S. P. Poudel et al., under review

*Work funded by the DOE (DE-SC0016139). Calculations were performed on Cori at NERSC (DE-AC02-05CH11231) and Trestles at Arkansas.*
1:39PM X53.00013: A spectrum of exfoliable 1D van der Waals materials and their electronic properties*  
YANBING ZHU (Presenter), Stanford University, DANIEL A REHN, Los Alamos National Laboratory, EVAN ANTONIUK, GOWOON CHEON, RODRIGO MOURA FREITAS, ADITI KRISHNAPRIYAN, EVAN J. REED, Stanford University — Data-mining efforts suggest there are hundreds of bulk materials with the potential to be exfoliated into one-dimensional (1D) structures. We combine data-mining with DFT calculations to elucidate the properties of 1D wires. We identify several materials that have the potential to be more readily exfoliable than the commonly studied 1D-like materials tellurium and selenium and examine the bulk and single-wire electronic characteristics. While layered materials have received significant attention, their 1D van der Waals counterparts have received relatively small amounts, yet are likely to have many of the same qualities that make layered materials of interest for a number of applications.

*This work was supported by NSF Grant DMREF-1174625

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X56 DCMP: Electronic Charge and Orbital Ordering  Mile High Ballroom

2C - Zhengqian Cheng, Columbia Univ

11:15AM X56.00001: Role of Coulomb correlations in the charge density wave of CuTe
SOORAN KIM (Presenter), Kyungpook National University, BONGJAE KIM, Kunsan National University, KYOO KIM, Max Planck POSTECH/Korea Research Initiative — A quasi-one-dimensional layered material CuTe undergoes a charge density wave (CDW) transition in Te chains with a modulation vector of \( q_{\text{CDW}} = (0.4, 0.0, 0.5) \). Here, using first-principles calculations, we demonstrate that the correlation effect of Cu is critical to stabilizing the 5 × 1 × 2 modulation of Te chains. The phonon calculation with the strong Coulomb correlation exhibits the imaginary phonon frequency at \( q_{\text{ph0}} = (0.4, 0.0, 0.5) \), indicating the structural instability. The corresponding lattice distortion of the soft mode agrees well with the experimental modulation. These results demonstrate that the CDW transition in CuTe originates from the interplay of the Coulomb correlation and electron-phonon interaction. Furthermore, we investigated the stability of the CDW state in a CuTe monolayer, Similarly to its bulk structure, we find the phonon soft mode at \( q = (0.4, 0.0) \), indicating structural instability, which only appears with the correlation effect on Cu. Interestingly, by reducing the interlayer interactions, tuning of the CDW modulation may be possible, as demonstrated by the modulation pattern in quasi-one-dimensional Te chains being different from that in the bulk counterpart.

Reference
**11:27AM X56.00002: Optical Enhancement of Superconductivity via Targeted Destruction of Charge Density Waves**

HOSSEIN DEHGHANI (Presenter), ZACHARY RAINES, VICTOR GALITSKI, MOHAMMAD HAFEZI, UMD, Joint Quantum Institute — It has been experimentally established that the occurrence of charge density waves is a common feature of various under-doped cuprate superconducting compounds. The observed states, which are often found in the form of bond density waves (BDW), often occur in a temperature regime immediately above the superconducting transition temperature. Motivated by recent optical experiments on superconducting materials, here, we propose a new approach for the enhancement of superconductivity by the targeted destruction of the BDW order. Since BDW states are usually found in competition with superconductivity, suppression of the BDW order enhances the tendency of electrons to form Cooper pairs after reaching a steady-state. By investigating the optical coupling of gapless, collective fluctuations of the BDW modes, we argue that the resonant excitation of these modes can melt the underlying BDW order parameter.

*This research was supported by supported by US- ARO (contract No. W911NF1310172) (Z.R.), NSF DMR-1613029, DARPA DRINQS project FP-017, “Long- term High Temperature Coherence in Driven Superconductors,” and Simons Foundation (V.G.), and AFOSR FA9550-16-1-0323, ARO W911NF-15-1-0397, and NSF Physics Frontier Center at the Joint Quantum Institute (H.D. & M.H.).

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**11:39AM X56.00003: Charge density waves in a quantum plasma**

ZHAOYU HAN (Presenter), Department of Physics, Stanford University, SHIWEI ZHANG, Center for Computational Quantum Physics, Flatiron Institute, XI DAI, Physics Department, Hong Kong University of Science and Technology — We analyze the instability of an unpolarized uniform quantum plasma consisting of two oppositely charged fermionic components with varying mass ratios against charge and spin density waves. Using density functional theory, we treat each component with the local spin density approximation and a rescaled exchange-correlation functional. Interactions between different components are treated with a mean-field approximation. In both two and three dimensions, we find leading unstable charge density wave modes in the second-order expansion of the energy functional, which would induce the transition to quantum liquid crystals. The transition point and the length of the wave vector are computed numerically. Discontinuous ranges of the wave vector are found for different mass ratios between the two components, indicating exotic quantum phase transitions. Phase diagrams are obtained, and a scaling relation is proposed to generalize the results to two-component fermionic plasmas with any mass scale. We discuss the implications of our results and directions for further improvement in treating quantum plasmas.
**11:51AM X56.00004: A Quantum Monte Carlo Study of the Effect of Strain on Charge Density Wave Order in the Holstein Model**

BENJAMIN COHEN-STEAD (Presenter), RICHARD THEODORE SCALETTAR, University of California, Davis, NATANAEL C. COSTA, International School for Advanced Studies, EHSAN KHATAMI, San Jose State University — We investigate charge ordering in the Holstein model in the presence of anisotropic hopping, $t_x t_y = (1-\delta)(1+\delta)$, as a model of the effect of strain on charge density wave (CDW) materials. Using Quantum Monte Carlo simulations, we show that the CDW transition temperature is relatively insensitive to moderate anisotropy $\delta \leq 0.3$, but begins to decrease more rapidly at $\delta \geq 0.4$. However, the density correlations change significantly for moderate $\delta$. Accompanying mean-field theory calculations show a similar qualitative structure, with the transition temperature relatively constant at small $\delta$ and a more rapid decrease for larger strains. We also obtain the density of states $N(\omega)$, which provides clear signal of the charge ordering transition at large strain, where finite size scaling of the charge structure factor is extremely difficult because of the small value of the order parameter.

*The work of B.C-S. and R.T.S. was supported by the Department of Energy under grant de-sc0014671. N.C.C. was supported by the Brazilian funding agencies CAPES and CNPq. E.K. and from the NSF Grant No. MR-1609560. Computations were performed in part on Spartan high-performance computing facility at San Jose State University, which is supported by the NSF under Grant No. OAC-1626645.

**12:03PM X56.00005: Charge Density Waves on a Decorated Honeycomb Lattice**

CHUNHAN FENG (Presenter), University of California, Davis, HUAIMING GUO, Beihang University, RICHARD THEODORE SCALETTAR, University of California, Davis — Tight binding models like the Hubbard Hamiltonian are most often explored in the context of uniform intersite hopping $t$. The electron-electron interactions, if sufficiently large compared to this translationally invariant $t$, can give rise to ordered magnetic phases and Mott insulator transitions, especially at commensurate filling. The more complex situation of non-uniform $t$ has been studied within a number of situations, perhaps most prominently in multi-band geometries where there is a natural distinction of hopping between orbitals of different degree of overlap. In this paper we explore related questions arising from the interplay of multiple kinetic energy scales and electron-phonon interactions. Specifically, we use Determinant Quantum Monte Carlo to solve the Holstein Hamiltonian on a \`decorated honeycomb lattice', consisting of hexagons with internal hopping $t$ coupled together by $t'$. This modulation of the hopping introduces a gap in the Dirac spectrum and affects the nature of the topological phases. We determine the range of $t/t'$ values which support a charge density wave phase about the Dirac point of uniform hopping $t = t'$ as well as the critical transition temperature $T_c$.

*CHF and RTS were supported by DOE grant DE-SC0014671. HG was supported by NSFC grant No. 11774019.
12:15PM X56.00006: Charge-density-wave melting in the one-dimensional Holstein model*
JAN STOLPP (Presenter), Institut for Theoretical Physics, Universität Göttingen, JACEK HERBRYCH, Wroclaw University of Science and Technology, FLORIAN DORFNER, Arnold Sommerfeld Center for Theoretical Physics, Universität München, ELBIO DAGOTTO, Department of Physics and Astronomy, University of Tennessee and ORNL, FABIAN HEIDRICH-MEISNER, Institut for Theoretical Physics, Universität Göttingen — We study the real-time dynamics in the half-filled Holstein model starting from different initial states that are charge-density-wave (CDW) ordered. The regime where the relaxation dynamics is dominated by electron-phonon coupling is considered (complementary to the case studied in [1] where strong electron interactions were present) and we focus on the far-from-equilibrium regime. Here, a clear separation of time scales between electron relaxation and phonon equilibration is identified. In the transient dynamics we observe effects like a temporal self trapping of the electrons. The study of such regimes is enabled by extending the time-evolving block decimation algorithm with local basis optimization, previously applied to single-polaron dynamics [2], to a half-filled system.


*DFG (Deutsche Forschungsgemeinschaft) Research Unit FOR 1807 and SFB 1073, Polish National Agency of Academic Exchange (NAWA), US Department of Energy (DOE)

12:27PM X56.00007: Tuning of physical properties through chemical intercalation in two dimensional Fe_xNbTe_2
SHENG LI (Presenter), HANLIN WU, University of Texas at Dallas, KEITH TADDEI, Oak Ridge National Laboratory, XIQI WANG, University of Houston, GARETH A OFENSTEIN, University of Texas at Dallas, CLARINA RELOJ DELA CRUZ, Oak Ridge National Laboratory, LI YANG, Washington University in St. Louis, BING LV, University of Texas at Dallas — The layered materials with weak van der Waals interlayer interaction have created a rich platform to exhibit exotic properties such as charge density wave (CDW), topological properties, 2D magnetism, and superconductivity. NbTe_2 is a layered materials with the same structure as 1T' WTe_2 phase. It has a CDW transition above 550K, and meanwhile exhibits superconducting transition below 0.74K. By intercalation of magnetic iron atoms, we are expecting to observe the interplay among superconductivity, CDW and magnetism in this NbTe_2 system. Indeed, through manipulation of the synthetic conditions, we observed drastic changes of crystal symmetry and physical properties in the same material Fe_xNbTe_2 with ground state from spin glass insulator to antiferromagnetic metal down to 2K, with more exotic magnetoresistivity and Hall behavior observed. The details of these results will be presented and the interplay of multiple orders in this system will be further elaborated.
12:39PM X56.00008: Unity-order refractive index tunability at room temperature in 1T-TaS$_2$, a strongly correlated material  WEIJIAN LI, MING YI, KEVIN F KELLY, GURURAJ NAIK (Presenter), Rice Univ — Strongly correlated materials could greatly respond to a stimulus due to their collective behavior. Thus, strongly correlated materials are well studied in the past for their tunable properties, especially electrical and thermal. However, their optical properties remain to be explored. In this work, we study the optical properties of 1T-TaS$_2$, a quasi-2D material supporting charge density waves (CDW). 1T-TaS$_2$ is the only material to exhibit a nearly commensurate CDW phase at room temperature and its electrical and thermal properties are shown to exhibit a large change with temperature, DC and AC biases, pressure, and light. Here, we study the optical properties of 1T-TaS$_2$ under DC and AC biases, different intensities of optical illumination, and at different temperatures. Under all these conditions, we observe a unity-order change in the refractive index of thin films of 1T-TaS$_2$. We hypothesize that the stacking of CDWs in this material changes with stimulus resulting in its optical constants to change. ARPES and STM measurements are underway to verify the hypothesis. Our discovery of the large tunability of optical constants of 1T-TaS$_2$ presents opportunities in studying light-matter interaction in strongly correlated materials and its application to nanophotonic devices.

12:51PM X56.00009: Probing Finite-Momentum Charge Collective Modes in Electron Doped SrTiO$_3$ * SAMANTHA RUBECK (Presenter), MELINDA S RAK, MATTEO MITRANO, ALI HUSAIN, JIN CHEN, University of Illinois at Urbana-Champaign, ALEXANDER EDELMAN, University of Chicago, PETER B LITTLEWOOD, Argonne National Lab, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — Electron doped strontium titanate, SrTiO$_3$, becomes a bulk superconductor at carrier densities as low as 5.5×10$^{17}$ cm$^{-3}$. The pairing mechanism in this dilute material, which is unconventional and widely debated, has recently been explained in terms of hybridization between the longitudinal optic phonons and the electronic plasmon collective modes. Using momentum-resolved inelastic electron scattering (M-EELS), we observed sub-200 meV acoustic and optic phonons, which have previously been implicated in the superconducting pairing, and a valence plasmon from the free carriers. For a carrier density of 2.137×10$^{20}$ cm$^{-3}$, the plasmon blueshifts with decreasing temperature, while its width and dispersion deviate from RPA predictions. In this talk, I will discuss evidence for hybridization of these modes for different carrier densities.

*This work was supported by DOE grant DE-FG02-06ER46285. S.R. acknowledges support from NSF Graduate Research Fellowship DGE-1746047. P.A. acknowledges support from Gordon and Betty Moore Foundation EPiQS grant GBMF-4542.
1:03PM X56.00010: Understanding the relationship between the structural and dielectric changes at the order-disorder transition in TEA(TCNQ)$_2$* ADAM BERLIE (Presenter), Rutherford Appleton Lab, IAN TERRY, MAREK SZABLEWSKI, Physics, Durham University, MARK TELLING, Rutherford Appleton Lab — Triethylammonium bis-7,7,8,8-tetracyanoquinodimethane (TEA(TCNQ)$_2$) shows an interesting dielectric behaviour, at approximately 220 K, where both the capacitance and the loss exhibit clear anomalies. This corresponds to the order-disorder transition where it is believed that the TEA cations freeze within the structure promoting both a structural change which manifests itself also as a change in dielectric properties. To understand this further, we have coupled quasi-elastic neutron scattering and other techniques to provide information on how these TEA cations are actually moving and what motions freeze out. We find that two things happen; firstly at 100 K we believe the methyl groups start rotating but at 220 K, the TEA cations rotate with a spherical radius of ~1.7 Angstroms.

*We would like to acknowledge the ISIS Neutron and Muon Source and the Institute Laue-Langevin for access to beam time.

1:15PM X56.00011: The Raman study of the structural transition in metallic LiOsO$_3$ single crystal under high pressure up to 40 GPa* JUNJIE GAO, SUYU FU, JUNG-FU LIN, Geological Sciences, University of Texas at Austin, KAZUNARI YAMAURA, Research Center for Functional Materials, National Institute for Materials Science, JIANSHI ZHOU (Presenter), Geological Sciences, University of Texas at Austin — LiOsO$_3$ is a novel metal that undergoes a second order phase transition from a centrosymmetric R-3c structure to a polar R3c structure at $T_s=140$ K [1]. In this work, we report the measurements of Raman scattering including polarized and unpolarized models on LiOsO$_3$ single crystal at different pressure up to 40 GPa with a diamond anvil cell. There are four phonon peaks in the phase at ambient condition; new peaks emerge for $P > 8.5$ GPa. The feature of the high-pressure phase resembles that of LiOsO$_3$ below $T_s$ at ambient condition [2]. The polar phase appears to be stabilized under high pressure, which is consistent with the observation of $dT_s/dP > 0$ from the resistivity measurement [3]. Results from the symmetry analysis and first-principles calculations will also be presented.

*This work was supported by NSF, DMR 1905598.
The interplay between electronic correlations and spin-orbit coupling often gives rise to novel quantum phases of matter. When spin-orbit coupling is strong and orbital degeneracies are present, the lattice also plays an important role in determining magnetic ground states. In the Lacunar spinel GaTa$_4$Se$_8$, electronic correlations localize a single unpaired electron on tetrahedral clusters of Ta ions, while spin-orbit coupling generates $J_{\text{eff}}=3/2$ magnetic degrees of freedom. At ambient pressures and $T=50$ K, GaTa$_4$Se$_8$ undergoes a magnetic transition to a valence bond solid state accompanied by a structural dimerization. Hydrostatic pressures can induce an insulator to metal transition, but the evolution of magnetic correlations and the crystal structure across this transition is not known. I will present a series of low temperature, high pressure x-ray diffraction measurements following the evolution of the structural dimerization in GaTa4Se8 across the pressure-induced insulator to metal transition. These measurements shed light on the coupling of spin-orbital pseudo spins with the crystal lattice.

NMR Investigation of Ferroquadrupolar Order in TmVO$_4$*  

TmVO$_4$ undergoes a tetragonal to orthorhombic structural phase transition below 2.2K due to a cooperative Jahn-Teller distortion. The Tm ions experience a crystal-field effect with a non-Kramer's ground state doublet, and undergo ferroquadrupolar order that breaks the C$_4$ symmetry of the lattice. This material is therefore is a model system to investigate Ising nematic ordering without competing phases. While previous $^{51}$V NMR has been hampered by significant line broadening due to demagnetization fields at low temperature, here we present improved results in a single crystal of ellipsoidal shape for which this broadening is absent. These are the first NMR measurements in which an ellipsoidal sample is used that has been carefully cut by a focused ion beam (FIB).

*Work at UC Davis was supported by the NSF under Grant DMR-1807889.
The interplay between competing ordered states and superconductivity has long been identified as key to understanding high-temperature superconductivity. In the case of the iron pnictide superconductors, superconductivity coexists with SDW order and electronic nematicity. BaNi$_2$As$_2$, a structural analogue of the high temperature pnictide superconductor BaFe$_2$As$_2$ has recently been reported to host CDW order and electronic nematicity in conjunction with superconductivity. Interestingly, as a function of Sr doping, CDW and nematicity in the system is suppressed. Upon suppression of this order to absolute zero, a dramatic, six-fold enhancement of the superconducting transition temperature is observed. This system could thus serve as a model system to study the enhancement of superconductivity in the vicinity of quantum critical fluctuations. Here we present detailed high-resolution ARPES measurements of the Sr$_x$Ba$_{1-x}$Ni$_2$As$_2$ series as a function of temperature, comparing the measured band dispersion and Fermi surfaces to density functional theory calculations of the electronic structure carried out in different phases. Utilizing both the experimental and theoretical data, we discuss various mechanisms for the CDW and electronic nematicity.

Effects of Electron Irradiation on Nematic-Like Phase Transition in BaNi$_2$P$_4$* ELIZABETH KRENKEL (Presenter), MAKARIY A TANATAR, ERIK I TIMMONS, JIAN WANG, LIN-LIN WANG, KIRILL KOVNIIR, RUSLAN PROZOROV, Ames Lab, MARCIN KONCZYKOWSKI, Ecole Polytechnique — We present the results of an experimental study of a tetragonal-to-orthorhombic phase transition with rather high transition temperature (T$_{TO} \sim 380$ K) in the clathrate material BaNi$_2$P$_4$. The transition is accompanied by formation of structural domain patterns which are revealed in polarized optics studies. The electrical resistivity shows metallic behavior both above and below T$_{TO}$. The transition temperature is notably affected by the low-temperature (20 K) irradiation with relativistic 2.5 MeV electrons. Additional insight into the nature of the transition is obtained from Hall effect measurements and band structure calculations. Similarity to the behavior found in the parent compounds of iron based superconductors will be discussed.

*This work was supported by the US DOE, Office of Science, BES Materials Science and Engineering Division under contract DE-AC02-07CH11358.
11:15AM X57.00001: First-principles studies of defect-induced electron-phonon interactions in 2D semiconductors* JUN-HO LEE (Presenter), Physics, UC Berkeley, LIANG TAN, Molecular Foundry, Lawrence Berkeley National Laboratory, JONAH HABER, Physics, UC Berkeley, KATHERINE COCHRANE, BRUNO SCHULER, ALEXANDER WEBER-BARGIONI, Molecular Foundry, Lawrence Berkeley National Laboratory, JEFFREY B NEATON, Physics, UC Berkeley — Point defects have played an important role in semiconductor physics to tune physical and chemical properties of the host material. A variety of point defects have been uncovered in monolayer transition-metal dichalcogenides (TMDs), showing unique fingerprints in structural, electronic, and vibronic properties. In this talk, I will summarize calculations of electron-phonon interactions in monolayer TMDs with point defects using density functional theory and density-functional perturbation theory. We find that local atomic-scale structure in the vicinity of point defects is distorted, leading to spatially-localized electronic states, which in turn possess strong electron-phonon coupling. We discuss our calculations in the context of ongoing scanning tunneling spectroscopy measurements.

This work was supported by the US Department of Energy. Computational resources are provided by NERSC.

11:27AM X57.00002: Defect hydrogenation in monolayer transition metal dichalcogenides LEHUA GU (Presenter), GUANQUN ZHANG, DI HUANG, SHUAI ZHANG, SHIWEI WU, Department of Physics, Fudan University — Structural defects in two-dimensional semiconducting transition metal dichalcogenides (TMDs) play an important role in modifying their physical properties. In this talk, we will present our optical spectroscopic study on the defect engineering of monolayer TMDs through hydrogenation. Photoluminescence spectra show the evolution of defect exciton upon hydrogenation, which behaves differently from that of free excitons. Time-resolved photoluminescence measurement further reveals the change of defect-induced exciton dynamics in monolayer TMDs after hydrogenation process. Based on the experimental observations, we propose a microscopic picture for the hydrogenation process in monolayer TMDs. Our work thus demonstrated the ability to tune the defect emission and gained the knowledge of structural defects in monolayer TMDs.
11:39AM X57.00003: Optical quantum emitters in monolayer MoS$_2$ fabricated with nm-precision by He ion microscopy*  ELMAR MITTERREITER, Walter-Schottky-Institut, TU Munich, BRUNO SCHULER, ALEXANDER WEBER-BARGIONI, Molecular Foundry, Lawrence Berkeley National Laboratory, ALEXANDER HOLLEITNER, CHRISTOPH KASTL (Presenter), Walter-Schottky-Institut, TU Munich — Atomistic defects in semiconductors can serve as single photon emitters for applications in quantum technologies. However, in conventional semiconductors, defects are often buried in the bulk hampering integration of defect centers into photonic circuits. Recently, it was demonstrated that color centers with narrow emission are generated in single layer MoS$_2$ by focused He-ion beam irradiation [1], opening a natural pathway for device integration. Here, we investigate atomistic defects in MoS$_2$ deliberately induced by focused He ion bombardment. We use scanning tunneling microscopy (STM) to resolve the atomistic defect states. By imaging line patterns with atomic resolution, we can quantify the lateral resolution of the defect patterning to be better than 7 nm.


*We acknowledge funding by the German Excellence Strategy MCQST - EXC-2111–390814868 and e-conversion – EXC 2089/1 – 390776260, BaCaTeC and International Graduate School of Science and Engineering (IGSSE). Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

11:51AM X57.00004: Crucial Role of many-body van der Waals interaction in understanding the stability of point defects in MoS$_2$ monolayer  ARUNIMA SINGH (Presenter), SASWATA BHATTACHARYA, Physics, Indian Institute of Technology Delhi — The present study investigates the stability of native point defects in MoS$_2$ monolayer by first-principles based approach under the framework of density functional theory (DFT). The property of band gap transition from indirect to direct on going from bulk to monolayer in MoS$_2$, establishes a huge potential in the optoelectronic industry. Defects being inevitable, their role in tuning the band gap for photovoltaics is an important approach. Initially, we have obtained the phase diagram that shows the most stable defect states with minimum Gibbs free energy of formation. We have considered charged and neutral states, of three vacancies and five antisites with the inclusion of many-body vdW interaction, which have posed a significant change in the stability pattern. The stable defect states as observed by HSE06 functional are, V$_S$ (-2,+2), V$_{Mo}$ (-2,+2), S$_{Mo}$ (-2) antisite and S$_{2Mo}$ (+2) antisite. They also have significant concentration at the finite temperature range of 50K-1000K, which is achieved by ab-initio atomistic thermodynamics along with the DFT input. Further, the S$_{Mo}$ (-2) and S$_{2Mo}$ (+2) antisites have tuned the band gap in the range 1.1 – 1.8 eV. These states have shown optical response in the visible region, hence increasing the absorption capability of MoS$_2$ monolayer.
12:03PM X57.00005: Electrical control of neutral and charged excitons in few-layer InSe*
ZHENGGUANG LU (Presenter), Natl High Magnetic Field Lab, DMITRY SHCHERBAKOV, Ohio State University, YUXUAN JIANG, SHAHRIAR MEMARAN, WENKAI ZHENG, Natl High Magnetic Field Lab, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, LUIS BALICAS, Natl High Magnetic Field Lab, CHUN NING LAU, Ohio State University, DMITRY SMIRNOV, Natl High Magnetic Field Lab — Indium selenide(InSe), a layered metal chalcogenide semiconductor with a layer dependent band structure, high electron mobility and strong light-matter interaction, has gained considerable interests as a promising material system for optoelectronics applications. Monolayer InSe is predicted to be an indirect band gap material. However, few-layer InSe maintains direct band gap optical properties and enables electrostatic gating. Here we report the observation of the electrical field controlled neutral and charged excitons in high-quality hBN encapsulated few-layer InSe devices. Near the charge neutrality point, the photoluminescence (PL) spectra display a strong and narrow peak with 4meV linewidth (at 20K) associated with the recombination of neutral excitons. By adjusting the Fermi energy, we can tune the PL emission so that the PL spectra are dominated either by positively charged or negatively charged trions. We found relatively large trion binding energies of about 8meV, which further indicates the potential of few-layer InSe for optoelectronics.

*The work at NHMFL was supported by the NSF-DMR 1644779 and the State of Florida, and DoE-BES DE-FG02-07ER46451.
CNL and DS acknowledge the support from NSF-DMR 1807928.
L.B. acknowledges support from NSF-DMR 807969.

12:15PM X57.00006: Trions in doped MoS2 monolayer. YAROSLAV V. ZHUMAGULOV, ITMO University, ALEXEI V. VAGOV, Institute for Theoretical Physics III, University of Bayreuth, DMITRY GULEVICH, ITMO University, VASILI PEREBEINOS (Presenter), State Univ of NY - Buffalo — Transition metal dichalcogenide monolayers are semiconductors with a direct transition at the K-point of the Brillouin zone. The band structure of these materials has unique features that makes them ideal candidates for valleytronics. Tightly bound negative trions, a quasiparticle composed of two electrons and a hole, can be optically optically created with valley and spin polarized holes. They possess a large binding energy and large oscillator strength, such that they dominate optical spectra even at room temperature. Here, we solve Bethe-Salpeter equation for the three particle wavefunction at finite momentum. Our results enable us to explain existing data on temperature and doping dependence and predict new spectroscopic features in doped MoS2.
12:27PM X57.00007: Visualizing Electrically Driven Photon Emission from Individual Defects in WS\textsubscript{2} with Atomic Resolution [Invited]  
BRUNO SCHULER (Presenter), KATHERINE COCHRANE, JUN-HO LEE, Lawrence Berkeley National Laboratory, CHRISTOPH KASTL, Technical University Munich, ED BARNARD, ED WONG, Lawrence Berkeley National Laboratory, NICHOLAS J BORYS, Montana State University, ADAM SCHWARTZBERG, FRANK OGLETREE, JEFFREY B NEATON, Lawrence Berkeley National Laboratory, JAVIER GARCIA DE ABAJO, ICFO – The Institute of Photonic Sciences, ALEXANDER WEBER-BARGIONI, Lawrence Berkeley National Laboratory — Point defects in two-dimensional semiconductors are exciting atomic quantum systems. Recently, we established the correlation of atomic structure, electronic and optical properties of native point defects in monolayer WS\textsubscript{2} [1] and MoSe\textsubscript{2} [2] using atomically resolved scanning probe microscopy techniques. We identified isoelectronic chalcogen and transition metal substitutions as the dominant defects based on their unique electronic fingerprint [1,2]. Sulfur vacancies that are absent in as-grown samples could be selectively generated by high temperature annealing in vacuum and exhibit strong spin-orbit splitting [3].

Here we demonstrate electrically driven photon emission from individual, atomically defined defects in a 2D semiconductor [4]. We show atomically resolved luminescence maps from sulfur vacancy defects and native chromium substituents. The widely tunable optical emission generated by charge carrier injection into localized defect states in a 2D material is a powerful platform for electrically driven single-photon emission.


1:03PM X57.00008: Unexpected symmetries in twisted bilayer MoSe\textsubscript{θ}  
PRIYA MAHADEVAN (Presenter), POONAM KUMARI, S N Bose Natl Ctr Basic Sci — Spin-orbit interactions lead to a large spin-splitting of the valence band maximum at K in MoSe\textsubscript{2} monolayers. However, on stacking a second layer of MoSe\textsubscript{2} in the same manner (2H) as found in the bulk, one finds that there is no spin splitting. This has been attributed to the presence of inversion symmetry. As exploiting the spin splitting at the K valleys allows us to increase the functionality, an obvious route to making the bilayers useful for exploring the coupled spin and valley physics is through breaking inversion symmetry. We examined this by rotating the top layer of the bilayer by an angle θ with respect to the lower layer. The choice of angles was restricted to those for which one had reasonable sized supercells and were otherwise arbitrary. Surprisingly, we found several instances where the spin splitting vanished, though there was no breaking of inversion symmetry. An unusual mechanism behind this is identified. Additionally, we found that while the spin splitting existed for theta, it vanished for 60 - θ. This unusual behavior, we find, is a consequence of the symmetry of the hexagonal Brillouin zone.
Twist-Angle Dependence of Moiré Excitons in MoSe$_2$/MoS$_2$ Twisted Heterobilayers

BO-HAN LIN (Presenter), YUNG-CHUN CHAO, CHIEN-JU LEE, FU-HSIEN CHU, LE-CHIH CHO, LI-SYUAN LU, JUNG-JUNG SU, WEN-HAO CHANG, Electrophysics, National Chiao Tung University — Twisted heterobilayers (hBLs) of transition metal dichalcogenides can form a moiré superlattice of periodically varying atomic registry between the two layers. The excitonic properties in twisted hBLs can be altered drastically by the formation of moiré minibands that depends sensitively on the moiré periodicity controlled by the twist angle. To study the twist-angle dependence, conventional methods based on mechanical exfoliation and transfer of individual crystals are tedious to fabricate many hBLs with various twist angles within 5°. Here we report on the study of moiré excitons in MoSe$_2$/MoS$_2$ hBLs fabricated by stacking a large MoSe$_2$ flake on an ensemble of highly-oriented MoS$_2$ flakes grown by chemical vapor deposition. The small angle variations in the MoS$_2$ flakes form a large number of hBLs with various small twist angles, enabling the study of twist-angle dependence of moiré excitons. We observed systematic energy shifts and fine structures in intralayer excitons with the twist angle, signifying the formation of moiré minibands. The polarization selection rules of moiré excitons were also investigated by photoluminescence excitation spectroscopy. Understanding the twist-angle dependent properties of moiré excitons provides insights for future developments of “twistronics”.

Twist-angle dependent interlayer exciton diffusion in MoS$_2$-MoSe$_2$ heterobilayers

CHIEN-JU LEE (Presenter), BO-HAN LIN, FU-HSIEN CHU, LE-CHIH CHO, LI-SYUAN LU, WEN-HAO CHANG, Department of Electrophysics, Natl Chiao Tung Univ — Heterobilayers (HBLs) of transition metal dichalcogenides can form a moiré superlattice with a periodic potential landscape, which can modulate the electronic structure and confine excitons. HBLs can host interlayer excitons (IXs) with electrons and holes separated in different layers, forming a dipolar exciton gas with repulsive Coulomb interactions among the aligned vertical dipoles. The presence of moiré superlattice further imposes an additional length scale that can change the dynamics and transport properties of IXs in HBLs. Here we study the influence of moiré periodicity on the IX diffusion in MoS$_2$-MoSe$_2$ HBLs. We prepared a series of HBLs with small twist angles by stacking monolayer MoSe$_2$ onto MoS$_2$ with well-aligned orientations grown by chemical vapor deposition. Twist-angle dependent photoluminescence (PL) energy of interlayer exciton (IX) were observed, signifying the formation of moiré potential. We further investigated the IX diffusion by time-resolved PL and spatially resolved PL imaging. The interplay between moiré potentials and dipole-dipole interactions of IX leads to exciton-density and twist-angle dependent diffusion length. Our results provide insights in understanding of the localization and delocalization of interlayer excitons in the moiré superlattice.
1:39PM X57.00011: Exciton physics in organic-inorganic 2D perovskites

JEAN-CHRISTOPHE BLANCON (Presenter), HAO ZHANG, WENBIN LI, Rice Univ, MERCOURI KANATZIDIS, Northwestern University, ANDREAS V. STIER, Walter Schottky Institute, Technical University of Munich, JACKY EVEN, PHOTON, INSA Rennes, ADITYA MOHITE, Rice Univ — Organic-inorganic (hybrid) 2D perovskites (2DPKs) is an emerging class of layered materials that feature unique structural characteristics related to the soft and dynamic nature of their lattice structure and organic-inorganic interfaces. There is still little knowledge of the interplay between the physical and structural characteristics. Here, using optical spectroscopy and magneto-absorption, coupled with structural probes, we report the dependence of the formation, dynamics, and recombination of exciton states on the structural and compositional details of 2DPKs. Our work reveals the changes in the exciton properties due to the tuning of the 2DPKs thickness and the size of the organic molecules in the lattice [1]. Moreover, we demonstrate the existence of unique electronic states located at the edge surfaces of 2DPKs that are beneficial for optoelectronic applications [2,3]. Finally, we provide insight into the hetero-coupling between 2D perovskites and monolayer WS$_2$, which yield photoluminescence enhancement by more than one order of magnitude as compared to their constituent [4].


1:51PM X57.00012: Plasmon-Resonant Enhancement of Photocatalysis on Monolayer WSe$_2$

JIHAN CHEN, STEVE CRONIN (Presenter), Univ of Southern California — We present plasmonic enhancement of photocatalysis by depositing 5 nm Au nanoislands onto tungsten diselenide (WSe$_2$) monolayer films.\textsuperscript{1} Under 532 nm wavelength illumination, the bare WSe$_2$ film produces a relatively small photocurrent (20 nA). With the addition of Au nanoparticles, we observe enhancements of up to 7X (0.14 μA) in the measured photocurrent. Despite these relatively small photocurrents, it is remarkable that adequate charge separating fields are generated over just 7.3 Å of material. Here, the improvement in the photocatalytic performance is caused by the local electric field enhancement produced in the monolayer WSe$_2$ monolayer by the plasmonic Au nanoislands, as verified by electromagnetic simulations using the finite different time domain (FDTD) method. The near-field optical enhancement increases the electron–hole pair generation rate at the surface of WSe$_2$, thus, increasing the amount of photogenerated charge contributing to photoelectrochemical reactions.

2:03PM X57.00013: First principles studies of magnetic ion-intercalated transition metal dichalcogenide bilayers*

JONATHAN REICHANADTER (Presenter), ELIZABETH A PETERSON, Physics, UC Berkeley, JEFFREY B NEATON, Lawrence Berkeley National Laboratory — Monolayer transition metal dichalcogenides (TMDs) offer a promising framework for valleytronic applications given their degenerate, yet non-equivalent K,K' points from broken inversion symmetry which exhibit significant spin-orbit interaction induced spin-valley coupling. Recent experimental work1,2 in transferring monolayer TMDs onto ferromagnetic substrates has shown splitting of the K-K' band degeneracy associated with the breaking of time-reversal symmetry. Here we perform ab initio density functional theory calculations of the structural, electronic, and magnetic properties of magnetic ion intercalated MoS2 bilayers. Through investigation of intercalant element, intercalant density, and bilayer spacing and registry, we assess the promise of intercalated bilayer architectures for valley splitting and valleytronic applications.


*This work is supported by supported by the Air Force Office of Scientific Research Hybrid Materials MURI under award number FA9550-18-1-0480. Computational resources provided by the Department of Energy via NERSC.

Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X58 DCMP: Topological Phases in Floquet Systems Mile High Ballroom 3B

11:15AM X58.00001: Phonon-assisted Floquet engineering of second-order topological phases*

SWATI CHAUDHARY (Presenter), ARBEL HAIM, YANG PENG, GIL REFAEL, Caltech — The co-existence of spatial and non-spatial symmetries together with appropriate commutation/anticommutation relations between them can give rise to static higher-order topological phases, which host gapless boundary modes of co-dimension higher than one. Alternative to spatial symmetries, space-time symmetries in a Floquet system can lead to anomalous Floquet boundary modes of higher co-dimensions, presumably with alterations in the commutation/anticommutation relations with respect to non-spatial symmetries. In this work, we discuss how a coherently excited phonon mode can be used to promote a spatial symmetry with which the static system is always trivial, to a space-time symmetry which supports non-trivial Floquet higher-order topological phase. We present two examples— one in class AIII and another in class D where a coherently excited phonon mode promotes the reflection symmetry to a time-glide symmetry such that the commutation/anticommutation relations between spatial and non-spatial symmetries are modified. These altered relations allow the previously trivial system to host gapless modes of co-dimension two at reflection-symmetric boundaries.

*This work was supported by ARO Grant No. W911NF-16-1-0361.
**11:27AM X58.00002: Majorana states in a spin or qubit chain with a resonantly modulated coupling**  
MARK DYKMAN (Presenter), Michigan State Univ — We show that a spin or qubit chain with the qubit coupling modulated close to twice the qubit frequency maps on the Kitaev chain. This is an example of topologically nontrivial Floquet dynamics induced in a trivial system by a simple sinusoidal modulation. The nontrivial regime exists in the frequency range with a width determined by the strength of the qubit coupling. Preparation of the system in this regime involves going through a quantum phase transition where the excitation gap closes, in the limit of an infinite chain. The results are compared with a quantum phase transition induced by a resonant parametric modulation of a system of coupled nonlinear mesoscopic oscillators, which remains topologically trivial [1].


*The work was supported in part by the NSF, DMR-1708331 and DMR-1806473, and by the Google faculty research award.

**11:39AM X58.00003: A periodic classification of local unitary operators**  
FENNER HARPER, XU LIU, RAHUL ROY (Presenter), University of California, Los Angeles — We present a complete topological classification of single particle local unitary operators, which are usually represented by local unitary matrices. The classification is performed in the ten symmetry classes and leads to a “periodic table”. Local unitary operators arise naturally in systems with an evolution generated by a quantum possibly time-varying (Hermitian) Hamiltonian. They also describe unitary operations in more general contexts, such as in quantum walks or models for information flow. The classification is complete in the sense that two local unitary operators have the same topological invariants if and only if they can be continuously deformed into each other. It allows one to distinguish “locally generated” unitary operators in a given symmetry class (generated by local Hamiltonians) from those that are not locally generated and provides a complete table of local operators which are not locally generated.

*NSF Career DMR-1455368

**11:51AM X58.00004: Classification of Interacting Floquet Phases with U(1) Symmetry**  
CAROLYN ZHANG (Presenter), MICHAEL LEVIN, University of Chicago — Recently, it has become clear that periodically driven many-body systems can support new types of topological phases that have no counterpart in static systems. These anomalous Floquet topological phases have been studied for both interacting and non-interacting systems in different symmetry classes. In this talk, we consider interacting Floquet topological phases with U(1) charge conservation symmetry in two spatial dimensions. We propose a complete classification of Floquet phases of this kind, in the case where the Floquet eigenstates are short-range entangled, and we show that each phase can be labeled by a topological invariant which can be computed either at the edge of an open system or in the bulk. The latter formula provides a way to measure the invariant and also reveals a connection to the bulk magnetization density discussed in previous work.

*This work is supported by the National Science Foundation Graduate Research Fellowship Program under Grant DGE-1746045 and the Simons Foundation through the “Ultra-Quantum Matter” Simons Collaboration.
Emergent topological phases in synthetic dimensions with low-frequency laser pumping

PEIZHE TANG (Presenter), SHUNSUKE SATO, ANGEL RUBIO, Theory Department, Max Planck Institute for the Structure and Dynamics of Matter — In the Floquet-Bloch theory, when a physical system is driven by a strong external optical field, its dynamics can be conveniently represented in a higher dimensional Floquet lattice. Here, we consider the 2D Dirac systems under strong external optical driving. In the low-frequency limit, new topological states of matter emerge in the synthetic 2+1D, including Dirac nodal line, helix nodal lines, and Weyl fermions. In contrast to conventional Floquet topological states under the high-frequency limit, there is no anomalous Hall signal observed in this system although the time-reversal symmetry is broken and the Floquet energy gap opens at the crossing point. Furthermore, we use the quantum Liouville equation with phenomenological dissipation to simulate the evolution of 2D Dirac fermions under the strong optical field with low frequency, we confirm the existence of the Floquet states and find the simulated transport properties consistent with our prediction from Floquet theory in synthetic 2+1D.

*This work was supported by the European Research Council (ERC-2015-AdG694097). We acknowledge funding from the European Unions Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 793609.

Floquet second-order topological insulator

RANJANI SESHADRI (Presenter), Physics, McGill University, ANIRBAN DUTTA, DIPTIMAN SEN, Centre for High Energy Physics, Indian Institute of Science — Higher-order topological insulators (HOTIs) are a recent entrant to the field of topology in condensed matter physics. Usually, two-dimensional topological insulators host robust one-dimensional edge modes. These are related to the bulk properties via topological invariants such as the Chern number. However, in HOTIs, there are zero-dimensional corner modes, which, in case of a square-shaped sample, say, are confined to the four vertices of the square. In this work, a variant of the well-known Bernevig-Hughes-Zhang (BHZ) model is used to construct a two-dimensional HOTI. When this system is driven periodically by varying one of the model parameters in time, i.e., using a Floquet drive, multiple corner states may appear depending on the driving frequency and other parameters. The system can be characterized by topological invariants such as the Chern number and a diagonal winding number. The behavior of these invariants can be understood in terms of the value of the Floquet operator at some special points in momentum space.
Out of equilibrium higher-order topological insulator: Floquet engineering and quench dynamics

TANAY NAG (Presenter), SISSA, VLADIMIR JURICIC, NORDITA, BITAN ROY, Lehigh University — Higher order topological (HOT) states, hosting topologically protected modes on lower-dimensional boundaries, such as hinges and corners, have recently extended the realm of the static topological phases. We here demonstrate the possibility of realizing a two-dimensional \textit{Floquet} second-order topological insulator, featuring corner localized zero quasienergy modes and characterized by quantized Floquet quadrupolar moment $Q_{xy}^{\text{Flq}} = 0.5$, by periodically kicking a quantum spin Hall insulator (QSHI) with a discrete four-fold ($C_4$) and time-reversal ($\mathcal{T}$) symmetry breaking mass perturbation. We also analyze the dynamics of a corner mode after a sudden quench, when the $C_4$ and $\mathcal{T}$ symmetry breaking perturbation is switched off, and find that the corresponding survival probability displays periodic appearances of complete, partial and no revival for long time, encoding the signature of corner modes in a QSHI. Our protocol is sufficiently general to explore the territory of dynamical HOT phases in insulators (electrical and thermal) and gapless systems.

Floquet topological flat bands in two-dimensional systems

MUHAMMAD TAHIR (Presenter), HUA CHEN, Colorado State University — Flat electronic bands in equilibrium condensed matter systems have been a common avenue to nontrivial correlation effects, with the twisted bilayer graphene being a most recent prominent example. It is expected that flat quasienergy bands can also enhance interaction effects in time-periodic Floquet systems and may lead to novel interaction driven metastable phases. Here, we propose a general approach to realizing Floquet flat bands with nontrivial topology in 2D or quasi-2D systems subject to circularly-polarized light. By using a simple model that can interpolate between Schrödinger and Dirac electrons, we demonstrate their different band flattening behaviors within Floquet theory. The flat band condition, determined by the ratio between the time-periodic electric field strength and its frequency, can be qualitatively obtained from perturbation theory. Moreover, flat bands argued in this work can be realized without the need of fine tuning in contrast to twisted bilayer graphene. Our proposal may pave the way to novel interaction-driven phases in nonequilibrium systems.

\*MT and HC were supported by the start-up funding of CSU.
12:51PM X58.00009: Topological Correspondence between Hermitian and Non-Hermitian Systems: Anomalous Dynamics*  JONG YEON LEE (Presenter), Harvard University, JUNYEONG AHN, Physics, Seoul National University, HENGYUN ZHOU, ASHVIN VISHWANATH, Harvard University — The hallmark of symmetry-protected topological (SPT) phases is the existence of anomalous boundary states, which can only be realized with the corresponding bulk system. In this work, we show that for every Hermitian anomalous boundary mode of the ten Altland-Zirnbauer classes, a non-Hermitian counterpart can be constructed, whose long time dynamics provides a realization of the anomalous boundary state. We prove that the non-Hermitian counterpart is characterized by a point-gap topological invariant, and furthermore, that the invariant exactly matches that of the corresponding Hermitian anomalous boundary mode. We thus establish a correspondence between the topological classifications of \((d + 1)\)-dimensional gapped Hermitian systems and \(d\)-dimensional point-gapped non-Hermitian systems. We illustrate this general result with a number of examples in different dimensions. This work provides a new perspective on point-gap topological invariants in non-Hermitian systems.

*J.Y.L. and A.V. are supported by a Simons Investigator Fellowship and by NSF-DMR 1411343. J.A. is supported by IBS-R009-D1. H.Z. is supported by NSF and ARO (W911NF-15-1-0548).

1:03PM X58.00010: Bulk-edge correspondence and robustness of edge states in a non-unitary three-step quantum walk with PT symmetry  HIDEAKI OBUSE (Presenter), MAKIO KAWASAKI, KEN MOCHIZUKI, Department of Applied Physics, Hokkaido University, NORIO KAWAKAMI, Department of Physics, Kyoto University — Topological phases in non-Hermitian systems have attracted great attention in recent years. It has been shown that a photonic quantum walk with effects of loss is an ideal platform to study topological phases in non-Hermitian systems with parity-time reversal symmetry (PT symmetry)[1]. In the present work, we study topological phases and the associated multiple edge states in non-unitary three-step quantum walks with PT symmetry in one dimension[2]. We show that the non-unitary quantum walk has large topological numbers and numerically confirm that multiple edge states appear as expected from the bulk-edge correspondence. We also study stability of the edge states and find extra stabilization mechanism of the edge states unique to non-unitary systems.


1:15PM X58.00011: A bulk edge connection for Class AIII Floquet insulators*  XU LIU (Presenter), FENNER HARPER, RAHUL ROY, University of California, Los Angeles — We propose edge and bulks invariants for Floquet systems in Class AIII in arbitrary dimensions. These indices are physically motivated and locally computable even in systems with disorder. Finally, we derive a bulk-edge correspondence which relates the nontrivial bulk behavior with the edge modes present on a boundary at the end of the evolution.

*NSF Career DMR-1455368
Kagome lattice network model as a chiral Floquet topological insulator

MATTEO WILCZAK (Presenter), ITAMAR KIMCHI, VICTOR GURARIE, University of Colorado, Boulder, DMITRY K. EFIMKIN, The School of Physics and Astronomy, Monash University — The magnetic proximity effect can open a gap in the spectrum of Dirac electrons at the surface of a topological insulator; on the other hand, topological defects in the magnetization can host topologically protected localized (isolated skyrmion) and propagating (domain walls) states. Here we argue that the electronic structure of Dirac electrons coupled to the skyrmion lattice phase in an insulating magnet (for example, Cu$_2$OSeO$_3$) can be described by the Chalker-Coddington network model (CCN) with the Kagome geometry. We study this model relying on a recent insight that CCN should be thought of as a chiral Floquet topological insulator. While in static systems the number of edge modes is completely determined by calculation of the Chern number for each energy band, in Floquet systems there may be edge modes even when the Chern number for each band is zero. We describe a new topological invariant which is a modified version of the chiral Floquet invariant proposed by Rudner et al. and does not require the construction of an effective Hamiltonian, and which correctly counts the number of edge modes in each spectral gap. We apply this invariant to the Kagome lattice network model and show that it includes both Chern and chiral Floquet phases.

Analysis of Topological States in a Floquet-driven Non-Hermitian System*

ANDREW HARTER (Presenter), NAOMICHI HATANO, Institute of Industrial Science, University of Tokyo — Non-Hermitian Hamiltonians offer a good description of many open systems in which gain and loss are present; crucially, in contrast to their Hermitian counterparts, they may have a complex eigenspectrum. Interestingly, non-Hermitian Hamiltonians which possess PT symmetry [1] can be shown to admit an entirely real eigenspectrum within a certain range of their parameters. It has been shown [2] that certain PT-symmetric lattices can admit topologically non-trivial phases; however, this phase only coincides with the PT-symmetry broken phase, and the topological edge states correspond to imaginary eigenvalues. We examine Floquet driving of this system which, for high enough driving frequencies [3], has been shown to stabilize the edge states. By using a simple two-step, pulsed time dependence, we explore the entire range of driving frequencies to highlight new regions of stability, including those which are explicitly below the high-frequency regime.


*This work was supported by the Japan Society for the Promotion of Science (JSPS)
X58.00014: Light-induced Topological Insulator with Superlattice Structure* 
HWANMUN KIM (Presenter), HOSSEIN DEHGHANI, University of Maryland, College Park, HIDEO AOKI, Department of Physics, The University of Tokyo, IVAR MARTIN, Material Science Division, Argonne National Laboratory, MOHAMMAD HAFEZI, University of Maryland, College Park — We study the superlattice structure created by light on 2D material. Specifically, we investigate the monolayer graphene irradiated by circularly-polarized (CP) beam where the beam amplitude has spatial periodicity. We numerically study the phase transition between the topological insulator and the normal insulator depending on the superlattice size. To examine the role of lattice shape in the topological property of the system, we investigate the topological phase transition happening in the sheared lattice. By superposing different kinds of beams, our scheme can create a more complicated lattice such as kagome lattice. This wide tunability of lattice can be used for further investigation of interesting dynamics of electrons.

*This research was supported by the Physics Frontier Center at the Joint Quantum Institute.

X58.00015: High-temperature Floquet fractional quantum Hall state in a Kagome lattice with photo-inverted hopping* HANG LIU (Presenter), GURJYOT SETHI, YINONG ZHOU, University of Utah, JIA-TAO SUN, SHENG MENG, Institute of Physics, Chinese Academy of Sciences, FENG LIU, University of Utah — High-temperature fractional quantum Hall (FQH) state is predicted to emerge from geometrically frustrated lattices with topological flat bands, but yet to be demonstrated in realistic systems due to very unusual lattice hopping requirements. Here we show that time-periodic circularly polarized laser (CPL) can effectively invert second-nearest-neighbor kinetic hopping in a Kagome lattice and simultaneously enhance spin-orbit coupling (SOC) in one spin channel, so as to produce an isolated flat Chern band exhibiting high-temperature Floquet FQH effect. CPL-driven monolayer HTT-Pt possesses an unprecedented high flatness ratio $\Delta/\nu \sim 40$, which paves the way to observing the high-temperature FQH state in realistic 2D systems. Meanwhile, the CPL decreases the SOC strength in the other spin channel to form a chiral Kagome band with a high Chern number. Our approach may be generally applicable to engineering exotic topological quantum states in other crystal lattices.

*U.S. DOE-BES (No. DE-FG02-04ER46148), National Key Research and Development Program of China (No. 2016YFA0300902 and No. 2016YFA0202300), National Basic Research Program of China (No. 2015CB921001), NSFC (No. 91850120 and 11774396), "Strategic Priority Research Program (B)" of CAS (No. XDB30000000).
**11:15AM X59.00001: Novel Magnetic Weyl Semimetallic State in Layered Material: Fe$_2$Sn**

BISHNU KARKI (Presenter), BISHNU PRASAD BELBASE, MADHAV PRASAD GHIMIRE, Central Department of Physics, Kirtipur, 44613, Kathmandu, Nepal, Tribhuvan University — Weyl Semimetals (WSMs) are the crystalline substances that are believed to be the sources for massless but charged particle called Weyl fermions. They are found to possess exotic properties such as high mobilities, magneto transport phenomenon, large magneto resistance and quantum hall phenomenon. These properties are expected to be highly applicable for high speed electronics and spintronics, quantum computing, hall effect devices and even in the catalysis. Here we focus on studying the electronic, magnetic and transport properties of hexagonal Fe$_2$Sn. From our density functional theory calculations, the magnetic ground state is found to be ferromagnetic with a total magnetic moment of 4.56μ$_B$/formula unit. The electronic state shows metallic behavior with the band crossing close to the Fermi level. Fe$_2$Sn is predicted to be magnetic WSM based on the identification of 16 Weyl points within an 0.01 eV around the Fermi level with chirality.

**11:27AM X59.00002: Engineering Weyl phases and nonlinear Hall effects in T$_d$-MoTe$_2$**

SOBHIT SINGH (Presenter), JINWOONG KIM, KARIN M RABE, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, New Brunswick, NJ, USA — MoTe$_2$ has recently attracted much attention due to the observation of pressure-induced superconductivity, exotic topological phase transitions, and nonlinear quantum effects. However, there is debate on the intriguing structural phase transitions among various observed phases of MoTe$_2$, and their connection to the underlying topological electronic properties. In this work, by means of density-functional theory (DFT+U) calculations, we describe the structural phase transition between the polar T$_d$ and nonpolar 1T’ phases of MoTe$_2$ in reference to a hypothetical high-symmetry structure T$_0$ that exhibits higher-order topological features. We obtain a total of 12 Weyl points, which can be created/annihilated, dynamically manipulated, and switched by tuning a zone-center polar phonon mode in the T$_d$ phase. We also report on the existence of a tunable nonlinear Hall effect in T$_d$-MoTe$_2$, and predict an emergent nonlinear surface current under the application of an external electric field. The potential technological applications of the tunable Weyl phase and nonlinear Hall effect will be discussed.

*Support from NSF DMREF Grant No. DMR-1629059, and ONR Grants N00014-16-1-2951 and N00014-17-1-2449 is acknowledged.
11:39 AM X59.00003: Multiple types of van Hove singularities induced by band inversion*

JIAWEI RUAN (Presenter), Nanjing University, University of California at Berkeley, and Lawrence Berkeley National Laboratory, HUAIQIANG WANG, Physics, Nanjing University, STEVEN LOUIE, University of California at Berkeley, and Lawrence Berkeley National Laboratory, HAI-JUN ZHANG, Physics, Nanjing University — Saddle-point Van Hove singularities in the electron density of states can cause system instabilities that lead to exotic phases of matter. Here, we show that such singularities are very common near the Fermi level of topological semimetals and insulators. Using a k.p model analysis, we find that multiple types of saddle points with different divergence behaviors can be induced by band inversion. In particular, we uncover a new type of saddle-like dispersion (called “saddle line”) that significantly enhances the divergence in the density of states. We present examples of ab initio electron band structures of topological materials including monolayer 1T'-WS₂, monolayer decorated stanene, and Dirac semimetal Na₃Bi. Our results suggest a new universal property of topological materials that can lead to further opportunities.

*Work at Nanjing University was supported by the National Natural Science Foundation of China (Grant No. 11674165), the Fok YingTong Education Foundation of China (Grant No. 161006), and the Fundamental Research Funds for the Central Universities (Grant No. 020414380038). Work at the University of California was supported by the National Science Foundation.

11:51 AM X59.00004: Cd₃As₂: Dirac semimetal to Weyl semimetal*

SANTU BAIDYA (Presenter), DAVID VANDERBILT, Department of Physics and Astronomy, Piscataway, NJ 08854, Rutgers University — Dirac and Weyl semimetals have attracted much attention in the past few years. The Dirac compound Cd₃As₂ has seen renewed interest due to reports of proximity-induced surface superconductivity [1] and quantum Hall effect in thin films [2]. Using first-principles based theoretical methods, we show that by breaking time-reversal symmetry upon the application of an external Zeeman magnetic field, the four-fold degenerate Dirac node in Cd₃As₂ splits into four non-degenerate Weyl nodes, of which two are simple Weyl nodes of chirality ±1 and other have chiral charges of ±2. We calculate the evolution of the Fermi surfaces and their contributions to the anomalous Hall conductivity as a function of magnetic field and Fermi level position. Our work forms a basis for understanding how the resulting hole and electron pockets may play a role in generating complex states such as unconventional forms of superconductivity.

References:

*This work was supported as part of the Institute for Quantum Matter, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0019331.
12:03PM X59.00005: Dirac and triple point semimetallic phases in Heusler alloys

CHIRANJIT MONDAL (Presenter), Discipline of Metallurgy Engineering and Materials Science, Indian Institute of Technology Indore, CHANCHAL BARMAN, Department of Physics, Indian Institute of Technology, Bombay, BISWARUP PATHAK, Discipline of Chemistry and Discipline of Metallurgy Engineering and Materials Science, Indian Institute of Technology Indore, AFTAB ALAM, Department of Physics, Indian Institute of Technology, Bombay — We predict full Heusler compounds XInPd$_2$ (X = Zr, Hf and Ti) to be potential candidates for type-II Dirac semimetals. The crystal symmetry of these compounds have appropriate chemical environment with a unique interplay of inversion, time reversal and mirror symmetry. These symmetries help to give six pairs of type-II Dirac nodes on the $C_4$ rotation axis, closely located at/near the Fermi level. Using first principle calculations, symmetry arguments and crystal field splitting analysis, we illustrate the occurrence of such Dirac nodes in these compounds. Bulk Fermi surfaces have been studied to understand the Lorentz symmetry breaking and Lifshitz transition (LT) of Fermi surfaces. Bulk nodes are projected on the (001) and (111) surfaces which form the surface Fermi arcs, that can further be detected by photo-emission and scanning tunneling spectroscopy. By analyzing the evolution of arcs with changing chemical potential, we prove the fragile nature and the absence of topological protection of the Dirac arcs. Our predicted compounds overcome the limitations of the previously reported PtTe$_2$ class of compounds. Further we show breaking of inversion symmetry leads to realize triply degenerate nodal points in Heusler family.

*We thank DST SERB and MHRD India for financial supports.

12:15PM X59.00006: First-Principles Study of Robust Magnetic Weyl Nodal Loops in 5d Cubic Double Perovskites

YOUNG-JOON SONG (Presenter), KWAN-WOO LEE, Division of Display and Semiconductor Physics, Korea University — Topological phenomena have been extensively studied due to their interesting properties in the condensed matter physics. In particular, topological nodal line phases have special features of dispersionless surface states, so-called drumhead surface states. These flat states lead to a large surface density of states, implying instabilities toward surface magnetism or superconductivity.

In this presentation, we will address a few Os-based cubic double perovskites possessing robust magnetic Weyl nodal lines (WNLs), protected by the mirror symmetry, even for considering spin-orbital coupling (SOC). Using first-principles and tight-binding approaches, we have investigated the nature of topological properties in the osmates. Our effective 3-band model of the isolated $t_{2g}$ orbitals indicates that the $dd\sigma$ and $dd\pi$ hoppings result in the nodal lines on the mirror planes. When including both correlation and SOC, these nodal lines are robust only in the broken time-reversal symmetry (TRS) case. Besides, remarkably, our calculated anomalous Hall conductivity shows a single sharp peak at the energy of WNLs due to a strong magnetic anisotropy, implying these WNLs to be experimentally observable.

*This research was supported by NRF-2019R1A2C1009588.
12:27PM X59.00007: A Dirac semimetal with surface hourglass fermions: BaHgSn  TAN ZHANG (Presenter), ZHIJUN WANG, HONGMING WENG, ZHONG FANG, Institute of Physics, Chinese Academy of Sciences — We proposed that BaHgSn is a Dirac semimetal which hosts hourglass-like surface states protected by glide symmetry. Compared with the topological crystalline insulators (TCI) K'HgSb, BaHgSn has the similar crystal structure, but it has an additional band inversion induced by the stronger bonding and antibonding state splitting at Γ point, which leads to the bulk Dirac point on AΓ path. Due to this additional band inversion, BaHgSn has the $M_2^z$ mirror Chern number $C_{\pm i}^\pm = \pm 3$, while K'HgSb has $Z_2^\prime = (0;000)$ and $C_{\pm i}^\prime = \pm 2$. BaHgSn has the same hourglass-like states as K'HgSb along the $\tilde{X}\tilde{U}$ path on (010) surface, but it has bulk Dirac cone projection along $\tilde{Z}\tilde{\Gamma}$ path and zigzag surface states protected by $C_{\pm i} = \pm 3$ along $\tilde{\Gamma}\tilde{X}$ path. When 5% pression is applied along the y axis, the bulk Dirac point is gapped, and BaHgSn becomes a strong topological insulator (TI) with $Z_2 = (1;000)$. The change of surface states is that bulk Dirac cone projection opens a gap and nontrival zigzag surface states protected by nontrivial $Z_2$ appear along $\tilde{Z}\tilde{\Gamma}$ path. We also calculate the Wilson-loop spectral for (010) surface, the results are consistent with the surface states.

12:39PM X59.00008: Computational search for Dirac and Weyl nodes in f-electron antiperovskites*  ANNA PERTSOVA (Presenter), R.M. GEILHUFE, NORDITA, MARTIN BREMHOLM, Aarhus University, ALEXANDER V BALATSKY, NORDITA — We present the results of a computational search for three-dimensional (3D) Dirac materials in the scarcely studied group of lanthanide antiperovskites [1]. There is no photoemission data available for these materials. We calculate electronic structures using density functional theory which accounts for spin-orbit coupling and strong correlations. We identify massive bulk Dirac states close to the Fermi level in $A_3B$, where $A=$Sm, Eu, Gd, Yb and $B=$Sn, Pb. The 3D Dirac nodes along the $\Gamma$-$M$ direction originate from the band inversion of the cation and anion bands at the $\Gamma$ point. This band inversion is also an indication of a topological crystalline insulator phase [2]. Most of the predicted materials display a finite magnetic moment due to unpaired electrons in the 4f shell. Specifically, in magnetic Eu$_3$BO the degeneracy of the Dirac nodes is lifted, leading to appearance of Weyl nodes. This offers intriguing possibilities of combining magnetism and Dirac/Weyl physics in pristine materials without doping or proximity effects.

[1] Pertsova et al., PRB 99 (20), 205126 (2019)

*We acknowledge support from VILLUM FONDEN via the Centre of Excellence for Dirac Materials (Grant No. 11744).
12:51PM X59.00009: Strain induced Kramers-Weyl Fermions  JINXIN HU (Presenter), YINGMING XIE, CHENGPING ZHANG, XI DAI, KAM TUEN LAW, Physics, Hong Kong University of Science and Technology — Kramers-Weyl fermions are recently found to be widely supported in chiral crystals and exhibit many novel properties. However, in achiral crystals due to the presence of mirror or roto-inversion symmetries, Kramers Weyl fermions are often obscured to emerge due to the presence of nodal lines. In this work, we show Kramers-Weyl fermions are easily generated by removing the degeneracy of these nodal lines through strain effects. Remarkably, based on realistic DFT calculations, in the strained Rashba semiconductor BiTeI, we find a single Kramers-Weyl fermion near Fermi energy. Moreover, a strain induced quantized circular photogalvanic effect (CPGE) is further established. Our work paved a way to study the topology, optoelectronics by the tuning the chirality of crystals.

1:03PM X59.00010: Insights from magnetic Weyl semimetals: the Berry phase and beyond* [Invited]  BINGHAI YAN (Presenter), Weizmann Institute of Science — It is known that Bloch electrons pick up an anomalous velocity because of the Berry curvature in the magnetic material. Recent discovery of magnetic Weyl semimetals (WSMs) provides a novel, ideal platform to examine the Berry curvature-induced transport phenomena, such as the anomalous Hall effect (AHE) and the thermal version of AHE. We focus on the Wideman-Franz law that governs the fundamental correlation between the charge and heat transport. We reveal a novel mechanism [1] to violate the Wideman-Franz law at the finite temperature by the Berry curvature distribution rather than the inelastic scattering effect, which is distinct from the ordinary (longitudinal) transport. Beyond the linear-response phenomena like AHE, WSMs can generate giant nonlinear optical response (such as the DC photocurrent), which is commonly attributed to the Berry curvature too. As a WSM turns magnetic, however, we find a new class of photocurrent [2,3] by re-examining the nonlinear response theory. It is contributed by the diabatic effect, instead of the Berry phase. Because this is a leading-order phenomena, the induced photocurrent is expected to be much larger compared to the non-magnetic case.


*We acknowledges the financial support by the Willner Family Leadership Institute for the Weizmann Institute of Science, the Benoziyo Endowment Fund for the Advancement of Science, Ruth and Herman Albert Scholars Program for New Scientists, the European Research Council (ERC) under the European Union Horizon 2020 research and innovation programme (grant agreement No. 815869) and by the collaborative Max Planck Lab.
1:39PM X59.00011: Pseudo Dirac Nodal Sphere and its Topological Phase Transitions in a Semimetallic Carbon Network  SHI-ZHANG CHEN (Presenter), Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, China, YUAN-PING CHEN, Faculty of Science, Jiangsu University, Zhenjiang, 212013, Jiangsu, China, WENHUI DUAN, Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, China — Because the global symmetry requirement is hard to achieved, topological nodal sphere is generally a pseudo phase, in which multiple nodal rings form the spherical backbone while the other points on the sphere are approximately degenerate. The physical understanding of nodal sphere, however, remains unclear. Here, we present a tight-binding (TB) model in a tetragonal crystal to simulate the evolution from a nodal sphere to a nodal surface. To provide clear picture, by performing first-principle calculations, a tetragonal carbon network, in which carbon nanotubes (CNTs) interconnected by graphene nanoribbons, is used to identify the pseudo nodal sphere phase. By applying strains, many topological phase transitions and novel semimetallic phases are achieved. The tensile strains lead to a transition from a nodal sphere to a nodal point, and eventually a trivial insulator; while a compressive strain leads to a transition to a nodal tube (uniaxial strains) or a nodal crossbar (biaxial strain), eventually to nodal surfaces, which is in good agreement with our TB modeling. Our results suggest that nodal sphere and nodal surface share the same origin, and their morphologies depend on the inter-CNTs hopping.

1:51PM X59.00012: Topological metals induced by Zeeman effect  SONG SUN (Presenter), ZHIDA SONG, HONGMING WENG, Chinese Academy of Sciences, Institute of Physics, XI DAI, Physics, Hong Kong University of Science and Technology — In the present work, we propose a new way to classify centrosymmetric metals by studying the Zeeman effect caused by an external magnetic field described by the momentum dependent g-factor tensor on the Fermi surfaces. Nontrivial U(1) Berry's phase and curvature can be generated once the otherwise degenerate Fermi surfaces are splitted by the Zeeman effect, which will be determined by both the intrinsic band structure and the structure of g-factor tensor on the manifold of the Fermi surfaces. Such Zeeman effect generated Berry's phase and curvature can lead to three important experimental effects, modification of spin-zero effect, Zeeman effect induced Fermi surface Chern number and the in-plane anomalous Hall effect. By first principle calculations, we study all these effects on two typical material, ZrTe$_5$ and TaAs$_2$ and the results are in good agreement with the existing experiments.

Friday, March 6, 2020 11:15 AM - 1:51 PM

Session X60 DMP: Weyl semimetal, Theory II  Mile High Ballroom 4A - Tag(s): Focus

11:15AM X60.00001: Topological semimetals: from classification to material realization  [Invited] JENNIFER CANO (Presenter), Department of Physics and Astronomy, Stony Brook University — The field of topological semimetals continues to reveal new insights. I will discuss recent developments in the field, starting with the classification of nodal fermions in both magnetic and non-magnetic space groups. I will then introduce new aspects of the bulk-edge correspondence, which elucidate the topological nature of certain non-chiral fermions. Finally, I will discuss routes to material realizations.
11:51AM X60.00002: Topological Vortices in Superconducting Time-Reversal Symmetric Weyl Semimetals  RAUF GIWA (Presenter), PAVAN HOSUR, Univ of Houston — Recent years have shown that superconducting vortices in topological insulators and strongly spin-orbit coupled semiconductors are natural platforms for obtaining Majorana zero modes. We ask the question, "under what conditions do superconducting vortices in Weyl semimetals trap protected Majorana zero modes on the surface?" We show that sufficient conditions for a time-reversal symmetric type I Weyl semimetal (TWSM) to host Majorana modes as above when ordinary BCS superconductivity is induced in them, are (i) the TWSM forms by perturbing a Dirac or a nodal line semimetal, so that kz=0,pi planes contain pairs of opposite chirality Weyl nodes with a small k-space separation (where z is the vortex axis), and (ii) the number of quadruplets of Weyl nodes in these planes is odd. We analytically calculate the topological invariant in this limit using Kitaev's Pfaffian criterion and support it with numerics on a cubic lattice model. Using our criteria, we predict TaAs and its isovalent counterparts to form topological trivial vortices, devoid of Majorana modes. Also, we propose Na(3-x)KxBi with broken inversion symmetry, where doping occurs via interstitial substitution, to be an ideal platform for realizing a non-trivial superconducting vortex with Majorana zero modes at its ends.

12:03PM X60.00003: Finite-Size Effects in the Dynamic Conductivity and Faraday Effect of Quantum Anomalous Hall Insulators  JUNJIE ZENG (Presenter), TAO HOU, ZHENHUA QIAO, Department of Physics, University of Science and Technology of China, WANG KONG TSE, Department of Physics and Astronomy, The University of Alabama — We theoretically study the finite-size effects in the dynamical response of a quantum anomalous Hall insulator in the disk geometry. Semi-analytic and numerical results are obtained for the wavefunctions and energies of the disk within a continuum Dirac Hamiltonian description subject to a topological infinite mass boundary condition. Using the Kubo formula, we obtain the frequency-dependent longitudinal and Hall conductivities and find that optical transitions between edge states contribute dominantly to the real part of the dynamic Hall conductivity for frequency values both within and beyond the bulk bandgap. We also find that the topological infinite mass boundary condition changes the low-frequency Hall conductivity to e^2/h in a finite-size system from the well-known value e^2/2h in an extended system. The magneto-optical Faraday rotation is then studied as a function of frequency for the setup of a quantum anomalous Hall insulator mounted on a dielectric substrate, showing both finite-size effects of the disk and Fabry-Perot resonances due to the substrate. Our work demonstrates the important role played by the boundary condition in the topological properties of finite-size systems through its effects on the electronic wavefunctions.
12:15PM X60.00004: Interplay of non-Abelian band topology with crystalline symmetry
TOMAS BZDUSEK (Presenter), Paul Scherrer Institute, QUANSHENG WU, EPFL Lausanne, ALEXEY SOLUYANOV, University of Zürich, ADRIEN BOUHON, NORDITA, ROBERT-JAN SLAGER, Harvard — We discuss the recently discovered non-Abelian topological invariant that characterizes band nodes inside the momentum space of certain non-interacting metals. This non-Abelian topology prominently arises in systems with PT symmetry (space-time inversion) or with C\textsubscript{2}\textsubscript{T} symmetry (composition of π-rotation with time-reversal). Given the prevalence of these symmetries in most space groups, one expects important implications of the non-Abelian invariant for real materials.

In this talk, we first introduce the quaternion formulation of this topological invariant as obtained by Ref. [1]. We subsequently reformulate the topology using frame rotations and Euler class [2] as developed recently by Ref. [3]. We finally present new results concerning the interplay of the non-Abelian band topology with point-group symmetry. We find that this interplay implies non-trivial conversions between Weyl points, nodal lines, and nodal chains as the system parameters (such as strain or tight-binding coefficients) are tuned.


*Work supported by Moore Foundation's EPIQS initiative and by SNSF Ambizione grant.

12:27PM X60.00005: Strain engineered higher order topological phases for spin-3/2 Luttinger fermions
ANDRAS SZABO (Presenter), RODERICH MOESSNER, Max Planck Inst, BITAN ROY, Lehigh University — Recently, the notion of topological phases of matter has been extended to higher order incarnations, supporting gapless modes on even lower dimensional boundaries, such as corners and hinges. We here identify a collection of cubic spin-3/2 fermions with bi-quadratic touching of Kramers degenerate valence and conduction bands as a platform to strain-engineer higher-order topological (HOT) phases: external uniaxial strain gives birth to a HOT Dirac semimetal or an insulator, depending on its sign, featuring topological \textit{hinge} modes in the strain direction. The insulator in fact exhibits \textit{mixed} topology, and in addition supports edge modes on orthogonal planes. These outcomes are germane when the external strain is applied along one of the C\textsubscript{4v} or coordinate axes, as well as C\textsubscript{3v} or body-diagonal, directions. Our findings place HgTe, gray-Sn, 227 pyrochlore iridates and half-Heusler compounds at the frontier of strain engineered electronic HOT phases.
12:39PM X60.00006: Wiedemann-Franz law and Mott relation for transport coefficients in the non-linear regime*  
CHUANCHANG ZENG (Presenter), Department of Physics and Astronomy, Clemson University, SNEHASISH NANDY, Department of Physics, University of Virginia, ARGHYA TARAPHDER, Department of Physics, Indian Institute of Technology Kharagpur, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University — In contrast to their counterparts in the linear regime, the non-linear anomalous Hall, Nernst, and thermal Hall effects can survive in time-reversal symmetric system in the presence of inversion symmetry breaking. Within the framework of semiclassical Boltzmann theory, we calculate the analytical expressions for the non-linear anomalous transport coefficients, namely, the non-linear anomalous Hall, Nernst, and thermal Hall coefficients. With these expressions, we predict the fundamental relations between the non-linear anomalous electric and thermo-electric transport coefficients, which are the analog of the Wiedemann-Franz law and the Mott relation in the non-linear regime. We also make several experimental predictions for non-linear anomalous Nernst Hall effect in bilayer WTe2 and for non-linear anomalous thermal Hall effect for monolayer transition metal dichalcogenide which can be verified in experiments.

References:

*We acknowledge support from ARO (W911NF-16-1-0182)

12:51PM X60.00007: Phonon induced topological phase transition in ZrTe5*  
NIRAJ ARYAL (Presenter), XILIAN JIN, WEIGUO YIN, Brookhaven National Laboratory — Layered crystalline material ZrTe5 is a unique material to study topological phase transitions; it is very close to the phase boundary between a weak and strong topological insulator (TI) and one can switch from one phase to another by small perturbations like strain. Recently, photoinduced topological transition from the TI regime to the Dirac semimetallic phase has been reported in this material. Motivated by the aforementioned work, using first-principles calculations and effective model Hamiltonian, we study the transition from the TI regime to the Dirac and Weyl semimetallic phases induced by various phonon modes. The experimental implications of our results are also discussed.

*U.S. Department of Energy
1:03PM X60.00008: Diagnosing and observing topological degeneracies in AI class systems
TIANTIAN ZHANG (Presenter), Department of physics, Tokyo Inst of Tech - Tokyo, HU MIAO, Brookhaven national lab, LING LU, Chinese academy of sciences, SHUICHI MURAKAMI, Department of physics, Tokyo Inst of Tech - Tokyo, ZHONG FANG, Chinese academy of sciences, MARK DEAN, Brookhaven national lab, HONGMING WENG, CHEN FANG, Chinese academy of sciences — Topological states have been widely studied in Fermionic systems for many years, wherever, they are sporadically explored in Bosonic systems, even both Fermions and Bosons are fundamental particles in condensed matter physics. Actually, Bosons can offer a better platform to get spinless band structures where nodal lines can be realized with only parity-time reversal (PT) symmetry, such as phonons. By combining first-principles calculations and meV-resolution inelastic x-ray scattering, we demonstrate the first realization of PT symmetry protected helical nodal lines of phonons in a real material. The combination of theoretical analysis and experimental measurements demonstrate the PT-protected helical nodal lines for the first time in phononic materials. This nodal line is robust because of the spinless nature of phonons, which will open a new route to explore exotic topological states in crystalline materials.

1:15PM X60.00009: Effects of Van der Waals interaction on the phonon and electron band structures of ZrTe$_5$
XILIAN JIN (Presenter), College of Physics, State Key Laboratory of Superhard Materials, Jilin University, NIRAJ ARYAL, WEIGUO YIN, Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory — Since the theoretical prediction of the existence of the topological insulating phase, ZrTe$_5$ has attracted a lot of interests in its topological nature, which may lead to the low-energy transport edge channels and the quantum spin Hall (QSH) effect in its two-dimensional form. Possible strain or photon induced topological transition from the topological insulator (TI) to the Dirac semimetal in ZrTe$_5$ has been recently suggested by experiments. Due to the layered structure of ZrTe$_5$, the van der Waals (vdW) interaction becomes an essential factor to study atomic vibrational behavior in the topological transition. In this theoretical work, phonon vibration modes and the corresponding electron band structures are explored systematically without and with vdw force correction to reveal the microscopic mechanism of the phase transition in ZrTe$_5$. 
1:27PM X60.00010: Bulk and surface polaritons in Weyl semimetals* ALEXEY BELYANIN, QIANFAN CHEN (Presenter), RYAN KUTAYIAH, Texas A&M University, MARIA ERUKHIMOVA, IVAN OLADYSHKIN, MIKHAIL TOKMAN, Institute of Applied Physics, Russian Academy of Sciences — We report theoretical studies of the optical properties and polariton modes of Type I Weyl semimetals with two Weyl nodes. We present rigorous quantum-mechanical derivation of bulk and surface conductivity tensors including both intraband and interband optical transitions and taking into account all possible combinations of bulk-to-bulk, bulk-to-surface, and surface-to-surface transitions. We show how the information about the electronic structure of Weyl semimetals, such as position and separation of Weyl nodes, Fermi energy, surface states etc. can be unambiguously extracted from their optical response, namely from the reflection, transmission, and polarization change of incident radiation. We predict the optical Hall effect and anomalous dispersion for surface polaritons excited by a nanotip. We show that Weyl semimetals represent a new class of gyrotropic materials with unique electrodynamics due to the combination of strongly anisotropic and gyrotropic bulk conductivity, surface conductivity, and surface dipole layer.

*This work has been supported in part by the Air Force Office for Scientific Research through Grant No. FA9550-17-1-0341.

1:39PM X60.00011: Hourglass Weyl loops in two dimensions: Theory and material realization in monolayer GaTel family WEIKANG WU (Presenter), YALONG JIAO, SI LI, XIAN-LEI SHENG, ZHIMING YU, SHENGYUAN YANG, Singapore University of Technology and Design — Nodal loops in two-dimensional (2D) systems are typically vulnerable against spin-orbit coupling (SOC). Here, we explore 2D systems with a type of doubly degenerate nodal loops that are robust under SOC and feature an hourglass type dispersion. We present symmetry conditions for realizing such hourglass Weyl loops, which involve nonsymmorphic lattice symmetries. Depending on the symmetry, the loops may exhibit different patterns in the Brillouin zone. Based on first-principles calculations, we identify the monolayer GaTel-family materials as a realistic material platform to realize such loops. These materials host a single hourglass Weyl loop circling around a high-symmetry point. Interestingly, there is also a spin-orbit Dirac point enabled by an additional screw axis. We show that the hourglass Weyl loop and the Dirac point are robust under a variety of applied strains. By breaking the screw axis, the Dirac point can be transformed into a second Weyl loop. Furthermore, by breaking the glide mirror, the hourglass Weyl loop and the spin-orbit Dirac point can both be transformed into a pair of spin-orbit Weyl points. Our work offers guidance and realistic material candidates for exploring fascinating physics of several novel 2D emergent fermions.
X60.00012: Fermionic analogue of Hawking radiation in bilayer black phosphorous*  
HANG LIU, JIATAO SUN (Presenter), Chinese Academy of Sciences, HUAQING HUANG, FENG LIU, Utah University, SHENG MENG, Chinese Academy of Sciences — **Topological matters upon the periodic driving of laser can lead to nonequilibrium topological states, which is not accessible in equilibrium topological materials.** Here we propose that the periodically driven two-dimensional black phosphorous (BP) thin film with a spatial gradient of Floquet-Dirac states can mimic the “gravity” felt by fermionic quasiparticles as that for a Schwarzschild black hole (SBH). Quantum tunneling of electrons from a type-II Dirac cone (inside BH) to a type-I Dirac cone (outside) emits a SBH-like Hawking radiation spectrum. The obtained $T_H$ of a fermionic analog of BH in BP is approximately 3 K, which is several orders of magnitude higher than previous works. Our work sheds some light on increasing the $T_H$ from the perspective of nonequilibrium topological states under periodic driving of laser. The obtained SBH accessible in nonequilibrium BP provides some clues to access the more Fermionic analogues of astronomy phenomena in solids.

*We thank financial support from the National Key Research and Development Program of China (Grants No. 2016YFA0300902 and No. 2016YFA0202300), National Basic Research Program of China (Grant No. 2015CB921001), NSF of China (Grants No. 11774396 and No. 11474328).

Friday, March 6, 2020 11:15 AM - 2:03 PM

Session X62 DCMP: Correlations - Measurement and Control Mile High

Ballroom 4C - Jing-Yuan Chen, Stanford Univ

11:15AM X62.00001: Domain wall spin-texture in quantum Hall magnets*  
NEMIN WEI (Presenter), CHUNLI HUANG, ALLAN MACDONALD, University of Texas at Austin — Recent experiments [Stepanov Petr, et al. *Nature Physics* 14.9,907; Wei et.al *Science* 362.229-233; Haoxin,arXiv:1904.11485] reported long range transport of spinful collective modes in single-layer graphene based quantum Hall magnets(QHMs), including transport across junctions between states with different Landau level filling factors. These experiments motivate a detailed study of the various junctions that can be formed between N=0 QHMs since the microscopic electronic and spin-texture structure near the junction influences the collective mode transmission rate. Using a self-consistent Hartree-Fock calculation, we show that the spin-textures around the junction of $\nu=0$ and $\nu=\pm 1$ QHMs are wide, reaching ~140nm at $B=8T$. For the junction of $\nu=-1$ and $\nu=1$ QHMs, however, the domain wall is narrower and the spin-texture depends on the sublattice potential. I will explain the microscopic physics that controls these junction properties.

*Work supported by DOE grant DE- FG02-02ER45958.
11:27AM X62.00002: Spin transport in quantum Hall magnets*  
CHUNLI HUANG (Presenter), NEMIN WEI, ALLAN MACDONALD, University of Texas at Austin — Recent nonlocal electrical measurements [Stepanov Petr, et al. Nature Physics 14.9, 907; Wei et.al Science 362, 229-233; Haoxin et.al, arXiv:1904.11485] have revealed remarkable spin transport properties in devices that host various graphene quantum Hall magnet (QHM) states. I will discuss our efforts to understand several different aspects of these experiments: 1) using an electric circuit model, we provide an explanation for the finite range of bias voltages over which nonlocal voltages are observed across insulating magnetic states and 2) using a microscopic spin-wave theory we estimate the transmission probabilities of magnon-like collective modes across junctions between QHMs that have different Landau level filling factors.

*Work supported by DOE grant DE- FG02-02ER45958.

11:39AM X62.00003: Enhanced thermal Hall effect in nearly ferroelectric insulators*  
JING-YUAN CHEN (Presenter), STEVEN KIVELSON, XIAO-QI SUN, Stanford Univ — In the context of recent experimental observations of an unexpectedly large thermal Hall conductivity in insulating La$_{2-x}$Sr$_x$CuO$_4$ and SrTiO$_3$, we theoretically explore conditions under which acoustic phonons can give rise to such a large thermal Hall effect. Both the intrinsic and extrinsic contributions to the thermal Hall conductivity are large in proportion to the dielectric constant and the flexoelectric coupling. While the intrinsic contribution is still orders of magnitude smaller than the observed effect, an extrinsic contribution proportional to the phonon mean free path appears likely to account for the observations, at least in SrTiO$_3$. We predict a larger intrinsic contribution to thermal Hall effect in certain insulating perovskites.

*J.-Y. C. is supported by the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant GBMF4302. Collaborator S. A. K. is supported in part by the U. S. Department of Energy (DOE) Office of Basic Energy Science, Division of Materials Science and Engineering at Stanford under contract No. DE-AC02-76SF00515. Collaborator X.-Q. S. is supported by the DOE Office of Science, Office of High Energy Physics, under the contract No. desc0019380.
11:51AM X62.00004: Probing quantum spin liquids in equilibrium using the inverse spin Hall effect  JOSHUA AFTERGOOD (Presenter), Physics, The Graduate Center - CUNY, SO TAKEI, Queens College CUNY — We propose an experimental method utilizing a spin orbit coupled metal to quantum magnet bilayer that will probe quantum magnets lacking long range magnetic order, e.g., quantum spin liquids, via a dc resistance measurement across the metal. The bilayer is held in thermal and chemical equilibrium, and spin fluctuations arising across the single interface are converted into voltage fluctuations in the metal as a result of the inverse spin Hall effect. In thermal equilibrium, changes to the voltage noise in the metal are measurable as changes to the resistance via the fluctuation dissipation theorem. We examine the theoretical workings of the proposed bilayer system, and offer predictions for the temperature scaling of the enhancement to the dc resistance measured across the metal for three quantum spin liquid models. We consider the Heisenberg spin-$\frac{1}{2}$ kagomé lattice model and extract the spinon gap. We find characteristic $T^3$ scaling of the dc resistance enhancement for the Kitaev model in the gapless phase. Finally, for fermionic spinons coupled to a $U(1)$ gauge field we find subdominant $T^{4/3}$ scaling of the dc resistance enhancement. We therefore show that our proposed bilayer can test the relevance of a quantum spin liquid model to a given candidate material.

12:03PM X62.00005: Improved quantum transport calculations for interacting nanostructures* EMMA MINARELLI (Presenter), ANDREW MITCHELL, Univ Coll Dublin — Nanoelectronics devices such as semiconductor quantum dots and single molecule transistors exhibit a rich range of physical behavior due to the interplay between orbital complexity, strong electronic correlations and device geometry. Understanding and simulating the quantum transport through such nanostructures is essential for rational design and technological applications. In this talk I present theoretical reformulations of the Kubo and Meir-Wingreen formulae for mesoscopic quantum transport calculations in linear response, and demonstrate the improvement over standard methods with several example applications using the numerical renormalization group.

*Emma Minarelli acknowledges funding from the Irish Research Council Enterprise Partnership Scheme, through Grant No. EPSPG/2017/343.
Resistive switching duality: insulator-to-metal vs. metal-to-insulator switching*  

PAVEL SALEV (Presenter), University of California, San Diego, RANI BERKOUN, Laboratoire de Physique des Solides, CNRS, DAYNE SASAKI, University of California, Davis, JAVIER DEL VALLE, YOAV KALCHEIM, University of California, San Diego, YAYOI TAKAMURA, University of California, Davis, MARCELO ROZENBERG, Laboratoire de Physique des Solides, CNRS, IVAN SCHULLER, University of California, San Diego — Electrical triggering of metal-insulator transitions offers an opportunity to build energy-efficient and scalable electronics. While insulator-to-metal (I-M) switching in materials such as VO$_2$ is thoroughly studied, much less is known about an opposite metal-to-insulator (M-I) switching. We present a detailed study of M-I switching in (La,Sr)MnO$_3$ (LSMO). Negative differential resistance (NDR) region in the I-V characteristic is necessary for the resistive switching. By comparing LSMO to VO$_2$, we observe an interesting duality: the N-type NDR in LSMO is a “mirror reflection” of the S-type NDR in VO$_2$. Using Kerr effect imaging, we found that an insulating blocking domain perpendicular to the current flow forms in the LSMO during the NDR. This behavior is reciprocal to VO$_2$ in which a conducting filament parallel to the current flow emerges during the NDR. M-I and I-M resistive switchings complement each other providing a broad range of nonlinear electrical properties, which could allow designing of complex electronic devices.

*This work was supported as part of the Quantum Materials for Energy Efficient Neuromorphic Computing (Q-MEEN-C) Energy Frontier Research Center (EFRC), funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award # DE-SC0019273.

Quantum aspects of “hydrodynamic” transport from weak electron-impurity scattering*  

AARON HUI (Presenter), SAMUEL LEDERER, Cornell University, VADIM OGANESYAN, The Graduate Center, City University of New York, EUN-AH KIM, Cornell University — Recent experimental observations of apparently hydrodynamic electronic transport have generated much excitement. However, theoretical understanding of the observed non-local transport (whirlpool) effects and parabolic current profiles has remained at the level of a phenomenological analogy with classical fluids. A more microscopic account of genuinely hydrodynamic electronic transport is difficult because such behavior requires strong interactions to diffuse momentum. Here, we show that the non-local conductivity effects can indeed occur for fermion systems in the presence of disorder. By explicit calculation of the conductivity at finite wavevector $\sigma(q)$ for selected weakly disordered free fermion systems, we propose experimental strategies for demonstrating distinctive quantum effects in non-local transport at odds with the expectations of classical kinetic theory. Our results imply that the observation of whirlpools or other "hydrodynamic" effects does not guarantee the dominance of electron-electron scattering over electron-impurity scattering.

*AH was supported by the NSF Fellowship. E-AK was supported by the W.M. Keck Foundation. VO was supported by NSF DMR Grant No. 1508538. We acknowledge support from NSF through PARADIM under Cooperative Agreement No. DMR-1539918.
12:39PM X62.00008: Integrable systems of heterogeneous qubits* NIKOLAI SINITSYN (Presenter), Los Alamos Natl Lab, VLADIMIR Y CHERNYAK, Mathermatics, Wayne State University, CHEN SUN, Physics, Brown University — We explore an unusual type of quantum spin matter that can be realized by qubits having different physical origin, such as in bound states near defects in Dirac materials. Interactions of different qubits in this matter are described by essentially different coupling operators that do not commute with each other. We show that at least the simplest such models satisfy integrability conditions that we use to describe pseudospin dynamics in a linearly time-dependent magnetic field. Generalizing to arbitrary numbers of qubits, we construct a spin Hamiltonian, which we call the gamma-magnet. For arbitrarily strong interactions, nonadiabatic dynamics, and any initial eigenstate, we find that quantum interference suppresses spin-flips, so that the system remains close to the initial state. This effect may not have a counterpart in classical physics and can be a signature of a new type of spin ordering, which is different from both disordered spin glasses and ordered phases of spin lattices.

*This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, Condensed Matter Theory Program.

12:51PM X62.00009: Looking into thermalization and localization through the lens of quantum coherence* SAYANDIP DHARA (Presenter), Univ of Central Florida, ALIOSCIA HAMMA, Physics, University of Massachusetts Boston, EDUARDO R MUCCIOLO, Univ of Central Florida — Quantum coherence quantifies the amount of superposition a quantum state can have in a basis. Since there is a difference in the structure of eigenstates of the ergodic and many-body localized systems, we expect them also to differ in terms of their coherences. Here, we numerically calculate different measures of quantum coherence in the excited eigenstates of an interacting disordered Hamiltonian as a function of the disorder. We show that these can be used as an order parameter to detect the well-studied ergodic to the many-body localized phase transition. We also perform quantum quench studies to distinguish the behavior of coherence in thermalized and localized phases. We present a protocol to calculate measurement-based localized coherence to investigate the thermal and many-body localized phases. The protocol allows looking at the correlation in a non-destructive way since tracing out a subsystem always destroys coherence and correlation.

*Support: NSF CCF-1844434
1:03PM X62.00010: Measurement-induced criticality in random quantum circuits  
CHAO-MING JIAN (Presenter), Station Q, Microsoft, Santa Barbara, YIZHUANG YOU, University of California, San Diego, ROMAIN VASSEUR, University of Massachusetts, Amherst, ANDREAS W LUDWIG, University of California, Santa Barbara — We investigate the critical behavior of the entanglement transition induced by projective measurements in (Haar) random unitary quantum circuits. Using a replica approach, we map the calculation of the entanglement entropies in such circuits onto a two-dimensional statistical mechanics model. In this language, the area- to volume-law entanglement transition can be interpreted as an ordering transition in the statistical mechanics model. We derive the general scaling properties of the entanglement entropies and mutual information near the transition using conformal invariance. We analyze in detail the limit of infinite on-site Hilbert space dimension in which the statistical mechanics model maps onto percolation. In particular, we compute the exact value of the universal coefficient of the logarithm of subsystem size in the nth Rényi entropies for n≥1 in this limit using relatively recent results for conformal field theory describing the critical theory of 2D percolation, and we discuss how to access the generic transition at finite on-site Hilbert space dimension from this limit, which is in a universality class different from 2D percolation.

1:15PM X62.00011: Temperature dependence of quantum information scrambling in gapped local systems*  
SUBHAYAN SAHU (Presenter), BRIAN SWINGLE, University of Maryland, College Park — We study temperature dependence of quantum information scrambling, specifically, in systems with a gap. Firstly, we perform large scale tensor network based numerics in gapped chaotic one dimensional spin chains to obtain scrambling data at different temperatures. We find that our numerics work very well even at low temperatures, and we are able to determine the temperature dependence of butterfly velocity to be √(T/m), where m is the mass, for T<m. From our numerics, we also observe a broadening of the operator wavefront at finite temperatures, which had been observed in the context of infinite T previously. Secondly, we perform a perturbative calculation to study scrambling in the paramagnetic phase of a 2+1 D non-linear sigma model to analytically understand the temperature dependence of the butterfly velocity. Using the ladder diagram techniques, we verify the √(T/m) behavior of the butterfly velocity at low temperatures, T<<m. Thirdly, we discuss these results in the context of a recently proposed state dependent bound on scrambling, and show that our results are in accordance with the bound, and in fact provides a clear physical picture of scrambling at low temperatures.

*This work is supported by the Air Force Office of Scientific Research (FA9550-17-1-0180).

1:27PM X62.00012: Magnetic Hamiltonian Engineering by Light-Matter Interaction*  
ZEXUN LIN (Presenter), MARTIN RODRIGUERZ-VEGA, GREGORY A FIETE, University of Texas at Austin — In this work, we explore the flexibility and magnitude of Hamiltonian engineering by considering photon-electron coupling and photon-phonon coupling. We compare the pros and cons of both routes in simple toy models, and extend our results to more realistic models.

*This work was supported by the NSF Materials Research Science and Engineering Center Grant No. DMR-1720595 and NSF Grant No. DMR-1949701.
Hydrogenated Rare-Earth Nickelate Nanojunctions with Synaptic Behavior Studied by X-ray Nanodiffraction

IVAN ZALUZHNYY (Presenter), PETER OLIVER SPRAU, University of California, San Diego, QI WANG, HAI-TIAN ZHANG, Purdue University, NELSON HUA, BOYAN STOYCHEV, University of California, San Diego, SHRIRAM RAMANATHAN, Purdue University, ALEX FRANO, OLEG SHPYRKO, University of California, San Diego — Rare-earth nickelates have been the target of intense fundamental and application-focused studies due to their rich phase diagram and possible utilization of these materials as novel sensors, memory devices and hardware elements for artificial intelligence. For example, hydrogenation of SmNiO$_3$ (SNO) drastically changes its electronical properties giving rise to a new insulating phase. Moreover, application of voltage pulses allows one to repeatedly switch the hydrogenated SNO films between the lower and higher resistance states. This allows one to create a device with synaptic behavior, which is a crucial hardware element for neuromorphic computing. With nanofocused x-ray diffraction and spectroscopy we performed in-situ spatially-resolved studies of the microscopic mechanism behind the potentiation and depression of an SNO-based device. We revealed changes in both electronic structure and crystal lattice between pristine and hydrogenated SNO films, as well as before and after electrical switch of the device.

*Quantum Materials for Energy Efficient Neuromorphic Computing, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences under award DE-SC0019273
Unveiling electron correlation in semiconducting Heusler FeVSb by angle-resolved photoemission and dynamical mean field theory

ESTIAQUE HAIDAR
SHOUROV (Presenter), PATRICK STROHBEEN, SEBASTIAN MANZO, DONGXUE DU, Materials Science and Engineering, University of Wisconsin Madison, FANNY RODOLAKIS, JESSICA L MCCHESENY, Advanced Photon Source, Argonne National Laboratory, ZACH KREBS, WYATT A BEHN, Physics, University of Wisconsin Madison, FELIPE CASTRO DE LIMA, Instituto de Física, Federal University of Uberlândia, Brazil, ABHISHEK SHARAN, Physics and Astronomy, University of Delaware, VICTOR BRAR, Physics, University of Wisconsin Madison, ANDERSON JANOTTI, Materials Science and Engineering, University of Delaware, TURAN BIROL, Chemical Engineering and Materials Science, University of Minnesota Twin Cities, FELIPE CASTRO DE LIMA, Instituto de Física, Federal University of Uberlândia, Brazil, ABHISHEK SHARAN, Physics and Astronomy, University of Delaware, VICTOR BRAR, Physics, University of Wisconsin Madison — Electron-electron correlations are responsible for many of the exotic properties of transition metal oxides and chalcogenides; however, the role of correlations in transition metal Heusler compounds is often overlooked. Here, combining angle-resolved photoemission spectroscopy (ARPES) and dynamical mean field theory (DMFT), we directly probe the single particle spectral function of the Heusler FeVSb. ARPES measurements on epitaxial FeVSb films reveal a mass renormalization of $m^* / m_{\text{bare}} = 1.4$, where $m_{\text{bare}}$ is the mass from DFT-LDA calculations that do not include a Hubbard $U$. This mass renormalization lies in dramatic contrast to other Heuslers LnPt(Sb,Bi) (Ln = lanthanide) [1-3] and CoTiSb [4], for which bare DFT calculations are in quantitative agreement with ARPES. By treating the many-body interactions more accurately at the level of DMFT, we quantitatively reproduce the measured electronic structure and comment on the differences between FeVSb and other Heuslers. Our work calls for a re-thinking of the role of correlations in FeVSb and in Heuslers more generally.


Friday, March 6, 2020 11:15 AM - 1:03 PM

Session X65 DCMP: 1D Materials: Nanowires, Nanotubes, and Nanoribbons Mile High Ballroom 4F - Paula Fekete, US Military Academy
Designing nano-biocomposite materials using CVD grown CNTs and ZnO nanostructures for hybrid interfaces and hydrogel environments with future biomedical applications

Nicholas Schaper (Presenter), Brannan Hutchinson, Silviya Zustiak, Irma Kuljanishvili, Saint Louis University — One dimensional (1D) nanostructures, carbon nanotubes (CNTs) and other nanowires, have been proven useful for many biomedical applications. Their high aspect ratio allows for functionalization with specific biological molecules or other nanoscale moieties through covalent bonding, physisorption or chemisorption. Controlled production of CNTs and zinc oxide nanowires (ZnO NWs) has been shown to provide avenues for tailoring interfaces at the nanoscale. These materials are excellent candidates for biomedical use due to unique physical/electrical properties and biocompatibility. When incorporated into nonconductive environments, CNTs/ZnO NW will efficiently transmit electrical signals to biological cells and improve the mechanical strength of composite materials. Here we investigate CVD-grown CNTs, ZnO NWs and CNTs/ZnO hybrid structures interfaced with hydrogels. We have demonstrated that sw-CNT/hydrogel interfaces guide healthy neuronal cell behaviors like cell attachment and neurite growth. Designing new hybrid nanomaterials such as CNTs/ZnO/Hydrogel composites with controlled morphology and functionalized interfaces provide a useful platform for investigating critical biomedical problems simultaneously targeting neural cell regeneration, cancer treatments, and drug delivery.

Unfolding the temperature induced dual bandgap in TiO$_2$ nanotubes with improved photocatalytic application

Sangita Bhowmick (Presenter), Physics, Shiv Nadar University, Chetan Prakash Saini, Saif Khan, Physics, Inter University Accelerator Centre, Mukul Gupta, Physics, UGC-DAE Consortium for Scientific Research, Khandwa Road, Rahul Singhal, Physics, Malaviya National Institute of Technology Jaipur, Raja Sen, Alok Kanjilal, Physics, Shiv Nadar University — Since the discovery of photocatalytic water splitting, TiO$_2$ has gained enormous interest in improving efficiency by generating stable electron-hole (e-h) pairs upon proper light illumination [1]. In particular, anodic TiO$_2$ nanotubes have attracted wide interest not only for their high surface-to-volume ratio with scalable structures [2]. However, the overall efficiency is limited by the recombination of the photo-generated (e-h) pairs in the bulk and electrode/electrolyte interfaces. To overcome this tuning the crystallinity and the bandgap of them are required. Among various approaches, thermal annealing dependent control over the anatase/rutile phase ratio of TiO$_2$ and their inter-granular charge transfer process exhibit a relatively high photocatalytic performance. Here, we report the efficacy of dual-phase mediated bandgap modulation and the subsequent improvement of photocatalytic activity of TiO2 nanotubes as a function of temperature by various complementary techniques like UV-Vis, XRD, XPS, XAS, Raman, etc. and supported by DFT calculations.

References
11:39AM X65.00003: Modulation Doping of Template-Defined InGaAs Nanowires*
KRISTOPHER CERVENY (Presenter), University of Basel, MARTIN FRIEDL, Ecole Polytechnique Federale de Lausanne, MOHAMMAD SAMANI, University of Basel, DIDEM DEDE, Ecole Polytechnique Federale de Lausanne, CHUNYI HUANG, LINCOLN J LAUHON, Northwestern University, ANNA FONTCUBERTA I MORRAL, Ecole Polytechnique Federale de Lausanne, DOMINIK ZUMBUHL, University of Basel — Templated semiconductor nanowires with strong Rashba spin-orbit interaction are a great platform to create and study novel quantum states of matter, such as helical states and spin helices, Majorana- and para-fermions. Here, we report recent results on templated InGaAs nanowire Y-junctions grown on GaAs nanomembranes[1] with modulation doping. Modulation doping has been successfully used in many high-performance systems to create structures with enhanced mobility and higher carrier concentrations. We investigate modulation doping in GaAs nanomembranes grown via molecular beam epitaxy in a selective area growth approach. In a novel process, the dopants migrate up through the GaAs membrane during growth. This remote doping process has enabled major improvements in notable system parameters such as mean free path, coherence length, and spin-orbit length. With a top gate, we can tune between weak localization and antilocalization. The improvements suggest ballistic transport may be within reach. Further, experiments with superconducting contacts for proximitizing and Majorana zero modes can be envisioned.


*Supported by Swiss NSF, NCCR QSIT, SNI, and European Microkelvin Platform (EMP)

11:51AM X65.00004: Reflection of light from gold coated InP NW arrays*
CHIAWEI TU (Presenter), Department of Physics, Univ of Cincinnati, QIAN GAO, HOE TAN, CHENNUPATI JAGADISH, Department of Electronic Materials Engineering, Research School of Physics and Engineering, Australian National University, MASOUD KAVEH, Department of Physics and Astronomy, James Madison University, HEIDRUN SCHMITZER, Department of Physics, Xavier University, MARTIN FRAENZL, Department of Physics, University of Leipzig, HANS-PETER WAGNER, Department of Physics, Univ of Cincinnati — To optimize light coupling into a plasmonic nanowire (NW) array as a function of incident angle and excitation wavelength, we investigated the reflection of light from two different bare and gold coated InP NW arrays. The NWs in the arrays have a diameter of 180 nm, heights of 2 and 1 micrometers and pitches of 666 and 500 nm. A nominally 10 nm thick gold film was deposited around the NWs to investigate the influence of plasmonic effects. The arrays were irradiated with s- and p- polarized light. The spectral reflectance was measured with an incandescent light source ranging from 500 to 1000 nm and the angle resolved reflectance was investigated with a cw laser at 880 nm. The p-polarized angle resolved reflectance of gold deposited NW arrays significantly differs from the reflectance of uncoated InP NW arrays. The differences are attributed to surface plasmon polariton effects. The measured spectrally and angle resolved reflectance was compared with finite-difference-time-domain (FDTD) simulations. The simulations show very good agreement when an air-gold effective medium according to the granularity of the deposited gold films was used.

*The support of the Australian Research Council and URC is kindly acknowledged.
We study theoretically the Dresselhaus SOI of electrons in zinc-blende NWs of various growth directions. We present qualitative and quantitative results for low-symmetry NW cross-sections modeled after sectors of rings or circles. Our analysis enables predictions for a variety of NW cross-sections, such as those of recently fabricated GaAs-InAs nanomembrane-NW structures (Friedl et al., Nano Lett. 18, 2666, 2018). While a specific configuration exists where the Dresselhaus SOI is suppressed, many configurations allow for a strong Dresselhaus coupling on the order of meV. By introducing dimensionless and material-independent functions, it is straightforward to recalculate the spin-orbit length and energy. The inclusion of a similarly strong, gate-induced Rashba term, enables electrical control of the overall SOI. Our results (arXiv:1910.00562) can serve as a guideline for NW-based setups with applications that rely on SOI.

*Supported by SNSF, SNI & EMP
12:15PM X65.00006: Investigating the magneto-optics in quantum wires for designing the optical amplifiers  MANVIR KUSHWAHA (Presenter), Physics, Rice Univ — Quantum wires occupy a unique status among the semiconducting nanostructures with reduced dimensionality -- no other system seems to have engaged researchers with as many appealing features to pursue. This paper aims at a core issue related with the magnetoplasmon excitations in the quantum wires characterized by the confining harmonic potential and subjected to a longitudinal electric field and a perpendicular magnetic field in the symmetric gauge. Crucial to this inquiry is an intersubband collective excitation that evolves into a magnetoroton -- above a threshold value of magnetic field -- which observes a negative group velocity between the maxon and the roton. The evidence of negative group velocity implies anomalous dispersion in a gain medium with the population inversion that forms the basis for the lasing action of lasers\(^1\)-\(^6\). Thus, the technological pathway that unfolds is the route to devices exploiting the magnetoroton features for designing the novel optical amplifiers at nanoscale and hence paving the way to a new generation of lasers. 1. M. S. Kushwaha, Phys. Rev. B \textbf{76}, 245315 (2007); 2. Phys. Rev. B \textbf{78}, 153306 (2008); 3. J. Appl. Phys. \textbf{109}, 106102 (2011); 4. Mod. Phys. Lett. B \textbf{28} 1430013 (2014); 5. Europhys. Lett. \textbf{123}, 34001 (2018); 6. Mod. Phys. Lett. B \textbf{33} 1950062 (2019).

12:27PM X65.00007: Mid-infrared photoconductivity of tellurium nanowire devices*  PENGKE LI (Presenter), IAN APPELBAUM, University of Maryland, College Park — Elemental tellurium is a narrow bandgap (0.34 eV) semiconductor, whose trigonal lattice is composed of weakly-bound, three-fold helical atomic chains. This unusual lattice allows the formation of nanowires with highly anisotropic electronic and optical properties. Here, we present photocurrent spectroscopy of single tellurium nanowire devices in the mid-infrared range close to the band gap, demonstrating interesting anisotropic features closely related to the linear polarization of the incident light and the resonant modes of the nanowires. It is found that the photosensitivity is strongly dependent on the temperature and the back-gate bias.

*We acknowledge support from the Office of Naval Research under Contract No. N000141712994.
12:39PM X65.00008: Quantum confinement and edge effects in zigzag green phosphorene nanoribbons*  
CHI MA (Presenter), TIANXING MA, Beijing Normal Univ, XIHONG PENG, Arizona State University — *Ab initio* calculations were carried out to study size and edge effects on the electronic properties of zigzag green phosphorene nanoribbons (ZGPNRs) with edge chemical functionalization including H, OH, F, Cl, O, and S for the ribbon width up to 3.7 nm. The electronic properties of the ZGPNRs are strongly dependent on the ribbon width and edge chemical species. The ribbons are either semiconducting or metallic depending on the edge functionalization species. The ZGPNRs demonstrate semiconducting behavior with the edge passivation of H, OH, F, or Cl (Group I), while show metallic feather with pristine or O, S edges (Group II). The conduction band minimum (CBM) and valence band maximum (VBM) of the ZGPNRs with the Group I edges are mainly contributed by the inner P atoms and the edge P and functionalization atoms have little contribution. However, for the Group II edges, the electronic bands crossing the Fermi level are dominantly located at the edge atoms. It was also found that the band gap and work function of the ZGPNRs are tunable by varying ribbon width and edge functionalization species.

*The authors acknowledge Beijing Normal University for the financial support and Arizona State University for the computational resources.

12:51PM X65.00009: Lifetime analysis of quasistationary states of an electron in open quantum wires*  
RUEI-FU JAO (Presenter), School of Information Technology, Guangdong Industry Polytechnic, HUA-YI HSU, Department of Mechanical Engineering, National Taipei University of Technology, MING-CHIEH LIN, Department of Electrical and Biomedical Engineering, Hanyang Univ — The quasistationary states of an electron in a cylindrically N-layered open quantum wire are investigated. A complex eigen-solver is developed to determine both the resonant states $E_R$ and the corresponding lifetimes $\tau$ of the system. Here, we solve the eigenvalue equations for the quasibound states of an electron in open quantum wires using the adaptive finite element method (FEM). We have carefully examined the convergence of this approach for the desired accuracy and efficiency. All the quasistationary states of the system can be determined via this eigen-solver. For illustration, the numerical calculations are carried out for the GaAs/Al$_x$Ga$_{1-x}$As/GaAs multi-layered open quantum wire. Both the energy levels and the lifetimes of the quasistationary states are found as functions of the geometric parameters of the system. The lifetime of an electron in such a system is very sensitive to the geometric characteristics. Figure 1 shows our preliminary results are in good agreement with a previous work done by M. Tkach et al. which analyzed the cases of the quasiparticle lifetimes using the $S$-matrix theory.

*This work was partially supported by Guangdong Industry Polytechnic, P. R. China (KYRC2018-001 and RC2016-005), Hanyang University, and National Research Foundation of Korea.

Friday, March 6, 2020 11:15 AM - 2:15 PM

Session X66 DCMP: Superconducting Electronics and Cryogenic Memory  
Four Seasons 1 - Nathan Satchell, Univ of Leeds - Tag(s): Invited
Superconducting circuits are under development as a solution to the demand for ultralow power computers. Logic technologies based in superconducting materials, such as Reciprocal Quantum Logic (RQL) require the development of a superconducting memory in order to build complex computers. Josephson Magnetic Random Access Memory (JMRAM) is a non-volatile memory utilizing the 0-π phase characteristics of pseudo-spin valve magnetic barrier Josephson junctions as a phase element within more traditional superconductor-insulator-superconductor (SIS) SQUIDs, which are used to read the phase state. Here, we present a demonstration of JMRAM from a single unit cell to 2x2 and 8x8 arrays. All arrays are built based on Ni/Cu/NiFe pseudo-spin valve junctions with 50-100 Oe switching field and high critical current of 0.5 mA. All array elements were functional with 100% switching between 0 and 1 state using external magnetic fields. This foundational demonstration serves as the basis for a more complete assessment of the progress of this technology toward practical implementation.

*This research is based upon work supported by the ODNI, IARPA, via ARO contract number W911NF-14-C-0115. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the ODNI, IARPA, or the U.S. Government.
Superconducting vortex-based memory cells

TARAS GOLOD, LISE MORLET-DECARIN, OLENA KAPRAN, ALESSANDRO PAGLIERO, ADRIAN IOVAN, VLADIMIR KRASNOV (Presenter), Department of Physics, Stockholm Univ — Non-volatile quantized states are ideal for the realization of classical Boolean logics. Abrikosov vortex represents the most compact magnetic object in superconductors with the size determined by the London penetration depth \( \sim 100 \text{ nm} \). Therefore, it can be utilized for creation of high-density digital cryoelectronics. In this talk we will describe operation of memory cells, in which a single vortex is used as an information bit [1]. The vortex is pinned at a nano-scale trap and is read-out by a nearby Josephson junction [2,3]. Unlike SQUID-based memory cells, such cells have non-degenerate 0 and 1 states, which greatly simplify the device architecture. Furthermore, SQUID-based devices have a problem with increasing write current upon decreasing the SQUID loop size, preventing a straightforward miniaturization. To the contrary, write current for a vortex is determined by the depinning current density and, therefore, scales with the size. All together this allows simple miniaturization down to sub-micron sizes. We demonstrate that vortex memory cells have a high-endurance operation, are characterized by an infinite magnetoresistance, do not require external magnetic field, have a short access time, and a low write energy. Non-volatility and perfect reproducibility are inherent for such devices due to the quantized nature of the vortex. We argue that vortex-based memory can be used in superconducting digital supercomputers.


*The work was supported by the European Union H2020-WIDESPREAD-05-2017-Twinning project SPINTECH under Grant Agreement No. 810144, the Russian Science Foundation, Grant No.19-19-00594 and the 5-top-100 program at Moscow Institute of Physics and Technology during a sabbatical period of V.K.

Superconducting nanowire-based memories

KARL BERGGREN (Presenter), Massachusetts Institute of Technology MIT — A persistent current in a superconductor provides a nearly perfect physical token for data storage. It is nonvolatile (so long as the loop remains cold), and can be read out precisely, thus enabling digital (and perhaps even multi-level) electronic memory. However, the quantisation of flux in units of \( \Phi_0 \), means that relatively large inductors (on the order of 10s of \( \mu \text{m} \)'s long) are typically required for such systems, somewhat limiting their potential. The solution until recently was to use Josephson junctions as a compact source of inductance, but even this approach resulted in memory-cell dimensions at the many-\( \mu \text{m}^2 \) level. Recently, however, high-quality thin superconducting films with long penetration depths (and thus high kinetic inductance) have become available. These materials enable much smaller persistent-current loops without requiring the use of a Josephson junction. Novel nanowire-based electronic devices, also not using Josephson junctions, have also emerged that can be used to read out the nanowire state. With this, working single-cell memories with negligible bit-error rates have been realized. I will describe these developments. I will also present a new family of novel superconducting electronic elements that can be used with these memories to enhance their capabilities and function.
Controlling supercurrents and their spatial distribution in ferromagnets

[Invited] JAN AARTS (Presenter), KAVEH LAHABI, REMKO FERMIN, Leiden University, MIKHAEL SILAEV, University of Jyväskylä — Spin-triplet Cooper pairs induced in ferromagnets form the centerpiece of the emerging field of superconducting spintronics. Control over the magnetization of the stacked ferromagnetic layers that generate the triplets allows, for instance, making controllable pi-junctions. In such stacks, crucial for triplet generation is the presence of different uniform magnetization directions. The mechanism at work is that the spin-dependent scattering of a singlet in one layer generates an $m_S = 0$ component of the triplet state, which, in the next ferromagnet with a different magnetization direction, manifest itself as an $m_S = 1$, or ‘equal-spin’ triplet. There are other configurations, however, which give rise to controllable triplet currents. Using more intricate magnetic texture even permits control over the spatial distribution of supercurrent. Here we discuss two types of experiments, both based on a disk-shaped ferromagnetic layer as supercurrent carrier. The in-plane magnetization forms a vortex, with in the center a core where the magnetic flux is forced out. In the first experiment, two superconductor / ferromagnet contacts on top of the disk allow us to generate a triplet supercurrent in the disk, and by using superconducting quantum interferometry, we show the existence of two channels. Moreover, we show how the supercurrent can be controlled by moving the vortex with an in-plane magnetic field. Micromagnetic simulations are used to make the connection between the behavior of the supercurrent and the magnetic texture of the disk. In the second experiment, we show that a triplet current can even be generated by placing the superconducting contacts directly on top of the disk, without the presence of the second ferromagnet. Again, the supercurrent is sensitive to the position of the magnetic vortex core. The rotating magnetization, combined with the edges of the structure, yields the correct kind of inhomogeneity. This is not entirely trivial as will be discussed.

Electromagnetic long ranged proximity effect in superconductor-ferromagnet structures

[Invited] ALEXANDRE BUZDIN (Presenter), LOMA UMR-CNRS 5798, University of Bordeaux, France — The spread of the Cooper pairs into the ferromagnet in proximity-coupled superconductor – ferromagnet (SF) structures is shown to cause a strong inverse electrodynamic phenomenon, namely, the long-range transfer of the magnetic field from the ferromagnet to the superconductor. Contrary to the previously investigated inverse proximity effect resulting from the spin polarization of superconducting surface layer, we found a very generic orbital mechanism of the magnetic moment transfer from a ferromagnet to a superconductor, which is unavoidable in S/F hybrids. It is related with the fact that the common superconducting wave function in S and F (near the interface) does not permit to exclude the vector-potential of the magnetization by gauge transformation. From the experimental point of view, this phenomenon reminds the Aharonov-Bohm effect since the current inside the attached superconductor is induced by the ferromagnetic layer, which cannot create the magnetic field in the outside in the absence of such superconducting environment. At the same time, the true physical key point is that the wave function penetrating the ferromagnet is responsible for this effect. Let us stress that the characteristic length of the proposed inverse electrodynamic effect is of the order of the London penetration depth.
11:15AM X67.00001: Higher order topology in superconducting and interacting electronic systems* [Invited] TITUS NEUPERT (Presenter), Univ of Zurich — Topological states with hinge and corner modes, so-called higher order topological insulators, have been predicted to exist in various crystalline materials such as elementary bismuth and WTe2. I will start with a review of the theoretical foundations of higher-order topology, introducing topological invariants to identify such phases as well as an explanation for their generalized topological bulk-boundary correspondence. Second, I will discuss venues for realizing higher order topology in superconductors, magnetic, and strongly interacting systems. To define (crystalline) topology in superconductors, I will discuss the question how theoretically a trivial reference state has to be defined (an atomic limit), and how a topological classification can be built up on this. For magnetic systems, the possibility of topological Kondo insulators hosting a phase with hinge states upon undergoing a magnetic instability is outlined. Finally, the generalization of the bulk-boundary correspondence of higher-order topology will be elevated to the interacting case, including the possibility of surface topological order.

*This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programm (ERC-StG-Neupert-757867-PARATOP).

11:51AM X67.00002: Probing the topological properties of Bismuth, a second order topological insulator [Invited] SOPHIE GUERON (Presenter), ANIL MURANI, BASTIEN DASSONNEVILLE, ALEXANDRE BERNARD, ALIK KASUMOV, RICHARD DEBLOCK, MEYDI FERRIER, HÉLÈNE BOUCHIAT, Laboratoire de Physique des Solides Orsay, U. Paris Sud, U. Paris Saclay, CNRS, France — Higher Order Topological Insulators are a new family of materials whose conduction paths are located not at the crystal boundaries but at the boundary of the boundaries: Thus, three dimensional Second Order Topological Insulators should conduct via one dimensional paths at the crystal hinges. In the talk I will demonstrate how mesoscopic physics experiments (along with some theory!) led to the discovery that Bismuth was the first example of a solid state Second Order Topological Insulators [1]. I will show how we detected such hinge states in monocristalline nanowires connected to superconducting contacts, and further used the supercurrent-versus-phase relation [2,3] to demonstrate their ballistic nature. I will also present our recent measurement of the nanowire's linear response to an ac phase difference excitation. I will argue that the response's sharp dissipation peak when the superconducting phase difference is π is a telltale sign of topological protection at the hinges [4,5].


12:27PM X67.00003: Sankar Das Sarma Invited Talk [Invited] —
Partial Lattice Defects in Higher-Order Topological Insulators

RAQUEL QUEIROZ (Presenter), Weizmann Institute of Science, ION COSMA FULGA, Institute for Theoretical Solid State Physics, IFW Dresden, NURIT AVRAHAM, HAIM BEIDENKOPF, Weizmann Institute of Science, JENNIFER CANO, Center for Computational Quantum Physics, Flatiron Institute — Nonzero weak topological indices are thought to be a necessary condition to bind a single helical mode to lattice dislocations. In this work we show that higher-order topological insulators (HOTIs) can, in fact, host a single helical mode along screw or edge dislocations (including step edges) in the absence of weak topological indices. When this occurs, the helical mode is necessarily bound to a dislocation characterized by a fractional Burgers vector, macroscopically detected by the existence of a stacking fault. The robustness of a helical mode on a partial defect is demonstrated by an adiabatic transformation that restores translation symmetry in the stacking fault. We present two examples of HOTIs, one intrinsic and one extrinsic, that show helical modes at partial dislocations. Since partial defects and stacking faults are commonplace in bulk crystals, the existence of such helical modes can measurably affect the expected conductivity in these materials.


Resolving the topological classification of bismuth using topological defects*

HAIM BEIDENKOPF (Presenter), ABHAY NAYAK, JONATHAN REINER, RAQUEL QUEIROZ, HUIXIA FU, Weizmann Institute of Science, CHANDRA SHEKHAR, Max Planck Institute for Chemical Physics of Solids, BINGHAI YAN, Weizmann Institute of Science, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, NURIT AVRAHAM, Weizmann Institute of Science — The growing diversity of topological classes leads to ambiguity between classes that share similar boundary phenomenology. This is the status of bulk bismuth. Recent studies have classified it as either a strong or a higher-order topological insulator, both of which host helical modes on their boundaries. We resolve the topological classification of bismuth by spectroscopically mapping the response of its boundary modes to a screw-dislocation. We find that the one-dimensional mode, on step-edges, extends over a wide energy range and does not open a gap near the screw-dislocations. This signifies that this mode binds to the screw-dislocation, as expected for a material with nonzero weak indices. We argue that the small energy gap, at the time reversal invariant momentum \( L \), positions bismuth within the critical region of a topological phase transition between a higher-order topological insulator and a strong topological insulator with nonzero weak indices.


*This study was supported by the United States–Israel Binational Science Foundation (BSF; grant number 2016389), the Helmsley Charitable Trust (grant number 2018PG-ISL006), the German-Israeli Foundation (GIF; I-1364-303.7/2016), and the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program (grant agreement no. 678702).
11:15AM X68.00001: Machine learning quantum states in the NISQ era [Invited]  
ROGER MELKO (Presenter), University of Waterloo — We discuss the development of machine learning techniques for the purpose of reconstructing quantum states from projective measurement data. Technology adapted from a branch of unsupervised learning, called generative models, are well-suited for learning representations of quantum states from real experimental data. We discuss quantum state reconstruction with several classes of generative model, and compare in particular the performance of tractable and approximate density models. We demonstrate their practical use for state reconstruction, moving systematically through increasingly complex classes of pure and mixed quantum states. As an example of a use case for a real experimental noisy intermediate-scale quantum (NISQ) device, we review recent efforts in reconstructing a cold atom wavefunction. Finally, we discuss the outlook for scalable experimental state reconstruction using machine learning, in the NISQ era and beyond.

11:51AM X68.00002: About that useful little corner of Hilbert space and its neural network representations [Invited]  
GIUSEPPE CARLEO (Presenter), Center for Computational Quantum Physics, Flatiron Institute — The vast majority of quantum states of interest for practical applications have distinctive features and intrinsic structure. These typically occupy only a very limited corner of the vast manifold of allowed quantum states, making them often amenable for compact classical representations.

In this talk I will overview a recently introduced classical representation of many-qubit states based on artificial neural networks.

First I will present results concerning their expressive power, reviewing representation theorems and arguing that these representations are not limited by the amount of entanglement they can encode. In this context, I will also show a new explicit and polynomially efficient mapping from contractible tensor-network states.

Then, I will show several applications of these variational representations, with a focus on quantum computing applications. Most notably, I will focus on a variational technique useful to simulate large structured quantum circuits, as well as applications of classical neural-network states to benchmark and improve NISQ quantum hardware.
12:27PM X68.00003: Machine Learning and Quantum [Invited] PENGFEI ZHANG (Presenter), Caltech — In this talk, I will first talk about “machine learning of quantum problems”. Since quantum problems are governed by well-defined physical rules, they are good platforms to investigate explainable machine learning. Here I will give one example of learning potential-to-density mapping by the recurrent neural network, from which we can extract the Schrodinger equation. Secondly, I will talk about “machine learning for quantum experiments”. Especially, I will describe how to use the idea of active learning to optimize quantum control, which requires minimal number of experimental data. Finally, I will talk about “machine learning on quantum compute”. I will bring together the concept information scrambling and quantum machine learning. I will show that the tripartite information developed for quantifying information scrambling can be used to diagnose the training dynamics of a quantum neural network.

1:03PM X68.00004: Machine Learning with Tensor Networks [Invited] EDWIN STOUDENMIRE (Presenter), CCQ, Flatiron Institute — Tensor networks are a technique developed to compress otherwise exponentially large, many-body wavefunctions into a form such that they can be optimized and their properties computed with only polynomial effort. Key examples including the matrix product state (MPS) and projected entangled pair state (PEPS) tensor networks, which give state-of-the-art results for challenging systems of strongly correlated electrons. But in recent years, it has been appreciated that tensor networks are a broader technique for compressing very large linear functions, which can appear in many different problem domains. One very promising domain is machine learning of real-world data, where certain powerful models closely resemble wavefunction tensors and where tensor networks can be directly applied, just as in physics.

I will give a progress update on work over the last few years bringing tensor network methods to bear on machine learning. In addition to empirical benchmark results on challenging data sets, there has been recent progress in obtaining theoretical results for machine learning too. I will discuss how a theory of generative modeling of data can be developed in the context of matrix product state models. Other interesting developments include a theoretical understanding of the expressive power of various families of models, and a direct connection between tensor networks and proposals for quantum machine learning.